APPENDIX B.

EVALUATION TABULATIONS AND FIGURES

This Appendix contains the table and figures giving the results of the evaluation of the mechanism against the individual environmental chamber experiments. Table B-1 lists all the environmental chamber experiments that were simulated in this study, and summarizes their major characteristics and selected experimental and calculated $\Delta(O_3\text{-}NO)$ results. Percentage differences between experimental and calculated data are also shown. Figure B-1 through Figure B-90 contain plots of the experimental and calculated data, or distribution plots of the errors in the simulations of the $\Delta(O_3\text{-}NO)$ data, for the various types of experiments that were modeled. The methods of procedure and the results of this evaluation are discussed in Section V of this report.

Table B-1. Summary of environmental chamber experiments used for mechanism evaluation.

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
Characterization Runs																	
ETC458	Pure Air		3			0.35	301	1	1	2	55	3	4	44	4	6	38
ETC485	Pure Air		3		0.00	0.35	300	1	1	2	51	3	5	46	3	7	49
DTC049A	Pure Air		1			0.39	301	1	1	1	37	2	3	28	4	4	20
ITC1009	Acetald - Air		11		0.42	0.35	302	1	1	2	34	4	4	2	7	7	-11
ITC627	Acetald - Air		5		0.23	0.35	300	1	1	2	41	3	4	23	6	7	9
ITC892	Acetald - Air		9		0.19	0.35	299	1	1	2	41	4	4	1	-		
ITC957	Acetald - Air		10		0.46	0.35	301	1	2	2	12	5	4	-7	8	7	-15
ETC319	Acetald - Air		2		0.30	0.35	298	1	0	1	69	1	3	49	3	5	49
ETC382	Acetald - Air		3		0.21	0.35	301	1	1	2	48	2	4	50	4	8	48
CTC019	Acetald - Air		1		0.34	0.20	304	2	1	0	-23	1	2	16	2	3	35
EC253	Acetald - Air		1		0.33	0.29	303	1	4	3	-20	9	9	-2	13	14	2
CTC031	CO - NOx		1	0.26	0.03	0.20	300	2	5	4	-26	10	8	-18	14	12	-17
CTC061	CO - NOx		2	0.23	0.03	0.19	300	2	4	4	13	7	9	15	-	12	
CTC090A	CO - NOx		4	0.26	0.03	0.19	294	2	-	4		8	8	1	-	11	
CTC090B	CO - NOx		4	0.26	0.03	0.19	294	2	-	4		9	8	-22	12	11	-12
ITC507	n-C4 - NOx		2	0.09	0.37	0.37	301	1	10	9	-6	16	16	3	23	25	10
ITC533	n-C4 - NOx		3	0.10	0.29	0.36	303	1	8	8	-3	14	14	-4	21	21	1
ITC939	n-C4 - NOx		10	0.53	0.48	0.35	301	1	5	4	-19	7	7	-2	10	10	0
ITC948	n-C4 - NOx		10	0.26	0.46	0.35	301	1	7	6	-12	12	11	-7	17	16	-6
ETC214	n-C4 - NOx		2	0.49	0.39	0.35	299	1	1	4	83	3	8	61	7	13	47
ETC318	n-C4 - NOx		2	0.52	0.42	0.35	298	1	1	3	61	3	6	48	6	9	35
DTC058A	n-C4 - NOx		1	0.24	0.38	0.39	301	1	4	4	-7	9	9	-7	14	13	-8
DTC058B	n-C4 - NOx		1	0.24	0.39	0.39	301	1	4	4	6	8	9	11	12	13	7
DTC145A	n-C4 - NOx		3	0.65	0.43	0.26	298	2	8	5	-39	13	11	-22	19	16	-18
DTC145B	n-C4 - NOx		3	0.66	0.43	0.26	298	2	6	7	16	13	14	7	20	20	2
DTC171A	n-C4 - NOx		3	0.59	0.51	0.24	298	2	9	7	-27	18	16	-17	-	23	
DTC171B	n-C4 - NOx		3	0.58	0.49	0.24	298	2	10	9	-11	21	18	-12	-	27	
DTC215A	n-C4 - NOx		3	0.54	0.44	0.23	299	2	4	6	28	-	13		-	19	
DTC215B	n-C4 - NOx		3	0.56	0.45	0.23	299	2	6	8	20	14	17	14	22	24	8
DTC228A	n-C4 - NOx		10	0.28	0.19	0.23	297	3	2	2	3	4	4	12	6	6	13
DTC228B	n-C4 - NOx		10	0.28	0.20	0.23	297	3	2	2	14	4	4	17	5	6	18
DTC236A	n-C4 - NOx		10	0.26	0.38	0.23	296	3	4	3	-23	7	6	-22	11	8	-28
DTC253A	n-C4 - NOx		10	0.27	0.41	0.23	297	3	3	3	-9	6	6	-1	10	10	-4
DTC253B	n-C4 - NOx		10	0.27	0.41	0.23	297	3	3	3	3	6	6	5	9	10	5
DTC285A	n-C4 - NOx		10	0.25	0.42	0.22	298	4	4	3	-21	8	6	-22	12	10	-23
DTC285B	n-C4 - NOx		10	0.25	0.41	0.22	298	4	3	3	-9	7	6	-8	11	10	-12
DTC299A	n-C4 - NOx		10	0.26	0.43	0.22	297	4	3	3	6	6	7	7	10	10	3
DTC299B	n-C4 - NOx		10	0.26	0.42	0.22	297	4	3	3	18	5	6	22	7	9	23
XTC085	n-C4 - NOx		1	0.55	0.39	0.26	302	1	4	4	-5	8	7	-10	11	11	-4
XTC098	n-C4 - NOx		1	0.57	0.42	0.25	303	1	4	4	4	8	8	0	-	12	
CTC013	n-C4 - NOx		1	0.45	0.30	0.20	303	2	2	2	40	3	5	39	-	8	
CTC020	n-C4 - NOx		1	0.26	0.40	0.20	304	2	2	3	32	4	6	32	7	9	28
CTC028	n-C4 - NOx		1	0.27	0.38	0.20	304	2	2	3	19	5	6	22	-	10	
CTC042	n-C4 - NOx		2	0.26	0.38	0.20	301	2	5	3	-61	9	6	-50	-	10	
CTC045	n-C4 - NOx		2	0.46	0.37	0.20	301	2	-	3		6	6	-10	8	8	0
CTC058	n-C4 - NOx		2	0.26	0.37	0.19	299	2	4	3	-34	8	6	-37	-	9	
CTC074	n-C4 - NOx		3	0.25	0.38	0.19	297	2	2	3	17	6	6	-3	-	10	
CTC084A	n-C4 - NOx		4	0.25	0.41	0.19	299	2	2	3	19	5	6	20	-	9	
CTC084B	n-C4 - NOx		4	0.25	0.41	0.19	299	2	2	3	12	5	6	22	8	9	10
CTC099A	n-C4 - NOx		4	0.27	0.36	0.19	295	2	3	2	-19	5	5	-6	-	8	
CTC099B	n-C4 - NOx		4	0.27	0.37	0.19	295	2	4	2	-65	8	5	-53	-	8	
CTC114A	n-C4 - NOx		5	0.24	0.38	0.19	296	2	3	2	-19	5	5	-6	-	8	
CTC114B	n-C4 - NOx		5	0.24	0.38	0.19	296	2	3	2	-19	5	5	-5	-	8	
CTC120A	n-C4 - NOx		5	0.26	0.37	0.19	294	2	2	2	26	4	5	27	-	8	
CTC120B	n-C4 - NOx		5	0.25	0.37	0.19	294	2	3	2	-2	5	5	11	-	8	
CTC135A	n-C4 - NOx		6	0.26	0.35	0.18	294	2	3	2	-15	5	5	-4	-	8	
CTC135B	n-C4 - NOx		6	0.26	0.35	0.18	294	2	3	2	-20	6	5	-11	-	8	
CTC241A	n-C4 - NOx		9	0.27	0.53	0.13	302	5	3	3	-3	8	7	-3	-	12	
CTC241B	n-C4 - NOx		9	0.27	0.53	0.13	302	5	3	3	7	7	7	1	12	12	-5

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC244A	n-C4 - NOx		9	0.26	0.60	0.13	293	6	4	3	-29	8	7	-16	15	12	-23
CTC244B	n-C4 - NOx		9	0.26	0.59	0.13	293	6	4	3	-18	8	7	-8	13	12	-11
CTC252A	n-C4 - NOx		9	0.25	0.61	0.13	293	6	3	3	18	6	8	20	11	12	15
CTC252B	n-C4 - NOx		9	0.25	0.58	0.13	293	6	3	3	6	6	7	18	9	11	17
EC162	n-C4 - NOx		1	0.54	0.20	0.34	301	1	21	16	-35	36	27	-31	44	37	-18
EC178	n-C4 - NOx		1	0.10	0.19	0.34	304	1	20	18	-10	36	36	1	45	50	10
EC304	n-C4 - NOx		1	0.51	0.42	0.40	302	1	29	30	1	49	51	4	63	71	11
EC305	n-C4 - NOx		1	0.11	0.42	0.41	302	1	28	30	6	43	52	18	48	64	26
EC307	n-C4 - NOx		1	0.11	0.63	0.41	302	1	30	35	14	46	60	24	50	71	29
EC355	n-C4 - NOx		1	0.50	0.41	0.35	302	1	20	26	25	33	43	22	46	59	22
EC356	n-C4 - NOx		1	0.50	0.43	0.35	302	1	20	27	27	33	44	24	45	60	25
OTC296A	n-C4 - NOx		11	0.53	0.46	0.00	310	7	8	7	-12	23	20	-13	-	31	
OTC296B	n-C4 - NOx		11	0.52	0.51	0.00	310	7	6	7	17	19	22	16	31	35	11
OTC303A	n-C4 - NOx		12	0.54	0.40	0.00	313	7	-	6		27	19	-40	-	28	
OTC303B	n-C4 - NOx		12	0.52	0.39	0.00	313	7	7	6	-23	20	19	-2	-	29	
OTC307A	n-C4 - NOx		12	0.46	0.38	0.00	319	7	14	12	-21	35	32	-9	-	43	
OTC307B	n-C4 - NOx		12	0.48	0.38	0.00	319	7	13	12	-4	32	33	4	44	44	0
Single VOC - NOx Runs																	
ITC1555	ETHENE		12	0.45	0.68	0.35	301	1	33	41	18	94	111	15	132	126	-5
ITC926	ETHENE		10	0.53	1.28	0.35	301	1	94	114	17	130	134	3	112	111	-1
ITC936	ETHENE		10	0.52	0.63	0.35	301	1	29	33	13	70	93	25	119	134	11
ETC220	ETHENE		2	0.51	0.20	0.35	299	1	5	5	8	12	13	14	20	23	11
ETC221	ETHENE		2	0.51	1.31	0.35	299	1	98	104	5	151	154	2	-	140	
ETC381	ETHENE		3	0.52	0.67	0.35	301	1	33	35	7	95	99	4	151	149	-1
ETC439	ETHENE		3	0.66	0.63	0.35	300	1	26	23	-17	66	61	-8	130	115	-13
ETC464	ETHENE		3	0.38	0.48	0.35	301	1	23	25	9	63	71	11	116	117	0
ETC466	ETHENE		3	0.41	0.48	0.35	300	1	22	23	4	55	63	12	108	112	3
ETC467	ETHENE		3	0.52	0.48	0.35	300	1	17	19	12	41	50	18	73	90	19
ETC469	ETHENE		3	0.46	0.58	0.35	301	1	22	29	25	58	82	30	114	133	14
ETC471	ETHENE		3	0.45	0.58	0.35	302	1	25	30	18	70	86	19	127	135	6
ETC473	ETHENE		3	0.46	0.61	0.35	301	1	25	31	21	66	89	26	123	137	10
ETC476	ETHENE		3	0.43	0.55	0.35	300	1	20	26	26	52	77	32	104	126	17
ETC479	ETHENE		3	0.42	0.57	0.35	301	1	22	30	26	59	86	31	115	131	12
ETC482	ETHENE		3	0.41	0.51	0.35	301	1	25	26	5	61	73	15	114	121	6
ETC486	ETHENE		3	0.44	0.51	0.35	301	1	20	24	17	54	66	19	108	118	9
ETC497	ETHENE		3	0.45	0.57	0.35	301	1	22	27	20	61	80	23	118	131	9
ETC505	ETHENE		3	0.40	0.53	0.35	300	1	23	25	10	59	75	21	108	122	11
DTC041B	ETHENE		1	0.17	0.57	0.39	300	1	30	47	36	79	88	10	88	92	4
DTC043A	ETHENE		1	0.47	0.55	0.39	300	1	17	23	23	49	65	25	101	122	18
DTC044B	ETHENE		1	0.16	0.59	0.39	300	1	33	50	35	81	88	7	89	91	2
DTC045A	ETHENE		1	0.48	0.57	0.39	301	1	19	24	22	54	70	24	113	130	13
DTC046B	ETHENE		1	0.17	0.57	0.19	300	1	10	14	33	36	48	24	58	64	10
DTC047A	ETHENE		1	0.48	0.59	0.39	301	1	20	24	16	55	70	22	113	131	14
DTC048B	ETHENE		1	0.17	0.59	0.39	301	1	35	49	28	82	88	7	89	92	3
DTC050A	ETHENE		1	0.16	0.59	0.39	301	1	34	50	33	80	87	9	86	90	4
DTC051A	ETHENE		1	0.48	0.59	0.39	301	1	20	25	20	56	73	23	117	134	13
DTC072B	ETHENE		1	0.47	0.56	0.39	302	1	18	24	24	49	64	24	102	117	13
XTC105	ETHENE		1	0.24	0.60	0.25	301	1	20	17	-17	71	57	-24	99	85	-16
XTC112	ETHENE		1	0.52	0.87	0.25	302	1	24	23	-3	74	71	-4	134	125	-7
EC142	ETHENE		1	0.49	0.31	0.31	301	1	40	32	-24	80	61	-31	109	91	-21
EC143	ETHENE		1	0.50	0.66	0.31	300	1	109	73	-49	145	124	-17	123	120	-2
EC156	ETHENE		1	0.47	0.65	0.33	301	1	110	75	-48	139	124	-12	117	121	3
EC285	ETHENE		1	1.01	0.63	0.38	302	1	66	77	14	115	151	24	165	193	15
EC286	ETHENE		1	0.97	1.22	0.38	302	1	144	172	17	169	192	12	141	163	14
EC287	ETHENE		1	0.54	1.30	0.37	302	1	137	148	7	116	133	13	97	110	13
OTC278B	ETHENE		11	0.46	0.25	0.00	313	8	12	8	-52	38	30	-27	62	48	-29
OTC279A	ETHENE		11	0.53	0.37	0.00	313	8	23	15	-49	87	56	-56	-	94	
OTC280B	ETHENE		11	0.54	0.39	0.00	312	8	23	19	-18	82	57	-44	-	85	
OTC297A	ETHENE		11	0.63	0.37	0.00	309	7	17	9	-96	60	39	-55	-	69	
OTC297B	ETHENE		11	0.28	0.37	0.00	309	7	24	18	-34	-	82		111	110	-1
OTC304A	ETHENE		12	0.60	0.36	0.00	316	7	18	14	-29	63	51	-23	-	79	
OTC304B	ETHENE		12	0.23	0.36	0.00	316	7	-	32		91	93	3	-	104	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ITC1550	PROPENE		12	0.49	0.98	0.35	301	1	70	71	1	106	106	0	-		
ITC1556	PROPENE		12	0.49	0.99	0.35	301	1	53	67	21	104	109	5	114	111	-3
ITC484	PROPENE		2	0.45	0.46	0.39	300	1	14	21	36	32	45	30	40	67	41
ITC510	PROPENE		2	0.59	0.95	0.53	302	1	57	69	17	107	134	20	127	157	19
ITC532	PROPENE		3	0.56	0.91	0.36	302	1	32	45	28	76	104	27	100	125	20
ITC569	PROPENE		4	0.48	0.94	0.36	299	1	44	53	17	96	109	12	-	117	
ITC693	PROPENE		6	0.48	1.07	0.35	301	1	62	73	16	110	117	6	115	118	2
ITC716	PROPENE		6	0.53	1.01	0.35	300	1	59	54	-8	101	115	13	108	124	13
ITC728	PROPENE		6	0.49	1.02	0.35	299	1	51	62	18	94	114	17	101	116	13
ITC736	PROPENE		7	0.49	0.50	0.35	299	1	21	19	-14	40	40	2	58	61	6
ITC754	PROPENE		7	0.57	0.95	0.35	299	1	56	43	-30	-	102		-	124	
ITC791	PROPENE		7	0.53	0.92	0.35	299	1	58	44	-32	103	102	-1	117	120	2
ITC792	PROPENE		8	0.50	0.95	0.35	296	1	50	50	-1	95	104	8	110	113	2
ITC810	PROPENE		8	0.52	0.90	0.35	298	1	52	43	-21	104	98	-6	122	117	-4
ITC860	PROPENE		9	0.52	0.98	0.35	298	1	42	50	17	86	109	21	99	120	18
ITC925	PROPENE		10	0.56	1.06	0.35	302	1	45	64	30	90	118	23	109	123	11
ITC938	PROPENE		10	0.54	0.81	0.35	301	1	43	36	-18	90	87	-3	105	109	4
ITC947	PROPENE		10	0.54	0.60	0.35	301	1	40	20	-98	81	49	-65	99	75	-31
ETC321	PROPENE		2	0.44	1.02	0.35	299	1	48	51	6	114	112	-2	117	116	0
ETC440	PROPENE		3	0.60	1.16	0.35	300	1	51	48	-6	123	123	0	133	138	4
ETC449	PROPENE		3	0.25	0.91	0.35	300	1	71	73	3	76	81	6	75	80	6
ETC475	PROPENE		3	0.26	0.89	0.35	300	1	79	73	-8	73	84	14	71	83	15
DTC026A	PROPENE		1	0.49	1.15	0.39	302	1	100	77	-29	126	128	1	125	128	3
DTC026B	PROPENE		1	0.49	1.16	0.39	302	1	98	78	-25	127	129	1	125	129	4
DTC052A	PROPENE		1	0.30	0.94	0.39	301	1	84	82	-2	83	92	10	82	92	10
DTC054A	PROPENE		1	0.29	0.98	0.39	301	1	80	82	3	80	88	10	79	88	10
DTC060A	PROPENE		1	0.24	0.93	0.39	301	1	75	76	2	73	84	13	-		
DTC060B	PROPENE		1	0.51	0.97	0.39	301	1	52	41	-27	118	111	-6	-		
DTC128A	PROPENE		3	0.48	0.89	0.29	299	2	45	36	-26	100	88	-13	110	106	-4
DTC128B	PROPENE		3	0.49	0.87	0.29	299	2	47	35	-34	101	82	-24	110	99	-11
DTC129A	PROPENE		3	0.47	0.96	0.29	299	2	51	42	-20	103	98	-5	-	109	
DTC129B	PROPENE		3	0.47	0.94	0.29	299	2	51	41	-25	102	91	-12	-	101	
DTC146A	PROPENE		3	0.51	1.06	0.26	298	2	36	36	0	95	98	2	110	113	3
DTC146B	PROPENE		3	0.52	1.05	0.26	298	2	38	36	-4	95	92	-3	108	107	0
DTC153A	PROPENE		3	0.51	1.12	0.25	297	2	41	36	-15	104	101	-3	110	112	2
DTC155B	PROPENE		3	0.10	0.43	0.25	298	2	18	23	24	37	40	7	38	42	9
DTC158B	PROPENE		3	0.51	0.78	0.25	298	2	48	21	-129	108	50	-117	109	77	-42
DTC159A	PROPENE		3	0.51	0.73	0.25	298	2	50	18	-172	109	45	-140	109	74	-48
DTC168A	PROPENE		3	0.52	1.20	0.24	299	2	49	39	-26	109	107	-2	110	113	2
DTC169A	PROPENE		3	0.55	1.20	0.24	299	2	44	37	-20	110	106	-3	114	117	2
DTC170B	PROPENE		3	0.51	1.13	0.24	299	2	53	34	-55	-	95		107	108	0
DTC179B	PROPENE		3	0.50	1.22	0.24	299	2	50	41	-23	106	104	-3	106	105	0
DTC187A	PROPENE		3	0.57	1.13	0.23	299	2	35	32	-12	101	94	-7	119	117	-2
DTC187B	PROPENE		3	0.59	1.08	0.23	299	2	38	30	-29	102	79	-29	117	107	-9
DTC190A	PROPENE		3	0.57	1.20	0.23	299	2	47	35	-33	113	103	-9	115	116	1
DTC205A	PROPENE		3	0.57	1.10	0.23	299	2	41	30	-38	105	88	-19	-	114	
DTC205B	PROPENE		3	0.60	1.15	0.23	299	2	45	32	-43	107	88	-21	116	111	-4
DTC246A	PROPENE		10	0.48	0.95	0.23	297	3	20	22	10	58	71	18	87	101	14
DTC288A	PROPENE		10	0.54	1.04	0.22	298	4	28	31	11	76	86	12	91	99	8
DTC288B	PROPENE		10	0.54	1.02	0.22	298	4	28	29	4	78	85	9	95	102	6
DTC301A	PROPENE		11	0.52	1.04	0.21	296	4	23	28	19	69	84	17	96	100	4
DTC301B	PROPENE		11	0.51	1.03	0.21	296	4	22	28	21	69	84	17	99	100	1
DTC331A	PROPENE		11	0.55	1.07	0.21	296	9	24	27	13	72	83	14	97	100	3
DTC331B	PROPENE		11	0.54	1.06	0.21	296	9	23	27	13	71	82	14	100	101	2
DTC346A	PROPENE		11	0.58	1.01	0.20	299	10	29	24	-24	82	72	-14	98	100	2
DTC346B	PROPENE		11	0.59	1.02	0.20	299	10	30	23	-30	83	71	-17	99	100	1
DTC371A	PROPENE		11	0.57	0.64	0.20	299	10	28	11	-156	82	26	-214	100	44	-127
DTC371B	PROPENE		11	0.57	0.64	0.20	299	10	28	11	-153	82	26	-214	101	44	-128
DTC393A	PROPENE		11	0.57	0.92	0.19	296	11	23	18	-27	62	49	-27	94	84	-11
DTC393B	PROPENE		11	0.56	0.91	0.19	296	11	23	18	-29	62	49	-26	91	84	-9
DTC405A	PROPENE		11	0.56	0.99	0.19	299	10	29	20	-43	83	65	-28	103	98	-5
DTC405B	PROPENE		11	0.56	0.98	0.19	299	10	30	20	-46	82	63	-31	102	96	-6
DTC417A	PROPENE		11	0.53	1.19	0.19	297	10	27	29	7	83	92	10	105	100	-4

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC417B	PROPENE		11	0.53	1.23	0.19	297	10	28	32	12	84	93	10	105	98	-7
DTC431A	PROPENE		11	0.56	1.11	0.18	297	12	31	25	-25	90	78	-15	104	98	-6
DTC431B	PROPENE		11	0.56	1.11	0.18	297	12	32	25	-28	91	78	-17	108	98	-10
DTC443A	PROPENE		11	0.53	1.20	0.17	297	13	26	29	8	83	90	7	103	96	-7
DTC443B	PROPENE		11	0.53	1.21	0.17	297	13	27	29	7	84	89	6	103	95	-9
DTC458A	PROPENE		12	0.53	1.19	0.16	298	14	34	32	-5	87	90	3	-	95	
DTC458B	PROPENE		11	0.53	1.23	0.16	298	14	26	27	4	80	86	8	-	93	
DTC472A	PROPENE		14	0.51	1.05	0.23	298	13	38	31	-21	99	90	-9	109	104	-5
DTC472B	PROPENE		15	0.51	1.05	0.23	298	13	37	30	-21	99	89	-11	110	104	-6
DTC483A	PROPENE		14	0.49	1.17	0.22	298	13	43	44	1	103	99	-4	108	99	-10
DTC483B	PROPENE		15	0.49	1.17	0.22	298	13	41	44	6	102	99	-2	108	100	-8
DTC503A	PROPENE		14	0.52	1.09	0.22	299	15	38	31	-23	102	93	-10	114	105	-8
DTC503B	PROPENE		15	0.51	1.09	0.22	299	15	36	30	-19	101	93	-8	113	105	-7
DTC526A	PROPENE		14	0.51	1.10	0.21	300	10	42	31	-32	104	94	-11	112	102	-9
DTC526B	PROPENE		15	0.51	1.11	0.21	300	10	41	31	-35	104	94	-11	112	103	-8
DTC578A	PROPENE		14	0.49	1.19	0.20	298	16	29	34	14	91	94	3	105	96	-9
DTC578B	PROPENE		15	0.49	1.19	0.20	298	16	27	33	18	89	96	7	104	98	-6
DTC597A	PROPENE		14	0.49	1.16	0.19	298	16	23	29	22	74	92	20	99	99	0
DTC597B	PROPENE		15	0.49	1.15	0.19	298	16	21	28	27	69	91	25	98	99	1
XTC081	PROPENE		1	0.56	1.10	0.26	302	1	43	27	-55	122	94	-31	134	121	-11
XTC082	PROPENE		1	0.54	1.06	0.26	302	1	45	27	-69	122	89	-37	131	116	-13
XTC097	PROPENE		1	0.56	1.20	0.25	302	1	42	29	-45	122	105	-16	131	125	-5
XTC113	PROPENE		1	0.53	1.19	0.25	302	1	44	27	-64	118	92	-28	123	113	-9
CTC012	PROPENE		1	0.42	0.79	0.20	302	2	18	15	-17	57	48	-20	-	80	
CTC018	PROPENE		1	0.47	1.00	0.20	303	2	25	20	-25	86	76	-13	105	99	-6
CTC023	PROPENE		1	0.50	1.14	0.20	301	2	32	24	-31	100	89	-13	110	102	-8
CTC049	PROPENE		2	0.50	1.18	0.20	301	2	38	25	-54	99	91	-8	-	102	
CTC059	PROPENE		2	0.49	1.07	0.19	300	2	26	21	-25	86	75	-15	-	99	
CTC078	PROPENE		3	0.47	1.16	0.19	298	2	30	22	-36	92	83	-11	-	98	
CTC083A	PROPENE		4	0.51	1.25	0.19	298	2	26	23	-12	83	79	-5	106	99	-7
CTC083B	PROPENE		4	0.51	1.23	0.19	298	2	28	22	-26	87	73	-19	-	98	
CTC086A	PROPENE		4	0.44	1.22	0.19	295	2	28	25	-10	88	83	-7	105	91	-15
CTC086B	PROPENE		4	0.44	1.23	0.19	295	2	30	26	-16	92	87	-6	105	93	-13
CTC102A	PROPENE		5	0.49	1.13	0.19	295	2	25	19	-32	77	66	-16	-	98	
CTC102B	PROPENE		5	0.49	1.14	0.19	295	2	27	19	-38	78	69	-13	-	98	
CTC115A	PROPENE		5	0.47	1.15	0.19	295	2	23	20	-16	73	71	-3	-	96	
CTC115B	PROPENE		5	0.47	1.14	0.19	295	2	24	20	-21	75	71	-5	-	96	
CTC132A	PROPENE		6	0.49	1.16	0.18	293	2	26	19	-41	80	61	-30	-	95	
CTC132B	PROPENE		6	0.49	1.15	0.18	293	2	27	19	-45	80	63	-27	-	96	
CTC147A	PROPENE		6	0.53	1.32	0.18	299	4	37	29	-27	102	95	-8	-	98	
CTC147B	PROPENE		6	0.53	1.32	0.18	299	4	36	29	-24	102	94	-9	107	97	-11
CTC153A	PROPENE		6	0.54	1.28	0.18	301	4	42	25	-69	107	94	-13	-	102	
CTC153B	PROPENE		6	0.54	1.26	0.18	301	4	43	24	-75	107	92	-16	-	102	
CTC163A	PROPENE		7	0.50		0.18	299	0	32	23	-41	99	87	-14	-	99	
CTC163B	PROPENE		7	0.50	1.25	0.18	299	0	33	23	-45	100	88	-14	-	98	
CTC170A	PROPENE		7	0.54		0.17	299	5	35	22	-59	105	85	-22	-	99	
CTC170B	PROPENE		7	0.53	1.32	0.17	299	5	36	23	-56	104	89	-17	-	98	
CTC191A	PROPENE		7	0.48	1.26	0.16	298	17	29	21	-41	95	80	-20	-	91	
CTC191B	PROPENE		7	0.47	1.25	0.16	298	17	29	20	-42	96	80	-19	105	90	-17
CTC203A	PROPENE		8	0.48	1.35	0.15	298	18	30	22	-35	96	83	-16	-	89	
CTC203B	PROPENE		8	0.47	1.39	0.15	298	18	30	24	-26	96	84	-15	100	87	-16
CTC219A	PROPENE		8	0.49	1.23	0.14	297	19	31	17	-76	94	65	-44	-	90	
CTC219B	PROPENE		8	0.48	1.22	0.14	297	19	28	18	-54	93	72	-28	100	89	-12
CTC234A	PROPENE		9	0.51	1.53	0.14	302	5	25	27	8	90	90	0	-	86	
CTC234B	PROPENE		9	0.51	1.54	0.14	302	5	25	28	14	90	89	-1	96	85	-13
CTC245A	PROPENE		9	0.49	1.52	0.13	295	6	25	19	-32	90	82	-10	108	91	-19
CTC245B	PROPENE		9	0.49	1.51	0.13	295	6	25	19	-29	89	76	-16	109	91	-19
CTC264A	PROPENE		10	0.50	1.39	0.12	294	20	21	13	-54	78	48	-62	100	92	-9
CTC264B	PROPENE		10	0.50	1.42	0.12	294	20	20	14	-40	74	49	-52	99	90	-11
EC121	PROPENE		1	0.51	0.48	0.27	302	1	64	37	-71	86	64	-33	90	80	-13
EC177	PROPENE		1	0.50	0.49	0.33	305	1	47	46	-2	74	84	12	89	105	15
EC216	PROPENE		1	0.52	0.50	0.43	301	1	50	54	8	77	86	11	93	102	9
EC230	PROPENE		1	0.50	0.55	0.29	302	1	35	43	20	55	73	25	67	87	23

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
EC256	PROPENE		1	0.53	0.11	0.29	303	1	11	10	-11	21	21	0	28	28	1
EC276	PROPENE		1	0.52	0.54	0.35	302	1	40	49	20	63	80	22	78	96	19
EC277	PROPENE		1	0.11	0.56	0.36	302	1	40	49	19	39	49	20	39	49	20
EC278	PROPENE		1	0.50	1.02	0.36	302	1	86	103	17	97	110	12	93	105	12
EC279	PROPENE		1	0.98	1.15	0.36	302	1	77	96	19	123	146	15	141	159	12
EC314	PROPENE		1	0.98	1.06	0.46	302	1	87	102	15	127	151	16	144	168	15
EC317	PROPENE		1	0.57	0.49	0.53	303	1	49	57	14	74	85	13	87	101	14
EC665	PROPENE		1	0.44	0.48	0.38	303	1	37	34	-7	50	55	9	57	67	15
EC684	PROPENE		1	0.44	1.13	0.38	303	1	66	92	28	72	107	33	69	105	35
EC687	PROPENE		1	0.47	1.04	0.37	303	1	64	82	22	95	107	12	89	110	19
EC691	PROPENE		1	0.49	1.08	0.37	304	1	63	87	27	90	111	19	86	113	24
EC863	PROPENE		1	0.57	0.52	0.22	302	1	33	25	-33	49	41	-20	56	52	-7
EC870	PROPENE		1	0.54	1.04	0.33	302	1	78	68	-14	91	101	10	84	107	21
EC885	PROPENE		1	0.52	0.93	0.29	301	1	61	53	-15	88	86	-2	87	93	7
EC899	PROPENE		1	0.48	1.06	0.27	302	1	60	63	6	83	95	12	77	96	20
OTC272A	PROPENE		11	0.54	1.08	0.00	311	7	134	88	-52	158	149	-6	158	153	-3
OTC272B	PROPENE		11	0.53	1.07	0.00	311	7	125	90	-39	152	149	-2	-	155	
OTC295A	PROPENE		11	0.54	1.51	0.00	313	7	135	129	-5	154	150	-3	-	153	
OTC295B	PROPENE		11	0.52	1.49	0.00	313	7	124	127	3	145	149	3	-	153	
OTC298A	PROPENE		11	0.58	1.29	0.00	311	7	136	92	-48	156	156	0	153	160	4
OTC298B	PROPENE		11	0.57	1.35	0.00	311	7	121	102	-18	151	155	3	-	159	
ITC927	1-BUTENE		10	0.54	1.27	0.35	301	1	38	41	7	81	84	3	98	105	7
ITC928	1-BUTENE		10	1.05	0.01	0.35	301	1	-2			13	16	18	42	54	23
ITC930	1-BUTENE		10	0.53	3.33	0.35	302	1	103	99	-4	88	76	-15	85	76	-11
ITC935	1-BUTENE		10	1.09	3.42	0.35	301	1	66	99	34	142	162	12	154	154	0
EC122	1-BUTENE		1	0.51	0.26	0.27	301	1	29	21	-40	45	37	-22	56	47	-18
EC123	1-BUTENE		1	0.51	0.48	0.27	300	1	48	35	-39	70	56	-27	86	68	-26
EC124	1-BUTENE		1	1.00	0.51	0.27	301	1	26	32	20	46	53	14	60	67	10
ITC929	1-HEXENE		10	0.52	1.19	0.35	302	1	13	14	10	34	38	9	60	65	8
ITC931	1-HEXENE		10	0.51	2.40	0.35	301	1	28	32	13	89	96	7	80	103	22
ITC934	1-HEXENE		10	1.07	2.27	0.35	303	1	20	15	-34	46	47	2	79	85	7
ITC937	1-HEXENE		10	1.08	0.01	0.35	301	1	-3			7	9	24	19	25	26
ITC694	ISOBUTEN		6	0.50	1.98	0.35	301	1	109	102	-6	126	142	11	126	144	12
DTC052B	ISOBUTEN		1	0.30	1.06	0.39	301	1	64	67	5	85	96	11	92	103	11
EC146	T-2-BUTE		1	0.51	0.56	0.32	301	1	41	43	5	52	53	2	60	60	-1
EC147	T-2-BUTE		1	0.96	1.01	0.32	301	1	66	72	9	79	86	8	89	95	7
EC157	T-2-BUTE		1	0.56	0.52	0.33	301	1	41	41	-1	50	51	1	58	57	-2
ITC511	ISOPRENE		2	0.60	3.83	0.53	300	1	135	146	8	125	135	7	-		
ITC811	ISOPRENE		8	0.46	2.42	0.35	297	1	121	90	-34	130	109	-19	-		
ITC812	ISOPRENE		8	0.53	1.28	0.35	297	1	59	32	-84	96	58	-65	114	75	-51
DTC053A	ISOPRENE		1	0.15	1.16	0.39	301	1	37	41	10	55	53	-4	56	52	-8
DTC053B	ISOPRENE		1	0.24	1.17	0.39	301	1	29	32	8	64	69	7	79	79	1
DTC056A	ISOPRENE		1	0.47	2.73	0.39	301	1	102	112	9	125	114	-10	122	110	-11
DTC056B	ISOPRENE		1	0.47	1.48	0.39	301	1	38	40	5	77	81	5	97	104	7
XTC093	ISOPRENE		1	0.16	1.07	0.25	301	1	20	16	-26	46	42	-8	-	45	
XTC101	ISOPRENE		1	0.53	1.55	0.25	302	1	28	27	-4	65	60	-8	89	89	1
EC520	ISOPRENE		1	0.49	1.69	0.31	302	1	63	67	6	86	93	7	89	99	11
EC522	ISOPRENE		1	0.96	1.72	0.32	304	1	66	69	3	89	94	5	102	110	7
EC524	ISOPRENE		1	1.00	3.34	0.33	302	1	133	144	8	157	168	7	148	164	10
EC527	ISOPRENE		1	0.53	1.61	0.34	301	1	65	62	-4	89	90	1	91	101	10
EC669	ISOPRENE		1	0.47	1.82	0.38	303	1	56	69	19	66	98	33	70	106	34
OTC309A	ISOPRENE		12	0.21	0.99	0.00	318	0	45	49	8	79	88	10	-	96	
OTC309B	ISOPRENE		12	0.37	0.99	0.00	318	0	40	39	-1	90	95	5	-	112	
OTC316A	ISOPRENE		12	0.42	0.86	0.00	310	0	31	25	-25	65	55	-20	77	66	-17
OTC316B	ISOPRENE		12	0.42	1.70	0.00	310	0	74	73	-1	120	115	-5	124	115	-8
ETC420	A-PINENE		3	0.29	0.54	0.35	299	1	36	39	6	51	50	-2	57	56	-1
ETC443	A-PINENE		3	0.26	0.57	0.35	300	1	41	46	10	54	55	2	61	62	2
ETC444	A-PINENE		3	0.30	0.56	0.35	300	1	40	44	9	51	52	2	58	59	2
ETC446	A-PINENE		3	0.53	0.56	0.35	300	1	19	20	4	43	44	2	55	54	-1
ETC447	A-PINENE		3	0.13	0.56	0.35	300	1	36	38	5	39	41	5	41	45	8
XTC095	A-PINENE		1	0.24	0.59	0.25	302	1	39	39	0	45	45	0	-	47	
OTC318A	A-PINENE		12	0.26	0.43	0.00	310	0	20	20	3	48	48	1	-	55	
ETC421	B-PINENE		3	0.25	0.82	0.35	299	1	7	5	-48	13	14	12	24	41	42

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC433	B-PINENE		3	0.27	0.80	0.35	300	1	4	5	15	11	13	21	21	32	35
ETC434	B-PINENE		3	0.29	2.92	0.35	300	1	16	11	-44	52	71	27	44	64	31
ETC435	B-PINENE		3	0.14	0.84	0.35	301	1	5	6	22	19	37	49	37	48	24
ETC442	B-PINENE		3	0.29	0.82	0.35	301	1	4	5	14	11	13	15	22	29	24
XTC099	B-PINENE		1	0.23	1.59	0.25	304	1	9	4	-101	33	17	-97	46	59	22
OTC318B	B-PINENE		12	0.26	0.53	0.00	310	0	17	5	-234	49	15	-223	-	26	
ETC424	3-CARENE		3	0.25	0.99	0.35	299	1	19	19	4	52	42	-24	57	49	-15
ETC456	3-CARENE		3	0.23	0.83	0.35	300	1	17	15	-7	48	36	-32	54	44	-24
ETC457	3-CARENE		3	0.16	0.88	0.35	301	1	29	24	-22	41	41	2	42	48	13
ETC459	3-CARENE		3	0.50	0.76	0.35	301	1	11	8	-37	30	19	-55	51	30	-72
ETC423	SABINENE		3	0.25	1.15	0.35	299	1	16	22	29	47	49	4	53	55	4
ETC436	SABINENE		3	0.29	1.14	0.35	300	1	12	18	36	43	47	8	51	53	4
ETC437	SABINENE		3	0.58	1.14	0.35	300	1	13	12	-13	34	28	-20	46	38	-19
ETC438	SABINENE		3	0.14	0.59	0.35	300	1	7	12	40	25	27	7	31	31	2
ETC425	D-LIMONE		3	0.25	1.97	0.35	299	1	48	49	1	56	57	1	62	63	3
ETC450	D-LIMONE		3	0.24	1.77	0.35	301	1	49	45	-8	57	54	-6	63	61	-4
ETC451	D-LIMONE		3	0.57	1.69	0.35	301	1	34	40	16	52	48	-8	58	51	-13
ETC452	D-LIMONE		3	0.16	1.76	0.35	301	1	45	43	-4	50	51	3	51	57	10
ITC560	BENZENE		3	0.11	2.84	0.36	301	1	38	46	17	-			-		
ITC561	BENZENE		3	0.11	0.34	0.36	301	1	35	33	-4	-			-		
ITC562	BENZENE		3	0.57	0.36	0.36	301	1	35	8	-340	75	19	-297	80	32	-150
ITC698	BENZENE		6	0.49	0.70	0.35	301	1	34	23	-44	76	61	-25	-		
ITC710	BENZENE		6	0.53	0.70	0.35	300	1	32	20	-58	71	50	-41	73	99	26
ITC831	BENZENE		8	1.01	0.01	0.35	298	1	-1	2		4	5	21	8	8	-5
CTC159A	BENZENE		6	0.26	1.74	0.18	303	0	31	31	-1	56	53	-5	-	49	
CTC159B	BENZENE		6	0.26	0.86	0.18	303	0	13	11	-20	50	38	-33	-	51	
CTC160A	BENZENE		6	0.49	0.96	0.18	302	0	4	8	50	16	22	30	-	45	
CTC160B	BENZENE		6	0.49	1.74	0.18	302	0	8	19	60	38	66	42	-	73	
ITC534	TOLUENE		3	0.53	0.49	0.36	302	1	61	58	-6	87	101	14	-		
ITC699	TOLUENE		6	0.49	0.37	0.35	300	1	59	41	-44	83	85	2	-		
ITC828	TOLUENE		8	1.01	0.01	0.35	297	1	-1	2		5	7	25	13	12	-2
DTC042A	TOLUENE		1	0.99	0.24	0.39	300	1	4	5	25	19	20	7	45	41	-10
DTC042B	TOLUENE		1	0.10	0.13	0.39	300	1	32	27	-19	35	37	7	34	38	9
DTC151A	TOLUENE		3	0.32	0.43	0.25	298	2	36	39	8	65	67	2	59	65	9
DTC155A	TOLUENE		3	0.10	0.16	0.25	298	2	25	21	-22	28	32	13	27	33	18
DTC158A	TOLUENE		3	0.50	0.57	0.25	298	2	41	45	10	87	86	-1	79	89	12
DTC170A	TOLUENE		3	0.49	0.58	0.24	299	2	42	45	8	89	86	-4	81	89	9
XTC106	TOLUENE		1	0.25	0.47	0.25	301	1	57	56	-2	58	61	5	-	60	
CTC026	TOLUENE		1	0.27	0.50	0.20	302	2	45	47	4	54	58	7	-	58	
CTC034	TOLUENE		1	0.52	0.50	0.20	305	2	36	41	14	83	88	6	-	92	
CTC048	TOLUENE		2	0.25	0.22	0.20	301	2	17	18	8	49	46	-7	48	53	9
CTC065	TOLUENE		2	0.66	0.23	0.19	300	2	5	6	6	22	23	4	-	46	
CTC079	TOLUENE		3	0.26	0.12	0.19	298	2	4	5	16	19	20	4	-	32	
EC264	TOLUENE		1	0.44	0.26	0.34	303	1	53	68	22	79	87	9	-		
EC266	TOLUENE		1	0.44	0.27	0.34	302	1	52	68	23	78	86	9	73	81	10
EC269	TOLUENE		1	0.48	0.13	0.34	302	1	32	34	6	51	60	15	69	83	17
EC270	TOLUENE		1	0.47	0.20	0.35	302	1	44	52	15	67	83	19	78	89	13
EC271	TOLUENE		1	0.21	0.26	0.35	302	1	47	57	18	42	54	21	40	50	21
EC273	TOLUENE		1	0.11	0.13	0.40	303	1	30	40	25	29	39	26	28	38	26
EC293	TOLUENE		1	0.49	0.24	0.40	302	1	74	69	-7	77	93	17	72	87	17
EC327	TOLUENE		1	0.49	0.13	0.41	302	1	33	39	17	57	69	17	76	89	15
EC340	TOLUENE		1	0.49	0.12	0.36	302	1	35	33	-4	57	59	3	-		
OTC299A	TOLUENE		11	0.51	0.28	0.00	312	7	56	50	-12	98	111	11	-	114	
OTC299B	TOLUENE		11	0.50	0.12	0.00	312	7	-	9		37	41	11	-	62	
OTC300A	TOLUENE		11	0.52	0.12	0.00	312	7	14	12	-13	54	48	-12	-	71	
OTC300B	TOLUENE		11	0.22	0.12	0.00	312	7	27	30	10	61	64	4	-	67	
DTC223A	C2-BENZ		3	0.26	0.43	0.22	299	2	19	24	24	49	51	3	-	58	
DTC223B	C2-BENZ		3	0.27	0.22	0.22	299	2	9	12	25	26	25	-7	42	35	-19
DTC224A	C2-BENZ		3	0.53	0.45	0.22	298	2	15	15	-3	41	37	-10	-	55	
DTC224B	C2-BENZ		3	0.55	0.20	0.22	298	2	7	7	2	20	17	-12	-	27	
CTC057	C2-BENZ		2	0.27	0.55	0.20	300	2	16	17	7	48	47	-1	50	57	11
CTC092A	C2-BENZ		4	0.27	0.29	0.19	295	2	7	5	-24	23	18	-28	-	29	
CTC092B	C2-BENZ		4	0.27	0.54	0.19	295	2	16	14	-10	43	39	-10	51	57	10

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC098B	C2-BENZ		4	0.49	0.51	0.19	295	2	5	8	29	20	25	21	-	43	
DTC073A	M-XYLENE		1	0.48	0.11	0.39	302	1	10	9	-12	31	27	-14	43	39	-10
DTC188A	M-XYLENE		3	0.55	0.12	0.23	299	2	7	7	0	22	21	-7	35	32	-8
DTC188B	M-XYLENE		3	0.57	0.22	0.23	299	2	24	18	-31	53	42	-26	67	55	-21
DTC189A	M-XYLENE		3	0.25	0.24	0.23	299	2	34	30	-11	56	51	-10	58	57	-3
DTC189B	M-XYLENE		3	0.26	0.11	0.23	299	2	16	13	-26	31	25	-24	40	33	-22
DTC191A	M-XYLENE		3	0.57	0.49	0.23	298	2	57	50	-13	96	87	-11	98	104	5
DTC191B	M-XYLENE		3	0.59	1.01	0.23	298	2	97	94	-4	97	99	3	85	94	9
DTC192A	M-XYLENE		3	0.30	0.49	0.23	298	2	61	56	-9	63	63	0	-	62	
DTC192B	M-XYLENE		3	0.15	0.49	0.23	298	2	40	43	8	37	42	12	35	40	13
DTC193A	M-XYLENE		3	0.13	0.27	0.23	299	2	36	35	-1	37	38	3	35	38	7
DTC193B	M-XYLENE		3	0.13	0.15	0.23	299	2	27	22	-20	39	34	-14	40	35	-13
CTC029	M-XYLENE		1	0.27	0.33	0.20	300	2	38	46	17	62	64	3	63	65	3
CTC035	M-XYLENE		1	0.28	0.15	0.20	301	2	20	18	-10	43	39	-9	57	54	-6
CTC036	M-XYLENE		1	0.51	0.15	0.20	302	2	7	8	15	30	29	-1	45	43	-3
CTC066	M-XYLENE		2	0.56	0.30	0.19	300	2	19	32	41	57	65	13	77	87	12
CTC080	M-XYLENE		3	0.51	0.48	0.19	298	2	52	64	18	93	97	4	92	98	6
CTC094A	M-XYLENE		4	0.49	0.51	0.19	294	2	41	62	33	77	93	18	-	93	
CTC094B	M-XYLENE		4	0.49	0.52	0.19	294	2	44	62	30	78	93	16	-	92	
DTC207A	O-XYLENE		3	0.28	0.17	0.23	299	2	21	24	12	47	43	-9	62	59	-4
DTC207B	O-XYLENE		3	0.30	0.36	0.23	299	2	48	54	11	65	67	4	-	65	
DTC208A	O-XYLENE		3	0.52	0.31	0.23	300	2	35	41	15	76	71	-7	-	98	
DTC208B	O-XYLENE		3	0.56	0.16	0.23	300	2	13	13	3	39	34	-14	53	47	-13
DTC209A	O-XYLENE		3	0.12	0.15	0.23	299	2	27	28	2	-	37		-	38	
DTC209B	O-XYLENE		3	0.13	0.09	0.23	299	2	15	16	11	-	28		-	35	
CTC038	O-XYLENE		1	0.25	0.16	0.20	301	2	16	16	0	47	40	-18	59	57	-4
CTC039	O-XYLENE		1	0.48	0.08	0.20	301	2	3	3	-20	11	10	-10	-	20	
CTC046	O-XYLENE		2	0.50	0.16	0.20	303	2	3	6	48	18	24	26	-	43	
CTC068	O-XYLENE		2	0.26	0.34	0.19	302	2	39	44	12	58	62	6	57	63	9
CTC081	O-XYLENE		3	0.26	0.29	0.19	298	2	35	34	-4	57	60	5	-	62	
CTC091A	O-XYLENE		4	0.28	0.25	0.19	295	2	23	25	7	54	52	-4	-	64	
EC288	O-XYLENE		1	0.50	0.10	0.38	302	1	42	33	-26	59	55	-8	69	68	-1
EC291	O-XYLENE		1	0.49	0.32	0.39	302	1	84	100	16	91	109	17	91	105	13
DTC198A	P-XYLENE		3	0.26	0.24	0.23	299	2	7	10	25	23	23	2	-	36	
DTC198B	P-XYLENE		3	0.27	0.47	0.23	299	2	15	20	26	-	46		-	57	
DTC199A	P-XYLENE		3	0.55	0.47	0.23	299	2	10	12	18	34	32	-6	-	50	
DTC199B	P-XYLENE		3	0.55	0.25	0.23	299	2	8	8	1	23	18	-26	41	29	-40
DTC200A	P-XYLENE		3	0.13	0.22	0.23	299	2	12	14	14	-	30		-	36	
DTC200B	P-XYLENE		3	0.13	0.12	0.23	299	2	8	8	7	19	16	-15	30	24	-26
CTC041	P-XYLENE		1	0.26	0.21	0.20	300	2	5	4	-35	17	13	-32	32	23	-41
CTC043	P-XYLENE		2	0.25	0.11	0.20	301	2	2	2	-17	7	5	-26	14	10	-40
CTC044	P-XYLENE		2	0.51	0.22	0.20	301	2	1	3	50	6	7	21	13	13	3
CTC047	P-XYLENE		2	0.28	0.54	0.20	301	2	9	12	26	37	39	5	-	59	
CTC069	P-XYLENE		2	0.24	1.11	0.19	302	2	17	35	52	57	56	-1	57	53	-8
CTC070	P-XYLENE		2	0.50	1.12	0.19	301	2	10	22	53	50	70	29	93	94	1
DTC201A	124-TMB		3	0.25	0.23	0.23	299	2	13	14	11	31	29	-6	-	41	
DTC203A	124-TMB		3	0.51	0.44	0.23	298	2	15	18	21	44	45	2	-	63	
DTC203B	124-TMB		3	0.54	0.23	0.23	298	2	10	9	-9	29	24	-18	44	36	-22
DTC204A	124-TMB		3	0.12	0.22	0.23	298	2	14	18	21	31	32	5	39	34	-13
DTC204B	124-TMB		3	0.12	0.13	0.23	298	2	9	11	15	20	20	-1	-	27	
CTC056	124-TMB		2	0.25	0.28	0.20	300	2	8	10	18	32	29	-9	50	45	-13
CTC091B	124-TMB		4	0.28	0.58	0.19	295	2	19	23	19	47	52	9	-	59	
CTC093A	124-TMB		4	0.48	0.60	0.19	294	2	13	15	11	43	42	-2	-	64	
CTC093B	124-TMB		4	0.49	1.42	0.19	294	2	35	48	27	74	86	15	-	83	
ITC703	135-TMB		6	0.49	1.23	0.35	301	1	107	105	-3	106	103	-3	-		
ITC706	135-TMB		6	0.47	0.61	0.35	300	1	70	78	10	94	102	7	101	104	3
ITC709	135-TMB		6	0.97	1.10	0.35	301	1	108	123	13	139	170	18	154	173	11
ITC742	135-TMB		7	0.52	1.09	0.35	300	1	-	107		-	106		-		
ITC826	135-TMB		8	0.90	0.01	0.35	297	1	-2	1		19	17	-13	35	34	-5
DTC194A	135-TMB		3	0.26	0.38	0.23	299	2	38	37	-4	57	54	-6	62	59	-5
DTC194B	135-TMB		3	0.28	0.76	0.23	299	2	58	58	1	57	57	-1	-	54	
DTC195A	135-TMB		3	0.55	0.77	0.23	300	2	60	59	-2	91	91	1	93	97	4
DTC195B	135-TMB		3	0.56	0.38	0.23	300	2	33	25	-30	53	43	-21	63	54	-16

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC196A	135-TMB		3	0.13	0.38	0.23	300	2	36	37	3	38	38	0	39	38	-1
DTC196B	135-TMB		3	0.14	0.19	0.23	300	2	27	23	-16	37	32	-14	-	37	
DTC206A	135-TMB		3	0.27	0.32	0.23	299	2	38	33	-18	58	48	-20	63	58	-7
XTC103	135-TMB		1	0.50	0.67	0.25	301	1	77	73	-5	107	102	-4	109	108	-1
CTC030	135-TMB		1	0.52	0.71	0.20	300	2	-	62		-	95		-	103	
CTC050	135-TMB		2	0.27	0.43	0.20	303	2	44	41	-7	56	60	7	-	66	
CTC071	135-TMB		2	0.52	0.73	0.19	300	2	64	62	-3	96	95	-1	-	102	
CTC073	135-TMB		3	0.26	0.39	0.19	297	2	32	36	10	52	55	5	56	60	6
CTC098A	135-TMB		4	0.48	0.44	0.19	295	2	32	32	0	58	55	-6	-	69	
EC901	135-TMB		1	0.49	0.68	0.27	303	1	67	82	19	74	93	21	63	92	32
EC903	135-TMB		1	1.01	1.21	0.27	302	1	111	131	16	127	153	17	124	148	16
DTC211A	123-TMB		3	0.25	0.17	0.23	299	2	28	26	-8	47	41	-15	-	52	
DTC211B	123-TMB		3	0.26	0.39	0.23	299	2	52	52	-1	63	55	-15	-	53	
DTC212A	123-TMB		3	0.51	0.40	0.23	299	2	49	50	1	-	77		-	94	
DTC212B	123-TMB		3	0.54	0.22	0.23	299	2	24	23	-4	49	45	-8	59	56	-5
DTC213A	123-TMB		3	0.11	0.19	0.23	299	2	31	30	-2	-	33		-	34	
DTC213B	123-TMB		3	0.11	0.12	0.23	299	2	18	21	15	30	31	3	35	32	-10
CTC054	123-TMB		2	0.23	0.27	0.20	302	2	35	37	6	53	53	1	54	56	3
CTC075	123-TMB		3	0.52	0.29	0.19	298	2	22	24	10	53	55	3	68	72	6
CTC076	123-TMB		3	0.26	0.23	0.19	297	2	29	27	-7	49	48	-3	58	56	-3
ITC751	NAPHTHAL		7	0.54	0.62	0.35	299	1	15	17	7	32	34	5	44	47	5
ITC755	NAPHTHAL		7	0.27	1.18	0.35	299	1	18	24	24	40	40	0	-	53	
ITC756	NAPHTHAL		7	0.25	2.28	0.35	299	1	28	26	-10	45	42	-5	-		
ITC798	NAPHTHAL		8	0.60	1.62	0.35	298	1	20	30	34	46	53	13	65	69	6
ITC802	NAPHTHAL		8	0.59	0.71	0.35	296	1	18	17	-6	39	35	-11	54	48	-12
ITC739	TETRALIN		7	0.54	0.36	0.35	299	1	8	6	-44	14	13	-10	18	19	6
ITC747	TETRALIN		7	0.54	15.10	0.35	299	1	29	37	22	63	72	13	90	82	-9
ITC748	TETRALIN		7	0.23	13.61	0.35	299	1	31	25	-23	52	47	-11	-		
ITC750	TETRALIN		7	0.54	7.12	0.35	299	1	25	32	22	50	65	23	88	79	-10
ITC832	TETRALIN		8	0.99	0.01	0.35	298	1	10	2	-333	29	49	40	65	98	34
ITC771	23-DMN		7	0.25	1.18	0.35	299	1	31	33	6	48	49	2	-		
ITC774	23-DMN		7	0.56	0.99	0.35	299	1	33	45	26	60	64	6	77	81	5
ITC775	23-DMN		7	0.26	0.42	0.35	299	1	21	22	7	38	34	-11	49	44	-10
ITC806	23-DMN		8	0.38	1.45	0.35	297	1	36	39	7	60	59	-1	63	64	1
ITC1000	ACETYLEN		11	0.10	0.01	0.35	302	1	2	2	-26	42	49	14	54	58	7
ITC1006	ACETYLEN		11	0.27	1.78	0.35	302	1	111	114	3	105	107	1	-		
ITC1007	ACETYLEN		11	0.23	1.92	0.35	301	1	104	106	2	96	99	3	-		
CTC188A	ACETYLEN		7	0.13	0.36	0.16	298	17	4	6	27	20	27	28	46	47	2
CTC188B	ACETYLEN		7	0.13	0.65	0.16	298	17	17	19	12	55	50	-10	-	59	
ITC1549	FORMALD		12	0.37	0.02	0.35	301	1	-1			12	18	33	19	26	26
ITC1554	FORMALD		12	0.44	0.38	0.35	300	1	26	42	39	37	56	34	-		
ITC864	FORMALD		9	0.54	0.01	0.35	299	1	1	1	38	18	25	28	-		
ETC378	FORMALD		3	0.24	0.08	0.35	301	1	5	9	39	9	12	28	11	13	21
ETC441	FORMALD		3	0.27	0.17	0.35	301	1	17	20	15	24	26	9	27	29	6
DTC149A	FORMALD		3	0.32	0.20	0.25	298	2	22	21	-6	32	30	-6	37	35	-6
DTC149B	FORMALD		3	0.34	0.21	0.25	298	2	23	22	-6	33	30	-8	38	35	-8
DTC218A	FORMALD		3	0.28	0.17	0.23	299	2	17	16	-7	26	23	-11	30	27	-12
DTC218B	FORMALD		3	0.29	0.19	0.23	299	2	18	18	-3	-	25		32	29	-10
DTC270A	FORMALD		10	0.28	0.14	0.22	298	3	14	11	-21	20	17	-18	24	21	-16
DTC270B	FORMALD		10	0.27	0.14	0.22	298	3	14	12	-16	20	18	-12	24	22	-11
DTC387A	FORMALD		11	0.26	0.20	0.19	299	11	19	18	-7	28	26	-6	34	32	-7
XTC086	FORMALD		1	0.16	0.21	0.26	302	1	23	23	0	36	36	0	45	45	-1
CTC016	FORMALD		1	0.24	0.34	0.20	303	2	26	29	10	40	44	9	51	54	6
CTC024	FORMALD		1	0.17	0.17	0.20	302	2	13	13	3	21	21	2	26	26	0
CTC077	FORMALD		3	0.16	0.15	0.19	299	2	12	10	-15	19	17	-13	24	21	-14
CTC095A	FORMALD		4	0.26	0.19	0.19	294	2	12	13	9	20	21	7	-	26	
CTC095B	FORMALD		4	0.26	0.19	0.19	294	2	12	13	5	20	21	4	-	26	
CTC116A	FORMALD		5	0.24	0.16	0.19	296	2	12	10	-10	18	17	-7	-	21	
CTC116B	FORMALD		5	0.26	0.16	0.19	296	2	12	10	-18	18	16	-12	-	21	
CTC133A	FORMALD		6	0.26	0.18	0.18	296	2	13	11	-13	20	18	-10	-	23	
CTC133B	FORMALD		6	0.25	0.18	0.18	296	2	13	11	-18	21	18	-12	-	23	
CTC176A	FORMALD		7	0.25	0.18	0.16	299	10	11	10	-12	18	17	-9	-	22	
CTC176B	FORMALD		7	0.25	0.18	0.16	299	10	11	10	-13	19	17	-11	-	22	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC055B	ACETALD		1	0.14	0.79	0.39	301	1	18	23	19	32	39	18	43	52	17
DTC150A	ACETALD		3	0.14	1.05	0.25	298	2	15	18	14	25	29	13	33	38	14
DTC150B	ACETALD		3	0.15	1.03	0.25	298	2	16	18	9	26	28	7	34	36	6
DTC152B	ACETALD		3	0.20	0.99	0.25	301	2	28	21	-34	49	33	-48	60	42	-42
DTC387B	ACETALD		11	0.26	0.30	0.19	299	11	8	10	15	15	17	10	21	23	8
XTC083	ACETALD		1	0.25	0.62	0.26	302	1	24	26	7	37	39	5	49	51	4
XTC092	ACETALD		1	0.25	0.69	0.25	301	1	20	22	8	31	34	9	41	46	10
CTC014	ACETALD		1	0.23	0.58	0.20	303	2	13	18	29	22	29	23	-	37	
CTC015	ACETALD		1	0.24	0.57	0.20	303	2	12	17	30	20	27	26	-	36	
CTC032	ACETALD		1	0.28	0.70	0.20	301	2	16	19	14	26	29	12	33	37	12
CTC072	ACETALD		3	0.26	0.66	0.19	298	2	15	17	14	24	27	12	-	34	
EC164	ACETALD		1	0.54	0.21	0.35	305	1	23	23	-1	35	36	5	41	46	11
EC254	ACETALD		1	0.11	0.28	0.29	303	1	16	17	7	26	28	6	34	37	8
OTC273B	ACETALD		11	0.30	0.72	0.00	315	8	50	53	6	100	109	8	113	126	10
OTC274A	ACETALD		11	0.28	0.69	0.00	308	8	49	40	-22	86	75	-15	-	95	
OTC305A	ACETALD		12	0.28	0.90	0.00	316	7	58	58	0	104	107	3	-	115	
OTC317B	ACETALD		12	0.26	0.78	0.00	305	0	27	28	4	47	46	-1	-	49	
ITC941	ACROLEIN		10	0.55	0.51	0.35	301	1	15	16	5	28	31	11	37	42	12
ITC944	ACROLEIN		10	0.27	1.24	0.35	301	1	25	23	-8	45	40	-12	65	58	-14
ITC945	ACROLEIN		10	0.52	0.01	0.35	301	1	1	3	61	17	20	16	-		
ITC946	ACROLEIN		10	0.54	1.20	0.35	302	1	68	36	-86	110	78	-42	107	105	-2
ITC513	METHACRO		2	0.57	3.22	0.53	301	1	68	82	17	111	116	4	105	110	5
ITC819	METHACRO		8	0.48	2.21	0.35	298	1	44	45	2	78	74	-6	110	95	-16
ITC823	METHACRO		8	0.51	41.39	0.35	298	1	64	60	-7	108	91	-19	98	80	-22
ETC386	METHACRO		3	0.56	2.83	0.35	301	1	56	57	2	105	97	-8	100	106	6
DTC075A	METHACRO		1	0.50	5.69	0.39	302	1	64	79	19	97	79	-23	85	73	-16
DTC075B	METHACRO		1	0.26	3.09	0.39	302	1	32	51	37	64	58	-9	63	56	-14
XTC094	METHACRO		1	0.49	5.06	0.25	302	1	51	46	-11	85	70	-21	-	70	
XTC102	METHACRO		1	0.24	2.00	0.25	301	1	31	24	-27	55	41	-32	-	57	
EC530	METHACRO		1	0.43	0.96	0.34	301	1	37	40	7	56	60	7	69	77	10
EC651	METHACRO		1	0.45	1.85	0.34	302	1	48	48	1	59	76	23	59	91	35
EC652	METHACRO		1	0.45	1.01	0.34	302	1	44	43	-2	55	64	14	62	83	26
EC655	METHACRO		1	0.80	1.88	0.34	302	1	67	72	7	88	99	10	104	125	16
OTC317A	METHACRO		12	0.25	0.64	0.00	305	0	24	17	-46	44	31	-41	51	36	-42
ETC445	ACETONE		3	0.14	0.08	0.35	300	1	13	15	15	23	28	18	33	41	21
DTC054B	ACETONE		1	0.29	0.13	0.39	301	1	15	20	22	27	35	23	39	51	24
DTC055A	ACETONE		1	0.15	0.17	0.39	301	1	20	25	19	36	46	21	50	61	18
XTC084	ACETONE		1	0.24	0.12	0.26	302	1	24	18	-34	40	31	-29	-	44	
XTC090	ACETONE		1	0.19	0.13	0.25	302	1	20	18	-8	34	31	-10	-	44	
OTC273A	ACETONE		11	0.30	0.14	0.00	315	8	51	42	-21	107	95	-12	-	120	
OTC274B	ACETONE		11	0.27	0.12	0.00	308	8	34	30	-11	71	64	-12	90	89	-2
DTC337A	MEK		11	0.29	0.39	0.21	296	10	26	27	5	39	42	6	51	56	8
DTC337B	MEK		11	0.11	0.39	0.21	296	10	19	20	8	-	33		-	38	
DTC361A	MEK		11	0.10	0.45	0.20	298	10	21	22	4	33	34	3	36	38	5
DTC361B	MEK		11	0.23	0.47	0.20	298	10	27	29	7	43	45	4	59	59	1
CTC178A	MEK		7	0.24	0.44	0.16	298	10	24	23	-5	36	34	-6	-	44	
CTC178B	MEK		7	0.09	0.44	0.16	298	10	17	16	-7	28	26	-7	-	33	
CTC256A	MPK		10	0.20		0.13	296	20	11	12	12	19	19	5	-	25	
CTC256B	C7-KET-2		10	0.20		0.13	296	20	4	4	8	8	8	6	13	13	-1
ITC512	MVK		2	0.60	1.44	0.53	301	1	69	82	16	-	106		100	105	5
ITC815	MVK		8	0.52	1.33	0.35	298	1	53	52	-2	100	93	-7	-		
ITC816	MVK		8	0.51	0.63	0.35	297	1	37	31	-19	64	58	-10	97	88	-10
EC529	MVK		1	0.48	0.70	0.34	301	1	44	52	16	77	87	12	91	97	6
EC644	MVK		1	0.49	0.42	0.34	303	1	54	44	-23	72	71	-2	-		
EC648	MVK		1	0.83	0.65	0.34	303	1	73	66	-11	103	102	-1	104	132	21
EC649	MVK		1	0.46	0.01	0.34	302	1	6	3	-89	51	58	12	62	90	31
EC281	O-CRESOL		1	0.49	0.64	0.37	302	1	18	15	-20	35	37	5	46	49	7
EC289	M-CRESOL		1	0.47	0.48	0.40	302	1	39	16	-137	49	34	-46	51	42	-21
EC290	P-CRESOL		1	0.50	0.59	0.39	302	1	17	18	5	32	37	14	41	46	11
Incremental Reactivity Runs -- VOC Added to Base Case Surrogate																	
ETC483	CO	MRE	3	0.42	1.95	0.35	300	1	45	42	-7	120	116	-3	148	152	3
ETC487	CO	MRE	3	0.46	1.52	0.35	301	1	41	38	-9	112	109	-2	143	152	6

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC416	CO	MR3	3	0.62	1.82	0.35	299	1	31	27	-15	68	65	-4	115	115	0
ETC418	CO	MR3	3	0.52	1.39	0.35	299	1	29	28	-3	66	68	3	114	121	6
DTC014A	CO	MR8	1	0.48	1.83	0.39	301	1	91	79	-14	130	120	-8	146	147	0
DTC015B	CO	MR8	1	0.50	1.89	0.39	301	1	102	80	-28	142	121	-17	153	148	-3
DTC016A	CO	MR8	1	0.48	1.08	0.39	300	1	65	56	-18	99	85	-17	122	111	-10
DTC020B	CO	MR8	1	0.50	1.33	0.39	300	1	66	49	-33	100	81	-23	125	111	-13
DTC029A	CO	R8	1	0.17	1.21	0.39	301	1	74	73	0	84	86	2	84	88	5
CTC105B	CO	MR3	5	0.30	0.45	0.19	296	2	18	21	13	44	53	17	69	80	14
CTC123A	CO	MR8	5	0.40	0.54	0.18	293	2	53	52	0	76	83	8	91	99	8
ETC506	ETHANE	MRE	3	0.41	1.03	0.35	300	1	32	37	13	83	92	10	121	128	5
ETC092	ETHANE	MR3	2	0.51	0.54	0.36	301	1	13	18	27	34	45	23	58	72	20
ETC099	ETHANE	MR3	2	0.50	0.53	0.36	300	1	14	17	17	35	43	19	56	69	18
ETC235	ETHANE	MR3	2	0.49	0.87	0.35	301	1	24	27	11	58	63	8	98	106	7
DTC242A	ETHANE	MR3	10	0.32	0.59	0.23	296	3	15	18	19	36	44	20	59	75	21
ETC226	PROPANE	MR3	2	0.48	0.92	0.35	299	1	14	20	29	40	54	27	71	100	29
ETC230	PROPANE	MR3	2	0.51	1.67	0.35	300	1	25	25	0	63	66	5	114	123	7
ETC305	PROPANE	MR3	2	0.54	1.27	0.35	301	1	19	19	-2	53	50	-5	100	92	-8
ETC484	N-C4	MRE	3	0.46	2.04	0.35	300	1	45	27	-65	121	89	-36	139	142	2
ETC488	N-C4	MRE	3	0.42	1.53	0.35	300	1	32	26	-24	95	78	-21	132	131	-1
ETC094	N-C4	MR3	2	0.48	1.02	0.36	301	1	13	16	23	33	42	21	57	72	21
ETC097	N-C4	MR3	2	0.50	0.94	0.36	301	1	14	16	10	35	42	17	62	72	14
ETC135	N-C4	MR3	2	0.52	0.89	0.35	301	1	11	13	16	31	35	12	53	60	11
ETC224	N-C4	MR3	2	0.50	1.41	0.35	300	1	20	18	-8	52	51	-3	93	93	0
ETC389	N-C4	R3	3	0.16	0.72	0.35	301	1	20	22	13	55	58	6	72	76	5
ETC393	N-C4	R3	3	0.16	0.69	0.35	300	1	19	21	11	56	56	0	74	75	2
DTC019B	N-C4	MR8	1	0.46	1.00	0.39	300	1	72	67	-7	107	103	-4	130	132	2
DTC031A	N-C4	R8	1	0.17	0.93	0.39	301	1	70	72	2	80	83	3	79	83	5
ETC201	N-C6	MR3	2	0.50		0.35	300	1	11	10	-9	30	29	-5	55	52	-5
ETC209	N-C6	MR3	2	0.51	0.74	0.35	299	1	-	9		25	27	7	47	49	3
DTC072A	N-C6	MRE	1	0.47	1.16	0.39	302	1	14	11	-23	41	33	-22	91	73	-26
ETC237	N-C8	MR3	2	0.48	0.95	0.35	301	1	6	5	-12	18	14	-25	34	26	-29
ETC239	N-C8	MR3	2	0.53	0.92	0.35	301	1	6	6	-6	18	15	-16	34	28	-21
DTC024B	N-C8	MR8	1	0.50	0.75	0.39	301	1	41	35	-16	72	63	-14	100	85	-17
DTC070A	N-C8	MR8	1	0.49	0.63	0.39	301	1	38	36	-6	66	63	-4	87	86	-1
DTC037B	N-C8	R8	1	0.18	0.77	0.39	301	1	54	55	1	66	73	9	67	76	12
DTC071B	N-C8	R8	1	0.18	0.56	0.39	302	1	52	49	-7	65	69	7	65	74	12
CTC110B	N-C8	MR3	5	0.30	0.57	0.19	296	2	8	9	11	26	30	13	-	55	
CTC131A	N-C8	MR8	5	0.39	0.87	0.18	293	2	32	26	-23	56	58	5	70	76	8
DTC271B	N-C12	MR3	10	0.30	0.57	0.22	298	4	7	7	2	23	23	2	38	43	13
DTC273A	N-C12	MR3	10	0.31	0.52	0.22	298	4	9	9	-5	28	26	-6	49	48	-1
DTC283B	N-C12	MR3	10	0.32	0.61	0.22	297	4	6	7	19	18	22	17	34	41	18
DTC272A	N-C12	MR8	10	0.14	0.42	0.22	298	4	24	28	16	36	42	14	26	48	45
DTC274B	N-C12	MR8	10	0.16	0.40	0.22	298	4	28	29	5	42	44	5	47	51	7
DTC284A	N-C12	MR8	10	0.15	0.48	0.22	298	4	28	32	13	42	45	8	47	49	6
DTC293A	N-C12	R8	10	0.08	0.50	0.22	297	4	26	29	9	31	31	0	31	30	-2
CTC150B	N-C12	MR8	6	0.42	0.68	0.18	299	4	30	24	-24	58	55	-5	74	73	-2
CTC154A	N-C12	MR8	6	0.42	0.87	0.18	301	4	32	22	-49	61	56	-9	77	74	-3
DTC275A	N-C14	MR3	10	0.32	0.58	0.22	298	4	6	6	-7	19	18	-7	35	34	-3
DTC277B	N-C14	MR3	10	0.31	0.57	0.22	298	4	7	12	40	23	35	35	42	64	34
DTC289B	N-C14	MR3	10	0.35	0.67	0.22	297	4	5	5	13	14	15	9	26	29	10
DTC276B	N-C14	MR8	10	0.17	0.48	0.22	298	4	29	29	0	44	45	3	50	53	5
DTC278A	N-C14	MR8	10	0.16	0.44	0.22	298	4	29	35	18	43	48	10	49	51	4
DTC290A	N-C14	MR8	10	0.17	0.48	0.22	298	4	24	31	20	39	46	15	45	52	14
CTC151A	N-C14	MR8	6	0.50	0.71	0.18	303	4	34	27	-22	55	54	-2	68	68	1
CTC158A	N-C14	MR8	6	0.36	0.92	0.18	304	4	22	18	-22	52	53	1	68	72	4
DTC279B	N-C15	MR3	10	0.32	0.64	0.22	298	4	4	6	30	15	19	20	31	36	16
DTC280A	N-C15	MR8	10	0.16	0.43	0.22	298	4	26	32	20	40	47	14	46	51	11
DTC282A	N-C16	MR3	10	0.33	0.56	0.22	299	4	8	10	21	23	29	22	40	52	23
DTC291B	N-C16	MR3	10	0.33	0.70	0.22	297	4	5	5	-4	14	14	-5	28	27	-4
DTC281B	N-C16	MR8	10	0.16	0.49	0.22	298	4	26	28	7	41	45	9	48	52	8
CTC152B	N-C16	MR8	6	0.37	0.65	0.18	301	4	22	17	-29	43	43	0	-	55	
CTC156B	N-C16	MR8	6	0.41	0.88	0.18	303	4	25	16	-52	52	49	-6	65	67	3
ETC228	2-ME-C3	MR3	2	0.51	0.67	0.35	300	1	14	18	23	41	49	18	72	90	20

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC232	2-ME-C3	MR3	2	0.51	2.31	0.35	299	1	21	19	-7	63	53	-19	133	114	-16
ETC241	2-ME-C3	MR3	2	0.48	1.32	0.35	301	1	17	20	13	54	54	0	119	115	-3
ETC303	2-ME-C3	MR3	2	0.45	0.96	0.35	300	1	13	18	29	41	49	17	88	100	11
ETC291	224TM-C5	MR3	2	0.50	1.81	0.35	303	1	13	13	2	43	41	-6	102	94	-8
ETC293	224TM-C5	MR3	2	0.49	1.92	0.35	302	1	12	12	-4	42	39	-8	99	90	-10
DTC733A	26DM-C8	MR4	18	0.30	0.53	0.16	296	21	4	3	-37	12	7	-76	23	12	-82
DTC749A	26DM-C8	MR4	18	0.38	0.55	0.16	298	21	6	5	-39	20	12	-72	36	22	-69
DTC738B	26DM-C8	MR8	18	0.31	0.41	0.16	293	21	18	13	-41	42	36	-19	55	49	-12
DTC747A	26DM-C8	MR8	18	0.29	0.42	0.16	299	21	16	13	-22	44	43	-4	59	58	-3
DTC739A	26DM-C8	R8	18	0.10	0.39	0.16	295	21	27	29	7	31	34	10	30	35	12
DTC734B	2-ME-C9	MR3	18	0.40	0.50	0.16	295	21	5	3	-70	13	6	-116	24	10	-133
DTC741A	2-ME-C9	MR3	18	0.38	0.48	0.16	295	21	5	4	-27	14	9	-52	27	17	-63
DTC737A	2-ME-C9	MR8	18	0.32	0.43	0.16	294	21	17	12	-37	42	36	-16	55	51	-7
DTC746B	2-ME-C9	MR8	18	0.30	0.44	0.16	298	21	13	12	-8	39	39	-1	53	54	3
DTC740B	2-ME-C9	R8	18	0.10	0.39	0.16	295	21	24	27	10	28	33	14	28	34	19
DTC725A	34-DE-C6	MR4	18		0.51	0.16	295	21	9	8	-14	29	22	-29	47	37	-28
DTC730A	34-DE-C6	MR4	18	0.30	0.51	0.16	296	21	6	4	-50	18	11	-69	32	20	-56
DTC726B	34-DE-C6	MR8	18	0.29	0.43	0.16	294	21	22	22	1	42	42	0	54	53	-2
DTC729B	34-DE-C6	MR8	18	0.24	0.40	0.16	294	21	15	15	-3	39	43	8	52	55	6
DTC732B	34-DE-C6	R8	18	0.08	0.41	0.16	296	21	-	26		30	30	2	29	30	5
DTC748B	34-DE-C6	R8	18	0.09	0.41	0.16	297	21	25	28	12	28	33	16	27	34	20
DTC541A	CYCC6	MR3	14	0.38	0.76	0.21	299	10	8	9	13	24	25	5	45	45	2
DTC551A	CYCC6	MR3	14	0.38	0.93	0.20	300	10	8	7	-10	21	18	-13	37	32	-14
DTC543B	CYCC6	MR8	15	0.30	0.96	0.21	299	10	42	38	-8	65	61	-6	81	77	-5
DTC552B	CYCC6	MR8	15	0.31	0.73	0.20	300	10	36	26	-39	64	52	-21	81	69	-18
DTC544A	CYCC6	R8	14	0.13	0.63	0.21	299	10	40	38	-5	49	48	-3	52	50	-3
DTC553A	CYCC6	R8	14	0.13	0.78	0.20	300	10	41	40	-4	51	50	-3	54	53	-3
DTC315B	C6-CYCC6	MR3	11	0.33	0.62	0.21	298	5	8	6	-19	21	18	-12	36	34	-5
DTC318B	C6-CYCC6	MR3	11	0.33	0.57	0.21	297	5	7	8	12	21	24	13	37	43	14
DTC317A	C6-CYCC6	MR8	11	0.17	0.54	0.21	297	5	27	28	3	41	44	6	46	52	11
DTC319B	C6-CYCC6	MR8	11	0.18	0.57	0.21	297	5	20	21	2	37	39	5	45	50	10
CTC167A	C6-CYCC6	MR8	7	0.41	0.95	0.18	300	5	28	22	-28	58	58	0	-	76	
CTC233A	C6-CYCC6	R8	9	0.17	0.85	0.14	299	5	37	40	7	44	47	7	-	48	
DTC324A	C8-CYCC6	MR3	11	0.32	0.59	0.21	298	5	9	10	18	25	30	16	44	55	20
DTC325B	C8-CYCC6	R8	11	0.18	0.68	0.21	299	5	25	29	12	40	46	14	46	55	16
CTC231A	C8-CYCC6	MR3	9	0.27	0.70	0.14	303	5	4	5	30	12	14	17	24	26	8
CTC168B	C8-CYCC6	MR8	7	0.41	0.96	0.18	300	5	27	22	-24	55	58	6	-	77	
CTC232B	C8-CYCC6	MR8	9	0.46	0.81	0.14	301	5	14	16	12	38	46	18	54	64	16
CTC239B	C8-CYCC6	MR8	9	0.44	1.01	0.13	301	5	18	17	-4	48	51	6	61	69	11
CTC240A	C8-CYCC6	R8	9	0.17	1.01	0.13	300	5	33	37	11	41	45	10	43	47	9
ETC199	ETHENE	MR3	2		0.52	0.35	301	1	23	22	-3	65	61	-7	120	108	-11
ETC203	ETHENE	MR3	2	0.52	0.46	0.35	301	1	20	19	-2	54	52	-2	96	90	-6
DTC017A	ETHENE	MR8	1	0.48	0.56	0.39	300	1	56	53	-5	94	88	-6	119	118	-1
DTC038A	ETHENE	R8	1	0.17	0.57	0.39	301	1	63	65	3	65	69	5	62	66	6
ETC496	PROPENE	MRE	3	0.38	0.82	0.35	301	1	45	57	22	111	117	5	123	121	-2
ETC500	PROPENE	MRE	3	0.42	0.76	0.35	300	1	35	43	19	100	113	12	127	131	3
ETC106	PROPENE	MR3	2	0.52	0.44	0.36	300	1	14	17	15	39	45	13	65	73	11
ETC108	PROPENE	MR3	2	0.52	0.45	0.36	300	1	14	16	12	37	43	16	59	71	17
ETC110	PROPENE	MR3	2	0.52	0.42	0.36	300	1	13	15	11	36	41	11	62	67	7
ETC118	PROPENE	MR3	2	0.50	0.49	0.36	302	1	14	20	28	39	53	26	70	90	23
DTC018A	PROPENE	MR8	1	0.48	0.71	0.39	301	1	73	65	-13	109	104	-6	117	124	6
DTC032B	PROPENE	R8	1	0.17	0.66	0.39	300	1	61	63	3	59	64	7	59	64	8
CTC142B	PROPENE	MR3	6	0.37	0.49	0.18	295	2	9	10	10	26	31	16	-	55	
CTC130B	PROPENE	MR8	5	0.39	0.86	0.18	293	2	52	53	3	79	83	5	84	87	4
ETC253	ISOBUTEN	MR3	2	0.48	0.81	0.35	301	1	29	26	-14	81	81	0	122	125	2
ETC255	ISOBUTEN	MR3	2	0.48	0.79	0.35	302	1	29	27	-10	80	83	4	121	127	5
ETC257	ISOBUTEN	MR3	2	0.48	0.62	0.35	301	1	22	20	-10	57	57	1	97	101	4
ETC493	T-2-BUTE	MRE	3	0.42	0.93	0.35	301	1	93	95	2	122	127	4	123	127	3
ETC501	T-2-BUTE	MRE	3	0.42	0.72	0.35	300	1	64	67	5	110	118	7	127	133	4
ETC307	T-2-BUTE	MR3	2	0.54	0.60	0.35	300	1	52	46	-12	81	73	-10	109	102	-7
ETC309	T-2-BUTE	MR3	2	0.52	0.53	0.35	301	1	44	37	-18	75	66	-14	105	93	-14
DTC043B	T-2-BUTE	MRE	1	0.47	0.79	0.39	300	1	72	73	2	122	125	2	141	146	3
DTC021B	T-2-BUTE	MR8	1	0.49	1.06	0.39	300	1	90	87	-3	107	110	3	112	124	10

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC069A	T-2-BUTE	MR8	1	0.48	0.72	0.39	302	1	69	66	-5	89	90	1	106	112	5
DTC041A	T-2-BUTE	RE	1	0.17	0.79	0.39	300	1	71	75	5	76	82	7	70	76	8
DTC033A	T-2-BUTE	R8	1	0.17	0.65	0.39	300	1	55	58	4	58	61	5	59	63	6
ETC495	ISOPRENE	MRE	3	0.42	1.28	0.35	300	1	42	55	24	106	119	11	131	126	-4
ETC503	ISOPRENE	MRE	3	0.42	1.61	0.35	301	1	65	80	20	119	119	0	126	113	-11
ETC510	ISOPRENE	MRE	3	0.41	1.43	0.35	300	1	45	64	30	109	118	8	127	118	-7
ETC271	ISOPRENE	MR3	2	0.49	0.98	0.35	299	1	31	31	2	78	73	-7	118	115	-3
ETC273	ISOPRENE	MR3	2	0.49	0.92	0.35	301	1	31	32	1	80	74	-8	121	115	-4
ETC275	ISOPRENE	MR3	2	0.49	0.79	0.35	302	1	29	27	-4	73	64	-14	117	106	-11
ETC277	ISOPRENE	MR3	2	0.50	0.67	0.35	302	1	26	25	-7	68	59	-16	113	97	-16
DTC047B	ISOPRENE	MRE	1	0.48	1.02	0.39	301	1	36	39	8	102	106	4	145	146	1
DTC046A	ISOPRENE	RE	1	0.17	1.04	0.19	300	1	14	18	22	48	53	9	55	55	-1
DTC050B	ISOPRENE	RE	1	0.16	0.99	0.39	301	1	50	55	11	78	76	-2	76	71	-7
ETC508	A-PINENE	MRE	3	0.41	0.82	0.35	301	1	54	66	19	103	111	8	121	124	2
DTC045B	A-PINENE	MRE	1	0.48	0.79	0.39	301	1	40	48	17	105	111	5	140	145	4
DTC044A	A-PINENE	RE	1	0.16	0.79	0.39	300	1	58	64	9	73	77	5	70	73	5
DTC034B	A-PINENE	R8	1	0.16	0.93	0.39	301	1	49	49	1	48	49	3	46	50	8
DTC051B	B-PINENE	MRE	1	0.48	0.92	0.39	301	1	16	18	9	52	73	28	118	134	12
DTC048A	B-PINENE	RE	1	0.17	0.91	0.39	301	1	18	36	50	66	78	15	70	80	12
ETC263	BENZENE	MR3	2	0.48	0.73	0.35	303	1	24	30	19	82	92	11	91	110	17
ETC265	BENZENE	MR3	2	0.49	0.69	0.35	300	1	23	26	11	67	76	12	96	114	16
DTC039B	BENZENE	R8	1	0.18	0.76	0.39	301	1	53	60	13	50	57	13	47	54	13
ETC101	TOLUENE	MR3	2	0.50	0.38	0.36	300	1	13	16	19	39	43	8	65	71	9
ETC103	TOLUENE	MR3	2	0.52	0.38	0.36	301	1	14	14	5	40	42	6	68	70	4
DTC023A	TOLUENE	MR8	1	0.47	0.52	0.39	301	1	60	57	-6	100	94	-7	108	114	6
DTC030B	TOLUENE	R8	1	0.17	0.64	0.39	300	1	50	55	9	48	54	10	47	53	11
CTC108B	TOLUENE	MR3	5	0.31	0.54	0.19	295	2	19	24	20	53	60	11	-	76	
CTC127B	TOLUENE	MR8	5	0.39	0.65	0.18	293	2	46	49	7	68	77	12	-	83	
ETC311	C2-BENZ	MR3	2	0.52	0.42	0.35	297	1	11	12	9	36	38	4	61	62	2
ETC313	C2-BENZ	MR3	2	0.53	0.40	0.35	298	1	13	12	-8	38	35	-7	64	58	-10
ETC315	C2-BENZ	MR3	2	0.53	0.44	0.35	298	1	14	14	3	45	42	-7	78	70	-12
ETC196	M-XYLENE	MR3	2	0.48		0.35	300	1	19	24	23	54	61	11	92	101	9
ETC207	M-XYLENE	MR3	2	0.51		0.35	299	1	21	23	10	59	58	0	98	96	-2
ETC301	M-XYLENE	MR3	2	0.46	0.43	0.35	300	1	19	23	17	56	58	4	97	98	1
DTC025A	M-XYLENE	MR8	1	0.47	0.50	0.39	302	1	57	56	-2	91	90	0	114	116	2
DTC068B	M-XYLENE	MR8	1	0.48	0.43	0.39	301	1	47	47	0	75	74	-1	100	101	2
DTC035A	M-XYLENE	R8	1	0.17	0.49	0.39	301	1	54	55	2	55	56	2	56	57	2
DTC067B	M-XYLENE	R8	1	0.17	0.52	0.39	301	1	54	55	4	54	56	4	53	56	5
CTC109A	M-XYLENE	MR3	5	0.31	0.51	0.19	295	2	37	25	-44	49	61	19	-	78	
CTC128A	M-XYLENE	MR8	5	0.41	0.64	0.18	294	2	43	49	11	66	76	12	-	87	
ETC259	O-XYLENE	MR3	2	0.49	0.44	0.35	300	1	22	20	-6	56	54	-3	95	93	-1
ETC261	O-XYLENE	MR3	2	0.48	0.44	0.35	301	1	21	22	1	57	57	0	100	100	0
ETC348	P-XYLENE	MR3	2	0.52	0.49	0.35	303	1	23	23	0	63	61	-4	107	104	-3
ETC267	124-TMB	MR3	2	0.49	0.45	0.35	300	1	21	18	-16	54	49	-9	93	85	-9
ETC269	124-TMB	MR3	2	0.48	0.45	0.35	302	1	23	20	-11	59	54	-9	102	93	-10
ETC249	135-TMB	MR3	2	0.49	0.57	0.35	301	1	35	35	1	85	83	-2	126	126	0
ETC297	123-TMB	MR3	2	0.46	0.45	0.35	301	1	34	32	-9	86	73	-17	122	113	-8
ETC299	123-TMB	MR3	2	0.48	0.44	0.35	301	1	29	27	-8	76	65	-17	117	105	-11
CTC246A	STYRENE	MR3	9	0.25	1.60	0.13	295	6	5	4	-9	15	13	-15	30	25	-19
CTC250B	STYRENE	MR3	9	0.23	0.96	0.13	296	6	4	6	27	15	18	13	29	32	8
CTC248B	STYRENE	MR8	9	0.31	1.72	0.13	292	6	37	45	18	54	61	12	61	62	1
CTC251A	STYRENE	MR8	9	0.35	2.22	0.13	294	6	37	46	20	52	64	19	58	62	7
CTC249A	STYRENE	R8	9	0.16	1.74	0.13	295	6	32	33	5	31	31	0	28	28	-2
CTC253B	STYRENE	R8	9	0.16	1.30	0.13	295	6	35	37	3	38	36	-3	36	34	-6
CTC184B	ACETYLEN	MR3	7	0.23	0.91	0.16	298	17	34	28	-22	74	66	-13	81	73	-11
CTC185A	ACETYLEN	MR3	7	0.27	0.95	0.16	301	17	42	31	-33	85	74	-15	92	82	-12
CTC192A	ACETYLEN	MR3	7	0.22	0.67	0.16	298	17	20	18	-16	61	52	-16	77	67	-14
CTC186B	ACETYLEN	MR8	7	0.37	0.77	0.16	298	17	41	42	3	74	74	0	89	86	-4
CTC193B	ACETYLEN	MR8	7	0.37	0.92	0.16	298	17	51	49	-3	85	82	-3	93	89	-4
CTC187A	ACETYLEN	R8	7	0.15	0.85	0.16	298	17	43	41	-4	47	44	-6	46	42	-8
CTC194A	ACETYLEN	R8	8	0.15	1.06	0.16	297	17	44	43	-3	48	46	-6	47	43	-9
ETC285	MEOH	MR3	2	0.52	0.66	0.35	303	1	24	24	-1	71	66	-7	127	120	-6
ETC287	MEOH	MR3	2	0.51	0.41	0.35	303	1	17	17	2	48	46	-5	85	77	-11

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC289	MEOH	MR3	2	0.50	0.47	0.35	304	1	20	20	0	58	53	-10	105	93	-14
ETC131	ETOH	MR3	2	0.54	0.70	0.35	302	1	14	15	8	37	41	9	60	64	7
ETC133	ETOH	MR3	2	0.53	0.66	0.35	302	1	13	15	12	38	39	5	60	62	3
ETC138	ETOH	MR3	2	0.54	0.70	0.35	300	1	13	14	10	35	38	9	56	60	8
ETC148	I-C3-OH	MR3	2	0.51	1.19	0.35	302	1	19	20	8	47	49	2	82	81	-1
ETC155	I-C3-OH	MR3	2	0.50	0.67	0.35	300	1	22	19	-12	55	50	-9	93	85	-10
ETC157	I-C3-OH	MR3	2	0.51	0.60	0.35	300	1	19	17	-7	46	47	1	78	79	2
ETC159	I-C3-OH	MR3	2	0.50	0.65	0.35	301	1	18	19	2	47	50	5	81	85	4
DTC395A	I-C3-OH	MR3	11	0.40	2.39	0.19	299	10	25	25	-3	64	57	-12	96	93	-3
DTC398B	I-C3-OH	MR3	11	0.43	0.98	0.19	297	10	19	15	-31	47	36	-30	80	61	-32
DTC396B	I-C3-OH	MR8	11	0.29	2.52	0.19	299	10	63	70	10	81	91	11	77	100	23
DTC399A	I-C3-OH	MR8	11	0.27	0.75	0.19	298	10	40	37	-10	62	55	-11	72	68	-6
DTC397A	I-C3-OH	R8	11	0.13	1.36	0.19	298	10	45	45	1	50	55	10	47	59	20
DTC400B	I-C3-OH	R8	11	0.11	0.79	0.19	298	10	39	37	-5	44	44	0	43	46	7
DTC233A	T-C4-OH	MR3	10	0.30	0.75	0.23	296	3	15	18	15	40	48	18	69	82	16
DTC241B	T-C4-OH	MR3	10	0.32	0.95	0.23	295	3	16	15	-8	39	41	6	68	78	14
DTC249A	T-C4-OH	MR8	10	0.25	0.82	0.23	297	3	40	54	26	61	80	24	72	91	20
DTC256A	T-C4-OH	MR8	10	0.26	0.62	0.23	297	3	33	42	21	51	67	25	54	82	34
DTC259A	T-C4-OH	R8	10	0.16	0.70	0.23	297	3	39	48	19	51	62	19	54	67	19
DTC268A	T-C4-OH	R8	10	0.16	0.59	0.22	299	3	39	46	14	52	60	13	54	64	15
DTC269A	T-C4-OH	R8	10	0.17	0.75	0.22	299	3	45	51	12	57	66	13	59	70	15
DTC508B	1-C8-OH	MR3	15	0.37	0.93	0.22	299	10	5	6	6	15	15	-1	30	28	-7
DTC529A	1-C8-OH	MR3	14	0.36	0.54	0.21	299	10	9	10	5	27	26	-2	49	46	-7
DTC509A	1-C8-OH	MR8	14	0.30	0.50	0.22	299	10	32	26	-23	55	49	-13	70	64	-10
DTC519B	1-C8-OH	R8	15	0.12	0.60	0.21	298	10	35	36	3	43	45	4	45	47	5
DTC517A	2-C8-OH	MR3	14	0.37		0.21	299	10	10	11	6	32	30	-6	60	54	-12
DTC521B	2-C8-OH	MR8	15	0.30		0.21	299	10	34	31	-11	59	57	-4	74	72	-2
DTC524B	2-C8-OH	R8	15	0.13		0.21	299	10	38	37	-1	45	46	1	46	48	4
DTC514B	3-C8-OH	MR3	15	0.38		0.21	299	10	9	10	9	28	27	-3	52	48	-7
DTC516B	3-C8-OH	MR8	15	0.32		0.21	299	10	34	33	-3	55	53	-3	70	68	-3
DTC520A	3-C8-OH	R8	14	0.13		0.21	299	10	38	38	0	46	47	3	46	49	7
DTC385A	PR-GLYCL	MR3	11	0.39	2.50	0.19	298	11	27	28	1	64	58	-10	94	87	-8
DTC389B	PR-GLYCL	MR3	11	0.36	1.31	0.19	299	11	20	20	3	48	46	-5	78	74	-5
DTC386B	PR-GLYCL	MR8	11	0.29	1.17	0.19	298	11	49	45	-8	69	63	-9	76	74	-3
DTC390A	PR-GLYCL	MR8	11	0.28	1.01	0.19	297	11	43	42	-2	64	60	-6	75	72	-3
DTC388A	PR-GLYCL	R8	11	0.11	1.26	0.19	298	11	39	38	-2	45	44	0	43	45	4
DTC391B	PR-GLYCL	R8	11	0.11	0.80	0.19	297	11	37	34	-8	42	40	-6	41	40	-3
ETC279	ME-O-ME	MR3	2	0.50	0.85	0.35	303	1	28	27	-5	75	67	-11	132	121	-9
ETC281	ME-O-ME	MR3	2	0.51	0.77	0.35	303	1	25	25	2	66	63	-5	121	114	-6
ETC283	ME-O-ME	MR3	2	0.51	0.63	0.35	303	1	24	23	-3	65	59	-11	117	103	-13
ETC295	ME-O-ME	MR3	2	0.48	0.62	0.35	301	1	21	24	11	56	59	4	102	103	1
DTC510B	ET-O-ET	MR3	15	0.39	0.84	0.22	299	10	19	21	11	53	56	4	99	97	-2
DTC522A	ET-O-ET	MR3	14	0.37	1.34	0.21	299	10	23	28	18	73	79	8	116	115	-1
DTC511A	ET-O-ET	MR8	14	0.31	1.30	0.21	299	10	78	88	11	107	114	6	109	120	10
DTC515A	ET-O-ET	MR8	14	0.31	0.65	0.21	299	10	57	49	-16	87	76	-15	101	93	-9
DTC513A	ET-O-ET	R8	14	0.13	0.72	0.21	298	10	49	50	2	57	59	3	57	60	5
DTC525A	ET-O-ET	R8	14	0.13	0.56	0.21	299	10	46	44	-3	53	53	-1	54	54	0
ETC120	MTBE	MR3	2	0.53		0.35	301	1	12	14	12	33	38	15	56	66	15
ETC123	MTBE	MR3	2	0.52		0.35	305	1	16	17	6	44	46	5	81	85	4
ETC125	MTBE	MR3	2	0.51		0.35	302	1	10	14	27	31	40	21	55	70	21
ETC127	MTBE	MR3	2	0.53		0.35	302	1	12	13	7	34	37	8	58	64	9
DTC489A	MEOC3OH	MR3	14	0.38	2.05	0.22	298	15	31	28	-11	71	63	-14	104	95	-10
DTC495A	MEOC3OH	MR3	14	0.38	1.33	0.22	299	15	25	25	-1	59	56	-5	94	88	-6
DTC492A	MEOC3OH	MR8	14	0.31	1.39	0.22	298	15	58	61	4	80	81	2	91	92	1
DTC500A	MEOC3OH	MR8	14	0.30	0.93	0.22	298	15	49	52	5	70	71	2	82	83	2
DTC496B	MEOC3OH	R8	15	0.12	1.13	0.22	299	15	47	45	-3	53	53	0	52	54	3
DTC501B	MEOC3OH	R8	15	0.13	0.85	0.22	299	15	45	43	-3	51	50	0	51	52	2
ETC163	ETO-ETOH	MR3	2	0.49		0.35	302	1	27	35	22	80	91	12	143	142	-1
ETC171	ETO-ETOH	MR3	2	0.49	1.03	0.35	301	1	21	27	20	62	71	13	122	122	0
ETC175	ETO-ETOH	MR3	2	0.50		0.35	298	1	18	21	15	49	57	14	91	99	8
DTC491B	BUO-ETOH	MR3	15	0.38	1.44	0.22	298	15	15	11	-34	42	34	-23	85	73	-17
DTC498B	BUO-ETOH	MR3	15	0.38	0.93	0.22	299	15	9	8	-14	24	22	-8	42	42	-1
DTC505B	BUO-ETOH	MR3	15	0.38	1.07	0.22	298	15	12	11	-1	35	34	-1	69	69	-1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC493B	BUO-ETOH	MR8	15	0.30	0.99	0.22	297	15	57	59	5	85	87	2	97	98	2
DTC502A	BUO-ETOH	MR8	14	0.30	0.67	0.22	299	15	52	47	-11	78	73	-7	91	88	-4
DTC497A	BUO-ETOH	R8	14	0.13	0.87	0.22	299	15	48	48	-2	57	57	0	57	59	3
DTC506A	BUO-ETOH	R8	14	0.12	0.70	0.22	298	15	44	43	-3	52	51	-2	53	52	-1
ETC166	CARBITOL	MR3	2	0.51	1.43	0.35	304	1	19	19	-1	56	56	0	112	109	-2
ETC169	CARBITOL	MR3	2	0.51	1.21	0.35	300	1	16	15	-11	44	44	-1	82	81	-1
ETC173	CARBITOL	MR3	2	0.51	2.29	0.35	300	1	15	14	-4	42	45	6	87	97	10
DTC327A	ME-ACET	MR3	11	0.34	0.64	0.21	297	9	15	18	18	40	44	11	67	76	11
DTC328B	ME-ACET	MR3	11	0.32	0.72	0.21	297	9	13	19	30	37	47	21	66	79	16
DTC336A	ME-ACET	MR3	11	0.32	0.77	0.21	296	9	17	18	9	42	46	9	69	77	11
DTC332A	ME-ACET	MR8	11	0.57	0.52	0.21	297	9	19	20	3	37	37	2	46	48	4
DTC335B	ME-ACET	MR8	11	0.42	0.55	0.21	297	9	26	30	12	45	50	11	57	65	13
DTC329A	ME-ACET	R8	11	0.17	0.64	0.21	296	9	41	47	13	55	59	6	59	63	6
DTC330B	ME-ACET	R8	11	0.17	0.55	0.21	296	9	38	43	12	53	56	5	58	60	4
DTC358A	ET-ACET	MR3	11	0.33	0.88	0.20	298	10	13	13	-1	28	28	3	40	42	5
DTC362B	ET-ACET	MR3	11	0.30	0.79	0.20	298	10	11	13	14	25	29	12	39	45	12
DTC364B	ET-ACET	MR3	11	0.32	0.78	0.20	298	10	12	13	2	28	28	2	41	42	4
DTC359B	ET-ACET	MR8	11	0.27	0.78	0.20	298	10	28	30	6	42	46	8	51	58	11
DTC408B	ET-ACET	MR8	11	0.28	1.03	0.19	298	10	32	28	-12	45	43	-4	55	54	-2
DTC415B	ET-ACET	R3	11	0.20	0.76	0.19	297	10	12	11	-11	26	23	-13	42	37	-13
DTC394A	ET-ACET	R8	11	0.11	0.75	0.19	296	10	25	24	-2	31	33	5	33	36	8
DTC409A	ET-ACET	R8	11	0.11	0.94	0.19	298	10	25	23	-6	31	32	3	33	36	7
CTC195B	ET-ACET	R8	8	0.14	0.85	0.15	297	10	34	31	-8	40	37	-9	42	38	-8
DTC688B	IPR-ACET	MR3	18	0.43	1.40	0.17	294	20	19	16	-19	51	42	-19	95	78	-23
DTC689A	IPR-ACET	MR8	18	0.32	1.06	0.16	294	20	70	65	-8	101	94	-8	114	104	-10
DTC697A	IPR-ACET	MR8	18	0.32	0.66	0.16	296	20	46	41	-12	75	67	-11	91	83	-9
DTC528B	ME-IBUAT	MR3	15	0.38	0.88	0.21	299	10	10	13	23	29	30	5	49	46	-5
DTC533A	ME-IBUAT	MR3	14	0.36	0.74	0.21	299	10	10	14	30	31	34	9	53	53	0
DTC530B	ME-IBUAT	MR8	15	0.31	0.76	0.21	299	10	33	33	-2	54	50	-9	71	64	-11
DTC534B	ME-IBUAT	MR8	15	0.29	0.94	0.21	299	10	32	35	8	56	53	-4	73	68	-9
DTC531A	ME-IBUAT	R8	14	0.12	0.77	0.21	299	10	34	33	-5	44	40	-9	47	42	-11
DTC539A	ME-IBUAT	R8	14	0.13	0.92	0.21	299	10	34	33	-1	44	42	-5	47	44	-6
DTC548A	ME-IBUAT	R8	14	0.13	1.09	0.20	299	10	34	32	-7	44	42	-5	48	46	-4
CTC216B	TBU-ACET	MR3	8	0.23		0.14	298	19	9	8	-13	30	29	-3	56	56	-1
CTC221A	TBU-ACET	MR3	8	0.24	0.80	0.14	299	19	8	7	-8	27	26	-4	54	53	-1
CTC217A	TBU-ACET	MR8	8	0.42	0.86	0.14	297	19	44	42	-4	77	85	9	96	102	6
CTC222B	TBU-ACET	MR8	8	0.43	0.71	0.14	299	19	39	34	-16	70	71	2	89	90	2
CTC220B	TBU-ACET	R8	8	0.16	0.82	0.14	298	19	46	47	1	54	55	1	55	55	1
CTC223A	TBU-ACET	R8	8	0.16	0.90	0.14	298	19	49	49	1	57	58	1	59	59	0
DTC365A	BU-ACET	MR3	11		1.45	0.20	298	22	9	9	2	20	21	5	33	35	7
DTC368B	BU-ACET	MR3	11		1.53	0.20	299	22	8	9	8	19	21	9	32	35	9
DTC402B	BU-ACET	MR3	11		1.10	0.19	299	22	9	10	5	24	24	0	39	39	0
DTC403A	BU-ACET	MR8	11	0.29	1.25	0.19	299	22	37	40	7	58	62	7	70	76	8
DTC410B	BU-ACET	MR8	11	0.26	1.63	0.19	298	22	41	39	-5	61	60	-1	71	73	2
DTC406A	BU-ACET	R8	11	0.12	1.00	0.19	299	22	35	36	3	42	44	3	44	46	4
DTC411A	BU-ACET	R8	11	0.11	1.63	0.19	297	10	34	34	1	41	43	4	43	46	7
DTC235B	PC	MR3	10	0.30	0.51	0.23	297	10	13	17	25	33	41	20	57	70	18
DTC239B	PC	MR3	10	0.31	0.68	0.23	297	10	14	17	22	32	37	13	56	60	7
DTC243A	PC	MR3	10	0.32	1.09	0.23	296	10	20	16	-29	37	33	-9	59	58	-1
DTC264B	PC	MR3	10	0.30	0.68	0.22	298	10	13	17	22	32	38	17	54	67	19
DTC250B	PC	MR8	10	0.26	0.70	0.23	297	10	39	44	12	56	66	15	67	82	18
DTC260B	PC	R8	10	0.17	0.55	0.22	297	10	37	42	13	49	58	16	53	65	18
DTC266A	PC	R8	10	0.16	0.65	0.22	298	22	36	44	19	47	60	23	51	67	25
DTC532B	PGME-ACT	MR3	15	0.36	0.98	0.21	299	22	10	10	4	25	24	-2	40	39	-4
DTC537A	PGME-ACT	MR3	14	0.35	0.73	0.21	299	22	11	11	2	29	27	-8	48	43	-11
DTC549B	PGME-ACT	MR3	15	0.37	1.06	0.20	300	22	12	10	-18	28	23	-20	45	37	-23
DTC538B	PGME-ACT	MR8	15	0.29	0.94	0.21	299	22	36	35	-4	54	53	-1	68	68	1
DTC547B	PGME-ACT	MR8	15	0.30	1.24	0.20	300	22	39	35	-12	58	55	-5	72	70	-3
CTC197B	DBE-4	MR3	8	0.25		0.15	297	22	9	9	0	27	27	-3	51	50	-2
CTC211B	DBE-4	MR3	8	0.22	0.96	0.15	298	22	8	10	19	26	30	12	50	52	3
CTC198A	DBE-4	MR8	8	0.39	1.52	0.15	298	22	57	62	7	93	89	-4	109	98	-11
CTC208A	DBE-4	MR8	8	0.43	1.14	0.15	298	22	47	54	14	80	84	5	99	96	-3
CTC199B	DBE-4	R8	8	0.15	1.07	0.15	298	22	48	44	-8	56	50	-10	56	51	-9

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC210A	DBE-4	R8	8	0.16	1.36	0.15	298	22	50	46	-9	59	53	-11	59	54	-9
CTC201A	DBE-5	MR3	8	0.25	1.60	0.15	298	3	4	4	-2	11	12	3	22	22	3
CTC209B	DBE-5	MR3	8	0.25	1.03	0.15	298	3	6	5	-5	18	17	-3	33	33	2
CTC204A	DBE-5	MR8	8	0.44	1.21	0.15	298	3	37	38	3	70	78	11	88	93	6
CTC212B	DBE-5	MR8	8			0.15	298	3	33	32	-4	64	74	13	81	90	10
CTC205B	DBE-5	R8	8	0.16	1.20	0.15	298	3	45	44	-1	53	52	-3	54	53	-2
CTC215A	DBE-5	R8	8	0.18	1.46	0.15	297	3	48	46	-3	57	55	-4	58	57	-3
ETC470	FORMALD	MRE	3	0.39	0.63	0.35	301	3	56	81	30	119	130	8	137	137	0
ETC489	FORMALD	MRE	3	0.42	0.64	0.35	301	10	51	81	37	118	133	11	138	142	3
ETC352	FORMALD	MR3	2	0.53	0.46	0.35	303	10	35	39	10	71	74	4	111	113	2
ETC357	FORMALD	MR3	2	0.53	0.52	0.35	303	10	46	56	18	86	102	16	120	136	12
DTC022B	FORMALD	MR8	1	0.51	0.56	0.39	300	10	62	66	6	89	96	7	108	118	8
DTC036A	FORMALD	R8	1	0.18	0.53	0.39	300	10	60	63	5	64	68	5	64	68	7
CTC138B	FORMALD	MR8	6	0.40	0.60	0.18	293	18	42	42	1	61	65	6	75	81	7
CTC140A	FORMALD	MR8	6	0.36	0.62	0.18	294	18	39	46	15	58	68	14	73	81	10
ETC335	ACETALD	MR3	2	0.54	0.80	0.35	303	18	41	41	-1	71	70	-2	103	101	-2
ETC338	ACETALD	MR3	2	0.52	1.14	0.35	303	18	46	46	0	74	75	2	102	105	2
DTC065A	ACETALD	MR8	1	0.45	1.31	0.39	301	18	54	58	6	79	87	10	98	109	10
DTC066B	ACETALD	R8	1	0.18	1.37	0.39	302	18	43	47	8	51	57	11	55	62	13
CTC107A	ACETALD	MR3	5	0.31	0.78	0.19	295	18	18	20	10	31	33	5	-	44	
CTC266A	BENZALD	MR4	10	0.23	0.53	0.12	299	18	4	2	-61	16	8	-100	30	16	-82
CTC267B	BENZALD	R8	10	0.16	0.65	0.12	300	18	31	31	2	35	36	4	35	36	5
ETC480	ACETONE	MRE	3	0.42	0.58	0.35	301	18	28	42	33	72	100	29	120	133	10
ETC481	ACETONE	MRE	3	0.42	0.57	0.35	301	18	31	45	31	72	101	28	119	132	10
ETC490	ACETONE	MRE	3	0.42	0.58	0.35	301	18	37	48	22	89	103	13	125	131	4
ETC243	ACETONE	MR3	2	0.49	0.38	0.35	301	1	17	18	1	47	45	-3	78	73	-6
ETC245	ACETONE	MR3	2	0.50	0.40	0.35	302	1	22	23	5	51	53	3	86	85	-1
ETC247	ACETONE	MR3	2	0.49	0.40	0.35	301	1	25	27	4	56	57	2	92	90	-2
DTC028A	ACETONE	MR8	1	0.48	0.49	0.39	301	1	51	55	8	78	86	9	103	113	9
DTC064B	ACETONE	MR8	1	0.49	0.52	0.39	302	1	59	63	5	90	100	10	115	130	11
OTC275A	ACETONE	R8	11	0.56	0.53	0.00	319	1	133	122	-9	170	175	3	159	178	11
OTC276B	ACETONE	R8	11	0.57	0.47	0.00	315	2	95	91	-5	150	151	1	-	166	
DTC338A	MEK	MR8	11	0.29	0.57	0.21	297	2	38	40	7	54	58	7	64	70	8
DTC345B	MEK	MRX	11	0.34	0.56	0.20	300	1	26	27	2	52	52	1	75	76	2
DTC363A	MEK	MRX	11	0.32	0.60	0.20	298	1	30	30	-1	54	54	1	75	75	1
CTC181A	MEK	MR3	7	0.23	0.56	0.16	298	1	24	22	-11	47	40	-16	62	55	-12
CTC180B	MEK	MR8	7	0.39	0.75	0.16	298	1	47	46	-1	67	66	-2	82	79	-4
CTC255A	MPK	MR3	9	0.22	0.44	0.13	296	2	11	14	21	25	26	7	39	38	-2
CTC260B	MPK	MR8	10	0.38	0.66	0.12	295	6	38	43	12	57	63	9	71	74	4
CTC263B	MPK	MR8	10	0.16	0.60	0.12	294	6	36	35	-4	41	40	-1	40	40	-2
CTC258B	MPK	R8	10	0.17		0.13	296	1	38	36	-4	43	43	-2	-	43	
DTC554B	CC6-KET	MR3	15	0.37		0.20	299	1	9	8	-21	22	19	-13	33	31	-7
DTC558A	CC6-KET	MR3	14	0.34		0.20	300	1	10	9	-7	23	23	-3	38	37	-3
DTC556A	CC6-KET	MR8	14	0.28		0.20	300	1	26	32	17	44	50	12	56	63	11
DTC559A	CC6-KET	MR8	14	0.29	0.42	0.20	299	1	28	32	13	46	49	6	60	62	3
DTC557B	CC6-KET	R8	15	0.12		0.20	300	1	28	31	12	37	39	6	39	41	6
CTC235A	CC6-KET	R8	9	0.16		0.14	301	1	31	35	12	38	41	8	-	42	
CTC238A	CC6-KET	R8	9	0.17		0.13	301	1	36	37	5	43	44	1	-	45	
DTC366B	MIBK	MR3	11	0.32		0.20	298	8	17	19	9	32	33	2	47	45	-3
DTC369A	MIBK	MR3	11	0.35		0.20	298	8	19	21	7	35	35	2	50	49	-4
DTC370B	MIBK	MR8	11	0.29		0.20	298	10	32	34	5	50	52	4	63	67	6
DTC414A	MIBK	MR8	11	0.27		0.19	298	10	37	36	-3	56	54	-4	67	68	1
DTC412B	MIBK	R8	11	0.11		0.19	297	10	27	26	-1	29	34	15	30	36	18
DTC418A	MIBK	R8	11	0.11		0.19	298	10	27	27	-1	32	34	5	33	36	6
CTC183A	MIBK	MR3	7	0.23		0.16	298	10	11	10	-9	22	19	-13	32	27	-20
CTC182B	MIBK	MR8	7	0.38		0.16	298	20	42	39	-9	63	60	-4	78	75	-3
CTC257A	C7-KET-2	MR3	10	0.24	0.45	0.13	297	20	4	4	11	11	11	0	20	19	-9
CTC262A	C7-KET-2	MR8	10	0.38	0.60	0.12	294	20	29	29	0	58	64	8	73	76	4
CTC259A	C7-KET-2	R8	10	0.17	0.64	0.12	295	20	38	40	4	45	47	4	44	48	8
DTC447A	TDI	MR3	12	0.42	0.99	0.17	297	10	2	4	46	7	9	17	15	15	0
DTC450A	TDI	MR3	12	0.37	0.64	0.17	297	10	8	8	4	25	21	-17	42	34	-25
DTC456A	TDI	MR8	12	0.28	0.53	0.17	297	10	15	14	-7	31	28	-9	39	35	-12
DTC459A	TDI	MR8	12	0.30	0.43	0.16	298	10	19	21	6	37	36	-2	46	45	-1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC453A	TDI	R8	12	0.16	0.86	0.17	295	10	9	8	-7	18	15	-17	21	20	-8
DTC454A	TDI	R8	12	0.13	0.51	0.17	297	10	20	22	8	26	26	0	26	25	-2
DTC462B	TDI	R8	13	0.14	0.54	0.16	299	10	19	23	15	28	27	-2	29	26	-9
DTC467A	TDI2	MR3	12	0.37	0.61	0.16	294	10	5	6	19	15	16	9	28	27	-5
DTC466A	TDI2	R8	12	0.15	0.46	0.16	297	10	21	21	0	-	27		27	27	-2
DTC601A	P-TI	MR3	16	0.39	0.58	0.19	298	10	11	16	27	33	37	11	57	57	1
DTC602A	P-TI	MR3	16	0.45	1.37	0.19	298	10	8	11	25	27	29	7	50	47	-6
DTC618A	P-TI	MR3	16	0.56	2.81	0.18	297	10	7	9	18	22	23	3	41	38	-8
DTC610A	P-TI	MR8	16	0.31	2.80	0.19	297	10	25	33	24	47	51	8	53	49	-8
DTC604B	P-TI	R8	17	0.20	1.24	0.19	298	10	31	31	1	33	33	0	32	32	1
DTC608A	P-TI	R8	16	0.15	2.05	0.19	297	10	29	34	14	32	33	3	30	32	5
DTC240A	NMP	MR3	10	0.31		0.23	296	20	9	8	-18	23	26	10	63	71	10
DTC244B	NMP	MR3	10	0.38		0.23	295	20	9	9	-8	24	30	20	-	76	
DTC252A	NMP	MR8	10	0.26		0.23	297	20	48	56	13	53	63	16	50	60	17
DTC255B	NMP	MR8	10	0.27		0.23	297	14	30	30	-1	55	60	8	54	61	11
DTC261A	NMP	R8	10	0.16		0.22	296	14	33	37	10	40	46	12	39	45	13
DTC267B	NMP	R8	10	0.16		0.22	299	14	39	42	7	43	47	7	41	45	9
DTC421A	C3-BR	MR3	11	0.38	0.81	0.19	297	14	18	17	-2	65	43	-50	66	73	10
DTC433A	C3-BR	MR3	11	0.39	0.60	0.18	297	14	17	13	-23	55	35	-55	82	59	-39
DTC423B	C3-BR	MR8	11	0.29	0.65	0.19	297	14	32	48	33	53	68	22	57	76	25
DTC427A	C3-BR	MR8	11	0.26	0.72	0.18	298	14	36	51	30	58	71	18	50	78	36
DTC424A	C3-BR	R8	11	0.10	0.55	0.18	297	14	31	32	5	30	34	13	28	34	18
DTC428B	C3-BR	R8	11	0.11	0.73	0.18	298	14	31	38	20	29	43	34	26	43	39
DTC401A	C4-BR	MR3	11	0.35	1.65	0.19	298	23	17	34	51	68	77	12	52	100	48
DTC426B	C4-BR	MR3	11	0.34	1.15	0.18	297	23	15	27	45	63	64	2	68	90	25
DTC419B	C4-BR	MR8	11	0.28	1.14	0.19	297	23	43	67	35	61	85	28	49	90	46
DTC430A	C4-BR	MR8	11	0.24	0.94	0.18	297	23	39	58	34	60	75	20	49	81	40
DTC420B	C4-BR	R8	11	0.11	1.16	0.19	297	23	32	42	22	29	48	39	26	48	47
DTC432B	C4-BR	R8	11	0.12	1.54	0.18	297	23	33	45	27	29	53	45	26	55	53
DTC303B	CL3-ETHE	MR3	11	0.33		0.21	298	3	24	35	31	91	79	-15	87	101	13
DTC305A	CL3-ETHE	MR3	11	0.33		0.21	299	3	12	20	42	39	51	23	76	81	6
DTC308B	CL3-ETHE	MR8	11	0.17		0.21	301	3	37	39	5	47	53	12	46	58	20
DTC311B	CL3-ETHE	MR8	11	0.29		0.21	298	3	33	35	8	60	55	-8	66	70	5
DTC320A	CL3-ETHE	MR8	11	0.30		0.21	297	3	28	32	11	48	49	3	59	64	8
DTC309A	CL3-ETHE	R8	11	0.17		0.21	299	3	46	50	8	45	57	21	43	57	26
DTC321B	CL3-ETHE	R8	11	0.11		0.21	298	12	33	37	9	34	42	19	33	43	23
DTC312A	CL3-ETHE	RX	11	0.32		0.21	299	12	18	17	-4	48	44	-9	76	74	-3
DTC692B	DMC	MR3	18	0.44	0.82	0.16	298	12	18	14	-30	46	34	-34	77	57	-36
DTC703B	DMC	MR3	18	0.42	1.04	0.16	296	12	18	16	-8	46	39	-16	79	68	-16
DTC693A	DMC	MR8	18	0.31	0.71	0.16	298	12	46	48	3	71	69	-2	86	82	-5
DTC705A	DMC	MR8	18	0.29	0.64	0.16	296	12	37	41	10	-	62		78	74	-5
DTC698B	DMC	R8	18	0.10	0.69	0.16	295	10	36	34	-4	41	40	-4	42	41	-1
DTC763B	DMC	R8	18	0.09		0.16	299	12	28	32	10	32	35	9	32	36	10
DTC750B	MIPR-CB	MR3	18	0.35		0.16	300	12	17	16	-12	44	41	-7	74	73	-1
DTC759A	MIPR-CB	MR3	18	0.37		0.16	299	12	12	14	12	37	36	-2	70	67	-5
DTC755A	MIPR-CB	MR8	18	0.29		0.16	299	12	50	51	2	77	74	-4	88	84	-4
DTC762A	MIPR-CB	MR8	18	0.30		0.16	299	12	39	37	-6	65	61	-6	78	75	-3
DTC758B	MIPR-CB	R8	18	0.09		0.16	299	24	35	35	0	40	40	0	40	40	1
DTC763B	MIPR-CB	R8	18	0.09		0.16	299	24	28	32	10	32	35	9	32	36	10
DTC694A	ME-PVAT	MR3	18	0.40	0.81	0.16	298	24	8	8	2	22	19	-14	38	32	-20
DTC701B	ME-PVAT	MR3	18	0.39	0.95	0.16	296	24	7	7	-2	18	16	-15	31	26	-21
DTC695B	ME-PVAT	MR8	18	0.31	0.81	0.16	299	24	28	31	8	54	56	5	69	71	2
DTC702A	ME-PVAT	MR8	18	0.32	1.01	0.16	297	24	27	27	-1	54	53	-1	71	67	-5
DTC700A	ME-PVAT	R8	18	0.11	0.96	0.16	296	24	30	29	-1	36	35	-5	39	35	-9
DTC707B	ME-PVAT	R8	18	0.11	1.21	0.16	297	24	27	28	5	35	36	2	38	38	1
DTC442A	MS-A	MR3	11	0.34		0.17	294	13	5	7	22	16	21	22	31	37	15
DTC486A	MS-A	MR8	14	0.30		0.22	298	13	33	27	-22	57	51	-11	72	68	-6
DTC487B	MS-A	R8	15	0.13		0.22	298	13	36	36	2	42	42	0	43	42	-2
DTC441B	MS-B	MR3	11	0.35		0.18	294	13	6	6	5	15	17	10	26	29	10
DTC480A	MS-B	MR8	14	0.29		0.22	298	13	27	22	-23	50	46	-10	66	61	-7
DTC481B	MS-B	R8	15	0.13		0.22	298	13	34	35	3	42	43	3	42	44	3
DTC440A	MS-C	MR3	11	0.36		0.18	296	13	6	7	10	18	19	6	32	34	4
DTC478A	MS-C	MR8	14	0.30		0.22	297	13	30	27	-11	52	50	-4	66	67	0

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC479B	MS-C	R8	15	0.14		0.22	297	13	36	38	4	45	46	3	46	47	2
DTC439B	MS-D	MR3	11	0.35		0.18	297	13	7	6	-9	21	19	-10	36	33	-8
DTC476A	MS-D	MR8	14	0.31		0.22	298	13	30	23	-30	53	46	-14	68	62	-10
DTC477B	MS-D	R8	15	0.13		0.22	297	13	36	38	4	43	44	3	43	44	3
DTC753A	D95	MR3	18	0.41		0.16	299	25	4	4	6	13	12	-12	26	22	-17
DTC757A	D95	MR3	18	0.38		0.16	299	25	6	6	-12	20	16	-30	37	29	-29
DTC754B	D95	MR8	18	0.30		0.16	299	25	17	17	2	40	40	1	51	52	2
DTC772B	D95	MR8	18	0.30		0.16	299	25	15	17	14	40	43	8	51	57	11
DTC756B	D95	R8	0	0.13		0.16	299	25	28	30	9	35	39	10	36	41	12
DTC778A	D95	R8	18	0.09		0.16	300	25	25	27	8	29	31	4	29	30	3
DTC719A	ISOPARM	MRX	18	0.40		0.16	294	25	8	7	-15	24	18	-31	42	32	-29
DTC724B	ISOPARM	MR3	18	0.33		0.16	294	25	4	4	1	12	10	-18	24	19	-27
DTC720B	ISOPARM	MR8	18	0.32		0.16	296	25	20	13	-56	43	33	-31	55	46	-20
DTC771A	ISOPARM	MR8	18	0.29		0.16	299	25	18	15	-19	44	40	-10	57	53	-6
DTC723A	ISOPARM	R8	18	0.11		0.16	295	25	29	28	-1	34	34	2	34	35	4
DTC775B	ISOPARM	R8	0	0.09		0.16	299	25	27	27	0	31	30	-2	30	30	0
DTC760B	OC10ACET	MR3	18	0.39		0.16	298	25	10	6	-75	23	14	-58	37	25	-46
DTC773A	OC10ACET	MR3	0	0.38		0.16	300	25	5	5	-17	16	12	-30	31	23	-35
DTC769A	OC10ACET	MR8	18	0.27		0.16	299	25	14	21	34	40	44	9	53	56	7
DTC776A	OC10ACET	MR8	18	0.30		0.16	300	25	21	19	-8	44	41	-9	57	53	-8
DTC770B	OC10ACET	R8	18	0.08		0.16	299	25	20	26	23	23	29	21	23	29	21
DTC771A	OC10ACET	R8	18	0.29		0.16	299	25	18	15	-19	44	40	-10	57	53	-6
VOC Mixture - NOx Runs (Including Base Case Reactivity Experiments)																	
EC166	MIX-A		1	0.11	0.25	0.35	301	1	26	18	-45	44	33	-36	53	44	-21
EC172	MIX-A		1	0.10	0.08	0.37	301	1	14	11	-24	23	20	-19	33	27	-23
EC144	MIX-E		1	0.51	0.88	0.31	301	1	130	94	-38	136	125	-9	116	113	-2
EC145	MIX-E		1	1.00	0.77	0.31	301	1	65	61	-7	107	103	-4	151	137	-11
EC149	MIX-E		1	1.00	0.89	0.31	301	1	77	65	-19	94	90	-4	107	103	-4
EC150	MIX-E		1	1.02	0.90	0.32	301	1	78	72	-8	116	108	-8	157	136	-16
EC151	MIX-E		1	2.06	1.47	0.31	301	1	91	94	3	128	136	6	152	161	5
EC152	MIX-E		1	0.51	0.96	0.32	301	1	93	86	-7	117	111	-5	108	109	1
EC153	MIX-E		1	0.99	1.70	0.33	302	1	153	140	-9	174	172	-1	157	160	1
EC160	MIX-E		1	1.01	0.73	0.34	301	1	75	57	-31	117	95	-23	163	125	-30
EC161	MIX-E		1	0.54	0.83	0.34	301	1	96	75	-29	123	104	-18	-		
XTC111	MIX-AE		1	0.22	1.14	0.25	303	1	7	5	-30	26	16	-65	65	39	-65
EC163	MIX-AO		1	0.51	0.47	0.34	300	1	40	33	-19	61	50	-21	80	63	-26
EC217	MIX-EO		1	0.48	0.19	0.43	301	1	12	20	41	19	32	39	26	40	36
EC257	MIX-EO		1	0.52	0.25	0.29	303	1	33	33	-1	46	47	2	52	53	3
EC272	MIX-RO		1	0.48	0.35	0.34	302	1	43	47	9	65	74	13	81	92	13
EC335	MIX-RO		1	0.50	0.42	0.38	302	1	54	63	15	77	96	20	73	93	22
EC336	MIX-RO		1	0.49	0.34	0.38	302	1	67	87	23	70	94	26	63	88	28
EC337	MIX-RO		1	0.51	0.30	0.38	302	1	34	35	2	66	72	8	62	77	19
EC338	MIX-RO		1	0.50	0.42	0.37	302	1	61	64	4	86	107	20	78	105	25
EC339	MIX-RO		1	0.50	0.21	0.37	302	1	19	16	-20	41	37	-13	60	54	-10
DTC073B	MIX-AR		1	0.49	0.44	0.39	302	1	5	6	20	12	13	6	23	22	-7
DTC076A	MIX-AR		1	0.48	0.31	0.39	302	1	6	9	38	18	22	20	33	35	7
EC328	MIX-AR		1	0.50	0.33	0.42	303	1	46	50	8	74	89	18	89	112	20
EC331	MIX-AR		1	0.52	0.65	0.41	302	1	91	110	17	81	103	21	73	94	22
ETC218	MIX-ER		2	0.47	0.61	0.35	299	1	79	75	-4	114	108	-6	106	101	-5
EC329	MIX-ER		1	0.50	0.22	0.41	302	1	42	46	10	69	80	14	76	95	20
EC330	MIX-ER		1	0.32	0.22	0.42	302	1	45	51	12	53	69	22	49	65	25
EC334	MIX-ER		1	0.50	0.32	0.39	302	1	63	70	10	75	96	22	69	91	24
ITC437	SURG-4		2	0.08	0.35	0.46	305	1	37	41	10	42	45	6	46	47	3
ITC438	SURG-4		2	0.08	0.37	0.46	302	1	30	40	25	33	43	23	36	45	22
ITC440	SURG-4		2	0.08	0.17	0.45	302	1	20	29	31	31	41	24	37	46	19
ITC442	SURG-4		2	0.14	0.34	0.45	303	1	37	49	25	55	62	11	60	66	9
ITC444	SURG-4		2	0.14	0.16	0.44	303	1	15	24	36	29	42	33	41	56	27
ITC446	SURG-4		2	0.07	0.39	0.44	302	1	29	36	20	29	37	20	30	36	17
ITC450	SURG-4		2	0.08	0.35	0.43	302	1	33	39	17	38	42	9	40	44	9
ITC452	SURG-4		2	0.08	0.33	0.43	302	1	31	39	21	38	43	12	40	45	11
ITC456	SURG-4		2	0.08	0.41	0.42	301	1	31	41	25	37	44	17	39	46	15
ITC459	SURG-4		2	0.08	0.35	0.42	301	1	31	38	19	37	40	7	39	42	8

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ITC461	SURG-4		2	0.09	0.35	0.41	302	1	30	39	23	37	42	12	39	44	12
ITC465	SURG-4		2	0.09	0.33	0.41	301	1	32	40	21	39	44	13	40	46	13
ITC467	SURG-4		2	0.09	0.33	0.40	302	1	29	41	30	36	46	20	38	47	21
ITC471	SURG-4		2	0.09	0.33	0.40	302	1	29	39	27	36	43	18	37	46	20
ITC483	SURG-4		2	0.08	0.34	0.39	302	1	30	38	22	35	41	15	39	43	8
ITC488	SURG-4		2	0.08	0.39	0.38	303	1	28	39	27	34	42	18	35	44	19
ITC489	SURG-4		2	0.09	0.35	0.38	302	1	28	38	27	34	41	17	36	43	16
ITC497	SURG-4		2	0.09	0.34	0.38	301	1	27	38	29	34	41	17	36	43	16
ITC501	SURG-4		2	0.09	0.34	0.38	302	1	30	39	23	37	42	13	39	44	12
ITC503	SURG-4		2	0.09	0.34	0.37	302	1	27	40	32	33	44	24	35	46	23
ITC571	SURG-4		4	0.11	0.33	0.36	298	1	28	38	28	39	46	16	-	48	
ITC572	SURG-4		4	0.12	0.34	0.36	299	1	34	39	14	40	48	16	45	50	9
ITC574	SURG-4		4	0.09	0.33	0.36	301	1	33	38	14	39	44	12	41	46	11
ITC578	SURG-4		4	0.09	0.32	0.36	299	1	30	36	17	38	40	5	42	42	0
ITC580	SURG-4		4	0.09	0.33	0.36	299	1	31	37	18	42	42	1	44	43	0
ITC581	SURG-4		4	0.09	0.48	0.35	300	1	37	41	10	41	41	1	43	42	-2
ITC584	SURG-4		4	0.09	0.36	0.35	300	1	34	38	11	43	42	-2	45	44	-4
ITC586	SURG-4		4	0.08	0.34	0.35	301	1	34	36	6	40	39	-3	43	41	-6
ITC590	SURG-4		4	0.09	0.33	0.35	302	1	31	37	17	40	42	4	44	44	-1
ITC598	SURG-4		4	0.10	0.37	0.35	300	1	34	39	14	42	43	4	44	45	1
ITC603	SURG-4		4	0.09	0.34	0.35	300	1	31	38	18	39	41	6	41	42	4
ITC607	SURG-4		4	0.10	0.37	0.35	302	1	34	40	15	43	44	3	45	46	1
ITC609	SURG-4		4	0.09	0.37	0.35	301	1	32	39	18	41	42	4	44	44	1
ITC613	SURG-4		4	0.08	0.37	0.35	301	1	31	37	17	38	40	5	40	42	3
EC676	SURG-4		1	0.09	0.40	0.37	301	1	20	38	47	19	39	50	16	41	61
ITC573	SURG-4R		4	0.11	0.18	0.36	300	1	24	26	7	-	40		43	47	8
EC231	SURG-7		1	0.68	0.97	0.29	302	1	78	105	26	104	131	21	96	119	19
EC232	SURG-7		1	0.48	0.47	0.29	302	1	37	33	-11	60	66	9	75	90	17
EC233	SURG-7		1	0.09	0.48	0.29	302	1	36	42	14	41	50	17	41	50	18
EC237	SURG-7		1	0.46	0.84	0.29	302	1	74	93	21	101	112	10	94	103	9
EC238	SURG-7		1	0.91	0.82	0.29	303	1	61	82	26	97	135	28	128	158	19
EC241	SURG-7		1	0.47	0.40	0.28	302	1	34	43	21	56	73	23	76	95	20
EC242	SURG-7		1	0.46	1.47	0.29	302	1	102	107	4	83	86	3	77	76	-1
EC243	SURG-7		1	0.47		0.29	302	1	107	111	4	-			-		
EC245	SURG-7		1	0.94	1.47	0.29	302	1	136	164	17	151	151	0	133	131	-2
EC246	SURG-7		1	0.48	0.44	0.29	302	1	35	37	5	55	62	11	73	84	13
EC247	SURG-7		1	0.48	0.72	0.29	302	1	77	94	18	100	106	5	-		
ITC626	SURG-8S		5	0.29	0.51	0.35	296	1	26	29	10	53	68	23	73	87	16
ITC630	SURG-8S		5	0.31	0.25	0.35	298	1	13	11	-17	22	23	4	31	35	11
ITC631	SURG-8S		5	0.32	0.14	0.35	300	1	8	5	-58	12	10	-19	17	15	-14
ITC633	SURG-8S		5	0.61	0.51	0.35	299	1	17	14	-20	31	34	9	42	53	20
ITC635	SURG-8S		5	1.19	0.52	0.35	300	1	13	8	-69	23	20	-19	31	32	3
ITC637	SURG-8S		5	0.30	0.51	0.35	299	1	28	28	1	54	68	20	71	88	19
ITC865	SURG-8S		9	0.31	0.63	0.35	296	1	30	33	10	62	79	21	80	95	16
ITC867	SURG-8S		9	0.28	0.52	0.35	297	1	29	47	39	52	80	35	68	93	27
ITC868	SURG-8S		9	0.37	0.39	0.35	296	1	28	13	-118	47	28	-65	61	44	-39
ITC871	SURG-8S		9	0.37	0.29	0.35	296	1	16	10	-67	29	21	-40	40	31	-31
ITC872	SURG-8S		9	0.36	0.25	0.35	297	1	16	16	-3	26	26	-1	34	33	-1
ITC873	SURG-8S		9	0.37	0.19	0.35	296	1	12	5	-119	20	11	-75	27	17	-63
ITC874	SURG-8S		9	0.36	0.22	0.35	296	1	11	6	-97	21	12	-74	28	18	-52
ITC877	SURG-8S		9	0.38	0.26	0.35	296	1	16	17	3	27	28	5	34	36	6
ITC880	SURG-8S		9	0.66	0.31	0.35	295	1	10	6	-71	20	13	-46	28	21	-31
ITC881	SURG-8S		9	0.67	0.25	0.35	296	1	10	10	5	18	18	1	25	24	-5
ITC885	SURG-8S		9	0.64	0.19	0.35	295	1	6	4	-59	11	7	-46	16	11	-38
ITC888	SURG-8S		9	0.32	0.40	0.35	296	1	19	11	-78	40	24	-64	57	38	-50
ITC891	SURG-8S		9	0.32	0.57	0.35	296	1	31	27	-17	64	66	3	81	89	9
DTC312B	SURG-X		11	0.31	0.68	0.21	299	24	21	18	-16	49	44	-12	77	72	-7
DTC345A	SURG-X		11	0.34	0.49	0.20	300	10	14	14	4	38	38	-2	65	64	-1
DTC363B	SURG-X		11	0.32	0.49	0.20	298	10	14	14	0	37	36	-1	62	62	1
DTC568B	SURG-X		15	0.46	0.51	0.20	298	16	8	13	41	25	34	27	44	54	19
DTC569B	SURG-X		15	0.36	0.49	0.20	298	16	9	14	40	-	40		58	66	12
DTC572B	SURG-X		15	0.38	0.44	0.20	298	16	7	10	30	25	28	12	46	47	3
DTC573B	SURG-X		15	0.13	0.38	0.20	297	16	32	33	4	40	40	1	41	42	1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC576B	SURG-X		15	0.41	0.49	0.20	299	16	8	12	28	28	32	13	50	54	9
DTC577B	SURG-X		15	0.33	0.37	0.20	298	16	22	23	8	40	40	1	51	51	0
DTC581B	SURG-X		15	0.40	0.50	0.20	298	16	7	13	45	25	35	28	43	57	24
DTC583B	SURG-X		15	0.35	0.51	0.19	298	16	-	13		26	33	23	46	58	21
DTC586B	SURG-X		15	0.32	0.43	0.19	297	16	22	30	25	41	47	12	52	59	12
DTC589B	SURG-X		15	0.42	0.53	0.19	298	16	6	12	45	21	30	32	37	53	31
DTC591B	SURG-X		15	0.35	0.42	0.19	296	16	20	27	24	40	45	12	50	57	12
DTC593B	SURG-X		15	0.45	0.52	0.19	297	16	6	11	45	22	32	31	40	53	24
DTC594B	SURG-X		15	0.32	0.42	0.19	298	16	-	29		42	46	9	54	58	8
DTC596B	SURG-X		15	0.29	0.52	0.19	297	16	9	15	36	29	38	24	55	65	16
DTC598A	SURG-X		14	0.03	0.15	0.19	298	16	11	12	15	12	14	16	13	15	18
DTC598B	SURG-X		15	0.14	0.15	0.19	298	16	8	10	23	15	18	14	21	23	11
DTC615B	SURG-X		17	0.72	0.41	0.19	298	23	23	13	-74	36	26	-36	43	36	-21
DTC719B	SURG-X		18	0.41	0.53	0.16	294	0	11	10	-10	32	27	-20	51	41	-24
ETC090	SURG-3M		2	0.55	0.37	0.36	301	1	9	13	31	27	37	26	46	60	22
ETC091	SURG-3M		2	0.51	0.33	0.36	301	1	9	12	27	27	34	22	43	55	21
ETC093	SURG-3M		2	0.51	0.34	0.36	301	1	11	13	16	30	36	18	47	58	18
ETC095	SURG-3M		2	0.51	0.35	0.36	301	1	9	13	28	28	36	23	46	59	21
ETC098	SURG-3M		2	0.51	0.33	0.36	301	1	10	12	17	29	34	15	44	54	18
ETC100	SURG-3M		2	0.51	0.34	0.36	300	1	9	12	24	27	34	21	45	55	18
ETC102	SURG-3M		2	0.51	0.34	0.36	300	1	12	12	0	29	34	14	48	55	12
ETC104	SURG-3M		2	0.50	0.34	0.36	300	1	10	12	19	27	33	21	44	54	19
ETC107	SURG-3M		2	0.50	0.36	0.36	300	1	12	13	5	31	37	17	47	59	20
ETC109	SURG-3M		2	0.52	0.34	0.36	300	1	8	11	32	24	33	28	41	53	24
ETC113	SURG-3M		2	0.51	0.35	0.36	300	1	9	12	28	26	34	24	42	55	24
ETC114	SURG-3M		2	0.49	0.34	0.36	300	1	8	12	32	26	34	24	41	54	25
ETC115	SURG-3M		2	0.53	0.33	0.36	300	1	8	11	31	24	32	25	40	51	21
ETC116	SURG-3M		2	0.51	0.37	0.36	301	1	12	15	24	34	42	20	56	69	18
ETC117	SURG-3M		2	0.52	0.33	0.36	301	1	9	12	25	27	34	20	43	55	21
ETC119	SURG-3M		2	0.52	0.35	0.35	302	1	11	13	19	31	37	15	50	60	16
ETC122	SURG-3M		2	0.53	0.31	0.35	304	1	9	11	18	28	33	13	48	53	10
ETC124	SURG-3M		2	0.50	0.31	0.35	303	1	8	11	24	27	33	17	45	53	15
ETC126	SURG-3M		2	0.52	0.31	0.35	302	1	8	11	25	27	32	18	43	52	18
ETC128	SURG-3M		2	0.53	0.31	0.35	301	1	8	10	20	24	30	19	40	49	17
ETC129	SURG-3M		2	0.53	0.31	0.35	301	1	7	10	27	24	30	19	41	49	16
ETC130	SURG-3M		2	0.52	0.30	0.35	302	1	8	10	21	26	31	17	43	50	14
ETC132	SURG-3M		2	0.54	0.31	0.35	302	1	8	10	26	24	30	18	43	48	11
ETC134	SURG-3M		2	0.53	0.31	0.35	303	1	8	11	29	25	32	20	43	51	15
ETC137	SURG-3M		2	0.52	0.29	0.35	300	1	8	9	10	23	27	13	39	44	12
ETC139	SURG-3M		2	0.53	0.31	0.35	301	1	9	10	11	25	30	15	42	48	13
ETC143	SURG-3M		2		0.29	0.35	301	1	11	11	0	30	32	7	48	51	5
ETC145	SURG-3M		2	0.51	0.28	0.35	301	1	8	10	20	23	28	19	39	45	14
ETC147	SURG-3M		2	0.50	0.28	0.35	301	1	8	10	15	23	28	16	38	44	13
ETC149	SURG-3M		2	0.51	0.28	0.35	302	1	8	10	22	24	28	14	41	45	10
ETC156	SURG-3M		2	0.51	0.40	0.35	300	1	16	16	-1	43	44	3	69	72	4
ETC158	SURG-3M		2	0.50	0.40	0.35	300	1	14	15	11	37	43	14	60	70	13
ETC160	SURG-3M		2	0.50	0.44	0.35	300	1	16	18	12	42	49	14	68	82	17
ETC161	SURG-3M		2	0.52	0.43	0.35	301	1	16	18	12	43	48	11	70	79	12
ETC162	SURG-3M		2	0.50	0.43	0.35	301	1	15	18	17	43	48	11	70	80	13
ETC165	SURG-3M		2	0.50	0.43	0.35	303	1	16	18	10	45	50	9	79	84	6
ETC168	SURG-3M		2	0.52	0.39	0.35	301	1	16	15	-7	44	42	-5	73	68	-8
ETC170	SURG-3M		2	0.51	0.40	0.35	301	1	16	16	3	43	44	3	72	72	0
ETC172	SURG-3M		2	0.50	0.41	0.35	300	1	14	16	10	40	44	9	68	73	7
ETC174	SURG-3M		2	0.50	0.44	0.35	299	1	13	16	19	40	46	15	67	79	15
ETC186	SURG-3M		2	0.40	0.08	0.35	299	1	13	3	-353	39	6	-561	67	9	-680
ETC188	SURG-3M		2		0.18	0.35	300	1	16	5	-200	44	18	-148	78	31	-153
ETC197	SURG-3M		2		0.17	0.35	300	1	28	5	-489	54	16	-236	84	28	-203
ETC208	SURG-3M		2	0.49	0.40	0.35	299	1	14	16	10	45	44	-2	-	71	
ETC210	SURG-3M		2	0.50	0.41	0.35	299	1	13	15	12	40	43	7	66	71	6
ETC215	SURG-3M		2	0.48	0.39	0.35	300	1	13	16	17	39	43	10	64	70	8
ETC223	SURG-3M		2	0.50	0.40	0.35	300	1	17	16	-6	44	44	0	71	71	1
ETC225	SURG-3M		2	0.50	0.40	0.35	299	1	11	15	23	34	41	19	55	67	19
ETC227	SURG-3M		2	0.50	0.43	0.35	300	1	12	17	26	37	46	19	62	77	20

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC229	SURG-3M		2	0.51	0.43	0.35	300	1	12	16	24	38	45	17	63	75	17
ETC231	SURG-3M		2	0.50	0.42	0.35	299	1	13	15	13	39	43	10	63	71	11
ETC234	SURG-3M		2	0.50	0.39	0.35	302	1	14	15	10	41	42	4	70	70	1
ETC236	SURG-3M		2	0.50	0.38	0.35	301	1	14	15	2	41	41	1	69	68	-3
ETC238	SURG-3M		2	0.47	0.37	0.35	301	1	13	15	8	39	41	4	67	67	0
ETC240	SURG-3M		2	0.48	0.37	0.35	300	1	12	14	15	36	39	9	62	64	3
ETC242	SURG-3M		2	0.48	0.38	0.35	301	1	15	15	1	41	42	1	72	69	-4
ETC244	SURG-3M		2	0.47	0.37	0.35	302	1	13	15	14	40	42	5	69	69	0
ETC246	SURG-3M		2	0.49	0.38	0.35	302	1	14	16	10	41	44	6	72	73	1
ETC248	SURG-3M		2	0.49	0.42	0.35	301	1	16	17	4	46	47	1	83	79	-4
ETC250	SURG-3M		2	0.50	0.44	0.35	299	1	14	15	8	42	44	4	73	74	1
ETC252	SURG-3M		2	0.50	0.41	0.35	300	1	13	16	16	39	45	14	67	75	11
ETC254	SURG-3M		2	0.42	0.37	0.35	299	1	12	14	17	34	40	14	59	67	13
ETC256	SURG-3M		2	0.49	0.41	0.35	302	1	17	16	-9	44	44	-1	77	75	-2
ETC258	SURG-3M		2	0.48	0.41	0.35	301	1	16	15	-4	44	44	0	76	75	0
ETC260	SURG-3M		2	0.49	0.41	0.35	300	1	15	15	1	41	42	3	70	72	3
ETC262	SURG-3M		2	0.47	0.40	0.35	302	1	17	17	1	44	46	5	75	78	4
ETC264	SURG-3M		2	0.49	0.41	0.35	301	1	17	15	-15	45	43	-4	75	74	-2
ETC266	SURG-3M		2	0.48	0.40	0.35	300	1	17	15	-17	44	42	-4	74	71	-4
ETC268	SURG-3M		2	0.48	0.39	0.35	302	1	19	16	-15	49	45	-9	83	76	-9
ETC270	SURG-3M		2	0.49	0.39	0.35	301	1	16	15	-7	44	42	-3	74	70	-6
ETC272	SURG-3M		2	0.48	0.40	0.35	301	1	16	15	-3	45	43	-4	76	72	-6
ETC274	SURG-3M		2	0.52	0.39	0.35	302	1	16	16	-1	49	45	-8	83	74	-13
ETC276	SURG-3M		2	0.49	0.38	0.35	302	1	16	16	-1	46	44	-4	80	72	-10
ETC278	SURG-3M		2	0.51	0.38	0.35	302	1	15	15	0	45	43	-5	80	70	-14
ETC280	SURG-3M		2	0.50	0.38	0.35	303	1	16	16	2	47	45	-4	84	75	-13
ETC282	SURG-3M		2	0.50	0.37	0.35	302	1	16	16	1	46	44	-5	81	72	-14
ETC284	SURG-3M		2	0.49	0.38	0.35	302	1	16	17	4	46	46	-2	83	75	-10
ETC286	SURG-3M		2	0.48	0.39	0.35	303	1	15	18	14	46	48	3	84	80	-5
ETC288	SURG-3M		2	0.49	0.37	0.35	303	1	16	17	4	48	45	-6	88	76	-16
ETC290	SURG-3M		2	0.49	0.39	0.35	304	1	17	18	4	51	48	-6	90	80	-13
ETC292	SURG-3M		2	0.49	0.38	0.35	301	1	16	16	1	46	44	-4	79	73	-8
ETC294	SURG-3M		2	0.48	0.38	0.35	301	1	15	17	10	45	45	-1	79	74	-8
ETC296	SURG-3M		2	0.47	0.37	0.35	301	1	16	16	2	47	44	-7	83	73	-13
ETC298	SURG-3M		2	0.49	0.40	0.35	302	1	18	19	7	51	51	-1	89	83	-6
ETC300	SURG-3M		2	0.48	0.40	0.35	300	1	16	18	8	47	48	2	80	79	-1
ETC302	SURG-3M		2	0.46	0.38	0.35	300	1	10	13	22	33	38	13	57	63	10
ETC304	SURG-3M		2	0.49	0.37	0.35	300	1	11	14	23	35	40	12	60	64	7
ETC306	SURG-3M		2	0.54	0.37	0.35	301	1	11	11	1	36	33	-9	61	55	-13
ETC308	SURG-3M		2	0.53	0.37	0.35	301	1	12	12	0	38	35	-7	65	58	-10
ETC310	SURG-3M		2	0.53	0.37	0.35	299	1	11	12	7	34	35	1	58	56	-3
ETC312	SURG-3M		2	0.52	0.38	0.35	297	1	10	10	9	32	33	3	55	55	0
ETC314	SURG-3M		2	0.53	0.37	0.35	298	1	11	11	-2	35	33	-5	59	54	-8
ETC316	SURG-3M		2	0.50	0.36	0.35	298	1	12	12	0	36	35	-4	60	56	-7
ETC323	SURG-3M		2	0.54	0.43	0.35	304	1	24	22	-6	59	55	-8	101	89	-14
ETC324	SURG-3M		2	0.62	0.42	0.35	302	1	15	16	5	43	45	4	68	70	2
ETC325	SURG-3M		2	0.53	0.42	0.35	302	1	18	19	2	49	49	0	81	80	-2
ETC326	SURG-3M		2	0.53	0.42	0.35	302	1	21	19	-12	52	50	-5	85	80	-6
ETC327	SURG-3M		2	0.49	0.44	0.35	302	1	19	21	8	51	54	5	88	91	3
ETC328	SURG-3M		2	0.52	0.42	0.35	303	1	18	19	8	49	50	2	80	81	1
ETC329	SURG-3M		2	0.52	0.41	0.35	303	1	19	19	3	51	50	-2	84	81	-5
ETC330	SURG-3M		2	0.50	0.41	0.35	303	1	20	20	-1	53	51	-4	88	83	-6
ETC331	SURG-3M		2	0.51	0.40	0.35	303	1	18	18	-1	49	47	-4	82	77	-7
ETC334	SURG-3M		2	0.52	0.41	0.35	303	1	19	19	-1	50	49	-1	84	81	-4
ETC336	SURG-3M		2	0.53	0.43	0.35	303	1	20	21	3	52	53	2	87	87	0
ETC339	SURG-3M		2	0.52	0.45	0.35	303	1	22	21	-3	55	54	-3	93	90	-3
ETC345	SURG-3M		2	0.52	0.44	0.35	303	1	21	21	-1	56	54	-3	91	89	-2
ETC347	SURG-3M		2	0.52	0.43	0.35	303	1	20	21	2	53	53	0	87	87	1
ETC349	SURG-3M		2	0.51	0.42	0.35	304	1	22	20	-7	56	52	-9	92	86	-7
ETC351	SURG-3M		2	0.57	0.42	0.35	303	1	18	18	0	49	48	-2	78	77	-2
ETC353	SURG-3M		2	0.51	0.42	0.35	303	1	18	19	2	49	49	0	84	81	-3
ETC356	SURG-3M		2	0.51	0.39	0.35	302	1	17	15	-15	47	41	-16	77	67	-16
ETC376	SURG-3M		3	0.50	0.41	0.35	302	1	17	19	11	46	48	4	78	79	1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC408	SURG-3M		3	0.53	0.41	0.35	300	1	17	16	-8	43	43	2	67	68	2
ETC411	SURG-3M		3	0.52	0.43	0.35	300	1	16	18	11	43	47	8	69	76	10
ETC413	SURG-3M		3	0.54	0.42	0.35	299	1	16	15	-7	42	42	1	66	68	3
ETC415	SURG-3M		3	0.53	0.42	0.35	298	1	12	16	23	37	44	16	60	69	14
ETC419	SURG-3M		3	0.54	0.45	0.35	299	1	15	18	18	42	49	14	66	78	16
DTC233B	SURG-3M		10	0.30	0.49	0.23	296	3	13	17	27	34	43	22	58	72	20
DTC235A	SURG-3M		10	0.31	0.46	0.23	297	3	13	16	20	34	40	14	59	68	14
DTC237B	SURG-3M		10	0.30	0.47	0.23	298	3	12	17	32	33	43	23	58	71	18
DTC239A	SURG-3M		10	0.33	0.49	0.23	297	3	13	17	21	34	40	13	59	65	10
DTC240B	SURG-3M		10	0.31	0.49	0.23	296	3	12	16	29	33	42	22	56	71	21
DTC241A	SURG-3M		10	0.33	0.48	0.23	295	3	14	15	8	33	38	13	54	65	17
DTC242B	SURG-3M		10	0.32	0.48	0.23	296	3	13	16	20	34	41	17	57	70	18
DTC243B	SURG-3M		10	0.31	0.47	0.23	296	3	12	14	17	31	37	16	52	64	19
DTC244A	SURG-3M		10	0.33	0.47	0.23	295	3	11	16	29	30	38	21	49	65	25
DTC264A	SURG-3M		10	0.31	0.47	0.22	298	3	11	16	31	32	40	21	53	69	23
DTC271A	SURG-3M		10	0.30	0.47	0.22	298	4	12	14	14	34	38	12	55	66	18
DTC273B	SURG-3M		10	0.31	0.48	0.22	298	4	14	14	5	37	37	2	63	66	4
DTC275B	SURG-3M		10	0.31	0.46	0.22	298	4	12	14	12	34	37	8	60	64	6
DTC277A	SURG-3M		10	0.33	0.51	0.22	298	4	13	22	42	35	51	31	61	80	24
DTC279A	SURG-3M		10	0.32	0.49	0.22	298	4	9	17	49	31	44	29	56	73	23
DTC282B	SURG-3M		10	0.34	0.48	0.22	299	4	15	16	5	39	40	2	68	68	1
DTC283A	SURG-3M		10	0.31	0.50	0.22	297	4	12	17	33	33	43	24	58	72	21
DTC289A	SURG-3M		10	0.35	0.50	0.22	297	4	12	16	28	33	40	19	55	68	20
DTC291A	SURG-3M		10	0.33	0.51	0.22	297	4	12	16	28	33	41	20	57	71	20
DTC302A	SURG-3M		11	0.35	0.47	0.21	297	24	8	14	42	27	35	25	46	60	23
DTC302B	SURG-3M		11	0.35	0.47	0.21	297	24	7	14	47	26	36	26	48	61	22
DTC303A	SURG-3M		11	0.33	0.51	0.21	298	24	11	16	35	33	41	19	59	70	17
DTC305B	SURG-3M		11	0.33	0.49	0.21	299	24	12	16	27	37	40	8	66	69	3
DTC315A	SURG-3M		11	0.33	0.47	0.21	298	5	15	15	-5	38	37	-2	62	63	2
DTC324B	SURG-3M		11	0.31	0.49	0.21	298	5	16	19	18	41	47	13	68	75	9
DTC327B	SURG-3M		11	0.33	0.51	0.21	297	9	12	16	24	34	40	14	60	69	13
DTC328A	SURG-3M		11	0.32	0.51	0.21	297	9	11	16	27	33	40	17	56	68	17
DTC336B	SURG-3M		11	0.32	0.50	0.21	296	9	13	15	16	33	38	12	57	65	13
DTC352B	SURG-3M		11	0.34	0.50	0.20	298	10	14	15	9	38	39	2	65	66	2
DTC358B	SURG-3M		11	0.33	0.50	0.20	298	10	15	16	4	39	40	3	64	67	3
DTC375B	SURG-3M		11	0.35	0.46	0.20	300	16	14	13	-7	34	34	0	57	58	2
DTC377A	SURG-3M		11	0.36	0.47	0.20	297	16	12	13	9	32	34	7	52	57	9
DTC380A	SURG-3M		11	0.37	0.47	0.20	298	16	11	10	-15	31	27	-14	52	46	-14
DTC385B	SURG-3M		11	0.39	0.44	0.19	298	11	11	11	-2	31	29	-6	50	47	-7
DTC389A	SURG-3M		11	0.37	0.45	0.19	299	11	13	11	-10	34	31	-12	56	51	-11
DTC395B	SURG-3M		11	0.41	0.45	0.19	299	10	14	11	-29	37	30	-24	61	48	-27
DTC398A	SURG-3M		11	0.43	0.47	0.19	297	10	13	11	-20	35	29	-19	57	47	-21
DTC401B	SURG-3M		11	0.36	0.44	0.19	298	10	11	12	2	32	31	-4	54	51	-6
DTC402A	SURG-3M		11	0.37	0.49	0.19	299	10	13	14	5	37	37	0	61	62	1
DTC426A	SURG-3M		11	0.36	0.53	0.18	297	12	10	14	24	33	36	9	56	62	10
DTC433B	SURG-3M		11	0.47	0.48	0.18	297	12	14	9	-60	39	24	-62	66	40	-67
DTC438B	SURG-3M		11	0.36	0.49	0.18	296	13	10	11	7	30	29	-5	50	46	-8
DTC439A	SURG-3M		11	0.35	0.48	0.18	297	13	11	11	7	31	31	0	51	51	-1
DTC440B	SURG-3M		11	0.35	0.48	0.18	296	13	10	12	13	30	30	2	50	49	-2
DTC441A	SURG-3M		11	0.35	0.48	0.18	294	13	9	10	13	25	27	6	40	44	8
DTC442B	SURG-3M		11	0.35	0.50	0.17	294	13	7	10	32	22	28	21	40	47	15
DTC447B	SURG-3M		11	0.39	0.51	0.17	297	14	11	11	1	32	29	-12	48	47	-1
DTC449A	SURG-3M		12	0.35	0.48	0.17	297	14	17	17	2	41	38	-7	64	61	-4
DTC449B	SURG-3M		11	0.35	0.48	0.17	297	14	13	10	-24	35	29	-19	55	47	-17
DTC450B	SURG-3M		11	0.37	0.52	0.17	297	14	12	11	-7	35	30	-16	57	49	-15
DTC467B	SURG-3M		13	0.36	0.48	0.16	294	14	9	12	20	26	27	2	39	43	9
DTC489B	SURG-3M		15	0.38		0.22	298	15	15	16	5	42	40	-3	74	70	-5
DTC491A	SURG-3M		14	0.38	0.52	0.22	298	15	17	17	-1	46	43	-7	81	74	-9
DTC495B	SURG-3M		15	0.38	0.51	0.22	299	15	15	17	11	42	43	1	75	74	-1
DTC498A	SURG-3M		14	0.38	0.31	0.22	299	15	8	8	0	26	23	-12	42	37	-12
DTC505A	SURG-3M		14	0.39	0.48	0.22	298	15	13	16	19	40	39	0	70	67	-5
DTC508A	SURG-3M		14	0.37	0.48	0.22	299	10	13	16	17	40	40	1	71	69	-3
DTC510A	SURG-3M		14	0.39	0.50	0.22	299	10	17	16	-5	46	40	-14	79	68	-16

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC512A	SURG-3M		14	0.38	0.47	0.21	299	10	14	14	6	40	36	-9	70	62	-14
DTC514A	SURG-3M		14	0.39	0.48	0.21	299	10	13	15	10	39	37	-7	71	61	-15
DTC517B	SURG-3M		15	0.37	0.49	0.21	299	10	12	14	15	37	37	1	68	65	-4
DTC522B	SURG-3M		15	0.37	0.48	0.21	299	10	12	14	10	36	36	-2	65	61	-5
DTC528A	SURG-3M		14	0.38	0.49	0.21	299	10	14	14	1	40	36	-10	71	62	-14
DTC529B	SURG-3M		15	0.36	0.45	0.21	299	10	12	12	-1	34	31	-11	63	54	-17
DTC532A	SURG-3M		14	0.36	0.49	0.21	299	10	11	14	24	34	37	7	64	65	2
DTC533B	SURG-3M		15	0.36	0.48	0.21	299	10	11	14	20	36	37	5	64	64	0
DTC537B	SURG-3M		15	0.35	0.46	0.21	299	10	10	13	20	33	34	2	61	59	-4
DTC541B	SURG-3M		15	0.38	0.49	0.21	299	10	11	13	17	35	34	-1	62	59	-6
DTC549A	SURG-3M		14	0.37	0.45	0.20	300	10	14	13	-8	39	33	-18	70	57	-23
DTC551B	SURG-3M		15	0.38	0.44	0.20	300	10	12	11	-4	35	29	-20	63	48	-31
DTC554A	SURG-3M		14	0.38	0.47	0.20	299	10	13	14	5	37	35	-4	66	60	-9
DTC558B	SURG-3M		15	0.34	0.49	0.20	300	10	11	13	18	33	35	8	61	63	3
DTC565B	SURG-3M		15	0.40	0.47	0.20	299	16	9	12	21	26	31	17	44	53	18
DTC570A	SURG-3M		14	0.37	0.51	0.20	298	16	11	14	18	34	36	4	59	61	2
DTC570B	SURG-3M		15	0.37	0.51	0.20	298	16	10	13	22	32	35	7	56	59	5
DTC590A	SURG-3M		14	0.42	0.56	0.19	297	16	10	15	32	31	38	18	52	63	18
DTC590B	SURG-3M		15	0.42	0.56	0.19	297	16	8	14	42	27	36	26	46	60	23
DTC600A	SURG-3M		14	0.37	0.49	0.19	298	23	10	13	23	31	33	7	54	55	2
DTC600B	SURG-3M		15	0.37	0.49	0.19	298	23	9	12	28	28	32	12	50	53	6
DTC601B	SURG-3M		15	0.38	0.49	0.19	298	23	-	12		30	31	4	52	52	1
DTC602B	SURG-3M		15	0.39	0.51	0.19	298	23	10	11	16	30	31	4	54	54	0
DTC603A	SURG-3M		16	0.38	0.49	0.19	298	23	14	16	17	36	39	7	62	64	3
DTC603B	SURG-3M		15	0.37	0.50	0.19	298	23	8	12	30	27	31	13	50	54	8
DTC618B	SURG-3M		17	0.42	0.50	0.18	297	23	8	9	1	27	25	-6	48	44	-9
DTC688A	SURG-3M		18	0.42	0.52	0.17	294	20	13	10	-29	37	29	-29	60	47	-28
DTC692A	SURG-3M		18	0.44	0.53	0.16	298	0	13	11	-21	38	28	-34	64	46	-38
DTC694B	SURG-3M		18	0.41	0.54	0.16	298	0	11	11	6	32	29	-10	55	47	-17
DTC701A	SURG-3M		18	0.40	0.49	0.16	296	0	11	9	-18	33	25	-32	56	40	-38
DTC703A	SURG-3M		18	0.43	0.52	0.16	296	0	10	10	-3	33	27	-24	57	44	-31
DTC724A	SURG-3M		18	0.34	0.46	0.16	294	0	7	10	29	27	28	7	47	47	1
DTC734A	SURG-3M		18	0.39	0.50	0.16	295	21	10	10	-1	32	28	-12	54	46	-16
DTC741B	SURG-3M		18	0.38	0.48	0.16	295	21	9	9	-3	29	25	-16	47	40	-17
DTC750A	SURG-3M		18	0.36	0.51	0.16	300	0	13	10	-21	34	29	-17	55	48	-13
DTC753B	SURG-3M		18	0.41	0.47	0.16	299	0	8	9	8	29	26	-12	48	42	-14
DTC757B	SURG-3M		18	0.38	0.47	0.16	299	0	10	9	-5	31	26	-17	51	43	-19
DTC759B	SURG-3M		18	0.37	0.47	0.16	299	0	9	10	6	29	26	-11	49	43	-13
DTC760A	SURG-3M		18	0.39	0.49	0.16	298	0	15	9	-61	33	23	-44	54	39	-38
DTC766B	SURG-3M		18	0.37	0.52	0.16	300	0	8	11	24	29	31	5	53	51	-3
DTC773B	SURG-3M		18	0.38	0.50	0.16	300	0	10	11	4	31	29	-5	51	48	-5
DTC783A	SURG-3M		18	0.40	0.55	0.16	300	0	13	12	-10	35	32	-10	55	54	-2
XTC104	SURG-3M		1	0.51	0.33	0.25	301	1	11	12	8	37	36	-1	58	55	-4
CTC100A	SURG-3M		4	0.45	0.35	0.19	295	2	5	6	26	16	22	27	-	37	
CTC100B	SURG-3M		4	0.45	0.36	0.19	295	2	5	7	28	18	24	24	-	40	
CTC101A	SURG-3M		4	0.36	0.44	0.19	295	2	8	12	33	26	35	26	43	58	25
CTC101B	SURG-3M		4	0.35	0.44	0.19	295	2	8	12	29	28	35	21	45	59	23
CTC103A	SURG-3M		5	0.30	0.46	0.19	295	2	10	16	34	30	41	27	-	66	
CTC103B	SURG-3M		5	0.30	0.46	0.19	295	2	11	16	34	31	44	29	-	69	
CTC104B	SURG-3M		5	0.29	0.45	0.19	295	2	11	15	28	31	42	26	52	68	24
CTC105A	SURG-3M		5	0.30	0.45	0.19	296	2	11	16	32	32	41	24	53	66	20
CTC107B	SURG-3M		5	0.30	0.44	0.19	295	2	10	15	29	32	40	20	-	65	
CTC108A	SURG-3M		5	0.31	0.44	0.19	295	2	10	13	29	30	38	21	-	63	
CTC109B	SURG-3M		5	0.31	0.43	0.19	295	2	11	13	16	33	38	14	-	64	
CTC110A	SURG-3M		5	0.30	0.46	0.19	296	2	11	15	26	34	43	20	-	69	
CTC112B	SURG-3M		5	0.29	0.43	0.19	296	2	11	14	22	31	39	20	-	64	
CTC113A	SURG-3M		5	0.30	0.20	0.19	297	2	13	6	-118	34	21	-61	-	33	
CTC113B	SURG-3M		5	0.30	0.21	0.19	297	2	12	6	-93	34	23	-47	-	35	
CTC119A	SURG-3M		5	0.31	0.43	0.19	294	2	12	12	6	30	34	12	-	57	
CTC121B	SURG-3M		5	0.31	0.42	0.19	292	2	9	12	25	27	34	20	-		
CTC142A	SURG-3M		6	0.37	0.34	0.18	295	2	6	6	9	18	21	16	-	35	
CTC172A	SURG-3M		7	0.32	0.44	0.17	294	10	7	9	22	26	28	8	-	49	
CTC172B	SURG-3M		7	0.32	0.44	0.17	294	10	8	9	11	27	28	3	-	50	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC181B	SURG-3M		7	0.23	0.43	0.16	298	10	13	11	-19	39	33	-17	63	54	-16
CTC183B	SURG-3M		7	0.23	0.43	0.16	298	10	12	11	-8	37	34	-9	61	55	-11
CTC184A	SURG-3M		7	0.23	0.43	0.16	298	17	11	10	-8	35	32	-11	60	53	-13
CTC185B	SURG-3M		7	0.28	0.43	0.16	301	17	12	11	-7	36	34	-5	60	56	-7
CTC192B	SURG-3M		7	0.22	0.41	0.16	298	17	9	9	-2	32	28	-14	57	49	-17
CTC196B	SURG-3M		8	0.22	0.42	0.15	297	10	10	11	6	34	34	-1	-	54	
CTC197A	SURG-3M		8	0.25		0.15	297	18	10	10	7	33	31	-5	57	53	-9
CTC201B	SURG-3M		8	0.24	0.54	0.15	298	18	9	8	-16	29	27	-8	51	49	-3
CTC209A	SURG-3M		8	0.25	0.45	0.15	298	18	10	10	9	32	32	0	55	53	-4
CTC211A	SURG-3M		8	0.23	0.46	0.15	298	18	8	11	27	30	34	10	54	54	-1
CTC216A	SURG-3M		8	0.24	0.44	0.14	298	19	10	10	1	33	31	-6	57	52	-10
CTC221B	SURG-3M		8	0.24	0.42	0.14	299	19	9	9	1	32	30	-6	55	51	-9
CTC231B	SURG-3M		9	0.27	0.51	0.14	303	5	8	14	47	27	39	32	-	58	
CTC246B	SURG-3M		9	0.25	0.48	0.13	295	6	6	10	36	30	31	4	53	50	-6
CTC250A	SURG-3M		9	0.24	0.45	0.13	296	6	7	10	30	27	29	8	50	48	-3
CTC255B	SURG-3M		9	0.22	0.44	0.13	296	20	7	10	33	26	30	14	48	48	1
CTC257B	SURG-3M		10	0.24	0.46	0.13	297	20	7	8	18	26	28	7	47	47	0
DTC725B	SURG-4M		18		0.51	0.16	295	21	10	10	4	30	27	-14	48	41	-16
DTC730B	SURG-4M		18	0.31	0.52	0.16	296	21	9	11	25	26	29	11	44	48	8
DTC733B	SURG-4M		18	0.30	0.53	0.16	296	21	9	12	29	27	30	10	47	50	7
DTC749B	SURG-4M		18	0.38	0.54	0.16	298	21	12	11	-1	34	30	-13	54	48	-12
CTC266B	SURG-4M		10	0.24	0.46	0.12	299	6	10	7	-49	33	23	-44	53	40	-32
ETC217	SURG-3		2	0.26	0.39	0.35	299	1	18	23	20	55	59	7	84	87	3
ETC219	SURG-3		2	0.25	0.38	0.35	300	1	20	22	10	58	58	0	85	85	0
ETC387	SURG-3		3	0.15	0.28	0.35	301	1	21	22	2	52	51	-1	62	65	5
ETC388	SURG-3		3	0.15	0.34	0.35	301	1	25	27	7	58	59	2	65	67	4
ETC390	SURG-3		3	0.14	0.34	0.35	300	1	23	26	15	56	57	3	64	65	2
ETC392	SURG-3		3	0.15	0.32	0.35	300	1	24	23	-4	58	55	-5	68	69	2
ETC395	SURG-3		3	0.14	0.34	0.35	299	1	24	26	9	57	57	-1	66	64	-2
ETC399	SURG-3		3	0.15	0.35	0.35	300	1	23	28	18	54	60	9	60	68	12
ETC401	SURG-3		3	0.15	0.35	0.35	300	1	20	27	27	53	59	10	60	66	9
ETC403	SURG-3		3	0.15	0.31	0.35	299	1	19	22	15	50	53	6	62	65	5
ETC405	SURG-3		3	0.13	0.33	0.35	299	1	21	26	17	53	55	5	61	63	2
ETC407	SURG-3		3	0.16	0.34	0.35	300	1	23	27	18	56	61	8	67	71	5
DTC318A	SURG-3		11	0.34	0.49	0.21	297	5	12	14	13	32	36	10	55	62	11
DTC360A	SURG-3		11	0.25	0.52	0.20	297	10	12	18	35	32	45	29	57	67	15
DTC360B	SURG-3		11	0.24	0.52	0.20	297	10	11	18	39	31	45	30	57	67	15
DTC362A	SURG-3		11	0.30	0.50	0.20	298	10	12	15	18	34	39	13	60	66	9
DTC364A	SURG-3		11	0.32	0.48	0.20	298	10	14	14	-5	37	36	-5	63	62	-2
DTC365B	SURG-3		11	0.32	0.49	0.20	298	10	13	15	12	35	38	6	61	65	5
DTC366A	SURG-3		11	0.33	0.50	0.20	298	10	13	15	15	35	39	10	60	67	10
DTC368A	SURG-3		11	0.35	0.49	0.20	299	10	13	14	6	35	35	0	61	60	-1
DTC369B	SURG-3		11	0.35	0.49	0.20	298	10	12	14	10	34	35	3	59	60	2
DTC415A	SURG-3		11	0.20	0.48	0.19	297	10	15	16	4	42	40	-5	61	58	-5
DTC421B	SURG-3		11	0.39	0.52	0.19	297	12	13	12	-11	37	32	-17	64	53	-21
DTC011A	SURG-8M		1	0.52	0.39	0.39	301	1	38	35	-7	60	56	-8	-	71	
DTC011B	SURG-8M		1	0.52	0.38	0.39	301	1	39	36	-9	61	55	-11	78	69	-13
DTC012A	SURG-8M		1	0.52	0.41	0.39	301	1	42	37	-14	63	57	-11	81	73	-11
DTC012B	SURG-8M		1	0.51	0.41	0.39	301	1	42	38	-12	64	58	-10	-	74	
DTC013A	SURG-8M		1	0.45	0.40	0.39	300	1	40	38	-5	61	58	-4	79	75	-4
DTC013B	SURG-8M		1	0.45	0.40	0.39	300	1	41	37	-9	62	57	-8	-	74	
DTC014B	SURG-8M		1	0.48	0.39	0.39	301	1	41	37	-12	62	57	-10	80	72	-11
DTC015A	SURG-8M		1	0.50	0.41	0.39	301	1	43	37	-16	66	58	-13	-	76	
DTC016B	SURG-8M		1	0.48	0.38	0.39	300	1	40	35	-14	62	55	-13	78	69	-13
DTC017B	SURG-8M		1	0.48	0.38	0.39	300	1	40	36	-11	61	55	-11	78	71	-10
DTC018B	SURG-8M		1	0.48	0.41	0.39	301	1	44	38	-14	66	59	-10	84	77	-9
DTC019A	SURG-8M		1	0.46	0.40	0.39	300	1	39	38	-3	60	59	-3	77	77	-1
DTC020A	SURG-8M		1	0.50	0.38	0.39	300	1	32	26	-24	53	48	-11	68	63	-8
DTC021A	SURG-8M		1	0.49	0.42	0.39	300	1	41	40	-2	61	60	-1	77	78	1
DTC022A	SURG-8M		1	0.50	0.40	0.39	300	1	40	37	-7	61	58	-6	77	74	-4
DTC023B	SURG-8M		1	0.47	0.40	0.39	301	1	40	39	-2	61	60	-2	80	78	-2
DTC024A	SURG-8M		1	0.50	0.41	0.39	301	1	41	38	-6	63	59	-6	82	77	-6
DTC025B	SURG-8M		1	0.47	0.42	0.39	302	1	40	41	1	64	64	0	85	85	0

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC028B	SURG-8M		1	0.49	0.41	0.39	301	1	39	40	3	61	62	1	80	80	1
DTC064A	SURG-8M		1	0.49	0.40	0.39	302	1	38	38	0	60	59	-1	77	78	1
DTC065B	SURG-8M		1	0.48	0.40	0.39	301	1	37	38	4	58	60	3	75	79	5
DTC068A	SURG-8M		1	0.48	0.38	0.39	301	1	34	36	4	56	56	1	72	74	2
DTC069B	SURG-8M		1	0.48	0.36	0.39	302	1	37	35	-6	58	55	-5	75	73	-3
DTC070B	SURG-8M		1	0.49	0.40	0.39	301	1	37	38	2	58	60	3	74	79	6
DTC249B	SURG-8M		10	0.26	0.36	0.23	297	3	24	28	16	36	44	16	47	57	18
DTC250A	SURG-8M		10	0.27	0.34	0.23	297	3	23	25	8	36	41	12	45	54	16
DTC251A	SURG-8M		10	0.26	0.34	0.23	297	3	24	26	9	37	41	10	46	53	13
DTC251B	SURG-8M		10	0.26	0.35	0.23	297	3	24	26	9	37	41	11	46	54	14
DTC252B	SURG-8M		10	0.26	0.37	0.23	297	3	25	29	13	38	45	16	48	58	19
DTC255A	SURG-8M		10	0.27	0.34	0.23	297	3	22	25	14	33	40	16	42	52	20
DTC256B	SURG-8M		10	0.27	0.36	0.23	297	3	24	27	12	35	42	17	46	56	17
DTC272B	SURG-8M		10	0.14	0.33	0.22	298	4	26	30	14	37	42	11	11	46	75
DTC274A	SURG-8M		10	0.16	0.35	0.22	298	4	30	31	5	43	45	5	47	50	6
DTC276A	SURG-8M		10	0.17	0.36	0.22	298	4	33	33	0	47	47	-1	51	52	2
DTC278B	SURG-8M		10	0.16	0.39	0.22	298	4	32	36	11	46	47	3	51	49	-2
DTC280B	SURG-8M		10	0.17	0.37	0.22	298	4	32	34	8	45	48	5	50	51	2
DTC281A	SURG-8M		10	0.16	0.37	0.22	298	4	30	34	11	44	46	6	48	50	5
DTC284B	SURG-8M		10	0.15	0.37	0.22	298	4	31	34	9	44	45	2	49	48	-3
DTC290B	SURG-8M		10	0.17	0.37	0.22	298	4	31	33	8	44	46	5	49	51	5
DTC292B	SURG-8M		10	0.16	0.56	0.22	297	4	23	27	13	38	44	14	46	51	11
DTC311A	SURG-8M		11	0.29	0.37	0.21	298	24	26	26	2	42	42	1	52	55	5
DTC317B	SURG-8M		11	0.18	0.37	0.21	297	5	30	33	8	43	46	7	48	52	8
DTC319A	SURG-8M		11	0.18	0.34	0.21	297	5	27	29	8	40	42	6	-	50	
DTC320B	SURG-8M		11	0.30	0.38	0.21	297	24	25	27	5	41	43	3	52	56	6
DTC332B	SURG-8M		11	0.57	0.38	0.21	297	9	15	16	10	29	31	8	37	40	8
DTC335A	SURG-8M		11	0.43	0.40	0.21	297	9	21	22	8	37	40	6	46	50	8
DTC338B	SURG-8M		11	0.29	0.39	0.21	297	10	24	28	14	40	44	10	50	57	11
DTC359A	SURG-8M		11	0.28	0.39	0.20	298	10	26	29	8	43	45	6	54	58	8
DTC370A	SURG-8M		11	0.28	0.36	0.20	298	10	24	24	2	40	40	1	50	52	3
DTC378A	SURG-8M		11	0.26	0.55	0.20	298	16	44	42	-6	63	63	0	71	74	4
DTC381B	SURG-8M		11	0.27	0.34	0.20	298	16	26	24	-7	41	38	-7	51	49	-5
DTC390B	SURG-8M		11	0.28	0.36	0.19	297	11	25	24	-6	41	39	-5	52	51	-2
DTC396A	SURG-8M		11	0.29	0.35	0.19	299	10	28	22	-26	44	37	-18	56	49	-15
DTC399B	SURG-8M		11	0.27	0.37	0.19	298	10	27	25	-7	42	39	-7	53	51	-5
DTC403B	SURG-8M		11	0.30	0.39	0.19	299	10	27	28	2	44	45	2	55	58	5
DTC408A	SURG-8M		11	0.28	0.36	0.19	298	10	30	24	-23	46	39	-18	57	51	-13
DTC410A	SURG-8M		11	0.28	0.37	0.19	298	10	29	26	-12	45	41	-10	56	53	-5
DTC414B	SURG-8M		11	0.27	0.39	0.19	298	10	28	27	-4	45	42	-6	56	53	-5
DTC419A	SURG-8M		11	0.29	0.45	0.19	297	12	31	32	2	47	49	5	58	63	8
DTC423A	SURG-8M		11	0.29	0.50	0.19	297	12	27	36	25	44	55	19	56	67	17
DTC427B	SURG-8M		11	0.26	0.47	0.18	298	12	28	36	21	47	54	13	59	64	8
DTC430B	SURG-8M		11	0.25	0.40	0.18	297	12	29	28	-4	46	43	-7	58	54	-7
DTC455A	SURG-8M		12	0.25	0.40	0.17	297	14	27	28	3	43	42	-1	52	53	2
DTC455B	SURG-8M		11	0.25	0.41	0.17	297	14	25	25	-1	42	40	-4	52	51	-2
DTC456B	SURG-8M		11	0.28	0.40	0.17	297	14	26	25	-3	41	41	-2	50	51	3
DTC459B	SURG-8M		11	0.29	0.41	0.16	298	14	24	24	1	41	40	-1	51	50	-1
DTC474A	SURG-8M		14	0.31	0.39	0.23	298	13	33	30	-11	51	46	-11	66	60	-10
DTC474B	SURG-8M		15	0.30	0.40	0.23	298	13	32	30	-8	51	46	-10	65	60	-9
DTC476B	SURG-8M		15	0.31	0.41	0.22	298	13	33	31	-8	52	48	-9	66	62	-7
DTC478B	SURG-8M		15	0.31	0.44	0.22	297	13	34	34	0	53	52	-2	67	66	-2
DTC480B	SURG-8M		15	0.30	0.41	0.22	298	13	33	31	-6	51	48	-7	66	63	-6
DTC486B	SURG-8M		15	0.30	0.41	0.22	298	13	33	31	-6	51	48	-8	66	62	-6
DTC488A	SURG-8M		14	0.30	0.38	0.22	298	13	32	23	-43	51	40	-26	66	53	-23
DTC488B	SURG-8M		15	0.30	0.38	0.22	298	13	32	22	-43	50	40	-25	64	53	-22
DTC492B	SURG-8M		15	0.30	0.38	0.22	298	15	29	28	-3	46	44	-4	59	58	-3
DTC493A	SURG-8M		14	0.30	0.38	0.22	297	15	29	28	-4	47	44	-5	61	58	-5
DTC500B	SURG-8M		15	0.30	0.42	0.22	298	15	32	32	0	50	49	-2	64	63	-1
DTC502B	SURG-8M		15	0.30	0.39	0.22	299	15	32	29	-11	50	46	-9	64	59	-7
DTC509B	SURG-8M		15	0.30	0.38	0.22	299	10	32	27	-18	50	44	-15	64	57	-13
DTC511B	SURG-8M		15	0.31	0.39	0.21	299	10	32	28	-16	51	45	-14	65	58	-12
DTC515B	SURG-8M		15	0.31	0.37	0.21	299	10	31	25	-24	49	41	-20	63	53	-18

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC516A	SURG-8M		14	0.32	0.40	0.21	299	10	31	28	-9	49	45	-10	64	59	-9
DTC521A	SURG-8M		14	0.30	0.39	0.21	299	10	32	28	-14	50	45	-12	64	58	-10
DTC530A	SURG-8M		14	0.31	0.37	0.21	299	10	29	26	-15	47	41	-13	60	54	-11
DTC534A	SURG-8M		14	0.29	0.38	0.21	299	10	29	27	-7	48	44	-9	62	57	-8
DTC538A	SURG-8M		14	0.29	0.37	0.21	299	10	28	27	-3	46	43	-6	59	56	-5
DTC547A	SURG-8M		14	0.31	0.36	0.20	300	10	31	25	-21	49	41	-18	63	54	-16
DTC552A	SURG-8M		14	0.31	0.37	0.20	300	10	32	26	-26	52	43	-21	67	56	-20
DTC556B	SURG-8M		15	0.28	0.42	0.20	300	10	26	33	20	44	50	11	58	63	9
DTC610B	SURG-8M		17	0.31	0.43	0.19	297	23	26	30	13	43	46	7	54	58	7
DTC616A	SURG-8M		16	0.81	0.37	0.19	297	23	9	11	18	19	22	14	26	30	13
DTC616B	SURG-8M		17	0.80	0.38	0.19	297	23	8	10	16	16	19	15	23	27	16
DTC689B	SURG-8M		18	0.33	0.44	0.16	294	20	27	25	-10	46	41	-12	58	50	-15
DTC693B	SURG-8M		18	0.31	0.45	0.16	298	0	29	29	0	48	46	-3	60	58	-3
DTC695A	SURG-8M		18	0.32	0.50	0.16	299	0	29	31	9	49	50	3	63	63	1
DTC697B	SURG-8M		18	0.32	0.42	0.16	296	20	30	24	-22	49	41	-17	60	52	-17
DTC702B	SURG-8M		18	0.32	0.44	0.16	297	0	26	25	-3	45	42	-6	57	53	-6
DTC705B	SURG-8M		18	0.29	0.45	0.16	296	0	25	27	9	42	44	4	56	55	-2
DTC720A	SURG-8M		18	0.33	0.40	0.16	296	0	28	21	-34	46	39	-18	58	50	-17
DTC726A	SURG-8M		18	0.29	0.42	0.16	294	21	24	24	1	43	42	-1	55	53	-3
DTC729A	SURG-8M		18	0.24	0.40	0.16	294	21	18	25	30	36	41	13	47	52	10
DTC737B	SURG-8M		18	0.32	0.43	0.16	294	21	24	22	-7	41	40	-5	51	49	-5
DTC738A	SURG-8M		18	0.31	0.42	0.16	293	21	25	23	-11	43	41	-4	54	52	-4
DTC746A	SURG-8M		18	0.30	0.44	0.16	298	21	25	28	11	42	45	6	54	57	6
DTC747B	SURG-8M		18	0.29	0.43	0.16	299	21	24	27	12	42	44	6	52	55	6
DTC754A	SURG-8M		18	0.31	0.43	0.16	299	0	26	27	5	44	44	1	56	56	0
DTC755B	SURG-8M		18	0.29	0.43	0.16	299	0	26	27	4	44	43	-1	55	54	-1
DTC762B	SURG-8M		18	0.30	0.42	0.16	299	0	25	25	-3	44	42	-4	54	53	-1
DTC769B	SURG-8M		18	0.28	0.43	0.16	299	0	19	28	32	39	45	13	50	57	11
DTC771B	SURG-8M		18	0.29	0.44	0.16	299	0	24	29	19	42	46	8	53	58	9
DTC772A	SURG-8M		18	0.30	0.44	0.16	299	0	26	27	4	45	44	-1	56	56	-1
DTC776B	SURG-8M		18	0.30	0.40	0.16	300	0	24	24	-3	43	42	-3	54	54	0
DTC780A	SURG-8M		18	0.30	0.42	0.16	300	0	25	24	-5	44	42	-5	56	53	-5
DTC786B	SURG-8M		18	0.30	0.47	0.16	300	0	23	30	24	39	47	16	47	58	19
CTC123B	SURG-8M		5	0.40	0.53	0.18	293	2	35	34	0	52	58	10	64	74	13
CTC124A	SURG-8M		5	0.39	0.51	0.18	293	2	33	33	0	49	54	9	-	69	
CTC126B	SURG-8M		5	0.38	0.51	0.18	294	2	32	33	2	50	54	9	-		
CTC127A	SURG-8M		5	0.39	0.51	0.18	293	2	33	31	-6	50	53	6	-	67	
CTC128B	SURG-8M		5	0.40	0.55	0.18	294	2	35	36	2	53	58	9	-	75	
CTC130A	SURG-8M		5	0.39	0.53	0.18	293	2	32	33	2	50	55	8	63	70	10
CTC131B	SURG-8M		5	0.40	0.54	0.18	293	2	33	34	3	51	56	9	64	72	11
CTC138A	SURG-8M		6	0.40	0.55	0.18	293	2	34	35	3	51	56	9	64	71	11
CTC140B	SURG-8M		6	0.37	0.55	0.18	294	2	30	37	18	49	59	18	-	74	
CTC149A	SURG-8M		6	0.42	0.47	0.18	299	4	25	23	-8	42	42	-1	-	51	
CTC149B	SURG-8M		6	0.42	0.46	0.18	299	4	25	22	-13	42	41	-2	-	52	
CTC150A	SURG-8M		6	0.43	0.54	0.18	299	4	36	33	-9	59	57	-3	75	73	-4
CTC151B	SURG-8M		6	0.51	0.54	0.18	303	4	37	33	-11	57	55	-4	71	68	-4
CTC152A	SURG-8M		6	0.38	0.45	0.18	301	4	27	25	-7	43	42	-3	52	51	-2
CTC154B	SURG-8M		6	0.42	0.54	0.18	301	4	41	35	-15	62	60	-4	78	77	-1
CTC156A	SURG-8M		6	0.41	0.52	0.18	303	4	36	34	-6	58	58	0	-	74	
CTC158B	SURG-8M		6	0.36	0.52	0.18	304	4	35	39	11	60	64	7	-	79	
CTC165A	SURG-8M		7	0.57	0.57	0.18	305	5	31	36	14	51	61	16	-	80	
CTC165B	SURG-8M		7	0.57	0.58	0.18	305	5	32	36	9	51	60	15	-	80	
CTC167B	SURG-8M		7	0.41	0.57	0.18	300	5	36	39	8	58	63	9	-	80	
CTC168A	SURG-8M		7	0.41	0.58	0.18	300	5	37	40	9	59	64	9	-	80	
CTC171A	SURG-8M		7	0.39	0.56	0.17	300	5	38	36	-5	61	60	-2	-	73	
CTC171B	SURG-8M		7	0.39	0.55	0.17	300	5	37	35	-6	61	59	-3	-	74	
CTC180A	SURG-8M		7	0.39	0.57	0.16	298	10	35	35	1	57	57	0	72	71	-2
CTC182A	SURG-8M		7	0.39	0.57	0.16	298	10	36	34	-5	58	56	-3	74	70	-5
CTC186A	SURG-8M		7	0.38	0.53	0.16	298	17	32	30	-5	54	53	-3	70	67	-4
CTC193A	SURG-8M		7	0.37	0.55	0.16	298	17	35	32	-11	57	54	-7	72	67	-8
CTC198B	SURG-8M		8	0.39	0.58	0.15	298	18	34	33	-5	56	56	0	71	71	0
CTC204B	SURG-8M		8	0.44	0.60	0.15	298	18	32	31	-5	56	57	1	71	72	3
CTC208B	SURG-8M		8	0.43	0.61	0.15	298	18	32	34	4	56	59	6	70	74	6

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC212A	SURG-8M		8			0.15	298	18	29	29	0	52	53	2	66	67	1
CTC217B	SURG-8M		8	0.43	0.58	0.14	297	19	31	28	-13	55	53	-3	70	67	-3
CTC222A	SURG-8M		8	0.45	0.55	0.14	299	19	32	26	-24	56	50	-11	71	64	-12
CTC232A	SURG-8M		9	0.46	0.57	0.14	301	5	20	27	27	42	51	17	-	65	
CTC239A	SURG-8M		9	0.44	0.59	0.13	301	5	28	30	7	52	55	6	-	69	
CTC248A	SURG-8M		9	0.32	0.60	0.13	292	6	32	41	22	54	62	13	66	70	5
CTC251B	SURG-8M		9	0.34	0.63	0.13	294	6	32	36	13	52	58	9	66	68	4
CTC260A	SURG-8M		10	0.40	0.65	0.12	295	20	28	32	12	50	57	13	63	70	10
CTC262B	SURG-8M		10	0.38	0.60	0.12	294	20	29	29	0	50	53	4	64	64	0
DTC027A	SURG-8		1	0.15	0.40	0.39	302	1	52	49	-6	61	59	-4	63	61	-3
DTC027B	SURG-8		1	0.15	0.41	0.39	302	1	52	50	-4	61	59	-4	63	61	-3
DTC029B	SURG-8		1	0.17	0.43	0.39	301	1	54	53	-2	63	64	2	64	66	3
DTC030A	SURG-8		1	0.17	0.40	0.39	300	1	50	50	-1	59	62	4	60	64	6
DTC031B	SURG-8		1	0.17	0.43	0.39	301	1	52	53	1	61	63	4	62	66	5
DTC032A	SURG-8		1	0.17	0.42	0.39	300	1	51	52	3	60	63	5	61	65	7
DTC033B	SURG-8		1	0.17	0.41	0.39	300	1	51	51	0	60	62	2	62	64	4
DTC034A	SURG-8		1	0.16	0.41	0.39	301	1	50	50	0	60	62	4	60	64	7
DTC035B	SURG-8		1	0.17	0.40	0.39	301	1	51	49	-3	60	62	4	61	65	6
DTC036B	SURG-8		1	0.18	0.44	0.39	300	1	54	53	-2	-	65		63	67	6
DTC037A	SURG-8		1	0.17	0.42	0.39	301	1	51	52	1	61	64	5	61	66	7
DTC038B	SURG-8		1	0.17	0.39	0.39	301	1	51	49	-4	59	62	4	61	64	6
DTC039A	SURG-8		1	0.18	0.41	0.39	301	1	52	51	-3	61	64	6	61	67	9
DTC066A	SURG-8		1	0.17	0.37	0.39	302	1	49	47	-4	59	62	5	60	66	9
DTC067A	SURG-8		1	0.17	0.38	0.39	301	1	48	48	-1	59	62	5	60	65	8
DTC071A	SURG-8		1	0.18	0.39	0.39	302	1	49	49	0	60	64	7	61	68	11
DTC258A	SURG-8		10	0.14	0.36	0.23	297	3	28	33	15	35	43	17	36	44	19
DTC258B	SURG-8		10	0.13	0.36	0.23	297	3	29	33	14	36	42	16	-	44	
DTC259B	SURG-8		10	0.16	0.35	0.23	297	3	27	32	16	37	44	16	41	49	16
DTC260A	SURG-8		10	0.17	0.36	0.22	297	3	28	32	14	39	46	16	42	52	18
DTC261B	SURG-8		10	0.16	0.34	0.22	296	3	25	31	18	36	44	18	39	48	19
DTC266B	SURG-8		10	0.16	0.34	0.22	298	3	25	31	18	36	44	20	39	50	21
DTC267A	SURG-8		10	0.16	0.36	0.22	299	3	29	33	12	40	46	13	43	51	16
DTC268B	SURG-8		10	0.16	0.47	0.22	299	3	34	40	15	46	54	14	49	58	15
DTC269B	SURG-8		10	0.17	0.36	0.22	299	3	30	33	7	42	46	9	45	52	13
DTC293B	SURG-8		10	0.08	0.39	0.22	297	4	28	29	4	32	30	-5	32	30	-6
DTC298A	SURG-8		10	0.09	0.38	0.22	298	4	29	30	4	31	31	0	31	31	1
DTC308A	SURG-8		11	0.17	0.37	0.21	301	24	32	33	3	45	48	6	48	54	11
DTC309B	SURG-8		11	0.17	0.53	0.21	299	24	42	45	5	49	52	6	49	53	6
DTC321A	SURG-8		11	0.11	0.38	0.21	298	24	30	32	7	33	36	8	32	37	12
DTC325A	SURG-8		11	0.18	0.42	0.21	299	5	31	37	17	44	50	13	47	54	13
DTC329B	SURG-8		11	0.18	0.39	0.21	296	9	29	34	13	43	47	8	49	51	5
DTC330A	SURG-8		11	0.17	0.39	0.21	296	9	30	34	12	43	46	6	48	49	4
DTC386A	SURG-8		11	0.29	0.34	0.19	298	11	26	20	-31	41	34	-21	52	44	-18
DTC388B	SURG-8		11	0.11	0.37	0.19	298	11	29	30	2	34	34	-1	34	34	0
DTC391A	SURG-8		11	0.11	0.36	0.19	297	11	30	29	-2	35	34	-3	35	34	-3
DTC394B	SURG-8		11	0.11	0.36	0.19	296	10	29	30	2	34	35	2	34	36	5
DTC397B	SURG-8		11	0.13	0.36	0.19	298	10	32	31	-3	38	39	3	38	41	8
DTC400A	SURG-8		11	0.12	0.36	0.19	298	10	31	30	-4	36	37	1	36	38	5
DTC406B	SURG-8		11	0.13	0.39	0.19	299	10	32	33	3	37	38	3	37	38	4
DTC409B	SURG-8		11	0.11	0.36	0.19	298	10	31	30	-3	35	36	2	34	37	7
DTC411B	SURG-8		11	0.11	0.36	0.19	297	10	30	29	-3	35	35	1	34	35	4
DTC412A	SURG-8		11	0.11	0.36	0.19	297	10	30	31	4	35	36	5	35	37	6
DTC418B	SURG-8		11	0.10	0.38	0.19	298	10	30	30	-1	34	34	-2	34	34	0
DTC420A	SURG-8		11	0.10	0.47	0.19	297	12	32	31	-3	35	31	-12	34	31	-11
DTC424B	SURG-8		11	0.10	0.44	0.18	297	12	31	30	-5	35	30	-15	34	30	-14
DTC428A	SURG-8		11	0.12	0.42	0.18	298	12	32	32	1	36	37	3	35	37	6
DTC432A	SURG-8		11	0.09	0.42	0.18	297	12	33	28	-18	37	29	-28	36	28	-27
DTC451A	SURG-8		12	0.10	0.43	0.17	297	14	31	30	-4	36	33	-9	36	33	-8
DTC451B	SURG-8		11	0.10	0.44	0.17	297	14	32	29	-8	37	31	-17	36	31	-17
DTC453B	SURG-8		11	0.14	0.40	0.17	295	14	29	30	3	35	37	5	35	38	10
DTC454B	SURG-8		11	0.12	0.40	0.17	297	14	29	29	1	34	34	-1	33	34	1
DTC462A	SURG-8		12	0.13	0.40	0.16	299	14	30	31	4	36	37	3	35	38	7
DTC466B	SURG-8		13	0.13	0.38	0.16	297	14	30	29	-5	-	34		34	34	2

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC477A	SURG-8		14	0.13	0.46	0.22	297	13	38	38	-1	43	42	-2	43	42	-2
DTC479A	SURG-8		14	0.14	0.44	0.22	297	13	37	38	2	44	44	0	44	44	0
DTC481A	SURG-8		14	0.13	0.41	0.22	298	13	37	36	-2	42	41	-2	42	41	-2
DTC487A	SURG-8		14	0.13	0.40	0.22	298	13	37	35	-3	42	41	-4	43	41	-4
DTC496A	SURG-8		14	0.13	0.41	0.22	299	15	37	36	-3	43	41	-4	44	42	-5
DTC497B	SURG-8		15	0.13	0.41	0.22	299	15	37	36	-3	43	42	-3	44	43	-3
DTC501A	SURG-8		14	0.13	0.40	0.22	299	15	37	35	-6	43	41	-5	44	42	-5
DTC506B	SURG-8		15	0.12	0.39	0.22	298	15	35	34	-2	41	40	-2	41	40	-2
DTC513B	SURG-8		15	0.13	0.36	0.21	298	10	35	33	-8	42	40	-4	43	42	-2
DTC519A	SURG-8		14	0.13	0.34	0.21	298	10	35	32	-8	41	39	-6	42	40	-5
DTC520B	SURG-8		15	0.12	0.39	0.21	299	10	35	34	-4	41	40	-2	42	41	-2
DTC524A	SURG-8		14	0.13	0.39	0.21	299	10	36	34	-6	42	40	-5	43	41	-4
DTC525B	SURG-8		15	0.13	0.38	0.21	299	10	37	34	-8	44	42	-6	45	43	-4
DTC531B	SURG-8		15	0.12	0.37	0.21	299	10	35	33	-7	42	39	-7	43	40	-6
DTC539B	SURG-8		15	0.13	0.38	0.21	299	10	34	34	-2	41	41	-1	42	42	0
DTC540A	SURG-8		14	0.12	0.37	0.21	299	10	35	33	-6	40	40	-2	42	41	-1
DTC543A	SURG-8		14	0.30	0.40	0.21	299	10	31	29	-5	48	45	-7	62	58	-7
DTC544B	SURG-8		15	0.13	0.38	0.21	299	10	36	34	-7	43	41	-3	44	43	-2
DTC548B	SURG-8		15	0.13	0.37	0.20	299	10	35	32	-9	42	41	-3	43	43	0
DTC553B	SURG-8		15	0.13	0.37	0.20	300	10	36	33	-7	43	42	-3	44	44	-1
DTC557A	SURG-8		14	0.12	0.42	0.20	300	10	35	35	0	42	40	-5	43	41	-6
DTC559B	SURG-8		15	0.28		0.20	299	10	26	32	17	43	50	15	54	64	15
DTC560B	SURG-8		15	0.12	0.41	0.20	299	16	30	33	11	37	37	1	38	37	-2
DTC604A	SURG-8		16	0.14	0.38	0.19	298	23	35	33	-6	40	41	3	41	43	5
DTC608B	SURG-8		17	0.15	0.43	0.19	297	23	32	35	9	40	43	7	41	44	7
DTC609A	SURG-8		16	0.14	0.42	0.19	298	23	31	35	10	37	41	10	-	42	
DTC609B	SURG-8		17	0.13	0.42	0.19	298	23	31	34	9	37	41	8	-	41	
DTC698A	SURG-8		18	0.10	0.43	0.16	295	0	30	29	-3	33	32	-1	33	32	-4
DTC700B	SURG-8		18	0.10	0.44	0.16	296	0	30	30	-2	33	32	-2	33	32	-2
DTC707A	SURG-8		18	0.10	0.41	0.16	297	0	30	28	-7	35	32	-8	35	32	-8
DTC723B	SURG-8		18	0.11	0.42	0.16	295	0	30	29	-1	33	33	-1	33	33	-1
DTC732A	SURG-8		18	0.08	0.42	0.16	296	21	26	25	-3	29	26	-9	29	26	-10
DTC739B	SURG-8		18	0.10	0.40	0.16	295	21	26	28	7	28	31	8	28	30	9
DTC740A	SURG-8		18	0.10	0.40	0.16	295	21	26	28	7	29	31	6	28	31	8
DTC748A	SURG-8		18	0.09	0.43	0.16	297	21	25	27	7	27	28	6	26	28	7
DTC758A	SURG-8		18	0.09	0.44	0.16	299	0	27	28	2	29	30	3	28	30	4
DTC763A	SURG-8		18	0.09	0.42	0.16	299	0	25	27	9	27	29	10	26	30	11
DTC763A	SURG-8		18	0.09	0.42	0.16	299	0	25	27	9	27	29	10	26	30	11
DTC770A	SURG-8		18	0.08	0.42	0.16	299	0	22	26	17	24	28	16	23	28	18
DTC778B	SURG-8		18	0.09	0.43	0.16	300	0	27	28	3	-	30		29	31	6
DTC782B	SURG-8		18	0.09	0.46	0.16	300	0	26	27	7	27	29	9	26	29	12
DTC787A	SURG-8		18	0.10	0.44	0.16	299	0	25	29	14	27	32	16	-	32	
XTC109	SURG-8		1	0.24	0.38	0.25	302	1	41	38	-7	63	60	-6	-	72	
XTC116	SURG-8		1	0.22	0.42	0.25	301	1	45	42	-6	64	62	-3	69	71	2
CTC187B	SURG-8		7	0.15	0.58	0.16	298	17	39	38	-3	44	42	-5	44	42	-5
CTC194B	SURG-8		8	0.15	0.58	0.16	297	17	39	38	-3	44	42	-5	44	42	-5
CTC195A	SURG-8		8	0.14	0.52	0.15	297	10	39	36	-9	44	41	-7	44	41	-5
CTC199A	SURG-8		8	0.16	0.58	0.15	298	18	39	39	-1	44	44	-1	44	44	-1
CTC205A	SURG-8		8	0.17	0.59	0.15	298	18	41	40	-2	46	45	-2	46	45	-3
CTC210B	SURG-8		8	0.16	0.60	0.15	298	18	40	39	-2	44	43	-3	44	43	-2
CTC215B	SURG-8		8	0.18	0.56	0.15	297	18	41	39	-5	47	46	-2	47	47	0
CTC220A	SURG-8		8	0.16	0.55	0.14	298	19	40	38	-4	46	44	-3	46	45	-2
CTC223B	SURG-8		8	0.17	0.56	0.14	298	19	40	39	-2	46	45	-1	46	46	0
CTC233B	SURG-8		9	0.17	0.62	0.14	299	5	38	40	5	43	44	4	43	45	5
CTC235B	SURG-8		9	0.15	0.60	0.14	301	10	36	37	3	40	41	2	41	42	4
CTC238B	SURG-8		9	0.16	0.58	0.13	301	10	37	39	4	43	44	4	43	45	5
CTC240B	SURG-8		9	0.16	0.60	0.13	300	5	37	39	6	42	44	3	-	44	
CTC249B	SURG-8		9	0.16	0.63	0.13	295	6	37	38	3	42	42	1	42	42	-1
CTC253A	SURG-8		9	0.16	0.63	0.13	295	6	39	39	-1	45	44	-3	45	44	-2
CTC258A	SURG-8		10	0.17	0.59	0.13	296	20	39	38	-1	44	44	0	43	45	5
CTC259B	SURG-8		10	0.17	0.64	0.12	295	20	37	39	4	43	44	2	43	44	3
CTC263A	SURG-8		10	0.16	0.62	0.12	294	20	37	38	1	42	43	1	41	43	4
CTC267A	SURG-8		10	0.16	0.59	0.12	300	6	36	37	2	40	42	6	39	43	8

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
OTC275B	SURG-8		11	0.63	0.44	0.00	319	8	84	75	-11	148	137	-8	-	158	
OTC276A	SURG-8		11	0.58	0.44	0.00	315	8	80	69	-15	135	120	-13	144	144	0
OTC277A	SURG-8		11	0.51	0.40	0.00	312	8	67	61	-10	121	109	-12	-	131	
OTC277B	SURG-8		11	0.52	0.39	0.00	312	8	63	60	-6	115	109	-6	133	132	-1

[a] See Table 45 for the definitions of the codes used to designate run type and incremental reactivity experiment category.

[b] Characterization set. Runs with the same chamber and characterization set number are assumed to have the same chamber effects and (for CTC runs) light spectrum.

[c] "Propene equivalent" for all VOCs injected in experiment. Sum of measured initial VOC concentration times OH rate constant, divided by the OH rate constant for propene.

[d] NO_2 photolysis rate assigned for this experiment.

[e] Average measured temperature for this experiment.

[f] References for reports describing chamber experiments. These reports are (or will be) available at http://cert.ucr.edu/~carter/bycarter.htm.

0 Unpublished results from this laboratory.
1 Carter et al. (1995d)
2 Carter et al. (1997a)
3 Carter et al. (1996c)
4 Carter et al. (1996a)
5 Carter et al. (2000c)
6 Carter et al. (1999b)
7 Carter et al. (1995c)
8 Carter et al. (1993b). See also Carter et al, (1995c).
9 Carter et al. (1996b)
10 Carter et al. (2000a)
11 Carter et al. (1997b)
12 Carter et al. (1997d)
13 Carter et al. (1997f)
14 Carter et al. (1997i)
15 Carter et al. (2000f)
16 Carter et al. (1999c)
17 Carter et al. (1997c)
18 Carter et al. (1997e)
19 Carter et al. (1997g)
20 Carter et al. (2000e)
21 Carter et al. (2000b)
22 Carter et al. (2000d)
23 Carter et al. (1999a)
24 Carter et al. (1996d)
25 Carter et al. (2000g)

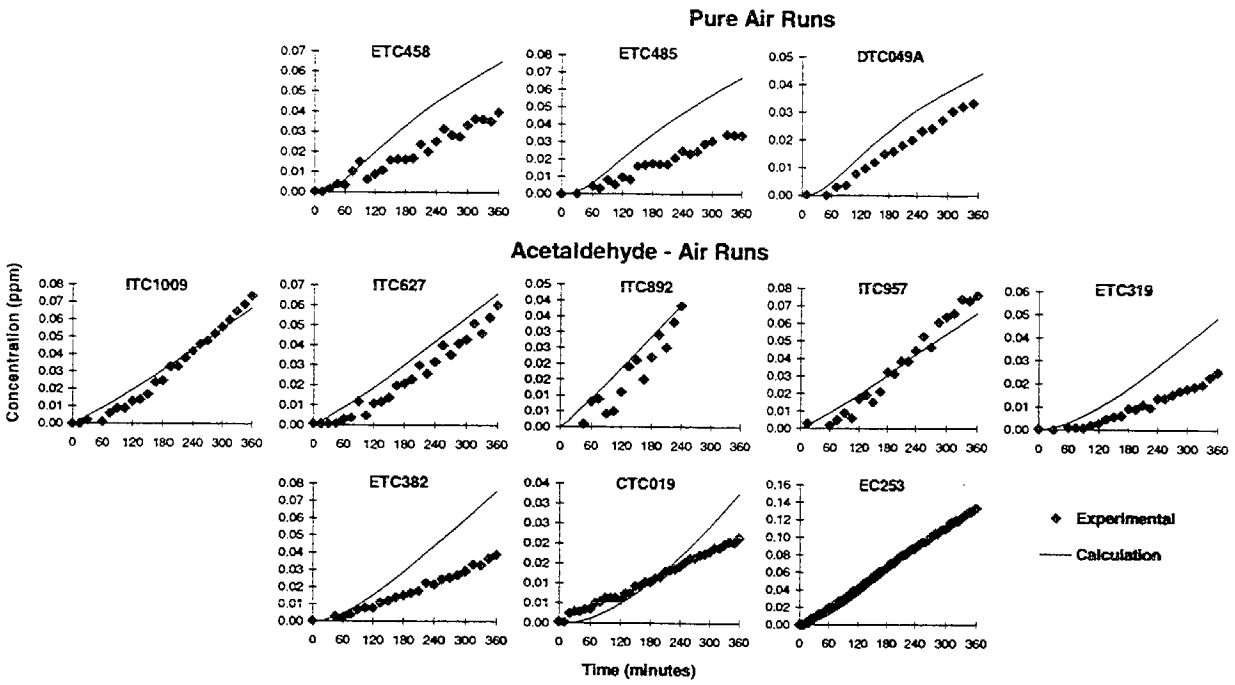


Figure B-1. Plots of experimental and calculated ozone data for the pure air and acetaldehyde - air runs.

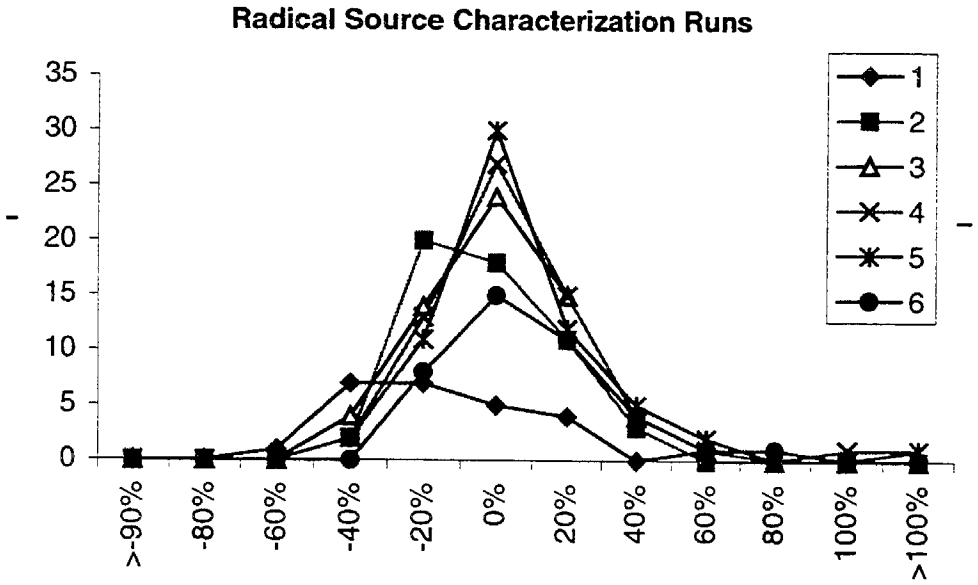


Figure B-2. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the radical source characterization (CO - NO_x and n-butane - NO_x) runs.

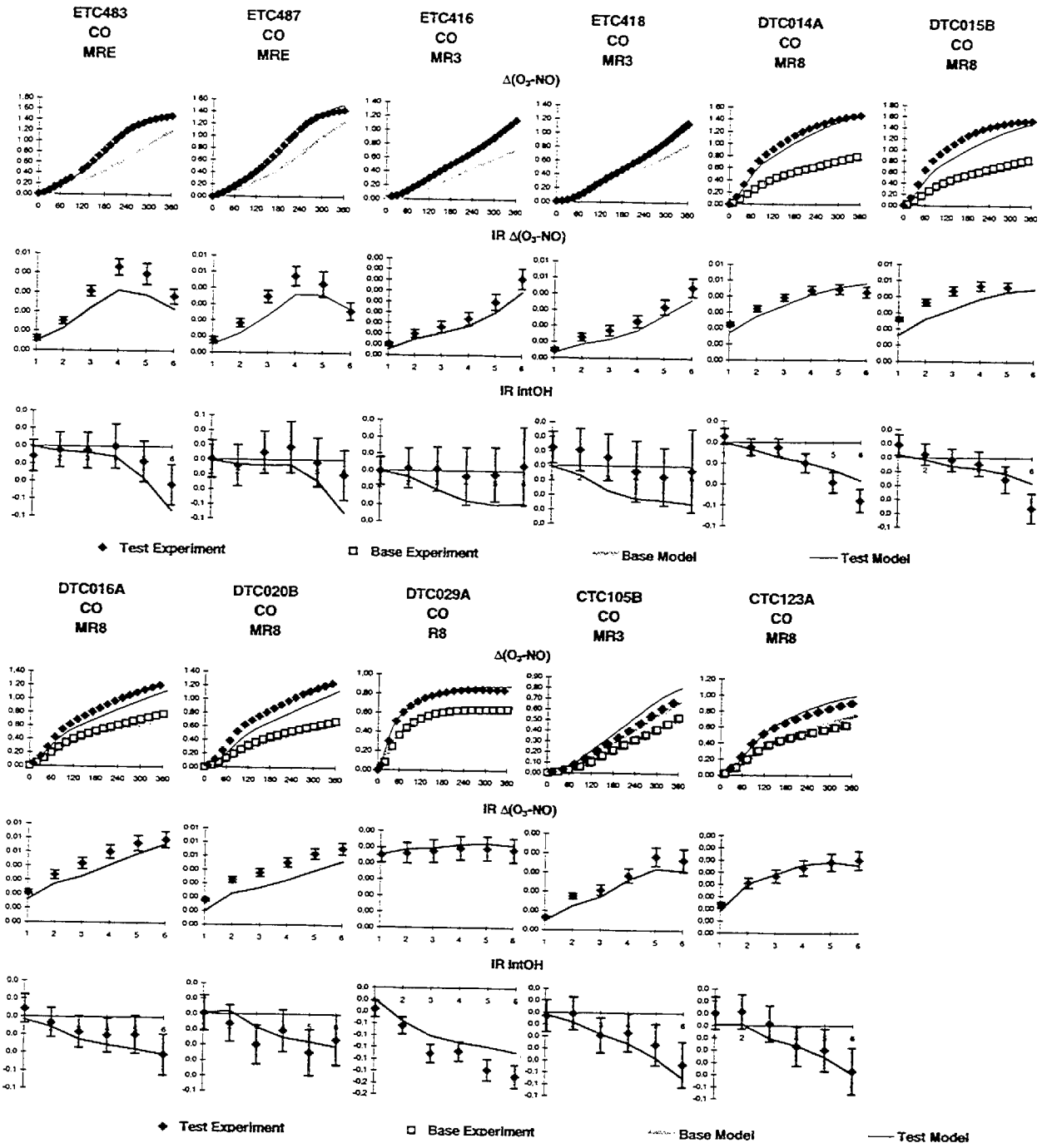


Figure B-3. Plots of experimental and calculated results of the incremental reactivity experiments with CO.

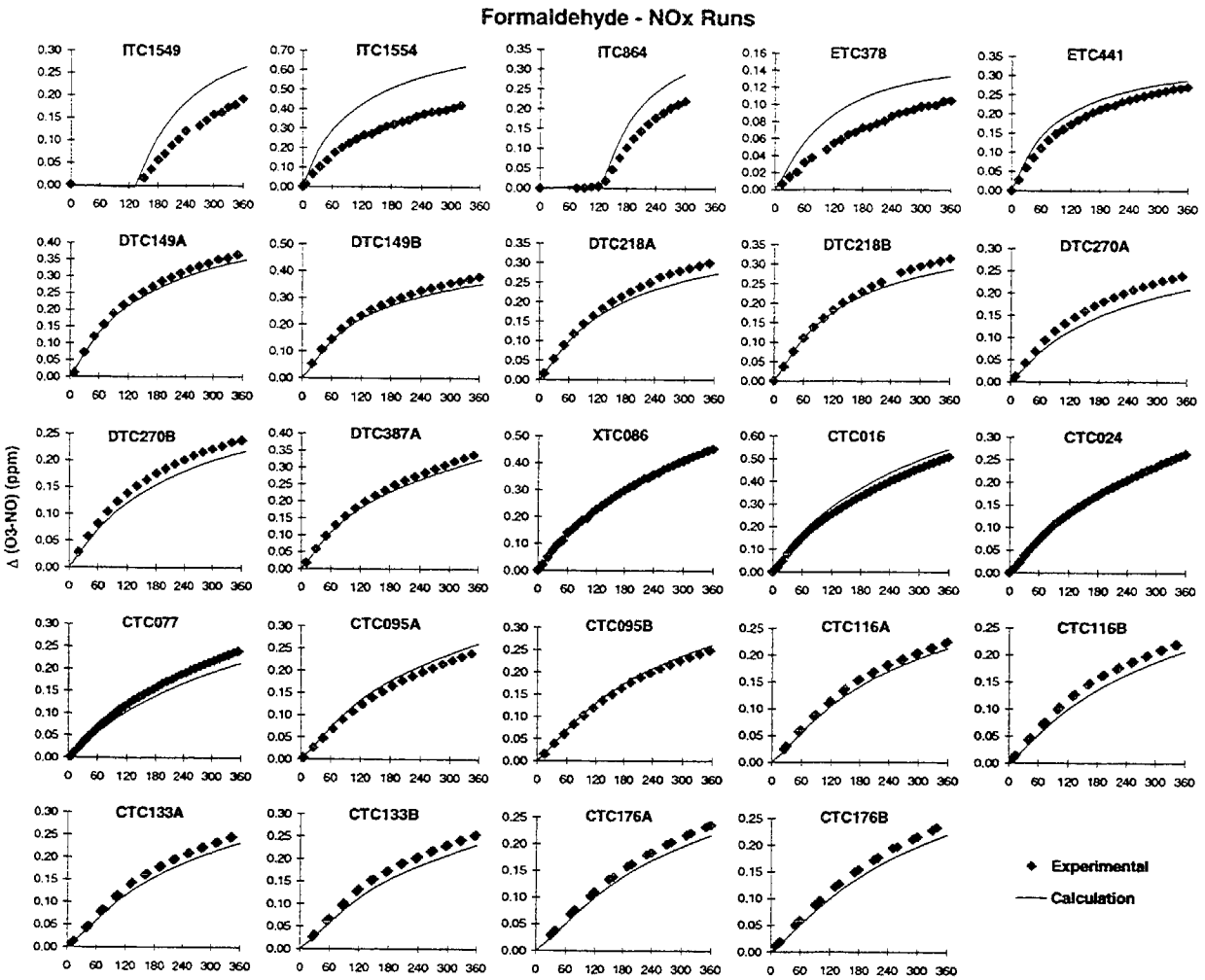


Figure B-4. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the formaldehyde - NO_x experiments.

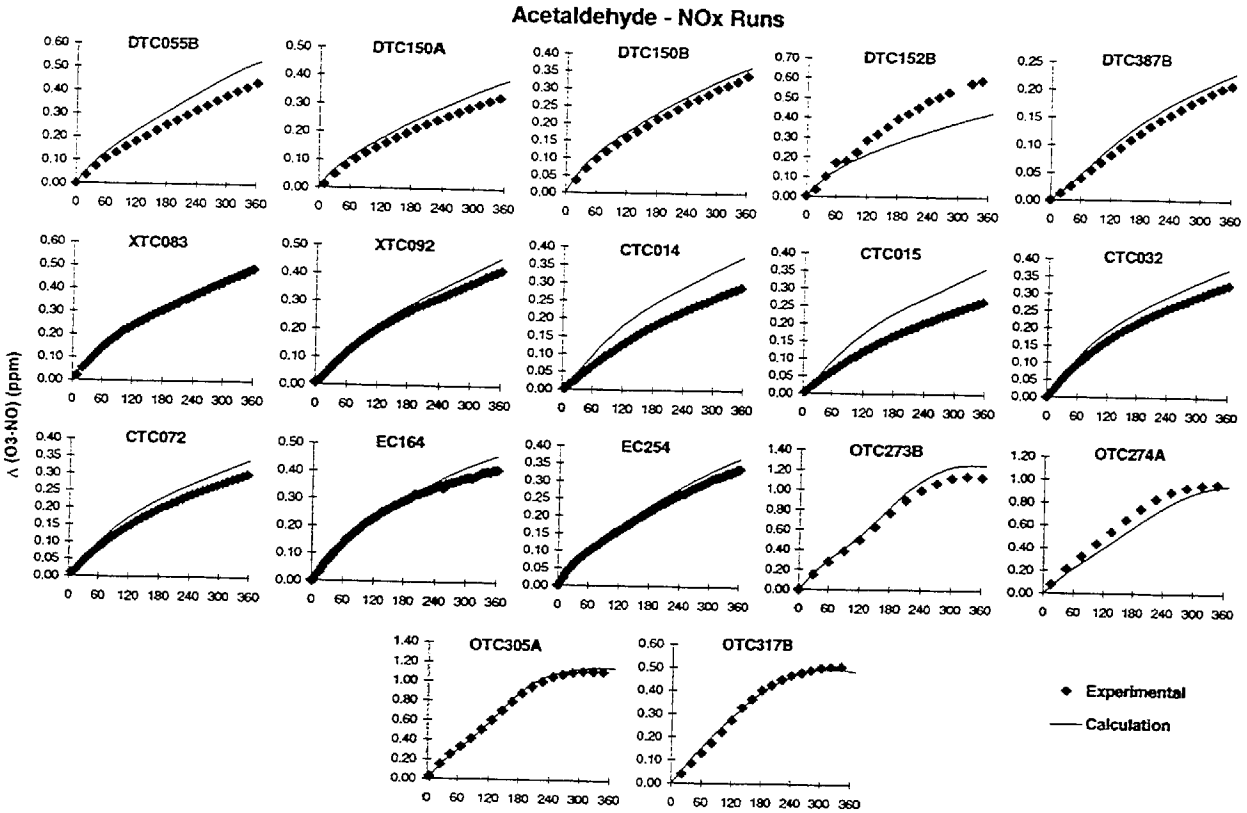


Figure B-5. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetaldehyde - NO_x experiments.

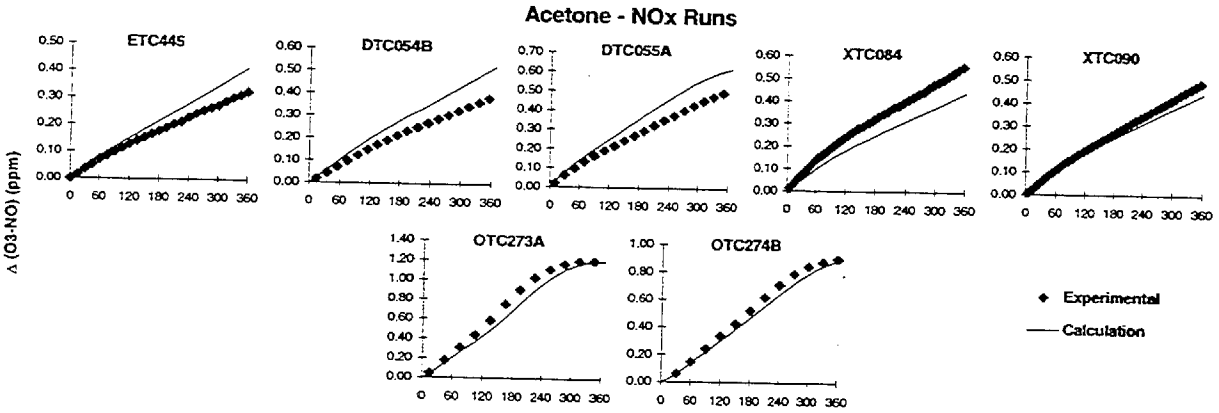


Figure B-6. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetone - NO_x experiments.

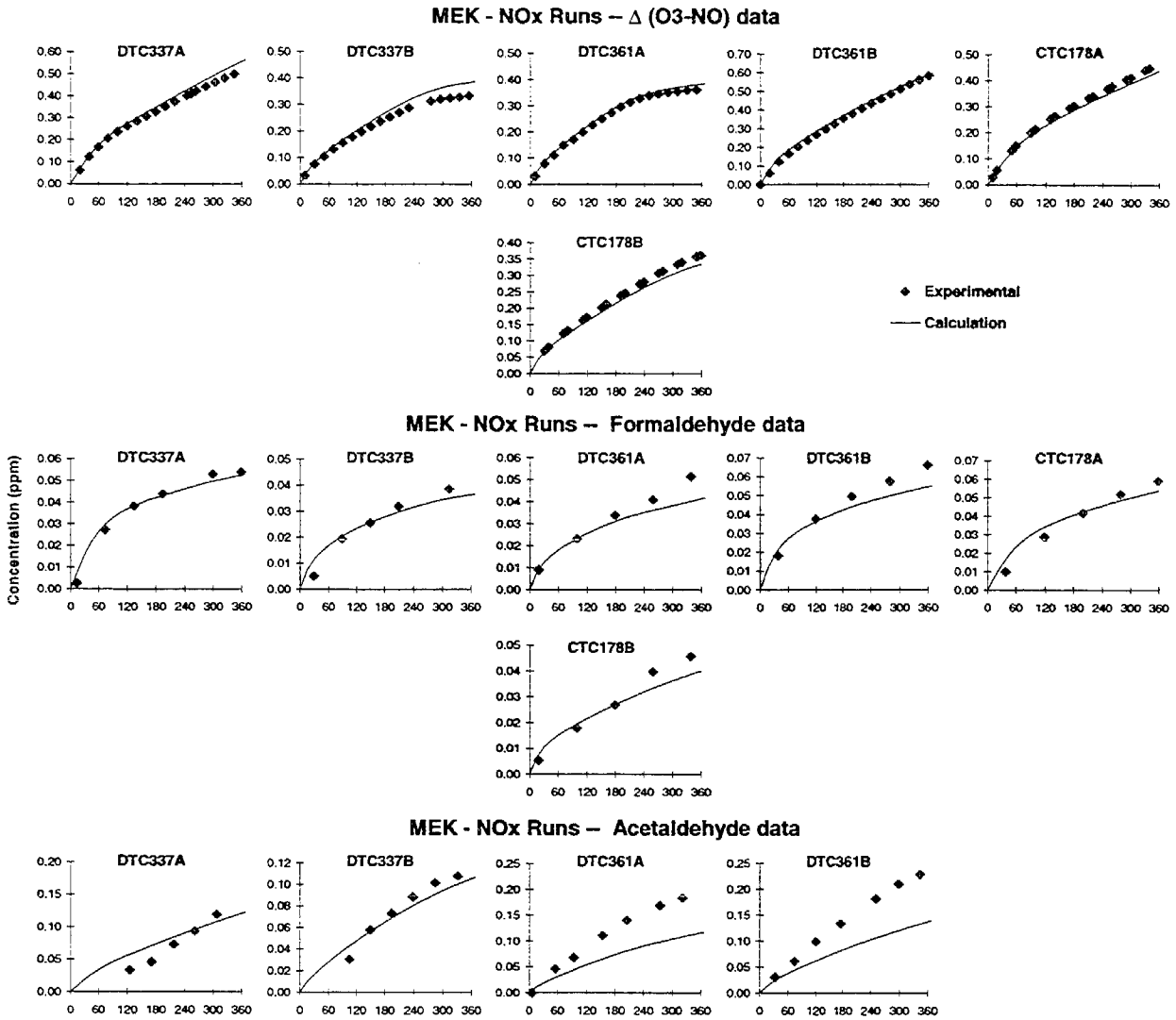


Figure B-7. Plots of experimental and calculated $\Delta([O_3]-[NO])$, formaldehyde, and acetaldehyde data for the methyl ethyl ketone (MEK) - NO_x experiments.

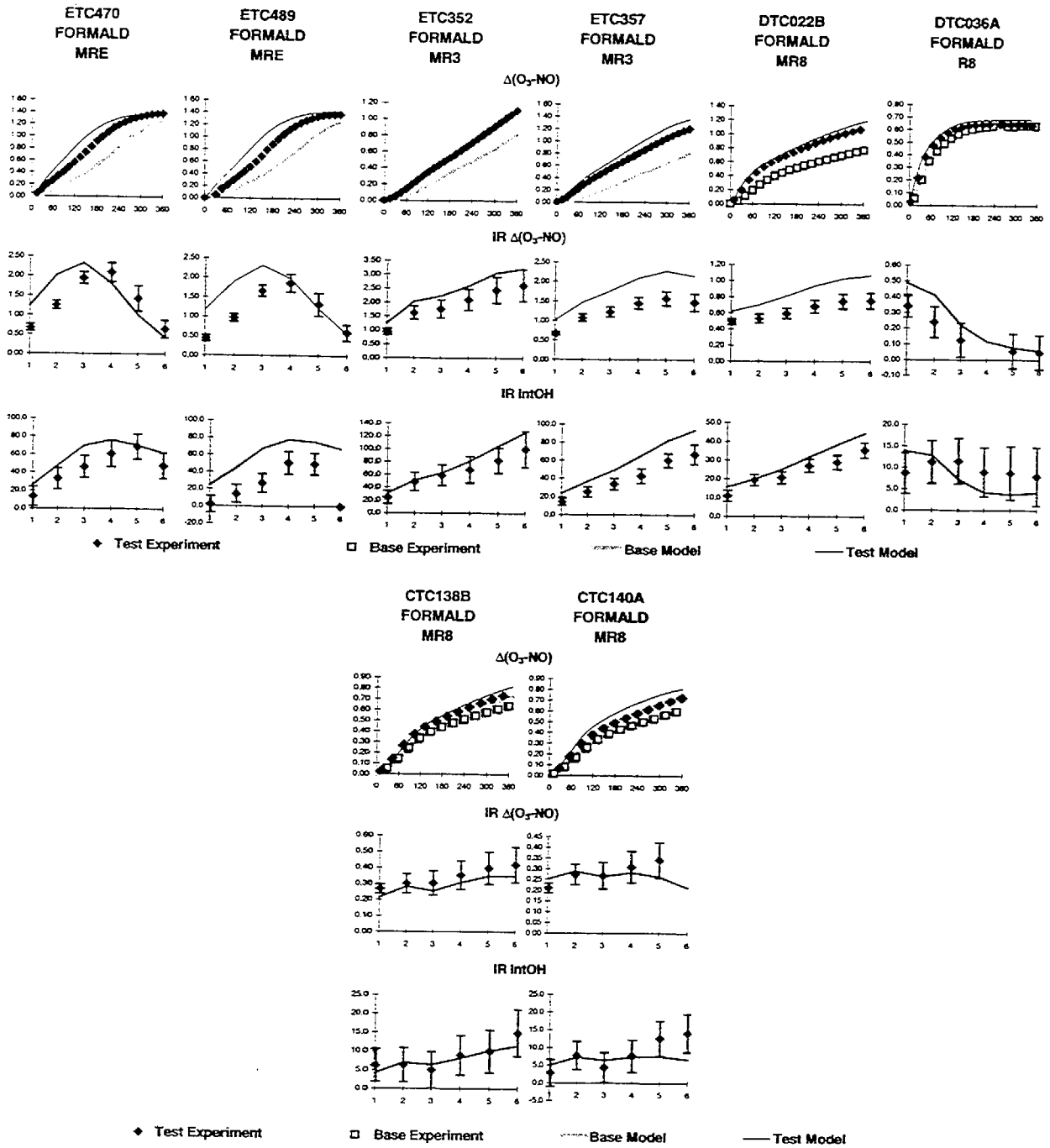


Figure B-8. Plots of experimental and calculated results of the incremental reactivity experiments with formaldehyde.

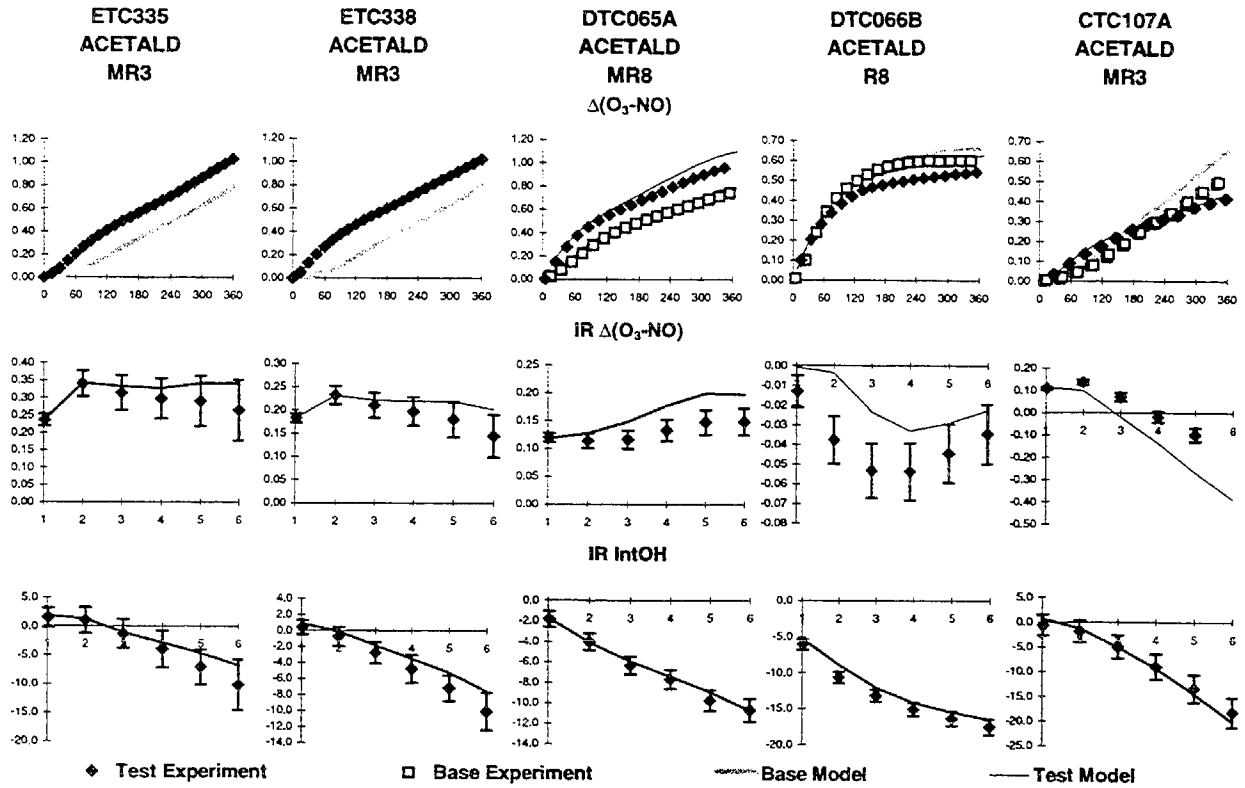


Figure B-9. Plots of experimental and calculated results of the incremental reactivity experiments with acetaldehyde.

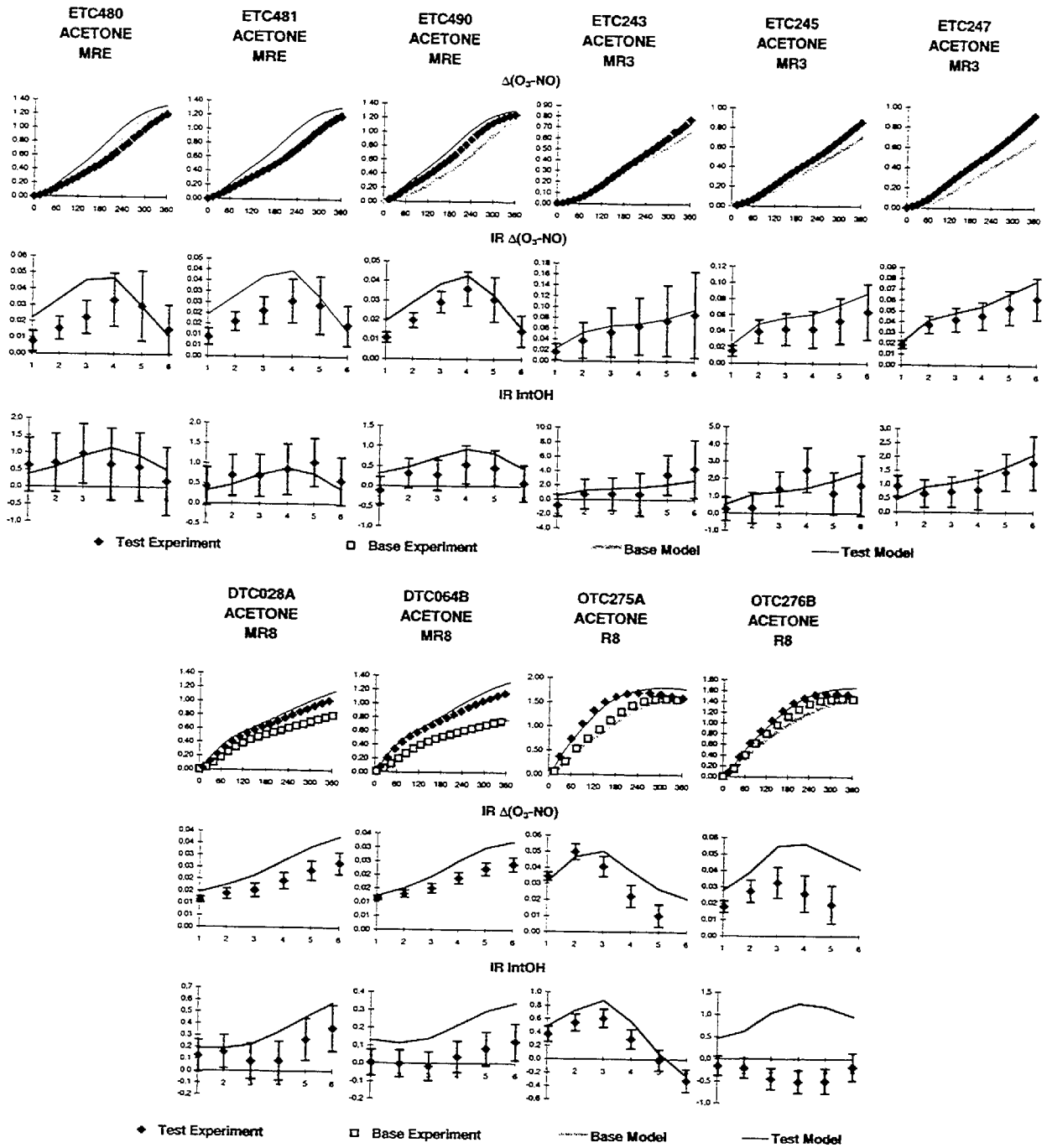


Figure B-10. Plots of experimental and calculated results of the incremental reactivity experiments with acetone.

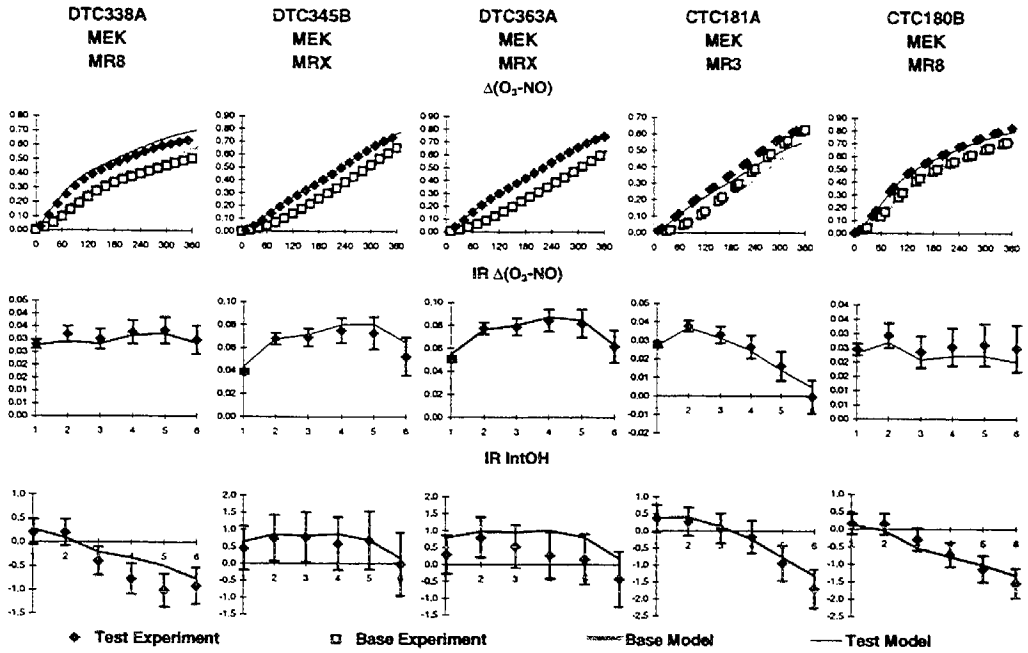


Figure B-11. Plots of experimental and calculated results of the incremental reactivity experiments with methyl ethyl ketone.

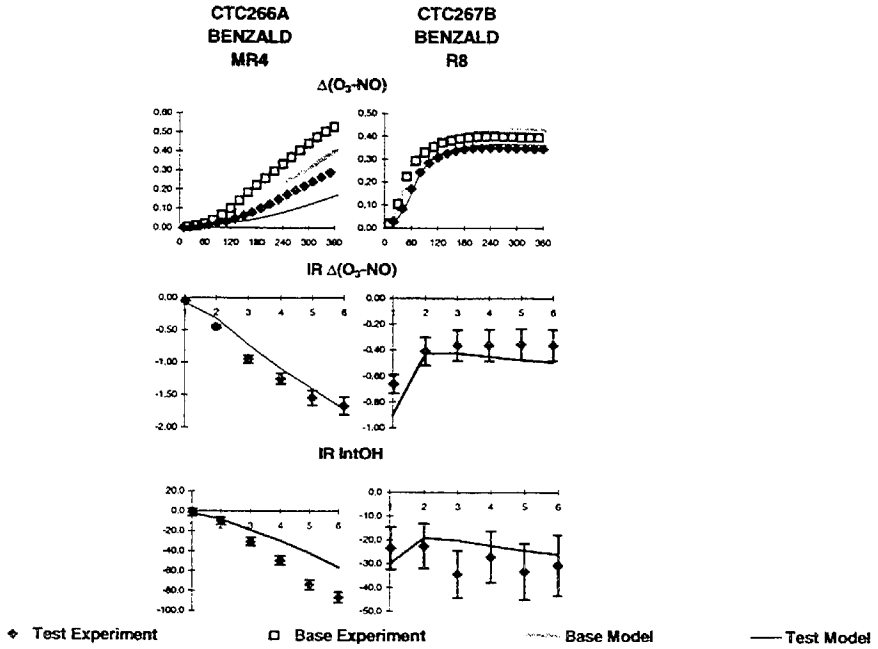


Figure B-12. Plots of experimental and calculated results of the incremental reactivity experiments with benzaldehyde.

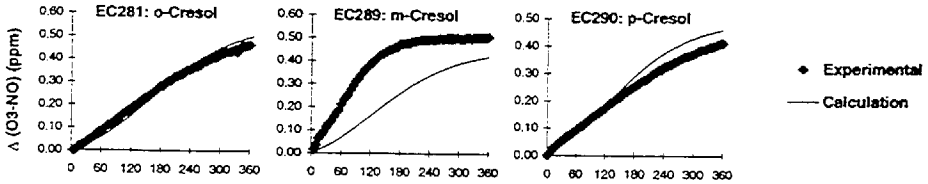


Figure B-13. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the cresol - NO_x experiments.

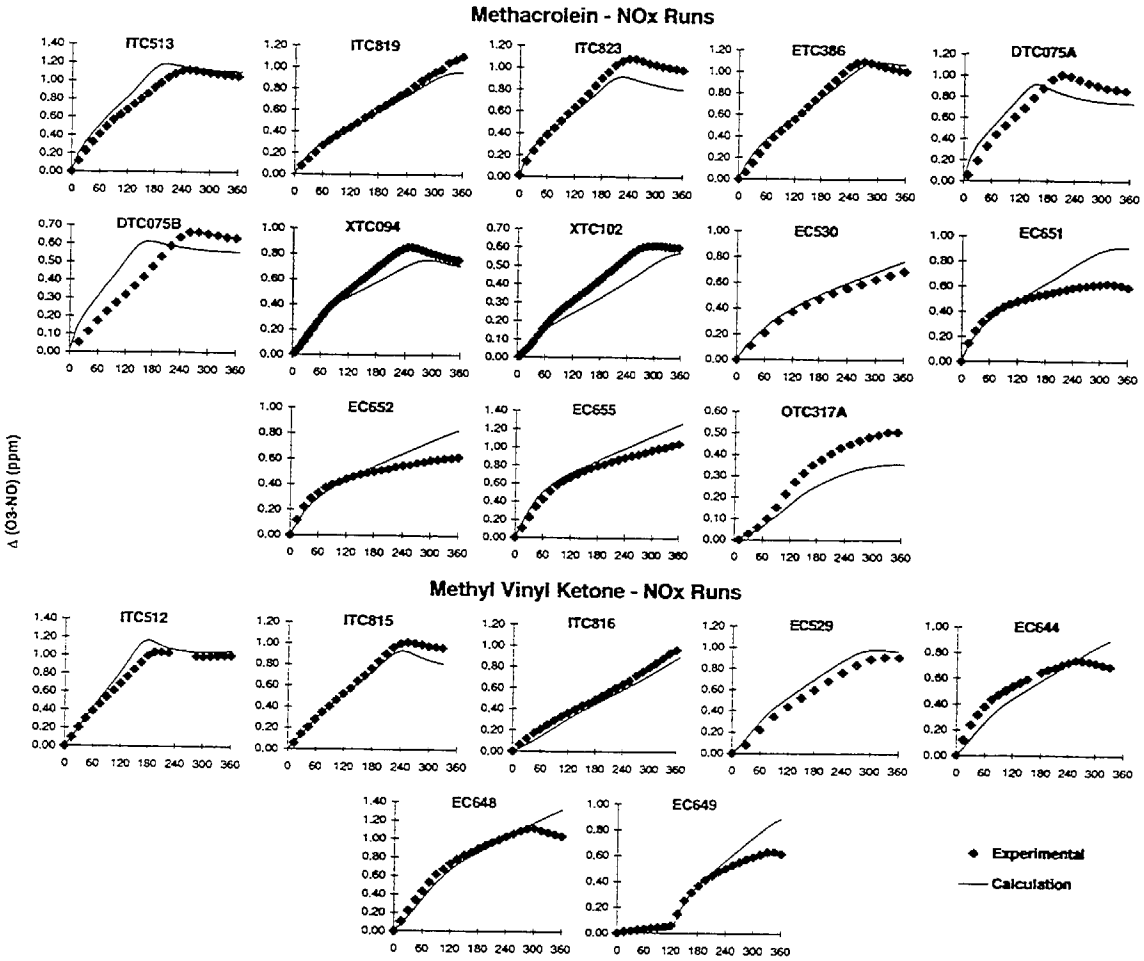


Figure B-14. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the methacrolein - NO_x and the methyl vinyl ketone - NO_x experiments.

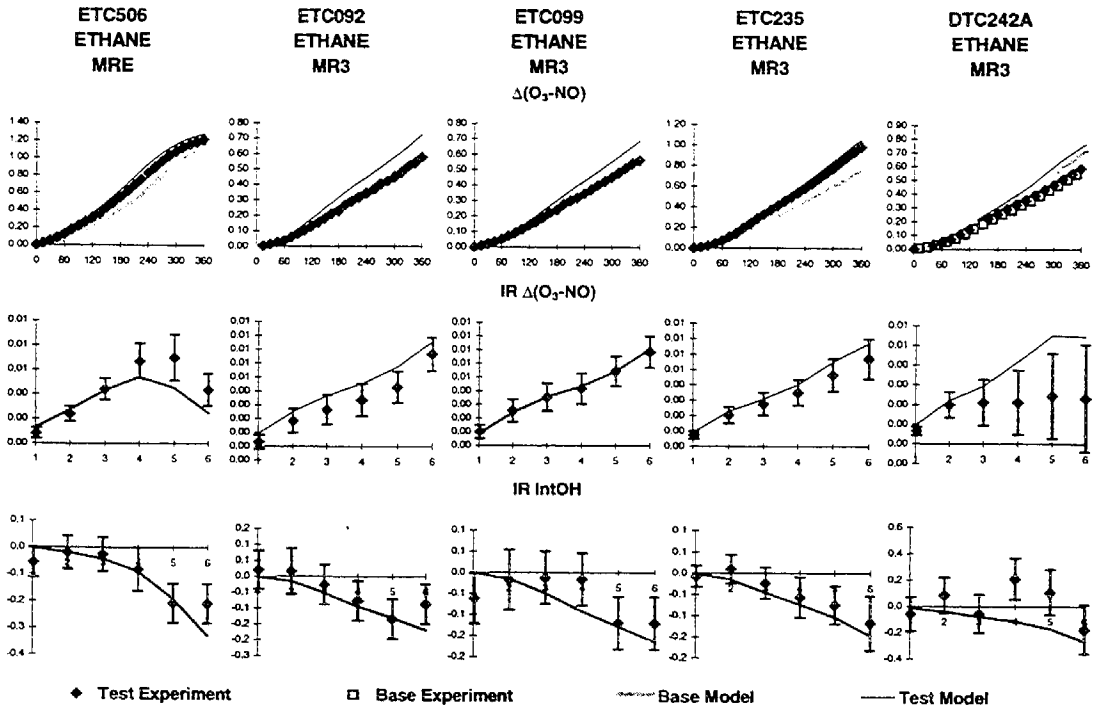


Figure B-15. Plots of experimental and calculated results of the incremental reactivity experiments with ethane

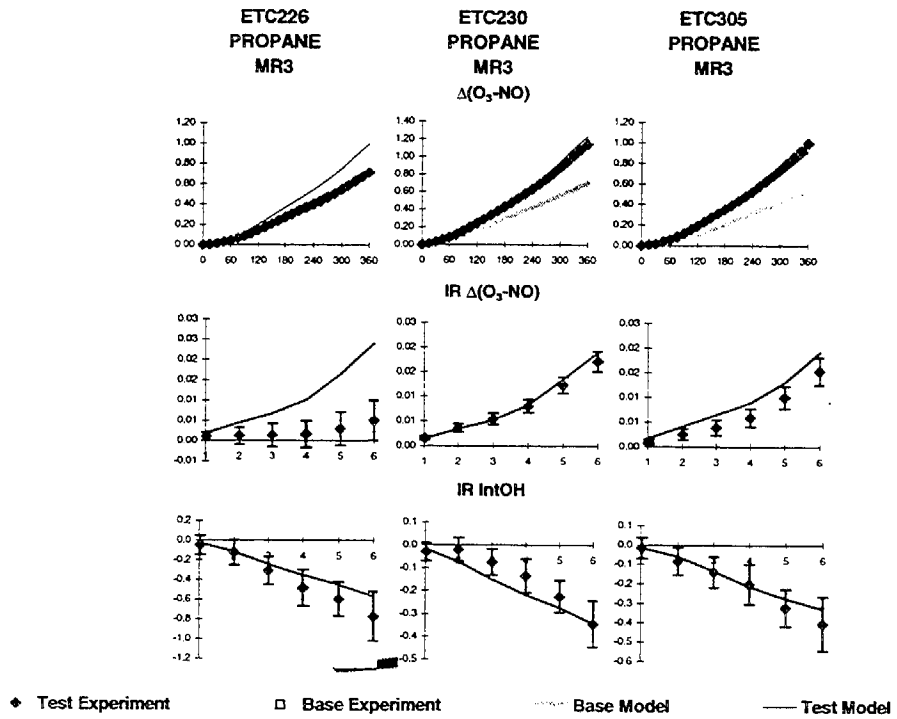


Figure B-16. Plots of experimental and calculated results of the incremental reactivity experiments with propane

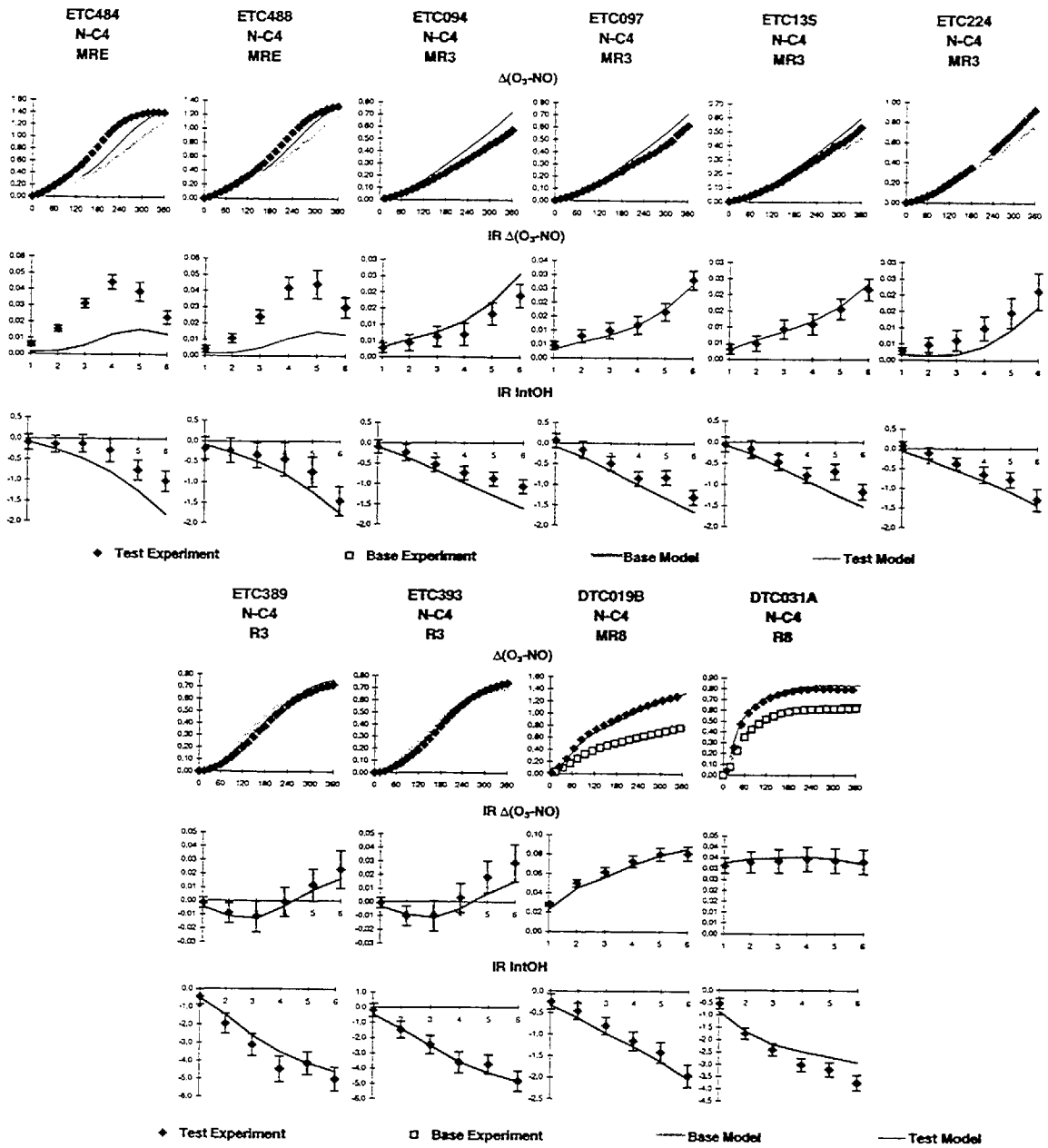


Figure B-17. Plots of experimental and calculated results of the incremental reactivity experiments with n-butane.

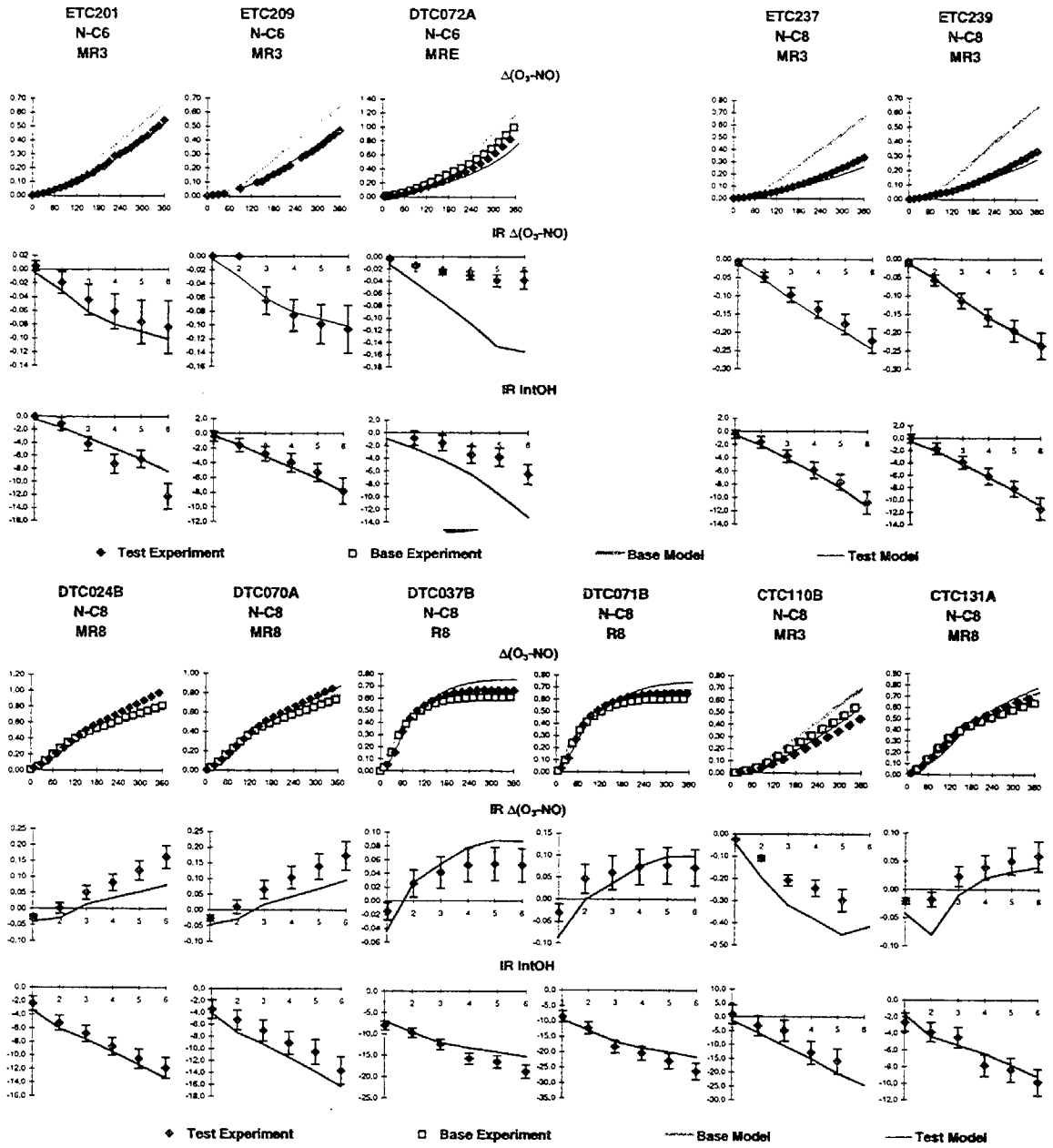


Figure B-18. Plots of experimental and calculated results of the incremental reactivity experiments with n-hexane and n-octane.

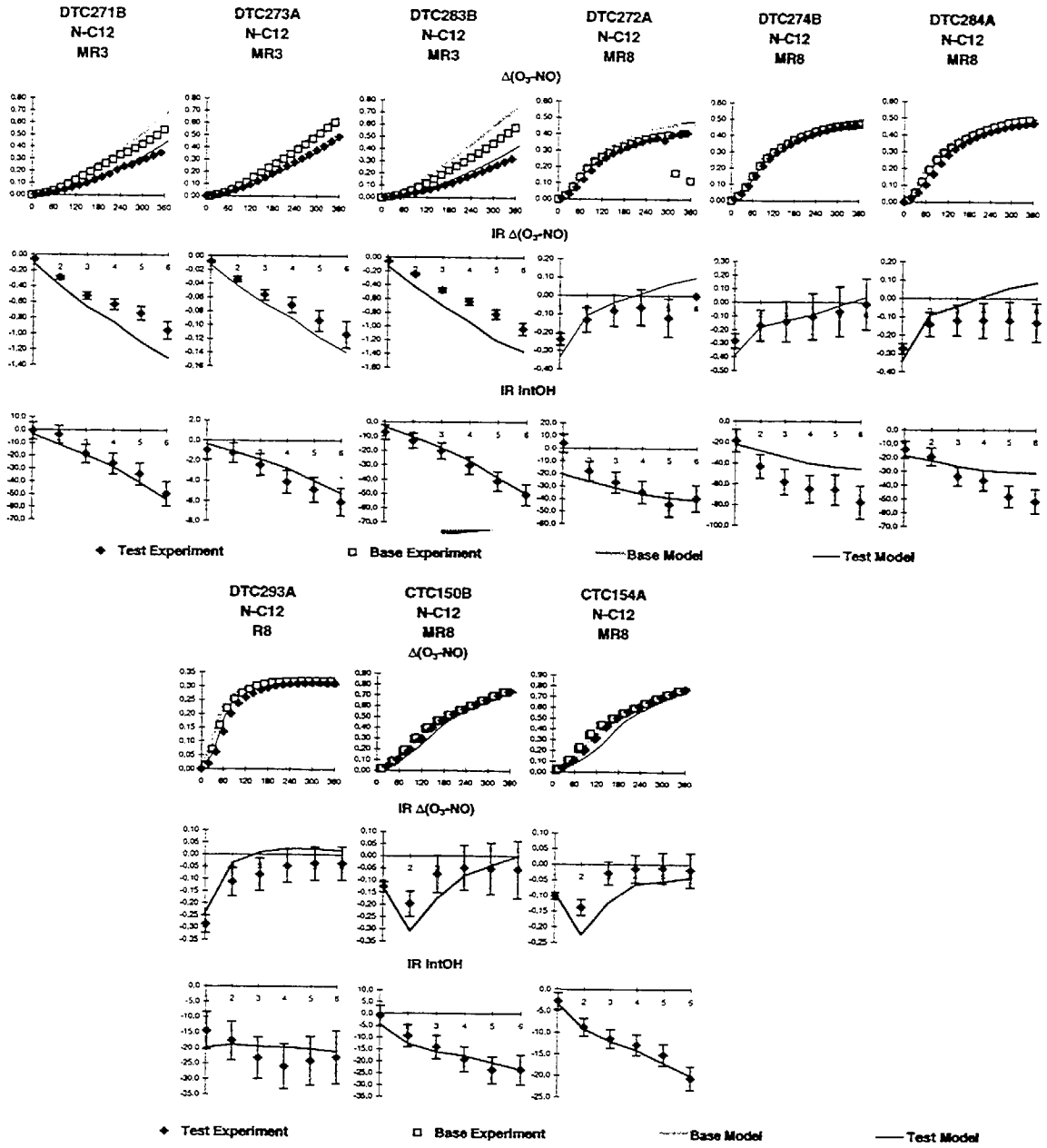


Figure B-19. Plots of experimental and calculated results of the incremental reactivity experiments with n-dodecane.

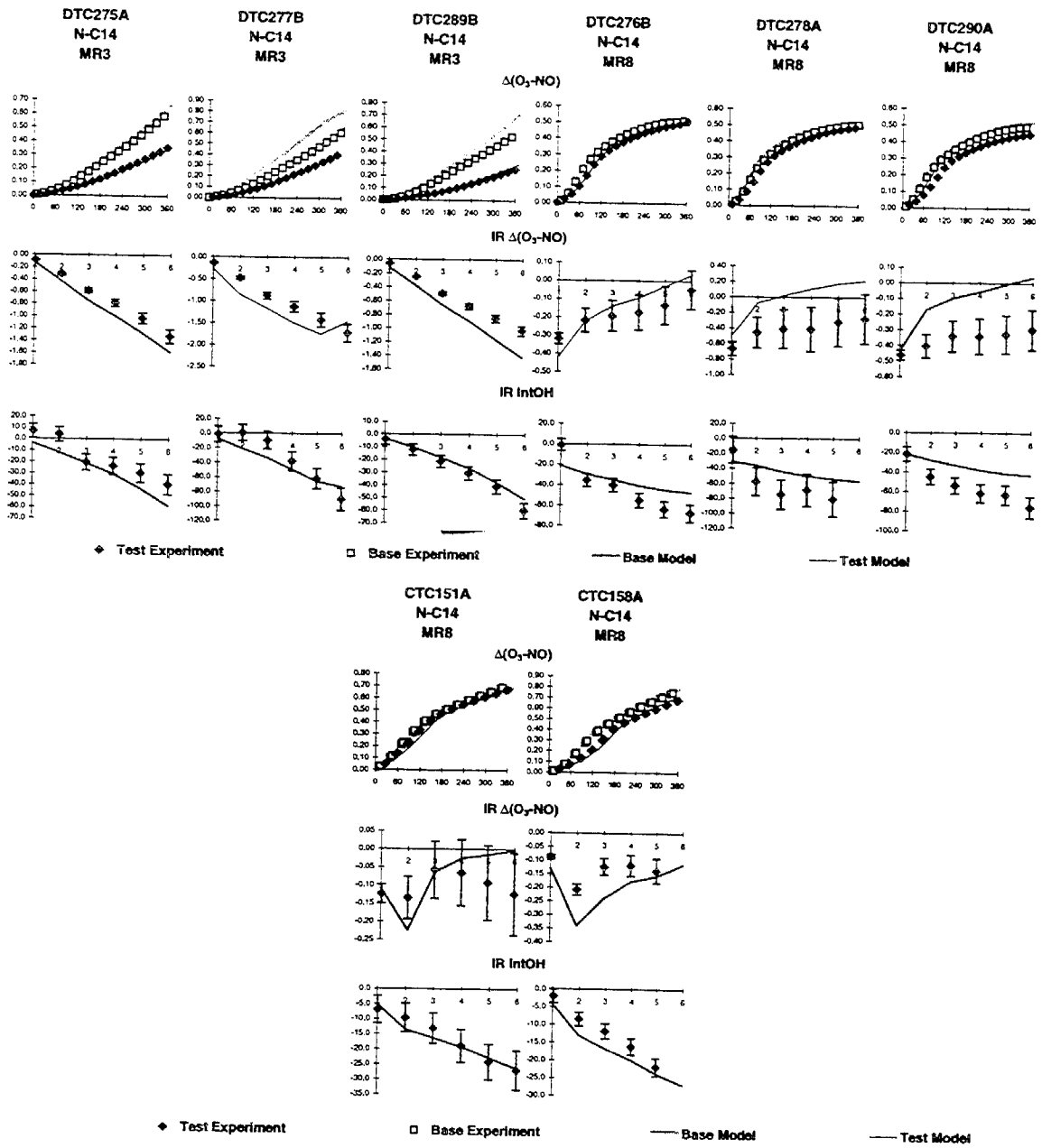


Figure B-20. Plots of experimental and calculated results of the incremental reactivity experiments with n-tetradecane.

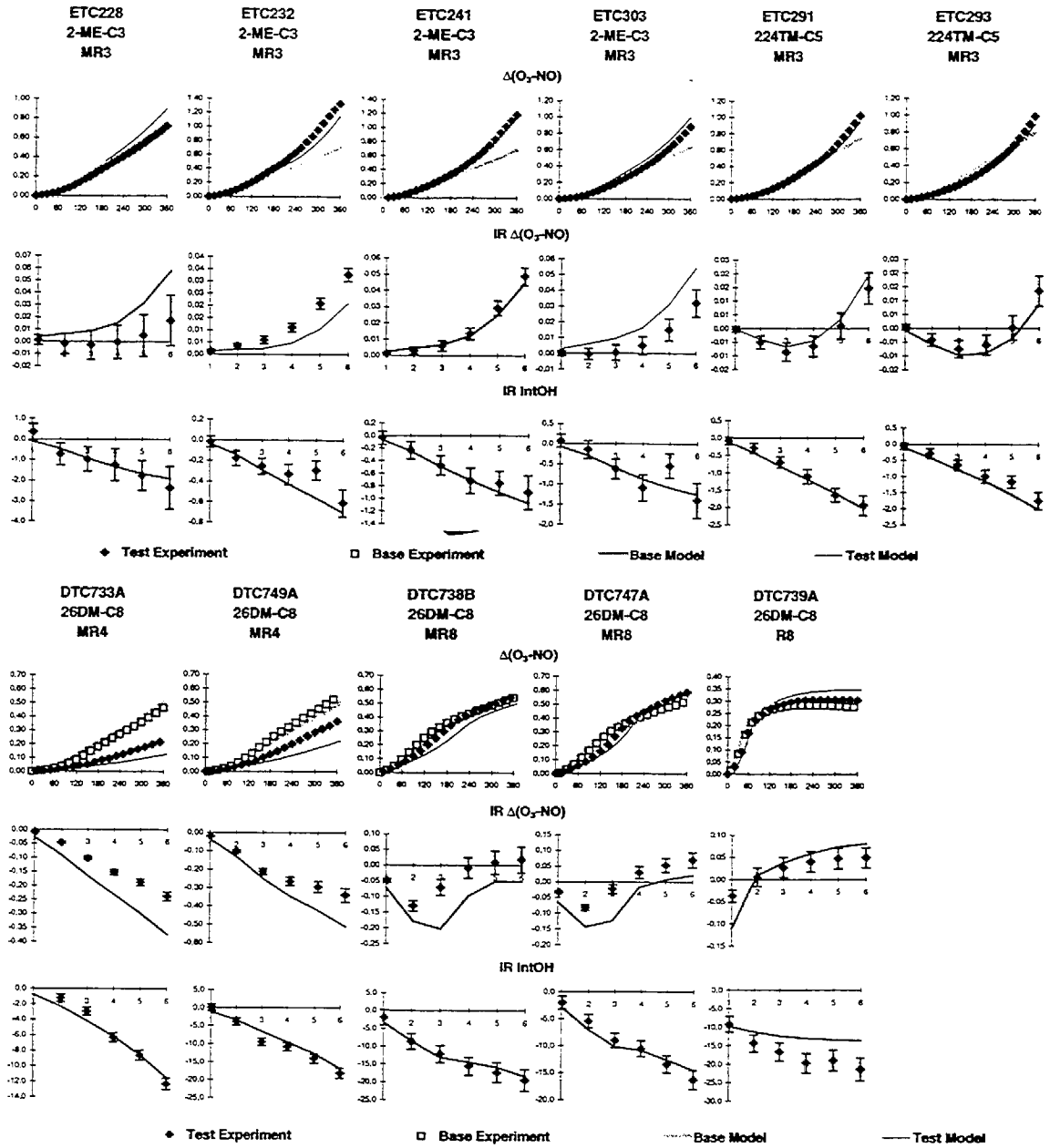


Figure B-22. Plots of experimental and calculated results of the incremental reactivity experiments with 2-methyl propene, 2,2,4-trimethyl butane and 2,5-dimethyl octane.

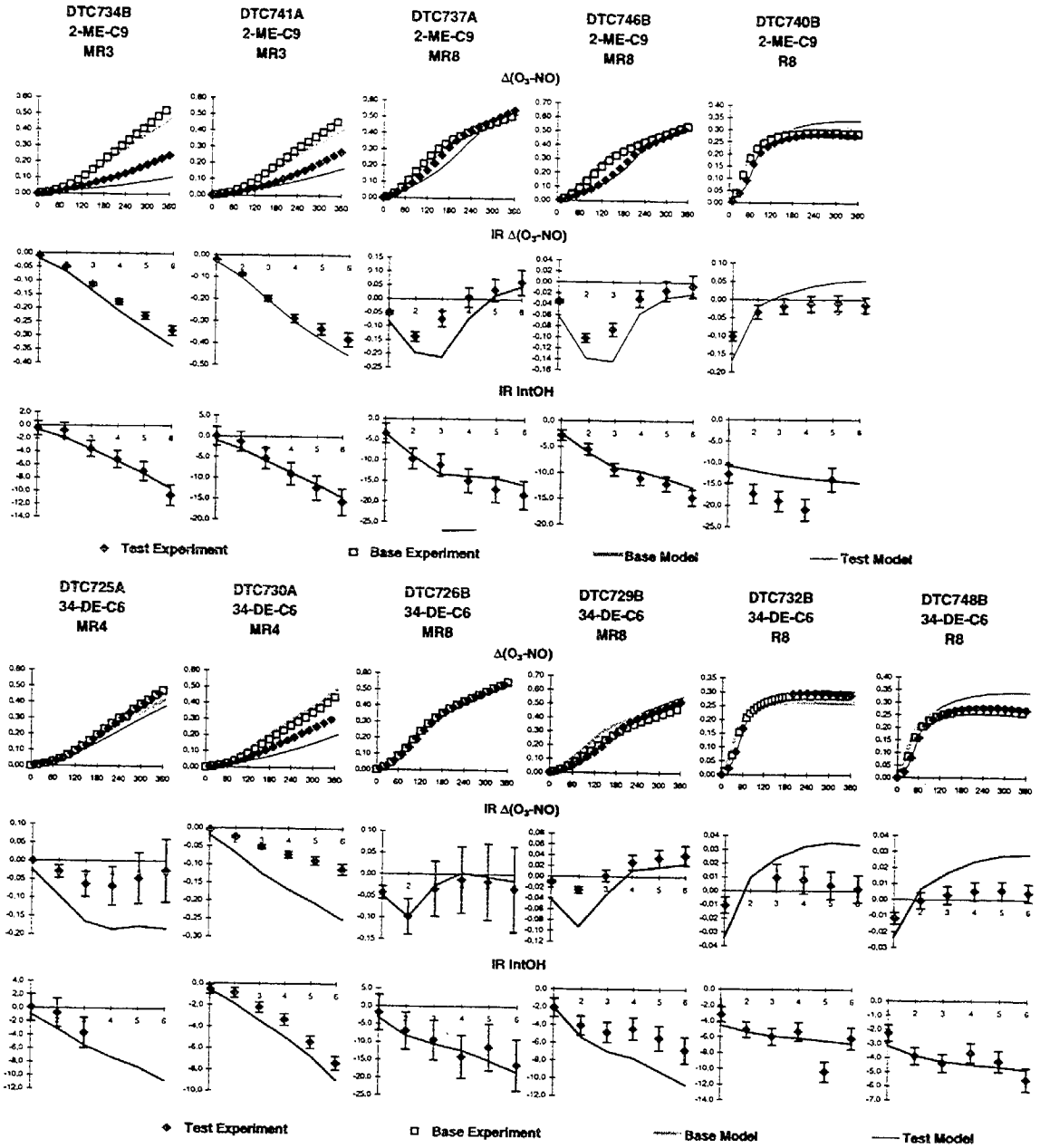


Figure B-23. Plots of experimental and calculated results of the incremental reactivity experiments with 2-methyl nonane and 3,4-diethyl hexane.

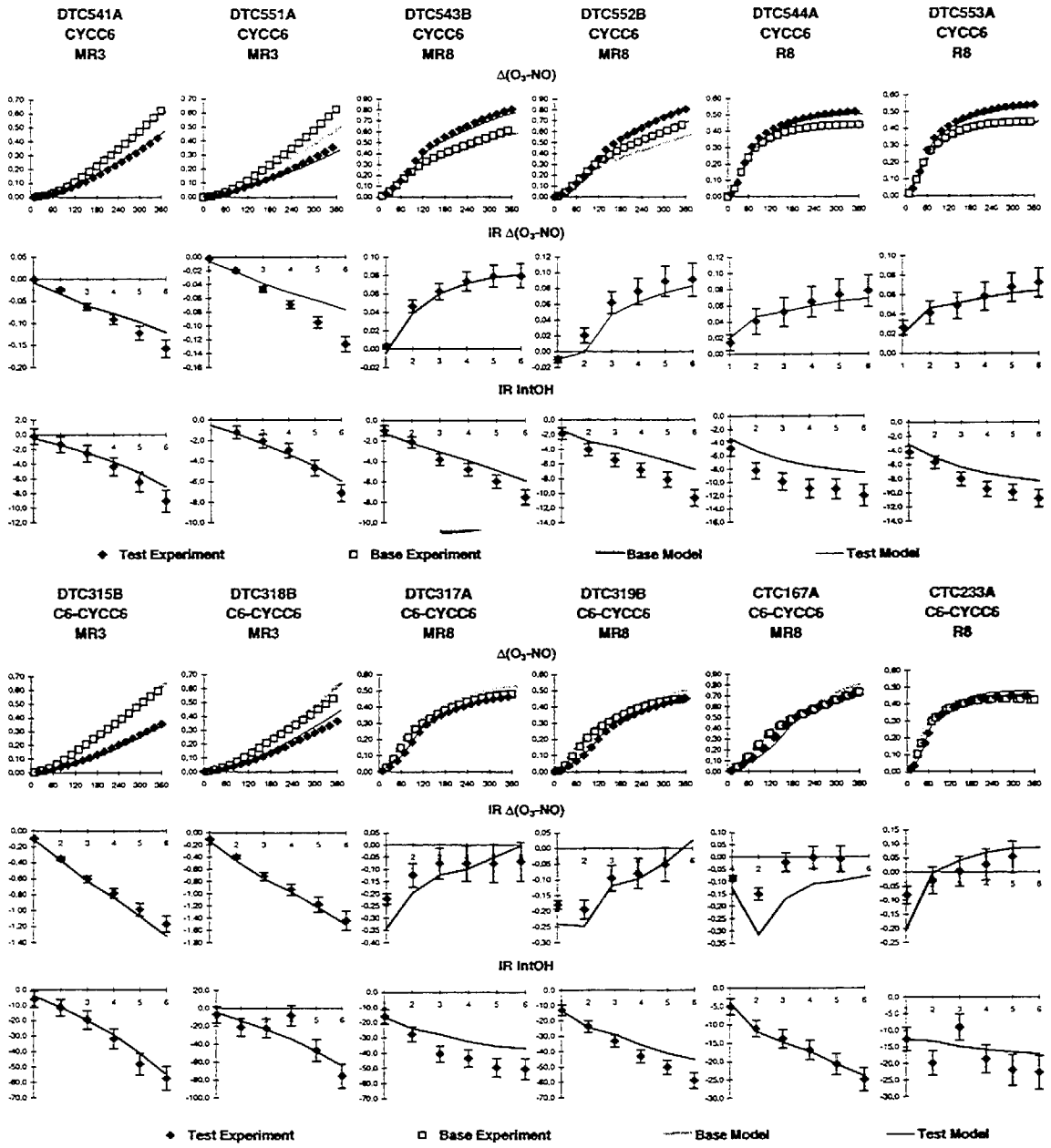


Figure B-24. Plots of experimental and calculated results of the incremental reactivity experiments with cyclohexane and n-hexyl cyclohexane.

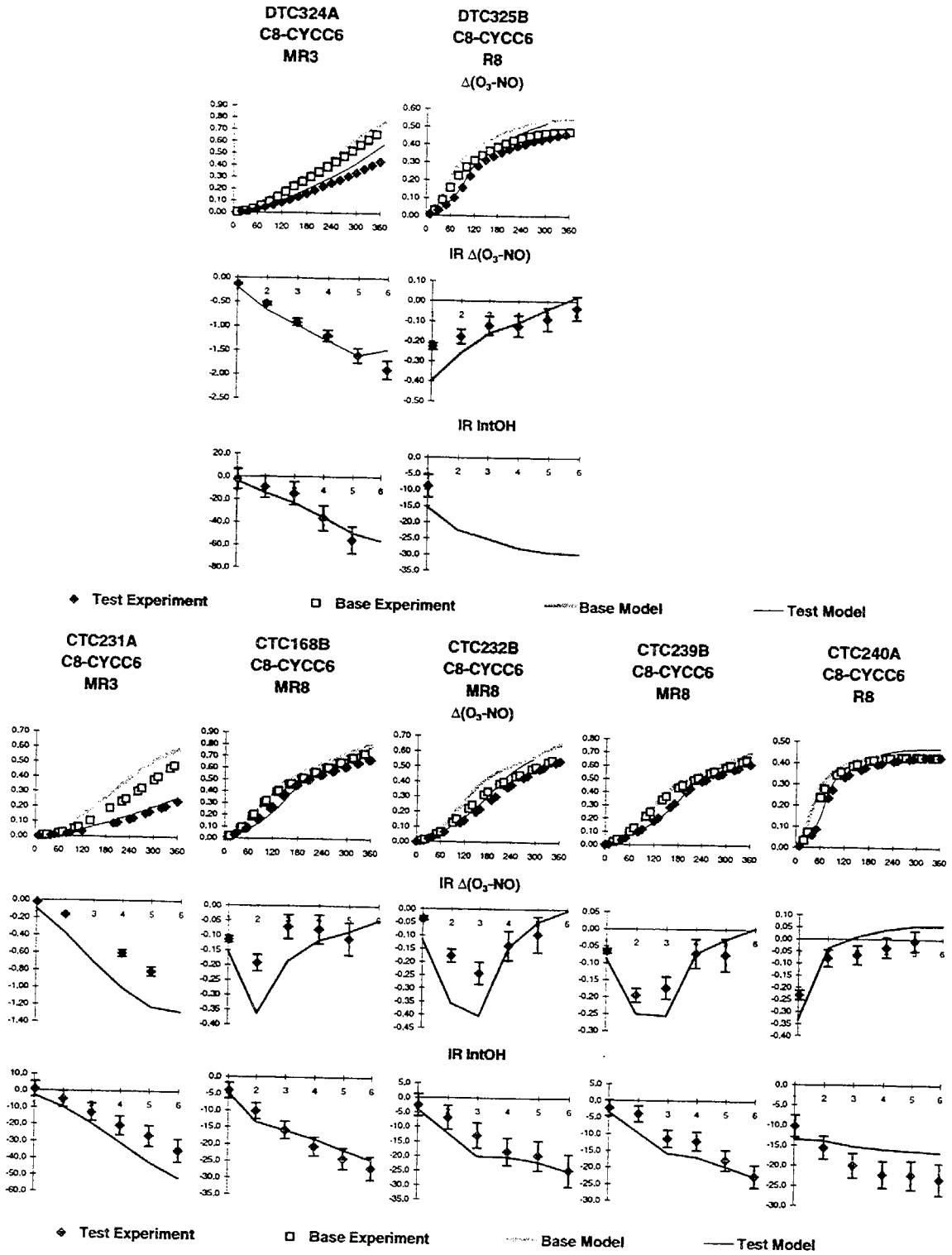


Figure B-25. Plots of experimental and calculated results of the incremental reactivity experiments with n-octyl cyclohexane.

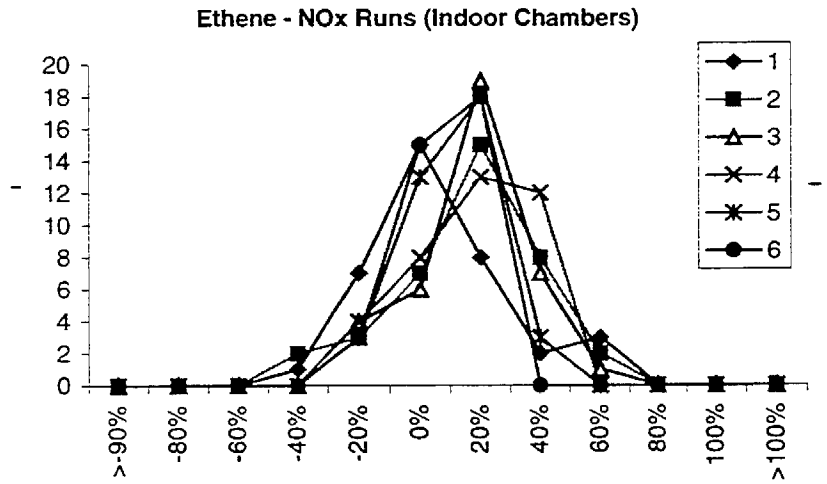


Figure B-26. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the ethene - NO_x runs carried out in indoor chambers.

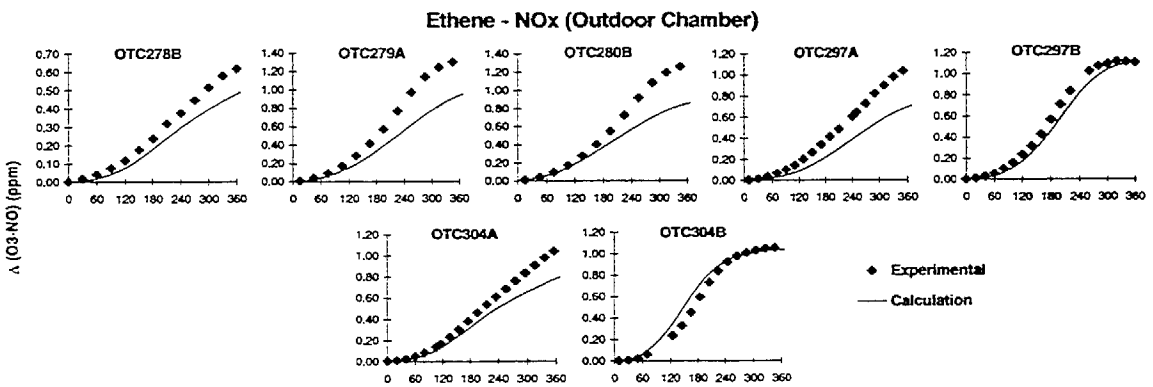


Figure B-27. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the ethene - NO_x runs carried out in the SAPRC outdoor chamber (OTC).

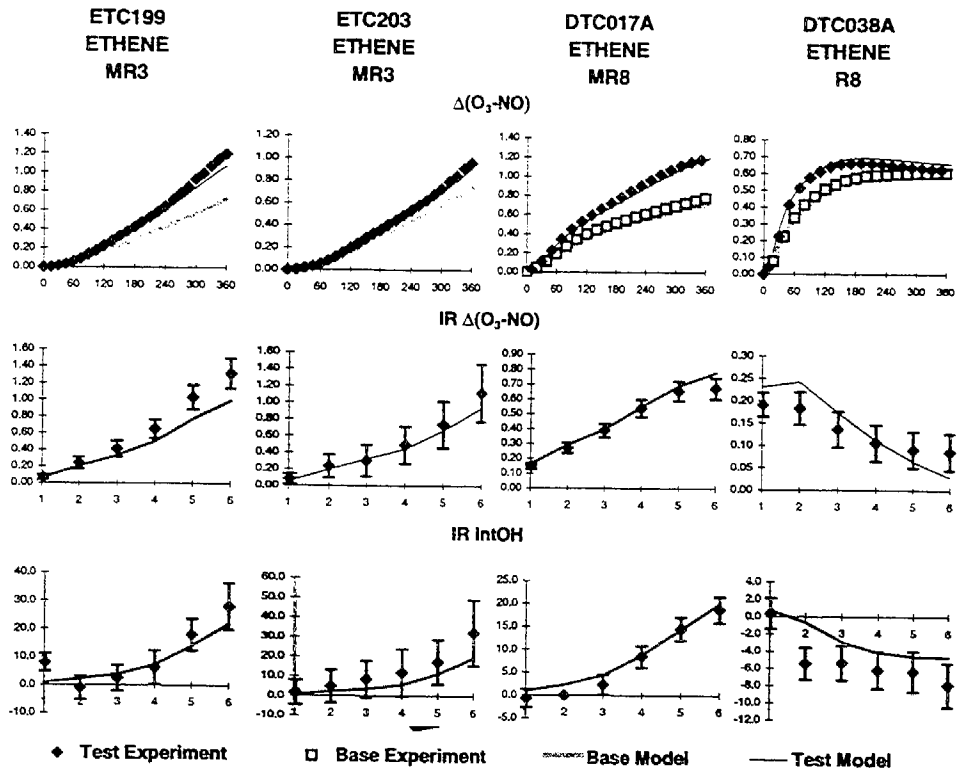


Figure B-28. Plots of experimental and calculated results of the incremental reactivity experiments with ethene.

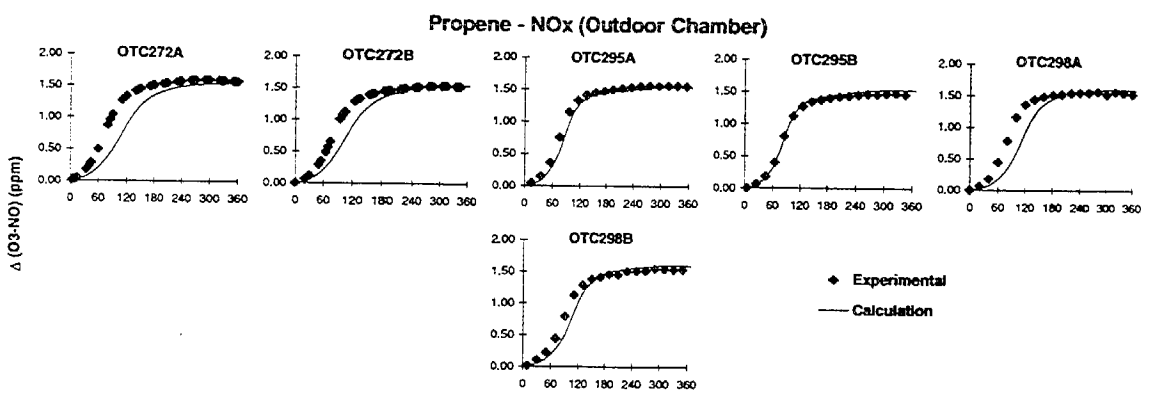


Figure B-29. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the propene - NO_x runs using the SAPRC outdoor chamber.

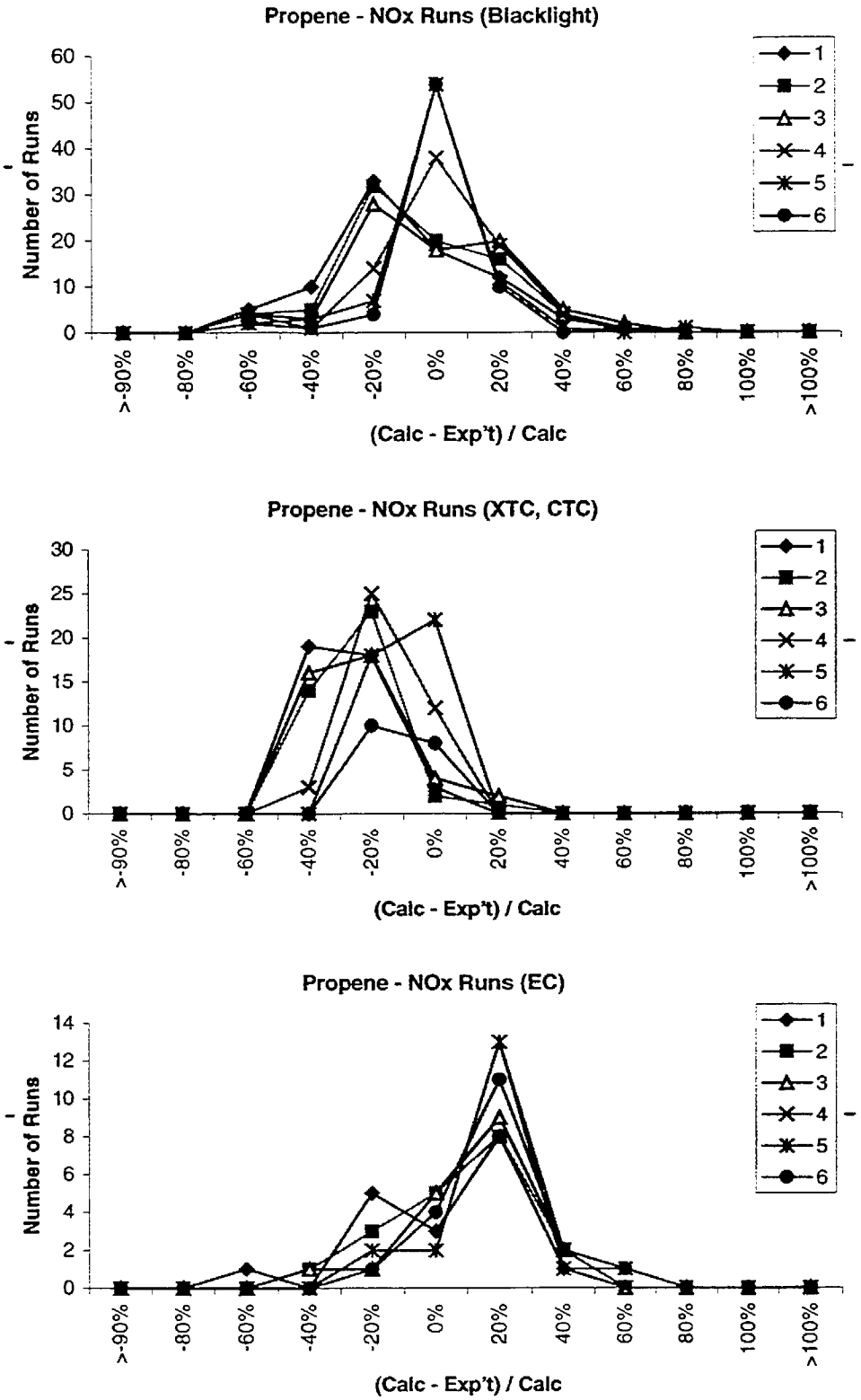


Figure B-30. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the propene - NO_x runs carried out using various chambers.

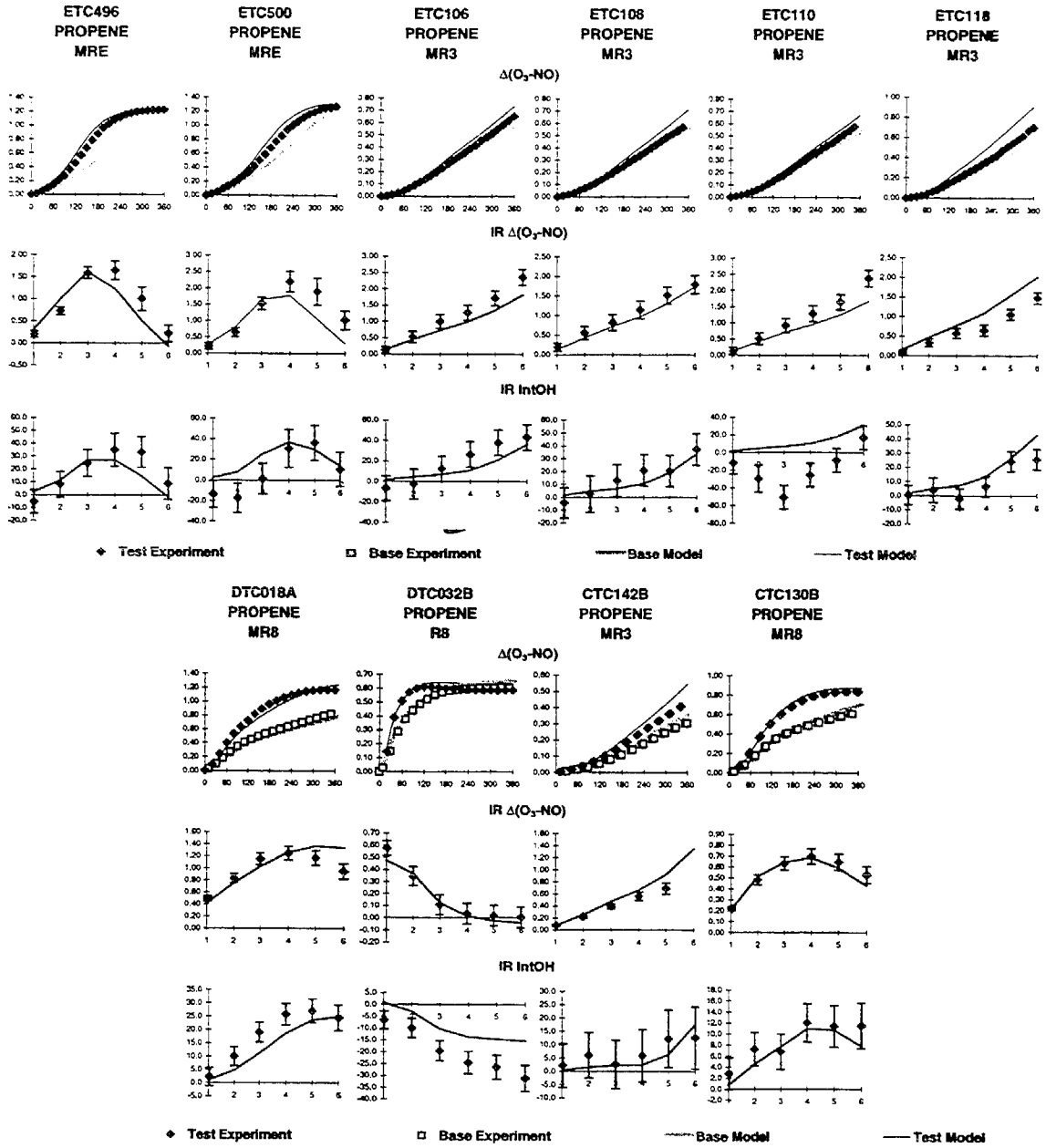


Figure B-31. Plots of experimental and calculated results of the incremental reactivity experiments with propene.

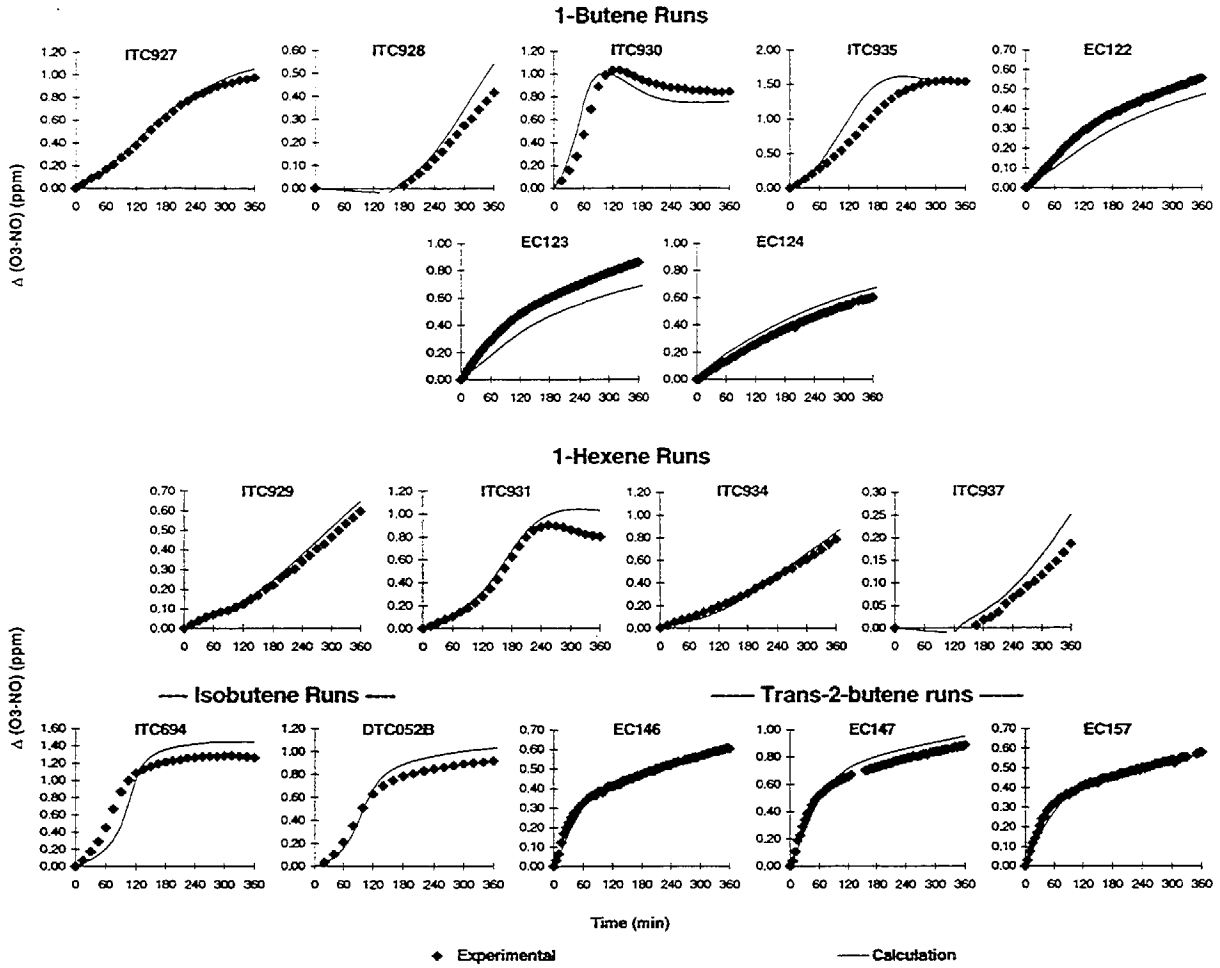


Figure B-32. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1-butene, 1-hexene, isobutene, and trans-2-butene - NO_x experiments.

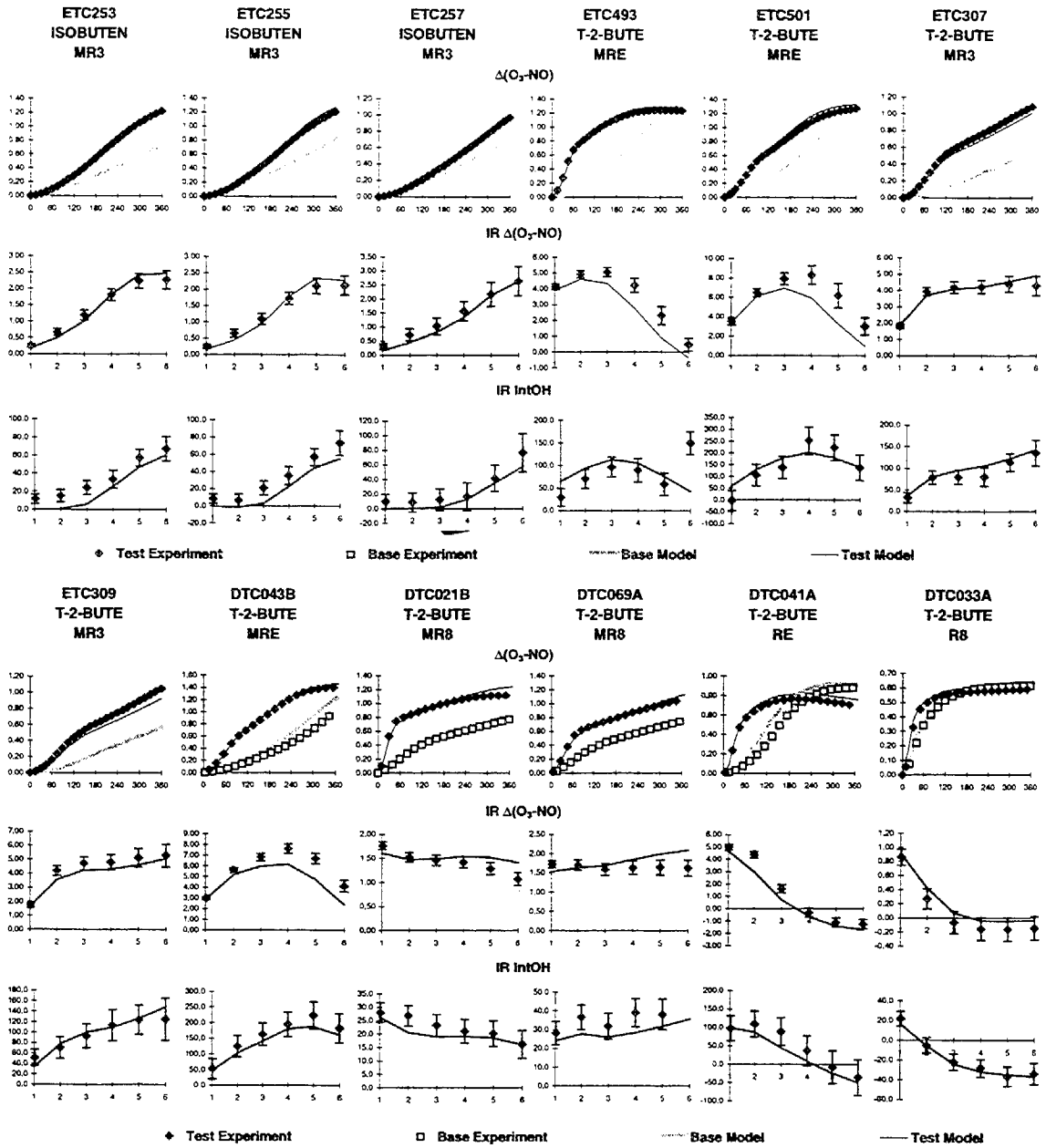


Figure B-33. Plots of experimental and calculated results of the incremental reactivity experiments with isobutene and trans-2-butene.

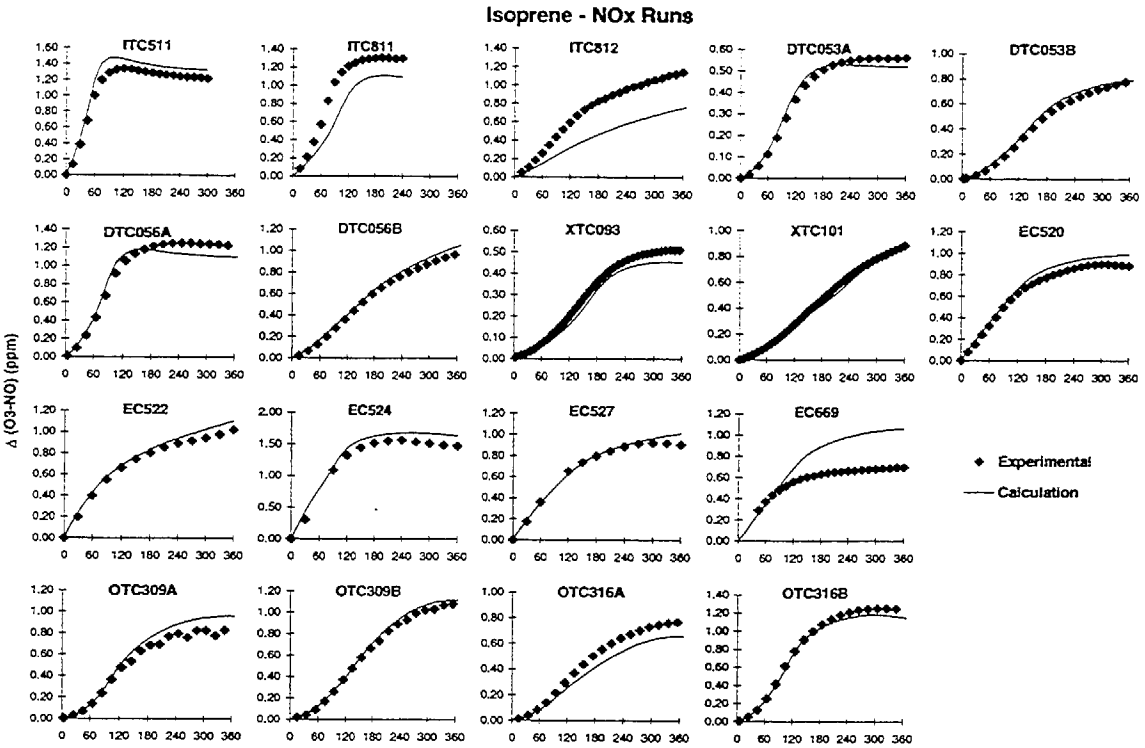


Figure B-34. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the isoprene - NO_x experiments.

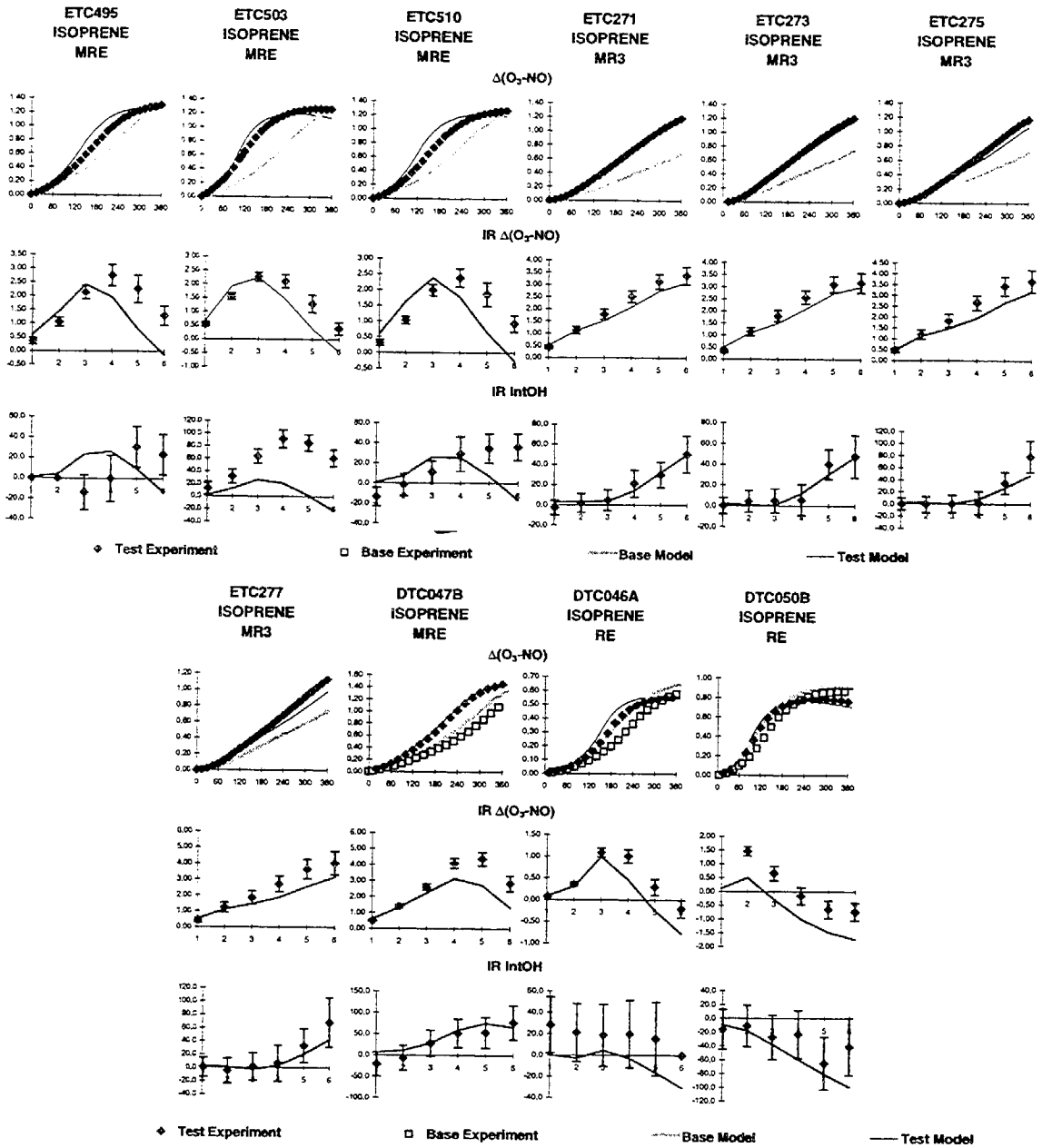


Figure B-35. Plots of experimental and calculated results of the incremental reactivity experiments with isoprene.

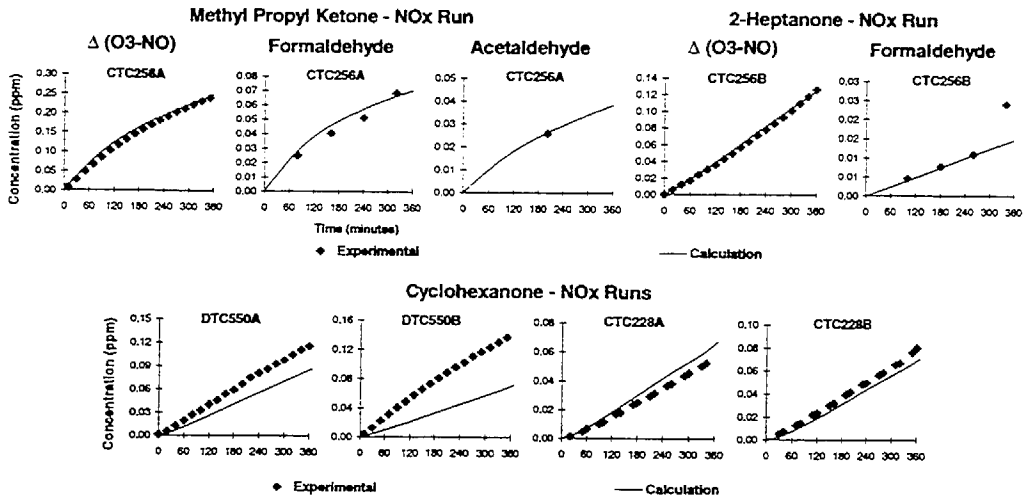


Figure B-36. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the methyl propyl ketone - NO_x, 2 -heptanone - NO_x and cyclohexanone - NO_x experiments.

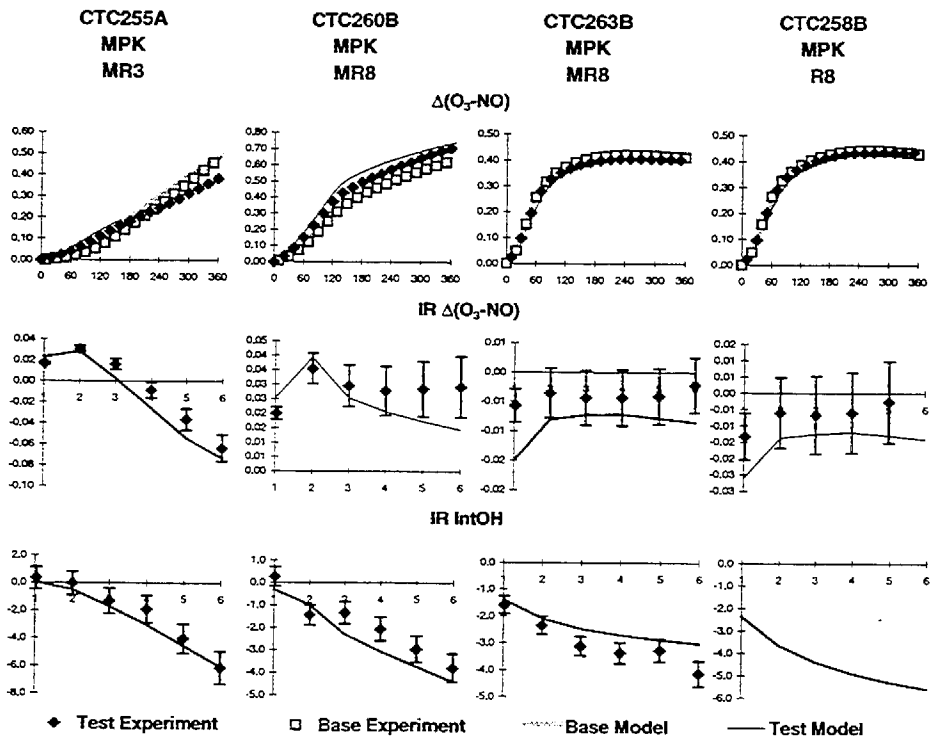


Figure B-37. Plots of experimental and calculated results of the incremental reactivity experiments with methyl propyl ketone.

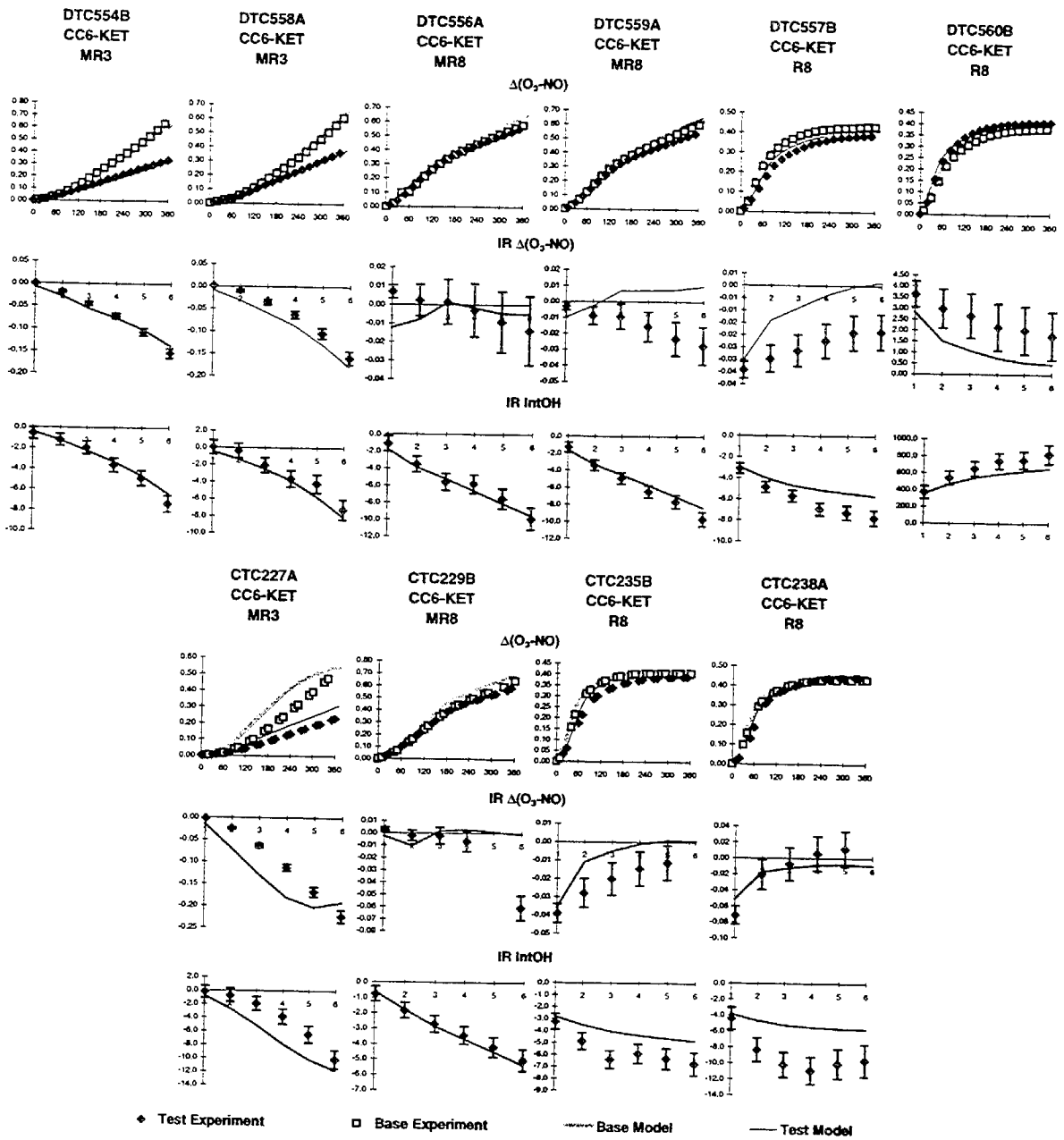


Figure B-38. Plots of experimental and calculated results of the incremental reactivity experiments with cyclohexanone.

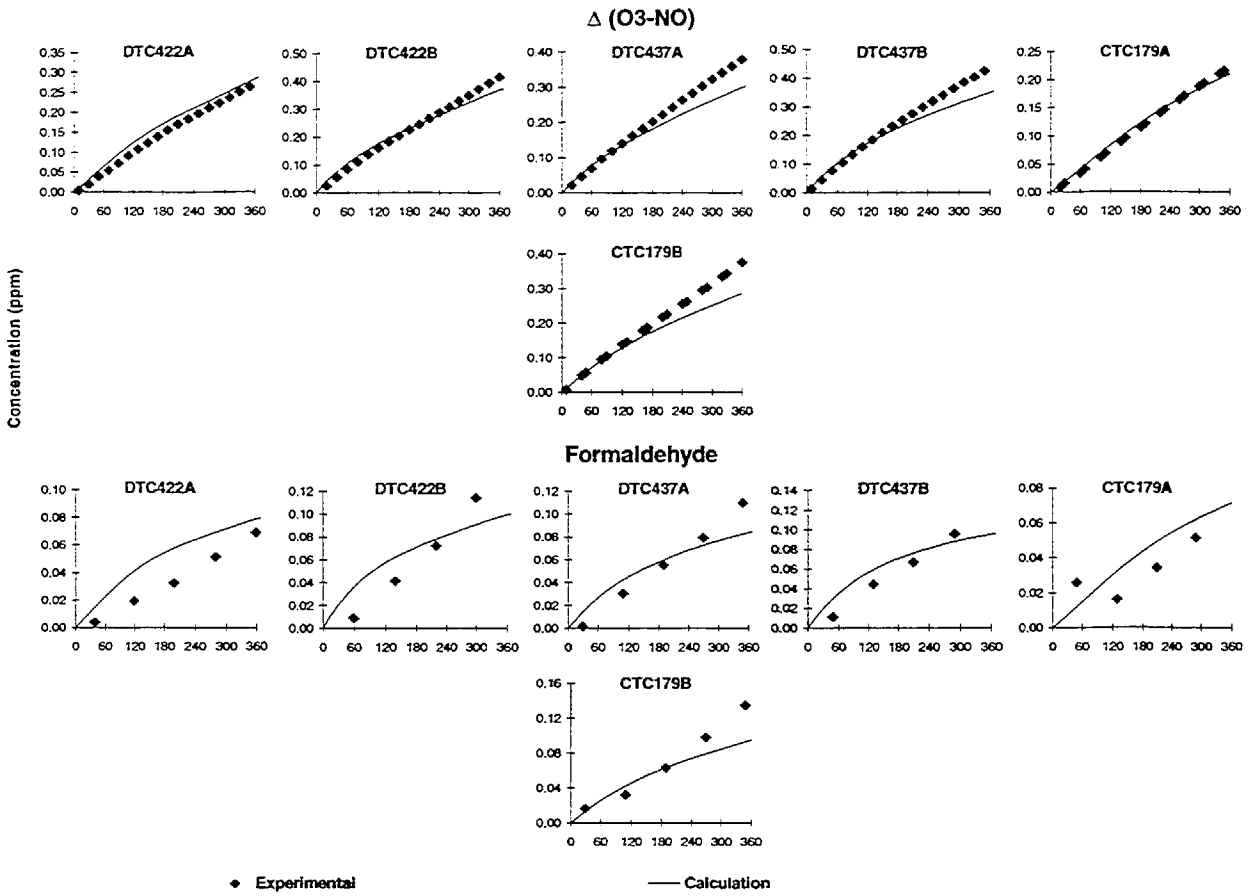


Figure B-39. Plots of experimental and calculated $\Delta([O_3]-[NO])$ and formaldehyde data for the methyl isobutyl ketone - NO_x experiments.

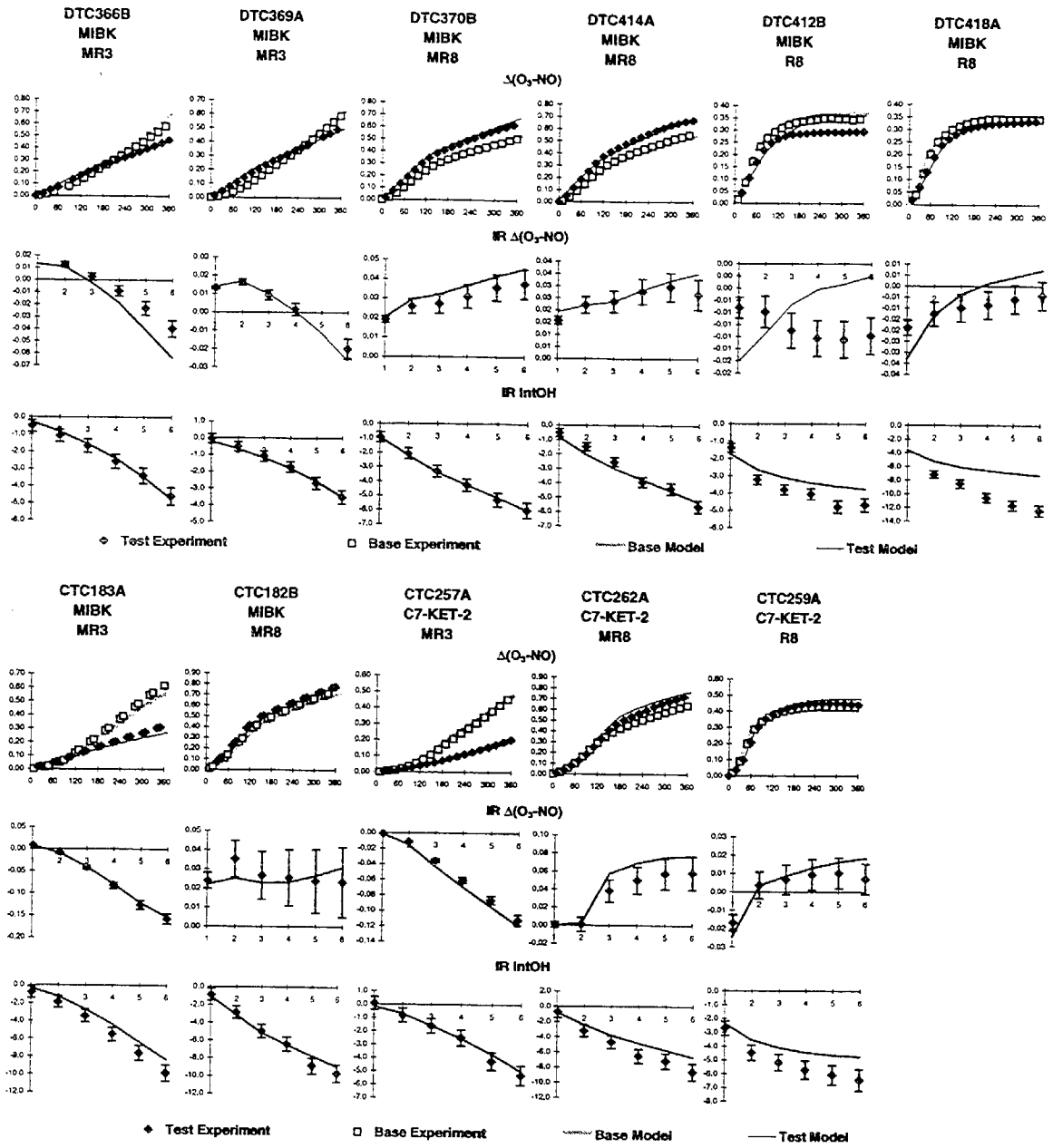


Figure B-40. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isobutyl ketone and 2-heptanone.

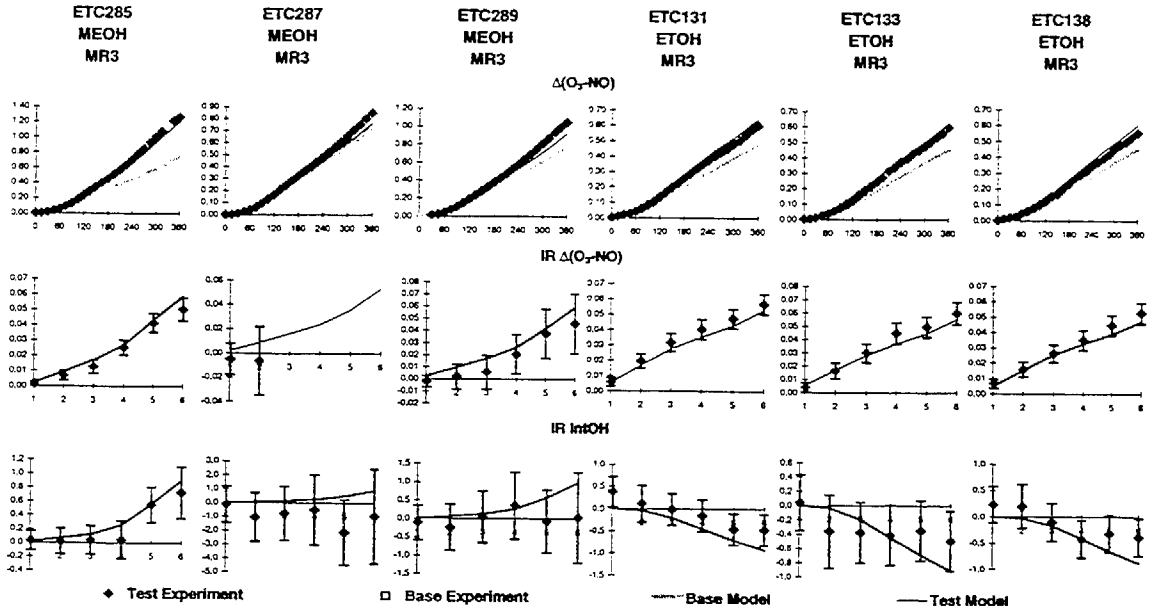


Figure B-41. Plots of experimental and calculated results of the incremental reactivity experiments with methanol and ethanol.

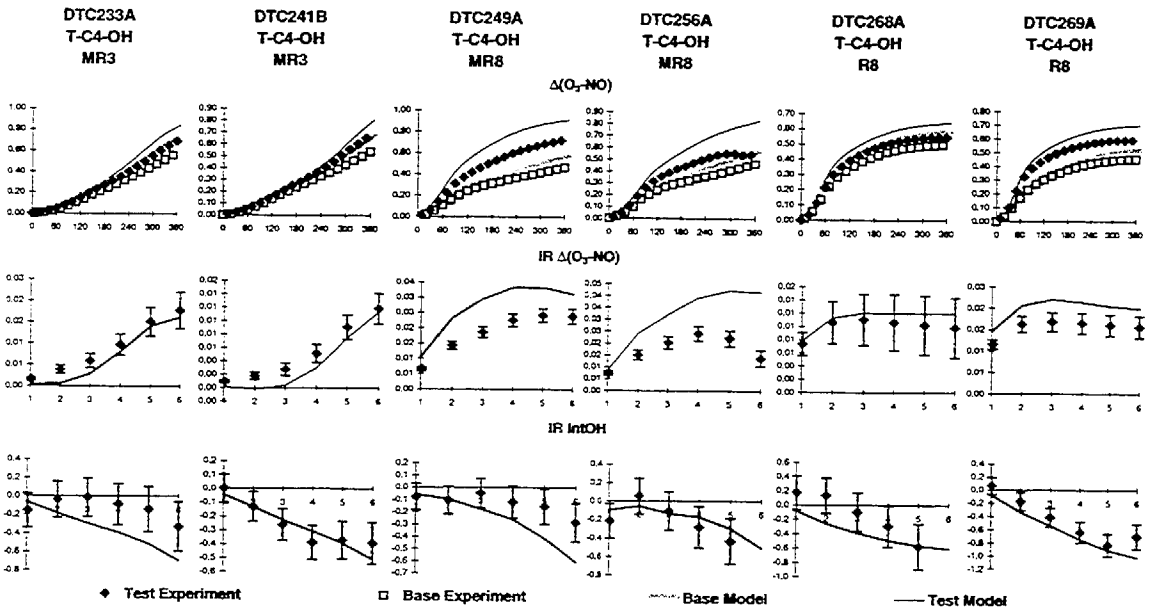


Figure B-42. Plots of experimental and calculated results of the incremental reactivity experiments with t-butyl alcohol. (Run DTC259A, whose results are very similar to those for run DTC269A, is not shown.)

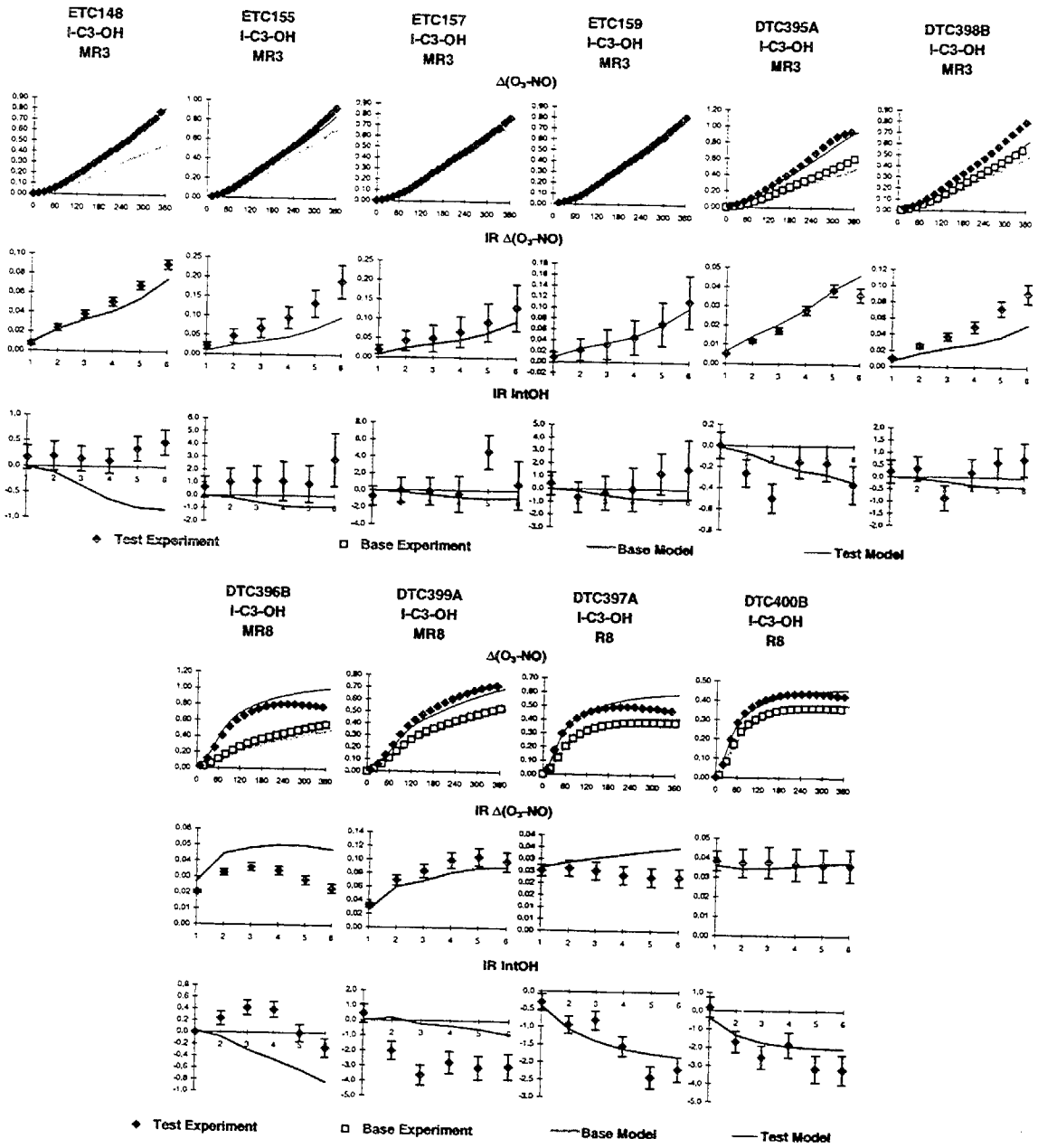
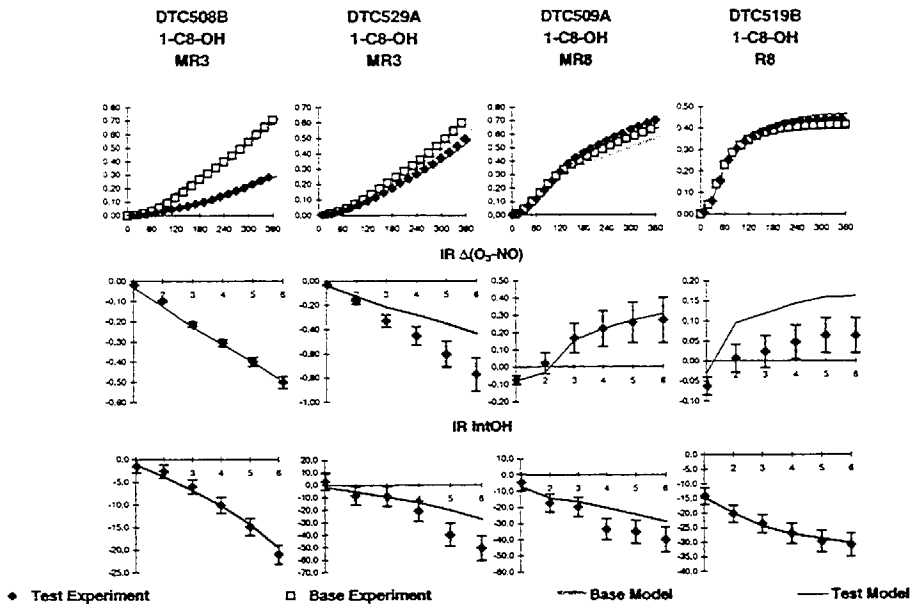


Figure B-43. Plots of experimental and calculated results of the incremental reactivity experiments with isopropyl alcohol.



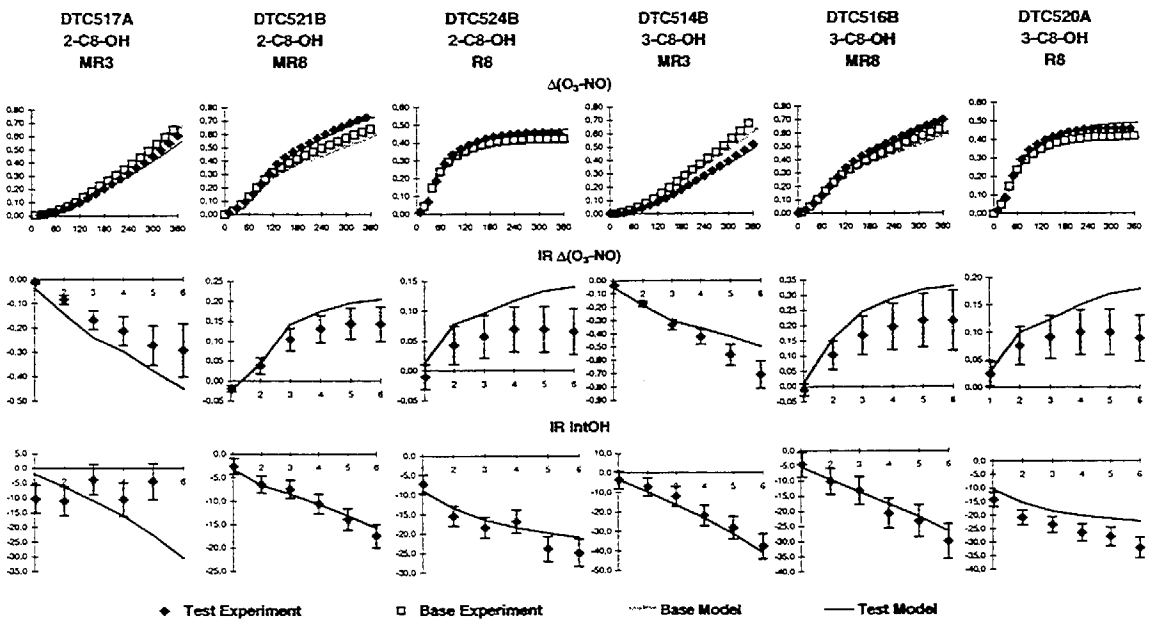


Figure B-44. Plots of experimental and calculated results of the incremental reactivity experiments with 1-, 2-, and 3-octanols.

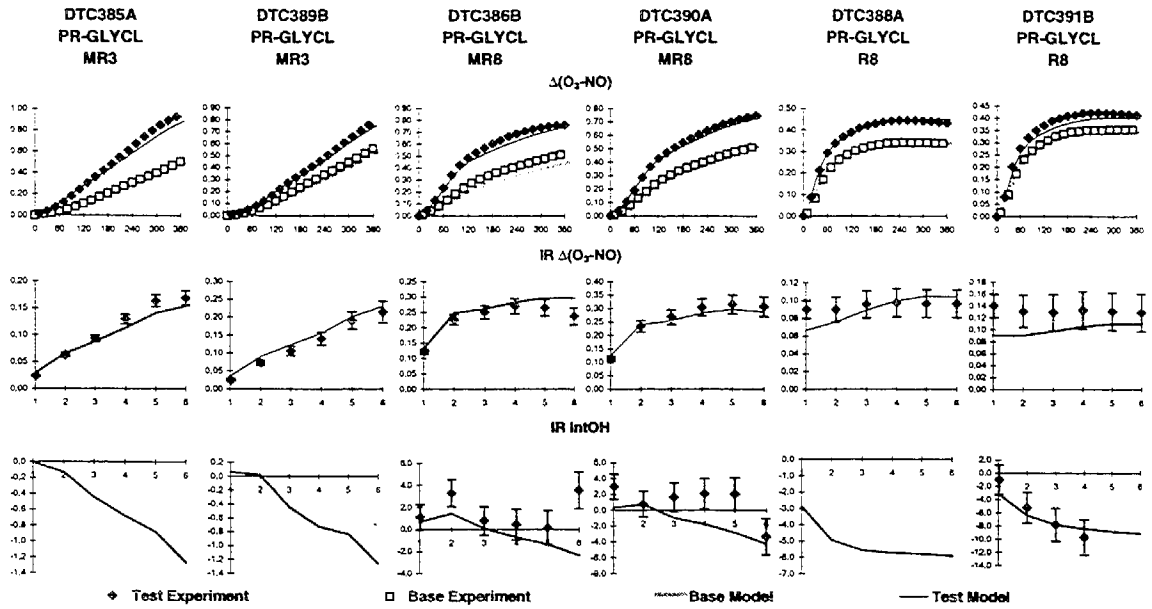


Figure B-45. Plots of experimental and calculated results of the incremental reactivity experiments with propylene glycol.

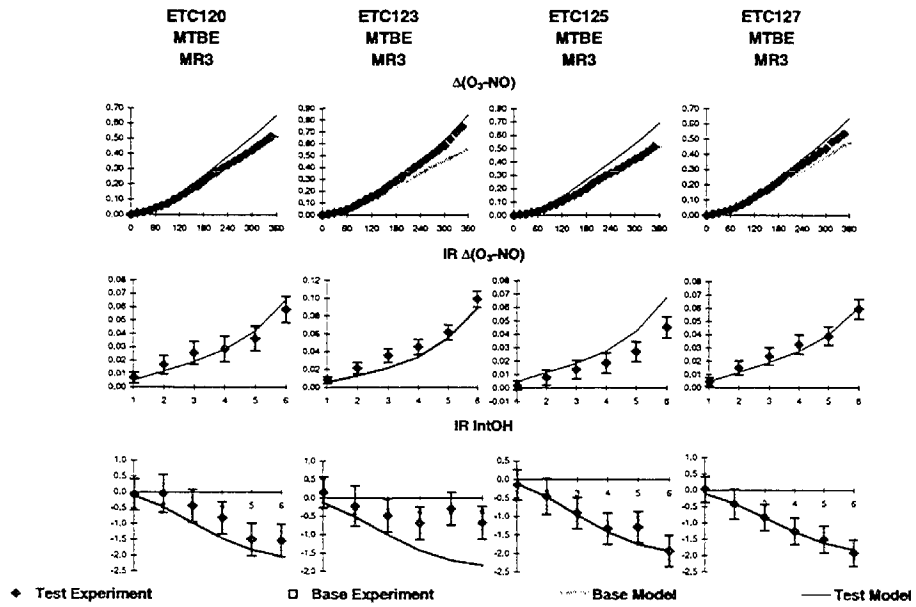


Figure B-46. Plots of experimental and calculated results of the incremental reactivity experiments with methyl t-butyl ether.

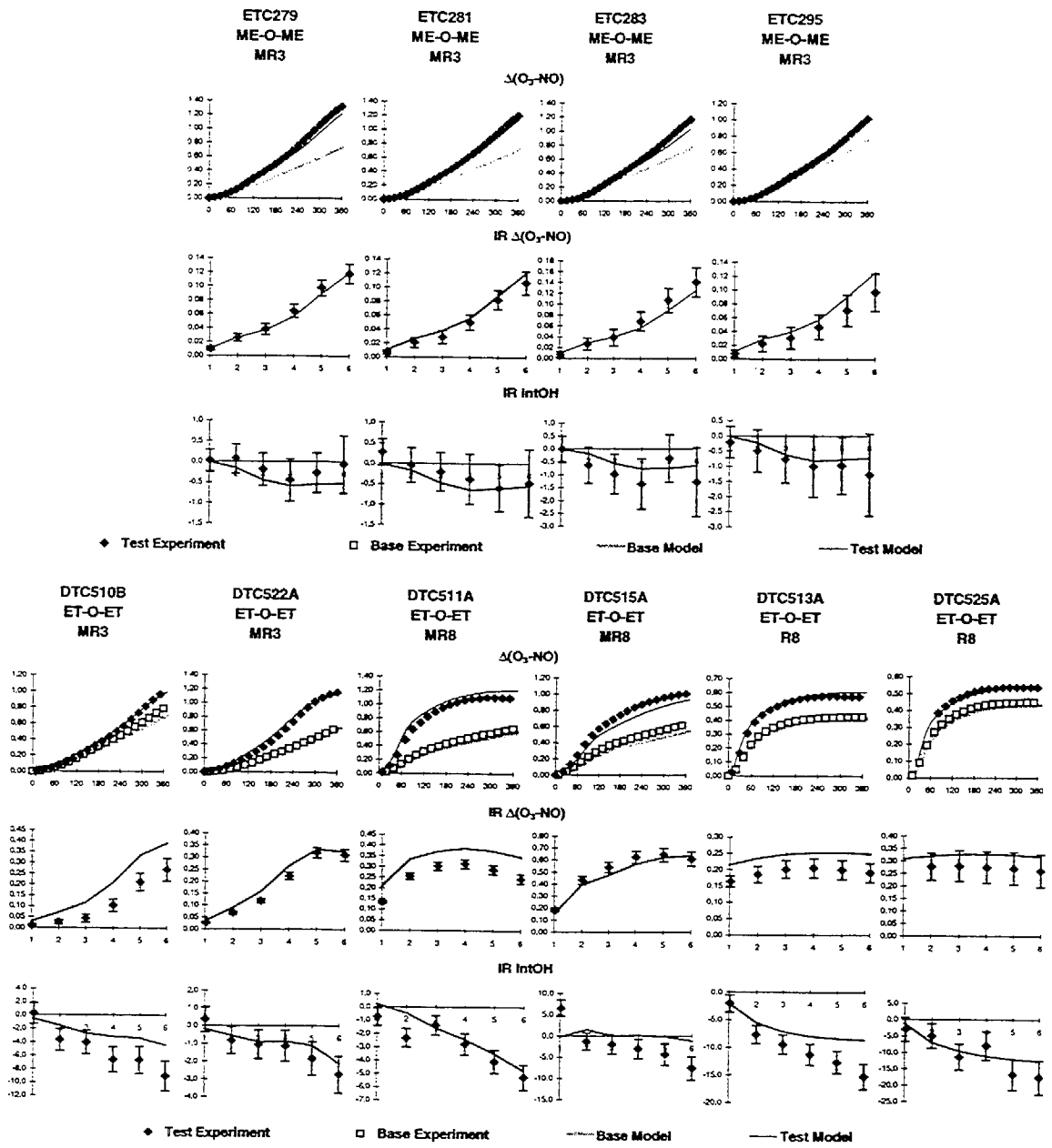


Figure B-47. Plots of experimental and calculated results of the incremental reactivity experiments with dimethyl ether and diethyl ether.

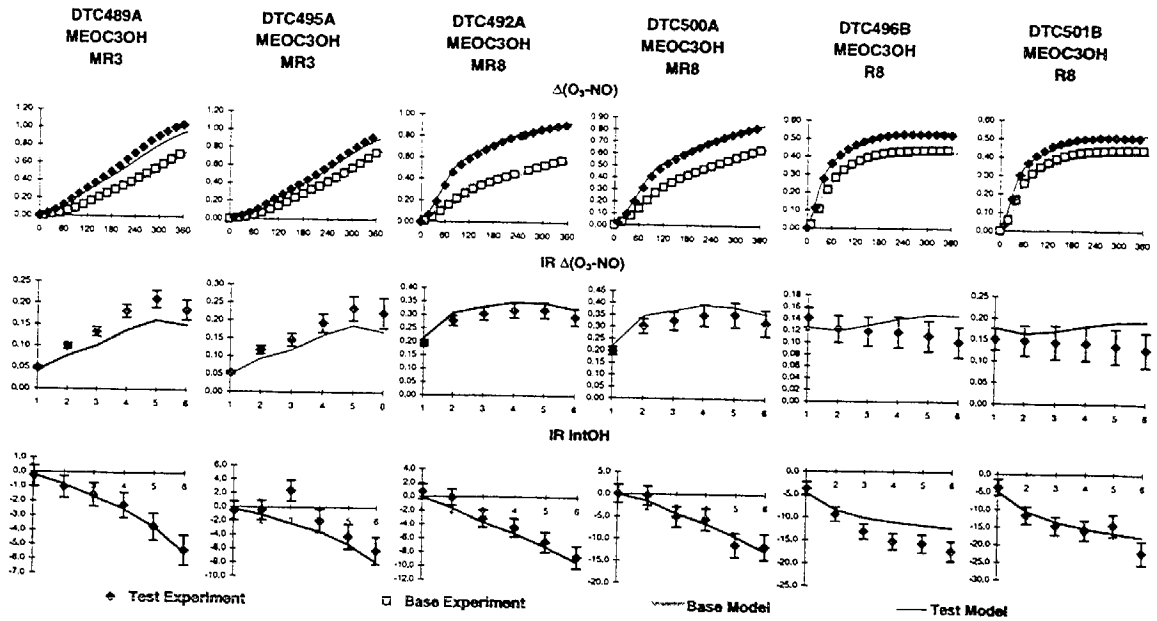


Figure B-48. Plots of experimental and calculated results of the incremental reactivity experiments with 1-Methoxy-2-Propanol

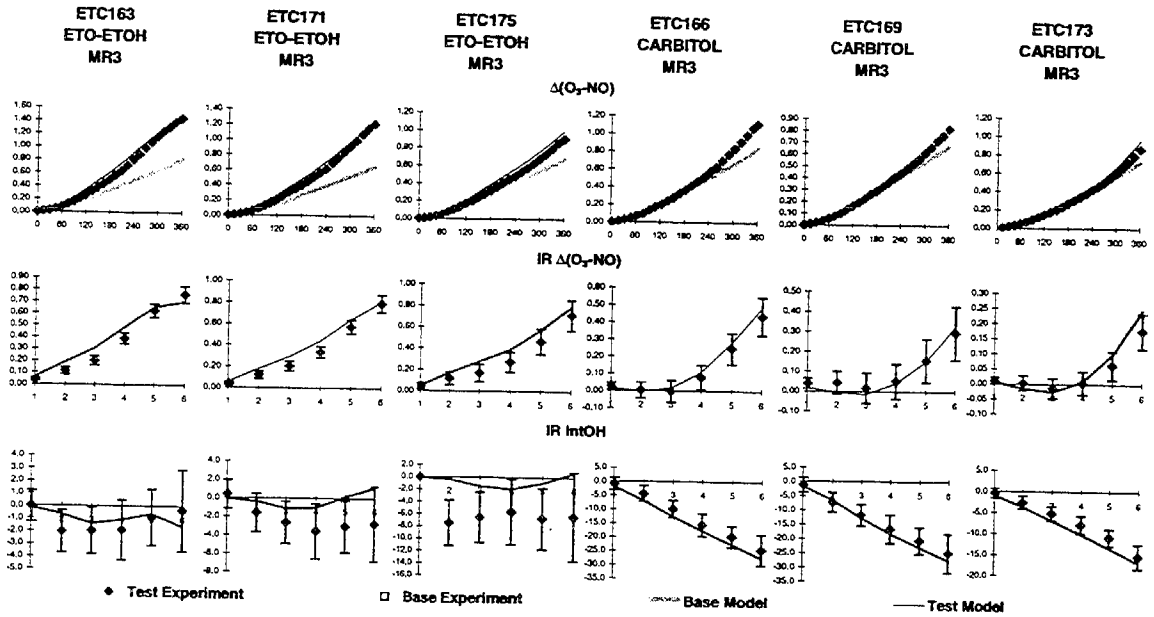
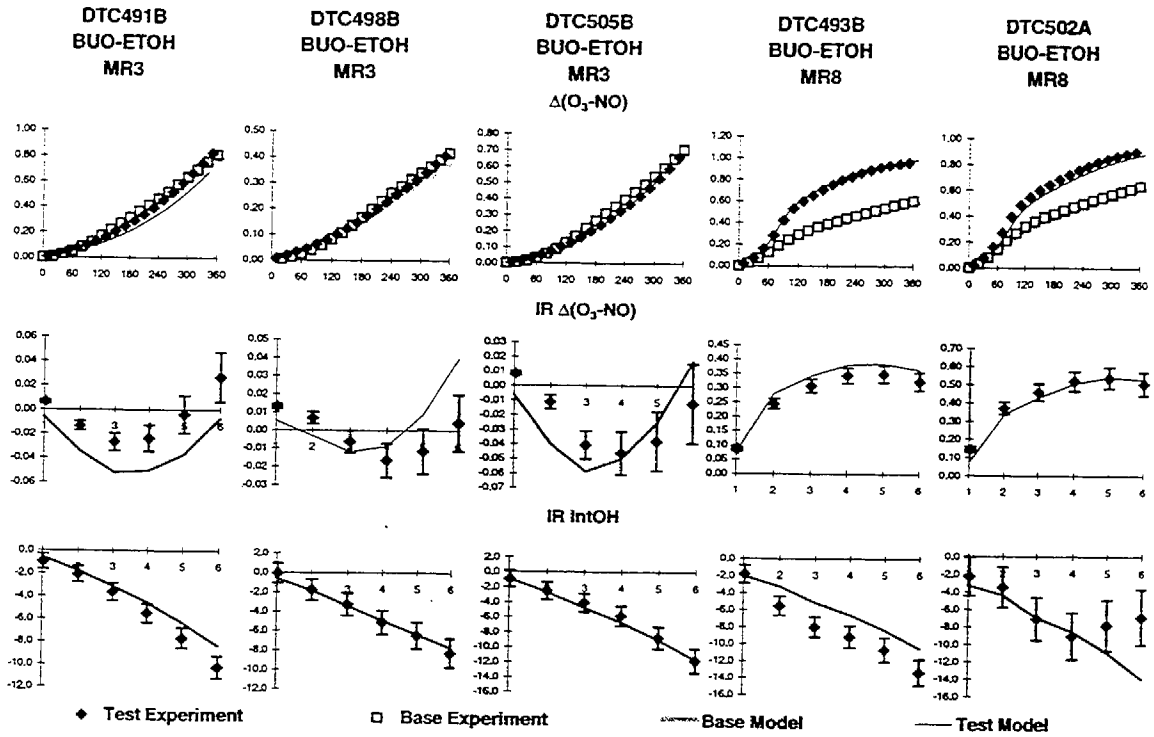


Figure B-49. Plots of experimental and calculated results of the incremental reactivity experiments with ethoxy ethanol and carbitol.



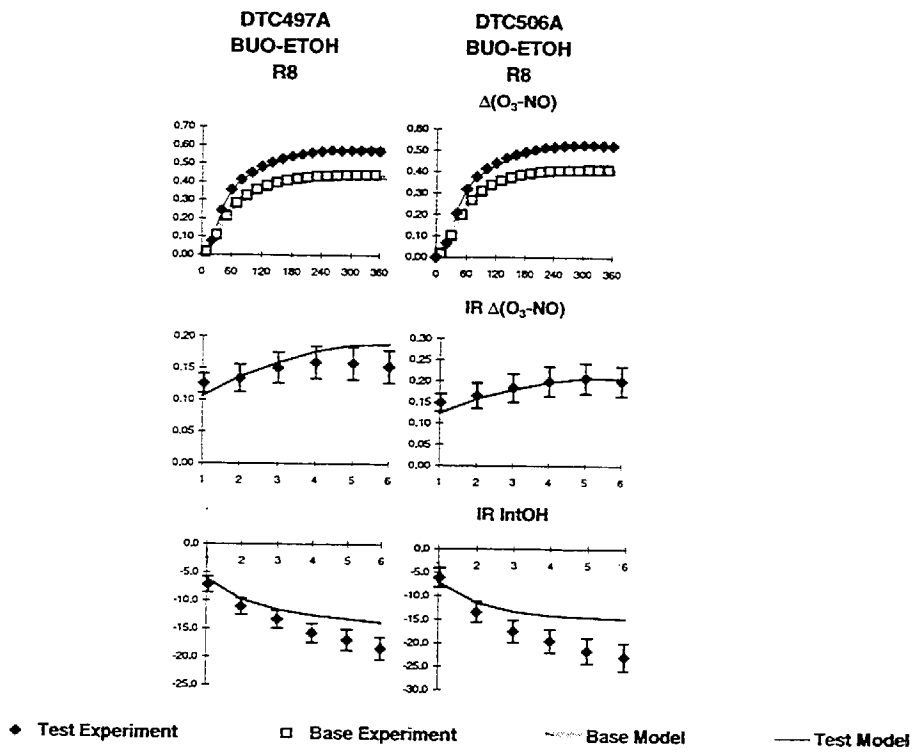
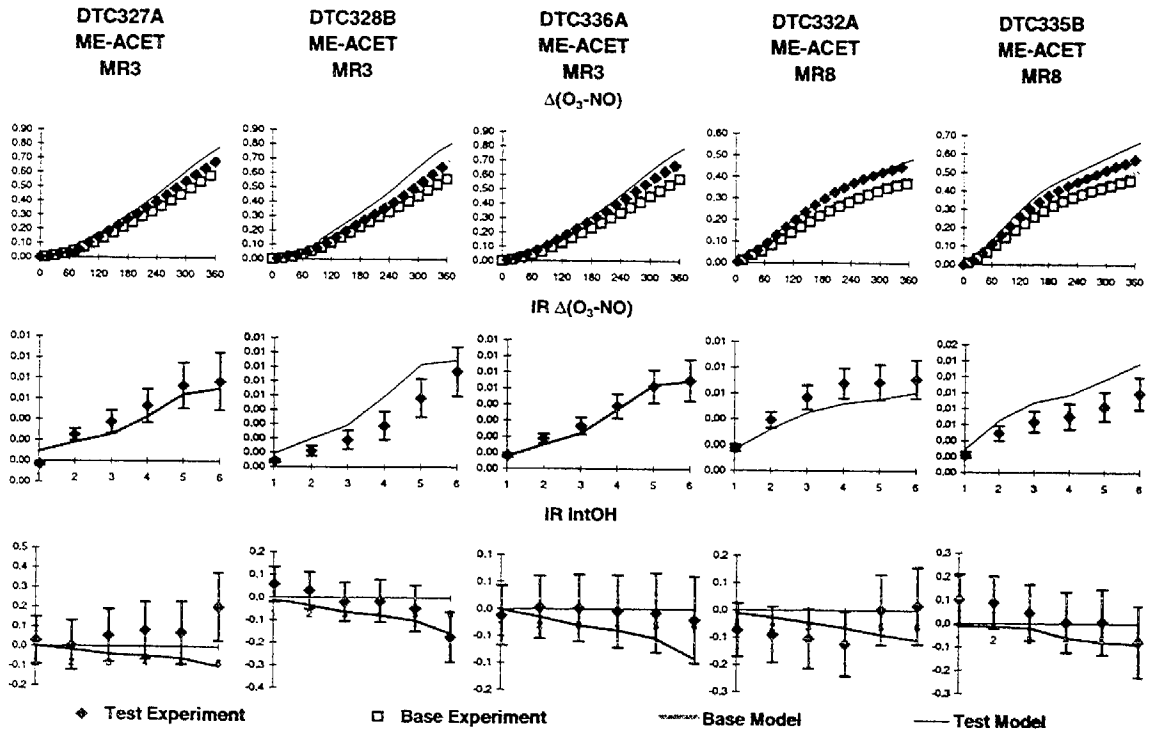


Figure B-50. Plots of experimental and calculated results of the incremental reactivity experiments with butoxy ethanol.



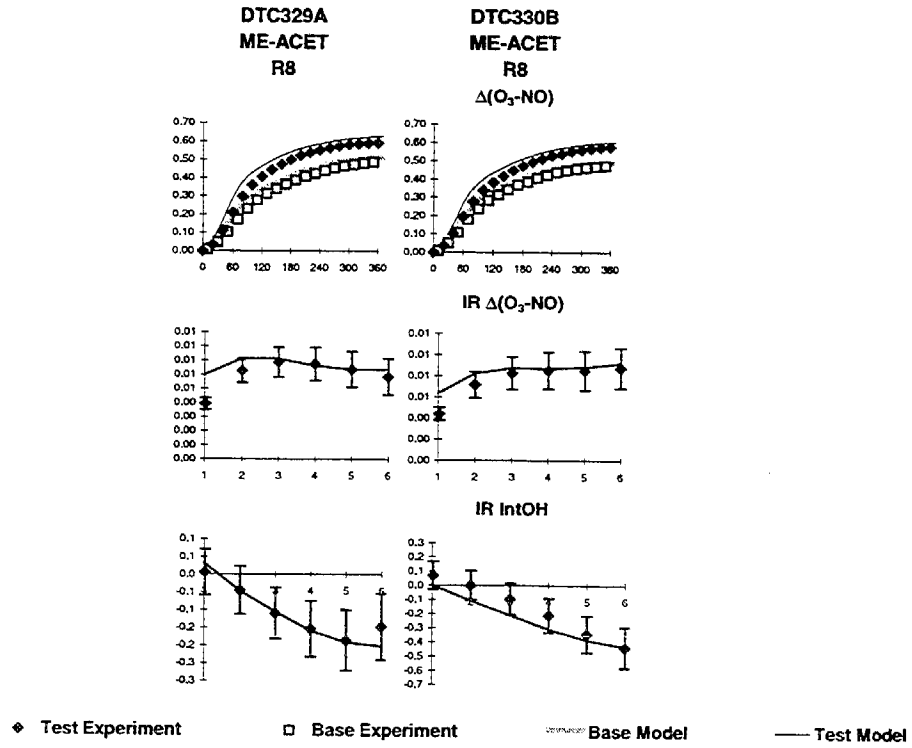
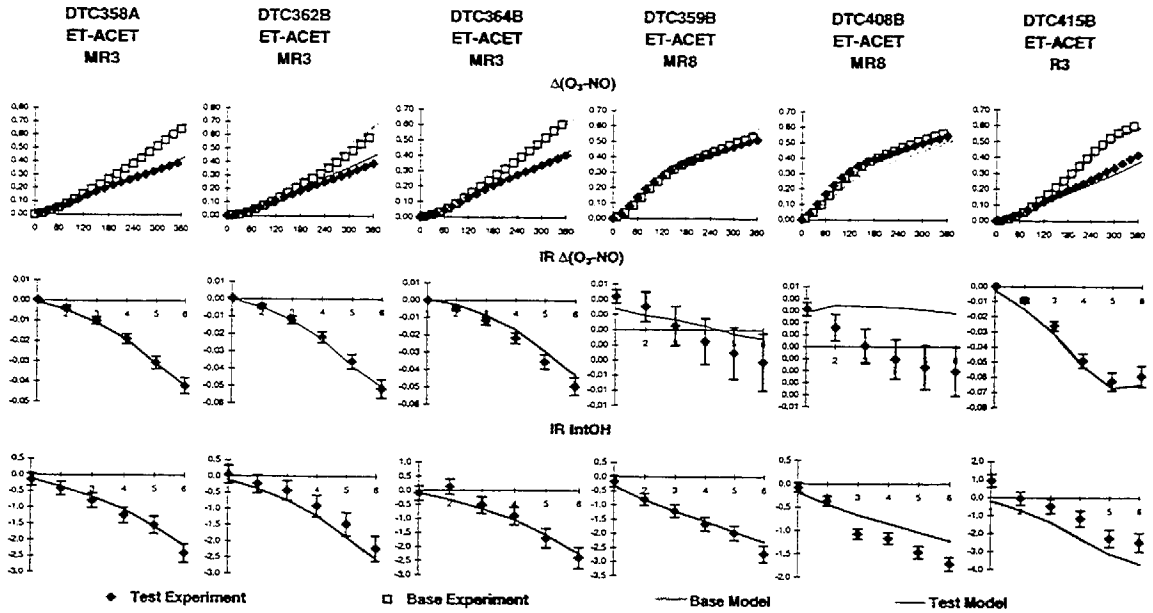


Figure B-51. Plots of experimental and calculated results of the incremental reactivity experiments with methyl acetate.



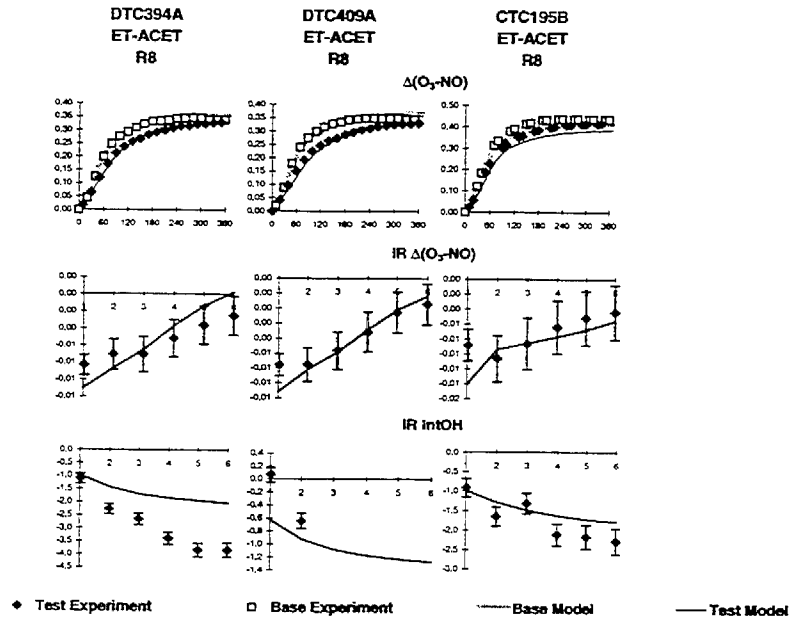
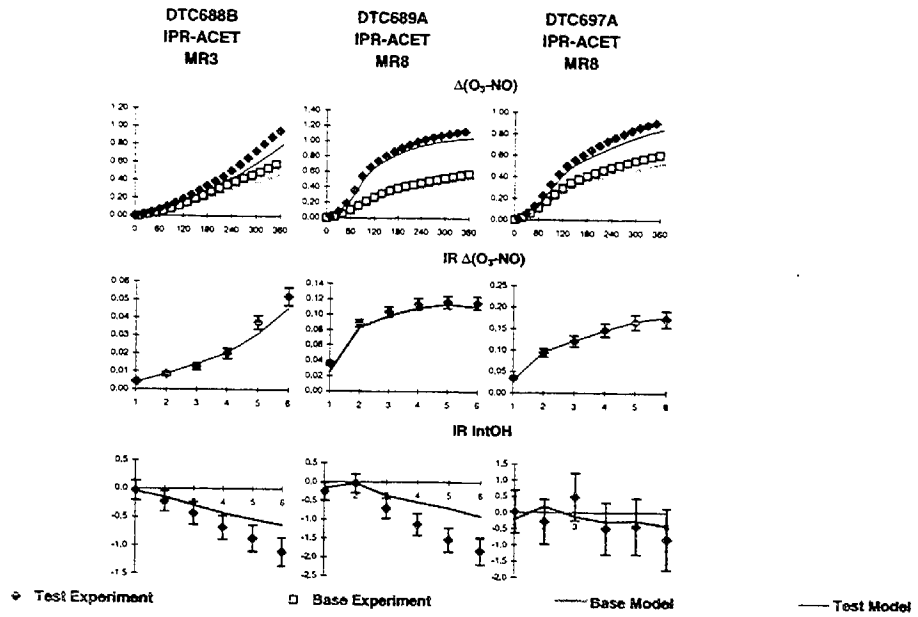


Figure B-52. Plots of experimental and calculated results of the incremental reactivity experiments with ethyl acetate.



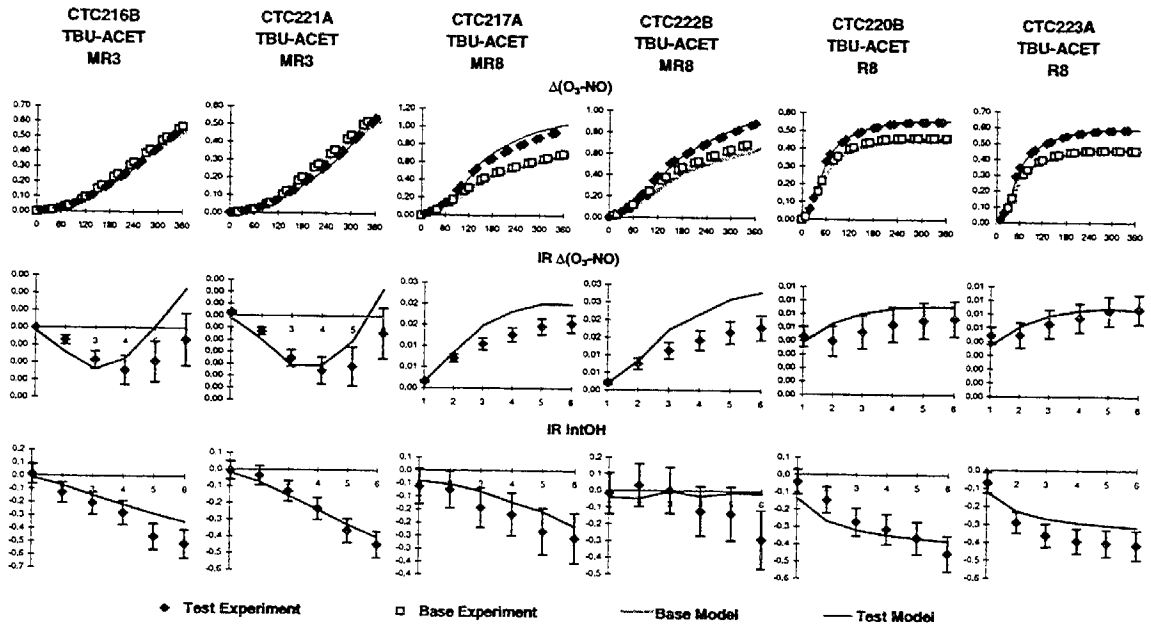


Figure B-53. Plots of experimental and calculated results of the incremental reactivity experiments with isopropyl and t-butyl acetates.

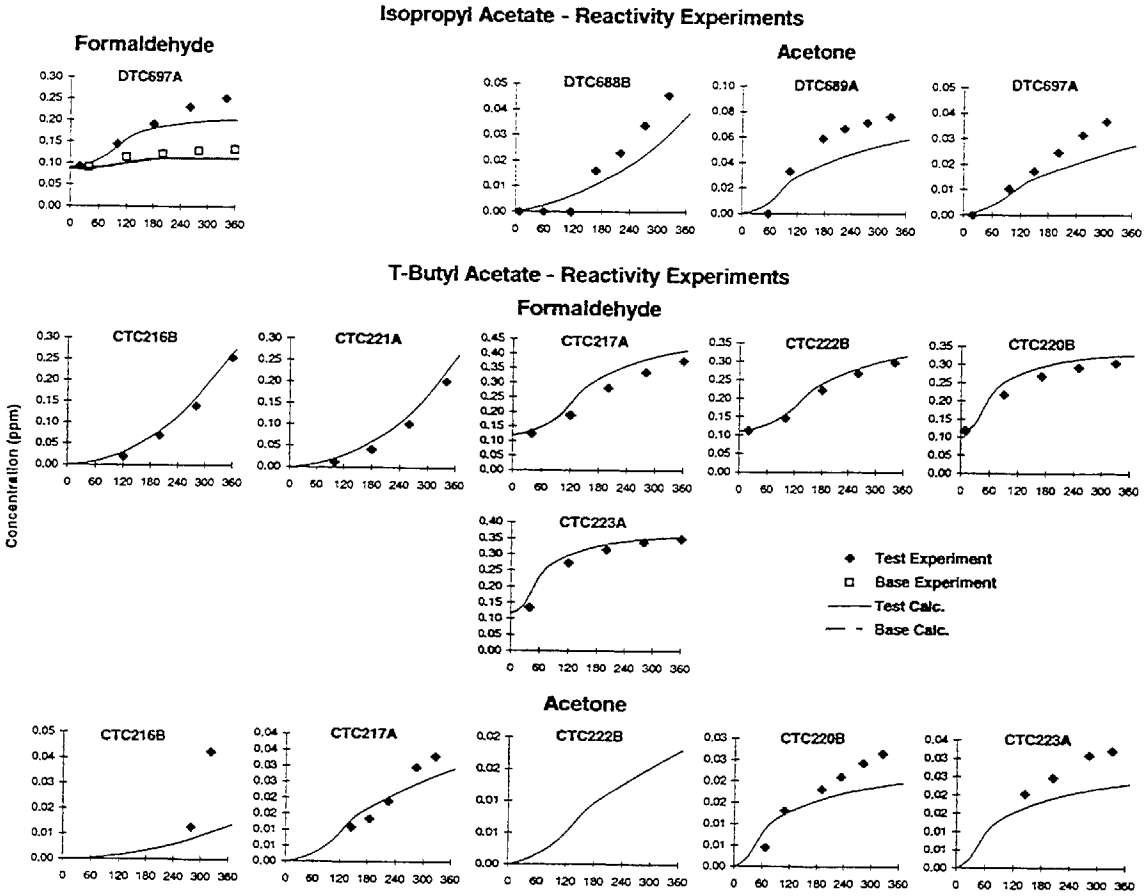


Figure B-54. Plots of experimental and calculated formaldehyde and acetone data for the isopropyl acetate and t-butyl acetate incremental reactivity experiments.

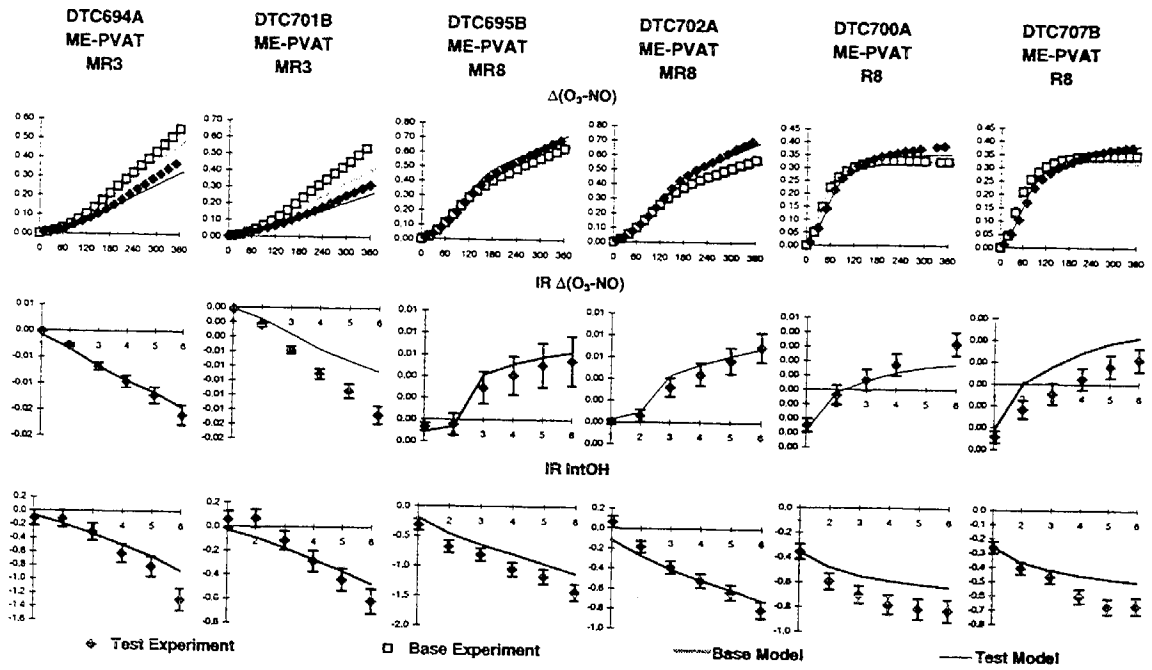


Figure B-55. Plots of experimental and calculated results of the incremental reactivity experiments with methyl pivalate.

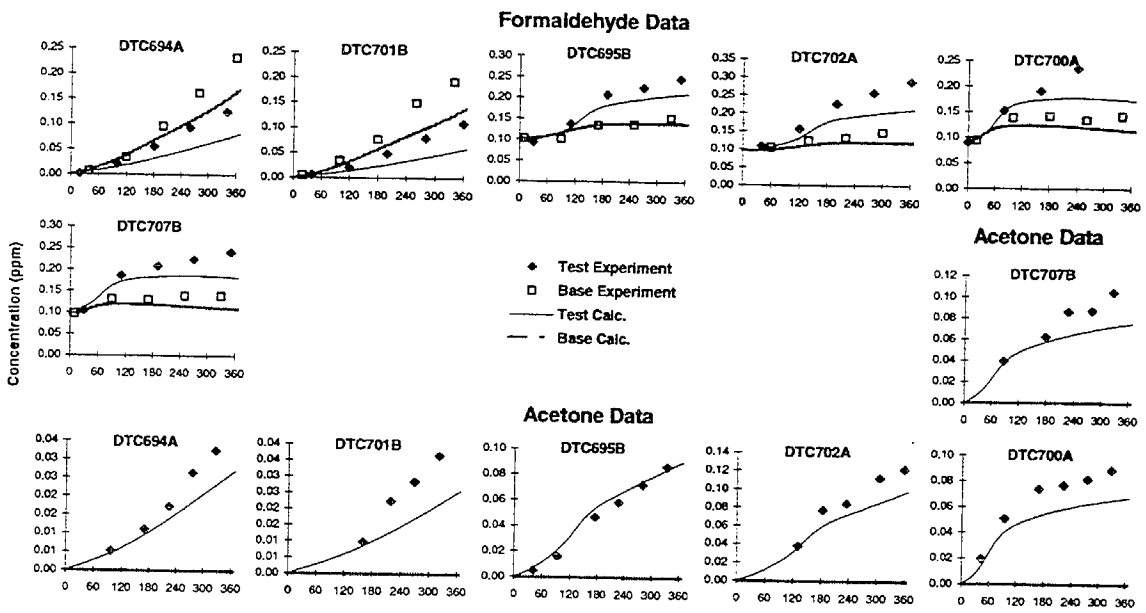
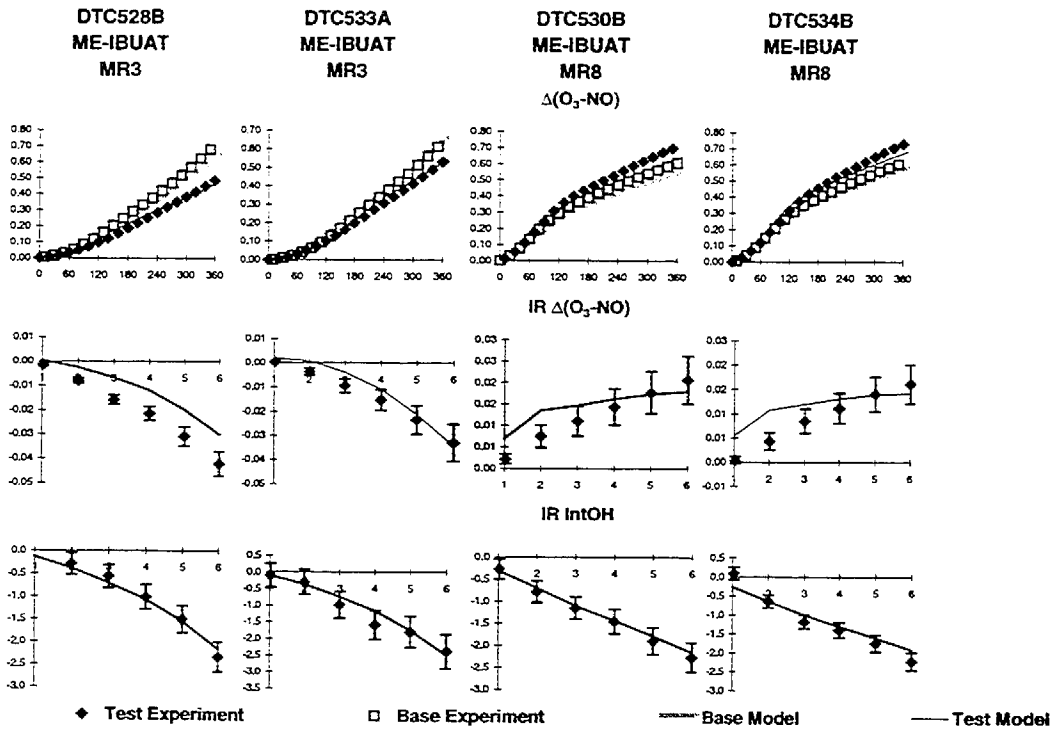


Figure B-56. Plots of experimental and calculated formaldehyde and acetone data for the methyl pivalate incremental reactivity experiments.



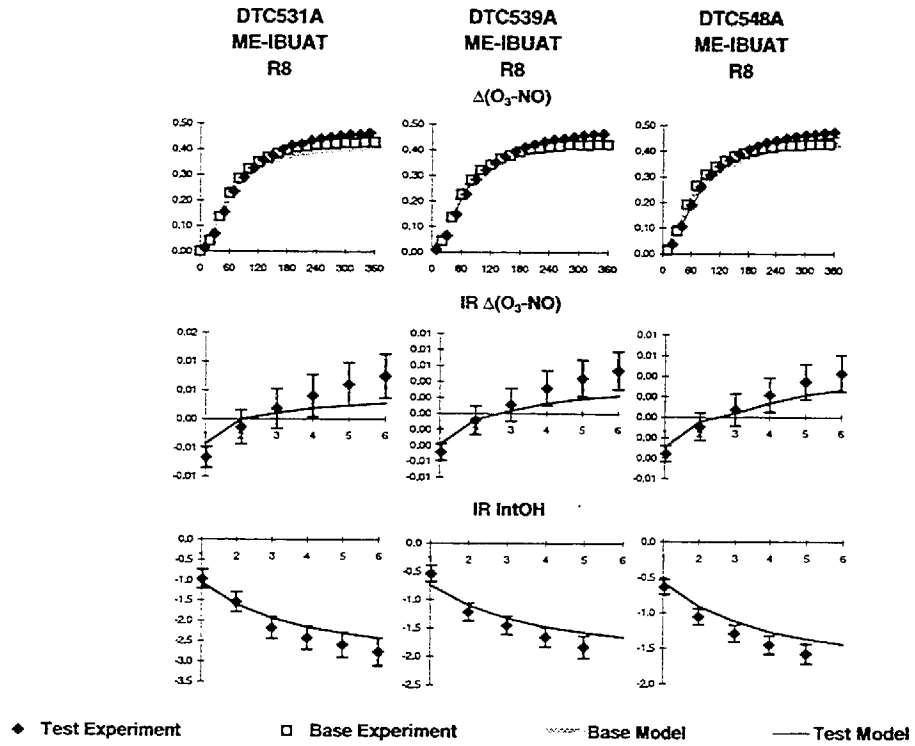


Figure B-57. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isobutyrate.

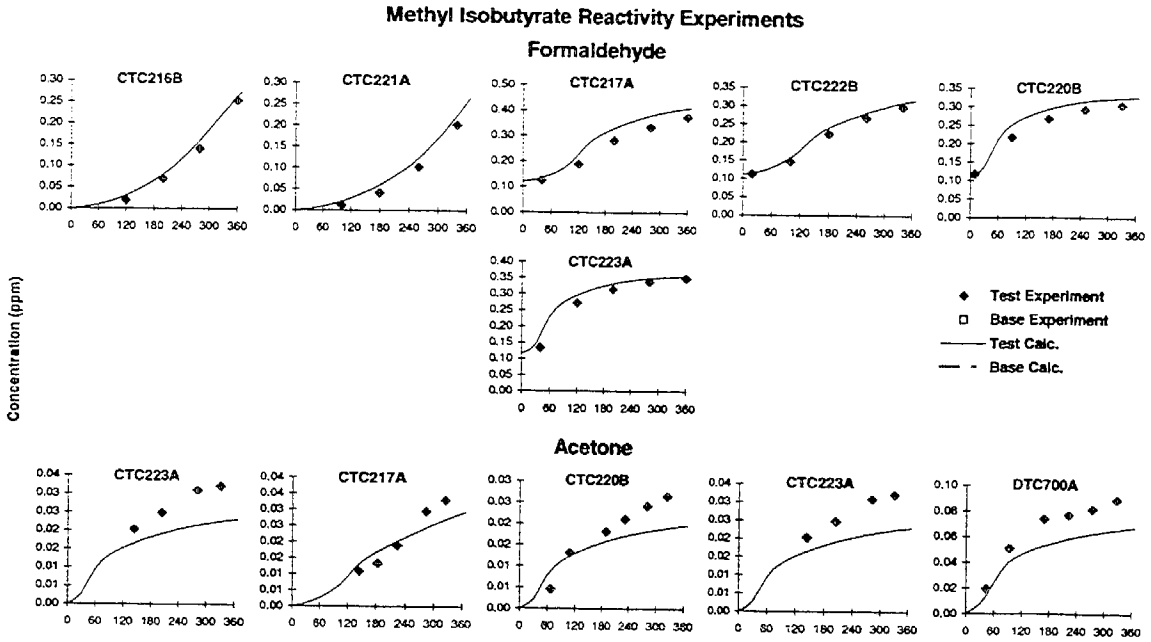


Figure B-58. Plots of experimental and calculated formaldehyde and acetone data for the methyl isobutyrate incremental reactivity experiments.

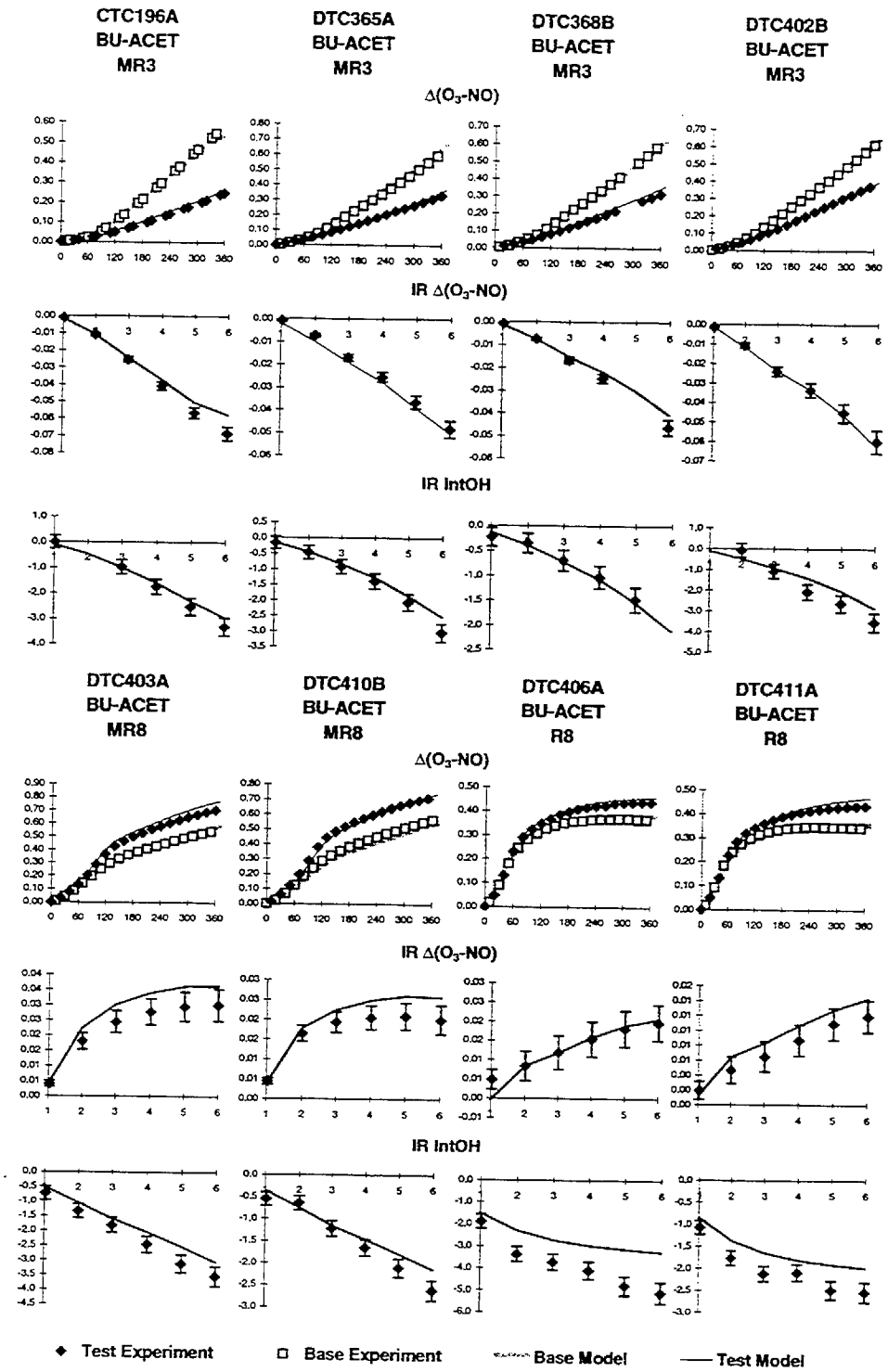


Figure B-59. Plots of experimental and calculated results of the incremental reactivity experiments with butyl acetate.

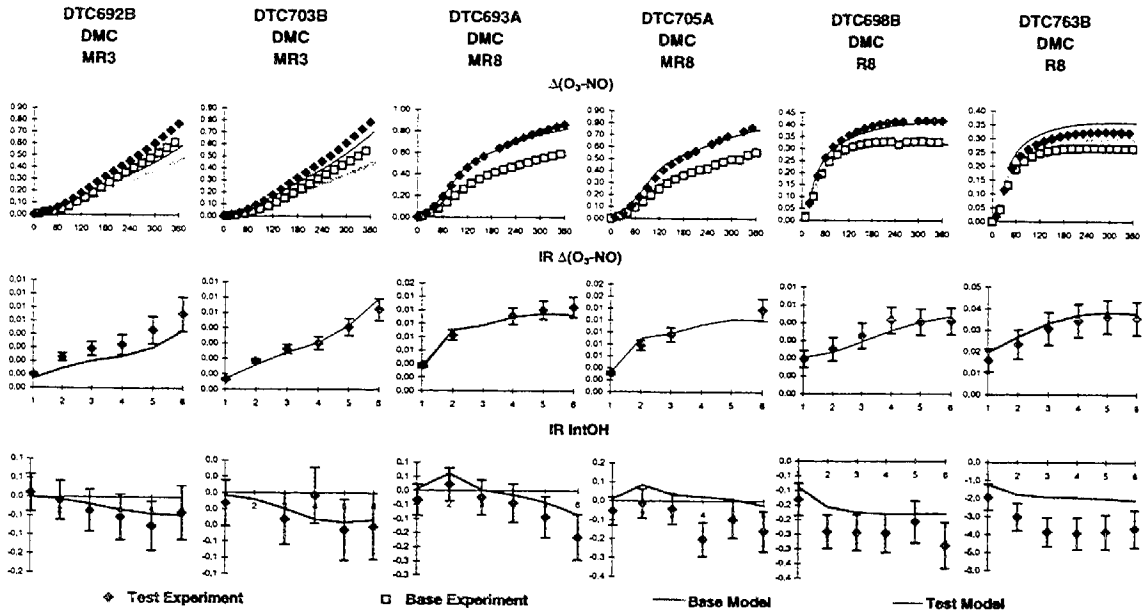


Figure B-60. Plots of experimental and calculated results of the incremental reactivity experiments with dimethyl carbonate.

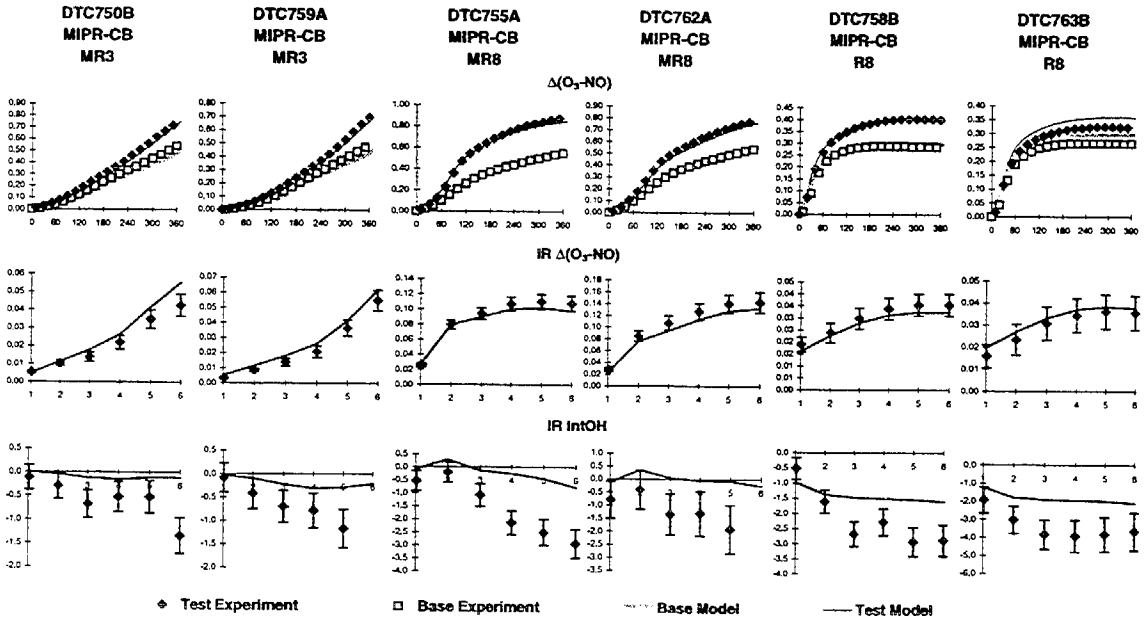
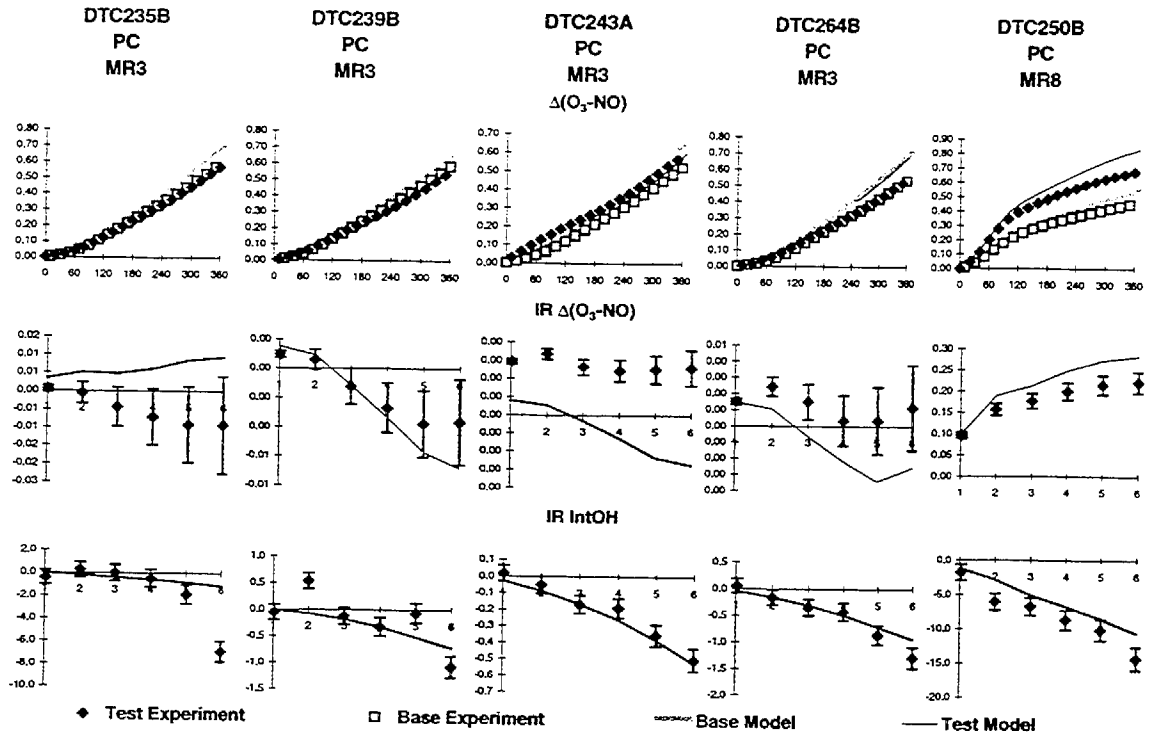


Figure B-61. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isopropyl carbonate.



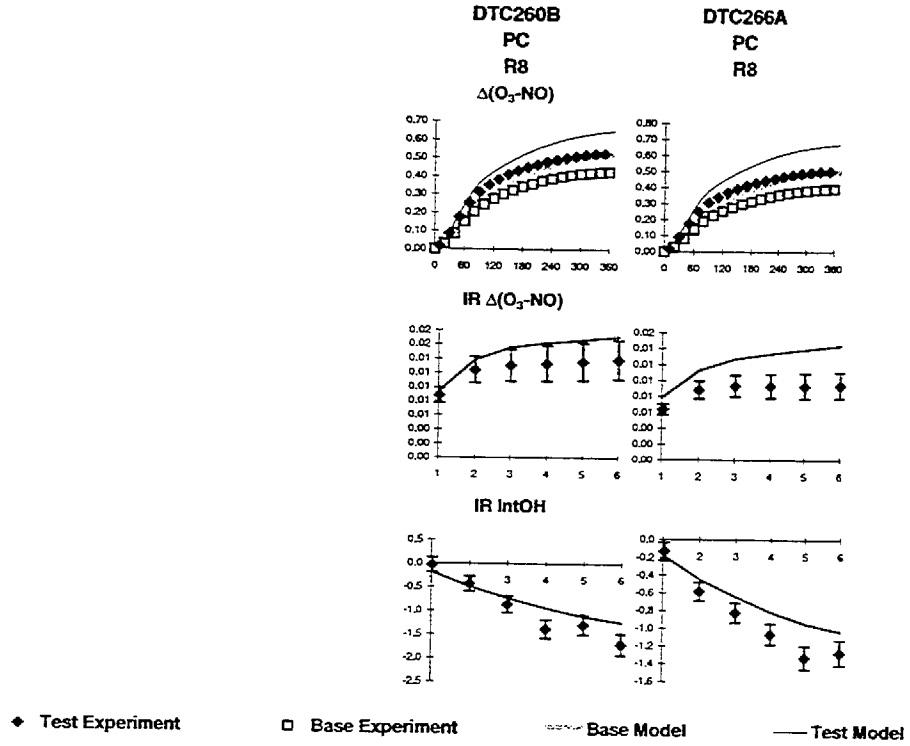


Figure B-62. Plots of experimental and calculated results of the incremental reactivity experiments with propylene carbonate.

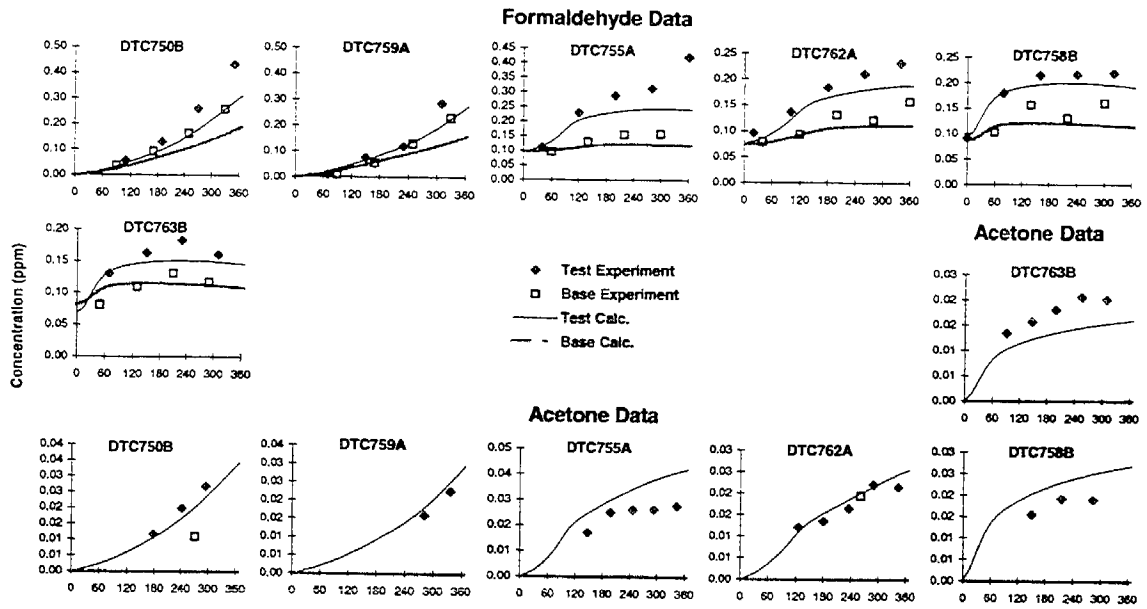


Figure B-63. Plots of experimental and calculated formaldehyde and acetone data for the methyl isopropyl carbonate incremental reactivity experiments.

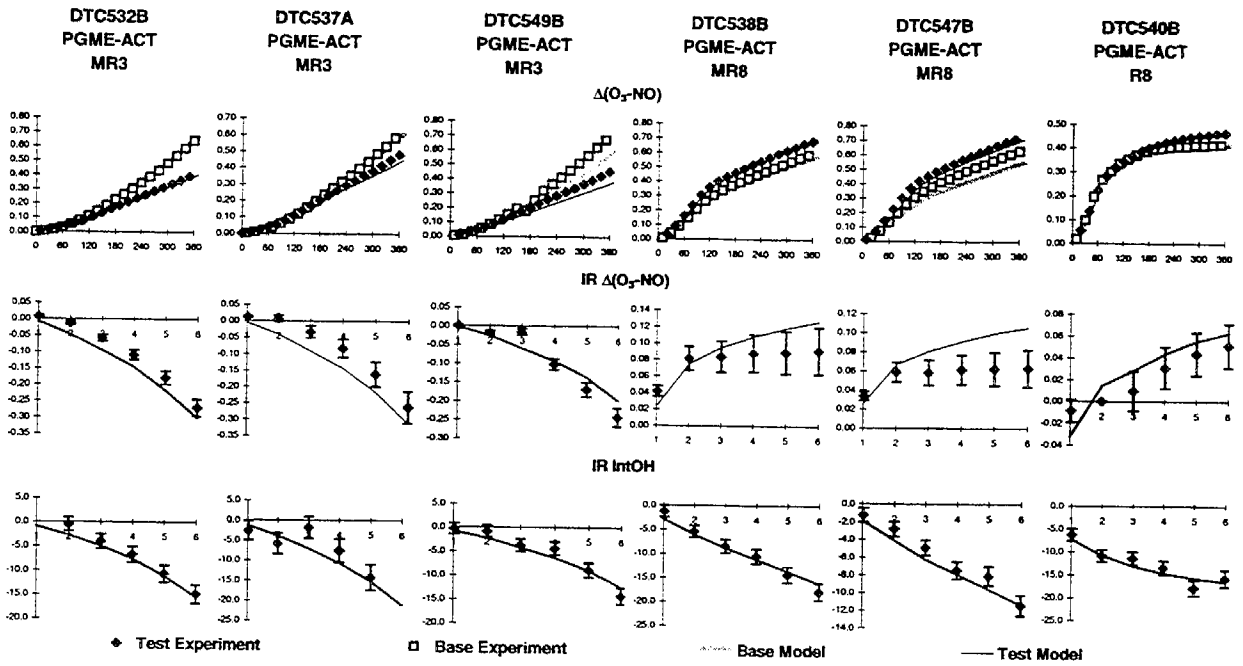


Figure B-64. Plots of experimental and calculated results of the incremental reactivity experiments with propylene glycol methyl ether acetate.

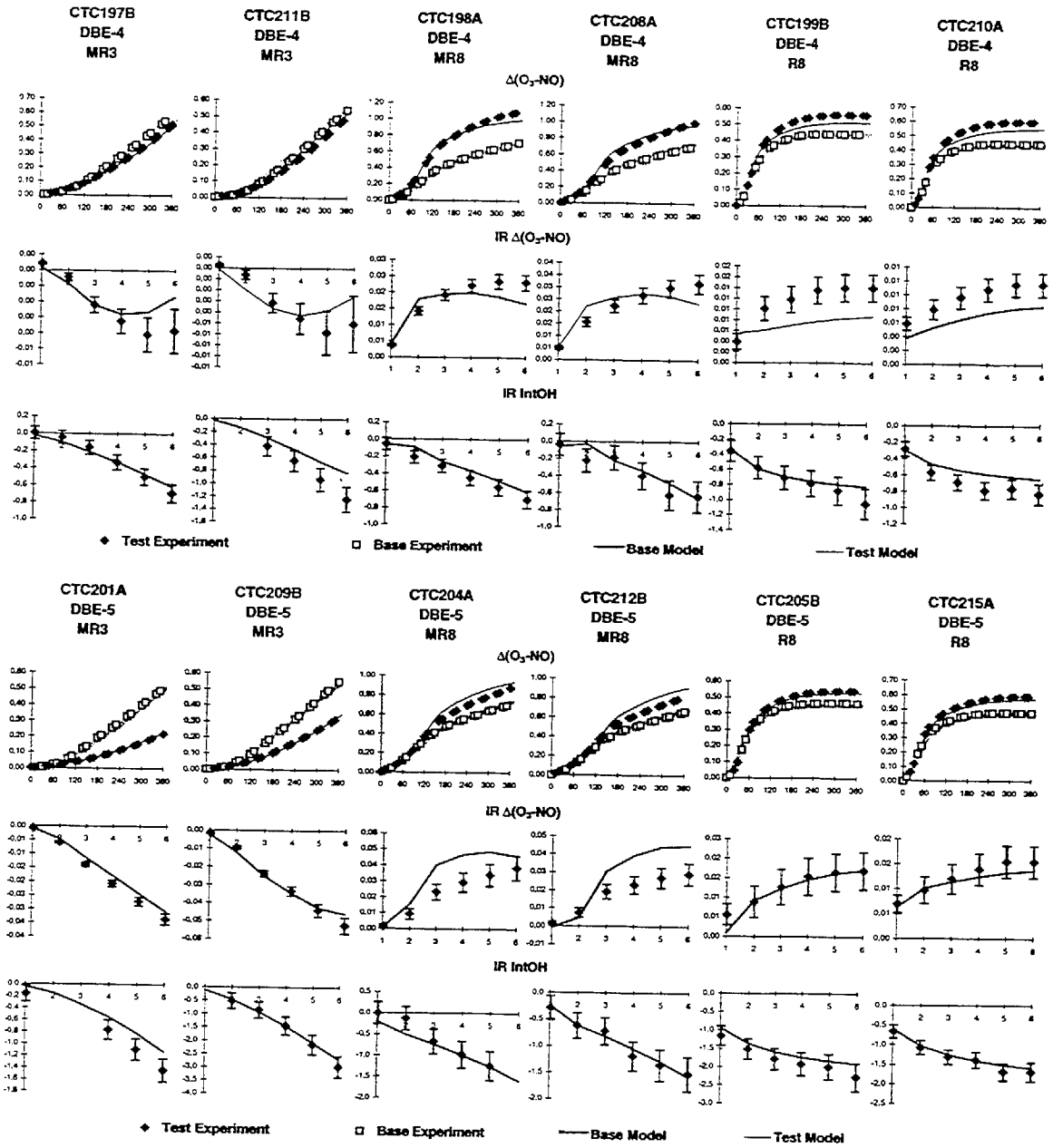


Figure B-65. Plots of experimental and calculated results of the incremental reactivity experiments with the dibasic esters Dimethyl Glutarate and Dimethyl Adipate.

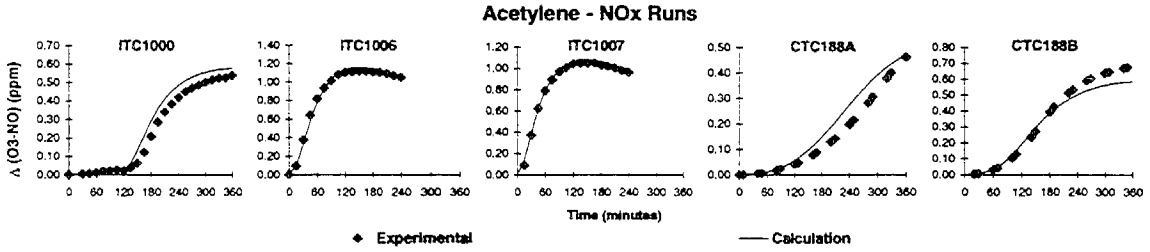


Figure B-66. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetylene - NO_x experiments.

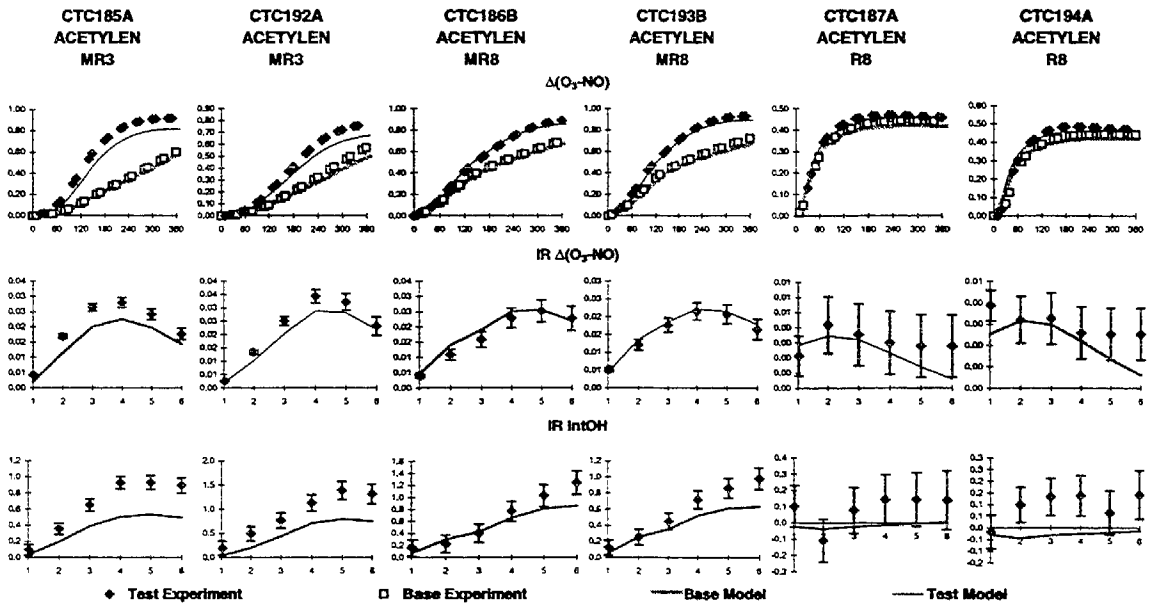


Figure B-67. Plots of experimental and calculated results of the incremental reactivity experiments with acetylene. (Run CTC184B, which has similar results as run CTC185A, is not shown.)

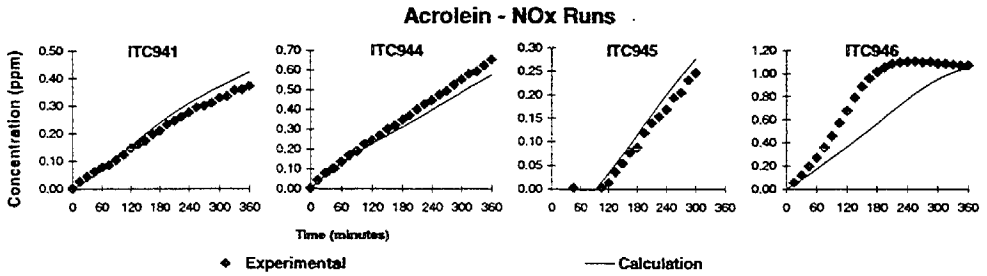


Figure B-68. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acrolein - NO_x experiments.

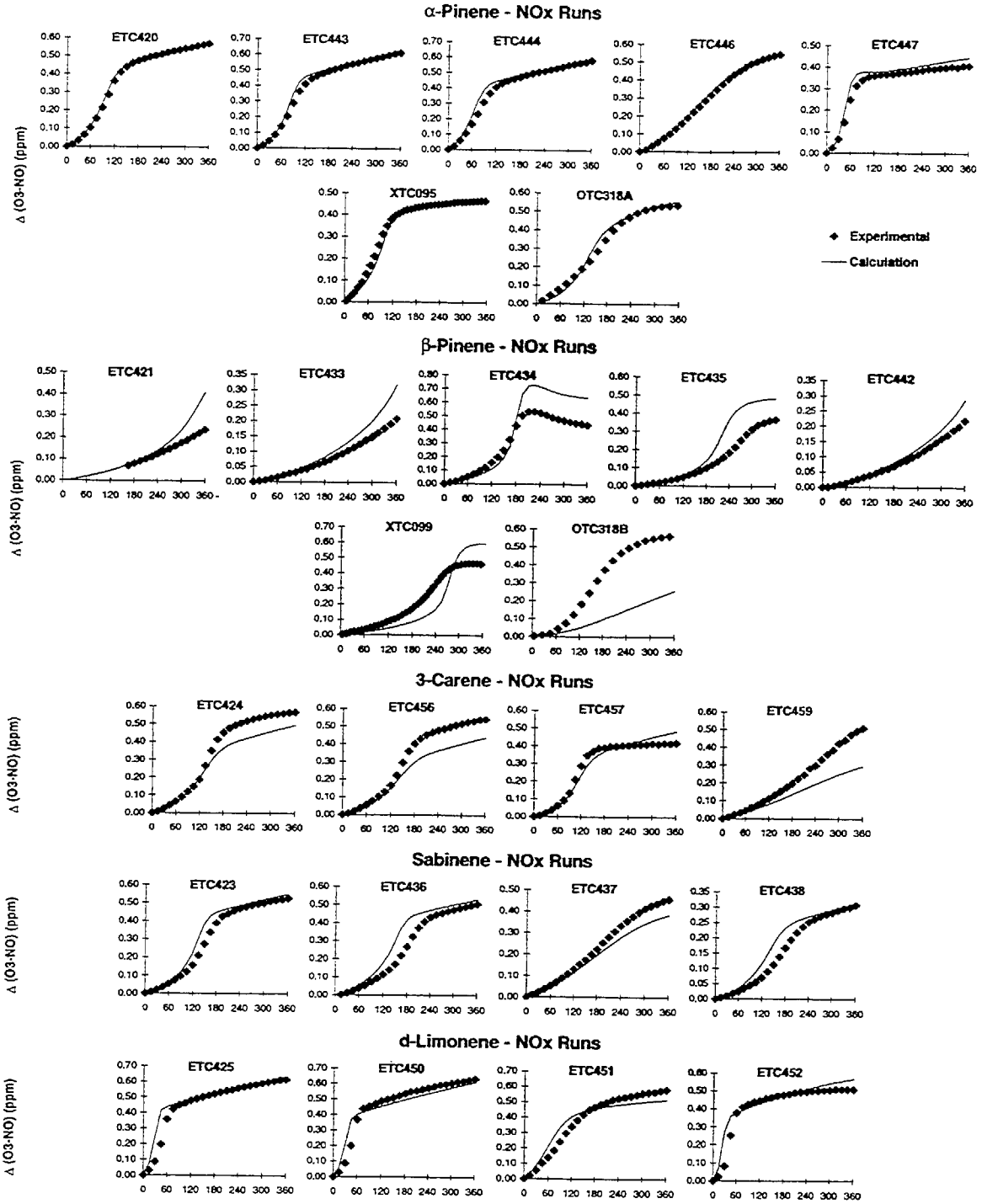


Figure B-69. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the terpene - NO_x experiments.

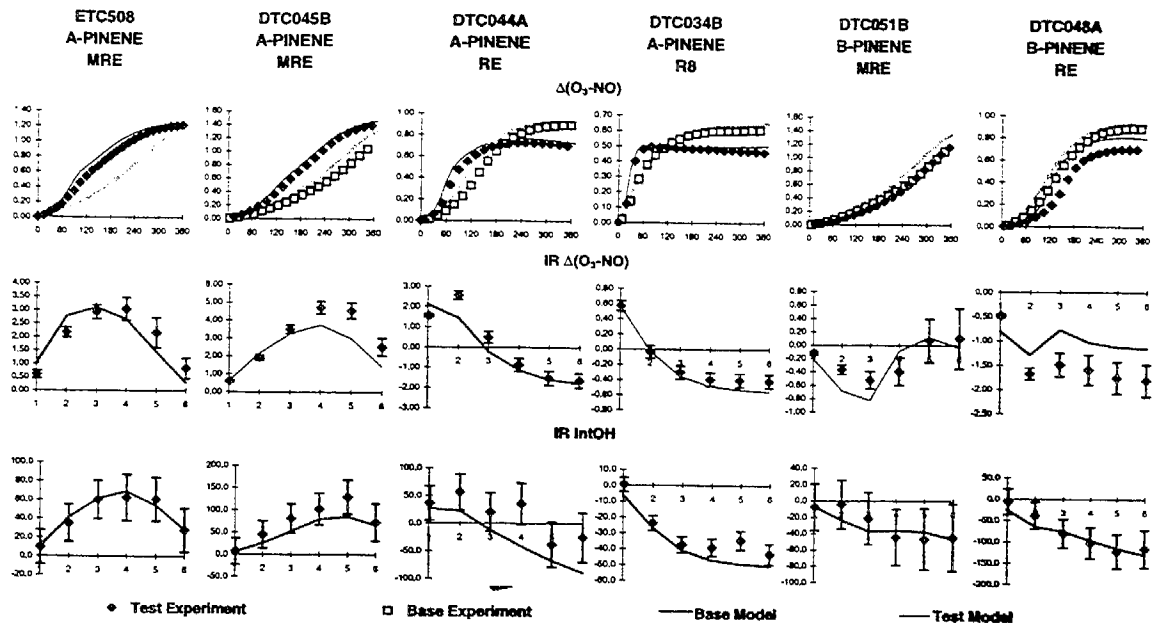


Figure B-70. Plots of experimental and calculated results of the incremental reactivity experiments with α- and β-pinenes.

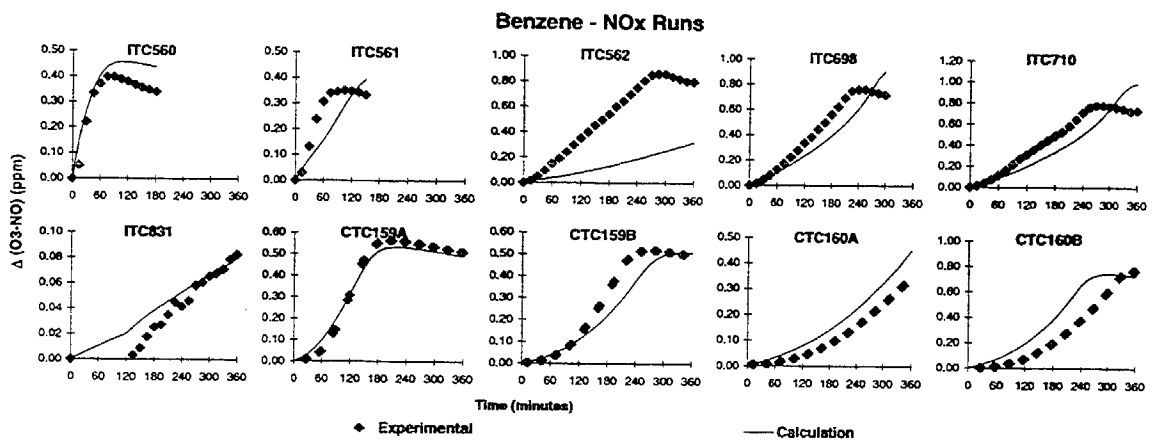


Figure B-71. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the benzene - NO_2 experiments.

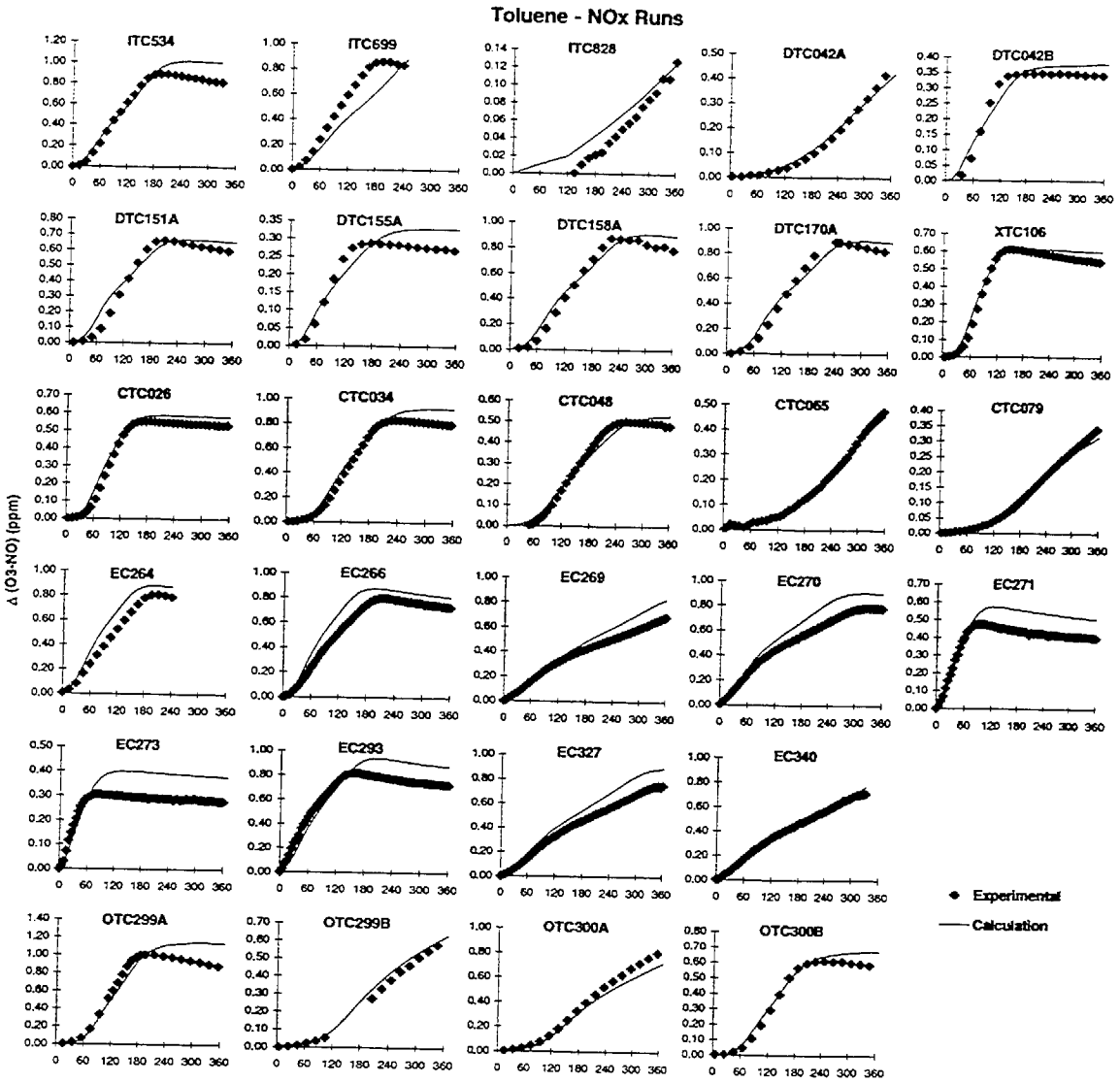


Figure B-72. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the toluene - NO_x experiments.

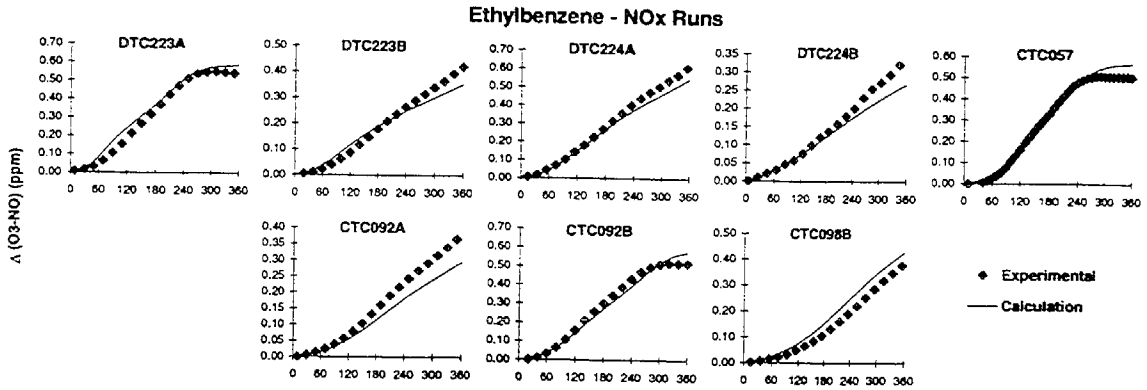


Figure B-73. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the ethylbenzene - NO_x experiments.

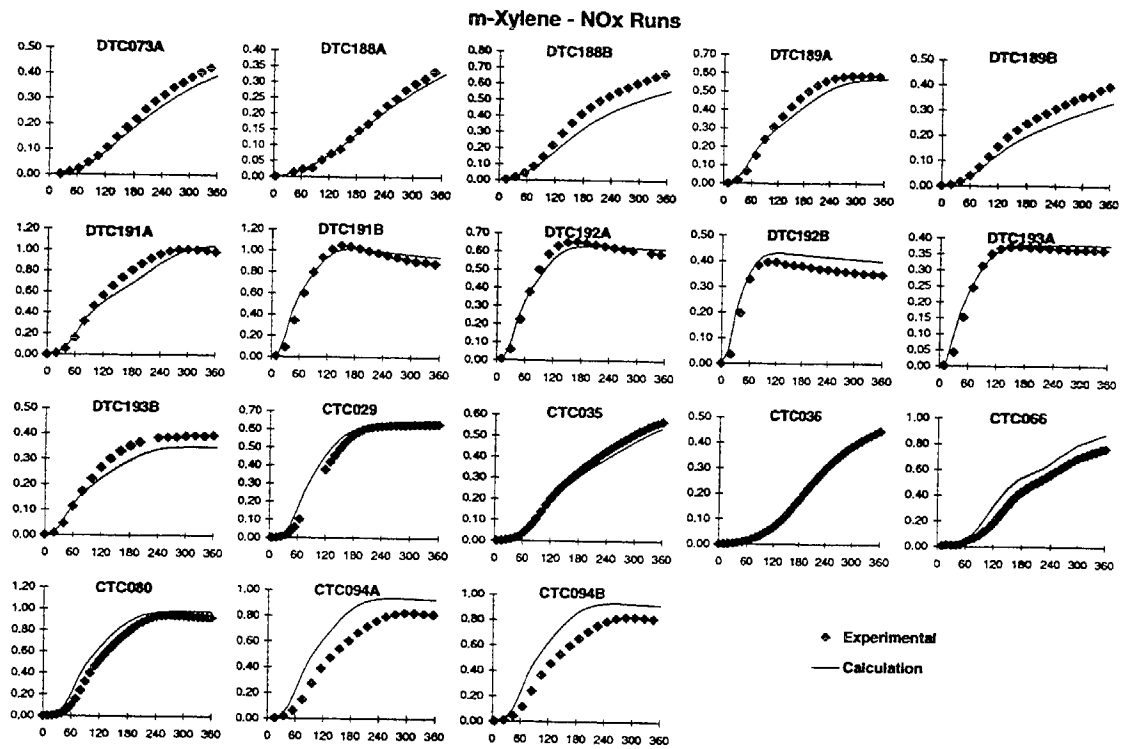


Figure B-74. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the m-xylene - NO_2 experiments.

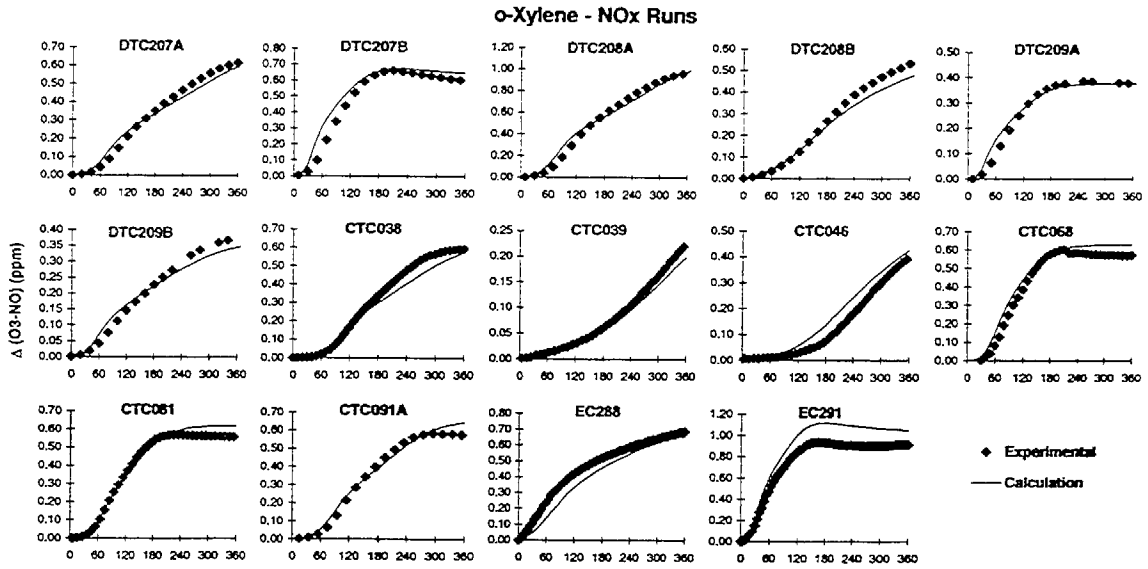


Figure B-75. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the o-xylene - NO_2 experiments.

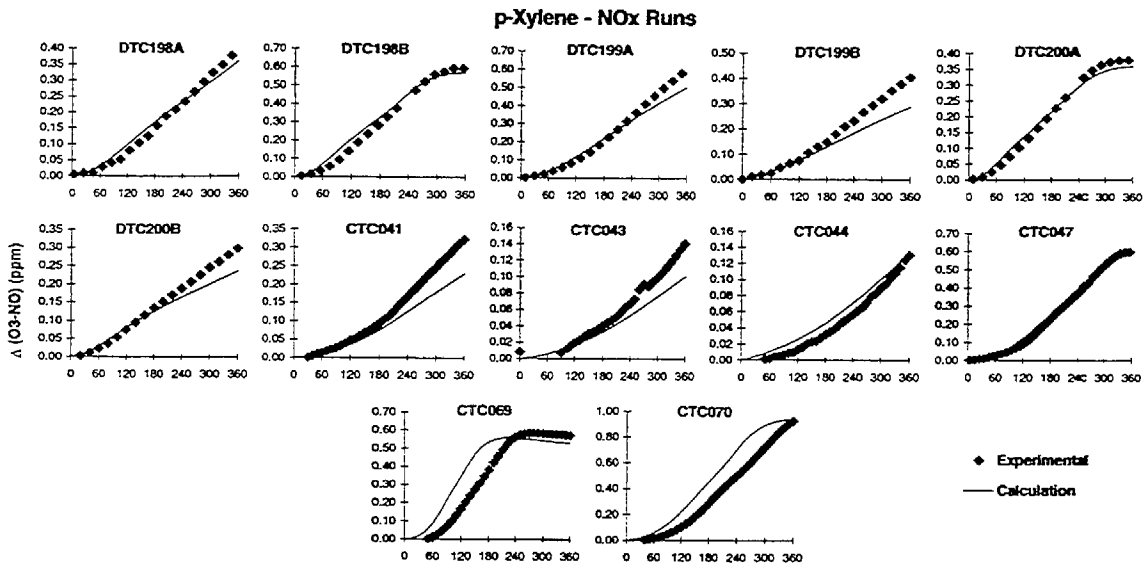


Figure B-76. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the p-xylene - NO_x experiments.

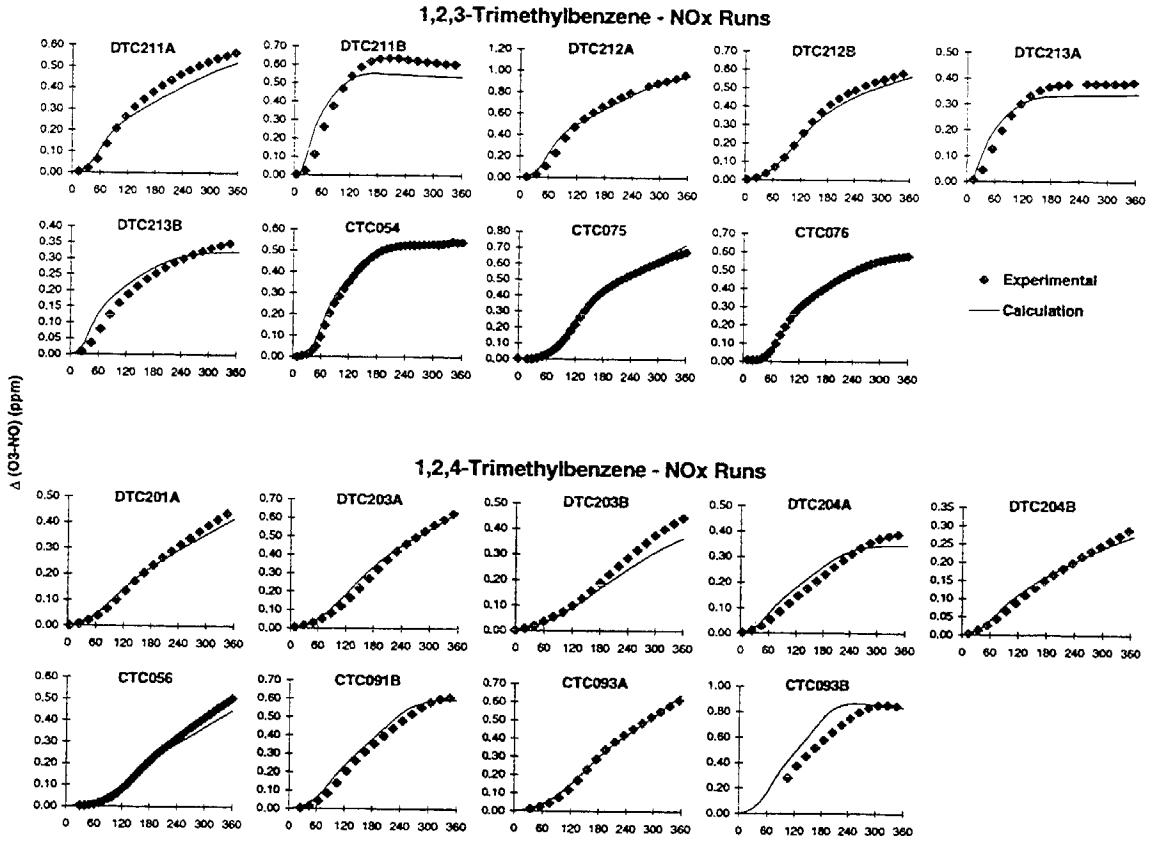


Figure B-77. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1,2,3-trimethylbenzene and 1,2,4-trimethylbenzene - NO_x experiments.

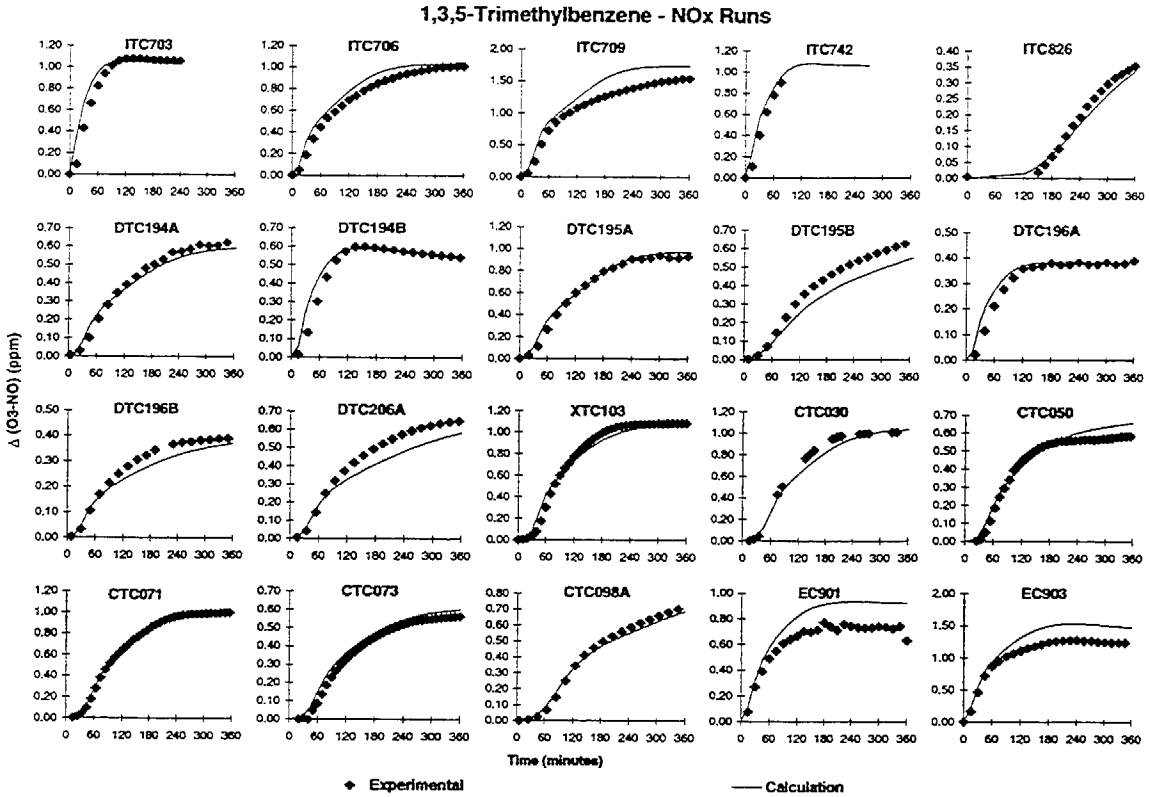


Figure B-78. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1,3,5-trimethylbenzene - NO_x experiments.

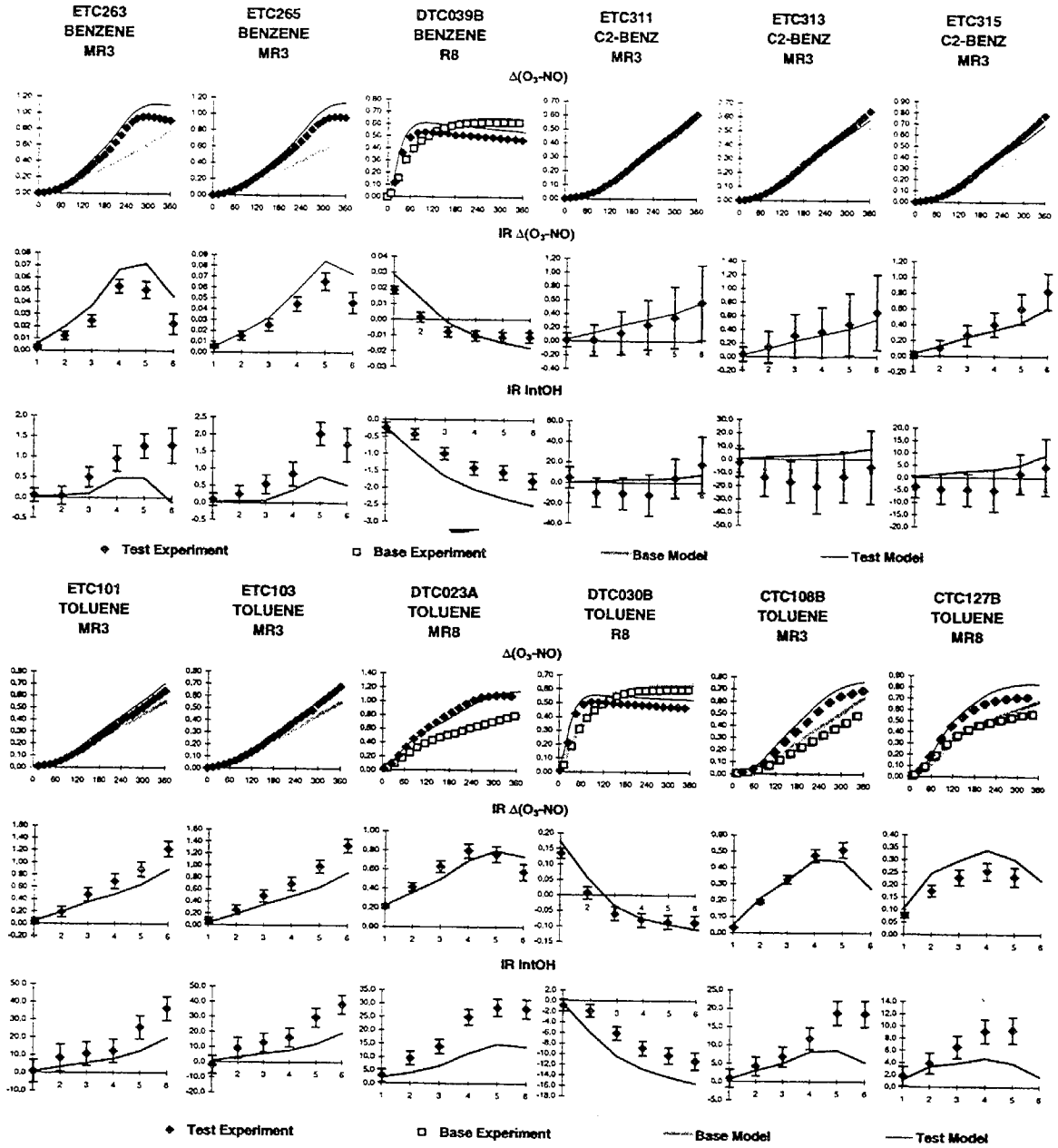


Figure B-79. Plots of experimental and calculated results of the incremental reactivity experiments with benzene, toluene, and ethylbenzene.

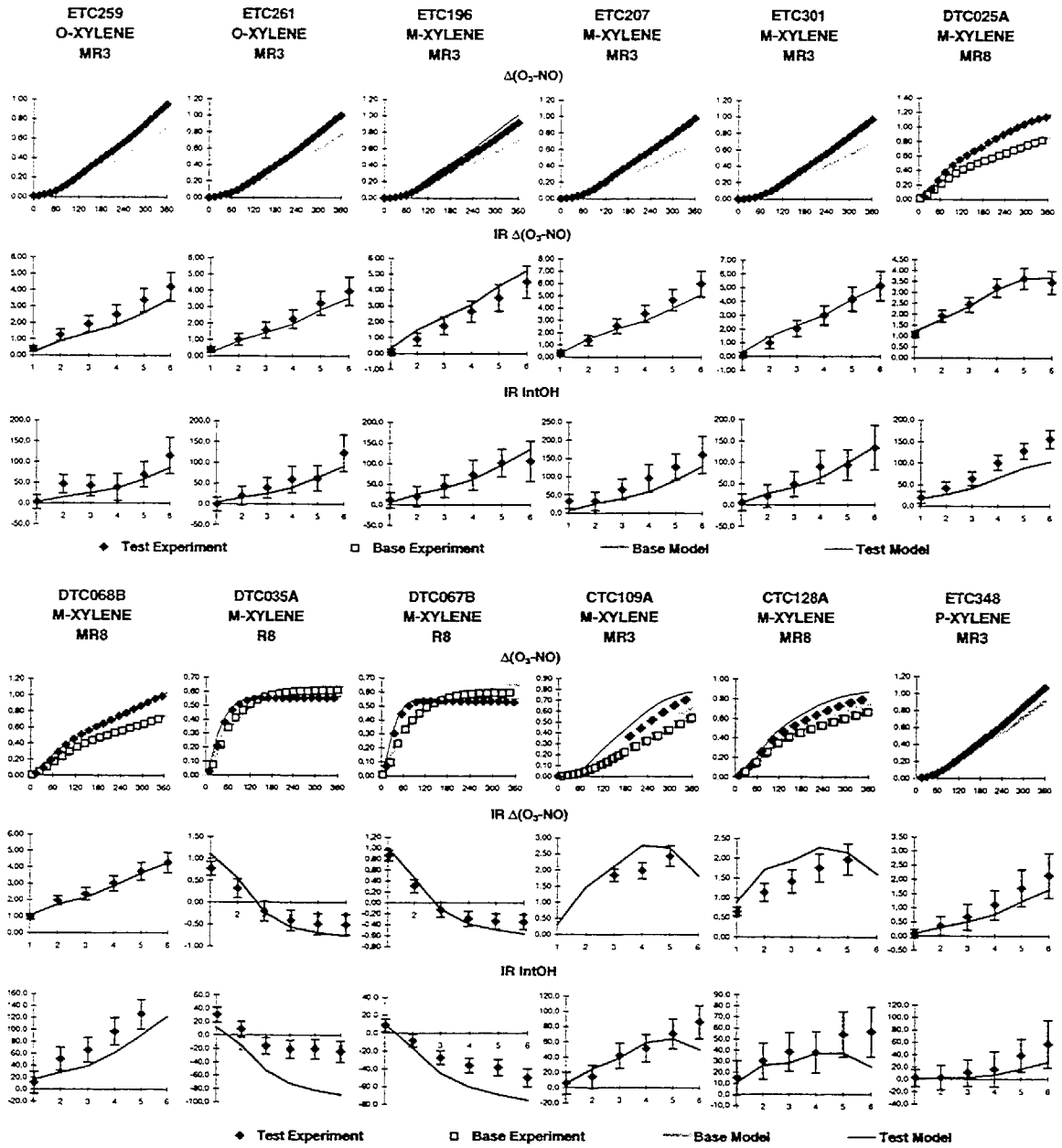


Figure B-80. Plots of experimental and calculated results of the incremental reactivity experiments with o-, m-, and p-xylenes.

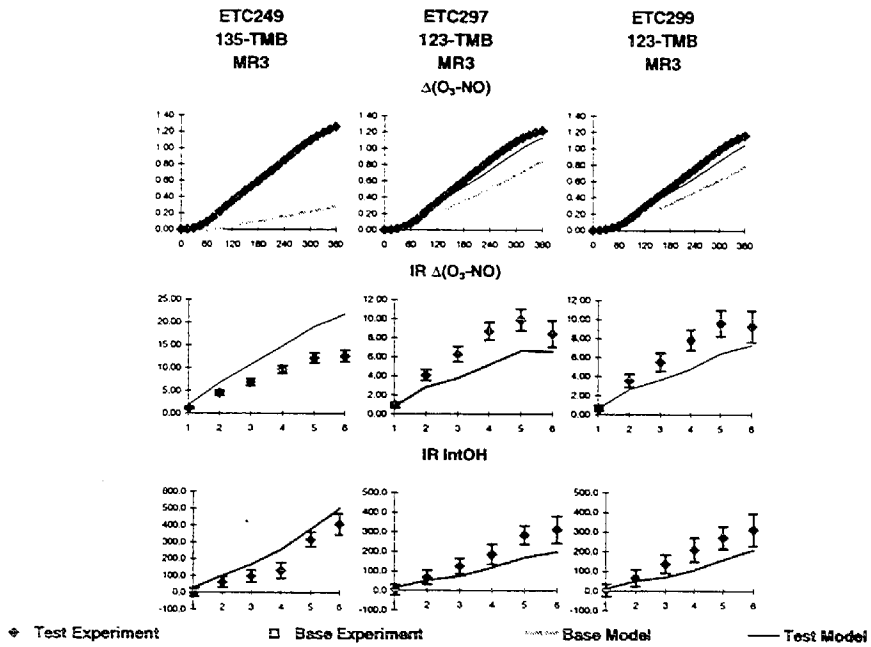


Figure B-81. Plots of experimental and calculated results of the incremental reactivity experiments with the trimethyl benzenes.

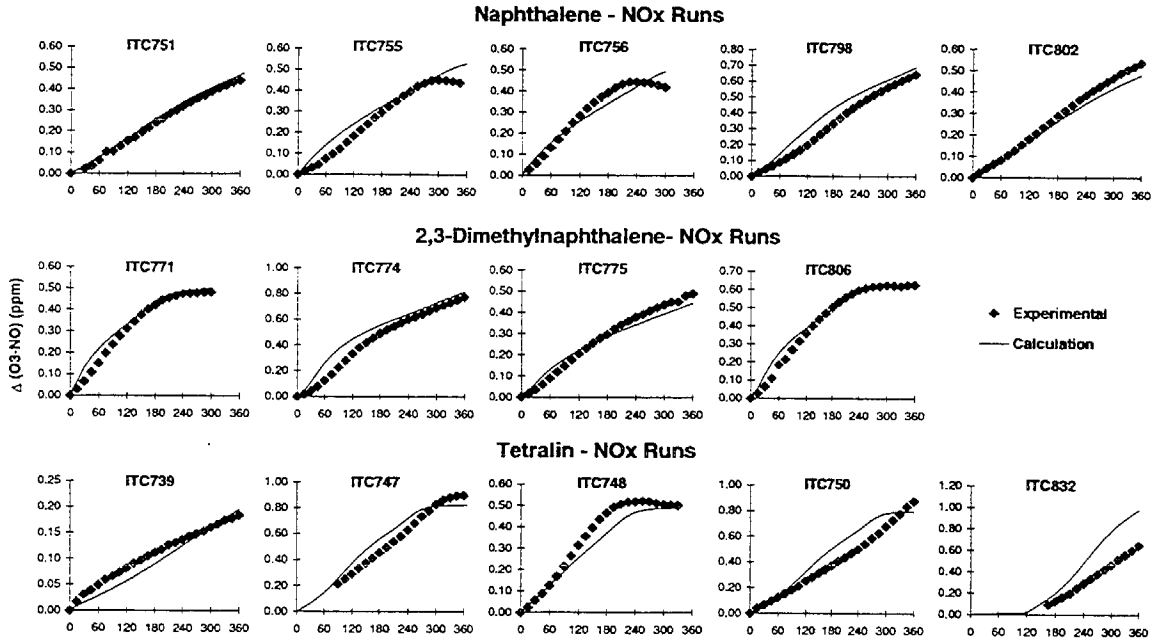


Figure B-82. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the naphthalene - NO_x, 2,3-dimethylnaphthalene - NO_x and tetralin - NO_x experiments.

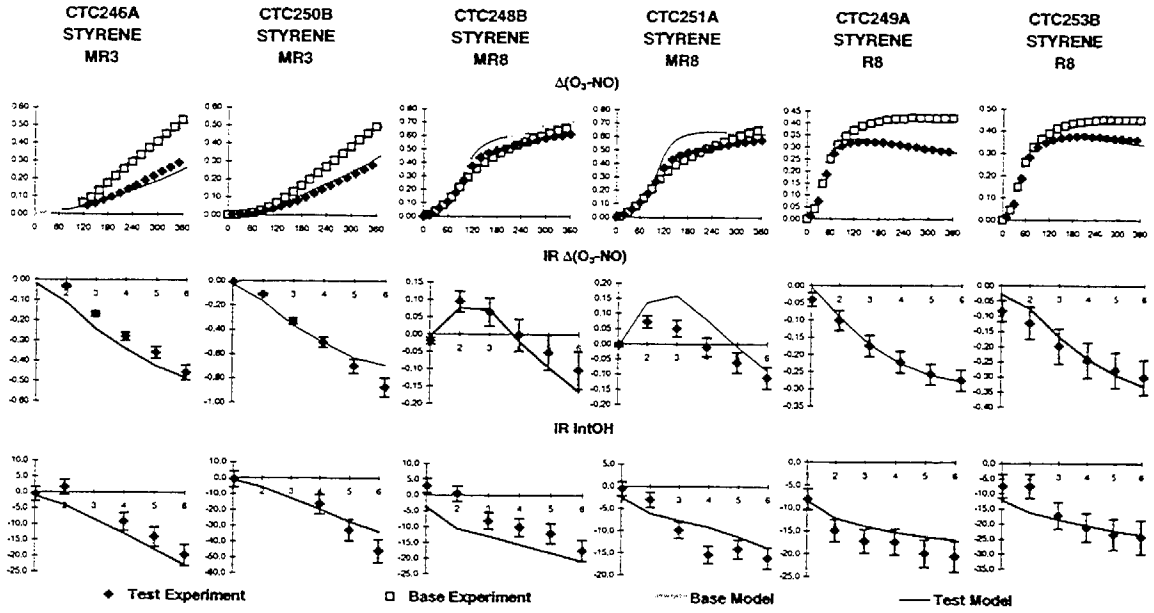


Figure B-83. Plots of experimental and calculated results of the incremental reactivity experiments with styrene.

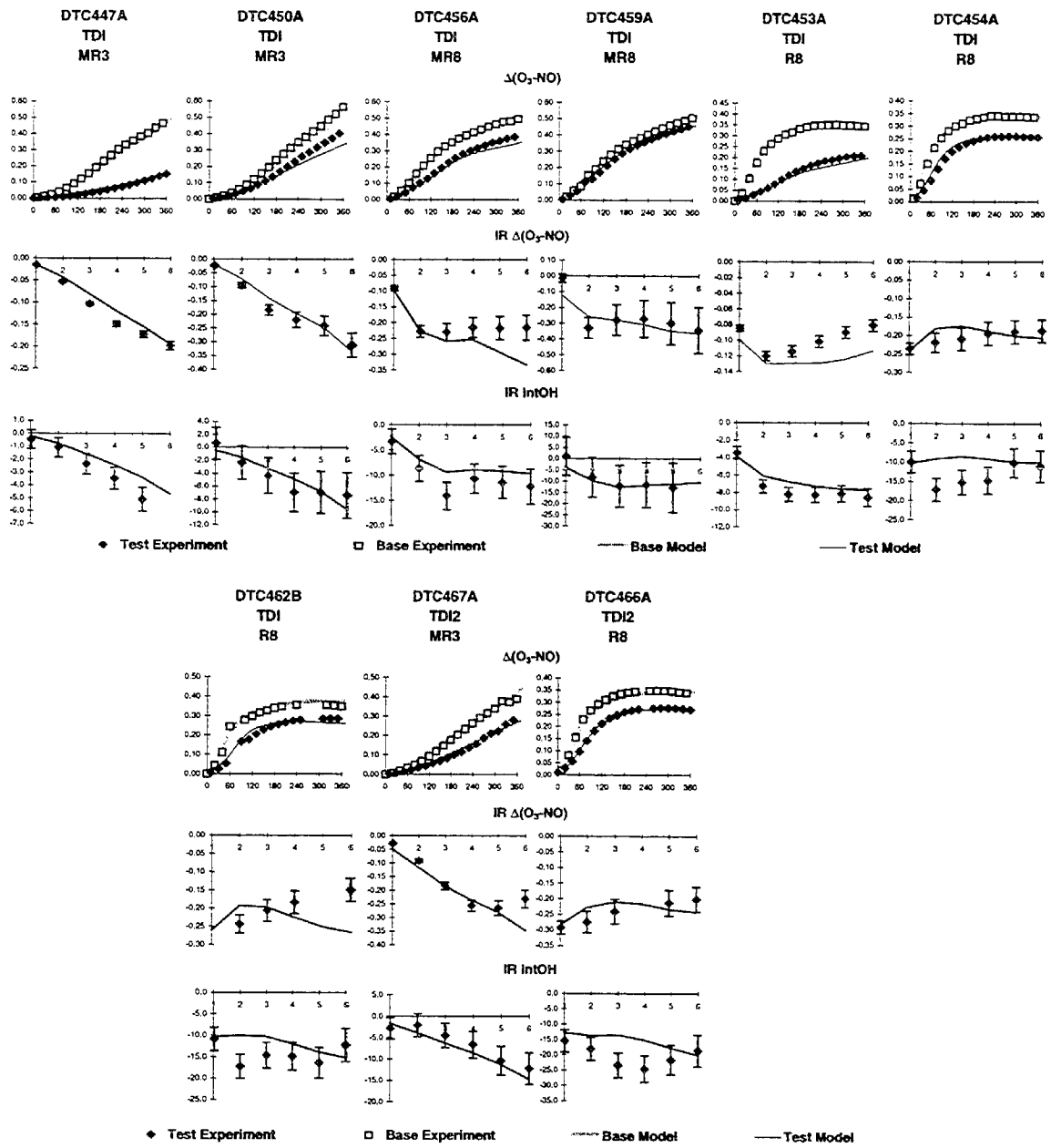


Figure B-84. Plots of experimental and calculated results of the incremental reactivity experiments with the toluene diisocyanate isomers (TDI and TDI2)

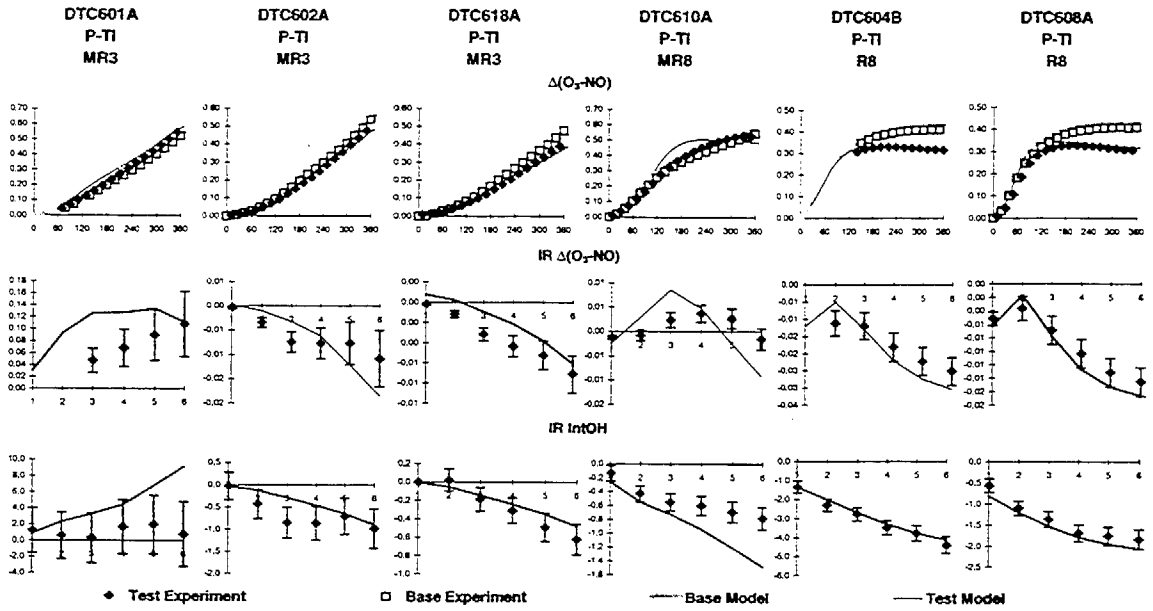


Figure B-85. Plots of experimental and calculated results of the incremental reactivity experiments with para toluene isocyanate.

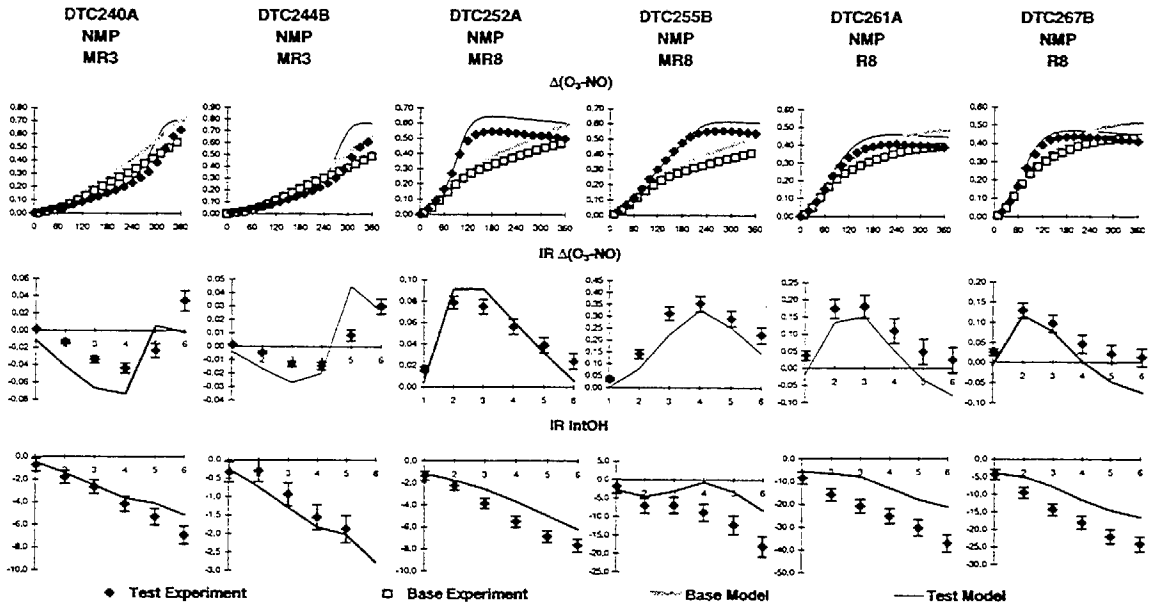


Figure B-86. Plots of experimental and calculated results of the incremental reactivity experiments with N-Methyl-2-Pyrrolidone.

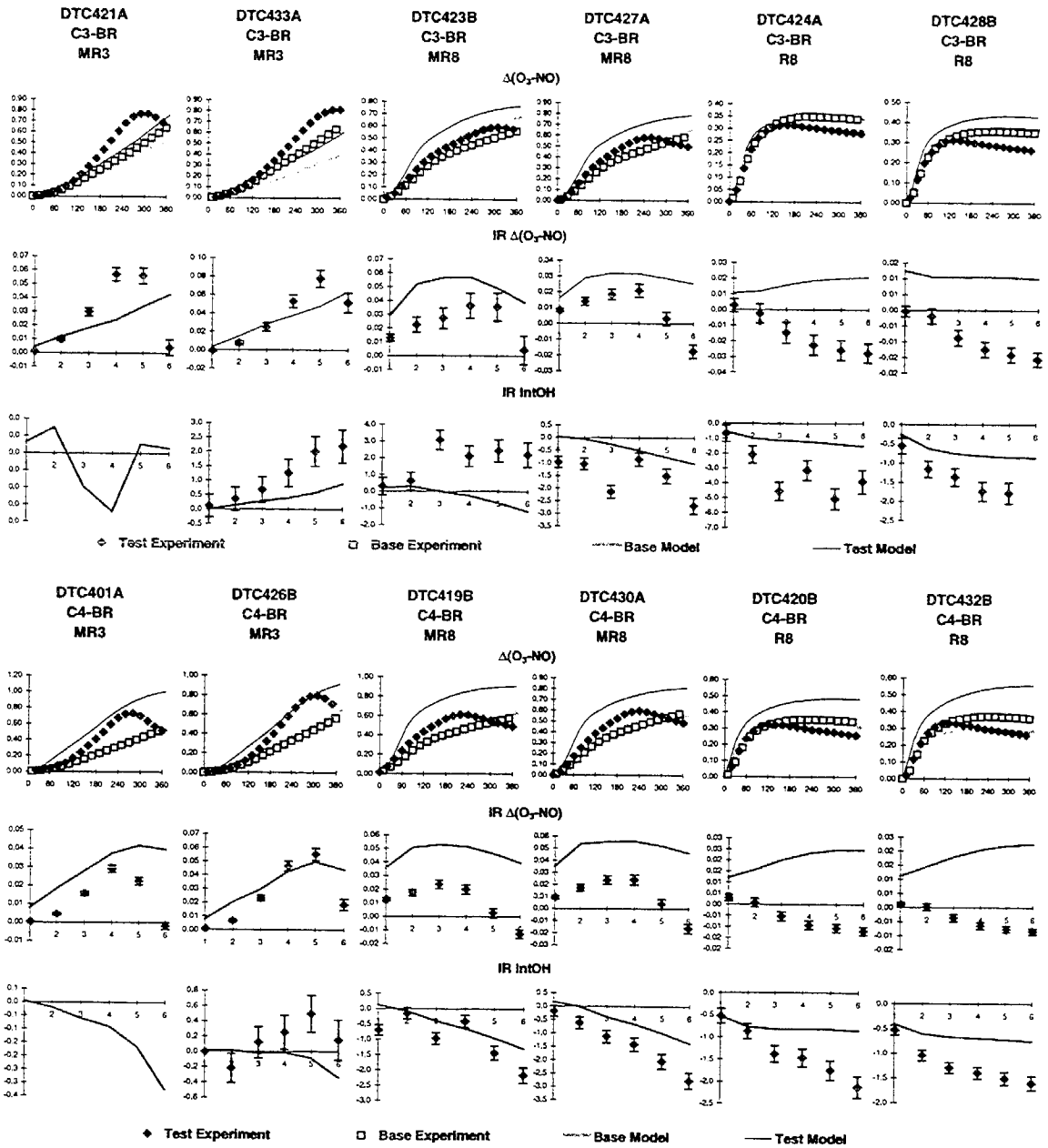
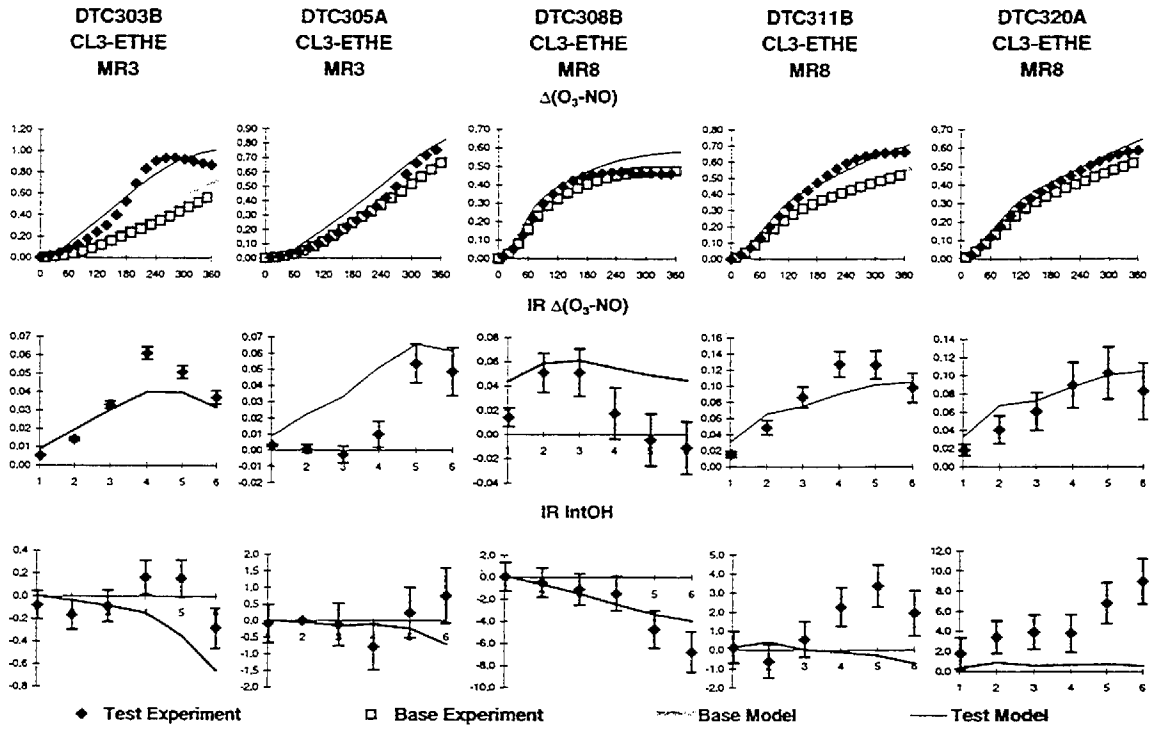


Figure B-87. Plots of experimental and calculated results of the incremental reactivity experiments with propyl and n-butyl bromides.



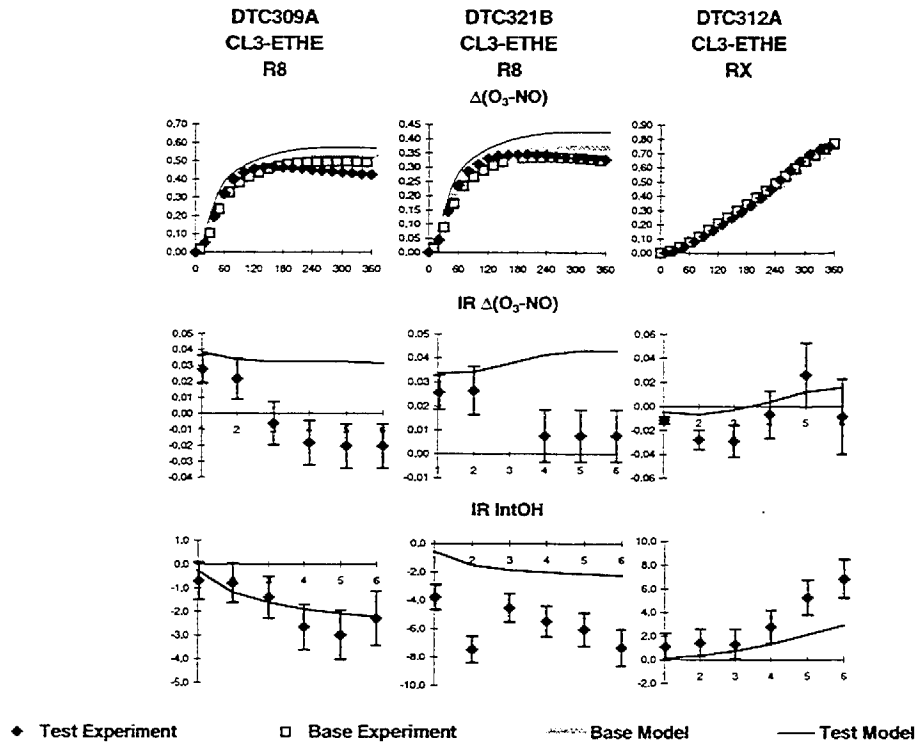


Figure B-88. Plots of experimental and calculated results of the incremental reactivity experiments with trichloroethylene.

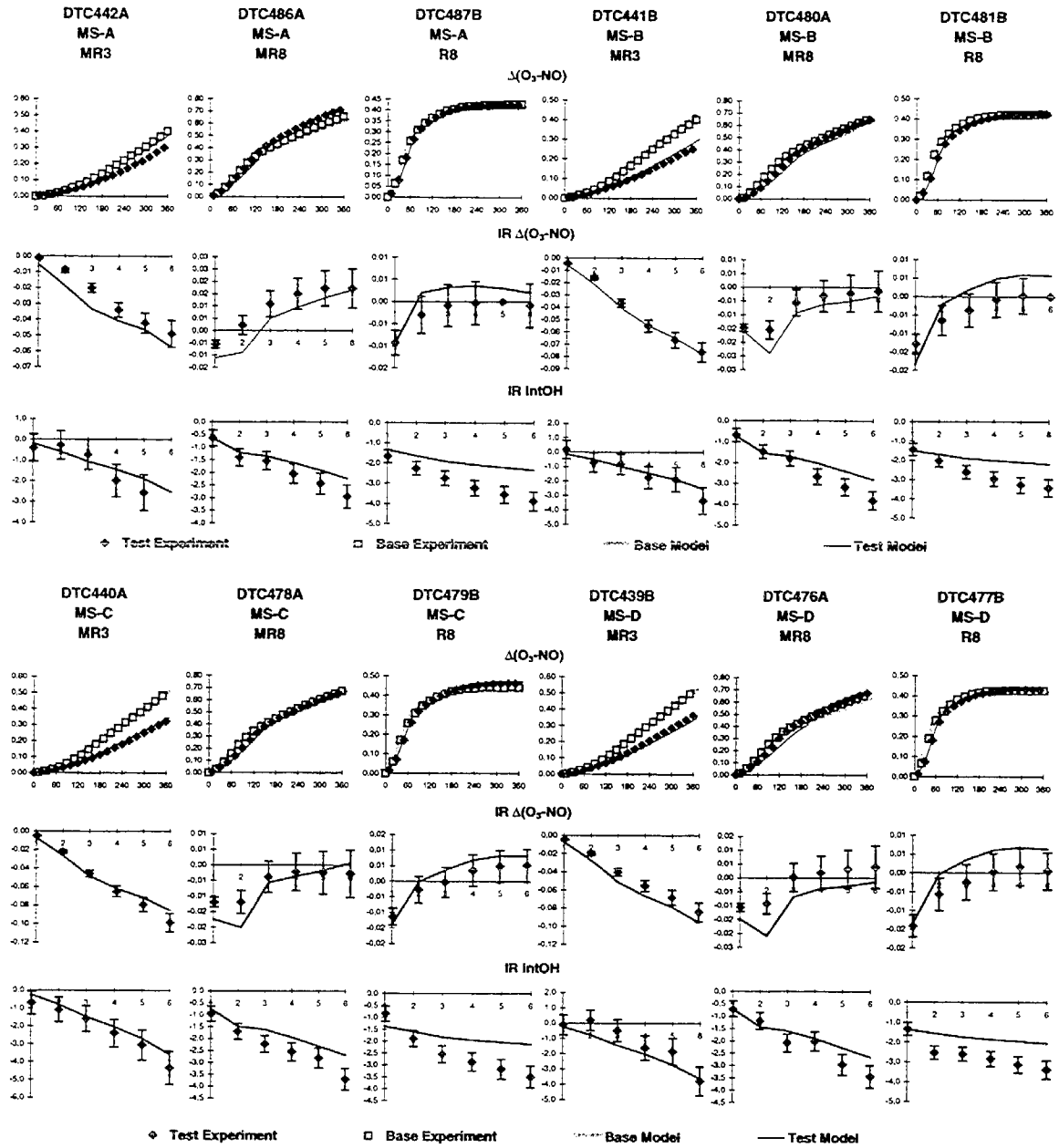


Figure B-89. Plots of experimental and calculated results of the incremental reactivity experiments with the mineral spirits samples used in the Safety-Kleen study (Carter et al, 1997f).

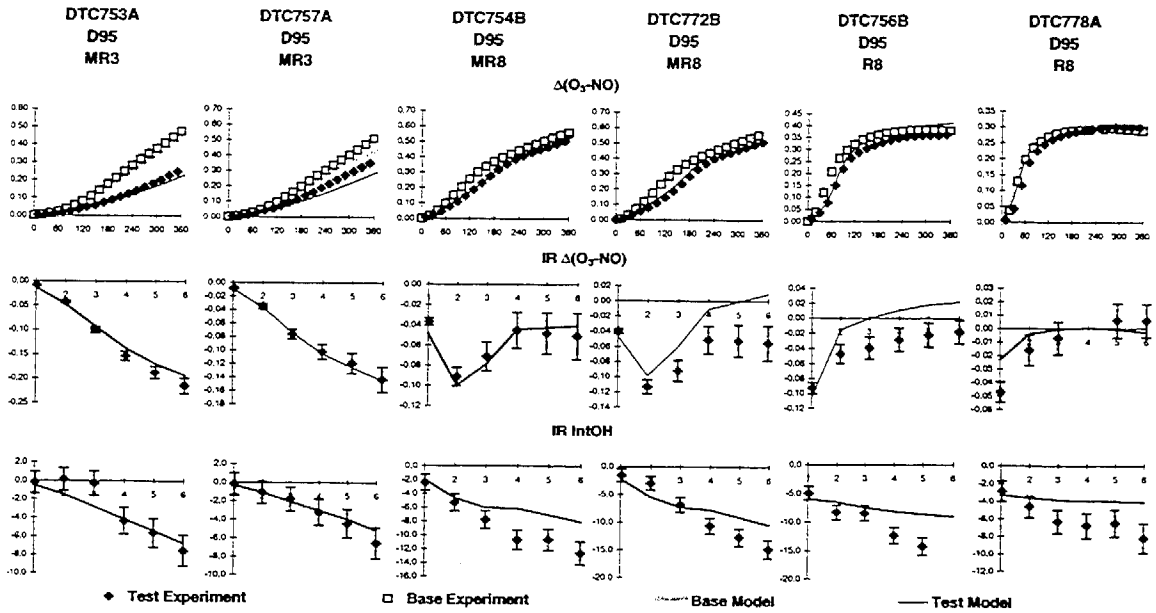


Figure B-90. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon D95® fluid..

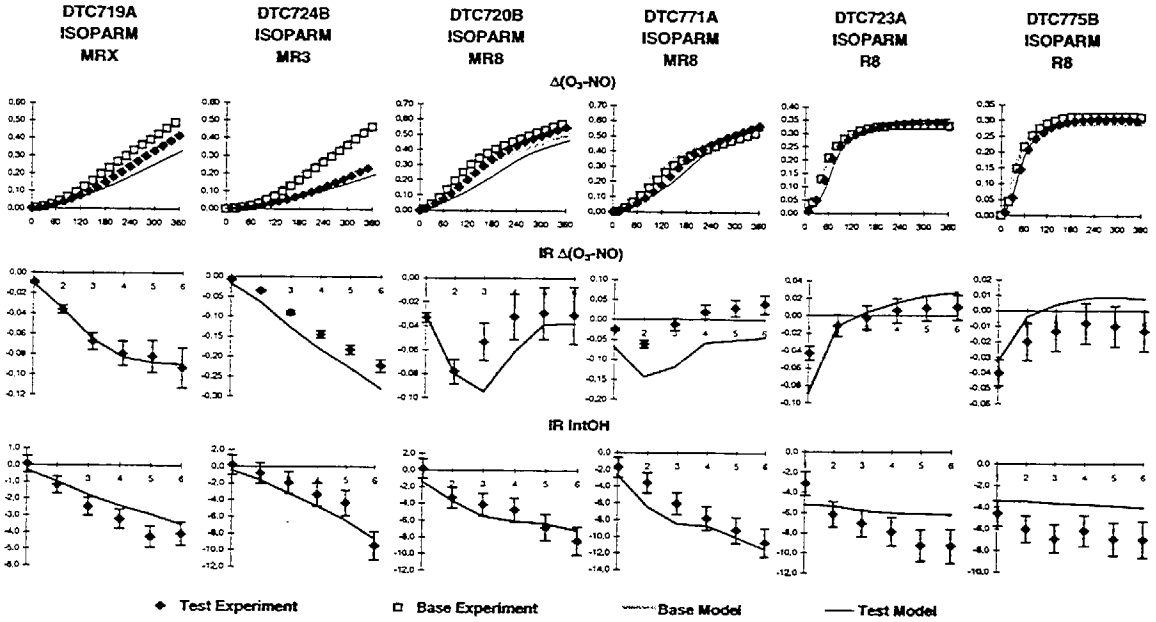


Figure B-91. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon Isopar-M® Fluid.

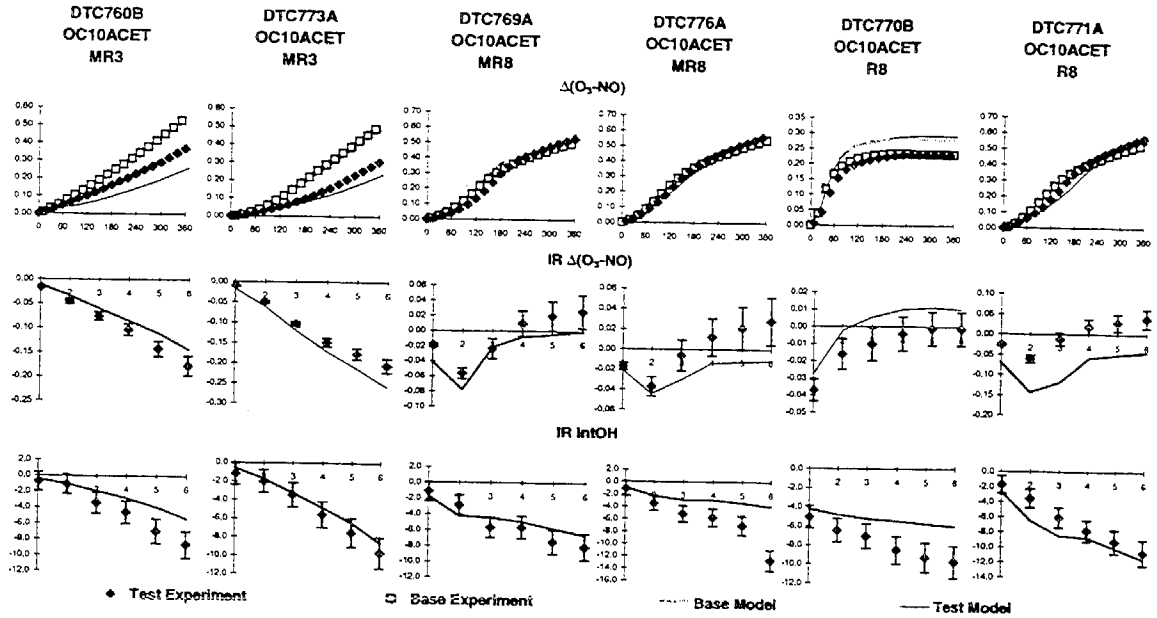


Figure B-92. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon Exxate-1000 Fluid (used to derive the reactivities of "oxo-decyl acetate").

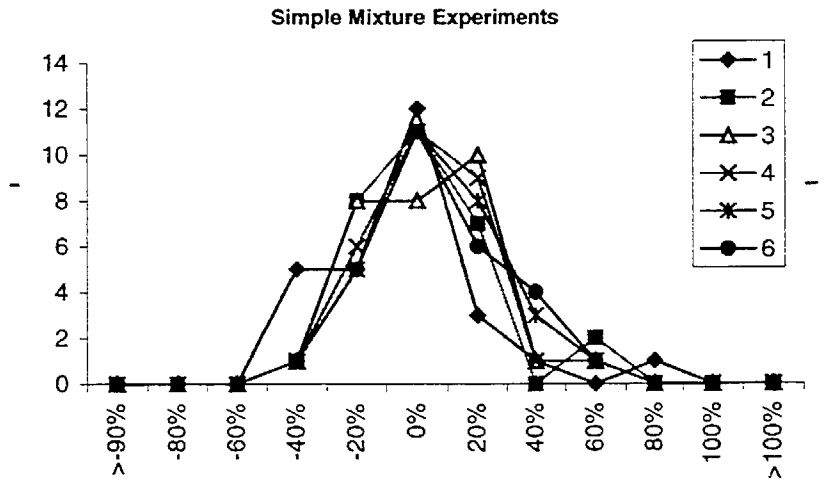


Figure B-93. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the simple mixture experiments (most carried out in the SAPRC EC).

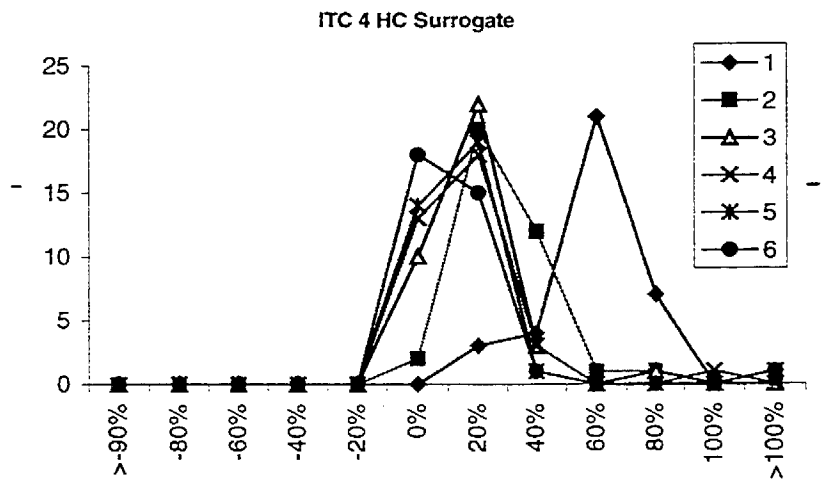


Figure B-94. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the four hydrocarbon surrogate experiments carried out in the ITC.

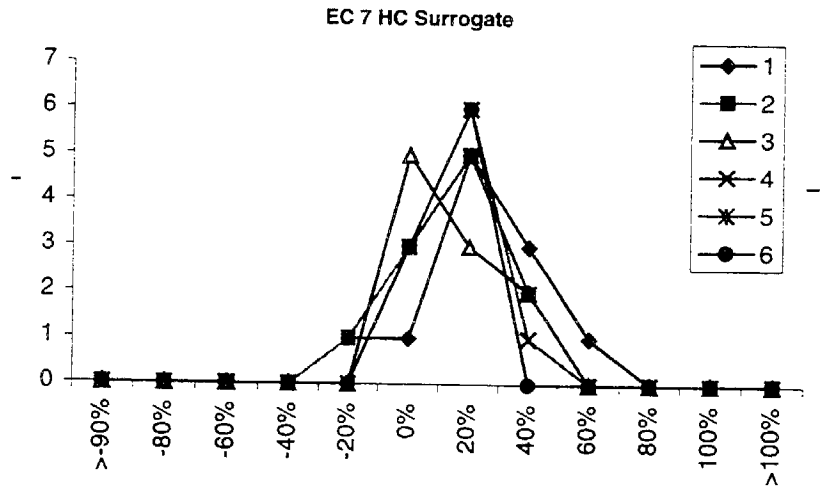


Figure B-95. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the seven hydrocarbon surrogate experiments carried out in the SAPRC EC.

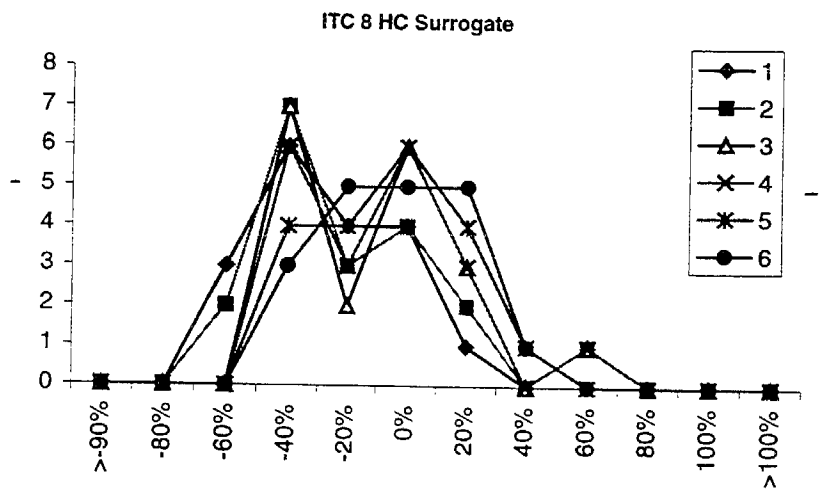


Figure B-96. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the eight hydrocarbon surrogate experiments carried out in the ITC.

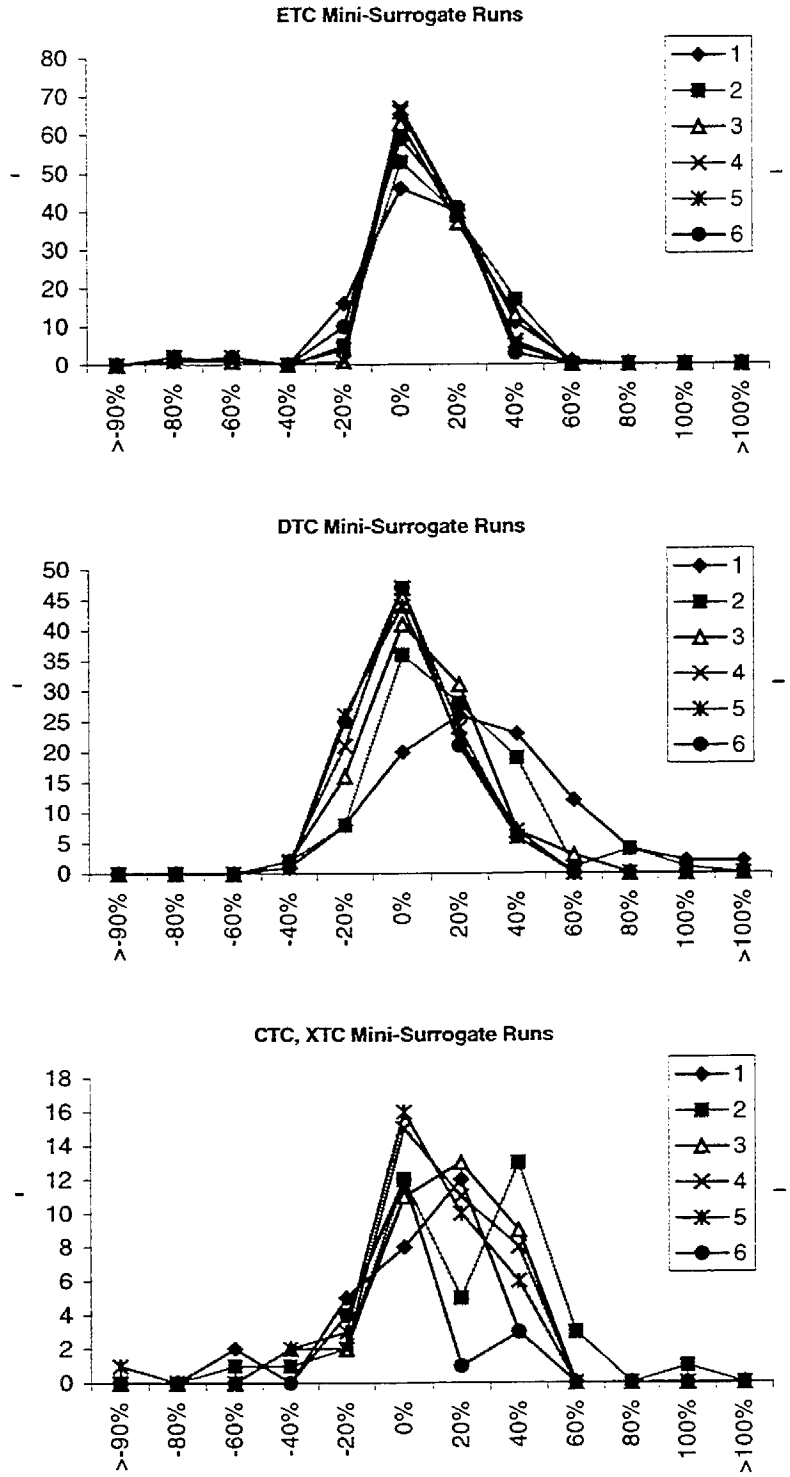


Figure B-97. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case mini-surrogate experiments carried out in various chambers.

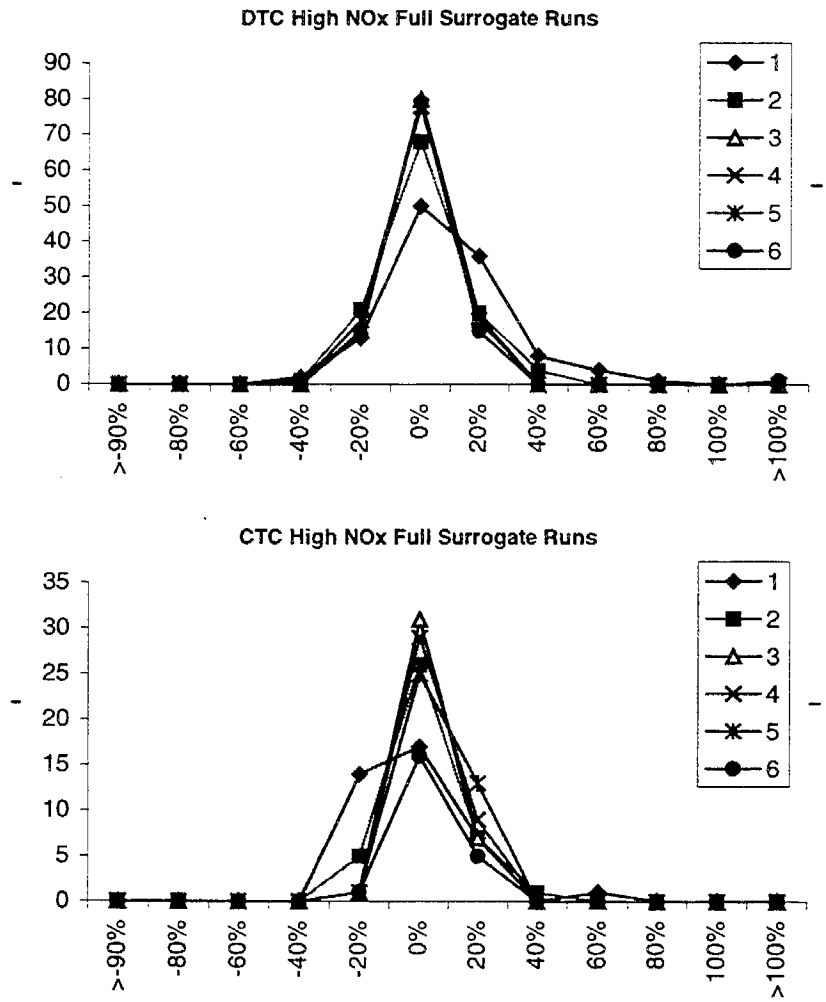
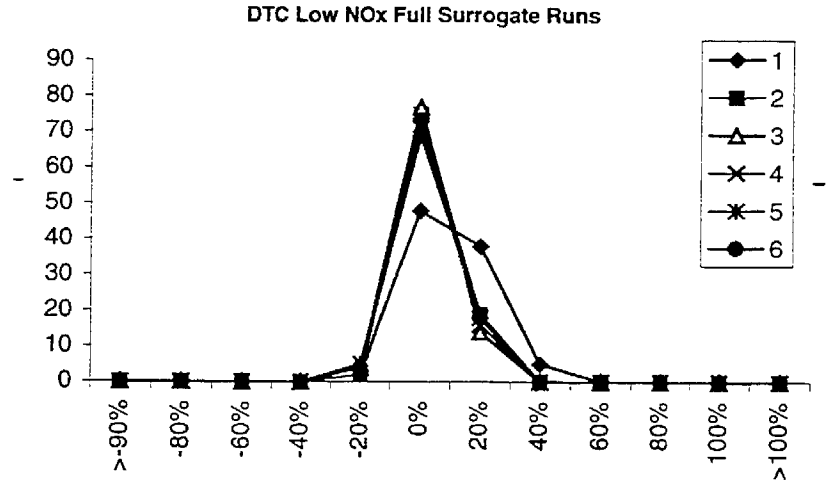


Figure B-98. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case high NO_x full surrogate experiments carried out in various chambers.



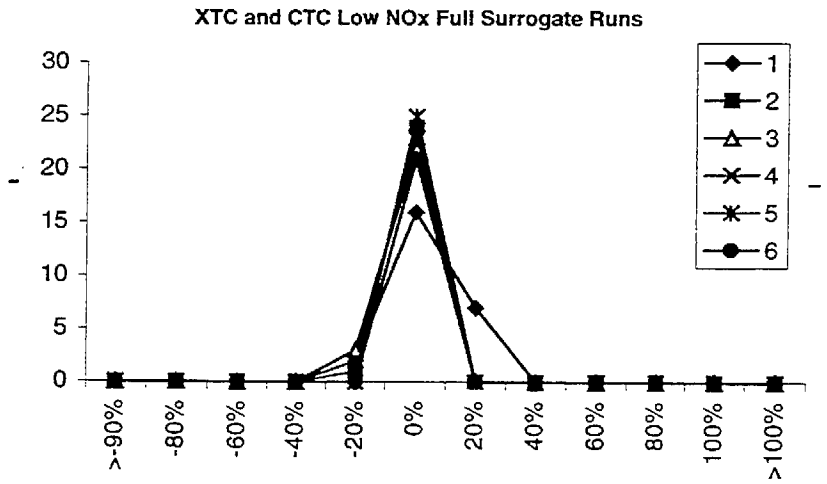


Figure B-99. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case low NO_x full surrogate experiments.

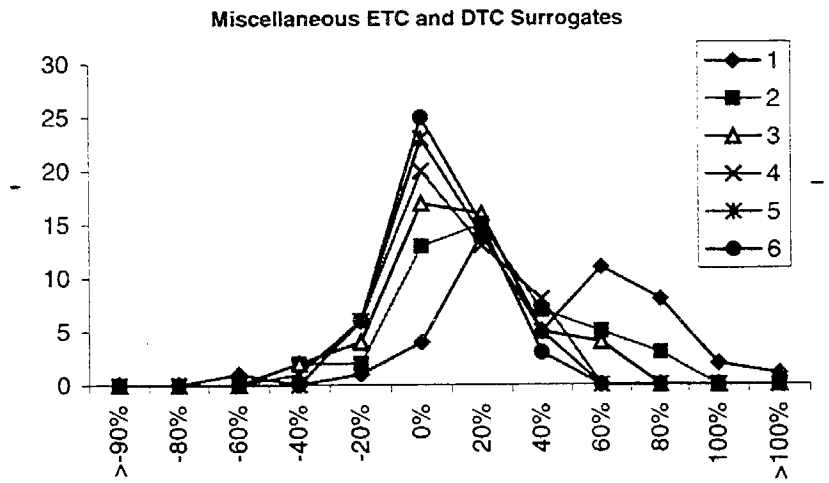


Figure B-100. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the miscellaneous non-standard surrogates used in various incremental reactivity experiments in the ETC and DTC.

APPENDIX C.

LISTING OF DETAILED MODEL SPECIES AND REACTIVITIES

This Appendix contains a complete listing and summary of all the detailed model species that are represented in the current mechanism, and gives the calculated reactivity results and the uncertainty assignments. Table C-1 lists all the detailed model species, indicates how they are represented in the model, gives their uncertainty classification and experimental availability codes, and other documentation notes and comments. It also gives the updated MIR values, calculated as discussed in Section VII, and the upper limit MIR values, derived as discussed in Appendix D. The uncertainty codes used in this table are defined in Table C-2, the experimental availability codes are defined in Table C-2, and the text for the comments footnotes is given in Table C-4. Table C-5 gives the compositions of the mixtures listed on Table C-1 whose reactivities are estimated, which were used as the basis for these estimates.

A summary of incremental and reactivity results using various scales in addition to MIR are given in Table C-6. The derivations of these scales are given in Section VII. This table includes averages of base case and adjusted NO_x reactivities calculated for the various 39 urban areas as discussed in Section VII. The reactivities calculated for the individual urban areas are given in Table C-7 and Table C-8, where the former has the O_3 yield reactivity data, and the latter has the reactivities relative to the maximum 8-hour average. Because of their length, Tables C-7 and C-8 are not included with the printed (or PDF) version of this report, but are available as supplementary material as Excel-97 files. They can be downloaded from a FTP site linked to http://cert.ucr.edu/~carter/reactdat.htm[1]

[1] This site may contain updated information when the mechanism and reactivity scale are updated in the future. However, it is expected that links and files will be retained so the version of the tables discussed in this report can still be downloaded.

Table C-1. Listing of detailed model species, their representation in the model, atmospheric reactivity estimates, and uncertainty assignments.

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
CO	Carbon Monoxide	28.01	1	1	1,2	0.058	(0.45)	Expl
METHANE	Methane	16.04	1	4	1	0.0139	(0.025)	Asn'd
ETHANE	Ethane	30.07	1	2	1,2	0.31	(0.92)	Gen'd CH3-CH3
PROPANE	Propane	44.10	1	2	1,2,3	0.56	(2.61)	Gen'd CH3-CH2-CH3
N-C4	n-Butane	58.12	1	1	1,2,4	1.33	(4.00)	Gen'd CH3-CH2-CH2-CH3
N-C5	n-Pentane	72.15	1	7	4	1.54	(4.82)	Gen'd CH3-CH2-CH2-CH2-CH3
N-C6	n-Hexane	86.18	2	2	2,4	1.45	(5.08)	Gen'd CH3-CH2-CH2-CH2-CH2-CH3
N-C7	n-Heptane	100.21	2	-	4	1.28	(5.20)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH3
N-C8	n-Octane	114.23	2	1	2,4	1.11	(5.21)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C9	n-Nonane	128.26	3a	7	4	0.95	(5.02)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C10	n-Decane	142.29	3a	-	4	0.83	(4.82)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C11	n-Undecane	156.31	3a	-	4	0.74	(4.70)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C12	n-Dodecane	170.34	3a	1	2,4	0.66	(4.43)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C13	n-Tridecane	184.37	3a	-	4	0.62	(4.37)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C14	n-Tetradecane	198.40	3a	1	2,4	0.58	(4.23)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C15	n-Pentadecane	212.42	3a	1	2,4	0.56	(4.17)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C16	n-C16	226.45	3a	1	2,4	0.52	(4.04)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C17	n-C17	240.46	3a			0.49	(3.80)	L.Mol N-C16
N-C18	n-C18	254.49	3a			0.46	(3.57)	L.Mol N-C16
N-C19	n-C19	268.51	3a			0.44	(3.39)	L.Mol N-C16
N-C20	n-C20	282.54	3a			0.42	(3.22)	L.Mol N-C16
N-C21	n-C21	296.57	3a			0.40	(3.07)	L.Mol N-C16
N-C22	n-C22	310.59	3a			0.38	(2.93)	L.Mol N-C16
2-ME-C3	Isobutane	58.12	1	2	2,4,5	1.35	(3.63)	Gen'd CH3-CH(CH3)-CH3
2-ME-C4	Iso-Pentane	72.15	2	7	4	1.68	(4.52)	Gen'd CH3-CH(CH3)-CH2-CH3
22-DM-C3	Neopentane	72.15	2	7	3	0.69	(1.23)	Gen'd CH3-C(CH3)(CH3)-CH3
BR-C5	Branched C5 Alkanes	72.15	3	-	6	1.68	(4.52)	L.Mol 2-ME-C4
22-DM-C4	2,2-Dimethyl Butane	86.18	2	-	4	1.33	(2.61)	Gen'd CH3-C(CH3)(CH3)-CH2-CH3
23-DM-C4	2,3-Dimethyl Butane	86.18	2	7	4	1.14	(5.28)	Gen'd CH3-CH(CH3)-CH(CH3)-CH3
2-ME-C5	2-Methyl Pentane	86.18	2	-	4	1.80	(4.98)	Gen'd CH3-CH(CH3)-CH2-CH2-CH3
3-ME-C5	3-Methylpentane	86.18	2	-	4	2.07	(5.05)	Gen'd CH3-CH2-CH(CH3)-CH2-CH3
BR-C6	Branched C6 Alkanes	86.18	3	6	6	1.53	(5.15)	L.Mol 0.5 23-DM-C4 +0.25 3-ME-C5 +0.25 2-ME-C5
223TM-C4	2,2,3-Trimethyl Butane	100.21	2	-	4	1.32	(3.62)	Gen'd CH3-C(CH3)(CH3)-CH(CH3)-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
22-DM-C5	2,2-Dimethyl Pentane	100.21	2	-	4	1.22	(3.03)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH3
23-DM-C5	2,3-Dimethyl Pentane	100.21	2	-	4	1.55	(7.65)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH3
24-DM-C5	2,4-Dimethyl Pentane	100.21	2	-	4	1.65	(4.09)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH3
2-ME-C6	2-Methyl Hexane	100.21	2	-	4	1.37	(7.51)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH3
33-DM-C5	3,3-Dimethyl Pentane	100.21	2	-	3	1.32	(4.66)	Gen'd	CH3-CH2-C(CH3)(CH3)-CH2-CH3
3-ME-C6	3-Methyl Hexane	100.21	2	-	4	1.86	(7.65)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH3
BR-C7	Branched C7 Alkanes	100.21	3	-	6	1.63	(5.83)	L.Mol	0.5 24-DM-C5 +0.25 3-ME-C6 +0.25 2-ME-C6
2233M-C4	2,2,3,3-Tetramethyl Butane	114.23	3	-	4	0.44	(0.94)	Gen'd	CH3-C(CH3)(CH3)-C(CH3)(CH3)-CH3
224TM-C5	2,2,4-Trimethyl Pentane	114.23	2	2	2,4,5	1.44	(2.78)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH(CH3)-CH3
22-DM-C6	2,2-Dimethyl Hexane	114.23	3	-	4	1.13	(3.50)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH2-CH3
234TM-C5	2,3,4-Trimethyl Pentane	114.23	3	-	3	1.23	(4.61)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH(CH3)-CH3
23-DM-C6	2,3-Dimethyl Hexane	114.23	3	-	4	1.34	(7.23)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH2-CH3
24-DM-C6	2,4-Dimethyl Hexane	114.23	3	-	4	1.80	(7.23)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH3
25-DM-C6	2,5-Dimethyl Hexane	114.23	3	-	4	1.68	(7.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH(CH3)-CH3
2-ME-C7	2-Methyl Heptane	114.23	3	-	4	1.20	(7.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH3
3-ME-C7	3-Methyl Heptane	114.23	3	-	4	1.35	(7.23)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH3
4-ME-C7	4-Methyl Heptane	114.23	3	-	4	1.48	(7.23)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH3
BR-C8	Branched C8 Alkanes	114.23	3	-	6	1.57	(7.19)	L.Mol	0.5 24-DM-C6 +0.25 4-ME-C7 +0.25 2-ME-C7
225TM-C6	2,2,5-Trimethyl Hexane	128.26	3a	-	4	1.33	(5.56)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH(CH3)-CH3
235TM-C6	2,3,5-Trimethyl Hexane	128.26	3a	-	4	1.33	(4.38)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH(CH3)-CH3
24-DM-C7	2,4-Dimethyl Heptane	128.26	3a	-	4	1.48	(6.80)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH3
2-ME-C8	2-Methyl Octane	128.26	3a	-	4	0.96	(5.05)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
33-DE-C5	3,3-Diethyl Pentane	128.26	3a	-	3	1.35	(3.15)	Gen'd	CH3-CH2-C(CH2-CH3)(CH2-CH3)-CH2-CH3
35-DM-C7	3,5-Dimethyl Heptane	128.26	3a	-	4	1.63	(6.87)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH3
4-ET-C7	4-Ethyl Heptane	128.26	3a	-	4	1.44	(6.87)	Gen'd	CH3-CH2-CH2-CH(CH2-CH3)-CH2-CH2-CH3
4-ME-C8	4-Methyl Octane	128.26	3a	-	4	1.08	(4.92)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH3
BR-C9	Branched C9 Alkanes	128.26	3a	-	6	1.25	(5.89)	L.Mol	0.5 24-DM-C7 +0.25 4-ME-C8 +0.25 2-ME-C8
24-DM-C8	2,4-Dimethyl Octane	142.29	3a	-	4	1.09	(6.38)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-CH3
26DM-C8	2,6-Dimethyl Octane	142.29	3a	1	2,4	1.27	(5.16)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH3
2-ME-C9	2-Methyl Nonane	142.29	3a	1	2,4	0.86	(5.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
34-DE-C6	3,4-Diethyl Hexane	142.29	3a	1a	2,4	1.20	(3.78)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH(CH2-CH3)-CH2-CH3
3-ME-C9	3-Methyl Nonane	142.29	3a	-	4	0.89	(6.38)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
4-ME-C9	4-Methyl Nonane	142.29	3a	-	4	0.99	(6.38)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
4-PR-C7	4-Propyl Heptane	142.29	3a	-	4	1.24	(6.44)	Gen'd	CH3-CH2-CH2-CH(CH2-CH2-CH3)-CH2-CH2-CH3
BR-C10	Branched C10 Alkanes	142.29	3a	6	6,7	1.09	(5.47)	L.Mol	0.5 26DM-C8 +0.25 4-ME-C9 +0.25 2-ME-C9
26DM-C9	2,6-Dimethyl Nonane	156.31	3a	-	4	0.95	(6.01)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
35-DE-C7	3,5-Diethyl Heptane	156.31	3a	-	4	1.21	(6.15)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C10	3-Methyl Decane	156.31	3a	-	4	0.77	(6.05)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
4-ME-C10	4-Methyl Decane	156.31	3a	-	4	0.80	(6.05)	Gen'd CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
BR-C11	Branched C11 alkanes	156.31	3a	-	6,7	0.87	(6.01)	L.Mol 0.5 26DM-C9 +0.25 4-ME-C10 +0.25 3-ME-C10
36-DE-C8	2,6-Diethyl Octane	170.34	3a	-	4	1.09	(5.78)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH3
36DM-C10	3,6-Dimethyl Decane	170.34	3a	-	4	0.88	(5.72)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH3
3-ME-C11	3-Methyl Undecane	170.34	3a	-	4	0.70	(5.68)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
5-ME-C11	5-Methyl Undecane	170.34	3a	-	4	0.72	(5.68)	Gen'd CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
BR-C12	Branched C12 Alkanes	170.34	3a	-	6,7	0.80	(5.72)	L.Mol 0.5 36DM-C10 +0.25 5-ME-C11 +0.25 3-ME-C11
36DM-C11	3,6-Dimethyl Undecane	184.37	3a	-	4	0.82	(5.42)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
37-DE-C9	3,7-Diethyl Nonane	184.37	3a	-	4	1.08	(5.48)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C12	3-Methyl Dodecane	184.37	3a	-	4	0.64	(5.38)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
5-ME-C12	5-Methyl Dodecane	184.37	3a	-	4	0.64	(5.38)	Gen'd CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C13	Branched C13 Alkanes	184.37	3a	-	6,7	0.73	(5.42)	L.Mol 0.5 36DM-C11 +0.25 5-ME-C12 +0.25 3-ME-C12
37DM-C12	3,7-Dimethyl Dodecane	198.40	3a	-	4	0.74	(5.15)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
38DE-C10	3,8-Diethyl Decane	198.40	3a	-	4	0.68	(5.18)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C13	3-Methyl Tridecane	198.40	3a	-	4	0.57	(5.12)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
6-ME-C13	6-Methyl Tridecane	198.40	3a	-	4	0.62	(5.12)	Gen'd CH3-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C14	Branched C14 Alkanes	198.40	3a	-	6,7	0.67	(5.12)	L.Mol 0.5 37DM-C12 +0.25 6-ME-C13 +0.25 3-ME-C13
37DM-C13	3,7-Dimethyl Tridecane	212.42	3a	-	4	0.64	(4.88)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
39DE-C11	3,9-Diethyl Undecane	212.42	3a	-	4	0.62	(4.92)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C14	3-Methyl Tetradecane	212.42	3a	-	4	0.53	(4.85)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
6-ME-C14	6-Methyl Tetradecane	212.42	3a	-	4	0.57	(4.85)	Gen'd CH3-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C15	Branched C15 Alkanes	212.42	3a	-	6,7	0.60	(4.88)	L.Mol 0.5 37DM-C13 +0.25 6-ME-C14 +0.25 3-ME-C14
3-ME-C15	3-Methyl Pentadecane	226.45	3a	-	4	0.50	(4.65)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
48DM-C14	4,8-Dimethyl Tetradecane	226.45	3a	-	4	0.58	(4.65)	Gen'd CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
7-ME-C15	7-Methyl Pentadecane	226.45	3a	-	4	0.51	(4.65)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C16	Branched C16 Alkanes	226.45	3a	-	6	0.54	(4.65)	L.Mol 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
BR-C17	Branched C17 Alkanes	240.46	3a	-	6	0.51	(4.38)	L.Mol 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
BR-C18	Branched C18 Alkanes	254.49	3a	-	6	0.48	(4.14)	L.Mol 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
CYCC3	Cyclopropane	42.08	3	-	4	0.103	(0.21)	Gen'd *CH2-CH2-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
CYCC4	Cyclobutane	56.11	3	-	3	1.05	(2.65)	Gen'd	*CH2-CH2-CH2-CH2-*
CYCC5	Cyclopentane	70.14	2	-	4	2.69	(5.92)	Gen'd	*CH2-CH2-CH2-CH2-CH2-*
CYCC6	Cyclohexane	84.16	2	1	2,4	1.46	(6.33)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-*
IPR-CC3	Isopropyl Cyclopropane	84.16	3	-	4	1.52	(2.97)	Gen'd	*CH(CH(CH3)-CH3)-CH2-CH2-*
ME-CYCC5	Methylcyclopentane	84.16	3	-	4	2.42	(8.18)	Gen'd	*CH(CH3)-CH2-CH2-CH2-CH2-*
CYC-C6	C6 Cycloalkanes	84.16	3	6	6	1.46	(6.33)	L.Mol	CYCC6
13DMCYC5	1,3-Dimeth. Cyclopentane	98.19	3	-	4	2.15	(7.63)	Gen'd	*CH(CH3)-CH2-CH(CH3)-CH2-CH2-*
CYCC7	Cycloheptane	98.19	3	-	4	2.26	(7.46)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-CH2-*
ET-CYCC5	Ethyl Cyclopentane	98.19	3	-	4	2.27	(7.87)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH2-CH2-*
ME-CYCC6	Methylcyclohexane	98.19	3	7	4	1.99	(6.54)	Gen'd	*CH(CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C7	C7 Cycloalkanes	98.19	3	-	6	1.99	(6.54)	L.Mol	ME-CYCC6
13DMCYC6	1,3-Dimethyl Cyclohexane	112.22	3	-	4	1.72	(8.21)	Gen'd	*CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
CYCC8	Cyclooctane	112.22	3	-	4	1.73	(6.78)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-*
ET-CYCC6	Ethylcyclohexane	112.22	3	-	4	1.75	(8.21)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
PR-CYCC5	Propyl Cyclopentane	112.22	3	-	4	1.91	(7.39)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-*
CYC-C8	C8 Cycloalkanes	112.22	3	-	6	1.75	(8.21)	L.Mol	ET-CYCC6
BCYC-C9	C9 Bicycloalkanes	124.23	3	-	6	1.57	(7.69)	L.Mol	0.5 C3-CYCC6 +0.5 1E4MCYC6
113MCYC6	1,1,3-Trimethyl Cyclohex.	126.24	3	-	4	1.37	(4.72)	Gen'd	*C(CH3)(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	126.24	3	-	4	1.62	(7.60)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C3-CYCC6	Propyl Cyclohexane	126.24	3	-	4	1.47	(7.56)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C9	C9 Cycloalkanes	126.24	3	-	6	1.55	(7.56)	L.Mol	0.5 C3-CYCC6 +0.5 1E4MCYC6
BCYC-C10	C10 Bicycloalkanes	138.25	3	-	6	1.29	(7.12)	L.Mol	0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
13DECYC6	1,3-Diethyl-Cyclohexane	140.27	3	-	4	1.34	(7.05)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH2-CH2-*
14DECYC6	1,4-Diethyl-Cyclohexane	140.27	3	-	4	1.49	(7.05)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-*
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	140.27	3	-	4	1.26	(7.02)	Gen'd	*CH(CH(CH3)-CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
C4-CYCC6	Butyl Cyclohexane	140.27	3	-	4	1.07	(6.98)	Gen'd	*CH(CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C10	C10 Cycloalkanes	140.27	3	6	6,7	1.27	(7.02)	L.Mol	0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
BCYC-C11	C11 Bicycloalkanes	152.28	3	-	6	1.01	(6.62)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
13E5MCC6	13-Dieth-5-Me. Cyclohex.	154.30	3	-	4	1.11	(6.57)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH3)-CH2-*
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	154.30	3	-	4	0.95	(6.57)	Gen'd	*CH(CH2-CH3)-CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-*
C5-CYCC6	Pentyl Cyclohexane	154.30	3	-	4	0.91	(6.50)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C11	C11 Cycloalkanes	154.30	3	-	6,7	0.99	(6.54)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
CYC-C11	C11 Cycloalkanes	154.30	3	-	6,7	0.99	(6.54)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
BCYC-C12	C12 Bicycloalkanes	166.30	3	-	6	0.88	(5.82)	L.Mol	0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
CYC-C12	C12 Cycloalkanes	168.32	3	6	6,7	0.87	(5.75)	L.Mol	0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
135ECYC6	1,3,5-Triethyl Cyclohex.	168.33	3	-	4	1.06	(6.16)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	168.33	3	-	3	0.81	(6.09)	Gen'd *CH(CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C6-CYCC6	Hexyl Cyclohexane	168.33	2	1	2,4	0.75	(4.96)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
BCYC-C13	C13 Bicycloalkanes	180.33	3	-	6	0.79	(5.81)	L.Mol 0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
13E5PCC6	13-Dieth-5-Pent Cyclohx.	182.35	3	-	4	0.99	(5.78)	Gen'd *CH(CH2-CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-*
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	182.35	3	-	4	0.70	(5.72)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH3)-CH(CH3)-CH2-CH2-CH2-CH2-*
C7-CYCC6	Heptyl Cyclohexane	182.35	3	-	4	0.66	(5.72)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C13	C13 Cycloalkanes	182.35	3	-	6,7	0.78	(5.75)	L.Mol 0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
BCYC-C14	C14 Bicycloalkanes	194.36	3	6	6	0.71	(5.46)	L.Mol 0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
13P5ECC6	13-Diprop-5-Eth Cyclohx.	196.38	3	-	4	0.94	(5.44)	Gen'd *CH(CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	196.38	3	-	3	0.58	(5.41)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C8-CYCC6	Octyl Cyclohexane	196.38	2	1	2,4	0.60	(5.37)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C14	C14 Cycloalkanes	196.38	3	-	6,7	0.71	(5.41)	L.Mol 0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
BCYC-C15	C15 Bicycloalkanes	208.39	3	-	6	0.69	(5.18)	L.Mol 0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
135PCYC6	135-Tripropyl Cyclohex.	210.41	3	-	4	0.90	(5.17)	Gen'd *CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	210.41	3	-	4	0.60	(5.10)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH(CH3)-CH2-CH2-CH2-CH2-*
C9-CYCC6	Nonyl Cyclohexane	210.41	3	-	4	0.54	(5.10)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C15	C15 Cycloalkanes	210.41	3	6	6,7	0.68	(5.13)	L.Mol 0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	224.43	3	-	4	0.77	(4.89)	Gen'd *CH(CH2-CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	224.43	3	-	4	0.55	(4.86)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C10CYCC6	Decyl Cyclohexane	224.43	3	-	4	0.50	(4.83)	Gen'd *CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C16	C16 Cycloalkanes	224.43	3	6	6,7	0.61	(4.86)	L.Mol 0.34 C10CYCC6 +0.33 13P5BCC6 +0.33 1M4C9CY6
ETHENE	Ethene	28.05	1	1a	2,4	9.08	(19.51)	Gen'd CH2=CH2
PROPENE	Propene	42.08	1	1	2,3,5	11.58	(23.89)	Gen'd CH2=CH-CH3
1-BUTENE	1-Butene	56.11	2	3	2,4,5	10.29	(23.92)	Gen'd CH2=CH-CH2-CH3
C4-OLE1	C4 Terminal Alkenes	56.11	2			10.29	(23.92)	L.Mol 1-BUTENE
1-PENTEN	1-Pentene	70.14	2	-	4	7.79	(23.92)	Gen'd CH2=CH-CH2-CH2-CH3
3M-1-BUT	3-Methyl-1-Butene	70.14	3	-	4	6.99	(23.92)	Gen'd CH2=CH-CH(CH3)-CH3
C5-OLE1	C5 Terminal Alkenes	70.14	2			7.79	(23.92)	L.Mol 1-PENTEN
1-HEXENE	1-Hexene	84.16	2	3	2,4,5	6.17	(19.95)	Gen'd CH2=CH-CH2-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
33M1-BUT	3,3-Dimethyl-1-Butene	84.16	3	-	4	6.06	(19.88)	Gen'd CH2=CH-C(CH3)(CH3)-CH3
3M1-C5E	3-Methyl-1-Pentene	84.16	3	-	4	6.22	(19.95)	Gen'd CH2=CH-CH(CH3)-CH2-CH3
4M1-C5E	4-Methyl-1-Pentene	84.16	3	-	4	6.26	(19.95)	Gen'd CH2=CH-CH2-CH(CH3)-CH3
C6-OLE1	C6 Terminal Alkenes	84.16	3			6.17	(19.95)	L.Mol 1-HEXENE
1-HEPTEN	1-Heptene	98.19	3	-	4	4.56	(17.11)	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH3
1-OCTENE	1-Octene	112.22	4	-	4	3.45	14.99	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH3
C8-OLE1	C8 Terminal Alkenes	112.22	4			3.45	14.99	L.Mol 1-OCTENE
1-C9E	1-Nonene	126.24	4	-	4	2.76	13.31	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C9-OLE1	C9 Terminal Alkenes	126.24	4			2.76	13.31	L.Mol 1-C9E
1-C10E	1-Decene	140.27	4	-	4	2.28	11.98	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C10-OLE1	C10 Terminal Alkenes	140.27	4			2.28	11.98	L.Mol 1-C10E
1-C11E	1-Undecene	154.30	4	-	4	1.95	10.88	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C11-OLE1	C11 Terminal Alkenes	154.30	4			1.95	10.88	L.Mol 1-C11E
C12-OLE1	C12 Terminal Alkenes	168.32	4			1.72	9.99	L.Mol 1-C12E
1-C12E	1-Dodecene	168.33	4	-	4	1.72	9.99	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
1-C13E	1-Tridecene	182.35	4	-	4	1.55	9.21	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C13-OLE1	C13 Terminal Alkenes	182.35	4			1.55	9.21	L.Mol 1-C13E
1-C14E	1-Tetradecene	196.38	4	-	4	1.48	8.56	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C14-OLE1	C14 Terminal Alkenes	196.38	4			1.48	8.56	L.Mol 1-C14E
1-C15E	1-Pentadecene	210.41	4	-	4	1.30	7.97	Gen'd CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C15-OLE1	C15 Terminal Alkenes	210.41	4			1.30	7.97	L.Mol 1-C15E
ISOBUTEN	Isobutene	56.11	1	2	2,4,5	6.35	(23.95)	Gen'd CH2=C(CH3)-CH3
2M-1-BUT	2-Methyl-1-Butene	70.14	3	-	4	6.51	(23.95)	Gen'd CH2=C(CH3)-CH2-CH3
23M1-BUT	23-Dimethyl-1-Butene	84.16	3	-	4	4.77	(19.95)	Gen'd CH2=C(CH3)-CH(CH3)-CH3
2E1-BUT	2-Ethyl-1-Butene	84.16	3	-	4	5.04	(19.95)	Gen'd CH2=C(CH2-CH3)-CH2-CH3
2M1-C5E	2-Methyl-1-Pentene	84.16	3	-	4	5.18	(19.95)	Gen'd CH2=C(CH3)-CH2-CH2-CH3
233M1BUT	2,3,3-trimethyl-1-Butene	98.19	3	-	4	4.62	(17.11)	Gen'd CH2=C(CH3)-C(CH3)(CH3)-CH3
C7-OLE1	C7 Terminal Alkenes	98.19	3			4.56	(17.11)	L.Mol 1-HEPTEN
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	112.22	4	-	4	3.29	14.99	Gen'd CH2=C(CH(CH3)-CH3)-CH(CH3)-CH3
C-2-BUTE	cis-2-Butene	56.11	2	7	3	13.22	(23.95)	Gen'd CH3-CH=CH-CH3
T-2-BUTE	trans-2-Butene	56.11	1	1	2,3	13.91	(23.95)	Gen'd CH3-CH=CH(CH3)
C4-OLE2	C4 Internal Alkenes	56.11	1			13.57	(23.95)	L.Mol 0.5 T-2-BUTE +0.5 C-2-BUTE
2M-2-BUT	2-Methyl-2-Butene	70.14	3	-	3	14.45	(23.95)	Gen'd CH3-C(CH3)=CH-CH3
C-2-PENT	cis-2-Pentene	70.14	3	-	3	10.24	(23.95)	Gen'd CH3-CH=CH-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
T-2-PENT	trans-2-Pentene	70.14	3	-	3	10.23	(23.95)	Gen'd	CH3-CH=CH(CH2-CH3)
2-C5-OLE	2-Pentenes	70.14	3			10.23	(23.95)	L.Mol	0.5 C-2-PENT +0.5 T-2-PENT
C5-OLE2	C5 Internal Alkenes	70.14	3			10.23	(23.95)	L.Mol	0.5 C-2-PENT +0.5 T-2-PENT
23M2-BUT	2,3-Dimethyl-2-Butene	84.16	3	-	3	13.32	(19.95)	Gen'd	CH3-C(CH3)=C(CH3)-CH3
2M-2-C5E	2-Methyl-2-Pentene	84.16	3	-	4	12.28	(19.95)	Gen'd	CH3-C(CH3)=CH-CH2-CH3
C-2-C6E	Cis-2-Hexene	84.16	3	-	4	8.44	(19.95)	Gen'd	CH3-CH=CH-CH2-CH2-CH3
C-3-C6E	Cis-3-Hexene	84.16	3	-	4	8.22	(19.95)	Gen'd	CH3-CH2-CH=CH-CH2-CH3
C3M2-C5E	Cis-3-Methyl-2-Hexene	84.16	3	-	4	13.38	(19.95)	Gen'd	CH3-CH=C(CH3)-CH2-CH3
T3M2-C5E	Trans 3-Methyl-2-Hexene	84.16	3	-	4	14.17	(19.95)	Gen'd	CH3-CH=C(CH3)-CH2-CH3
T4M2-C5E	Trans 4-Methyl-2-Hexene	84.16	3	-	4	7.88	(19.95)	Gen'd	CH3-CH(CH3)-CH=CH-CH3
T-2-C6E	Trans-2-Hexene	84.16	3	-	4	8.44	(19.95)	Gen'd	CH3-CH=CH(CH2-CH2-CH3)
T-3-C6E	Trans-3-Hexene	84.16	3	-	4	8.16	(19.95)	Gen'd	CH3-CH2-CH=CH(CH2-CH3)
2-C6-OLE	2-Hexenes	84.16	3			8.44	(19.95)	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
C6-OLE2	C6 Internal Alkenes	84.16	3			8.44	(19.95)	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
23M2-C5E	2,3-Dimethyl-2-Hexene	98.19	4	-	3	10.41	17.11	Gen'd	CH3-C(CH3)=C(CH3)-CH2-CH3
C-3-C7E	Cis-3-Heptene	98.19	4	-	4	6.96	17.11	Gen'd	CH3-CH2-CH=CH-CH2-CH2-CH3
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	98.19	4	-	4	6.99	17.11	Gen'd	CH3-C(CH3)(CH3)-CH=CH-CH3
T-2-C7E	Trans-2-Heptene	98.19	4	-	4	7.33	17.11	Gen'd	CH3-CH=CH(CH2-CH2-CH2-CH3)
T-3-C7E	Trans-3-Heptene	98.19	4	-	4	6.96	17.11	Gen'd	CH3-CH2-CH=CH(CH2-CH2-CH3)
2-C7-OLE	2-Heptenes	98.19	3			6.96	(17.11)	L.Mol	0.5 T-3-C7E +0.5 C-3-C7E
C7-OLE2	C7 Internal Alkenes	98.19	3			6.96	(17.11)	L.Mol	T-3-C7E
C-4-C8E	Cis-4-Octene	112.22	4	-	4	5.94	14.99	Gen'd	CH3-CH2-CH2-CH=CH-CH2-CH2-CH3
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	112.22	4	-	4	5.97	14.99	Gen'd	CH3-C(CH3)(CH3)-CH=CH(CH2-CH3)
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	112.22	4	-	4	5.44	14.99	Gen'd	CH3-CH(CH3)-CH=CH(CH(CH3)-CH3)
T-3-C8E	Trans-3-Octene	112.22	4	-	4	6.13	14.99	Gen'd	CH3-CH2-CH=CH(CH2-CH2-CH2-CH3)
T-4-C8E	Trans-4-Octene	112.22	4	-	4	5.90	14.99	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH3)
3-C8-OLE	3-Octenes	112.22	4			6.13	14.99	L.Mol	T-3-C8E
C8-OLE2	C8 Internal Alkenes	112.22	4			5.90	14.99	L.Mol	T-4-C8E
244M2C5E	2,4,4-trimethyl-2-Pentene	126.24	4	-	4	5.85	13.32	Gen'd	CH3-C(CH3)=CH-C(CH3)(CH3)-CH2-CH3
3-C9-OLE	3-Nonenes	126.24	4			5.31	13.31	L.Mol	T-4-C9E
C9-OLE2	C9 Internal Alkenes	126.24	4			5.31	13.31	L.Mol	T-4-C9E
T-4-C9E	Trans-4-Nonene	128.26	4	-	4	5.23	13.10	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH2-CH3)
34E2-C6E	3,4-Diethyl-2-Hexene	140.27	4	-	4	3.95	11.98	Gen'd	CH3-CH=C(CH2-CH3)-CH(CH2-CH3)-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
C-5-C10E	Cis-5-Decene	140.27	4	-	4	4.89	11.98	Gen'd	CH3-CH2-CH2-CH2-CH=CH-CH2-CH2-CH2-CH3
T-4-C10E	Trans-4-Decene	140.27	4	-	4	4.50	11.98	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH3)
3C10-OLE	C10 3-Alkenes	140.27	4			4.50	11.98	L.Mol	T-4-C10E
C10-OLE2	C10 Internal Alkenes	140.27	4			4.50	11.98	L.Mol	T-4-C10E
T-5-C11E	Trans-5-Undecene	154.30	4	-	4	4.23	10.88	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH3)
3C11-OLE	C11 3-Alkenes	154.30	4			4.23	10.88	L.Mol	T-5-C11E
C11-OLE2	C11 Internal Alkenes	154.30	4			4.23	10.88	L.Mol	T-5-C11E
2C12-OLE	C12 2-Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
3C12-OLE	C12 3-Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
C12-OLE2	C12 Internal Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
T-5-C12E	Trans-5-Dodecene	168.33	4	-	4	3.74	9.99	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH3)
T-5-C13E	Trans-5-Tridecene	182.35	4	-	4	3.38	9.21	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C13-OLE	C13 3-Alkenes	182.35	4			3.38	9.21	L.Mol	T-5-C13E
C13-OLE2	C13 Internal Alkenes	182.35	4			3.38	9.21	L.Mol	T-5-C13E
T-5-C14E	Trans-5-Tetradecene	196.38	4	-	4	3.08	8.56	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C14-OLE	C14 3-Alkenes	196.38	4			3.08	8.56	L.Mol	T-5-C14E
C14-OLE2	C14 Internal Alkenes	196.38	4			3.08	8.56	L.Mol	T-5-C14E
T-5-C15E	Trans-5-Pentadecene	210.41	4	-	4	2.82	7.97	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C15-OLE	C15 3-Alkenes	210.41	4			2.82	7.97	L.Mol	T-5-C15E
C15-OLE2	C15 Internal Alkenes	210.41	4			2.82	7.97	L.Mol	T-5-C15E
C4-OLE	C4 Alkenes	56.11	4b	-	6	11.93	23.92	L.Mol	0.5 1-BUTENE +0.25 T-2-BUTE +0.25 C-2-BUTE
C5-OLE	C5 Alkenes	70.14	4b	-	6	9.01	23.92	L.Mol	0.5 1-PENTEN +0.25 C-2-PENT +0.25 T-2-PENT
C6-OLE	C6 Alkenes	84.16	4b	-	6	6.88	19.95	L.Mol	0.5 1-HEPTEN +0.25 C-2-C6E +0.25 T-2-C6E
C7-OLE	C7 Alkenes	98.19	4b	-	6	5.76	17.11	L.Mol	0.5 1-HEPTEN +0.5 T-3-C7E
C8-OLE	C8 Alkenes	112.22	4b	-	6	4.68	14.99	L.Mol	0.5 1-OCTENE +0.5 T-4-C8E
C9-OLE	C9 Alkenes	126.24	4b	-	6	4.03	13.31	L.Mol	0.5 1-C9E +0.5 T-4-C9E
C10-OLE	C10 Alkenes	140.27	4b	-	6	3.39	11.98	L.Mol	0.5 1-C10E +0.5 T-4-C10E
C11-OLE	C11 Alkenes	154.30	4b	-	6	3.09	10.88	L.Mol	0.5 1-C11E +0.5 T-5-C11E
C12-OLE	C12 Alkenes	168.32	4b	-	6	2.73	9.99	L.Mol	0.5 1-C12E +0.5 T-5-C12E
C13-OLE	C13 Alkenes	182.35	4b	-	6	2.46	9.21	L.Mol	0.5 1-C13E +0.5 T-5-C13E
C14-OLE	C14 Alkenes	196.38	4b	-	6	2.28	8.56	L.Mol	0.5 1-C14E +0.5 T-5-C14E
C15-OLE	C15 Alkenes	210.41	4b	-	6	2.06	7.97	L.Mol	0.5 1-C15E +0.5 T-5-C15E
CYC-PNTE	Cyclopentene	68.12	4	-	4	7.38	24.66	Gen'd	*CH=CH-CH2-CH2-CH2-*
1M-CC5E	1-Methyl cyclopentene	82.15	4	-	4	13.95	20.45	Gen'd	*C(CH3)=CH-CH2-CH2-CH2-*
CYC-HEXE	Cyclohexene	82.15	4	-	4	5.45	20.44	Gen'd	*CH=CH-CH2-CH2-CH2-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1M-CC6E	1-Methyl Cyclohexene	96.17	4	-	4	7.81	17.47	Gen'd	*C(CH3)=CH-CH2-CH2-CH2-CH2-*
4M-CC6E	4-Methyl Cyclohexene	96.17	4	-	4	4.48	17.47	Gen'd	*CH(CH3)-CH2-CH=CH-CH2-CH2-*
12M-CC6E	1,2-Dimethyl Cyclohexene	110.20	4	-	4	6.77	15.26	Gen'd	*C(CH3)=C(CH3)-CH2-CH2-CH2-CH2-*
13-BUTDE	1,3-Butadiene	54.09	3	-	4	13.58	(24.85)	Gen'd	CH2=CH-CH=CH2
ISOPRENE	Isoprene	68.12	1	1	2,3,5	10.69	(24.66)	Gen'd	CH2=CH-C(CH3)=CH2
C6-OL2D	C6 Cyclic or di-olefins	82.15	5b	-	6,8	8.65	20.44	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
C7-OL2D	C7 Cyclic or di-olefins	96.18	5b	-	6,8	7.49	17.47	L.Mol	T-2-C7E
C8-OL2D	C8 Cyclic or di-olefins	110.20	5b	-	6,8	6.01	15.26	L.Mol	T-4-C8E
C9-OL2D	C9 Cyclic or di-olefins	124.23	5b	-	6,8	5.40	13.53	L.Mol	T-4-C9E
C10-OL2D	C10 Cyclic or di-olefins	138.26	5b	-	6,8	4.56	12.15	L.Mol	T-4-C10E
C11-OL2D	C11 Cyclic or di-olefins	152.29	5b	-	6,8	4.29	11.03	L.Mol	T-5-C11E
C12-OL2D	C12 Cyclic or di-olefins	166.31	5b	-	6,8	3.79	10.11	L.Mol	T-5-C12E
C13-OL2D	C13 Cyclic or di-olefins	180.34	5b	-	6,8	3.42	9.31	L.Mol	T-5-C13E
C14-OL2D	C14 Cyclic or di-olefins	194.37	5b	-	6,8	3.11	8.64	L.Mol	T-5-C14E
C15-OL2D	C15 Cyclic or di-olefins	208.39	5b	-	6,8	2.85	8.05	L.Mol	T-5-C15E
CYC-PNDE	Cyclopentadiene	66.10	5	-	8	7.61	25.42	L.Mol	CYC-PNTE
3-CARENE	3-Carene	136.24	2c	3	2,9	3.21	(12.33)	Trp	
A-PINENE	a-Pinene	136.24	2c	1	2,9	4.29	(12.33)	Trp	
B-PINENE	b-Pinene	136.24	3c	1a	2,9	3.28	(12.33)	Trp	
D-LIMONE	d-Limonene	136.24	2c	3	2,9	3.99	(12.33)	Trp	
SABINENE	Sabinene	136.24	2c	3	2,9	3.67	(12.33)	Trp	
TERPENE	Terpene	136.24	4b	-	10	3.79	12.33	L.Mol	0.4 A-PINENE +0.25 B-PINENE +0.1 D-LIMONE +0.15 3-CARENE +0.1 SABINENE
STYRENE	Styrene	104.15	2	1	11	1.95	(16.15)	Asn'd	
AME-STYR	a-Methyl Styrene	118.18	4	-	8	1.72	14.22	L.Mol	STYRENE
C9-STYR	C9 Styrenes	118.18	4	-	8	1.72	14.22	L.Mol	STYRENE
C10-STYR	C10 Styrenes	132.21	4	-	8	1.53	12.71	L.Mol	STYRENE
BENZENE	Benzene	78.11	3c	1a	2,9	0.81	(4.39)	Asn'd	
TOLUENE	Toluene	92.14	2c	1	2,9	3.97	(12.07)	Asn'd	
C2-BENZ	Ethyl Benzene	106.17	2c	1	2,9	2.79	(11.54)	Asn'd	
I-C3-BEN	Isopropyl Benzene (cumene)	120.20	3c	-	8	2.32	(9.74)	Asn'd	
N-C3-BEN	n-Propyl Benzene	120.20	3c	-	8	2.20	(9.34)	Asn'd	
C9-BEN1	C9 Monosub. Benzenes	120.20	3c	-	8	2.20	(9.34)	L.Mol	N-C3-BEN
S-C4-BEN	s-Butyl Benzene	134.22	3c	-	8	1.97	(8.37)	Asn'd	
C10-BEN1	C10 Monosub. Benzenes	134.22	3c	-	8	1.97	(8.37)	L.Mol	N-C3-BEN

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
N-C4-BEN	n-Butyl Benzene	134.22	3c	-	8	1.97	(8.37)	L.Mol N-C3-BEN
C11-BEN1	C11 Monosub. Benzenes	148.25	3c	-	8	1.78	(7.55)	L.Mol N-C3-BEN
C12-BEN1	C12 Monosub. Benzenes	162.28	3c	-	8	1.63	(6.92)	L.Mol N-C3-BEN
C13-BEN1	C13 Monosub. Benzenes	176.30	3c	-	8	1.50	(6.37)	L.Mol N-C3-BEN
M-XYLENE	m-Xylene	106.17	2c	1	2,9	10.61	(15.62)	Asn'd
O-XYLENE	o-Xylene	106.17	2c	1	2,9	7.49	(14.54)	Asn'd
P-XYLENE	p-Xylene	106.17	2c	1	2,9	4.25	(14.68)	Asn'd
C8-BEN2	C8 Disub. Benzenes	106.17	3b	6	6	5.16	(13.27)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C9-BEN2	C9 Disub. Benzenes	120.20	3b	-	6	6.61	(13.19)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C10-BEN2	C10 Disub. Benzenes	134.22	3b	-	6	5.92	(11.84)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C11-BEN2	C11 Disub. Benzenes	148.25	3b	-	6	5.35	(10.72)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C12-BEN2	C12 Disub. Benzenes	162.28	3b	-	6	4.90	(9.80)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C13-BEN2	C13 Disub. Benzenes	176.30	3b	-	6	4.50	(8.99)	L.Mol 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C8-BEN2	Isomers of Ethylbenzene	106.17	4b	-	6	5.16	13.27	L.Mol 0.17 M-XYLENE +0.17 O-XYLENE+0.17 P-XYLENE +0.49 C2-BENZ
123-TMB	1,2,3-Trimethyl Benzene	120.20	2c	2	2,9	11.26	(13.94)	Asn'd
124-TMB	1,2,4-Trimethyl Benzene	120.20	2c	2	2,9	7.18	(13.94)	Asn'd
135-TMB	1,3,5-Trimethyl Benzene	120.20	2c	2	2,9	11.22	(13.98)	Asn'd
C9-BEN	Isomers of Propylbenzene	120.20	4b	-	6	6.12	11.68	L.Mol 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C9-BEN3	C9 Trisub. Benzenes	120.20	3b	6	6	9.90	(13.94)	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C10-BEN	Isomers of Butylbenzene	134.22	4b	-	6	5.48	10.48	L.Mol 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C10-BEN4	C10 Tetrasub. Benzenes	134.22	4b	-	6	8.86	12.48	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C10-BEN3	C10 Trisub. Benzenes	134.22	3b	-	6	8.86	(12.48)	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN	Isomers of Pentylbenzene	148.25	4b	-	6	4.96	9.47	L.Mol 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C11-BEN5	C11 Pentasub. Benzenes	148.25	4b	-	6	8.03	11.33	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN4	C11 Tetrasub. Benzenes	148.25	4b	-	6	8.03	11.33	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN3	C11 Trisub. Benzenes	148.25	3b	-	6	8.03	(11.33)	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN	Isomers of Hexylbenzene	162.28	4b	-	6	4.53	8.66	L.Mol 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C12-BEN5	C11 Pentasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN6	C12 Hexaasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN4	C12 Tetrasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN3	C12 Trisub. Benzenes	162.28	3b	-	6	7.33	(10.33)	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C13-BEN3	C13 Trisub. Benzenes	176.30	3b	-	6	6.75	(9.52)	L.Mol 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
INDAN	Indan	118.18	5c	-	8	3.17	14.18	L.Mol TETRALIN
NAPHTHAL	Naphthalene	128.17	3c	3a,b	2,9	3.26	(12.85)	Asn'd
TETRALIN	Tetralin	132.21	3c	3a	2,9	2.83	(12.67)	Asn'd
ME-NAPH	Methyl Naphthalenes	142.20	3c	-a	9	4.61	(11.81)	Asn'd

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1ME-NAPH	1-Methyl Naphthalene	142.20	3c	-	9	4.61	(11.81)	L.Mol	ME-NAPH
2ME-NAPH	2-Methyl Naphthalene	142.20	3c,h	-	9	4.61	(11.81)	L.Mol	ME-NAPH
C11-TET	C11 Tetralin or Indane	146.24	5c	-	8	2.56	11.48	L.Mol	TETRALIN
23-DMN	2,3-Dimethyl Naphth.	156.23	3c	3	2,9	5.54	(10.77)	Asn'd	
C12-NAP2	C12 Disub. Naphthalenes	156.23	3c	-	8	5.54	(10.77)	L.Mol	23-DMN
DM-NAPH	Dimethyl Naphthalenes	156.23	3c	-	8	5.54	(10.77)	L.Mol	23-DMN
C12-NAP1	C12 Monosub. Naphth.	156.23	3c	-	8	4.20	(10.77)	L.Mol	ME-NAPH
C13-NAP2	C13 Disub. Naphthalenes	170.26	4c	-	8	5.08	9.86	L.Mol	23-DMN
C13-NAP3	C13 Trisub. Naphthalenes	170.26	4c	-	8	5.08	9.86	L.Mol	23-DMN
C13-NAP1	C13 Monosub. Naphth.	170.26	4c	-	8	3.86	9.86	L.Mol	ME-NAPH
ACETYLEN	Acetylene	26.04	2	1	2,3,5	1.25	(3.98)	Gen'd	HC::CH
ME-ACTYL	Methyl Acetylene	40.07	4	-	3	6.45	16.64	Gen'd	HC::C-CH3
2-BUTYNE	2-Butyne	54.09	4	-	3	16.33	24.67	Gen'd	CH3-C::C-CH3
ET-ACTYL	Ethyl Acetylene	54.09	4	-	4	6.20	19.13	Gen'd	HC::C-CH2-CH3
MEOH	Methanol	32.04	1	2	2,3	0.71	(1.65)	Gen'd	CH3-OH
ETOH	Ethanol	46.07	1	2	2,3	1.69	(6.40)	Gen'd	CH3-CH2-OH
I-C3-OH	Isopropyl Alcohol	60.10	1	1	2,3	0.71	(7.14)	Gen'd	CH3-CH(OH)-CH3
N-C3-OH	n-Propyl Alcohol	60.10	2	-	4	2.74	(7.36)	Gen'd	CH3-CH2-CH2-OH
I-C4-OH	Isobutyl Alcohol	74.12	3	-	4	2.24	(10.18)	Gen'd	CH3-CH(CH3)-CH2-OH
N-C4-OH	n-Butyl Alcohol	74.12	3	-	4	3.34	(7.95)	Gen'd	CH3-CH2-CH2-CH2-OH
S-C4-OH	s-Butyl Alcohol	74.12	3	-	3	1.60	(11.73)	Gen'd	CH3-CH(OH)-CH2-CH3
T-C4-OH	t-Butyl Alcohol	74.12	3	1a	2,3,5	0.45	(1.54)	Gen'd	CH3-C(CH3)(OH)-CH3
CC5-OH	Cyclopentanol	86.13	3	-	4	1.96	(7.75)	Gen'd	*CH(OH)-CH2-CH2-CH2-CH2-*
2-C5OH	2-Pentanol	88.15	3	-	4	1.74	(7.95)	Gen'd	CH3-CH(OH)-CH2-CH2-CH3
3-C5OH	3-Pentanol	88.15	3	-	3	1.73	(8.09)	Gen'd	CH3-CH2-CH(OH)-CH2-CH3
C5OH	Pentyl Alcohol	88.15	3	-	4	3.35	(7.71)	Gen'd	CH3-CH2-CH2-CH2-CH2-OH
CC6-OH	Cyclohexanol	100.16	3	-	4	2.25	(10.18)	Gen'd	*CH(OH)-CH2-CH2-CH2-CH2-CH2-*
1-C6OH	1-Hexanol	102.18	3	-	4	2.74	(7.05)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-OH
2-C6OH	2-Hexanol	102.18	3	-	4	2.46	(6.93)	Gen'd	CH3-CH(OH)-CH2-CH2-CH2-CH3
1-C7OH	1-Heptanol	116.20	3	-	4	2.21	(6.48)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-OH
1-C8-OH	1-Octanol	130.23	2	1	2,4	2.01	(6.72)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-OH
2-ETC6OH	2-Ethyl-1-Hexanol	130.23	3	-	4	2.20	(7.28)	Gen'd	CH3-CH2-CH(CH2-OH)-CH2-CH2-CH2-CH3
2-C8-OH	2-Octanol	130.23	2	1	2,4	2.16	(7.20)	Gen'd	CH3-CH(OH)-CH2-CH2-CH2-CH2-CH2-CH3
3-C8-OH	3-Octanol	130.23	2	1	2,4	2.57	(7.64)	Gen'd	CH3-CH2-CH(OH)-CH2-CH2-CH2-CH2-CH3
4-C8-OH	4-Octanol	130.23	3	-	4	3.07	(7.46)	Gen'd	CH3-CH2-CH2-CH(OH)-CH2-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	158.29	3	-	4	1.18	(6.25)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-OH
ET-GLYCL	Ethylene Glycol	62.07	2	-	3	3.36	(10.10)	Gen'd	HO-CH2-CH2-OH
PR-GLYCL	Propylene Glycol	76.10	1	1	2,4	2.75	(11.71)	Gen'd	CH3-CH(OH)-CH2-OH
12-C4OH2	1,2-Butandiol	90.12	2	-	4	2.21	(11.06)	Gen'd	CH3-CH2-CH(OH)-CH2-OH
GLYCERL	Glycerol	92.10	2	-	4	3.27	(10.93)	Gen'd	HO-CH2-CH(OH)-CH2-OH
C6-GLYCL	1,2-Dihydroxy Hexane	118.18	3	-	4	2.75	(8.77)	Gen'd	CH3-CH2-CH2-CH2-CH(OH)-CH2-OH
2M24C5OH	2-Methyl-2,4-Pentanediol	118.18	3	-	4	1.04	(5.63)	Gen'd	CH3-C(CH3)(OH)-CH2-CH(OH)-CH3
ME-O-ME	Dimethyl Ether	46.07	1	2	2,3	0.93	(5.96)	Gen'd	CH3-O-CH3
TME-OX	Trimethylene Oxide	58.08	3	-	4	5.22	(11.26)	Gen'd	*CH2-CH2-CH2-O-*
THF	Tetrahydrofuran	72.11	3	-	4	4.95	(11.16)	Gen'd	*CH2-CH2-CH2-CH2-O-*
ET-O-ET	Diethyl Ether	74.12	2	1	2,3	4.01	(9.92)	Gen'd	CH3-CH2-O-CH2-CH3
METHYLAL	Dimethoxy methane	76.10	1	-	4	1.04	(5.32)	Gen'd	CH3-O-CH2-O-CH3
AM-THF	Alpha-Methyltetrahydro-furan	86.13	3	-	4	4.62	(10.42)	Gen'd	*CH(CH3)-CH2-CH2-CH2-O-*
THP	Tetrahydropyran	86.13	3	-	4	3.81	(8.75)	Gen'd	*CH2-CH2-CH2-CH2-CH2-O-*
ET-O-IPR	Ethyl Isopropyl Ether	88.15	3	-	3	3.86	(12.42)	Gen'd	CH3-CH(CH3)-O-CH2-CH3
MNBE	Methyl n-Butyl Ether	88.15	3	-	4	3.66	(8.82)	Gen'd	CH3-CH2-CH2-CH2-O-CH3
MTBE	Methyl t-Butyl Ether	88.15	1	2	2,3,5	0.78	(3.05)	Gen'd	CH3-C(CH3)(CH3)-O-CH3
PR-O-PR	Di n-Propyl Ether	102.18	3	-	4	3.24	(8.29)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-CH3
ENBE	Ethyl n-Butyl Ether	102.18	3	-	4	3.86	(8.71)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH3
ETBE	Ethyl t-Butyl Ether	102.18	3	8	3	2.11	(5.86)	Gen'd	CH3-C(CH3)(CH3)-O-CH2-CH3
MTAE	Methyl t-Amyl Ether	102.18	3	-	3	2.14	(5.50)	Gen'd	CH3-CH2-C(CH3)(CH3)-O-CH3
2BU-THF	2-Butyl Tetrahydrofuran	128.22	3	-	4	2.53	(8.72)	Gen'd	*CH(CH2-CH2-CH2-CH3)-CH2-CH2-CH2-O-*
IBU2-O	Di-Isobutyl Ether	130.23	3	-	3	1.29	(7.25)	Gen'd	CH3-CH(CH3)-CH2-O-CH2-CH(CH3)-CH3
BU-O-BU	Di-n-butyl Ether	130.23	3	-	4	3.17	(7.46)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-CH2-CH3
C5-O-C5	Di-n-Pentyl Ether	158.29	3	-	4	2.64	(6.43)	Gen'd	CH3-CH2-CH2-CH2-CH2-O-CH2-CH2-CH2-CH2-CH3
MEO-ETOH	2-Methoxyethanol	76.10	3	-	4	2.98	(9.75)	Gen'd	CH3-O-CH2-CH2-OH
MEOC3OH	1-Methoxy-2-Propanol	90.12	1	1	2,4,5	2.62	(9.65)	Gen'd	CH3-CH(OH)-CH2-O-CH3
ETO-ETOH	2-Ethoxyethanol	90.12	2	2	2,4,5	3.78	(9.44)	Gen'd	CH3-CH2-O-CH2-CH2-OH
2MEOC3OH	2-Methoxy-1-Propanol	90.12	3	-	4	3.01	(12.23)	Gen'd	CH3-O-CH(CH3)-CH2-OH
ETOC3OH	1-Ethoxy-2-Propanol	104.15	3	-	4	3.25	(10.65)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH3
2PROETOH	2-Propoxyethanol	104.15	3	-	4	3.52	(10.53)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-OH
3ETOC3OH	3-Ethoxy-1-Propanol	104.15	3	-	4	4.24	(8.62)	Gen'd	CH3-CH2-O-CH2-CH2-CH2-OH
3MEOC4OH	3-Methoxy-1-Butanol	104.15	3	-	4	0.97	(8.83)	Gen'd	CH3-O-CH(CH3)-CH2-CH2-OH
DET-GLCL	Diethylene Glycol	106.12	3	-	4	3.55	(10.53)	Gen'd	HO-CH2-CH2-O-CH2-CH2-OH

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
PROXC3OH	1-Propoxy-2-Propanol	118.18	3	-	4	2.86	(8.24)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH2-CH3
BUO-ETOH	2-Butoxyethanol	118.18	1	1	2,4,5	2.90	(7.97)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-OH
3MOMC4OH	3 methoxy -3 methyl-Butanol	118.18	3	-	4	1.74	(6.46)	Gen'd	CH3-O-C(CH3)(CH3)-CH2-CH2-OH
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	120.15	3	-	4	2.90	(9.61)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-OH
PG-1TB-E	1-tert-Butoxy-2-Propanol	132.20	3	-	4	1.71	(7.83)	Gen'd	CH3-C(CH3)(CH3)-O-CH2-CH(OH)-CH3
PG-2TB-E	2-tert-Butoxy-1-Propanol	132.20	3	-	4	1.81	(8.29)	Gen'd	CH3-C(CH3)(CH3)-O-CH(CH3)-CH2-OH
BUOC3OH	n-Butoxy-2-Propanol	132.20	3	-	4	2.70	(8.59)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH2-CH2-CH3
CARBITOL	2-(2-Ethoxyethoxy) EtOH	134.18	2	2	2,4,5	3.19	(8.22)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-OH
DPR-GLCL	Dipropylene Glycol	134.18	3	-	4	2.48	(8.67)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH(OH)-CH3
EGHE	2-Hexyloxyethanol	146.23	3	-	3	2.45	(7.69)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-O-CH2-CH2-OH
DGPE	2-(2-Propoxyethoxy) ethanol	148.20	3	-	3	3.00	(8.00)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
DPRGOME	Dipropylene Glycol Methyl Ether	148.20	3	-	4	2.21	(8.07)	Gen'd	CH3-CH(OH)-CH2-O-CH(CH3)-CH2-O-CH3
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	162.23	3	-	4	2.70	(7.31)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	164.20	3	-	3	2.62	(7.31)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
EGEHE	2-(2-Ethylhexyloxy) ethanol	174.29	3	-	3	1.71	(6.58)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-O-CH2-CH2-OH
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	178.23	3	-	3	2.66	(6.77)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
DGHE	2-(2-Hexyloxyethoxy) ethanol	190.29	3	-	3	2.03	(6.28)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	192.26	3	-	3	2.46	(6.29)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	206.28	3	-	3	2.24	(5.86)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TPRGOME	Tripropylene Glycol Monomethyl Ether	206.28	3	-	4	1.90	(5.89)	Gen'd	CH3-CH(OH)-CH2-O-CH(CH3)-CH2-O-CH(CH3)-CH2-O-CH3
TETRAGME	2,5,8,11-Tetraoxatridecan-13-ol	208.26	3	-	3	2.15	(5.83)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TETRAGBE	3,6,9,12-Tetraoxahexadecan-1-ol	250.34	3	-	3	1.90	(4.86)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
ME-FORM	Methyl Formate	60.05	3	-	3	0.066	(0.46)	Gen'd	CH3-O-CHO

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
ET-FORM	Ethyl Formate	74.08	3	-	3	0.52	(1.92)	Gen'd CH3-CH2-O-CHO
ME-ACET	Methyl Acetate	74.08	1	1	2,3,5	0.073	(0.68)	Gen'd CH3-O-CO-CH3
ET-ACET	Ethyl Acetate	88.11	1	1	2,4,5	0.64	(2.46)	Gen'd CH3-CH2-O-CO-CH3
ME-PRAT	Methyl Propionate	88.11	3	-	4	0.71	(1.63)	Gen'd CH3-CH2-CO-O-CH3
C3-FORM	n-Propyl Formate	88.11	3	-	4	0.93	(3.51)	Gen'd CH3-CH2-CH2-O-CHO
ET-PRAT	Ethyl Propionate	102.13	3	-	4	0.79	(2.75)	Gen'd CH3-CH2-O-CO-CH2-CH3
IPR-ACET	Isopropyl Acetate	102.13	2	2	2,4	1.24	(4.09)	Gen'd CH3-CH(CH3)-O-CO-CH3
ME-BUAT	Methyl Butyrate	102.13	3	-	4	1.18	(3.74)	Gen'd CH3-CH2-CH2-CO-O-CH3
ME-IBUAT	Methyl Isobutyrate	102.13	2	1	2,4,5	0.70	(2.28)	Gen'd CH3-CH(CH3)-CO-O-CH3
C4-FORM	n-Butyl Formate	102.13	3	-	4	0.95	(3.81)	Gen'd CH3-CH2-CH2-CH2-O-CHO
PR-ACET	Propyl Acetate	102.13	3	-	4	0.87	(4.09)	Gen'd CH3-CH2-CH2-O-CO-CH3
ET-BUAT	Ethyl Butyrate	116.16	3	-	4	1.25	(4.84)	Gen'd CH3-CH2-CH2-CO-O-CH2-CH3
IBU-ACET	Isobutyl Acetate	116.16	3	-	3	0.67	(7.31)	Gen'd CH3-CH(CH3)-CH2-O-CO-CH3
ME-PVAT	Methyl Pivalate	116.16	2	1	2,3,5	0.41	(1.51)	Gen'd CH3-C(CH3)(CH3)-CO-O-CH3
BU-ACET	n-Butyl Acetate	116.16	2	1	2,4,5	0.89	(4.26)	Gen'd CH3-CH2-CH2-CH2-O-CO-CH3
PR-PRAT	n-Propyl Propionate	116.16	3	-	4	0.93	(4.12)	Gen'd CH3-CH2-CH2-O-CO-CH2-CH3
SBU-ACET	s-Butyl Acetate	116.16	3	-	3	1.43	(5.23)	Gen'd CH3-CH2-CH(CH3)-O-CO-CH3
TBU-ACET	t-Butyl Acetate	116.16	2	1	2,4,5	0.22	(0.53)	Gen'd CH3-C(CH3)(CH3)-O-CO-CH3
BU-PRAT	Butyl Propionate	130.19	3	-	4	0.89	(6.89)	Gen'd CH3-CH2-CH2-CH2-O-CO-CH2-CH3
AM-ACET	Amyl Acetate	130.19	3	-	4	0.96	(7.56)	Gen'd CH3-CH2-CH2-CH2-CH2-O-CO-CH3
PR-BUAT	n-Propyl Butyrate	130.19	3	-	4	1.17	(5.73)	Gen'd CH3-CH2-CH2-O-CO-CH2-CH2-CH3
23MC4ACT	2,3-Dimethylbutyl Acetate	144.22	3	-	3	0.84	(10.97)	Gen'd CH3-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
2MC5-ACT	2-Methylpentyl Acetate	144.22	3	-	3	1.11	(10.97)	Gen'd CH3-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
3MC5-ACT	3-Methylpentyl Acetate	144.22	3	-	3	1.31	(10.97)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
4MC5-ACT	4-Methylpentyl Acetate	144.22	3	-	3	0.92	(10.89)	Gen'd CH3-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
IBU-IBTR	Isobutyl Isobutyrate	144.22	3	-	3	0.64	(6.52)	Gen'd CH3-CH(CH3)-CH2-O-CO-CH(CH3)-CH3
BU-BUAT	n-Butyl Butyrate	144.22	3	-	4	1.12	(6.36)	Gen'd CH3-CH2-CH2-CH2-O-CO-CH2-CH2-CH3
NC6-ACET	n-Hexyl Acetate	144.22	3	-	3	0.87	(10.89)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
E3EOC3OH	Ethyl 3-Ethoxy Propionate	146.19	3	-	4	3.61	(10.07)	Gen'd CH3-CH2-O-CH2-CH2-CO-O-CH2-CH3
24MC5ACT	2,4-Dimethylpentyl Acetate	158.24	3	-	3	0.98	(10.24)	Gen'd CH3-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
2MC6-ACT	2-Methylhexyl Acetate	158.24	3	-	3	0.89	(10.24)	Gen'd CH3-CH2-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
3EC5-ACT	3-Ethylpentyl Acetate	158.24	3	-	3	1.24	(10.29)	Gen'd CH3-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
3MC6-ACT	3-Methylhexyl Acetate	158.24	3	-	3	1.01	(10.24)	Gen'd CH3-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
4MC6-ACT	4-Methylhexyl Acetate	158.24	3	-	3	0.91	(10.24)	Gen'd CH3-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC6-ACT	5-Methylhexyl Acetate	158.24	3	-	3	0.79	(10.21)	Gen'd CH3-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
IC5IBUAT	Isoamyl Isobutyrate	158.24	3	-	4	0.89	(6.63)	Gen'd CH3-CH(CH3)-CH2-CH2-O-CO-CH(CH3)-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
NC7-ACET	n-Heptyl Acetate	158.24	3	-	3	0.73	(10.21)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
24MC6ACT	2,4-Dimethylhexyl Acetate	172.27	3	-	3	0.93	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
2ETHXACT	2-Ethyl-Hexyl Acetate	172.27	3	-	4	0.79	(7.27)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-O-CO-CH3
34MC6ACT	3,4-Dimethylhexyl Acetate	172.27	3	-	3	1.16	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-O-CO-CH3
35MC6ACT	3,5-Dimethylhexyl Acetate	172.27	3	-	3	1.09	(9.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3EC6-ACT	3-Ethylhexyl Acetate	172.27	3	-	3	1.03	(9.59)	Gen'd	CH3-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
3MC7-ACT	3-Methylheptyl Aceate	172.27	3	-	3	0.76	(9.56)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
45MC6ACT	4,5-Dimethylhexyl Acetate	172.27	3	-	3	0.86	(9.56)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
4MC7-ACT	4-Methylheptyl Acetate	172.27	3	-	3	0.72	(9.56)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC7-ACT	5-Methylheptyl Aceate	172.27	3	-	3	0.73	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
NC8-ACET	n-Octyl Acetate	172.27	3	-	3	0.64	(9.53)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
235M6ACT	2,3,5-Teimethylhexyl Acetate	186.30	3	-	3	0.86	(8.93)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
23MC7ACT	2,3-Dimethylheptyl Acetate	186.30	3	-	3	0.84	(8.93)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
24MC7ACT	2,4-Dimethylheptyl Acetate	186.30	3	-	3	0.88	(8.93)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
25MC7ACT	2,5-Dimethylheptyl Acetate	186.30	3	-	3	0.86	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
2MC8-ACT	2-Methyloctyl Acetate	186.30	3	-	3	0.63	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
35MC7ACT	3,5-Dimethylheptyl Acetate	186.30	3	-	3	1.01	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
36MC7ACT	3,6-Dimethylheptyl Acetate	186.30	3	-	3	0.87	(8.90)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3EC7-ACT	3-Ethylheptyl Acetate	186.30	3	-	3	0.71	(8.93)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
45MC7ACT	4,5-Dimethylheptyl Acetate	186.30	3	-	3	0.96	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
46MC7ACT	4,6-Dimethylheptyl Acetate	186.30	3	-	3	0.83	(8.90)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
4MC8-ACT	4-Methyloctyl Acetate	186.30	3	-	3	0.68	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC8-ACT	5-Methyloctyl Acetate	186.30	3	-	3	0.67	(8.90)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
NC9-ACET	n-Nonyl Acetate	186.30	3	-	3	0.58	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
36MC8ACT	3,6-Dimethyloctyl Acetate	200.32	3	-	3	0.88	(8.34)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3IPC7ACT	3-Isopropylheptyl Acetate	200.32	3	-	3	0.71	(8.34)	Gen'd	CH3-CH2-CH2-CH2-CH(CH(CH3)-CH3)-CH2-CH2-O-CO-CH3
46MC8ACT	4,6-Dimethyloctyl Acetate	200.32	3	-	3	0.85	(8.34)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
357M8ACT	3,5,7-Trimethyloctyl Acetate	214.35	3	-	3	0.83	(7.80)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	214.35	3	-	3	0.80	(7.80)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
47MC9ACT	4,7-Dimethylnonyl Acetate	214.35	3	-	3	0.64	(7.80)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	228.38	3	-	3	0.74	(7.36)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
357M9ACT	3,5,7-Trimethylnonyl Acetate	228.38	3	-	3	0.76	(7.36)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
368M9ACT	3,6,8-Trimethylnonyl Acetate	228.38	3	-	3	0.72	(7.33)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	242.41	3	-	3	0.63	(6.92)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	242.41	3	-	3	0.76	(6.92)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
479M10AC	4,7,9-Trimethyldecyl Acetate	242.41	3	-	3	0.55	(6.92)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	256.43	3	-	3	0.74	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	256.43	3	-	3	0.58	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	256.43	3	-	3	0.77	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH2-CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
DMC	Dimethyl Carbonate	90.08	2	1	2,3	0.059	(0.53)	Gen'd	CH3-O-CO-O-CH3
PC	Propylene Carbonate	102.09	2	1	2,4,5	0.25	(0.96)	Gen'd	*CH(CH3)-CH2-O-CO-O-*
ME-LACT	Methyl Lactate	104.11	3	-	4	2.75	(3.38)	Gen'd	CH3-CH(OH)-CO-O-CH3
MCSVACET	2-Methoxyethyl Acetate	118.13	3	-	3	1.18	(11.07)	Gen'd	CH3-O-CH2-CH2-O-CO-CH3
ET-LACT	Ethyl Lactate	118.13	3	-	4	2.71	(3.96)	Gen'd	CH3-CH(OH)-CO-O-CH2-CH3
MIPR-CB	Methyl Isopropyl Carbonate	118.13	2	1	2,3,5	0.69	(2.78)	Gen'd	CH3-CH(CH3)-O-CO-O-CH3
PGME-ACT	1-Methoxy-2-Propyl Acetate	132.16	2	1	2,4	1.71	(8.09)	Gen'd	CH3-O-CH2-CH(CH3)-O-CO-CH3
CSV-ACET	2-Ethoxyethyl Acetate	132.16	3	-	4	1.90	(11.09)	Gen'd	CH3-CH2-O-CH2-CH2-O-CO-CH3
2PGMEACT	2-Methyoxy-1-propyl Acetate	132.16	3	-	3	1.12	(11.53)	Gen'd	CH3-O-CH(CH3)-CH2-O-CO-CH3
DBE-4	Dimethyl Succinate	146.14	3	1a	2,4,5	0.25	(1.40)	Gen'd	CH3-O-CO-CH2-CH2-CO-O-CH3
ETGLDACT	Ethylene Glycol Diacetate	146.14	3	-	3	0.72	(5.16)	Gen'd	CH3-CO-O-CH2-CH2-O-CO-CH3
DIPR-CB	Diisopropyl Carbonate	146.19	3	-	4	1.04	(7.15)	Gen'd	CH3-CH(CH3)-O-CO-O-CH(CH3)-CH3
DBE-5	Dimethyl Glutarate	160.17	3	1a	2,4,5	0.49	(2.66)	Gen'd	CH3-O-CO-CH2-CH2-CH2-CO-O-CH3
2BUETACT	2-Butoxyethyl Acetate	160.21	3	-	4	1.67	(9.59)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CO-CH3
DBE-6	Dimethyl Adipate	174.20	3	-	4	1.95	(4.76)	Gen'd	CH3-O-CO-CH2-CH2-CH2-CH2-CO-O-CH3
DGEEA	2-(2-Ethoxyethoxy) ethyl acetate	176.21	3	-	3	1.50	(9.41)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-O-CO-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
DGBEA	2-(2-Butoxyethoxy) ethyl acetate	204.27	3	-	3	1.38	(8.22)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CO-CH3
SC7ESC12	Substituted C7 ester (C12)	211.19	4	-	12	0.92	6.52	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
TEXANOL2	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	216.32	3	-	4	0.92	(6.10)	Gen'd	CH3-CH(CH3)-CO-O-CH(CH(CH3)-CH3)-C(CH3)(CH3)-CH2-OH
TEXANOL1	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	216.32	3	-	4	0.88	(6.50)	Gen'd	CH3-CH(CH3)-CH(OH)-C(CH3)(CH3)-CH2-O-CO-CH(CH3)-CH3
TEXANOL	Texanol isomers	216.32	3	-	13	0.89	(6.36)	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
SC9ESC12	Substituted C9 Ester (C12)	218.24	4	-	12	0.89	6.31	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
ETOX	Ethylene Oxide	44.05	3	-	3	0.045	(0.185)	Gen'd	*CH2-CH2-O-*
PROX	Propylene Oxide	58.08	3	-	3	0.32	(0.94)	Gen'd	*CH(CH3)-CH2-O-*
12BUOX	1,2-Epoxybutane	72.11	3	-	3	1.02	(2.56)	Gen'd	*CH(CH2-CH3)-CH2-O-*
FORMACID	Formic Acid	46.03	3	-	3	0.076	(0.58)	Gen'd	HCO-OH
ACETACID	Acetic Acid	60.05	3	-	4	0.71	(1.37)	Gen'd	CH3-CO-OH
ACYRACID	Acrylic Acid	72.06	5	-	4	11.66	13.97	Gen'd	CH2=CH-CO-OH
PROPACID	Propionic Acid	74.08	3	-	4	1.16	(1.58)	Gen'd	CH3-CH2-CO-OH
ME-ACRYL	Methyl Acrylate	86.09	5	-	4	12.24	15.61	Gen'd	CH2=CH-CO-O-CH3
VIN-ACET	Vinyl Acetate	86.09	5	-	4	3.26	15.61	Gen'd	CH2=CH-O-CO-CH3
MBUTENOL	2-Methyl-2-Butene-3-ol	86.13	3	-	4	4.12	(15.60)	Gen'd	CH2=CH-C(CH3)(OH)-CH3
ET-ACRYL	Ethyl Acrylate	100.11	5	-	4	8.78	16.78	Gen'd	CH2=CH-CO-O-CH2-CH3
ME-MACRT	Methyl Methacrylate	100.12	5	-	3	15.84	16.78	Gen'd	CH2=C(CH3)-CO-O-CH3
BU-MACRT	Butyl Methacrylate	142.20	5	-	3	9.09	11.83	Gen'd	CH2=C(CH3)-CO-O-CH2-CH2-CH2-CH3
IBUMACRT	Isobutyl Methacrylate	142.20	5	-	3	8.99	11.83	Gen'd	CH2=C(CH3)-CO-O-CH2-CH(CH3)-CH3
FURAN	Furan	68.08	4	3c	8	16.54	24.37	L.Mol	M-XYLENE
FORMALD	Formaldehyde	30.03	2a	1	1,2,14	8.97	(15.81)	Expl	
ACETALD	Acetaldehyde	44.05	1	1	1,2,14	6.84	(21.36)	Expl	
PROPALD	Propionaldehyde	58.08	2	7	14	7.89	(24.64)	Expl	
2MEC3AL	2-Methylpropanal	72.11	3	-	3	5.87	(26.57)	Gen'd	CH3-CH(CHO)-CH3
1C4RCHO	Butanal	72.11	3	-	4	6.74	(26.55)	Gen'd	CH3-CH2-CH2-CHO
C4-RCHO	C4 aldehydes	72.11	3			6.74	(26.55)	L.Mol	1C4RCHO
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	86.13	3	-	3	5.40	(22.24)	Gen'd	CH3-C(CH3)(CHO)-CH3
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	86.13	3	-	4	5.52	(22.26)	Gen'd	CH3-CH(CH3)-CH2-CHO

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1C5RCHO	Pentanal (Valeraldehyde)	86.13	3	-	4	5.76	(22.26)	Gen'd	CH3-CH2-CH2-CH2-CHO
C5-RCHO	C5 Aldehydes	86.14	3			5.76	(22.26)	L.Mol	1C5RCHO
GLTRALD	Glutaraldehyde	100.12	3	-	3	4.79	(19.18)	Gen'd	HCO-CH2-CH2-CH2-CHO
1C6RCHO	Hexanal	100.16	3	-	4	4.98	(19.18)	Gen'd	CH3-CH2-CH2-CH2-CH2-CHO
C6-RCHO	C6 Aldehydes	100.16	3			4.98	(19.18)	L.Mol	1C6RCHO
1C7RCHO	Heptanal	114.19	3	-	4	4.23	(16.80)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CHO
C7-RCHO	C7 Aldehydes	114.19	3			4.23	(16.80)	L.Mol	1C7RCHO
1C8RCHO	Octanal	128.22	3	-	4	3.65	(14.97)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CHO
C8-RCHO	C8 Aldehydes	128.22	3			3.65	(14.97)	L.Mol	1C8RCHO
GLYOXAL	Glyoxal	58.04	3	5	5,14	14.22	(16.54)	Expl	
MEGLYOX	Methyl Glyoxal	72.07	3	-	14	16.21	(19.98)	Expl	
ACROLEIN	Acrolein	56.06	3	3a	2,4,5	7.60	(25.69)	Gen'd	CH2=CH-CHO
CROTALD	Crotonaldehyde	70.09	3	-	4	10.07	(27.39)	Gen'd	CH3-CH=CH(CHO)
METHACRO	Methacrolein	70.09	1	3	2,5,14	6.23	(27.39)	Gen'd	CH2=C(CHO)-CH3
HOMACR	Hydroxy Methacrolein	86.09	3	-	4	6.61	(22.30)	Gen'd	CH2=C(CHO)-CH2-OH
BENZALD	Benzaldehyde	106.13	2			-0.61	(18.08)	Expl	
TOLUALD	Tolualdehyde	120.15	3			-0.54	(15.98)	L.Mol	BENZALD
ACETONE	Acetone	58.08	1			0.43	(8.28)	Expl	
CC4-KET	Cyclobutanone	70.09	4	-	3	0.68	11.40	Gen'd	*CH2-CH2-CH2-CO-*
MEK	Methyl Ethyl Ketone	72.11	1	1	2,3,5	1.49	(11.96)	Gen'd	CH3-CH2-CO-CH3
CC5-KET	Cyclopentanone	84.12	4	-	4	1.43	13.69	Gen'd	*CH2-CH2-CH2-CH2-CO-*
KET5C	C5 Cyclic Ketones	84.12	4b	-	8	1.43	13.69	L.Mol	CC5-KET
MPK	2-Pentanone	86.13	2	1	2,4,5	3.07	(15.69)	Gen'd	CH3-CH2-CH2-CO-CH3
DEK	3-Pentanone	86.13	3	-	4	1.45	(11.70)	Gen'd	CH3-CH2-CO-CH2-CH3
KET5	C5 Ketones	86.13	3	-	8	3.07	(15.69)	L.Mol	MPK
CC6-KET	Cyclohexanone	98.15	3	1a	2,4,5	1.61	(15.40)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CO-*
KET6C	C6 Cyclic Ketones	98.15	4b	-	8	1.61	15.40	L.Mol	CC6-KET
MIBK	4-Methyl-2-Pentanone	100.16	2	1	2,4,5	4.31	(18.17)	Gen'd	CH3-CH(CH3)-CH2-CO-CH3
MNBK	Methyl n-Butyl Ketone	100.16	3	-	4	3.55	(16.71)	Gen'd	CH3-CH2-CH2-CH2-CO-CH3
MTBK	Methyl t-Butyl Ketone	100.16	3	-	3	0.78	(8.66)	Gen'd	CH3-C(CH3)(CH3)-CO-CH3
KET6	C6 Ketones	100.16	3	-	8	3.55	(16.71)	L.Mol	MNBK
KET7C	C7 Cyclic Ketones	112.17	4b	-	8	1.41	13.48	L.Mol	CC6-KET
C7-KET-2	2-Heptanone	114.19	2	1	2,4,5	2.80	(15.48)	Gen'd	CH3-CH2-CH2-CH2-CH2-CO-CH3
2M-3-HXO	2-Methyl-3-Hexanone	114.19	3	-	4	1.79	(16.01)	Gen'd	CH3-CH(CH3)-CO-CH2-CH2-CH3
DIPK	Di-Isopropyl Ketone	114.19	3	-	4	1.63	(12.53)	Gen'd	CH3-CH(CH3)-CO-CH(CH3)-CH3
KET7	C7 Ketones	114.19	3	-	8	2.80	(15.48)	L.Mol	C7-KET-2

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
KET8C	C8 Cyclic Ketones	126.20	4b	-	8	1.25	11.99	L.Mol	CC6-KET
C8-KET-2	2-Octanone	128.22	3	-	4	1.66	(13.63)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CO-CH3
KET8	C8 Ketones	128.22	4	-	8	1.66	13.63	L.Mol	C8-KET-2
KET9C	C9 Cyclic Ketones	140.23	4b	-	8	1.13	10.78	L.Mol	CC6-KET
C9-KET-2	2-Nonanone	142.24	3	-	4	1.30	(12.51)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CO-CH3
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	142.24	3	-	4	2.94	(13.42)	Gen'd	CH3-CH(CH3)-CH2-CO-CH2-CH(CH3)-CH3
KET9	C9 Ketones	142.24	4	-	8	1.30	12.51	L.Mol	C9-KET-2
KET10C	C10 Cyclic Ketones	154.25	4b	-	8	1.02	9.80	L.Mol	CC6-KET
C10-K-2	2-Decanone	156.27	3	-	4	1.06	(11.55)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CO-CH3
KET10	C10 Ketones	156.27	4	-	8	1.06	11.55	L.Mol	C10-K-2
BIACETYL	Biacetyl	86.09	3	7	14	20.73	(22.30)	Expl	
MVK	Methylvinyl ketone	70.09	1	3	2,5,14	8.73	(27.39)	Gen'd	CH2=CH-CO-CH3
HOACET	Hydroxy Acetone	74.08	3	-	3	3.08	(11.78)	Gen'd	CH3-CO-CH2-OH
MEOACET	Methoxy Acetone	88.11	3	-	3	2.14	(17.48)	Gen'd	CH3-O-CH2-CO-CH3
DIACTALC	Diacetone Alcohol	116.16	3	9	4	0.68	(9.97)	Gen'd	CH3-C(CH3)(OH)-CH2-CO-CH3
PHENOL	Phenol	94.11	4	-	14	1.82	17.72	Expl	
CRESOL	Alkyl Phenols	108.14	3c	6	8	2.34	(15.54)	L.Mol	O-CRESOL
M-CRESOL	m-Cresol	108.14	3c	4a	8	2.34	(15.54)	L.Mol	O-CRESOL
P-CRESOL	p-Cresol	108.14	3c	4	8	2.34	(15.54)	L.Mol	O-CRESOL
O-CRESOL	o-Cresol	108.14	3c	4	2,5,14	2.34	(15.54)	Expl	
NO2-BENZ	Nitrobenzene	123.11	6c	-	8	0.067	0.37	Asn'd	
P-TI	Para Toluene Isocyanate	134.15	2c	1	2,9	0.93	(8.29)	Asn'd	
TDI	Toluene Diisocyanate	174.16	2c	1	2,9	-0.132	(7.17)	Asn'd	
MDI	Methylene Diphenylene Diisocyanate	250.26	3c	-	15	0.79	(5.96)	Asn'd	
DM-AMINE	Dimethyl Amine	45.09	6d	-	16	9.37	14.90	Asn'd	
ET-AMINE	Ethyl Amine	45.09	6d	8	16	7.80	14.80	Asn'd	
TM-AMINE	Trimethyl Amine	59.11	6d	8	16	7.06	17.05	Asn'd	
ME-NITRT	Methyl Nitrite	61.04	-	-	17			-	
ETOH-NH2	Ethanolamine	61.08	6d	-	16	5.97	10.97	Asn'd	
DMAE	Dimethylaminoethanol	89.14	6d	8	16	4.76	13.33	Asn'd	
ETOH2-NH	Diethanol Amine	105.14	6d	-	16	4.05	12.78	Asn'd	
ETOH3-N	Triethanolamine	149.19	6d	-	16	2.76	11.25	Asn'd	
ACRYLNIT	Acrylonitrile	53.06	-					-	
NMP	N-Methyl-2-Pyrrolidone	99.13	2	1	18	2.56	(16.66)	Asn'd	

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
CH3-CL	Methyl Chloride	50.49	6d			0.034	0.055	Asn'd	
CL-ETHE	Vinyl Chloride	62.50	6d			2.92	7.73	Asn'd	
C2-CL	Ethyl Chloride	64.52	6d			0.25	0.77	Asn'd	
CL2-ME	Dichloromethane	84.94	6d			0.066	0.104	Asn'd	
C4-CL	1-Chlorobutane	92.57	-					-	
ME-BR	Methyl Bromide	94.95	6d			0.0169	0.027	Asn'd	
11CL2-C2	1,1-Dichloroethane	98.97	6d			0.101	0.32	Asn'd	
12CL2-C2	1,2-Dichloroethane	99.00	6d			0.098	0.31	Asn'd	
C2-BR	Ethyl Bromide	108.97	6d			0.108	0.34	Asn'd	
12CL2-C3	1,2-Dichloropropane	112.99	-					-	
CHCL3	Chloroform	119.39	6d			0.034	0.054	Asn'd	
C3-BR	n-Propyl Bromide	123.00	6d	1a,d	2,19	0.35	1.59	Asn'd	
111-TCE	1,1,1-Trichloroethane	133.42	6d			0.0036	0.0114	Asn'd	
112CL3C2	1,1,2-Trichloroethane	133.42	6d			0.058	0.181	Asn'd	
C4-BR	n-Butyl Bromide	137.03	6d	1a,d	2,19	0.60	3.57	Asn'd	
3CLME-C8	3-(Chloromethyl)-Heptane	148.68	-					-	
CCL4	Carbon Tetrachloride	153.84	1					L.Mol	INERT
ME-BR2	Methylene Bromide	173.85	-					L.Mol	INERT
11BR2-C2	1,2-Dibromoethane	187.88	6d			0.046	0.146	Asn'd	
11CL2ETH	1,1-Dichloroethene	96.95	-					-	
T-12-DCE	Trans-1,2-Dichloroethene	96.95	6d	-	19	0.81	2.41	Asn'd	
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	125.00	6d	2a,d	19	1.13	10.72	Gen'd	CH2=C(CH2-Cl)-CH2-Cl
CL3-ETHE	Trichloroethylene	131.40	6d	1d	2,19	0.60	1.78	Asn'd	
CL4-ETHE	Perchloroethylene	165.85	6d	-	19	0.040	0.126	Asn'd	
CL-BEN	Monochlorobenzene	112.56	6d	-	9	0.36	1.97	Asn'd	
CF3-BEN	Benzotrifluoride	146.11	6d	-	9	0.26	0.93	Asn'd	
CL2-BEN	p-Dichlorobenzene	147.01	6d	-	9	0.20	1.11	Asn'd	
PCBTF	p-Trifluoromethyl-Cl-Benzene	180.56	6d	-	9	0.113	0.40	Asn'd	
CCL3NO2	Chloropicerin	164.38	-	-	20			-	
DMS	Dimethyl Sulfide	62.13	-					-	
DMSO	Dimethyl Sulfoxide	78.13	-	1e	21			-	
SI2OME6	Hexamethyldisiloxane	162.39	-e	1c	22			-	
SI2OMEOH	Hydroxymethyldisiloxane	164.36	-e	1c	22			-	
(SIOME)4	D4 Cyclosiloxane	296.64	-e	1c	22			-	
(SIOME)5	D5 Cyclosiloxane	370.80	-e	1c	22			-	

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
Mixtures									
ARBROG	Base ROG Mixture	14.44		0	23	3.71		Mix	See Table C-5a
RFA-TLEV	TLEV Exhaust -- RFA	14.04		0	24	4.09		Mix	See Table C-5a
PH2-TLEV	TLEV Exhaust -- Phase 2	14.12		0	24	4.05		Mix	See Table C-5a
LPG-TLEV	TLEV Exhaust -- LPG	14.86		0	24	2.11		Mix	See Table C-5a
CNG-TLEV	TLEV Exhaust -- CNG	15.22		0	24	0.75		Mix	See Table C-5a
E85-TLEV	TLEV Exhaust -- E-85	20.74		0	24	2.70		Mix	See Table C-5a
M85-TLEV	TLEV Exhaust -- M-85	27.45		0	24	1.57		Mix	See Table C-5a
RFA-LEV	Final LEV -- RFA	14.03		0	25	3.64		Mix	See Table C-5a
PH2-LEV	Final LEV -- Phase 2	14.22		0	25	3.55		Mix	See Table C-5a
MS-D	Mineral Spirits "D" (Type II-C)	14.08	3a	1	26	0.79		Mix	See Table C-5b
MS-A	Mineral Spirits "A" (Type I-B, 91% Alkanes)	14.10	3a	1	26	1.27		Mix	See Table C-5b
MS-B	Mineral Spirits "B" (Type II-C)	14.11	3a	1	26	0.78		Mix	See Table C-5b
MS-C	Mineral Spirits "C" (Type II-C)	14.12	3a	1	26	0.78		Mix	See Table C-5b
D95	Exxon Exxol(r) D95 Fluid	14.11	3a	1	27	0.67		Mix	See Table C-5b
ISOPARM	Exxon Isopar(r) M Fluid	14.15	3a	1a	27	0.65		Mix	See Table C-5b
OC6-ACET	Oxo-Hexyl Acetate	18.02	3	-	28	1.03		Mix	See Table C-5c
OC7-ACET	Oxo-Heptyl Acetate	17.58	3	-	28	0.97		Mix	See Table C-5c
OC8-ACET	Oxo-Octyl Acetate	17.23	3	-	28	0.96		Mix	See Table C-5c
OC9-ACET	Oxo-Nonyl Acetate	16.89	3a	-	28	0.85		Mix	See Table C-5c
OC10ACET	Oxo-Decyl Acetate	16.71	3a	1	28	0.83		Mix	See Table C-5c
OC12ACET	Oxo-Dodecyl Acetate	16.30	3a	-	28	0.72		Mix	See Table C-5c
OC13ACET	Oxo-Tridecyl Acetate	16.19	3a	-	28	0.67		Mix	See Table C-5c

[a] Uncertainty codes are given in Table C-2.

[b] Experimental data availability codes are given in Table C-3.

[c] Notes on representation of the detailed model species are given in Table C-4.

[d] Maximum incremental reactivity in units of grams O_3 per gram VOC.

[e] Upper limit maximum incremental reactivity in units of grams O_3 per gram VOC. Parentheses indicate that the MIR is not considered to be sufficiently uncertain that use of upper limit values are appropriate.

Table C-1 (continued)

[f] Representation in the mechanism: "Expl" = explicit in the base mechanism; "Asn'd" = mechanistic parameters assigned; "Gen'd" = mechanistic parameters generated using the mechanism generation system, using the structure shown; "L.Mol" = represented on a mole for mole basis by the model species or mixture shown; "-" = not represented in current version of the mechanism; "Mix" = mixture.

Table C-2 Uncertainty codes used in the listing of detailed model species.

No.	Description
-	No representation of this compound has been developed for this version of the mechanism.
0	Compound believed to be unreactive.
1	Considered to be relatively uncertain, or some uncertainties but reactivity is not expected to change significantly.
2	Uncertain mechanism may change somewhat if refined, but change is expected to be less than a factor of two. If the compound is predicted to inhibit O3, changes are not expected to affect predicted inhibition, but may affect magnitude of inhibition. This code is also used for compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
3	Uncertain and may change if compound is studied (or studied further) or estimation methods are updated. Change in MIR could be as much as a factor of two. This code is also used for (1) compounds whose reactivities are expected to be sensitive to the representation of the reactive products, whose accuracy is difficult to test experimentally and (2) compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
4	Uncertain and is expected to change if compound is studied or estimation methods are updated. It is recommended that uncertainty adjustments be employed in regulatory applications.
5	Non-negligible chance of the estimate being incorrect in significant respects. It is recommended that uncertainty adjustments be employed in regulatory applications.
6	Current mechanism is probably incorrect, but biases in atmospheric reactivity predictions are uncertain. It is recommended that uncertainty adjustments be employed in regulatory applications.
a	The reactivity of this compound is expected to be sensitive to ambient conditions and/or changes in the base mechanism.
b	Some uncertainty due to differences in reactivities of compounds represented by this class. Look at differences among compounds in this class for the magnitude of this uncertainty.
c	Parameterized mechanism used, with uncertain portions adjusted to fit chamber data for representative compounds.
d	Highly simplified "Placeholder" mechanism used to represent the approximate range of reactivity of this compound. Mechanism does not represent an estimate of the actual mechanism of the compound.
e	The current version of this mechanism does not represent these compounds, but based on previous studies they are expected to be O_3 inhibitors under all conditions.

Table C-3 Notes on availability of experimental data for evaluating mechanisms for the listed detailed model species.

No.	Description
-	No data available to test ozone predictions for this compound.
1	Tested under MIR and other conditions; well tested.
2	Tested under MIR conditions. There may be limited data for other conditions in some cases.
3	Tested under some conditions, but not MIR reactivity.
4	Tested under some conditions, but data are limited, or are of low quality or precision.
5	This compound has not been studied by itself, but its mechanism has been evaluated using experiments where it is formed as the major reactive product, for which model simulations are highly sensitive to assumed mechanisms for this compound.
6	Experimental data are available for some members of this class or for complex mixtures containing significant amounts of compounds of this class.
7	Chamber data may be available to test mechanisms for this compound, but were not used in this evaluation. Data are believed to be limited, of low precision, not well characterized or difficult to characterize, or highly sensitive to chamber effects.
8	There may be chamber data available to test mechanisms for this compound, but their availability and utility for mechanism evaluation have not been assessed.
9	Attempts to conduct chamber experiments with this compound have been unsuccessful because of experimental difficulties. Probably not possible to study this compound using current methods.
a	Model does not successfully simulate results of all chamber experiments. This may be due to experimental difficulties, though mechanism problems cannot be completely ruled out.
b	Reactivity of this compound may be sensitive to the nature of the light source, but data are available only from blacklight chambers. Effect of changing light source is uncertain and needs to be evaluated.
c.	The current version of the mechanism does not represent this compound or the available data were not used to evaluate how it is currently represented.
d	Although there are chamber data available for this compound and the model performance has been evaluated using them, the current mechanism does not represent halogen chemistry and the predictions of the mechanism may be inaccurate in ambient simulations.
e	Chamber data are available that will be used to develop a mechanism for this compound, which is not represented in the current version of the mechanism.

Table C-4. Notes and comments for the listed detailed model species.

No.	Documentation or Comment
1	Mechanism believed to be fairly well established. See Atkinson (1990, 1994, 1997a) reviews.
2	Evaluation of the mechanism for this compound against chamber data is discussed in this report. See Section V and Appendix B.
3	Mechanism was derived using the mechanism generation system discussed in Section III. Lumped product version of the mechanism used for all simulations.
4	Mechanism was derived using the mechanism generation system discussed in Section III. Adjusted product version of the mechanism used when representing this compound in reactivity or mechanism evaluation simulations, and the lumped product version of the mechanism is used when representing this compound in mixtures. See documentation of product lumping approaches.
5	Adjustments were made to mechanism to improve fits to chamber data.
6	It is uncertain whether the compound(s) used to represent this class is most appropriate for all complex mixtures containing this class.
7	The current mechanism gives reasonably good simulations of incremental reactivity experiments of mineral spirits samples believed to contain significant amounts of these compounds (Carter et al, 1997f). See Section V and Appendix B.
8	The appropriateness of the lumped molecule representation for this class is uncertain.
9	Parameterized mechanism used, with uncertain portions adjusted to fit chamber data for representative compounds. See Section IV.
10	Mixture based roughly on terpenes in estimated North American annual biogenic rates given by Guenther et al (2000).
11	An estimated mechanism was derived as discussed in Section IV.B.2.
12	These are present in relatively large amounts in emissions inventories. The specific compound(s) referred to in these classes are unknown. They are assumed to be similar to the Texanol isomers, though the molecular weights are slightly different.
13	Mixture composition for commercial Texanol samples based on information provided by David Morgott of Eastman Kodak Company (private communication, 1999).
14	The reactions of this compound is represented explicitly in the base mechanism. See Section II.C.
15	Mechanism for this compound estimated by analogy from para toluene isocyanate.
16	Mechanisms for amines have not been developed. A placeholder mechanism used to represent their approximate range of reactivity, given the OH rate constant. See Section IV.B.6
17	The reactions for this compound can be added to the mechanism if needed, but this has not been done for the current version of the mechanism.
18	An estimated mechanism was derived as discussed in Section IV.B.3.

Table C-4 (continued)

No.	Documentation or Comment
19	The current version of the mechanism does not provide for representing reactions of ClO_x or BrO_x species. However, earlier versions of the mechanism that did represent these reactions did not perform well simulating chamber data for most of the halogenated compounds that were studied (Carter et al, 1996d, 1997d). A placeholder mechanism is used to estimate the approximate MIR given the compound's OH rate constant. This mechanism probably overestimates the reactivity of these compounds under low NO_x conditions.
20	The current version of the mechanism does not provide for representing reactions of ClO_x species, and this compound is not currently represented. However, an earlier version of the mechanism that did represent these reactions gave reasonably good fits to the chamber data for this compound (Carter et al, 1997h).
21	An experimental and modeling study of the reactivity of this compound is underway at our laboratories.
22	Volatile silicone compounds are not represented in the current version of the mechanism. They have previously been shown to be ozone inhibitors under all conditions likely to occur in the atmosphere (Carter et al, 1992).
23	The Base ROG mixture is used to represent reactive VOCs from all sources in the atmospheric reactivity calculations, as discussed in Section VII.A.1. It is derived from the "all city average" mixture derived by Jeffries et al (1989) from analysis of air quality data, with minor modifications as discussed by Carter (1994a,b). The compositions of this mixture is given on Table C-5a.
24	These are the "Transitional Low Emissions Vehicle" exhaust mixtures used by the California ARB to calculate reactivity adjustment factors for its Clean Fuels, Low-Emissions Vehicle regulations. Composition obtained from the CARB. The compositions of these mixtures are given on Table C-5a.
25	These are "Low Emissions Vehicle" exhaust mixtures provided by the California ARB. The compositions of these mixtures are given on Table C-5a.
26	These are the mineral spirits samples provided by Safety-Kleen Corporation for environmental chamber reactivity studies (Carter et al, 1997f). Contrary to the earlier version of the mechanism discussed by in that report, the current mechanism performs reasonably well in simulating the chamber results for these samples (see Section V and Appendix B). The assumed compositions of these mixtures are given on Table C-5b.
27	These are commercial solvents produced by Exxon Chemical company. The assumed compositions of these solvents were derived as discussed by Carter et al (2000g), and are given in Table C-5b.
28	These represent commercial solvents produced by Exxon Chemical company, and also similar mixtures consisting of esters of C_{6+} branched alcohols. Their assumed compositions were derived as discussed by Carter et al (2000g), and are given in Table C-5e.
29	This was used in part to derive the mechanism for the ISO-PROD model species, as discussed in the documentation of the base mechanism.
30	This was used in part to derive the mechanism for the PROD2 model species, as discussed in the documentation of the base mechanism.

Table C-4 (continued)

No.	Documentation or Comment
31	This was used in part to derive the mechanism for the RNO3 model species, as discussed in the documentation of the base mechanism.

Table C-5. Compositions of mixtures for which model species have been assigned and reactivities have been estimated.

Table C-5a. Compositions of the ambient reactive organic gas (ROG) surrogate and exhaust mixtures.

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
ETHANE	1.69e-2	1.86e-2	1.45e-2	2.37e-3	4.00e-2	4.44e-1	1.13e-2	2.42e-2	1.98e-2
PROPANE	1.41e-2	1.05e-3	5.44e-4	1.24e-4	2.21e-1	1.72e-2	8.46e-4	1.08e-3	2.13e-3
N-C4	1.81e-2	1.07e-2	2.79e-3	4.44e-3	2.45e-3	1.62e-3	4.39e-3	1.24e-2	3.86e-3
N-C5	6.13e-3	5.21e-3	2.29e-3	1.41e-3	1.26e-3	5.06e-4	1.90e-3	5.91e-3	2.46e-3
N-C6	1.32e-3	2.98e-3	2.23e-3	6.05e-4	3.97e-4	1.77e-5	7.70e-4	4.12e-3	1.77e-3
N-C7	1.20e-3	1.81e-3	1.18e-3	2.19e-4	2.22e-4	6.07e-5	2.69e-4	1.93e-3	1.42e-3
N-C8	7.40e-4	6.14e-4	5.19e-4	2.40e-5	-	-	1.82e-5	8.72e-4	5.48e-4
N-C9	7.43e-4	1.75e-4	1.32e-4	-	-	-	-	2.73e-4	1.66e-4
N-C10	1.84e-3	5.92e-5	5.95e-5	-	-	-	-	7.89e-5	2.40e-4
N-C11	1.65e-4	6.29e-5	4.52e-5	1.76e-5	-	-	-	1.35e-4	3.64e-5
N-C12	3.26e-4	-	3.31e-5	-	-	-	-	-	-
N-C13	1.47e-5	-	-	-	-	-	-	-	-
2-ME-C3	7.88e-3	1.18e-3	-	9.45e-5	2.81e-3	7.07e-4	2.14e-4	-	-
2-ME-C4	1.52e-2	-	-	-	-	-	-	-	-
BR-C5	-	8.35e-3	-	2.21e-3	2.59e-3	8.23e-4	2.27e-3	-	-
22-DM-C4	4.62e-4	1.12e-3	-	1.59e-4	-	-	1.44e-4	-	-
23-DM-C4	9.55e-4	1.91e-3	-	1.27e-4	1.38e-4	-	-	-	-
2-ME-C5	3.55e-3	-	4.86e-3	-	-	-	-	8.28e-3	5.41e-3
3-ME-C5	2.53e-3	-	2.37e-3	-	-	-	-	4.07e-3	2.66e-3
BR-C6	2.39e-4	7.39e-3	-	1.24e-3	5.17e-4	5.30e-5	4.81e-4	-	-
223TM-C4	-	-	2.82e-5	-	-	-	-	-	-
23-DM-C5	1.12e-3	-	1.32e-3	-	-	-	-	-	4.11e-4
24-DM-C5	6.00e-4	-	7.89e-4	-	-	-	-	1.40e-5	2.41e-4
2-ME-C6	-	-	5.35e-4	-	-	-	-	-	1.13e-4
33-DM-C5	-	-	7.04e-5	-	-	-	-	-	-
3-ME-C6	1.27e-3	-	1.63e-3	-	-	-	-	2.10e-3	2.01e-3
BR-C7	2.09e-3	6.79e-3	5.55e-3	1.15e-3	1.16e-3	2.89e-4	8.90e-4	5.75e-3	9.36e-3
234TM-C5	-	-	1.36e-3	-	-	-	-	7.00e-4	1.41e-3
23-DM-C6	-	-	8.77e-4	-	-	-	-	6.26e-4	9.09e-4
24-DM-C6	-	-	4.57e-4	-	-	-	-	-	1.12e-4
25-DM-C6	-	-	3.21e-4	-	-	-	-	-	7.47e-5
2-ME-C7	-	-	2.84e-4	-	-	-	-	-	3.73e-5
3-ME-C7	-	-	3.83e-4	-	-	-	-	-	6.22e-5
4-ME-C7	-	-	1.11e-4	-	-	-	-	-	-
BR-C8	4.03e-3	7.25e-3	2.36e-3	1.30e-3	2.21e-4	7.99e-5	5.81e-4	3.28e-3	3.01e-3
225TM-C6	-	-	8.25e-4	-	-	-	-	6.12e-4	9.53e-4
24-DM-C7	-	-	5.50e-5	-	-	-	-	-	-
BR-C9	1.71e-3	8.54e-4	8.03e-4	1.71e-4	-	-	1.62e-5	7.11e-4	4.88e-4
BR-C10	1.56e-3	3.95e-5	1.98e-4	3.86e-5	-	-	-	3.94e-5	4.00e-5
BR-C11	1.65e-4	-	-	-	-	-	-	-	-
BR-C12	3.26e-4	-	-	-	-	-	-	-	-
BR-C13	1.47e-5	-	-	-	-	-	-	-	-
CYCC5	7.07e-4	1.80e-4	1.01e-4	3.13e-4	-	-	-	2.00e-5	-
CYCC6	6.84e-4	-	2.01e-4	-	-	-	-	3.17e-4	1.52e-4
CYC-C6	-	5.67e-4	-	-	-	-	1.23e-4	-	-
ME-CYCC5	1.61e-3	1.18e-3	1.02e-3	2.61e-4	4.24e-4	1.81e-5	3.20e-4	1.57e-3	8.11e-4
13DMCYC5	-	-	1.58e-4	-	-	-	-	-	1.45e-5
CYC-C7	1.23e-4	7.15e-5	-	-	-	-	-	-	4.34e-5
ME-CYCC6	6.82e-4	6.58e-4	6.18e-4	2.80e-5	1.51e-5	-	1.48e-4	8.71e-4	4.63e-4
CYC-C8	-	8.38e-4	9.43e-4	7.34e-5	1.32e-5	-	7.39e-5	1.12e-3	5.32e-4
ET-CYCC6	1.79e-4	-	7.55e-5	-	-	-	-	-	-
CYC-C10	-	1.80e-4	-	3.91e-5	2.12e-5	-	2.96e-5	-	-
ETHENE	1.35e-2	4.40e-2	3.08e-2	8.90e-3	3.45e-2	5.59e-3	3.59e-2	2.64e-2	2.76e-2
PROPENE	3.18e-3	1.02e-2	1.45e-2	2.87e-3	1.49e-2	7.23e-4	2.17e-3	8.40e-3	1.14e-2
1-BUTENE	1.15e-3	1.33e-3	1.43e-3	1.47e-4	6.35e-4	1.36e-4	3.70e-4	1.02e-3	9.63e-4
1-PENTEN	8.02e-4	2.80e-4	2.41e-4	-	-	-	-	-	-
3M-1-BUT	3.25e-4	2.00e-5	1.01e-4	-	-	-	-	-	-

Table C-5a (continued)

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
1-HEXENE	3.34e-4	3.34e-4	5.03e-5	-	-	-	-	-	-
C4-OLE1	1.43e-4	-	-	-	-	-	-	-	-
ISOBUTEN	1.15e-3	3.85e-3	1.15e-2	9.78e-4	7.41e-4	2.44e-4	8.87e-4	2.87e-3	1.00e-2
2M-1-BUT	9.17e-4	2.00e-5	3.02e-4	-	-	-	-	4.00e-5	6.08e-5
C5-OLE1	4.39e-4	-	-	-	-	-	-	-	-
C6-OLE1	2.23e-3	-	3.69e-4	-	-	-	-	5.33e-4	3.89e-4
C7-OLE1	1.19e-3	-	1.44e-5	1.12e-4	-	-	-	1.29e-4	7.24e-5
C8-OLE1	2.39e-4	1.10e-3	8.80e-5	1.96e-4	7.94e-5	4.07e-5	1.85e-4	-	-
C9-OLE1	5.20e-4	3.34e-5	1.68e-4	-	1.18e-5	-	-	8.89e-5	6.76e-5
C10-OLE1	9.55e-5	-	-	-	-	-	-	-	-
C11-OLE1	1.91e-4	-	-	-	-	-	-	-	-
C-2-BUTE	9.07e-4	-	4.28e-4	-	-	-	-	-	1.27e-4
C4-OLE2	1.43e-4	-	-	-	-	-	-	-	-
T-2-BUTE	1.15e-3	1.75e-4	2.26e-4	-	-	-	-	-	7.60e-5
2M-2-BUT	5.16e-4	1.60e-4	4.23e-4	7.83e-5	-	-	-	-	8.11e-5
C5-OLE2	3.17e-3	5.40e-4	4.23e-4	-	-	-	-	1.80e-4	2.03e-5
C6-OLE2	1.00e-3	5.34e-4	8.39e-4	-	-	-	-	8.83e-4	5.41e-4
C7-OLE2	4.37e-4	-	5.75e-5	-	-	-	-	-	-
C8-OLE2	2.15e-4	1.10e-3	1.01e-4	1.96e-4	7.94e-5	4.07e-5	1.85e-4	-	-
C9-OLE2	2.44e-4	3.34e-5	3.35e-5	-	1.18e-5	-	-	8.89e-5	6.76e-5
C10-OLE2	9.55e-5	-	-	-	-	-	-	-	-
C11-OLE2	1.91e-4	-	-	-	-	-	-	-	-
CYC-PNTE	-	4.53e-4	2.49e-4	2.42e-4	1.09e-4	-	-	4.12e-5	2.09e-5
CYC-HEXE	1.75e-4	5.13e-5	6.87e-5	-	-	-	-	-	-
13-BUTDE	6.21e-4	8.82e-4	1.28e-3	2.54e-4	1.37e-4	8.44e-5	2.68e-4	7.52e-4	8.15e-4
ISOPRENE	1.30e-3	1.24e-4	3.94e-4	-	-	-	-	-	6.26e-5
C7-OL2D	1.91e-4	-	-	-	-	-	-	-	-
A-PINENE	5.06e-4	-	-	-	-	-	-	-	-
3-CARENE	1.91e-4	-	-	-	-	-	-	-	-
STYRENE	-	5.66e-4	8.94e-4	1.05e-4	-	-	3.98e-5	7.81e-4	6.83e-4
C9-STYR	4.77e-4	-	-	-	-	-	-	-	-
C10-STYR	3.63e-4	-	-	-	-	-	-	-	-
BENZENE	3.29e-3	1.23e-2	6.52e-3	3.41e-3	7.80e-4	1.95e-5	1.49e-3	1.04e-2	7.88e-3
TOLUENE	9.23e-3	1.53e-2	1.24e-2	4.83e-3	1.37e-3	2.64e-4	1.96e-3	1.10e-2	1.28e-2
C2-BENZ	1.28e-3	3.75e-3	3.48e-3	1.01e-3	1.96e-4	7.17e-5	3.52e-4	3.57e-3	3.23e-3
C9-BEN1	1.59e-4	-	-	-	-	-	-	-	-
I-C3-BEN	1.91e-4	4.79e-4	1.88e-4	2.51e-4	-	-	1.73e-5	1.63e-4	1.42e-4
N-C3-BEN	3.61e-4	-	5.40e-4	-	-	-	-	5.60e-4	4.85e-4
C10-BEN1	1.81e-4	3.66e-5	-	2.05e-5	-	-	-	-	6.36e-5
S-C4-BEN	2.29e-4	-	1.05e-5	-	-	-	-	-	-
C11-BEN1	6.51e-4	-	1.90e-5	-	-	-	-	-	-
C12-BEN1	2.39e-5	-	-	-	-	-	-	-	-
M-XYLENE	2.18e-3	4.97e-3	3.54e-3	1.22e-3	4.76e-4	4.30e-5	6.44e-4	4.47e-3	3.17e-3
O-XYLENE	1.83e-3	3.15e-3	2.62e-3	8.79e-4	1.82e-4	2.87e-5	2.93e-4	3.54e-3	2.41e-3
P-XYLENE	2.18e-3	4.32e-3	3.54e-3	1.22e-3	4.76e-4	4.30e-5	6.44e-4	4.47e-3	3.17e-3
C9-BEN2	2.47e-3	2.80e-3	2.63e-3	7.31e-4	9.89e-5	-	2.93e-4	4.25e-3	2.74e-3
C10-BEN2	1.54e-3	5.75e-5	3.05e-4	4.09e-5	-	-	-	-	-
C11-BEN2	9.55e-5	-	3.81e-5	-	-	-	-	-	-
C12-BEN2	8.75e-5	-	-	-	-	-	-	-	-
123-TMB	7.53e-4	7.01e-5	2.35e-5	-	-	-	-	-	1.18e-5
124-TMB	-	2.22e-3	1.60e-3	5.71e-4	3.71e-5	-	2.59e-4	3.12e-3	1.17e-3
135-TMB	7.21e-4	6.54e-4	7.52e-4	2.28e-4	-	-	1.21e-4	1.21e-3	6.74e-4
C9-BEN3	2.36e-3	-	-	-	-	-	-	-	-
C10-BEN3	1.60e-3	-	1.16e-4	-	-	-	-	-	-
C10-BEN4	4.20e-4	-	6.31e-5	4.50e-4	-	-	-	-	1.06e-5
C11-BEN3	9.55e-5	-	-	-	-	-	-	-	-
C12-BEN3	8.75e-5	-	8.70e-6	-	-	-	-	-	-
INDAN	-	2.38e-5	2.39e-5	-	-	-	-	-	-
NAPHTHAL	-	2.19e-5	5.51e-5	6.42e-5	-	-	-	-	-
ACETYLEN	9.74e-3	1.71e-2	1.63e-2	3.79e-3	1.06e-2	9.35e-4	1.48e-2	1.04e-2	1.16e-2
ME-ACTYL	-	-	1.76e-4	-	-	-	-	-	-
ET-ACTYL	-	-	2.61e-4	-	-	-	-	-	-
MEOH	-	-	-	7.03e-1	-	-	-	-	-

Table C-5a (continued)

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
ETOH	-	-	-	-	-	-	3.28e-1	-	-
MTBE	-	-	2.03e-3	-	-	-	-	-	4.27e-3
FORMALD	7.92e-3	6.92e-3	7.66e-3	4.81e-2	1.48e-2	1.35e-2	1.25e-2	5.00e-3	9.04e-3
ACETALD	4.77e-3	3.09e-3	1.63e-3	1.31e-3	2.97e-3	1.59e-3	3.62e-2	1.88e-3	1.97e-3
PROPALD	7.00e-4	3.87e-4	2.43e-5	-	1.02e-4	-	2.50e-4	-	-
C4-RCHO	3.10e-4	5.84e-5	-	-	-	-	-	-	1.97e-5
C5-RCHO	1.07e-3	1.63e-5	-	-	-	-	-	-	-
C6-RCHO	7.32e-4	-	-	1.37e-4	-	-	-	-	-
ACROLEIN	-	4.51e-4	2.27e-4	9.79e-5	1.85e-4	-	1.11e-4	-	5.07e-5
CROTALD	-	8.01e-5	-	7.83e-5	-	-	-	-	-
BENZALD	1.64e-4	1.45e-4	2.93e-4	7.76e-5	-	-	-	1.32e-5	1.61e-4
ACETONE	3.09e-3	1.76e-3	1.09e-3	2.46e-3	2.15e-3	8.91e-4	1.86e-3	4.11e-4	7.59e-4
MEK	1.10e-3	1.36e-4	1.96e-5	3.81e-5	-	-	-	-	-

[a] ARBROG is ambient mixture used to represent the base ROG in the reactivity simulations, derived as discussed by Carter (1994a,b). The other mixtures are transitional low emissions vehicle (TLEV) or low emissions vehicle (LEV) compositions provided by the California Air Resources Board (Croes, personal communications, 1990-1991).

Table C-5b. Compositions of mineral spirits and solvent mixtures.

Model Name	Mixture Names and Compositions					
	MS-A [a]	MS-B [a]	MS-C [a]	MS-D [a]	D95 [b]	ISOPARM [b]
N-C8	2.47e-4	-	-	-	-	-
N-C9	2.59e-3	-	-	-	-	-
N-C10	7.04e-3	-	-	-	-	-
N-C11	7.46e-3	-	1.06e-2	1.29e-2	-	9.07e-7
N-C12	2.61e-3	1.22e-3	1.13e-2	7.87e-3	8.06e-4	1.27e-5
N-C13	1.77e-4	1.07e-3	4.04e-4	1.63e-4	6.33e-3	3.41e-5
N-C14	-	1.22e-3	-	-	9.19e-3	7.07e-5
N-C15	-	-	-	-	1.02e-3	2.16e-5
N-C16	-	-	-	-	-	5.01e-6
24-DM-C6	4.93e-5	-	-	-	-	-
2-ME-C7	2.47e-5	-	-	-	-	-
4-ME-C7	2.47e-5	-	-	-	-	-
24-DM-C7	6.04e-4	-	-	-	-	-
2-ME-C8	3.02e-4	-	-	-	-	-
4-ME-C8	3.02e-4	-	-	-	-	-
26DM-C8	3.90e-3	1.73e-4	-	-	-	-
2-ME-C9	1.95e-3	8.67e-5	-	-	-	-
4-ME-C9	1.95e-3	8.67e-5	-	-	-	-
26DM-C9	4.29e-3	1.88e-3	1.07e-3	1.50e-3	-	1.90e-4
3-ME-C10	2.14e-3	9.39e-4	5.37e-4	7.52e-4	-	9.51e-5
4-ME-C10	2.14e-3	9.39e-4	5.37e-4	7.52e-4	-	9.51e-5
36DM-C10	3.42e-3	4.63e-3	5.51e-3	8.72e-3	5.74e-4	2.65e-3
3-ME-C11	1.71e-3	2.31e-3	2.75e-3	4.36e-3	2.87e-4	1.33e-3
5-ME-C11	1.71e-3	2.31e-3	2.75e-3	4.36e-3	2.87e-4	1.33e-3
36DM-C11	8.63e-4	6.77e-3	2.68e-3	2.12e-3	4.51e-3	7.16e-3
3-ME-C12	4.32e-4	3.38e-3	1.34e-3	1.06e-3	2.25e-3	3.58e-3
5-ME-C12	4.32e-4	3.38e-3	1.34e-3	1.06e-3	2.25e-3	3.58e-3
37DM-C12	3.58e-5	2.74e-3	-	-	6.54e-3	1.48e-2
3-ME-C13	1.79e-5	1.37e-3	-	-	3.27e-3	7.42e-3
6-ME-C13	1.79e-5	1.37e-3	-	-	3.27e-3	7.42e-3
37DM-C13	-	4.41e-4	-	-	7.28e-4	4.53e-3
3-ME-C14	-	2.21e-4	-	-	3.64e-4	2.27e-3
6-ME-C14	-	2.21e-4	-	-	3.64e-4	2.27e-3
3-ME-C15	-	-	-	-	-	5.25e-4
48DM-C14	-	-	-	-	-	1.05e-3
7-ME-C15	-	-	-	-	-	5.25e-4
ME-CYCC6	1.86e-5	-	-	-	-	-
ET-CYCC6	5.27e-5	-	-	-	-	-
1E4MCYC6	1.11e-3	-	-	-	-	-
C3-CYCC6	1.11e-3	-	-	-	-	-
14DECYC6	3.46e-3	9.00e-4	-	-	-	-
1M3IPCY6	3.46e-3	9.00e-4	-	-	-	-
C4-CYCC6	3.57e-3	9.27e-4	-	-	-	-
13E5MCC6	5.22e-3	3.32e-3	3.79e-3	4.05e-3	-	2.38e-5
1E2PCYC6	5.22e-3	3.32e-3	3.79e-3	4.05e-3	-	2.38e-5
C5-CYCC6	5.37e-3	3.42e-3	3.90e-3	4.17e-3	-	2.45e-5
135ECYC6	2.73e-3	5.33e-3	8.65e-3	7.56e-3	4.82e-4	3.32e-4
1M4C5CY6	2.73e-3	5.33e-3	8.65e-3	7.56e-3	4.82e-4	3.32e-4
C6-CYCC6	2.82e-3	5.49e-3	8.91e-3	7.79e-3	4.97e-4	3.42e-4
13E5PCC6	3.28e-4	3.67e-3	1.96e-3	1.36e-3	3.79e-3	8.96e-4
1M2C6CC6	3.28e-4	3.67e-3	1.96e-3	1.36e-3	3.79e-3	8.96e-4
C7-CYCC6	3.38e-4	3.78e-3	2.02e-3	1.40e-3	3.91e-3	9.23e-4
13P5ECC6	-	1.20e-3	-	-	5.50e-3	1.86e-3
1M4C7CC6	-	1.20e-3	-	-	5.50e-3	1.86e-3
C8-CYCC6	-	1.23e-3	-	-	5.67e-3	1.91e-3
135PCYC6	-	1.30e-4	-	-	6.12e-4	5.67e-4
1M2C8CC6	-	1.30e-4	-	-	6.12e-4	5.67e-4
C9-CYCC6	-	1.34e-4	-	-	6.31e-4	5.84e-4
13P5BCC6	-	-	-	-	-	1.31e-4
1M4C9CY6	-	-	-	-	-	1.31e-4
C10CYCC6	-	-	-	-	-	1.35e-4
1-OCTENE	2.51e-6	-	-	-	-	-

Table C-5b (continued)

Model Name	Mixture Names and Compositions					
	MS-A [a]	MS-B [a]	MS-C [a]	MS-D [a]	D95 [b]	ISOPARM [b]
1-C9E	9.37e-5	-	-	-	-	-
1-C10E	4.42e-4	-	-	-	-	-
1-C11E	6.65e-4	-	-	-	-	-
1-C12E	3.49e-4	-	-	-	-	-
1-C13E	4.17e-5	-	-	-	-	-
T-4-C9E	2.34e-5	-	-	-	-	-
T-4-C10E	1.10e-4	-	-	-	-	-
T-5-C11E	1.66e-4	-	-	-	-	-
T-5-C12E	8.70e-5	-	-	-	-	-
T-5-C13E	1.08e-5	-	-	-	-	-
TOLUENE	1.88e-4	-	-	-	-	-
I-C3-BEN	2.34e-5	-	-	-	-	-
N-C3-BEN	2.76e-4	-	-	-	-	-
M-XYLENE	5.80e-4	-	-	-	-	-
O-XYLENE	6.41e-4	-	-	-	-	-
P-XYLENE	5.67e-4	-	-	-	-	-
123-TMB	1.27e-3	-	-	-	-	-
124-TMB	1.27e-3	-	-	-	-	-
135-TMB	1.31e-3	-	-	-	-	-
NAPHTHAL	2.14e-4	-	-	-	-	-
INERT	1.67e-3	-	-	-	-	-

[a] See Carter et al (1997f) for a discussion of how these compositions were derived.

[b] See Carter et al (2000g) for a discussion of how these compositions were derived.

Table C-5c. Compositions of iso-acetate solvents.

Model Name	Mixture Names and Compositions [a]						
	OC6-ACET	OC7-ACET	OC8-ACET	OC9-ACET	OC10ACET	OC12ACET	OC13ACET
NC6-ACET	4.62e-2	5.57e-3	-	-	-	-	-
2MC5-ACT	2.37e-2	-	-	-	-	-	-
3MC5-ACT	2.87e-2	5.57e-3	-	-	-	-	-
4MC5-ACT	2.12e-2	-	-	-	-	-	-
23MC4ACT	1.87e-3	-	-	-	-	-	-
2MC6-ACT	-	8.18e-3	-	-	-	-	-
3MC6-ACT	-	1.52e-2	-	-	-	-	-
4MC6-ACT	2.85e-3	2.71e-2	3.81e-3	-	-	-	-
5MC6-ACT	-	8.18e-3	-	-	-	-	-
24MC5ACT	-	1.69e-2	-	-	-	-	-
3EC5-ACT	-	5.08e-3	-	-	-	-	-
NC7-ACET	-	7.33e-3	-	-	-	-	-
34MC6ACT	-	1.19e-2	2.00e-2	3.43e-3	7.76e-4	-	-
35MC6ACT	-	-	1.75e-2	-	-	-	-
3EC6-ACT	-	-	1.35e-2	-	-	-	-
4MC7-ACT	-	-	9.75e-3	-	-	-	-
45MC6ACT	-	-	9.75e-3	-	-	-	-
5MC7-ACT	-	-	8.00e-3	-	-	-	-
3MC7-ACT	-	-	7.00e-3	-	-	-	-
24MC6ACT	-	-	7.00e-3	-	-	-	-
NC8-ACET	-	-	1.50e-3	-	-	-	-
36MC7ACT	-	-	-	5.21e-3	-	-	-
35MC7ACT	-	-	2.31e-3	1.86e-2	3.05e-3	-	-
45MC7ACT	-	-	-	5.21e-3	3.05e-3	-	-
46MC7ACT	-	-	-	5.21e-3	-	-	-
24MC7ACT	-	-	-	1.81e-3	-	-	-
2MC8-ACT	-	-	-	1.81e-3	-	-	-
4MC8-ACT	-	-	-	8.39e-3	-	-	-
5MC8-ACT	-	-	-	8.39e-3	-	-	-
3EC7-ACT	-	-	-	5.21e-3	-	-	-
23MC7ACT	-	-	-	1.36e-3	-	-	-
25MC7ACT	-	-	-	3.40e-3	-	-	-
235M6ACT	-	-	-	3.40e-3	-	-	-
NC9-ACET	-	-	-	4.53e-4	-	-	-
36MC8ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
46MC8ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
3IPC7ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
357M8ACT	-	-	-	-	2.49e-3	3.55e-3	2.52e-4
47MC9ACT	-	-	-	-	-	3.55e-3	2.52e-4
3E6M8ACT	-	-	-	-	-	3.55e-3	2.52e-4
368M9ACT	-	-	-	-	-	1.38e-2	4.96e-3
357M9ACT	-	-	-	-	-	1.38e-2	4.96e-3
2357M8AC	-	-	-	-	-	1.38e-2	4.96e-3
2468M8AC	-	-	-	-	-	5.38e-3	1.56e-2
479M10AC	-	-	-	-	-	5.38e-3	1.56e-2
3E67M9AC	-	-	-	-	-	5.38e-3	1.56e-2
3579M10A	-	-	-	-	-	4.24e-4	1.47e-3
5E368M9A	-	-	-	-	-	4.24e-4	1.47e-3
23568M9A	-	-	-	-	-	4.24e-4	1.47e-3

[a] See Carter et al (2000g) for a discussion of how these compositions were derived.

Table C-6. Summary of calculated incremental and relative reactivities in various scales.

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
ARBROG	Base ROG Mixture	3.71	0.63	17%	3.79	2%	1.46	0.28	19%	0.85	0.25	30%	1.00	2.07	0.25	0.41	41%	1.00	1.62	0.40	0.31	31%
CO	Carbon Monoxide	0.06	0.01	21%	0.06	2%	0.04	0.01	20%	0.03	0.01	25%	0.03	0.07	0.01	0.01	34%	0.02	0.04	0.01	0.01	28%
METHANE	Methane	0.01	0.00	20%	0.01	1%	0.01	0.00	19%	0.01	0.00	25%	0.01	0.01	0.00	0.00	30%	0.01	0.01	0.00	0.00	23%
ETHANE	Ethane	0.31	0.08	26%	0.31	1%	0.20	0.06	29%	0.15	0.05	34%	0.16	0.28	0.05	0.04	28%	0.10	0.15	0.04	0.02	23%
PROPANE	Propane	0.56	0.14	24%	0.56	1%	0.36	0.09	26%	0.26	0.08	31%	0.29	0.51	0.10	0.08	27%	0.19	0.27	0.09	0.04	22%
N-C4	n-Butane	1.33	0.34	25%	1.34	1%	0.83	0.24	29%	0.58	0.20	34%	0.64	1.03	0.22	0.15	24%	0.40	0.56	0.19	0.08	20%
N-C5	n-Pentane	1.54	0.40	26%	1.55	1%	0.95	0.28	29%	0.65	0.23	36%	0.70	0.99	0.25	0.16	22%	0.44	0.59	0.22	0.08	18%
N-C6	n-Hexane	1.45	0.40	28%	1.44	0%	0.93	0.30	32%	0.60	0.24	39%	0.63	0.84	0.21	0.15	24%	0.38	0.56	0.17	0.07	20%
N-C7	n-Heptane	1.28	0.38	29%	1.27	0%	0.82	0.28	35%	0.51	0.23	45%	0.51	0.74	0.07	0.16	30%	0.28	0.46	0.05	0.08	29%
N-C8	n-Octane	1.11	0.35	32%	1.11	0%	0.71	0.27	38%	0.42	0.22	52%	0.40	0.64	-0.13	0.17	43%	0.19	0.38	-0.11	0.10	52%
N-C9	n-Nonane	0.95	0.32	34%	0.95	0%	0.61	0.26	42%	0.34	0.21	60%	0.31	0.56	-0.27	0.19	60%	0.12	0.29	-0.23	0.12	98%
N-C10	n-Decane	0.83	0.30	36%	0.82	-1%	0.54	0.24	44%	0.29	0.19	68%	0.25	0.49	-0.36	0.19	78%	0.06	0.23	-0.30	0.12	193%
N-C11	n-Undecane	0.74	0.28	38%	0.73	-1%	0.48	0.23	48%	0.25	0.19	75%	0.21	0.45	-0.45	0.20	98%	0.03	0.20	-0.36	0.13	-
N-C12	n-Dodecane	0.66	0.26	40%	0.66	1%	0.43	0.21	49%	0.22	0.18	80%	0.18	0.41	-0.42	0.19	106%	0.01	0.18	-0.38	0.13	-
N-C13	n-Tridecane	0.62	0.26	42%	0.61	-1%	0.41	0.20	50%	0.21	0.17	82%	0.17	0.40	-0.48	0.19	115%	-0.01	0.16	-0.38	0.13	-
N-C14	n-Tetradecane	0.58	0.25	43%	0.57	-2%	0.38	0.19	51%	0.20	0.17	83%	0.16	0.38	-0.48	0.18	117%	-0.02	0.15	-0.38	0.13	-
N-C15	n-Pentadecane	0.56	0.25	44%	0.56	0%	0.37	0.19	52%	0.20	0.16	81%	0.16	0.37	-0.43	0.18	114%	-0.02	0.15	-0.40	0.13	-
N-C16	n-C16	0.52	0.24	46%	0.51	-2%	0.35	0.18	52%	0.18	0.15	84%	0.14	0.35	-0.44	0.17	120%	-0.03	0.14	-0.37	0.13	-
N-C17	n-C17	0.49	0.23	46%	0.48	-2%	0.33	0.17	52%	0.17	0.14	84%	0.13	0.33	-0.42	0.16	120%	-0.03	0.13	-0.35	0.12	-
N-C18	n-C18	0.46	0.21	46%	0.45	-2%	0.31	0.16	52%	0.16	0.14	84%	0.13	0.31	-0.39	0.15	120%	-0.03	0.13	-0.33	0.11	-
N-C19	n-C19	0.44	0.20	46%	0.43	-2%	0.29	0.15	52%	0.16	0.13	83%	0.12	0.30	-0.37	0.14	120%	-0.03	0.12	-0.31	0.11	-
N-C20	n-C20	0.42	0.19	46%	0.41	-2%	0.28	0.15	52%	0.15	0.12	84%	0.11	0.28	-0.35	0.14	120%	-0.02	0.11	-0.30	0.10	-
N-C21	n-C21	0.40	0.18	46%	0.39	-2%	0.26	0.14	52%	0.14	0.12	84%	0.11	0.27	-0.34	0.13	120%	-0.02	0.11	-0.29	0.10	-
N-C22	n-C22	0.38	0.18	46%	0.37	-2%	0.25	0.13	52%	0.13	0.11	84%	0.10	0.26	-0.32	0.12	120%	-0.02	0.10	-0.27	0.09	-
2-ME-C3	Isobutane	1.35	0.27	20%	1.36	1%	0.80	0.16	20%	0.57	0.14	25%	0.65	1.22	0.26	0.17	26%	0.48	0.71	0.24	0.10	21%
2-ME-C4	Iso-Pentane	1.68	0.39	23%	1.68	0%	1.02	0.26	26%	0.72	0.22	31%	0.80	1.33	0.30	0.19	23%	0.52	0.74	0.27	0.10	19%
22-DM-C3	Neopentane	0.69	0.14	20%	0.71	1%	0.42	0.08	20%	0.29	0.07	25%	0.34	0.62	0.14	0.09	27%	0.24	0.36	0.13	0.05	21%
BR-C5	Branched C5 Alkanes	1.68	0.39	23%	1.68	0%	1.02	0.26	26%	0.72	0.22	31%	0.80	1.33	0.30	0.19	23%	0.52	0.74	0.27	0.10	19%
22-DM-C4	2,2-Dimethyl Butane	1.33	0.31	23%	1.34	1%	0.80	0.20	25%	0.55	0.17	31%	0.61	0.98	0.24	0.13	21%	0.40	0.53	0.21	0.07	17%
23-DM-C4	2,3-Dimethyl Butane	1.14	0.24	21%	1.15	1%	0.69	0.15	21%	0.48	0.13	27%	0.53	0.92	0.21	0.13	24%	0.40	0.58	0.20	0.08	20%
2-ME-C5	2-Methyl Pentane	1.80	0.44	25%	1.82	1%	1.03	0.30	29%	0.68	0.25	36%	0.74	1.00	0.32	0.15	20%	0.47	0.62	0.28	0.07	15%
3-ME-C5	3-Methylpentane	2.07	0.50	24%	2.10	1%	1.21	0.33	27%	0.83	0.28	34%	0.91	1.37	0.37	0.19	21%	0.58	0.78	0.32	0.10	17%
BR-C6	Branched C6 Alkanes	1.53	0.35	23%	1.55	1%	0.91	0.23	25%	0.62	0.19	31%	0.68	1.04	0.28	0.14	21%	0.46	0.62	0.25	0.08	17%
223TM-C4	2,2,3-Trimethyl Butane	1.32	0.26	20%	1.34	1%	0.76	0.15	19%	0.51	0.13	26%	0.58	0.96	0.26	0.13	22%	0.44	0.61	0.23	0.08	18%
22-DM-C5	2,2-Dimethyl Pentane	1.22	0.29	24%	1.23	1%	0.72	0.20	28%	0.47	0.17	35%	0.52	0.68	0.22	0.10	19%	0.33	0.45	0.19	0.05	15%
23-DM-C5	2,3-Dimethyl Pentane	1.55	0.37	24%	1.57	1%	0.90	0.24	26%	0.60	0.20	33%	0.65	0.89	0.27	0.13	20%	0.43	0.60	0.24	0.07	16%
24-DM-C5	2,4-Dimethyl Pentane	1.65	0.38	23%	1.66	1%	0.94	0.24	26%	0.62	0.21	33%	0.68	0.94	0.31	0.13	19%	0.46	0.60	0.28	0.06	14%
2-ME-C6	2-Methyl Hexane	1.37	0.36	27%	1.38	0%	0.83	0.26	31%	0.52	0.21	40%	0.54	0.74	0.21	0.13	25%	0.33	0.49	0.15	0.07	21%
33-DM-C5	3,3-Dimethyl Pentane	1.32	0.34	26%	1.34	1%	0.80	0.23	28%	0.54	0.19	35%	0.59	0.86	0.23	0.12	21%	0.36	0.49	0.20	0.06	17%
3-ME-C6	3-Methyl Hexane	1.86	0.48	26%	1.87	1%	1.06	0.32	31%	0.69	0.27	39%	0.73	0.99	0.32	0.16	21%	0.44	0.62	0.27	0.08	18%
BR-C7	Branched C7 Alkanes	1.63	0.40	24%	1.64	1%	0.94	0.27	28%	0.61	0.22	36%	0.66	0.86	0.29	0.13	20%	0.42	0.58	0.25	0.07	15%
2233M-C4	2,2,3,3-Tetramethyl Butane	0.44	0.10	22%	0.45	1%	0.27	0.06	23%	0.18	0.05	30%	0.19	0.33	0.08	0.05	23%	0.14	0.19	0.07	0.02	16%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
224TM-C5	2,2,4-Trimethyl Pentane	1.44	0.30	21%	1.45	1%	0.81	0.18	23%	0.54	0.16	29%	0.60	0.91	0.28	0.11	18%	0.43	0.55	0.25	0.06	14%
22-DM-C6	2,2-Dimethyl Hexane	1.13	0.29	25%	1.14	0%	0.67	0.21	31%	0.41	0.17	40%	0.43	0.58	0.17	0.10	23%	0.26	0.39	0.12	0.05	19%
234TM-C5	2,3,4-Trimethyl Pentane	1.23	0.31	25%	1.25	2%	0.72	0.19	27%	0.47	0.16	35%	0.50	0.74	0.21	0.10	21%	0.32	0.47	0.18	0.06	18%
23-DM-C6	2,3-Dimethyl Hexane	1.34	0.34	25%	1.35	1%	0.78	0.23	30%	0.50	0.19	39%	0.52	0.74	0.22	0.12	23%	0.32	0.48	0.16	0.07	21%
24-DM-C6	2,4-Dimethyl Hexane	1.80	0.45	25%	1.83	1%	1.01	0.30	30%	0.63	0.25	39%	0.67	0.89	0.32	0.14	21%	0.40	0.60	0.19	0.08	21%
25-DM-C6	2,5-Dimethyl Hexane	1.68	0.41	24%	1.70	1%	0.93	0.27	29%	0.59	0.22	38%	0.62	0.83	0.28	0.13	22%	0.39	0.58	0.19	0.08	20%
2-ME-C7	2-Methyl Heptane	1.20	0.35	29%	1.20	0%	0.74	0.26	36%	0.44	0.21	49%	0.43	0.65	-0.06	0.16	37%	0.22	0.39	-0.06	0.09	42%
3-ME-C7	3-Methyl Heptane	1.35	0.38	29%	1.36	1%	0.82	0.28	35%	0.50	0.23	47%	0.50	0.73	0.03	0.16	32%	0.26	0.45	-0.01	0.09	35%
4-ME-C7	4-Methyl Heptane	1.48	0.41	28%	1.49	1%	0.86	0.29	34%	0.53	0.24	45%	0.54	0.76	0.12	0.16	29%	0.29	0.47	0.03	0.09	31%
BR-C8	Branched C8 Alkanes	1.57	0.41	26%	1.59	1%	0.90	0.29	32%	0.56	0.24	42%	0.58	0.79	0.18	0.15	26%	0.33	0.51	0.09	0.09	26%
225TM-C6	2,2,5-Trimethyl Hexane	1.33	0.32	24%	1.33	1%	0.73	0.21	29%	0.46	0.18	39%	0.48	0.63	0.23	0.10	21%	0.30	0.43	0.15	0.05	18%
235TM-C6	2,3,5-Trimethyl Hexane	1.33	0.34	26%	1.34	1%	0.79	0.23	29%	0.49	0.19	39%	0.51	0.73	0.20	0.12	24%	0.30	0.47	0.12	0.07	23%
24-DM-C7	2,4-Dimethyl Heptane	1.48	0.40	27%	1.50	1%	0.84	0.28	34%	0.50	0.23	47%	0.50	0.73	0.01	0.16	32%	0.26	0.45	-0.05	0.10	39%
2-ME-C8	2-Methyl Octane	0.96	0.32	33%	0.96	0%	0.60	0.25	41%	0.33	0.20	61%	0.30	0.54	-0.31	0.19	63%	0.11	0.29	-0.25	0.12	105%
33-DE-C5	3,3-Diethyl Pentane	1.35	0.37	27%	1.37	2%	0.79	0.25	31%	0.51	0.20	40%	0.54	0.71	0.22	0.12	21%	0.30	0.44	0.16	0.06	21%
35-DM-C7	3,5-Dimethyl Heptane	1.63	0.44	27%	1.65	1%	0.92	0.31	33%	0.57	0.25	44%	0.58	0.82	0.13	0.17	29%	0.30	0.52	-0.01	0.11	37%
4-ET-C7	4-Ethyl Heptane	1.44	0.41	29%	1.45	0%	0.84	0.30	36%	0.51	0.25	48%	0.51	0.75	0.02	0.17	34%	0.25	0.44	-0.07	0.11	44%
4-ME-C8	4-Methyl Octane	1.08	0.34	32%	1.06	-1%	0.67	0.27	40%	0.38	0.21	56%	0.36	0.59	-0.21	0.18	51%	0.15	0.33	-0.19	0.11	75%
BR-C9	Branched C9 Alkanes	1.25	0.36	29%	1.26	0%	0.74	0.27	37%	0.43	0.22	51%	0.42	0.65	-0.12	0.17	42%	0.20	0.38	-0.13	0.11	55%
24-DM-C8	2,4-Dimethyl Octane	1.09	0.34	31%	1.09	0%	0.65	0.26	41%	0.37	0.21	59%	0.34	0.59	-0.26	0.19	57%	0.13	0.30	-0.25	0.13	98%
26DM-C8	2,6-Dimethyl Octane	1.27	0.37	29%	1.28	1%	0.72	0.27	38%	0.42	0.22	53%	0.41	0.64	-0.14	0.18	45%	0.17	0.37	-0.20	0.13	74%
2-ME-C9	2-Methyl Nonane	0.86	0.31	36%	0.85	0%	0.55	0.25	45%	0.30	0.20	68%	0.26	0.51	-0.36	0.20	78%	0.06	0.25	-0.34	0.13	-
34-DE-C6	3,4-Diethyl Hexane	1.20	0.33	27%	1.19	0%	0.69	0.24	35%	0.42	0.19	46%	0.43	0.61	0.08	0.13	29%	0.22	0.37	0.00	0.08	35%
3-ME-C9	3-Methyl Nonane	0.89	0.31	35%	0.88	-1%	0.56	0.24	44%	0.30	0.20	67%	0.26	0.51	-0.37	0.20	77%	0.07	0.25	-0.33	0.13	187%
4-ME-C9	4-Methyl Nonane	0.99	0.33	34%	0.98	-1%	0.61	0.26	42%	0.34	0.21	63%	0.30	0.55	-0.30	0.20	65%	0.10	0.28	-0.28	0.13	130%
4-PR-C7	4-Propyl Heptane	1.24	0.38	31%	1.25	0%	0.73	0.28	39%	0.42	0.23	55%	0.41	0.65	-0.13	0.19	46%	0.17	0.35	-0.19	0.12	74%
BR-C10	Branched C10 Alkanes	1.09	0.35	32%	1.10	0%	0.65	0.26	40%	0.37	0.21	58%	0.34	0.58	-0.23	0.19	55%	0.12	0.31	-0.25	0.13	103%
26DM-C9	2,6-Dimethyl Nonane	0.95	0.31	33%	0.95	0%	0.56	0.24	43%	0.31	0.20	64%	0.28	0.51	-0.29	0.19	68%	0.08	0.26	-0.30	0.13	162%
35-DE-C7	3,5-Diethyl Heptane	1.21	0.37	31%	1.22	1%	0.69	0.27	39%	0.40	0.23	57%	0.38	0.62	-0.19	0.19	51%	0.12	0.34	-0.30	0.15	124%
3-ME-C10	3-Methyl Decane	0.77	0.29	38%	0.77	1%	0.49	0.23	47%	0.26	0.19	73%	0.22	0.46	-0.42	0.20	92%	0.03	0.21	-0.37	0.13	-
4-ME-C10	4-Methyl Decane	0.80	0.30	37%	0.80	0%	0.51	0.23	46%	0.27	0.19	73%	0.23	0.48	-0.41	0.20	89%	0.04	0.21	-0.36	0.13	-
BR-C11	Branched C11 alkanes	0.87	0.30	35%	0.87	1%	0.53	0.24	45%	0.29	0.19	68%	0.25	0.49	-0.35	0.20	78%	0.06	0.24	-0.33	0.13	-
36-DE-C8	2,6-Diethyl Octane	1.09	0.35	32%	1.11	1%	0.64	0.26	40%	0.38	0.22	58%	0.35	0.59	-0.19	0.19	53%	0.11	0.31	-0.26	0.13	117%
36DM-C10	3,6-Dimethyl Decane	0.88	0.32	36%	0.88	0%	0.54	0.24	45%	0.30	0.20	69%	0.26	0.52	-0.37	0.20	78%	0.05	0.24	-0.36	0.14	-
3-ME-C11	3-Methyl Undecane	0.70	0.28	39%	0.70	0%	0.45	0.22	49%	0.23	0.18	77%	0.19	0.43	-0.42	0.20	104%	0.01	0.19	-0.38	0.14	-
5-ME-C11	5-Methyl Undecane	0.72	0.28	39%	0.71	-2%	0.46	0.22	48%	0.24	0.19	79%	0.19	0.43	-0.45	0.20	107%	0.01	0.18	-0.39	0.14	-
BR-C12	Branched C12 Alkanes	0.80	0.30	37%	0.79	0%	0.50	0.23	46%	0.27	0.19	73%	0.22	0.47	-0.40	0.20	90%	0.03	0.21	-0.37	0.14	-
36DM-C11	3,6-Dimethyl Undecane	0.82	0.30	37%	0.82	0%	0.50	0.23	46%	0.27	0.20	72%	0.24	0.47	-0.39	0.20	83%	0.03	0.21	-0.38	0.14	-
37-DE-C9	3,7-Diethyl Nonane	1.08	0.34	32%	1.08	0%	0.61	0.25	41%	0.35	0.21	60%	0.33	0.56	-0.20	0.18	54%	0.09	0.28	-0.29	0.14	146%
3-ME-C12	3-Methyl Dodecane	0.64	0.26	41%	0.63	-2%	0.41	0.21	50%	0.21	0.17	81%	0.17	0.40	-0.47	0.19	115%	-0.01	0.16	-0.39	0.13	-
5-ME-C12	5-Methyl Dodecane	0.64	0.27	42%	0.64	0%	0.42	0.21	50%	0.21	0.18	83%	0.17	0.41	-0.48	0.20	116%	-0.01	0.16	-0.39	0.14	-
BR-C13	Branched C13 Alkanes	0.73	0.28	39%	0.73	0%	0.46	0.22	48%	0.24	0.19	76%	0.20	0.44	-0.43	0.20	96%	0.01	0.19	-0.39	0.14	-
37DM-C12	3,7-Dimethyl Dodecane	0.74	0.28	38%	0.75	0%	0.46	0.22	48%	0.24	0.18	76%	0.21	0.44	-0.43	0.19	93%	0.01	0.19	-0.37	0.14	-
38DE-C10	3,8-Diethyl Decane	0.68	0.28	41%	0.67	-2%	0.43	0.21	49%	0.23	0.18	76%	0.19	0.42	-0.41	0.19	98%	-0.01	0.18	-0.40	0.14	-
3-ME-C13	3-Methyl Tridecane	0.57	0.25	43%	0.57	0%	0.37	0.20	53%	0.19	0.16	85%	0.15	0.38	-0.42	0.18	123%	-0.02	0.15	-0.39	0.13	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
6-ME-C13	6-Methyl Tridecane	0.62	0.26	42%	0.62	0%	0.40	0.20	51%	0.21	0.17	83%	0.16	0.40	-0.48	0.19	119%	-0.01	0.16	-0.40	0.13	-
BR-C14	Branched C14 Alkanes	0.67	0.27	40%	0.67	0%	0.42	0.21	50%	0.22	0.18	79%	0.18	0.41	-0.44	0.19	104%	0.00	0.17	-0.38	0.14	-
37DM-C13	3,7-Dimethyl Tridecane	0.64	0.26	41%	0.65	0%	0.41	0.20	50%	0.21	0.17	80%	0.17	0.40	-0.45	0.19	109%	-0.01	0.16	-0.40	0.14	-
39DE-C11	3,9-Diethyl Undecane	0.62	0.26	42%	0.61	-1%	0.39	0.20	51%	0.21	0.17	82%	0.16	0.39	-0.46	0.18	111%	-0.02	0.15	-0.40	0.14	-
3-ME-C14	3-Methyl Tetradecane	0.53	0.24	44%	0.53	0%	0.35	0.18	52%	0.18	0.15	85%	0.14	0.35	-0.45	0.18	128%	-0.03	0.14	-0.39	0.13	-
6-ME-C14	6-Methyl Tetradecane	0.57	0.25	43%	0.57	-1%	0.38	0.19	51%	0.19	0.16	86%	0.15	0.37	-0.48	0.19	125%	-0.02	0.15	-0.40	0.13	-
BR-C15	Branched C15 Alkanes	0.60	0.25	42%	0.60	0%	0.39	0.20	50%	0.20	0.17	82%	0.16	0.38	-0.46	0.18	117%	-0.02	0.15	-0.40	0.13	-
3-ME-C15	3-Methyl Pentadecane	0.50	0.23	45%	0.50	-1%	0.33	0.18	53%	0.17	0.15	87%	0.13	0.33	-0.48	0.17	133%	-0.03	0.13	-0.39	0.13	-
48DM-C14	4,8-Dimethyl Tetradecane	0.58	0.25	43%	0.57	-2%	0.37	0.19	51%	0.20	0.16	83%	0.16	0.36	-0.44	0.18	112%	-0.02	0.14	-0.39	0.13	-
7-ME-C15	7-Methyl Pentadecane	0.51	0.23	45%	0.51	-2%	0.34	0.18	52%	0.18	0.15	87%	0.13	0.34	-0.43	0.17	130%	-0.03	0.13	-0.40	0.13	-
BR-C16	Branched C16 Alkanes	0.54	0.24	44%	0.53	-2%	0.36	0.18	52%	0.18	0.16	85%	0.14	0.34	-0.45	0.17	121%	-0.03	0.14	-0.39	0.13	-
BR-C17	Branched C17 Alkanes	0.51	0.23	44%	0.50	-2%	0.33	0.17	52%	0.17	0.15	85%	0.14	0.32	-0.42	0.16	121%	-0.03	0.13	-0.37	0.12	-
BR-C18	Branched C18 Alkanes	0.48	0.21	44%	0.48	-2%	0.32	0.16	52%	0.16	0.14	85%	0.13	0.31	-0.40	0.15	121%	-0.03	0.12	-0.35	0.11	-
CYCC3	Cyclopropane	0.10	0.03	27%	0.10	1%	0.07	0.02	32%	0.05	0.02	37%	0.05	0.08	0.02	0.01	27%	0.03	0.05	0.02	0.01	22%
CYCC4	Cyclobutane	1.05	0.30	29%	1.06	1%	0.68	0.23	33%	0.48	0.19	40%	0.52	0.78	0.17	0.14	27%	0.29	0.42	0.15	0.07	24%
CYCC5	Cyclopentane	2.69	0.65	24%	2.72	1%	1.53	0.41	27%	1.03	0.35	34%	1.13	1.60	0.49	0.22	20%	0.74	0.97	0.43	0.12	16%
CYCC6	Cyclohexane	1.46	0.39	26%	1.47	1%	0.90	0.28	31%	0.57	0.23	40%	0.60	0.83	0.23	0.14	24%	0.36	0.54	0.20	0.08	21%
IPR-CC3	Isopropyl Cyclopropane	1.52	0.37	25%	1.53	1%	0.94	0.27	28%	0.66	0.23	34%	0.73	1.12	0.27	0.17	23%	0.45	0.63	0.24	0.08	19%
ME-CYCC5	Methylcyclopentane	2.42	0.58	24%	2.46	1%	1.33	0.38	28%	0.87	0.31	36%	0.94	1.23	0.45	0.17	18%	0.59	0.80	0.39	0.09	16%
CYC-C6	C6 Cycloalkanes	1.46	0.39	26%	1.47	1%	0.90	0.28	31%	0.57	0.23	40%	0.60	0.83	0.23	0.14	24%	0.36	0.54	0.20	0.08	21%
13DMCYC5	1,3-Dimeth. Cyclopentane	2.15	0.52	24%	2.18	2%	1.15	0.34	29%	0.72	0.28	39%	0.77	0.99	0.40	0.15	20%	0.46	0.67	0.20	0.10	21%
CYCC7	Cycloheptane	2.26	0.58	26%	2.30	2%	1.21	0.38	31%	0.78	0.32	41%	0.81	1.11	0.41	0.20	24%	0.46	0.75	0.13	0.14	31%
ET-CYCC5	Ethyl Cyclopentane	2.27	0.58	26%	2.30	1%	1.24	0.38	31%	0.78	0.32	41%	0.83	1.12	0.40	0.18	22%	0.48	0.71	0.19	0.11	24%
ME-CYCC6	Methylcyclohexane	1.99	0.51	26%	2.01	1%	1.11	0.34	31%	0.69	0.28	41%	0.72	0.99	0.25	0.18	25%	0.42	0.66	0.12	0.11	26%
CYC-C7	C7 Cycloalkanes	1.99	0.51	26%	2.01	1%	1.11	0.34	31%	0.69	0.28	41%	0.72	0.99	0.25	0.18	25%	0.42	0.66	0.12	0.11	26%
13DMCYC6	1,3-Dimethyl Cyclohexane	1.72	0.46	27%	1.75	2%	0.94	0.32	34%	0.56	0.27	48%	0.56	0.83	-0.01	0.20	35%	0.29	0.52	-0.10	0.14	48%
CYCC8	Cyclooctane	1.73	0.48	28%	1.75	1%	0.94	0.33	35%	0.57	0.28	49%	0.57	0.86	0.00	0.21	37%	0.26	0.53	-0.17	0.16	61%
ET-CYCC6	Ethylcyclohexane	1.75	0.48	27%	1.77	1%	0.99	0.33	34%	0.60	0.27	45%	0.61	0.88	0.09	0.19	32%	0.32	0.56	-0.03	0.13	40%
PR-CYCC5	Propyl Cyclopentane	1.91	0.51	27%	1.94	1%	1.03	0.35	33%	0.63	0.29	45%	0.65	0.91	0.15	0.18	28%	0.34	0.56	-0.03	0.13	38%
CYC-C8	C8 Cycloalkanes	1.75	0.48	27%	1.77	1%	0.99	0.33	34%	0.60	0.27	45%	0.61	0.88	0.09	0.19	32%	0.32	0.56	-0.03	0.13	40%
BCYC-C9	C9 Bicycloalkanes	1.57	0.45	29%	1.59	1%	0.88	0.32	37%	0.52	0.27	51%	0.51	0.79	-0.09	0.21	41%	0.23	0.46	-0.19	0.15	65%
113MCYC6	1,1,3-Trimethyl Cyclohex.	1.37	0.38	28%	1.38	1%	0.76	0.27	35%	0.44	0.22	51%	0.42	0.66	-0.17	0.18	44%	0.20	0.39	-0.18	0.13	63%
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	1.62	0.46	28%	1.64	1%	0.89	0.32	36%	0.53	0.27	51%	0.52	0.81	-0.06	0.21	40%	0.23	0.47	-0.20	0.15	67%
C3-CYCC6	Propyl Cyclohexane	1.47	0.43	29%	1.49	1%	0.84	0.31	37%	0.49	0.25	52%	0.48	0.75	-0.12	0.20	42%	0.22	0.43	-0.18	0.14	64%
CYC-C9	C9 Cycloalkanes	1.55	0.44	29%	1.57	1%	0.86	0.32	37%	0.51	0.26	51%	0.50	0.78	-0.09	0.21	41%	0.22	0.45	-0.19	0.15	65%
BCYC-C10	C10 Bicycloalkanes	1.29	0.40	31%	1.29	0%	0.74	0.29	39%	0.43	0.24	56%	0.40	0.67	-0.20	0.21	52%	0.15	0.38	-0.28	0.15	102%
13DECYC6	1,3-Diethyl-Cyclohexane	1.34	0.41	30%	1.36	1%	0.75	0.29	39%	0.43	0.24	57%	0.41	0.69	-0.23	0.22	53%	0.13	0.38	-0.32	0.16	122%
14DECYC6	1,4-Diethyl-Cyclohexane	1.49	0.44	30%	1.49	0%	0.82	0.31	38%	0.48	0.26	53%	0.47	0.74	-0.12	0.21	45%	0.18	0.43	-0.26	0.16	89%
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	1.26	0.38	30%	1.26	0%	0.72	0.27	37%	0.42	0.22	53%	0.40	0.66	-0.16	0.19	48%	0.16	0.39	-0.22	0.14	84%
C4-CYCC6	Butyl Cyclohexane	1.07	0.36	33%	1.07	0%	0.64	0.27	43%	0.36	0.23	63%	0.32	0.59	-0.35	0.22	68%	0.09	0.30	-0.33	0.15	158%
CYC-C10	C10 Cycloalkanes	1.27	0.39	31%	1.27	0%	0.73	0.28	39%	0.42	0.24	56%	0.40	0.66	-0.20	0.21	52%	0.15	0.37	-0.27	0.15	102%
BCYC-C11	C11 Bicycloalkanes	1.01	0.35	35%	1.01	0%	0.59	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
13E5MCC6	13-Dieth-5-Me. Cyclohex.	1.11	0.37	33%	1.11	0%	0.62	0.27	43%	0.34	0.22	66%	0.31	0.58	-0.42	0.22	72%	0.05	0.28	-0.43	0.18	-
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	0.95	0.35	36%	0.95	0%	0.58	0.26	45%	0.32	0.22	69%	0.27	0.55	-0.48	0.23	84%	0.03	0.26	-0.44	0.17	-
C5-CYCC6	Pentyl Cyclohexane	0.91	0.32	36%	0.91	0%	0.55	0.25	45%	0.30	0.21	70%	0.26	0.52	-0.41	0.21	83%	0.04	0.24	-0.39	0.15	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
CYC-C11	C11 Cycloalkanes	0.99	0.35	35%	0.99	0%	0.58	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
CYC-C11	C11 Cycloalkanes	0.99	0.35	35%	0.99	0%	0.58	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
BCYC-C12	C12 Bicycloalkanes	0.88	0.32	37%	0.89	1%	0.52	0.24	46%	0.28	0.20	71%	0.24	0.50	-0.43	0.21	86%	0.02	0.22	-0.43	0.16	-
CYC-C12	C12 Cycloalkanes	0.87	0.32	37%	0.88	1%	0.52	0.24	46%	0.28	0.20	71%	0.24	0.50	-0.43	0.21	86%	0.02	0.22	-0.42	0.16	-
135ECYC6	1,3,5-Triethyl Cyclohex.	1.06	0.36	34%	1.07	1%	0.60	0.26	44%	0.33	0.22	67%	0.30	0.57	-0.42	0.22	74%	0.03	0.26	-0.45	0.18	-
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	0.81	0.31	39%	0.83	3%	0.49	0.22	46%	0.27	0.19	70%	0.23	0.46	-0.37	0.19	82%	0.02	0.21	-0.37	0.14	-
C6-CYCC6	Hexyl Cyclohexane	0.75	0.30	39%	0.75	0%	0.47	0.23	49%	0.25	0.19	79%	0.20	0.45	-0.51	0.21	107%	0.00	0.19	-0.44	0.15	-
BCYC-C13	C13 Bicycloalkanes	0.79	0.31	39%	0.80	1%	0.48	0.23	48%	0.26	0.20	78%	0.21	0.46	-0.50	0.21	100%	-0.01	0.20	-0.45	0.16	-
13E5PCC6	13-Dieth-5-Pent Cyclohx.	0.99	0.35	35%	1.01	1%	0.56	0.25	45%	0.31	0.21	68%	0.28	0.54	-0.45	0.22	78%	0.02	0.25	-0.46	0.17	-
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	0.70	0.29	42%	0.70	0%	0.44	0.22	51%	0.23	0.19	82%	0.18	0.44	-0.51	0.21	114%	-0.03	0.19	-0.46	0.16	-
C7-CYCC6	Heptyl Cyclohexane	0.66	0.27	42%	0.66	-1%	0.42	0.21	51%	0.22	0.19	86%	0.17	0.42	-0.52	0.21	119%	-0.02	0.17	-0.44	0.15	-
CYC-C13	C13 Cycloalkanes	0.78	0.30	39%	0.79	1%	0.48	0.23	48%	0.25	0.20	78%	0.21	0.46	-0.49	0.21	100%	-0.01	0.20	-0.45	0.16	-
BCYC-C14	C14 Bicycloalkanes	0.71	0.28	40%	0.72	1%	0.44	0.21	49%	0.24	0.18	77%	0.19	0.43	-0.47	0.20	100%	-0.02	0.18	-0.43	0.15	-
13P5ECC6	13-Diprop-5-Eth Cyclohx.	0.94	0.33	35%	0.94	0%	0.53	0.24	46%	0.30	0.20	69%	0.26	0.51	-0.43	0.20	78%	0.01	0.23	-0.45	0.17	-
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	0.58	0.27	46%	0.60	4%	0.38	0.19	51%	0.20	0.16	80%	0.16	0.37	-0.42	0.18	109%	-0.03	0.15	-0.40	0.14	-
C8-CYCC6	Octyl Cyclohexane	0.60	0.26	44%	0.60	0%	0.39	0.20	52%	0.20	0.18	87%	0.16	0.39	-0.53	0.20	128%	-0.03	0.15	-0.44	0.15	-
CYC-C14	C14 Cycloalkanes	0.71	0.28	40%	0.71	1%	0.43	0.21	49%	0.23	0.18	77%	0.19	0.42	-0.46	0.19	100%	-0.02	0.18	-0.43	0.15	-
BCYC-C15	C15 Bicycloalkanes	0.69	0.28	41%	0.69	0%	0.42	0.21	50%	0.23	0.18	78%	0.19	0.41	-0.45	0.19	101%	-0.02	0.17	-0.42	0.15	-
135PCYC6	135-Tripropyl Cyclohex.	0.90	0.32	35%	0.90	0%	0.51	0.23	46%	0.29	0.20	69%	0.25	0.50	-0.37	0.19	75%	0.01	0.21	-0.42	0.16	-
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	0.60	0.27	44%	0.60	-1%	0.39	0.20	51%	0.21	0.17	80%	0.16	0.38	-0.47	0.18	112%	-0.03	0.15	-0.42	0.14	-
C9-CYCC6	Nonyl Cyclohexane	0.54	0.26	47%	0.54	1%	0.36	0.19	54%	0.18	0.16	90%	0.14	0.37	-0.48	0.19	137%	-0.04	0.13	-0.43	0.14	-
CYC-C15	C15 Cycloalkanes	0.68	0.28	41%	0.68	0%	0.42	0.21	50%	0.23	0.18	78%	0.18	0.41	-0.44	0.19	101%	-0.02	0.16	-0.42	0.15	-
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	0.77	0.29	38%	0.77	0%	0.45	0.22	48%	0.25	0.18	74%	0.21	0.44	-0.44	0.19	90%	-0.01	0.19	-0.45	0.15	-
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	0.55	0.26	47%	0.55	-1%	0.35	0.19	55%	0.19	0.17	88%	0.14	0.36	-0.48	0.18	129%	-0.05	0.13	-0.44	0.14	-
C10CYCC6	Decyl Cyclohexane	0.50	0.24	48%	0.51	1%	0.33	0.18	54%	0.17	0.16	90%	0.13	0.34	-0.48	0.18	136%	-0.05	0.14	-0.42	0.14	-
CYC-C16	C16 Cycloalkanes	0.61	0.26	43%	0.61	0%	0.38	0.20	52%	0.20	0.17	83%	0.16	0.38	-0.47	0.18	114%	-0.04	0.15	-0.43	0.15	-
ETHENE	Ethene	9.08	1.39	15%	9.28	2%	3.70	0.52	14%	2.34	0.52	22%	2.85	4.86	2.43	0.49	17%	2.73	3.74	2.35	0.33	12%
PROPENE	Propene	11.58	1.74	15%	11.91	3%	4.43	0.67	15%	2.83	0.65	23%	3.46	5.83	2.93	0.52	15%	3.41	4.32	3.16	0.26	8%
1-BUTENE	1-Butene	10.29	1.71	17%	10.54	2%	4.03	0.76	19%	2.60	0.69	27%	3.12	4.85	2.65	0.42	14%	2.85	3.30	2.65	0.18	6%
C4-OLE1	C4 Terminal Alkenes	10.29	1.71	17%	10.54	2%	4.03	0.76	19%	2.60	0.69	27%	3.12	4.85	2.65	0.42	14%	2.85	3.30	2.65	0.18	6%
1-PENTEN	1-Pentene	7.79	1.34	17%	7.97	2%	3.11	0.61	20%	2.00	0.55	28%	2.38	3.58	2.01	0.31	13%	2.09	2.41	1.95	0.12	6%
3M-1-BUT	3-Methyl-1-Butene	6.99	1.17	17%	7.19	3%	2.83	0.54	19%	1.85	0.50	27%	2.21	3.44	1.82	0.32	14%	1.97	2.34	1.82	0.13	7%
C5-OLE1	C5 Terminal Alkenes	7.79	1.34	17%	7.97	2%	3.11	0.61	20%	2.00	0.55	28%	2.38	3.58	2.01	0.31	13%	2.09	2.41	1.95	0.12	6%
1-HEXENE	1-Hexene	6.17	1.08	18%	6.33	3%	2.58	0.53	21%	1.69	0.48	28%	1.98	2.93	1.63	0.27	14%	1.70	2.10	1.54	0.12	7%
33M1-BUT	3,3-Dimethyl-1-Butene	6.06	1.01	17%	6.23	3%	2.51	0.45	18%	1.64	0.42	26%	1.95	3.06	1.61	0.28	14%	1.75	2.25	1.58	0.15	8%
3M1-C5E	3-Methyl-1-Pentene	6.22	1.08	17%	6.37	2%	2.54	0.51	20%	1.64	0.46	28%	1.93	2.81	1.61	0.24	12%	1.64	1.91	1.47	0.09	6%
4M1-C5E	4-Methyl-1-Pentene	6.26	1.05	17%	6.43	3%	2.51	0.49	20%	1.61	0.44	28%	1.91	2.81	1.61	0.24	12%	1.65	1.92	1.48	0.09	5%
C6-OLE1	C6 Terminal Alkenes	6.17	1.08	18%	6.33	3%	2.58	0.53	21%	1.69	0.48	28%	1.98	2.93	1.63	0.27	14%	1.70	2.10	1.54	0.12	7%
1-HEPTEN	1-Heptene	4.56	0.85	19%	4.69	3%	1.95	0.45	23%	1.25	0.40	32%	1.43	1.80	1.16	0.17	12%	1.13	1.34	0.79	0.10	9%
1-OCTENE	1-Octene	3.45	0.67	19%	3.53	2%	1.50	0.38	25%	0.94	0.33	35%	1.06	1.37	0.84	0.14	13%	0.77	0.94	0.43	0.11	14%
C8-OLE1	C8 Terminal Alkenes	3.45	0.67	19%	3.53	2%	1.50	0.38	25%	0.94	0.33	35%	1.06	1.37	0.84	0.14	13%	0.77	0.94	0.43	0.11	14%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
1-C9E	1-Nonene	2.76	0.56	20%	2.83	2%	1.22	0.33	27%	0.75	0.29	38%	0.83	1.07	0.56	0.14	17%	0.55	0.75	0.20	0.13	23%
C9-OLE1	C9 Terminal Alkenes	2.76	0.56	20%	2.83	2%	1.22	0.33	27%	0.75	0.29	38%	0.83	1.07	0.56	0.14	17%	0.55	0.75	0.20	0.13	23%
1-C10E	1-Decene	2.28	0.49	21%	2.33	2%	1.02	0.30	29%	0.61	0.25	41%	0.66	0.88	0.33	0.14	21%	0.41	0.60	0.05	0.13	32%
C10-OLE1	C10 Terminal Alkenes	2.28	0.49	21%	2.33	2%	1.02	0.30	29%	0.61	0.25	41%	0.66	0.88	0.33	0.14	21%	0.41	0.60	0.05	0.13	32%
1-C11E	1-Undecene	1.95	0.42	22%	1.97	1%	0.87	0.27	31%	0.52	0.23	44%	0.55	0.77	0.20	0.14	25%	0.32	0.49	-0.04	0.13	42%
C11-OLE1	C11 Terminal Alkenes	1.95	0.42	22%	1.97	1%	0.87	0.27	31%	0.52	0.23	44%	0.55	0.77	0.20	0.14	25%	0.32	0.49	-0.04	0.13	42%
C12-OLE1	C12 Terminal Alkenes	1.72	0.38	22%	1.75	2%	0.77	0.24	31%	0.46	0.21	45%	0.48	0.69	0.10	0.14	29%	0.26	0.43	-0.10	0.13	51%
1-C12E	1-Dodecene	1.72	0.38	22%	1.75	2%	0.77	0.24	31%	0.46	0.21	45%	0.48	0.69	0.10	0.14	29%	0.26	0.43	-0.10	0.13	51%
1-C13E	1-Tridecene	1.55	0.35	23%	1.59	3%	0.69	0.22	32%	0.41	0.19	47%	0.42	0.61	0.03	0.14	32%	0.22	0.38	-0.13	0.13	58%
C13-OLE1	C13 Terminal Alkenes	1.55	0.35	23%	1.59	3%	0.69	0.22	32%	0.41	0.19	47%	0.42	0.61	0.03	0.14	32%	0.22	0.38	-0.13	0.13	58%
1-C14E	1-Tetradecene	1.48	0.33	22%	1.50	1%	0.66	0.20	31%	0.40	0.17	43%	0.43	0.59	0.18	0.10	24%	0.23	0.36	-0.06	0.10	44%
C14-OLE1	C14 Terminal Alkenes	1.48	0.33	22%	1.50	1%	0.66	0.20	31%	0.40	0.17	43%	0.43	0.59	0.18	0.10	24%	0.23	0.36	-0.06	0.10	44%
1-C15E	1-Pentadecene	1.30	0.30	23%	1.31	1%	0.59	0.19	33%	0.34	0.17	49%	0.35	0.52	-0.06	0.13	36%	0.17	0.31	-0.16	0.12	70%
C15-OLE1	C15 Terminal Alkenes	1.30	0.30	23%	1.31	1%	0.59	0.19	33%	0.34	0.17	49%	0.35	0.52	-0.06	0.13	36%	0.17	0.31	-0.16	0.12	70%
ISOBUTEN	Isobutene	6.35	0.75	12%	6.57	3%	2.19	0.27	13%	1.26	0.28	23%	1.56	2.18	1.22	0.23	15%	2.03	2.51	1.66	0.19	9%
2M-1-BUT	2-Methyl-1-Butene	6.51	0.83	13%	6.71	3%	2.35	0.34	15%	1.39	0.33	24%	1.70	2.39	1.42	0.19	11%	2.08	2.56	1.77	0.16	8%
23M1-BUT	23-Dimethyl-1-Butene	4.77	0.63	13%	4.93	3%	1.76	0.27	15%	1.03	0.26	25%	1.25	1.58	1.08	0.11	8%	1.48	1.77	1.25	0.11	7%
2E1-BUT	2-Ethyl-1-Butene	5.04	0.67	13%	5.20	3%	1.85	0.29	16%	1.10	0.27	25%	1.33	1.77	1.16	0.12	9%	1.54	1.82	1.31	0.11	7%
2M1-C5E	2-Methyl-1-Pentene	5.18	0.68	13%	5.34	3%	1.88	0.30	16%	1.11	0.28	25%	1.34	1.73	1.17	0.13	9%	1.59	1.88	1.34	0.12	7%
233M1BUT	2,3,3-trimethyl-1-Butene	4.62	0.69	15%	4.76	3%	1.83	0.31	17%	1.14	0.30	26%	1.35	1.71	1.19	0.12	9%	1.49	1.92	1.22	0.15	10%
C7-OLE1	C7 Terminal Alkenes	4.56	0.85	19%	4.69	3%	1.95	0.45	23%	1.25	0.40	32%	1.43	1.80	1.16	0.17	12%	1.13	1.34	0.79	0.10	9%
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	3.29	0.59	18%	3.35	2%	1.42	0.33	23%	0.87	0.29	33%	0.98	1.19	0.81	0.09	10%	0.85	0.99	0.54	0.09	10%
C-2-BUTE	cis-2-Butene	13.22	1.83	14%	13.79	4%	4.75	0.67	14%	2.95	0.67	23%	3.66	6.26	3.07	0.55	15%	4.27	5.31	3.73	0.29	7%
T-2-BUTE	trans-2-Butene	13.91	1.90	14%	14.51	4%	4.89	0.66	14%	2.98	0.66	22%	3.72	6.29	3.04	0.56	15%	4.63	5.82	4.02	0.33	7%
C4-OLE2	C4 Internal Alkenes	13.57	1.87	14%	14.13	4%	4.82	0.67	14%	2.97	0.67	22%	3.69	6.27	3.06	0.55	15%	4.45	5.56	3.87	0.31	7%
2M-2-BUT	2-Methyl-2-Butene	14.45	1.86	13%	15.26	6%	4.65	0.58	13%	2.63	0.62	23%	3.35	5.23	2.23	0.68	20%	5.31	6.98	4.16	0.59	11%
C-2-PENT	cis-2-Pentene	10.24	1.68	16%	10.61	4%	3.87	0.68	18%	2.49	0.65	26%	3.03	5.02	2.58	0.44	15%	2.94	3.28	2.58	0.17	6%
T-2-PENT	trans-2-Pentene	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.57	0.17	6%
2-C5-OLE	2-Pentenes	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.58	0.17	6%
C5-OLE2	C5 Internal Alkenes	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.58	0.17	6%
23M2-BUT	2,3-Dimethyl-2-Butene	13.32	1.89	14%	14.06	6%	3.97	0.51	13%	2.06	0.56	27%	2.69	4.77	1.36	0.86	32%	5.28	7.46	3.58	0.86	16%
2M-2-C5E	2-Methyl-2-Pentene	12.28	1.67	14%	12.87	5%	4.18	0.62	15%	2.37	0.59	25%	2.97	4.27	2.27	0.44	15%	4.29	5.13	3.39	0.42	10%
C-2-C6E	Cis-2-Hexene	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
C-3-C6E	Cis-3-Hexene	8.22	1.52	18%	8.45	3%	3.21	0.68	21%	2.10	0.62	29%	2.52	4.07	2.01	0.42	17%	2.10	2.49	1.65	0.19	9%
C3M2-C5E	Cis-3-Methyl-2-Hexene	13.38	1.81	14%	14.00	5%	4.60	0.66	14%	2.63	0.64	24%	3.29	4.92	2.40	0.54	16%	4.90	6.18	3.87	0.50	10%
T3M2-C5E	Trans 3-Methyl-2-Hexene	14.17	1.92	14%	14.85	5%	4.84	0.68	14%	2.75	0.67	24%	3.45	5.17	2.46	0.60	17%	5.27	6.77	4.15	0.54	10%
T4M2-C5E	Trans 4-Methyl-2-Hexene	7.88	1.25	16%	8.14	3%	3.03	0.54	18%	1.95	0.51	26%	2.36	3.91	2.03	0.34	15%	2.29	2.53	1.94	0.14	6%
T-2-C6E	Trans-2-Hexene	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
T-3-C6E	Trans-3-Hexene	8.16	1.50	18%	8.38	3%	3.18	0.67	21%	2.07	0.61	29%	2.48	4.04	1.99	0.41	17%	2.09	2.47	1.66	0.18	9%
2-C6-OLE	2-Hexenes	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
C6-OLE2	C6 Internal Alkenes	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
23M2-C5E	2,3-Dimethyl-2-Hexene	10.41	1.43	14%	10.98	5%	3.27	0.41	12%	1.75	0.44	25%	2.24	3.47	1.39	0.54	24%	3.91	5.18	2.86	0.52	13%
C-3-C7E	Cis-3-Heptene	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	6.99	1.09	16%	7.22	3%	2.63	0.46	17%	1.65	0.43	26%	2.01	3.12	1.75	0.24	12%	2.03	2.20	1.76	0.10	5%
T-2-C7E	Trans-2-Heptene	7.33	1.22	17%	7.56	3%	2.89	0.56	19%	1.85	0.51	27%	2.22	3.51	1.87	0.31	14%	2.01	2.23	1.53	0.14	7%
T-3-C7E	Trans-3-Heptene	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
2-C7-OLE	2-Heptenes	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
C7-OLE2	C7 Internal Alkenes	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
C-4-C8E	Cis-4-Octene	5.94	1.15	19%	6.09	2%	2.38	0.56	23%	1.57	0.49	31%	1.85	2.80	1.40	0.31	17%	1.39	1.66	0.86	0.17	12%
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	5.97	1.06	18%	6.16	3%	2.37	0.50	21%	1.54	0.45	29%	1.83	2.67	1.49	0.26	14%	1.53	1.82	1.13	0.13	8%
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	5.44	1.04	19%	5.58	3%	2.27	0.53	23%	1.53	0.48	31%	1.80	2.77	1.35	0.33	18%	1.33	1.61	0.81	0.17	13%
T-3-C8E	Trans-3-Octene	6.13	1.17	19%	6.30	3%	2.50	0.57	23%	1.64	0.51	31%	1.94	2.99	1.47	0.33	17%	1.46	1.73	0.91	0.17	12%
T-4-C8E	Trans-4-Octene	5.90	1.13	19%	6.09	3%	2.34	0.54	23%	1.53	0.48	31%	1.82	2.80	1.39	0.30	17%	1.39	1.68	0.89	0.17	12%
3-C8-OLE	3-Octenes	6.13	1.17	19%	6.30	3%	2.50	0.57	23%	1.64	0.51	31%	1.94	2.99	1.47	0.33	17%	1.46	1.73	0.91	0.17	12%
C8-OLE2	C8 Internal Alkenes	5.90	1.13	19%	6.09	3%	2.34	0.54	23%	1.53	0.48	31%	1.82	2.80	1.39	0.30	17%	1.39	1.68	0.89	0.17	12%
244M2C5E	2,4,4-trimethyl-2-Pentene	5.85	0.88	15%	6.11	5%	2.08	0.38	18%	1.21	0.33	28%	1.47	1.86	1.21	0.14	10%	1.76	2.16	1.15	0.23	13%
3-C9-OLE	3-Nonenes	5.31	1.03	19%	5.48	3%	2.17	0.52	24%	1.43	0.46	32%	1.68	2.49	1.24	0.28	17%	1.21	1.46	0.66	0.17	14%
C9-OLE2	C9 Internal Alkenes	5.31	1.03	19%	5.48	3%	2.17	0.52	24%	1.43	0.46	32%	1.68	2.49	1.24	0.28	17%	1.21	1.46	0.66	0.17	14%
T-4-C9E	Trans-4-Nonene	5.23	1.01	19%	5.39	3%	2.14	0.51	24%	1.40	0.45	32%	1.65	2.45	1.22	0.28	17%	1.19	1.43	0.65	0.17	14%
34E2-C6E	3,4-Diethyl-2-Hexene	3.95	0.87	22%	4.04	2%	1.81	0.52	29%	1.14	0.45	39%	1.27	1.73	0.83	0.22	17%	0.82	1.16	0.10	0.22	27%
C-5-C10E	Cis-5-Decene	4.89	0.95	20%	5.03	3%	2.04	0.50	24%	1.35	0.44	32%	1.57	2.32	1.15	0.27	17%	1.10	1.33	0.54	0.17	15%
T-4-C10E	Trans-4-Decene	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
3C10-OLE	C10 3-Alkenes	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
C10-OLE2	C10 Internal Alkenes	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
T-5-C11E	Trans-5-Undecene	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
3C11-OLE	C11 3-Alkenes	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
C11-OLE2	C11 Internal Alkenes	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
2C12-OLE	C12 2-Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
3C12-OLE	C12 3-Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
C12-OLE2	C12 Internal Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
T-5-C12E	Trans-5-Dodecene	3.74	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
T-5-C13E	Trans-5-Tridecene	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
3C13-OLE	C13 3-Alkenes	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
C13-OLE2	C13 Internal Alkenes	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
T-5-C14E	Trans-5-Tetradecene	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
3C14-OLE	C14 3-Alkenes	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
C14-OLE2	C14 Internal Alkenes	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
T-5-C15E	Trans-5-Pentadecene	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
3C15-OLE	C15 3-Alkenes	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
C15-OLE2	C15 Internal Alkenes	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
C4-OLE	C4 Alkenes	11.93	1.77	15%	12.35	4%	4.43	0.70	16%	2.78	0.67	24%	3.41	5.57	2.95	0.45	13%	3.65	4.42	3.39	0.20	6%
C5-OLE	C5 Alkenes	9.01	1.51	17%	9.31	3%	3.49	0.65	19%	2.25	0.60	27%	2.71	4.31	2.32	0.37	14%	2.52	2.78	2.26	0.13	5%
C6-OLE	C6 Alkenes	6.88	1.18	17%	7.08	3%	2.75	0.56	20%	1.76	0.50	29%	2.09	3.07	1.78	0.25	12%	1.85	2.06	1.44	0.12	6%
C7-OLE	C7 Alkenes	5.76	1.08	19%	5.92	3%	2.36	0.53	23%	1.53	0.47	31%	1.80	2.59	1.43	0.26	14%	1.42	1.63	1.00	0.13	9%
C8-OLE	C8 Alkenes	4.68	0.89	19%	4.79	2%	1.92	0.45	24%	1.23	0.40	32%	1.44	1.94	1.12	0.20	14%	1.08	1.26	0.66	0.13	12%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
C9-OLE	C9 Alkenes	4.03	0.79	20%	4.14	3%	1.70	0.42	25%	1.09	0.37	34%	1.25	1.67	0.95	0.18	14%	0.88	1.05	0.43	0.14	16%
C10-OLE	C10 Alkenes	3.39	0.68	20%	3.46	2%	1.44	0.38	26%	0.91	0.33	36%	1.04	1.40	0.77	0.16	15%	0.69	0.86	0.25	0.14	20%
C11-OLE	C11 Alkenes	3.09	0.63	20%	3.15	2%	1.33	0.36	27%	0.85	0.31	36%	0.96	1.30	0.71	0.15	16%	0.61	0.79	0.17	0.14	22%
C12-OLE	C12 Alkenes	2.73	0.56	21%	2.80	3%	1.18	0.32	27%	0.75	0.28	37%	0.84	1.14	0.61	0.13	16%	0.52	0.69	0.11	0.13	25%
C13-OLE	C13 Alkenes	2.46	0.51	21%	2.53	3%	1.06	0.30	28%	0.67	0.26	38%	0.75	1.02	0.54	0.12	17%	0.46	0.62	0.06	0.13	28%
C14-OLE	C14 Alkenes	2.28	0.47	21%	2.32	2%	0.98	0.27	28%	0.62	0.23	38%	0.70	0.96	0.50	0.12	17%	0.42	0.57	0.06	0.12	27%
C15-OLE	C15 Alkenes	2.06	0.43	21%	2.10	2%	0.90	0.26	29%	0.56	0.22	40%	0.61	0.85	0.44	0.11	18%	0.36	0.51	0.01	0.12	33%
CYC-PNTE	Cyclopentene	7.38	1.30	18%	7.65	4%	2.81	0.57	20%	1.81	0.52	29%	2.19	3.70	1.70	0.37	17%	1.90	2.23	1.54	0.17	9%
1M-CC5E	1-Methyl cyclopentene	13.95	1.94	14%	14.55	4%	4.87	0.69	14%	2.81	0.68	24%	3.50	5.18	2.72	0.49	14%	4.99	6.24	4.04	0.43	9%
CYC-HEXE	Cyclohexene	5.45	1.04	19%	5.64	4%	2.24	0.50	22%	1.51	0.46	30%	1.79	2.85	1.32	0.34	19%	1.38	1.75	0.91	0.17	12%
1M-CC6E	1-Methyl Cyclohexene	7.81	1.21	16%	8.18	5%	2.89	0.52	18%	1.73	0.47	27%	2.10	2.91	1.76	0.19	9%	2.44	2.91	1.87	0.23	10%
4M-CC6E	4-Methyl Cyclohexene	4.48	0.88	20%	4.61	3%	1.86	0.44	24%	1.25	0.40	32%	1.47	2.26	1.05	0.28	19%	1.07	1.37	0.59	0.16	15%
12M-CC6E	1,2-Dimethyl Cyclohexene	6.77	1.11	16%	7.07	4%	2.56	0.50	19%	1.46	0.43	29%	1.73	2.05	1.42	0.14	8%	2.14	2.45	1.65	0.23	11%
13-BUTDE	1,3-Butadiene	13.58	1.88	14%	13.99	3%	4.83	0.73	15%	2.90	0.70	24%	3.59	5.36	3.10	0.42	12%	4.03	4.85	3.71	0.24	6%
ISOPRENE	Isoprene	10.69	1.62	15%	11.03	3%	3.95	0.64	16%	2.48	0.62	25%	3.01	4.52	2.60	0.36	12%	3.04	3.44	2.77	0.16	5%
C6-OL2D	C6 Cyclic or di-olefins	8.65	1.42	16%	8.94	3%	3.31	0.62	19%	2.11	0.57	27%	2.57	4.16	2.20	0.36	14%	2.43	2.68	2.02	0.14	6%
C7-OL2D	C7 Cyclic or di-olefins	7.49	1.24	17%	7.72	3%	2.95	0.57	19%	1.89	0.52	27%	2.27	3.59	1.91	0.31	14%	2.05	2.27	1.56	0.15	7%
C8-OL2D	C8 Cyclic or di-olefins	6.01	1.15	19%	6.20	3%	2.39	0.55	23%	1.56	0.48	31%	1.85	2.85	1.42	0.31	17%	1.42	1.71	0.90	0.17	12%
C9-OL2D	C9 Cyclic or di-olefins	5.40	1.04	19%	5.56	3%	2.21	0.53	24%	1.45	0.47	32%	1.71	2.53	1.26	0.29	17%	1.23	1.48	0.67	0.17	14%
C10-OL2D	C10 Cyclic or di-olefins	4.56	0.90	20%	4.69	3%	1.89	0.47	25%	1.23	0.41	33%	1.44	2.11	1.03	0.25	17%	0.99	1.20	0.45	0.16	16%
C11-OL2D	C11 Cyclic or di-olefins	4.29	0.85	20%	4.37	2%	1.81	0.46	25%	1.19	0.40	34%	1.37	1.93	0.99	0.23	17%	0.92	1.12	0.38	0.16	17%
C12-OL2D	C12 Cyclic or di-olefins	3.79	0.76	20%	3.91	3%	1.61	0.41	26%	1.05	0.36	34%	1.21	1.66	0.86	0.20	17%	0.80	0.98	0.30	0.15	19%
C13-OL2D	C13 Cyclic or di-olefins	3.42	0.69	20%	3.53	3%	1.45	0.38	26%	0.94	0.33	35%	1.08	1.48	0.79	0.18	16%	0.70	0.88	0.23	0.14	20%
C14-OL2D	C14 Cyclic or di-olefins	3.11	0.63	20%	3.18	2%	1.32	0.35	27%	0.85	0.30	36%	0.97	1.34	0.69	0.16	16%	0.62	0.80	0.17	0.14	22%
C15-OL2D	C15 Cyclic or di-olefins	2.85	0.58	20%	2.91	2%	1.21	0.32	27%	0.78	0.28	36%	0.89	1.23	0.64	0.15	17%	0.56	0.72	0.13	0.13	24%
CYC-PNDE	Cyclopentadiene	7.61	1.34	18%	7.88	4%	2.89	0.59	20%	1.86	0.53	29%	2.26	3.81	1.75	0.38	17%	1.96	2.29	1.59	0.17	9%
3-CARENE	3-Carene	3.21	0.63	19%	3.36	5%	1.27	0.30	24%	0.79	0.26	34%	0.91	1.13	0.64	0.10	11%	0.79	1.00	0.21	0.15	19%
A-PINENE	a-Pinene	4.29	0.68	16%	4.51	5%	1.56	0.29	19%	0.90	0.26	29%	1.08	1.21	0.88	0.08	8%	1.23	1.42	0.76	0.16	13%
B-PINENE	b-Pinene	3.28	0.62	19%	3.39	3%	1.37	0.32	24%	0.83	0.28	34%	0.94	1.12	0.75	0.09	10%	0.82	0.96	0.42	0.11	13%
D-LIMONE	d-Limonene	3.99	0.72	18%	4.19	5%	1.48	0.31	21%	0.89	0.27	30%	1.06	1.25	0.76	0.09	9%	1.15	1.44	0.46	0.19	17%
SABINENE	Sabinene	3.67	0.65	18%	3.81	4%	1.45	0.32	22%	0.84	0.28	34%	0.96	1.10	0.73	0.09	9%	0.97	1.15	0.48	0.14	14%
TERPENE	Terpene	3.79	0.65	17%	3.95	4%	1.45	0.30	21%	0.86	0.27	31%	1.00	1.14	0.78	0.07	7%	1.02	1.21	0.54	0.14	13%
STYRENE	Styrene	1.95	0.39	20%	2.04	5%	-0.62	0.18	-29%	-1.57	0.56	-36%	-1.86	0.53	-9.07	1.78	-96%	-0.59	0.55	-3.01	0.86	-145%
AME-STYR	a-Methyl Styrene	1.72	0.34	20%	1.80	5%	-0.55	0.16	-29%	-1.38	0.50	-36%	-1.64	0.47	-8.00	1.57	-96%	-0.52	0.49	-2.64	0.76	-145%
C9-STYR	C9 Styrenes	1.72	0.34	20%	1.80	5%	-0.55	0.16	-29%	-1.38	0.50	-36%	-1.64	0.47	-8.00	1.57	-96%	-0.52	0.49	-2.64	0.76	-145%
C10-STYR	C10 Styrenes	1.53	0.31	20%	1.61	5%	-0.49	0.14	-29%	-1.24	0.44	-36%	-1.47	0.42	-7.14	1.40	-96%	-0.46	0.43	-2.37	0.68	-145%
BENZENE	Benzene	0.81	0.19	24%	0.82	1%	0.34	0.13	38%	0.16	0.12	74%	0.17	0.28	-0.31	0.11	63%	0.17	0.22	0.05	0.03	19%
TOLUENE	Toluene	3.97	0.72	18%	4.05	2%	1.17	0.32	28%	0.36	0.31	86%	0.44	1.06	-1.79	0.51	116%	0.78	1.01	0.15	0.17	22%
C2-BENZ	Ethyl Benzene	2.79	0.56	20%	2.83	2%	1.00	0.30	30%	0.43	0.27	64%	0.48	0.80	-0.97	0.31	63%	0.58	0.71	0.14	0.10	17%
I-C3-BEN	Isopropyl Benzene (cumene)	2.32	0.47	20%	2.36	2%	0.84	0.26	31%	0.36	0.23	65%	0.40	0.67	-0.83	0.26	65%	0.48	0.59	0.11	0.09	18%
N-C3-BEN	n-Propyl Benzene	2.20	0.45	20%	2.23	1%	0.79	0.25	31%	0.34	0.22	66%	0.38	0.64	-0.81	0.25	67%	0.45	0.56	0.09	0.08	18%
C9-BENI	C9 Monosub. Benzenes	2.20	0.45	20%	2.23	1%	0.79	0.25	31%	0.34	0.22	66%	0.38	0.64	-0.81	0.25	67%	0.45	0.56	0.09	0.08	18%
S-C4-BEN	s-Butyl Benzene	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%
C10-BENI	C10 Monosub. Benzenes	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
N-C4-BEN	n-Butyl Benzene	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%
C11-BEN1	C11 Monosub. Benzenes	1.78	0.36	20%	1.81	1%	0.64	0.20	31%	0.27	0.18	66%	0.31	0.52	-0.66	0.20	67%	0.36	0.45	0.07	0.07	18%
C12-BEN1	C12 Monosub. Benzenes	1.63	0.33	20%	1.65	1%	0.59	0.18	31%	0.25	0.17	66%	0.28	0.47	-0.60	0.19	67%	0.33	0.42	0.07	0.06	18%
C13-BEN1	C13 Monosub. Benzenes	1.50	0.31	20%	1.52	1%	0.54	0.17	31%	0.23	0.15	66%	0.26	0.44	-0.55	0.17	67%	0.31	0.38	0.06	0.06	18%
M-XYLENE	m-Xylene	10.61	1.49	14%	10.89	3%	3.19	0.47	15%	1.55	0.47	31%	1.95	3.30	0.53	0.51	26%	2.88	3.38	2.26	0.27	9%
O-XYLENE	o-Xylene	7.49	1.19	16%	7.67	2%	2.46	0.46	19%	1.22	0.42	34%	1.50	2.02	0.34	0.32	21%	1.84	2.03	1.57	0.13	7%
P-XYLENE	p-Xylene	4.25	0.75	18%	4.34	2%	1.36	0.35	25%	0.55	0.33	60%	0.63	1.10	-1.47	0.44	70%	0.88	1.07	0.23	0.15	17%
C8-BEN2	C8 Disub. Benzenes	5.16	0.84	16%	5.28	2%	1.68	0.35	21%	0.77	0.33	43%	0.93	1.37	-0.58	0.34	37%	1.24	1.37	0.84	0.12	10%
C9-BEN2	C9 Disub. Benzenes	6.61	1.00	15%	6.76	2%	2.07	0.37	18%	0.98	0.35	36%	1.21	1.88	-0.17	0.36	29%	1.66	1.88	1.34	0.14	9%
C10-BEN2	C10 Disub. Benzenes	5.92	0.90	15%	6.04	2%	1.85	0.33	18%	0.88	0.32	36%	1.08	1.69	-0.15	0.32	29%	1.49	1.68	1.20	0.13	9%
C11-BEN2	C11 Disub. Benzenes	5.35	0.81	15%	5.49	2%	1.68	0.30	18%	0.79	0.29	36%	0.98	1.53	-0.14	0.29	30%	1.35	1.52	1.09	0.12	9%
C12-BEN2	C12 Disub. Benzenes	4.90	0.74	15%	5.01	2%	1.53	0.27	18%	0.73	0.26	36%	0.89	1.39	-0.13	0.26	30%	1.23	1.39	0.99	0.11	9%
C13-BEN2	C13 Disub. Benzenes	4.50	0.68	15%	4.60	2%	1.41	0.25	18%	0.67	0.24	36%	0.82	1.28	-0.12	0.24	29%	1.13	1.28	0.91	0.10	9%
C8-BEN2	Isomers of Ethylbenzene	5.16	0.84	16%	5.28	2%	1.68	0.35	21%	0.77	0.33	43%	0.93	1.37	-0.58	0.34	37%	1.24	1.37	0.84	0.12	10%
123-TMB	1,2,3-Trimethyl Benzene	11.26	1.58	14%	11.57	3%	3.49	0.50	14%	1.81	0.49	27%	2.28	3.57	1.63	0.41	18%	3.12	3.70	2.51	0.26	8%
124-TMB	1,2,4-Trimethyl Benzene	7.18	1.09	15%	7.37	3%	2.32	0.41	18%	1.18	0.39	33%	1.44	2.14	0.27	0.30	21%	1.83	2.15	1.45	0.14	8%
135-TMB	1,3,5-Trimethyl Benzene	11.22	1.55	14%	11.57	3%	3.44	0.44	13%	1.80	0.46	26%	2.29	3.74	1.68	0.42	18%	3.34	4.07	2.70	0.30	9%
C9-BEN	Isomers of Propylbenzene	6.12	0.91	15%	6.29	3%	1.96	0.33	17%	0.98	0.32	33%	1.21	1.83	0.24	0.27	22%	1.63	1.89	1.34	0.12	8%
C9-BEN3	C9 Trisub. Benzenes	9.90	1.40	14%	10.17	3%	3.09	0.44	14%	1.60	0.44	28%	2.00	3.14	1.26	0.36	18%	2.77	3.32	2.26	0.23	8%
C10-BEN	Isomers of Butylbenzene	5.48	0.82	15%	5.62	3%	1.76	0.30	17%	0.88	0.29	33%	1.08	1.64	0.22	0.24	22%	1.46	1.69	1.20	0.11	8%
C10-BEN4	C10 Tetrasub. Benzenes	8.86	1.26	14%	9.12	3%	2.76	0.40	14%	1.43	0.40	28%	1.79	2.82	1.13	0.32	18%	2.48	2.97	2.02	0.20	8%
C10-BEN3	C10 Trisub. Benzenes	8.86	1.26	14%	9.12	3%	2.76	0.40	14%	1.43	0.40	28%	1.79	2.82	1.13	0.32	18%	2.48	2.97	2.02	0.20	8%
C11-BEN	Isomers of Pentylbenzene	4.96	0.74	15%	5.09	3%	1.59	0.27	17%	0.79	0.26	33%	0.98	1.48	0.20	0.22	22%	1.32	1.54	1.09	0.10	8%
C11-BEN5	C11 Pentasub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C11-BEN4	C11 Tetrasub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C11-BEN3	C11 Trisub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C12-BEN	Isomers of Hexylbenzene	4.53	0.68	15%	4.65	3%	1.45	0.25	17%	0.72	0.24	33%	0.89	1.35	0.18	0.20	22%	1.21	1.40	1.00	0.09	8%
C12-BEN5	C11 Pentasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN6	C12 Hexaasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN4	C12 Tetrasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN3	C12 Trisub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C13-BEN3	C13 Trisub. Benzenes	6.75	0.96	14%	6.94	3%	2.10	0.30	14%	1.09	0.30	28%	1.37	2.14	0.86	0.24	18%	1.89	2.26	1.54	0.15	8%
INDAN	Indan	3.17	0.48	15%	3.26	3%	0.41	0.29	70%	-0.39	0.42	-109%	-0.46	0.83	-5.80	1.13	-	0.29	0.84	-1.68	0.49	170%
NAPHTHAL	Naphthalene	3.26	0.57	17%	3.35	3%	1.02	0.27	27%	0.44	0.27	60%	0.53	0.84	-0.96	0.31	60%	0.68	0.82	0.07	0.14	21%
TETRALIN	Tetralin	2.83	0.43	15%	2.91	3%	0.37	0.26	70%	-0.35	0.38	-109%	-0.41	0.75	-5.18	1.01	-	0.26	0.75	-1.51	0.43	170%
ME-NAPH	Methyl Naphthalenes	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
1ME-NAPH	1-Methyl Naphthalene	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
2ME-NAPH	2-Methyl Naphthalene	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
C11-TET	C11 Tetralin or Indane	2.56	0.39	15%	2.63	3%	0.33	0.23	70%	-0.31	0.34	-109%	-0.37	0.67	-4.68	0.91	-	0.23	0.68	-1.37	0.39	170%
23-DMN	2,3-Dimethyl Naphth.	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
C12-NAP2	C12 Disub. Naphthalenes	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
DM-NAPH	Dimethyl Naphthalenes	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
C12-NAP1	C12 Monosub. Naphth.	4.20	0.63	15%	4.31	3%	1.21	0.21	17%	0.50	0.22	44%	0.64	1.26	-0.70	0.32	50%	1.03	1.34	0.47	0.18	18%
C13-NAP2	C13 Disub. Naphthalenes	5.08	0.73	14%	5.24	3%	1.47	0.22	15%	0.67	0.23	34%	0.86	1.59	-0.12	0.29	34%	1.39	1.76	0.92	0.18	13%
C13-NAP3	C13 Trisub. Naphthalenes	5.08	0.73	14%	5.24	3%	1.47	0.22	15%	0.67	0.23	34%	0.86	1.59	-0.12	0.29	34%	1.39	1.76	0.92	0.18	13%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
C13-NAPI	C13 Monosub. Naphth.	3.86	0.58	15%	3.96	3%	1.11	0.19	17%	0.46	0.20	44%	0.59	1.16	-0.65	0.29	50%	0.95	1.23	0.43	0.17	18%
ACETYLEN	Acetylene	1.25	0.22	18%	1.26	1%	0.49	0.10	20%	0.28	0.08	29%	0.34	0.47	0.28	0.04	12%	0.30	0.38	0.27	0.03	9%
ME-ACTYL	Methyl Acetylene	6.45	1.15	18%	6.58	2%	2.35	0.49	21%	1.38	0.42	30%	1.68	2.41	1.08	0.19	11%	1.44	1.68	1.08	0.12	8%
2-BUTYNE	2-Butyne	16.33	2.36	14%	16.72	2%	5.30	0.76	14%	3.08	0.71	23%	3.90	6.48	3.03	0.64	17%	4.38	5.26	3.61	0.40	9%
ET-ACTYL	Ethyl Acetylene	6.20	1.20	19%	6.28	1%	2.39	0.61	25%	1.43	0.52	36%	1.68	2.21	0.70	0.26	15%	1.32	1.60	0.86	0.15	12%
MEOH	Methanol	0.71	0.14	19%	0.72	1%	0.34	0.06	18%	0.22	0.05	25%	0.26	0.44	0.16	0.05	21%	0.21	0.30	0.14	0.03	15%
ETOH	Ethanol	1.69	0.42	25%	1.71	1%	0.93	0.27	29%	0.65	0.23	35%	0.73	1.16	0.31	0.17	24%	0.45	0.66	0.27	0.08	18%
I-C3-OH	Isopropyl Alcohol	0.71	0.14	19%	0.72	1%	0.39	0.07	18%	0.28	0.07	23%	0.33	0.63	0.15	0.09	27%	0.26	0.41	0.14	0.06	22%
N-C3-OH	n-Propyl Alcohol	2.74	0.65	24%	2.76	1%	1.39	0.41	30%	0.94	0.35	37%	1.05	1.52	0.56	0.23	22%	0.67	0.95	0.48	0.10	15%
I-C4-OH	Isobutyl Alcohol	2.24	0.48	22%	2.26	1%	1.10	0.28	26%	0.73	0.24	33%	0.83	1.24	0.48	0.15	18%	0.58	0.75	0.44	0.07	11%
N-C4-OH	n-Butyl Alcohol	3.34	0.74	22%	3.37	1%	1.62	0.44	27%	1.09	0.38	35%	1.24	1.82	0.73	0.25	20%	0.84	1.14	0.66	0.11	13%
S-C4-OH	s-Butyl Alcohol	1.60	0.35	22%	1.62	2%	0.84	0.21	25%	0.59	0.18	30%	0.67	1.11	0.33	0.14	21%	0.48	0.66	0.30	0.08	17%
T-C4-OH	t-Butyl Alcohol	0.45	0.09	20%	0.46	1%	0.25	0.05	19%	0.17	0.04	26%	0.19	0.34	0.09	0.05	25%	0.14	0.21	0.08	0.03	18%
CC5-OH	Cyclopentanol	1.96	0.42	21%	1.98	1%	0.99	0.25	25%	0.68	0.21	31%	0.77	1.19	0.42	0.15	20%	0.55	0.74	0.39	0.08	14%
2-C5OH	2-Pentanol	1.74	0.36	21%	1.76	1%	0.89	0.22	25%	0.61	0.19	31%	0.69	1.11	0.37	0.14	20%	0.50	0.69	0.34	0.08	15%
3-C5OH	3-Pentanol	1.73	0.38	22%	1.77	2%	0.88	0.22	25%	0.61	0.19	32%	0.69	1.10	0.37	0.14	20%	0.49	0.66	0.34	0.07	15%
C5OH	Pentyl Alcohol	3.35	0.73	22%	3.40	2%	1.60	0.42	27%	1.08	0.37	34%	1.22	1.79	0.74	0.24	19%	0.84	1.10	0.67	0.10	12%
CC6-OH	Cyclohexanol	2.25	0.52	23%	2.27	1%	1.20	0.33	27%	0.81	0.28	34%	0.89	1.21	0.43	0.17	19%	0.61	0.78	0.40	0.09	14%
1-C6OH	1-Hexanol	2.74	0.61	22%	2.77	1%	1.36	0.37	27%	0.91	0.31	34%	1.02	1.40	0.58	0.19	19%	0.69	0.87	0.53	0.09	13%
2-C6OH	2-Hexanol	2.46	0.60	24%	2.48	0%	1.37	0.38	28%	0.93	0.32	34%	1.03	1.53	0.43	0.22	21%	0.66	0.89	0.38	0.11	17%
1-C7OH	1-Heptanol	2.21	0.51	23%	2.23	1%	1.12	0.32	28%	0.73	0.27	37%	0.80	1.09	0.45	0.15	18%	0.52	0.68	0.39	0.07	14%
1-C8-OH	1-Octanol	2.01	0.48	24%	2.05	2%	1.02	0.31	30%	0.66	0.26	40%	0.71	0.97	0.38	0.15	21%	0.43	0.62	0.22	0.09	21%
2-ETC6OH	2-Ethyl-1-Hexanol	2.20	0.49	22%	2.23	1%	1.08	0.31	28%	0.69	0.26	37%	0.76	1.02	0.46	0.13	17%	0.50	0.64	0.36	0.06	13%
2-C8-OH	2-Octanol	2.16	0.51	23%	2.19	1%	1.13	0.33	29%	0.73	0.27	38%	0.79	1.06	0.41	0.15	20%	0.50	0.70	0.30	0.09	18%
3-C8-OH	3-Octanol	2.57	0.59	23%	2.61	2%	1.28	0.37	29%	0.85	0.32	37%	0.93	1.29	0.53	0.18	19%	0.59	0.79	0.36	0.10	17%
4-C8-OH	4-Octanol	3.07	0.70	23%	3.13	2%	1.49	0.42	28%	0.98	0.36	37%	1.09	1.53	0.65	0.21	19%	0.69	0.89	0.41	0.11	16%
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	1.18	0.33	28%	1.21	2%	0.63	0.21	34%	0.38	0.18	46%	0.39	0.57	0.09	0.12	30%	0.20	0.33	-0.03	0.08	42%
ET-GLYCL	Ethylene Glycol	3.36	0.70	21%	3.43	2%	1.57	0.35	22%	1.08	0.31	29%	1.27	2.19	0.76	0.26	21%	0.90	1.22	0.69	0.13	14%
PR-GLYCL	Propylene Glycol	2.75	0.52	19%	2.80	2%	1.23	0.28	22%	0.83	0.24	29%	0.97	1.57	0.67	0.17	18%	0.76	0.98	0.63	0.08	11%
12-C4OH2	1,2-Butandiol	2.21	0.44	20%	2.24	1%	1.03	0.24	23%	0.69	0.21	30%	0.80	1.29	0.51	0.15	18%	0.60	0.79	0.47	0.07	12%
GLYCERL	Glycerol	3.27	0.65	20%	3.33	2%	1.41	0.33	23%	0.91	0.28	31%	1.07	1.62	0.74	0.17	16%	0.81	1.04	0.64	0.08	10%
C6-GLYCL	1,2-Dihydroxy Hexane	2.75	0.57	21%	2.78	1%	1.28	0.32	25%	0.84	0.27	32%	0.97	1.43	0.58	0.16	17%	0.69	0.88	0.52	0.08	11%
2M24C5OH	2-Methyl-2,4-Pentanediol	1.04	0.21	20%	1.05	0%	0.53	0.13	25%	0.36	0.11	31%	0.41	0.65	0.22	0.08	19%	0.30	0.40	0.20	0.04	14%
ME-O-ME	Dimethyl Ether	0.93	0.18	19%	0.95	2%	0.58	0.09	16%	0.44	0.09	21%	0.52	1.11	0.18	0.18	34%	0.40	0.68	0.18	0.11	27%
TME-OX	Trimethylene Oxide	5.22	1.18	23%	5.33	2%	2.74	0.66	24%	2.01	0.61	30%	2.32	4.21	1.06	0.61	26%	1.59	2.50	1.00	0.33	21%
THF	Tetrahydrofuran	4.95	1.03	21%	5.03	2%	2.40	0.57	24%	1.67	0.51	30%	1.91	3.01	1.13	0.38	20%	1.43	2.03	1.07	0.21	15%
ET-O-ET	Diethyl Ether	4.01	0.68	17%	4.12	3%	1.86	0.30	16%	1.26	0.29	23%	1.48	2.64	1.00	0.29	19%	1.33	1.92	0.97	0.21	16%
METHYLAL	Dimethoxy methane	1.04	0.20	19%	1.06	2%	0.66	0.11	16%	0.50	0.11	21%	0.59	1.26	0.20	0.20	34%	0.45	0.76	0.19	0.12	27%
AM-THF	Alpha-Methyltetrahydrofuran	4.62	0.92	20%	4.74	2%	2.17	0.50	23%	1.48	0.45	30%	1.70	2.48	1.11	0.30	18%	1.30	1.82	1.06	0.17	13%
THP	Tetrahydropyran	3.81	0.81	21%	3.87	2%	1.96	0.46	24%	1.34	0.41	30%	1.51	2.24	0.81	0.28	19%	1.12	1.58	0.75	0.17	15%
ET-O-IPR	Ethyl Isopropyl Ether	3.86	0.63	16%	3.98	3%	1.66	0.26	16%	1.10	0.26	23%	1.30	2.12	1.04	0.21	16%	1.25	1.71	1.04	0.16	13%
MNBE	Methyl n-Butyl Ether	3.66	0.76	21%	3.73	2%	1.81	0.42	23%	1.26	0.38	30%	1.43	2.23	0.81	0.28	20%	1.06	1.49	0.76	0.15	15%
MTBE	Methyl t-Butyl Ether	0.78	0.17	21%	0.79	2%	0.47	0.10	21%	0.32	0.09	27%	0.36	0.64	0.15	0.09	24%	0.26	0.38	0.14	0.05	19%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
PR-O-PR	Di n-Propyl Ether	3.24	0.65	20%	3.33	3%	1.62	0.36	22%	1.13	0.32	28%	1.29	2.08	0.72	0.25	20%	0.97	1.42	0.67	0.15	15%
ENBE	Ethyl n-Butyl Ether	3.86	0.73	19%	3.95	2%	1.80	0.39	22%	1.21	0.35	29%	1.39	2.12	0.93	0.23	17%	1.11	1.51	0.89	0.13	12%
ETBE	Ethyl t-Butyl Ether	2.11	0.39	18%	2.16	2%	1.04	0.18	17%	0.69	0.17	24%	0.80	1.35	0.48	0.15	18%	0.67	0.93	0.46	0.10	15%
MTAE	Methyl t-Amyl Ether	2.14	0.44	20%	2.19	2%	1.11	0.23	20%	0.75	0.20	27%	0.86	1.40	0.45	0.16	18%	0.65	0.88	0.42	0.09	14%
2BU-THF	2-Butyl Tetrahydrofuran	2.53	0.60	24%	2.59	2%	1.22	0.36	30%	0.79	0.31	39%	0.86	1.20	0.54	0.18	21%	0.50	0.77	0.08	0.14	28%
IBU2-O	Di-Isobutyl Ether	1.29	0.32	24%	1.34	3%	0.69	0.19	27%	0.46	0.16	35%	0.49	0.73	0.25	0.10	20%	0.36	0.54	0.21	0.08	21%
BU-O-BU	Di-n-butyl Ether	3.17	0.67	21%	3.24	2%	1.50	0.39	26%	1.01	0.34	34%	1.13	1.53	0.74	0.20	17%	0.79	1.05	0.51	0.11	14%
C5-O-C5	Di-n-Pentyl Ether	2.64	0.63	24%	2.69	2%	1.36	0.40	29%	0.91	0.34	37%	0.99	1.35	0.53	0.19	20%	0.61	0.89	0.29	0.13	21%
MEO-ETOH	2-Methoxyethanol	2.98	0.48	16%	3.05	2%	1.30	0.21	16%	0.87	0.20	23%	1.04	1.87	0.78	0.20	19%	0.95	1.33	0.76	0.13	13%
MEOC3OH	1-Methoxy-2-Propanol	2.62	0.51	19%	2.68	3%	1.28	0.26	21%	0.90	0.24	26%	1.05	1.87	0.58	0.23	22%	0.81	1.16	0.55	0.13	16%
ETO-ETOH	2-Ethoxyethanol	3.78	0.64	17%	3.86	2%	1.65	0.30	18%	1.09	0.27	25%	1.29	2.16	0.98	0.21	16%	1.15	1.54	0.95	0.13	11%
2MEOC3OH	2-Methoxy-1-Propanol	3.01	0.41	14%	3.09	2%	1.18	0.15	13%	0.75	0.16	21%	0.91	1.52	0.77	0.15	16%	0.98	1.35	0.86	0.11	11%
ETOC3OH	1-Ethoxy-2-Propanol	3.25	0.59	18%	3.32	2%	1.52	0.30	19%	1.04	0.27	26%	1.21	2.02	0.76	0.23	19%	0.99	1.36	0.73	0.13	14%
2PROETOH	2-Propoxyethanol	3.52	0.63	18%	3.60	2%	1.60	0.33	20%	1.08	0.29	27%	1.25	2.01	0.87	0.21	17%	1.05	1.41	0.84	0.12	12%
3ETOC3OH	3-Ethoxy-1-Propanol	4.24	0.70	16%	4.33	2%	1.82	0.32	18%	1.19	0.30	25%	1.40	2.24	1.13	0.20	14%	1.27	1.65	1.11	0.13	10%
3MEOC4OH	3-Methoxy-1-Butanol	0.97	0.19	20%	0.98	1%	0.52	0.10	20%	0.35	0.09	26%	0.41	0.72	0.20	0.09	22%	0.31	0.43	0.19	0.05	17%
DET-GLCL	Diethylene Glycol	3.55	0.61	17%	3.62	2%	1.53	0.30	20%	1.00	0.27	27%	1.17	1.82	0.94	0.17	14%	1.05	1.33	0.93	0.10	9%
PROXC3OH	1-Propoxy-2-Propanol	2.86	0.57	20%	2.92	2%	1.41	0.31	22%	0.97	0.28	28%	1.12	1.84	0.62	0.22	20%	0.84	1.20	0.58	0.12	15%
BUO-ETOH	2-Butoxyethanol	2.90	0.52	18%	2.95	2%	1.28	0.28	22%	0.83	0.25	30%	0.96	1.35	0.73	0.12	13%	0.80	0.98	0.70	0.06	8%
3MOMC4OH	3 methoxy -3 methyl-Butanol	1.74	0.37	22%	1.76	1%	0.88	0.23	26%	0.59	0.19	33%	0.66	1.00	0.37	0.12	18%	0.46	0.59	0.34	0.06	12%
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	2.90	0.51	18%	2.96	2%	1.35	0.26	19%	0.93	0.24	26%	1.08	1.79	0.71	0.20	19%	0.97	1.38	0.72	0.14	15%
PG-1TB-E	1-tert-Butoxy-2-Propanol	1.71	0.37	21%	1.74	1%	0.88	0.22	26%	0.59	0.19	32%	0.66	0.95	0.35	0.12	18%	0.45	0.60	0.31	0.06	13%
PG-2TB-E	2-tert-Butoxy-1-Propanol	1.81	0.26	14%	1.84	2%	0.71	0.11	16%	0.43	0.11	24%	0.51	0.77	0.45	0.05	10%	0.51	0.63	0.46	0.03	6%
BUOC3OH	n-Butoxy-2-Propanol	2.70	0.56	21%	2.75	2%	1.31	0.32	24%	0.89	0.28	32%	1.01	1.47	0.60	0.18	18%	0.72	0.99	0.55	0.10	13%
CARBITOL	2-(2-Ethoxyethoxy) EtOH	3.19	0.59	19%	3.26	2%	1.47	0.31	21%	0.99	0.28	29%	1.14	1.64	0.76	0.18	16%	0.97	1.35	0.76	0.12	12%
DPR-GLCL	Dipropylene Glycol	2.48	0.51	20%	2.53	2%	1.23	0.28	23%	0.85	0.25	29%	0.96	1.51	0.52	0.19	19%	0.72	1.00	0.48	0.10	14%
EGHE	2-Hexyloxyethanol	2.45	0.52	21%	2.50	2%	1.20	0.32	26%	0.78	0.27	35%	0.86	1.12	0.53	0.14	16%	0.61	0.80	0.44	0.08	13%
DGPE	2-(2-Propoxyethoxy) ethanol	3.00	0.58	19%	3.06	2%	1.42	0.32	22%	0.96	0.28	29%	1.09	1.60	0.69	0.18	17%	0.87	1.22	0.67	0.11	13%
DPRGOME	Dipropylene Glycol Methyl Ether	2.21	0.41	18%	2.26	3%	1.05	0.21	20%	0.73	0.19	27%	0.83	1.25	0.49	0.15	18%	0.71	1.06	0.48	0.11	16%
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	2.70	0.55	20%	2.77	3%	1.28	0.31	24%	0.86	0.27	32%	0.97	1.27	0.61	0.15	16%	0.72	0.98	0.53	0.09	13%
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	2.62	0.51	19%	2.66	2%	1.26	0.27	22%	0.86	0.25	28%	0.98	1.42	0.58	0.17	17%	0.83	1.22	0.57	0.13	15%
EGEHE	2-(2-Ethylhexyloxy) ethanol	1.71	0.44	26%	1.74	2%	0.89	0.29	33%	0.56	0.25	44%	0.58	0.81	0.24	0.15	27%	0.32	0.53	0.02	0.11	36%
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	2.66	0.54	20%	2.74	3%	1.28	0.30	23%	0.86	0.26	31%	0.97	1.29	0.58	0.16	16%	0.77	1.11	0.55	0.11	15%
DGHE	2-(2-Hexyloxyethoxy) ethanol	2.03	0.48	23%	2.07	2%	1.03	0.29	28%	0.68	0.25	37%	0.73	0.98	0.40	0.14	19%	0.47	0.69	0.21	0.10	21%
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	2.46	0.52	21%	2.52	2%	1.19	0.30	25%	0.80	0.26	33%	0.90	1.16	0.52	0.15	17%	0.66	0.97	0.41	0.11	16%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	2.24	0.49	22%	2.29	2%	1.09	0.29	27%	0.73	0.25	35%	0.80	1.07	0.47	0.14	18%	0.55	0.79	0.25	0.10	18%
TPRGOME	Tripropylene Glycol Monomethyl Ether	1.90	0.41	21%	1.95	3%	0.93	0.23	25%	0.62	0.20	33%	0.69	0.91	0.39	0.12	17%	0.52	0.80	0.25	0.11	20%
TETRAGME	2,5,8,11-Tetraoxatridecan-13-ol	2.15	0.47	22%	2.20	2%	1.07	0.26	25%	0.72	0.23	32%	0.80	1.06	0.44	0.14	18%	0.61	0.94	0.36	0.11	18%
TETRAGBE	3,6,9,12-Tetraoxahexa-decan-1-ol	1.90	0.45	24%	1.94	2%	0.94	0.27	29%	0.63	0.23	37%	0.68	0.93	0.37	0.14	20%	0.43	0.68	0.07	0.11	27%
ME-FORM	Methyl Formate	0.07	0.01	21%	0.07	2%	0.05	0.01	20%	0.04	0.01	24%	0.04	0.09	0.01	0.01	36%	0.03	0.05	0.01	0.01	29%
ET-FORM	Ethyl Formate	0.52	0.13	25%	0.53	2%	0.31	0.09	29%	0.23	0.08	35%	0.26	0.44	0.10	0.07	27%	0.15	0.24	0.09	0.03	22%
ME-ACET	Methyl Acetate	0.07	0.02	22%	0.07	2%	0.05	0.01	20%	0.04	0.01	25%	0.05	0.10	0.01	0.02	36%	0.03	0.05	0.01	0.01	29%
ET-ACET	Ethyl Acetate	0.64	0.15	24%	0.65	1%	0.37	0.10	28%	0.26	0.09	34%	0.29	0.48	0.12	0.07	24%	0.18	0.26	0.11	0.03	19%
ME-PRAT	Methyl Propionate	0.71	0.16	23%	0.71	1%	0.35	0.10	28%	0.22	0.08	36%	0.25	0.34	0.14	0.04	16%	0.17	0.22	0.13	0.02	10%
C3-FORM	n-Propyl Formate	0.93	0.26	28%	0.93	1%	0.55	0.19	34%	0.39	0.16	41%	0.43	0.66	0.15	0.12	29%	0.23	0.36	0.13	0.06	25%
ET-PRAT	Ethyl Propionate	0.79	0.19	24%	0.80	1%	0.44	0.13	29%	0.30	0.11	35%	0.34	0.52	0.15	0.07	22%	0.21	0.29	0.13	0.04	17%
IPR-ACET	Isopropyl Acetate	1.24	0.23	18%	1.25	1%	0.65	0.12	18%	0.44	0.11	24%	0.51	0.89	0.27	0.11	21%	0.40	0.56	0.25	0.07	16%
ME-BUAT	Methyl Butyrate	1.18	0.26	22%	1.19	1%	0.60	0.16	26%	0.38	0.13	34%	0.43	0.61	0.23	0.07	16%	0.31	0.39	0.21	0.03	11%
ME-IBUAT	Methyl Isobutyrate	0.70	0.18	25%	0.71	1%	0.40	0.12	31%	0.27	0.10	39%	0.29	0.43	0.13	0.07	23%	0.18	0.25	0.11	0.03	18%
C4-FORM	n-Butyl Formate	0.95	0.25	27%	0.96	1%	0.57	0.18	32%	0.40	0.16	38%	0.44	0.65	0.16	0.11	26%	0.25	0.37	0.14	0.06	22%
PR-ACET	Propyl Acetate	0.87	0.23	26%	0.88	1%	0.52	0.16	31%	0.36	0.14	37%	0.40	0.60	0.15	0.10	25%	0.23	0.33	0.13	0.05	21%
ET-BUAT	Ethyl Butyrate	1.25	0.28	22%	1.27	1%	0.65	0.17	26%	0.43	0.14	33%	0.48	0.72	0.24	0.08	18%	0.32	0.40	0.22	0.04	13%
IBU-ACET	Isobutyl Acetate	0.67	0.15	22%	0.69	2%	0.43	0.09	20%	0.30	0.08	26%	0.34	0.59	0.12	0.09	26%	0.25	0.36	0.11	0.05	21%
ME-PVAT	Methyl Pivalate	0.41	0.11	26%	0.41	1%	0.24	0.07	30%	0.16	0.06	37%	0.17	0.23	0.07	0.04	20%	0.10	0.14	0.06	0.02	16%
BU-ACET	n-Butyl Acetate	0.89	0.23	26%	0.90	1%	0.54	0.16	31%	0.37	0.14	37%	0.40	0.55	0.15	0.09	23%	0.24	0.32	0.13	0.04	18%
PR-PRAT	n-Propyl Propionate	0.93	0.24	26%	0.93	1%	0.53	0.17	32%	0.36	0.14	39%	0.39	0.57	0.16	0.09	23%	0.23	0.30	0.14	0.05	20%
SBU-ACET	s-Butyl Acetate	1.43	0.34	24%	1.46	2%	0.81	0.20	25%	0.57	0.17	31%	0.64	1.07	0.27	0.14	22%	0.42	0.60	0.24	0.07	17%
TBU-ACET	t-Butyl Acetate	0.22	0.04	20%	0.22	1%	0.13	0.03	21%	0.08	0.02	28%	0.09	0.16	0.04	0.02	21%	0.07	0.10	0.04	0.01	15%
BU-PRAT	Butyl Propionate	0.89	0.23	26%	0.89	0%	0.52	0.16	32%	0.34	0.14	40%	0.36	0.50	0.14	0.08	22%	0.21	0.30	0.12	0.04	19%
AM-ACET	Amyl Acetate	0.96	0.25	26%	0.96	0%	0.59	0.18	31%	0.38	0.15	39%	0.40	0.53	0.15	0.09	23%	0.24	0.35	0.12	0.05	19%
PR-BUAT	n-Propyl Butyrate	1.17	0.29	25%	1.18	1%	0.63	0.19	30%	0.42	0.16	37%	0.46	0.64	0.21	0.10	21%	0.27	0.37	0.18	0.05	19%
23MC4ACT	2,3-Dimethylbutyl Acetate	0.84	0.21	25%	0.85	2%	0.50	0.13	27%	0.33	0.11	34%	0.35	0.55	0.14	0.07	22%	0.23	0.34	0.13	0.04	18%
2MC5-ACT	2-Methylpentyl Acetate	1.11	0.30	27%	1.13	2%	0.64	0.20	32%	0.40	0.17	42%	0.42	0.56	0.17	0.10	24%	0.24	0.37	0.09	0.06	23%
3MC5-ACT	3-Methylpentyl Acetate	1.31	0.35	27%	1.33	1%	0.75	0.23	31%	0.48	0.19	40%	0.51	0.69	0.22	0.11	22%	0.30	0.43	0.17	0.06	19%
4MC5-ACT	4-Methylpentyl Acetate	0.92	0.26	28%	0.94	2%	0.53	0.17	33%	0.34	0.14	43%	0.35	0.48	0.12	0.09	26%	0.19	0.31	0.05	0.05	29%
IBU-IBTR	Isobutyl Isobutyrate	0.64	0.16	26%	0.65	2%	0.39	0.11	27%	0.25	0.09	35%	0.27	0.43	0.11	0.06	23%	0.17	0.25	0.09	0.03	18%
BU-BUAT	n-Butyl Butyrate	1.12	0.28	25%	1.13	1%	0.61	0.19	31%	0.39	0.16	40%	0.42	0.56	0.19	0.09	21%	0.25	0.36	0.13	0.05	22%
NC6-ACET	n-Hexyl Acetate	0.87	0.26	30%	0.88	1%	0.55	0.19	34%	0.33	0.15	45%	0.33	0.48	0.02	0.11	32%	0.18	0.31	0.02	0.06	31%
E3EOC3OH	Ethyl 3-Ethoxy Propionate	3.61	0.59	16%	3.68	2%	1.47	0.27	19%	0.91	0.25	27%	1.08	1.49	0.95	0.09	9%	0.97	1.11	0.91	0.04	4%
24MC5ACT	2,4-Dimethylpentyl Acetate	0.98	0.27	28%	1.00	2%	0.56	0.18	33%	0.33	0.15	45%	0.33	0.48	-0.02	0.11	33%	0.18	0.31	-0.02	0.07	38%
2MC6-ACT	2-Methylhexyl Acetate	0.89	0.27	31%	0.91	2%	0.54	0.19	35%	0.32	0.16	48%	0.32	0.48	-0.04	0.12	37%	0.16	0.29	-0.05	0.07	44%
3EC5-ACT	3-Ethylpentyl Acetate	1.24	0.34	28%	1.26	2%	0.70	0.23	33%	0.44	0.19	43%	0.46	0.62	0.19	0.11	25%	0.25	0.39	0.08	0.06	26%
3MC6-ACT	3-Methylhexyl Acetate	1.01	0.30	29%	1.03	2%	0.59	0.20	35%	0.36	0.17	46%	0.36	0.52	0.03	0.11	31%	0.19	0.32	-0.01	0.07	36%
4MC6-ACT	4-Methylhexyl Acetate	0.91	0.27	30%	0.93	2%	0.53	0.18	35%	0.32	0.15	47%	0.32	0.47	0.02	0.11	34%	0.15	0.28	-0.05	0.07	47%
5MC6-ACT	5-Methylhexyl Acetate	0.79	0.25	32%	0.81	2%	0.49	0.18	37%	0.29	0.15	51%	0.28	0.43	-0.10	0.12	43%	0.13	0.26	-0.08	0.07	53%
IC5IBUAT	Isoamyl Isobutyrate	0.89	0.23	26%	0.90	1%	0.50	0.17	33%	0.31	0.14	44%	0.32	0.45	0.11	0.08	27%	0.18	0.28	0.04	0.05	29%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
NC7-ACET	n-Heptyl Acetate	0.73	0.24	33%	0.74	2%	0.47	0.18	38%	0.27	0.14	53%	0.25	0.41	-0.13	0.12	48%	0.12	0.24	-0.10	0.07	62%
24MC6ACT	2,4-Dimethylhexyl Acetate	0.93	0.29	32%	0.95	2%	0.55	0.20	37%	0.32	0.17	52%	0.30	0.49	-0.12	0.14	45%	0.13	0.28	-0.14	0.09	73%
2ETHXACT	2-Ethyl-Hexyl Acetate	0.79	0.25	32%	0.79	1%	0.49	0.20	40%	0.27	0.16	58%	0.25	0.43	-0.19	0.15	58%	0.10	0.24	-0.18	0.09	97%
34MC6ACT	3,4-Dimethylhexyl Acetate	1.16	0.34	29%	1.18	2%	0.67	0.23	34%	0.41	0.19	45%	0.42	0.60	0.10	0.12	29%	0.22	0.37	0.01	0.07	35%
35MC6ACT	3,5-Dimethylhexyl Acetate	1.09	0.32	29%	1.11	2%	0.62	0.22	35%	0.37	0.18	49%	0.36	0.54	-0.03	0.13	36%	0.18	0.32	-0.07	0.08	47%
3EC6-ACT	3-Ethylhexyl Acetate	1.03	0.31	30%	1.04	2%	0.59	0.21	36%	0.36	0.17	49%	0.35	0.53	-0.01	0.12	35%	0.17	0.31	-0.06	0.08	47%
3MC7-ACT	3-Methylheptyl Aceate	0.76	0.26	34%	0.77	2%	0.47	0.18	39%	0.27	0.15	57%	0.25	0.42	-0.17	0.13	54%	0.10	0.23	-0.16	0.08	87%
45MC6ACT	4,5-Dimethylhexyl Acetate	0.86	0.26	31%	0.87	2%	0.51	0.18	36%	0.30	0.15	49%	0.29	0.45	-0.05	0.11	39%	0.14	0.27	-0.08	0.08	55%
4MC7-ACT	4-Methylheptyl Acetate	0.72	0.24	34%	0.74	2%	0.44	0.17	39%	0.25	0.14	56%	0.23	0.39	-0.14	0.12	52%	0.09	0.21	-0.16	0.08	98%
5MC7-ACT	5-Methylheptyl Aceate	0.73	0.25	34%	0.74	2%	0.46	0.18	39%	0.26	0.15	57%	0.24	0.41	-0.17	0.13	54%	0.09	0.22	-0.16	0.08	89%
NC8-ACET	n-Octyl Acetate	0.64	0.23	36%	0.65	2%	0.41	0.17	41%	0.23	0.14	61%	0.21	0.37	-0.21	0.13	63%	0.07	0.20	-0.17	0.08	112%
235M6ACT	2,3,5-Teimethylhexyl Acetate	0.86	0.28	32%	0.88	2%	0.52	0.20	37%	0.31	0.16	53%	0.29	0.47	-0.12	0.13	46%	0.13	0.28	-0.12	0.09	68%
23MC7ACT	2,3-Dimethylheptyl Acetate	0.84	0.27	33%	0.86	2%	0.51	0.19	38%	0.30	0.16	53%	0.29	0.46	-0.11	0.13	45%	0.12	0.26	-0.12	0.08	69%
24MC7ACT	2,4-Dimethylheptyl Acetate	0.88	0.29	33%	0.90	2%	0.52	0.21	40%	0.29	0.17	59%	0.27	0.47	-0.20	0.15	56%	0.09	0.24	-0.22	0.11	115%
25MC7ACT	2,5-Dimethylheptyl Acetate	0.86	0.28	33%	0.88	2%	0.52	0.20	38%	0.30	0.16	53%	0.29	0.47	-0.13	0.14	47%	0.12	0.27	-0.14	0.09	77%
2MC8-ACT	2-Methyloctyl Acetate	0.63	0.23	37%	0.64	2%	0.40	0.17	43%	0.22	0.14	65%	0.19	0.36	-0.25	0.14	74%	0.05	0.18	-0.23	0.09	189%
35MC7ACT	3,5-Dimethylheptyl Acetate	1.01	0.32	32%	1.03	2%	0.58	0.22	38%	0.34	0.19	55%	0.32	0.53	-0.14	0.15	47%	0.12	0.28	-0.19	0.11	89%
36MC7ACT	3,6-Dimethylheptyl Acetate	0.87	0.29	33%	0.89	2%	0.52	0.20	39%	0.30	0.17	56%	0.28	0.47	-0.17	0.14	52%	0.10	0.25	-0.18	0.10	93%
3EC7-ACT	3-Ethylheptyl Acetate	0.71	0.25	35%	0.72	2%	0.44	0.18	41%	0.24	0.15	61%	0.22	0.40	-0.21	0.14	63%	0.07	0.20	-0.20	0.09	135%
45MC7ACT	4,5-Dimethylheptyl Acetate	0.96	0.30	31%	0.98	2%	0.56	0.21	36%	0.34	0.17	50%	0.33	0.51	-0.05	0.13	39%	0.14	0.29	-0.10	0.09	60%
46MC7ACT	4,6-Dimethylheptyl Acetate	0.83	0.27	33%	0.85	2%	0.48	0.19	39%	0.28	0.16	56%	0.26	0.44	-0.13	0.13	50%	0.10	0.23	-0.18	0.09	99%
4MC8-ACT	4-Methyloctyl Acetate	0.68	0.24	35%	0.70	2%	0.42	0.17	42%	0.23	0.14	61%	0.21	0.38	-0.19	0.13	62%	0.06	0.19	-0.20	0.09	146%
5MC8-ACT	5-Methyloctyl Acetate	0.67	0.24	36%	0.68	2%	0.42	0.17	42%	0.23	0.14	62%	0.21	0.38	-0.22	0.14	65%	0.06	0.20	-0.20	0.09	142%
NC9-ACET	n-Nonyl Acetate	0.58	0.22	38%	0.59	2%	0.38	0.16	43%	0.20	0.14	66%	0.18	0.35	-0.25	0.14	77%	0.04	0.17	-0.22	0.09	198%
36MC8ACT	3,6-Dimethyloctyl Acetate	0.88	0.29	33%	0.89	2%	0.52	0.20	39%	0.30	0.17	55%	0.28	0.47	-0.13	0.14	49%	0.10	0.25	-0.18	0.10	94%
3IPC7ACT	3-Isopropylheptyl Acetate	0.71	0.25	35%	0.73	2%	0.44	0.18	41%	0.25	0.15	59%	0.23	0.40	-0.17	0.13	58%	0.07	0.21	-0.19	0.09	122%
46MC8ACT	4,6-Dimethyloctyl Acetate	0.85	0.29	34%	0.87	2%	0.49	0.20	40%	0.28	0.16	58%	0.27	0.45	-0.15	0.14	54%	0.08	0.23	-0.21	0.10	128%
357M8ACT	3,5,7-Trimethyloctyl Acetate	0.83	0.28	34%	0.85	2%	0.48	0.20	42%	0.27	0.17	62%	0.25	0.44	-0.20	0.15	61%	0.06	0.21	-0.25	0.11	181%
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	0.80	0.27	34%	0.82	3%	0.47	0.19	40%	0.27	0.16	58%	0.26	0.44	-0.15	0.14	54%	0.08	0.23	-0.20	0.10	128%
47MC9ACT	4,7-Dimethylnonyl Acetate	0.64	0.24	38%	0.66	3%	0.39	0.17	44%	0.22	0.14	66%	0.19	0.37	-0.22	0.14	72%	0.03	0.17	-0.26	0.10	-
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	0.74	0.26	36%	0.76	3%	0.44	0.18	42%	0.25	0.15	62%	0.23	0.41	-0.19	0.14	62%	0.05	0.20	-0.23	0.10	190%
357M9ACT	3,5,7-Trimethylnonyl Acetate	0.76	0.27	35%	0.78	2%	0.44	0.19	43%	0.25	0.16	63%	0.23	0.42	-0.20	0.15	64%	0.04	0.19	-0.26	0.11	-
368M9ACT	3,6,8-Trimethylnonyl Acetate	0.72	0.25	35%	0.74	3%	0.42	0.18	42%	0.24	0.15	63%	0.22	0.40	-0.20	0.14	65%	0.05	0.19	-0.24	0.10	-
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	0.63	0.24	38%	0.64	3%	0.37	0.17	45%	0.21	0.14	69%	0.18	0.36	-0.26	0.14	78%	0.02	0.16	-0.28	0.11	-
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	0.76	0.26	34%	0.78	3%	0.45	0.18	40%	0.27	0.15	56%	0.25	0.42	-0.11	0.13	51%	0.07	0.22	-0.18	0.09	129%
479M10AC	4,7,9-Trimethyldecyl Acetate	0.55	0.22	40%	0.57	3%	0.34	0.16	46%	0.19	0.13	71%	0.16	0.32	-0.26	0.13	84%	0.01	0.14	-0.28	0.10	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	0.74	0.27	36%	0.76	2%	0.45	0.19	42%	0.26	0.16	60%	0.24	0.42	-0.16	0.14	58%	0.06	0.21	-0.22	0.10	182%
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	0.58	0.23	40%	0.60	3%	0.36	0.16	46%	0.20	0.14	70%	0.17	0.35	-0.27	0.14	82%	0.00	0.15	-0.29	0.11	-
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	0.77	0.28	36%	0.79	3%	0.46	0.20	43%	0.27	0.16	61%	0.24	0.44	-0.17	0.15	60%	0.05	0.21	-0.25	0.11	-
DMC	Dimethyl Carbonate	0.06	0.01	21%	0.06	2%	0.04	0.01	20%	0.03	0.01	24%	0.04	0.08	0.01	0.01	37%	0.03	0.05	0.01	0.01	30%
PC	Propylene Carbonate	0.25	0.05	22%	0.26	2%	0.17	0.04	22%	0.13	0.04	27%	0.15	0.29	0.05	0.04	30%	0.10	0.15	0.04	0.02	25%
ME-LACT	Methyl Lactate	2.75	0.58	21%	2.79	1%	1.10	0.30	27%	0.63	0.24	39%	0.73	0.94	0.21	0.12	17%	0.59	0.73	0.38	0.07	11%
MCSVACET	2-Methoxyethyl Acetate	1.18	0.23	19%	1.22	3%	0.64	0.11	17%	0.46	0.11	23%	0.53	0.96	0.25	0.13	25%	0.45	0.70	0.25	0.10	21%
ET-LACT	Ethyl Lactate	2.71	0.59	22%	2.74	1%	1.15	0.31	27%	0.68	0.26	38%	0.79	1.02	0.31	0.12	16%	0.59	0.72	0.38	0.06	11%
MIPR-CB	Methyl Isopropyl Carbonate	0.69	0.13	19%	0.71	2%	0.39	0.07	18%	0.27	0.06	24%	0.32	0.60	0.15	0.08	26%	0.24	0.36	0.14	0.05	20%
PGME-ACT	1-Methoxy-2-Propyl Acetate	1.71	0.31	18%	1.75	3%	0.82	0.15	19%	0.57	0.15	26%	0.66	1.13	0.39	0.14	21%	0.53	0.78	0.38	0.08	15%
CSV-ACET	2-Ethoxyethyl Acetate	1.90	0.34	18%	1.93	2%	0.92	0.18	20%	0.62	0.16	27%	0.71	1.05	0.44	0.12	17%	0.61	0.85	0.43	0.09	14%
2PGMEACT	2-Methyoxy-1-propyl Acetate	1.12	0.20	18%	1.16	4%	0.56	0.09	16%	0.40	0.09	23%	0.46	0.82	0.26	0.10	22%	0.46	0.72	0.27	0.10	21%
DBE-4	Dimethyl Succinate	0.25	0.06	23%	0.25	0%	0.14	0.04	26%	0.10	0.03	33%	0.11	0.16	0.04	0.02	21%	0.07	0.09	0.04	0.01	15%
ETGLDACT	Ethylene Glycol Diacetate	0.72	0.21	29%	0.73	2%	0.42	0.14	34%	0.29	0.12	41%	0.31	0.48	0.12	0.08	27%	0.17	0.23	0.09	0.04	26%
DIPR-CB	Diisopropyl Carbonate	1.04	0.19	19%	1.06	1%	0.54	0.11	20%	0.35	0.09	27%	0.40	0.63	0.23	0.07	18%	0.32	0.42	0.21	0.04	14%
DBE-5	Dimethyl Glutarate	0.49	0.12	24%	0.50	0%	0.28	0.08	29%	0.17	0.06	38%	0.18	0.24	0.08	0.04	20%	0.12	0.16	0.07	0.02	14%
2BUETACT	2-Butoxyethyl Acetate	1.67	0.36	21%	1.70	2%	0.83	0.21	26%	0.56	0.19	33%	0.62	0.82	0.36	0.11	18%	0.44	0.63	0.30	0.07	16%
DBE-6	Dimethyl Adipate	1.95	0.43	22%	1.98	1%	0.91	0.25	28%	0.56	0.21	38%	0.63	0.85	0.43	0.10	16%	0.42	0.50	0.30	0.05	12%
DGEEA	2-(2-Ethoxyethoxy) ethyl acetate	1.50	0.31	21%	1.54	2%	0.76	0.18	24%	0.52	0.16	31%	0.57	0.79	0.31	0.10	17%	0.45	0.69	0.30	0.08	18%
DGBEA	2-(2-Butoxyethoxy) ethyl acetate	1.38	0.32	24%	1.41	2%	0.71	0.20	29%	0.48	0.18	37%	0.52	0.70	0.27	0.10	20%	0.33	0.51	0.11	0.08	24%
SC7ESC12	Substituted C7 ester (C12)	0.92	0.22	24%	0.92	0%	0.48	0.15	32%	0.29	0.12	43%	0.30	0.41	0.08	0.08	25%	0.18	0.27	0.04	0.05	26%
TEXANOL2	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	0.92	0.20	22%	0.93	1%	0.44	0.13	29%	0.26	0.11	40%	0.28	0.37	0.12	0.06	20%	0.18	0.25	0.06	0.04	22%
TEXANOL1	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	0.88	0.23	26%	0.88	0%	0.48	0.16	34%	0.29	0.13	44%	0.30	0.42	0.07	0.08	27%	0.17	0.26	0.02	0.05	28%
TEXANOL	Texanol isomers	0.89	0.22	24%	0.89	0%	0.47	0.15	32%	0.28	0.12	43%	0.30	0.40	0.08	0.07	25%	0.18	0.26	0.04	0.05	26%
SC9ESC12	Substituted C9 Ester (C12)	0.89	0.22	24%	0.89	0%	0.46	0.15	32%	0.28	0.12	43%	0.29	0.40	0.08	0.07	25%	0.18	0.26	0.04	0.05	26%
ETOX	Ethylene Oxide	0.05	0.01	22%	0.05	2%	0.04	0.01	20%	0.03	0.01	25%	0.03	0.07	0.01	0.01	36%	0.02	0.04	0.01	0.01	31%
PROX	Propylene Oxide	0.32	0.07	22%	0.32	1%	0.23	0.05	21%	0.17	0.05	26%	0.20	0.39	0.06	0.06	32%	0.13	0.20	0.05	0.03	27%
12BUOX	1,2-Epoxybutane	1.02	0.25	24%	1.04	2%	0.69	0.17	24%	0.51	0.15	29%	0.58	1.06	0.18	0.16	28%	0.37	0.57	0.16	0.09	24%
FORMACID	Formic Acid	0.08	0.02	21%	0.08	2%	0.05	0.01	20%	0.04	0.01	24%	0.04	0.09	0.01	0.01	34%	0.03	0.05	0.01	0.01	28%
ACETACID	Acetic Acid	0.71	0.13	19%	0.71	1%	0.34	0.07	20%	0.22	0.06	27%	0.26	0.44	0.15	0.05	18%	0.21	0.28	0.14	0.03	13%
ACYRACID	Acrylic Acid	11.66	1.63	14%	11.93	2%	3.99	0.56	14%	2.33	0.53	23%	2.93	4.56	2.34	0.43	15%	3.56	4.45	3.03	0.29	8%
PROPACID	Propionic Acid	1.16	0.25	21%	1.17	1%	0.55	0.14	25%	0.35	0.12	33%	0.40	0.59	0.24	0.06	15%	0.30	0.38	0.22	0.03	10%
ME-ACRYL	Methyl Acrylate	12.24	1.84	15%	12.51	2%	4.21	0.66	16%	2.43	0.60	25%	3.03	4.45	2.50	0.36	12%	3.39	3.90	2.89	0.23	7%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
VIN-ACET	Vinyl Acetate	3.26	0.44	14%	3.35	3%	1.19	0.15	13%	0.73	0.16	21%	0.90	1.39	0.75	0.13	15%	1.07	1.42	0.96	0.11	10%
MBUTENOL	2-Methyl-2-Butene-3-ol	4.12	0.65	16%	5.37	30%	1.65	0.30	18%	1.10	0.28	26%	1.30	2.10	1.07	0.21	16%	1.18	1.53	1.05	0.10	8%
ET-ACRYL	Ethyl Acrylate	8.78	1.37	16%	8.99	2%	3.21	0.55	17%	1.93	0.50	26%	2.36	3.51	2.07	0.24	10%	2.37	2.65	2.18	0.10	4%
ME-MACRT	Methyl Methacrylate	15.84	2.09	13%	16.30	3%	4.95	0.58	12%	2.86	0.60	21%	3.66	6.02	2.61	0.73	20%	4.89	6.11	3.96	0.50	10%
BU-MACRT	Butyl Methacrylate	9.09	1.21	13%	9.37	3%	2.91	0.35	12%	1.67	0.36	22%	2.11	3.20	1.59	0.36	17%	2.69	3.32	2.22	0.25	9%
IBUMACRT	Isobutyl Methacrylate	8.99	1.19	13%	9.26	3%	2.87	0.34	12%	1.63	0.35	22%	2.07	3.15	1.54	0.37	18%	2.67	3.29	2.20	0.26	10%
FURAN	Furan	16.54	2.32	14%	16.98	3%	4.97	0.73	15%	2.41	0.74	31%	3.05	5.13	0.83	0.79	26%	4.49	5.29	3.51	0.42	9%
FORMALD	Formaldehyde	8.97	1.32	15%	9.24	3%	2.56	0.32	12%	1.27	0.31	24%	1.71	3.51	0.88	0.56	33%	2.95	4.18	2.08	0.48	16%
ACETALD	Acetaldehyde	6.84	1.14	17%	7.06	3%	2.56	0.44	17%	1.70	0.42	25%	2.09	3.83	1.64	0.42	20%	1.79	2.16	1.42	0.17	9%
PROPALD	Propionaldehyde	7.89	1.43	18%	8.13	3%	2.97	0.59	20%	1.95	0.55	28%	2.37	4.02	1.84	0.43	18%	2.00	2.60	1.60	0.21	11%
2MEC3AL	2-Methylpropanal	5.87	1.05	18%	6.07	3%	2.25	0.43	19%	1.51	0.41	27%	1.83	3.22	1.40	0.36	20%	1.57	1.92	1.24	0.16	10%
1C4RCHO	Butanal	6.74	1.22	18%	6.92	3%	2.55	0.52	20%	1.67	0.47	28%	2.03	3.41	1.57	0.37	18%	1.70	2.20	1.36	0.18	11%
C4-RCHO	C4 aldehydes	6.74	1.22	18%	6.92	3%	2.55	0.52	20%	1.67	0.47	28%	2.03	3.41	1.57	0.37	18%	1.70	2.20	1.36	0.18	11%
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	5.40	0.96	18%	5.57	3%	2.03	0.39	19%	1.35	0.37	27%	1.64	2.87	1.26	0.32	19%	1.41	1.80	1.12	0.15	10%
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	5.52	0.96	17%	5.68	3%	2.08	0.39	19%	1.37	0.37	27%	1.66	2.79	1.30	0.30	18%	1.46	1.82	1.17	0.14	10%
1C5RCHO	Pentanal (Valeraldehyde)	5.76	1.04	18%	5.94	3%	2.20	0.44	20%	1.45	0.40	28%	1.76	2.98	1.35	0.33	19%	1.47	1.86	1.15	0.16	11%
C5-RCHO	C5 Aldehydes	5.76	1.04	18%	5.94	3%	2.20	0.44	20%	1.45	0.40	28%	1.76	2.98	1.35	0.33	19%	1.47	1.86	1.15	0.16	11%
GLTRALD	Glutaraldehyde	4.79	0.89	19%	4.96	3%	1.84	0.36	19%	1.25	0.34	27%	1.52	2.74	1.12	0.33	22%	1.27	1.55	0.92	0.15	12%
1C6RCHO	Hexanal	4.98	0.89	18%	5.12	3%	1.89	0.38	20%	1.23	0.35	28%	1.48	2.44	1.17	0.25	17%	1.25	1.61	1.01	0.13	10%
C6-RCHO	C6 Aldehydes	4.98	0.89	18%	5.12	3%	1.89	0.38	20%	1.23	0.35	28%	1.48	2.44	1.17	0.25	17%	1.25	1.61	1.01	0.13	10%
1C7RCHO	Heptanal	4.23	0.76	18%	4.36	3%	1.61	0.33	21%	1.04	0.30	29%	1.26	1.97	0.98	0.20	16%	1.05	1.35	0.82	0.11	11%
C7-RCHO	C7 Aldehydes	4.23	0.76	18%	4.36	3%	1.61	0.33	21%	1.04	0.30	29%	1.26	1.97	0.98	0.20	16%	1.05	1.35	0.82	0.11	11%
1C8RCHO	Octanal	3.65	0.67	18%	3.74	3%	1.40	0.30	21%	0.90	0.27	29%	1.08	1.64	0.83	0.17	15%	0.89	1.15	0.65	0.10	11%
C8-RCHO	C8 Aldehydes	3.65	0.67	18%	3.74	3%	1.40	0.30	21%	0.90	0.27	29%	1.08	1.64	0.83	0.17	15%	0.89	1.15	0.65	0.10	11%
GLYOXAL	Glyoxal	14.22	2.15	15%	14.72	3%	4.05	0.54	13%	2.02	0.51	25%	2.72	5.26	1.33	0.94	35%	5.19	7.64	3.30	0.91	17%
MEGLYOX	Methyl Glyoxal	16.21	2.37	15%	16.82	4%	4.67	0.54	12%	2.49	0.56	23%	3.31	5.95	1.92	0.94	28%	5.63	7.77	4.00	0.88	16%
ACROLEIN	Acrolein	7.60	1.43	19%	7.78	2%	2.78	0.60	22%	1.80	0.55	31%	2.19	3.61	1.60	0.41	19%	1.71	2.12	1.23	0.24	14%
CROTALD	Crotonaldehyde	10.07	1.52	15%	10.33	3%	3.50	0.54	15%	2.13	0.51	24%	2.67	4.40	2.14	0.40	15%	2.75	3.25	2.29	0.19	7%
METHACRO	Methacrolein	6.23	1.02	16%	6.41	3%	2.24	0.40	18%	1.42	0.37	26%	1.75	2.94	1.38	0.30	17%	1.62	1.92	1.26	0.15	9%
HOMACR	Hydroxy Methacrolein	6.61	1.06	16%	6.78	3%	2.37	0.41	17%	1.46	0.38	26%	1.81	2.90	1.49	0.26	14%	1.76	1.98	1.46	0.11	6%
BENZALD	Benzaldehyde	-0.61	0.23	-37%	-0.60	-1%	-1.64	0.24	-15%	-2.32	0.66	-29%	-2.79	-0.32	- 11.54	2.06	-74%	-1.67	-0.44	-4.95	1.05	-63%
TOLUALD	Tolualdehyde	-0.54	0.20	-37%	-0.53	-1%	-1.45	0.22	-15%	-2.05	0.59	-29%	-2.47	-0.28	- 10.19	1.82	-74%	-1.47	-0.38	-4.37	0.93	-63%
ACETONE	Acetone	0.43	0.08	19%	0.43	2%	0.17	0.04	21%	0.11	0.03	29%	0.13	0.19	0.10	0.02	13%	0.10	0.13	0.08	0.01	9%
CC4-KET	Cyclobutanone	0.68	0.18	26%	0.69	1%	0.41	0.12	30%	0.29	0.11	37%	0.31	0.48	0.12	0.08	24%	0.19	0.27	0.11	0.04	19%
MEK	Methyl Ethyl Ketone	1.49	0.31	21%	1.52	2%	0.66	0.18	26%	0.43	0.15	35%	0.49	0.72	0.35	0.08	16%	0.34	0.44	0.28	0.03	10%
CC5-KET	Cyclopentanone	1.43	0.37	26%	1.44	1%	0.84	0.25	30%	0.59	0.22	37%	0.65	0.96	0.25	0.16	24%	0.39	0.54	0.22	0.08	20%
KET5C	C5 Cyclic Ketones	1.43	0.37	26%	1.44	1%	0.84	0.25	30%	0.59	0.22	37%	0.65	0.96	0.25	0.16	24%	0.39	0.54	0.22	0.08	20%
MPK	2-Pentanone	3.07	0.65	21%	3.12	2%	1.50	0.37	25%	1.01	0.32	31%	1.16	1.87	0.71	0.22	19%	0.80	1.06	0.64	0.10	12%
DEK	3-Pentanone	1.45	0.36	25%	1.46	1%	0.73	0.24	32%	0.49	0.20	41%	0.54	0.80	0.32	0.13	24%	0.32	0.45	0.21	0.06	18%
KET5	C5 Ketones	3.07	0.65	21%	3.12	2%	1.50	0.37	25%	1.01	0.32	31%	1.16	1.87	0.71	0.22	19%	0.80	1.06	0.64	0.10	12%
CC6-KET	Cyclohexanone	1.61	0.43	26%	1.62	1%	0.90	0.29	32%	0.61	0.24	40%	0.65	0.94	0.28	0.15	23%	0.36	0.52	0.22	0.08	23%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
KET6C	C6 Cyclic Ketones	1.61	0.43	26%	1.62	1%	0.90	0.29	32%	0.61	0.24	40%	0.65	0.94	0.28	0.15	23%	0.36	0.52	0.22	0.08	23%
MIBK	4-Methyl-2-Pentanone	4.31	0.73	17%	4.40	2%	1.83	0.32	17%	1.21	0.30	25%	1.45	2.49	1.13	0.25	18%	1.21	1.58	1.07	0.11	9%
MNBK	Methyl n-Butyl Ketone	3.55	0.76	21%	3.62	2%	1.71	0.43	25%	1.15	0.37	32%	1.32	2.00	0.80	0.25	19%	0.90	1.17	0.73	0.11	13%
MTBK	Methyl t-Butyl Ketone	0.78	0.17	21%	0.80	2%	0.39	0.09	24%	0.26	0.08	31%	0.29	0.44	0.19	0.04	15%	0.20	0.25	0.17	0.02	9%
KET6	C6 Ketones	3.55	0.76	21%	3.62	2%	1.71	0.43	25%	1.15	0.37	32%	1.32	2.00	0.80	0.25	19%	0.90	1.17	0.73	0.11	13%
KET7C	C7 Cyclic Ketones	1.41	0.37	26%	1.42	1%	0.79	0.25	32%	0.53	0.21	40%	0.57	0.82	0.24	0.13	23%	0.32	0.46	0.19	0.07	23%
C7-KET-2	2-Heptanone	2.80	0.64	23%	2.85	2%	1.40	0.39	28%	0.93	0.33	36%	1.03	1.41	0.58	0.19	18%	0.66	0.85	0.47	0.10	15%
2M-3-HXO	2-Methyl-3-Hexanone	1.79	0.44	24%	1.82	2%	0.94	0.28	30%	0.62	0.24	38%	0.69	0.97	0.35	0.15	21%	0.41	0.54	0.25	0.08	19%
DIPK	Di-Isopropyl Ketone	1.63	0.41	25%	1.65	1%	0.87	0.28	32%	0.58	0.23	40%	0.63	0.91	0.30	0.14	23%	0.36	0.48	0.20	0.08	22%
KET7	C7 Ketones	2.80	0.64	23%	2.85	2%	1.40	0.39	28%	0.93	0.33	36%	1.03	1.41	0.58	0.19	18%	0.66	0.85	0.47	0.10	15%
KET8C	C8 Cyclic Ketones	1.25	0.33	26%	1.26	1%	0.70	0.22	32%	0.47	0.19	40%	0.51	0.73	0.21	0.12	23%	0.28	0.41	0.17	0.06	23%
C8-KET-2	2-Octanone	1.66	0.43	26%	1.68	1%	0.92	0.29	32%	0.58	0.24	41%	0.61	0.81	0.29	0.14	23%	0.35	0.52	0.12	0.09	25%
KET8	C8 Ketones	1.66	0.43	26%	1.68	1%	0.92	0.29	32%	0.58	0.24	41%	0.61	0.81	0.29	0.14	23%	0.35	0.52	0.12	0.09	25%
KET9C	C9 Cyclic Ketones	1.13	0.30	26%	1.13	1%	0.63	0.20	32%	0.42	0.17	40%	0.46	0.66	0.19	0.11	23%	0.26	0.37	0.15	0.06	23%
C9-KET-2	2-Nonanone	1.30	0.36	28%	1.32	1%	0.74	0.26	35%	0.45	0.22	48%	0.45	0.67	0.04	0.15	34%	0.22	0.40	-0.06	0.10	45%
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	2.94	0.59	20%	3.00	2%	1.29	0.31	24%	0.85	0.28	33%	0.97	1.31	0.69	0.16	16%	0.65	0.85	0.31	0.11	17%
KET9	C9 Ketones	1.30	0.36	28%	1.32	1%	0.74	0.26	35%	0.45	0.22	48%	0.45	0.67	0.04	0.15	34%	0.22	0.40	-0.06	0.10	45%
KET10C	C10 Cyclic Ketones	1.02	0.27	26%	1.03	1%	0.57	0.18	32%	0.39	0.15	40%	0.42	0.60	0.18	0.10	23%	0.23	0.33	0.14	0.05	23%
C10-K-2	2-Decanone	1.06	0.33	31%	1.07	1%	0.62	0.24	39%	0.36	0.20	55%	0.34	0.57	-0.12	0.16	47%	0.14	0.31	-0.18	0.11	82%
KET10	C10 Ketones	1.06	0.33	31%	1.07	1%	0.62	0.24	39%	0.36	0.20	55%	0.34	0.57	-0.12	0.16	47%	0.14	0.31	-0.18	0.11	82%
BIACETYL	Biacetyl	20.73	3.02	15%	21.50	4%	6.09	0.69	11%	3.38	0.75	22%	4.44	7.37	2.68	1.17	26%	7.45	10.51	5.49	1.14	15%
MVK	Methylvinyl ketone	8.73	1.34	15%	8.96	3%	3.31	0.55	17%	2.11	0.52	25%	2.59	4.39	2.17	0.40	15%	2.35	2.70	2.10	0.14	6%
HOACET	Hydroxy Acetone	3.08	0.54	18%	3.15	2%	1.13	0.23	20%	0.66	0.19	30%	0.80	1.12	0.61	0.08	10%	0.70	0.82	0.60	0.05	7%
MEOACET	Methoxy Acetone	2.14	0.43	20%	2.18	2%	1.01	0.21	21%	0.70	0.19	28%	0.82	1.45	0.52	0.17	21%	0.60	0.82	0.49	0.08	13%
DIACTALC	Diacetone Alcohol	0.68	0.16	24%	0.69	1%	0.36	0.11	31%	0.23	0.09	39%	0.26	0.36	0.14	0.05	20%	0.16	0.21	0.11	0.02	14%
PHENOL	Phenol	1.82	0.28	15%	1.88	3%	-0.74	0.28	-38%	-1.67	0.65	-39%	-1.99	0.37	-11.6	2.09	-105%	-0.72	0.32	-4.54	0.99	-137%
CRESOL	Alkyl Phenols	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
M-CRESOL	m-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
P-CRESOL	p-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
O-CRESOL	o-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
NO2-BENZ	Nitrobenzene	0.07	0.02	24%	0.07	0%	0.03	0.01	40%	0.01	0.01	77%	0.01	0.02	-0.03	0.01	65%	0.01	0.02	0.00	0.00	21%
P-TI	Para Toluene Isocyanate	0.93	0.20	21%	0.95	2%	-0.85	0.33	-39%	-1.44	0.61	-42%	-1.69	0.16	-9.22	1.63	-97%	-0.58	0.13	-3.01	0.60	-104%
TDI	Toluene Diisocyanate	-0.13	0.07	-55%	-0.13	1%	-1.02	0.26	-25%	-1.38	0.51	-37%	-1.63	-0.10	-8.19	1.39	-86%	-0.77	-0.13	-2.98	0.53	-69%
MDI	Methylene Diphenylene Diisocyanate	0.79	0.15	19%	0.81	3%	-0.48	0.21	-44%	-0.91	0.40	-44%	-1.07	0.15	-6.35	1.12	-104%	-0.38	0.13	-2.20	0.44	-118%
DM-AMINE	Dimethyl Amine	9.37	1.48	16%	9.69	3%	3.60	0.56	16%	2.36	0.56	24%	2.88	4.78	2.39	0.48	17%	3.03	3.85	2.68	0.29	10%
ET-AMINE	Ethyl Amine	7.80	1.29	17%	8.01	3%	3.20	0.55	17%	2.14	0.53	25%	2.57	4.34	2.07	0.44	17%	2.42	3.16	2.12	0.26	11%
TM-AMINE	Trimethyl Amine	7.06	1.11	16%	7.31	3%	2.73	0.43	16%	1.79	0.42	24%	2.18	3.64	1.82	0.36	17%	2.27	2.90	2.01	0.22	10%
ETOH-NH2	Ethanolamine	5.97	0.98	16%	6.15	3%	2.42	0.41	17%	1.62	0.39	24%	1.94	3.28	1.57	0.33	17%	1.86	2.43	1.64	0.20	11%
DMAE	Dimethylaminoethanol	4.76	0.76	16%	4.93	4%	1.81	0.29	16%	1.17	0.29	25%	1.42	2.24	1.20	0.21	15%	1.48	1.84	1.34	0.12	8%
ETOH2-NH	Diethanol Amine	4.05	0.65	16%	4.20	4%	1.54	0.25	16%	1.00	0.24	24%	1.21	1.90	1.02	0.18	15%	1.26	1.57	1.14	0.10	8%
ETOH3-N	Triethanolamine	2.76	0.46	17%	2.86	4%	1.05	0.19	18%	0.67	0.18	26%	0.81	1.17	0.69	0.11	13%	0.80	0.99	0.62	0.06	8%
NMP	N-Methyl-2-Pyrrolidone	2.56	0.59	23%	2.59	1%	1.23	0.36	29%	0.80	0.31	39%	0.89	1.24	0.56	0.17	19%	0.56	0.71	0.37	0.08	15%
CH3-CL	Methyl Chloride	0.03	0.01	24%	0.03	1%	0.02	0.01	27%	0.01	0.00	33%	0.02	0.03	0.01	0.00	25%	0.01	0.02	0.01	0.00	19%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.		Sdev		Δ%	Avg.		Sdev	Avg.		Sdev	Avg.	Max	Min		Sdev	Avg.	Max	Min		Sdev
CL-ETHE	Vinyl Chloride	2.92	0.59	20%	2.98	2%	1.43	0.31	21%	0.98	0.27	28%	1.14	1.96	0.66	0.23	20%	0.87	1.17	0.62	0.13	14%
C2-CL	Ethyl Chloride	0.25	0.06	24%	0.25	1%	0.14	0.04	27%	0.10	0.03	33%	0.11	0.19	0.05	0.03	24%	0.07	0.11	0.04	0.01	18%
CL2-ME	Dichloromethane	0.07	0.02	24%	0.07	1%	0.04	0.01	27%	0.03	0.01	33%	0.03	0.05	0.01	0.01	24%	0.02	0.03	0.01	0.00	19%
ME-BR	Methyl Bromide	0.02	0.00	24%	0.02	1%	0.01	0.00	27%	0.01	0.00	33%	0.01	0.01	0.00	0.00	25%	0.01	0.01	0.00	0.00	19%
11CL2-C2	1,1-Dichloroethane	0.10	0.02	24%	0.10	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.04	0.02	0.01	18%
12CL2-C2	1,2-Dichloroethane	0.10	0.02	24%	0.10	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.04	0.02	0.01	18%
C2-BR	Ethyl Bromide	0.11	0.03	24%	0.11	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.05	0.02	0.01	18%
CHCL3	Chloroform	0.03	0.01	24%	0.03	1%	0.02	0.01	27%	0.01	0.00	33%	0.02	0.03	0.01	0.00	25%	0.01	0.02	0.01	0.00	19%
C3-BR	n-Propyl Bromide	0.35	0.08	23%	0.35	1%	0.20	0.05	26%	0.14	0.04	32%	0.16	0.26	0.07	0.04	23%	0.10	0.15	0.06	0.02	18%
111-TCE	1,1,1-Trichloroethane	0.00	0.00	24%	0.00	1%	0.00	0.00	27%	0.00	0.00	33%	0.00	0.00	0.00	0.00	25%	0.00	0.00	0.00	0.00	19%
112CL3C2	1,1,2-Trichloroethane	0.06	0.01	24%	0.06	1%	0.03	0.01	27%	0.02	0.01	33%	0.03	0.05	0.01	0.01	24%	0.02	0.03	0.01	0.00	19%
C4-BR	n-Butyl Bromide	0.60	0.13	22%	0.61	1%	0.33	0.08	24%	0.23	0.07	31%	0.26	0.44	0.12	0.06	22%	0.18	0.25	0.11	0.03	17%
11BR2-C2	1,2-Dibromoethane	0.05	0.01	24%	0.05	1%	0.03	0.01	27%	0.02	0.01	33%	0.02	0.04	0.01	0.01	24%	0.01	0.02	0.01	0.00	18%
T-12-DCE	Trans-1,2-Dichloroethene	0.81	0.18	22%	0.82	1%	0.44	0.11	25%	0.31	0.10	31%	0.35	0.60	0.16	0.08	22%	0.24	0.34	0.15	0.04	17%
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	1.13	0.31	28%	1.18	4%	0.61	0.17	29%	0.47	0.15	32%	0.53	0.94	0.27	0.18	33%	0.22	0.70	-0.15	0.13	61%
CL3-ETHE	Trichloroethylene	0.60	0.13	22%	0.61	1%	0.33	0.08	25%	0.23	0.07	31%	0.26	0.44	0.12	0.06	22%	0.18	0.25	0.11	0.03	17%
CL4-ETHE	Perchloroethylene	0.04	0.01	24%	0.04	1%	0.02	0.01	27%	0.02	0.01	33%	0.02	0.03	0.01	0.00	24%	0.01	0.02	0.01	0.00	18%
CL-BEN	Monochlorobenzene	0.36	0.09	24%	0.36	0%	0.15	0.06	39%	0.07	0.05	75%	0.08	0.13	-0.14	0.05	64%	0.08	0.10	0.02	0.02	20%
CF3-BEN	Benzotrifluoride	0.26	0.06	21%	0.27	1%	0.08	0.03	36%	0.02	0.03	131%	0.02	0.08	-0.15	0.04	173%	0.05	0.07	0.00	0.01	29%
CL2-BEN	p-Dichlorobenzene	0.20	0.05	24%	0.20	1%	0.09	0.03	39%	0.04	0.03	76%	0.04	0.07	-0.08	0.03	64%	0.04	0.05	0.01	0.01	20%
PCBTF	p-Trifluoromethyl-Cl-Benzene	0.11	0.02	21%	0.11	1%	0.04	0.01	36%	0.01	0.01	133%	0.01	0.03	-0.07	0.02	176%	0.02	0.03	0.00	0.01	29%
Mixtures																						
ARBROG	Base ROG Mixture	3.71	0.63	17%	3.79	2%	1.46	0.28	19%	0.85	0.25	30%	1.00	1.00	1.00			1.00	1.00	1.00		
RFA-TLEV	TLEV Exhaust -- RFA	4.09	0.68	17%	4.21	3%	1.58	0.30	19%	0.89	0.27	30%	1.06	1.12	0.93	0.04	4%	1.10	1.15	1.06	0.02	2%
PH2-TLEV	TLEV Exhaust -- Phase 2	4.05	0.66	16%	4.15	2%	1.57	0.29	18%	0.90	0.26	29%	1.07	1.12	1.01	0.03	3%	1.11	1.16	1.08	0.02	2%
LPG-TLEV	TLEV Exhaust -- LPG	2.11	0.35	16%	2.15	2%	0.91	0.15	17%	0.58	0.15	25%	0.69	1.11	0.57	0.10	14%	0.64	0.83	0.58	0.06	9%
CNG-TLEV	TLEV Exhaust -- CNG	0.75	0.13	18%	0.76	2%	0.35	0.07	20%	0.23	0.06	28%	0.27	0.44	0.20	0.04	16%	0.23	0.30	0.21	0.02	10%
E85-TLEV	TLEV Exhaust -- E-85	2.70	0.53	20%	2.75	2%	1.24	0.28	23%	0.82	0.25	30%	0.96	1.51	0.66	0.16	16%	0.74	0.94	0.64	0.07	9%
M85-TLEV	TLEV Exhaust -- M-85	1.57	0.24	16%	1.61	2%	0.61	0.09	15%	0.35	0.09	25%	0.43	0.60	0.35	0.05	12%	0.47	0.60	0.41	0.04	8%
RFA-LEV	Final LEV -- RFA	3.64	0.62	17%	3.73	2%	1.43	0.28	20%	0.81	0.25	31%	0.95	1.00	0.77	0.04	4%	0.96	1.01	0.92	0.02	2%
PH2-LEV	Final LEV -- Phase 2	3.55	0.60	17%	3.65	3%	1.42	0.27	19%	0.82	0.24	30%	0.96	1.01	0.92	0.02	2%	0.97	1.02	0.92	0.02	2%
MS-D	Mineral Spirits "D" (Type II-C)	0.79	0.30	38%	0.81	3%	0.48	0.22	45%	0.27	0.18	68%	0.23	0.46	-0.32	0.18	78%	0.03	0.21	-0.34	0.13	-
MS-A	Mineral Spirits "A" (Type I-B, 91% Alkanes)	1.27	0.36	28%	1.30	2%	0.65	0.24	36%	0.36	0.20	54%	0.35	0.56	-0.20	0.17	49%	0.17	0.33	-0.17	0.12	73%
MS-B	Mineral Spirits "B" (Type II-C)	0.78	0.30	38%	0.80	3%	0.48	0.21	45%	0.26	0.18	68%	0.23	0.45	-0.31	0.18	77%	0.03	0.21	-0.34	0.13	-
MS-C	Mineral Spirits "C" (Type II-C)	0.78	0.30	38%	0.80	3%	0.48	0.21	45%	0.26	0.18	68%	0.23	0.45	-0.32	0.18	79%	0.03	0.21	-0.34	0.13	-
D95	Exxon Exxol(r) D95 Fluid	0.67	0.27	40%	0.68	2%	0.42	0.19	47%	0.23	0.16	71%	0.20	0.40	-0.32	0.17	84%	0.01	0.18	-0.33	0.12	-
ISOPARM	Exxon Isopar(r) M Fluid	0.65	0.26	40%	0.67	3%	0.41	0.19	46%	0.23	0.16	71%	0.19	0.39	-0.31	0.16	84%	0.01	0.18	-0.32	0.12	-
OC6-ACET	Oxo-Hexyl Acetate	1.03	0.29	28%	1.04	2%	0.61	0.20	33%	0.38	0.16	42%	0.39	0.54	0.13	0.10	26%	0.22	0.35	0.07	0.06	25%
OC7-ACET	Oxo-Heptyl Acetate	0.97	0.29	29%	0.99	2%	0.57	0.20	34%	0.35	0.16	46%	0.35	0.50	0.02	0.11	32%	0.18	0.31	-0.02	0.07	38%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
OC8-ACET	Oxo-Octyl Acetate	0.96	0.29	31%	0.98	2%	0.56	0.20	36%	0.33	0.16	50%	0.33	0.50	-0.05	0.12	38%	0.15	0.29	-0.09	0.08	53%
OC9-ACET	Oxo-Nonyl Acetate	0.85	0.28	33%	0.87	2%	0.50	0.20	39%	0.29	0.16	56%	0.27	0.46	-0.15	0.14	51%	0.10	0.25	-0.18	0.10	95%
OC10ACET	Oxo-Decyl Acetate	0.83	0.28	33%	0.85	2%	0.49	0.19	40%	0.28	0.16	57%	0.27	0.45	-0.15	0.14	52%	0.09	0.24	-0.19	0.10	108%
OC12ACET	Oxo-Dodecyl Acetate	0.72	0.26	36%	0.74	2%	0.43	0.18	42%	0.24	0.15	63%	0.22	0.40	-0.19	0.14	64%	0.05	0.19	-0.24	0.11	-
OC13ACET	Oxo-Tridecyl Acetate	0.67	0.25	37%	0.69	3%	0.40	0.17	43%	0.23	0.15	64%	0.21	0.38	-0.20	0.14	66%	0.04	0.18	-0.25	0.10	-

[a] Maximum, minimum, and standard deviations for base ROG mixture are incremental reactivities relative to the average.

Table C-7. Ozone yield incremental reactivities in the individual base case and adjusted NO_x scenarios. (This table is included with the electronic version of the report only.)

Table C-8. Maximum 8-hour average incremental reactivities in the individual base case and adjusted NO_x scenarios. (This table is included with the electronic version of the report only.)

APPENDIX D

ESTIMATION OF UPPER LIMIT MAXIMUM INCREMENTAL REACTIVITIES

A. Abstract

A procedure is presented for estimating upper limit Maximum Incremental ozone Reactivities (MIR's) for volatile organic compounds (VOCs) whose atmospheric ozone impacts are uncertain. This might be applicable for including compounds of unknown reactivity in reactivity-based regulations which employ the MIR scale for quantifying ozone impacts. The procedure is based on deriving upper limits for the two factors that determine the ozone impact of a compound in pollution episode. These are the fraction of emitted VOC that reacts during the episode (the kinetic reactivity), and the amount of ozone formed per molecule of VOC that reacts (the mechanistic reactivity). Upper limit kinetic reactivities are derived from the rate constants for the atmospheric reactions of the VOCs if they are known, otherwise a maximum kinetic reactivity of unity is assumed. Upper limit mechanistic reactivities are obtained from calculated relative mechanistic reactivities for a variety of VOCs for MIR scenarios, with lower upper limits being obtained for compounds known not to photolyze, or for alkanes or saturated compounds containing only alcohol, ether or ester groups. The information needed for making such estimates is discussed, and examples are given for representative VOCs whose reactivities are reasonably well known.

B. Introduction

In recognition of the fact that volatile organic compounds (VOCs) differ in their impacts on photochemical ozone formation, The California Air Resources Board (CARB) has implemented ozone reactivity adjustments in vehicle emissions regulations (CARB, 1993), and is now considering use or reactivity adjustments in regulations of VOCs from consumer products. The reactivity adjustments currently used in the CARB vehicle regulations are based on the Maximum Incremental Reactivity (MIR) scale (Carter, 1994a), and an updated version of this scale would likely be used in any consumer product reactivity-based regulations. Although ozone impacts of VOCs depend on atmospheric conditions (Carter and Atkinson; 1989; Carter, 1994a; Jeffries and Crouse, 1991), the MIR scale was chosen for this purpose because it reflects ozone impacts under conditions where ozone is most sensitive to VOC emissions. In addition, the MIR scale has been shown to correlate reasonably well to effects of VOCs on integrated ozone and ozone exposure (Carter, 1994a; McNair et al 1992, 1994; CARB, 1993).

One problem with implementing reactivity adjustments in VOC regulations for consumer products and other stationary sources is that a wide variety of VOCs are involved, including many whose ozone impacts are highly uncertain or unknown. Some means is necessary to incorporate such compounds in reactivity-based regulations which provides incentives for using compounds of known low reactivity, but which is not unduly burdensome to the producers and users of compounds of unknown reactivity, some of which may also turn out to be beneficial. One approach is to use "default" reactivity factors for compounds whose reactivities are unknown, which would be the upper limit of their actual likely ozone impact. This approach allows regulations to cover compounds of both known and unknown reactivity in a relatively simple and consistent manner, and provides incentives for producers or users to reduce the uncertainties concerning the environmental effects of the emissions they cause. For this

approach to be acceptable, the default reactivity factors must not be so high that they cause an unfair burden to producers and users of new or unstudied compounds, which may turn out to have relatively low reactivity. Ideally, they should incorporate, to the maximum extent possible, any knowledge we have concerning the likely upper limit ozone impacts of the compounds, so they will not be higher than absolutely necessary, given the limitations in our knowledge. In addition, the procedures for deriving them should not be so complex that they cannot be applied to large numbers of unstudied compounds that might be covered by reactivity-based regulations.

Given below is a suggested set of procedures that can be employed to estimate upper limit MIR's for VOCs for which limited kinetic or mechanistic information is available. The procedures take into account our current knowledge concerning the general factors that affect ozone reactivities of all VOCs. This provides a means for appropriate upper limit values to be derived for compounds whose atmospheric reaction rate constants are known, or which belongs to classes of compounds where the range of possible oxidation products and mechanisms are reasonably well understood.

C. Methods

1. Factors Affecting Reactivity

a. Kinetic and Mechanistic Reactivities

For regulatory applications, the appropriate quantification of ozone impact is the *incremental reactivity*, which is the amount of additional ozone formation caused by adding a small amount of the compound to the emissions, divided by the amount emitted (Carter and Atkinson, 1989; Carter, 1994a). For upper limit estimation purposes, it is useful to think of incremental reactivities as being a product of three factors, as follows (Carter and Atkinson, 1989):

$$\begin{array}{c}\text{Incremental}\\\text{Reactivity}\\\text{(Ozone per}\\\text{mass VOC}\\\text{emitted)}\end{array} = \begin{array}{c}\text{Kinetic}\\\text{Reactivity}\\\text{(VOC reacted}\\\text{/VOC emitted)}\end{array} = \begin{array}{c}\text{Mechanistic}\\\text{Reactivity}\\\text{(moles } O_3\\\text{/mole VOC}\\\text{reacted)}\end{array} \cdot \begin{array}{c}\text{Mass Conv-}\\\text{ersion Factor}\\\text{(moles VOC}\\\text{/mass VOC)}\end{array} \qquad \text{(I)}$$

The *kinetic reactivity* is the fraction of the emitted VOC which undergoes chemical reaction in the atmosphere during the time period being considered. It depends primarily on the rate constants for the VOCs atmospheric reactions, but also on the overall levels of OH radicals, ozone, or light in the scenario, depending on how the VOC reacts. Being a fraction, it is a unitless number. Note that kinetic reactivity is *not* the same as the atmospheric reaction rate, which is the speed at which it reacts. Although they are approximately proportional for slowly reacting compounds, for rapidly reacting compounds the kinetic reactivity is approximately unity, and thus almost independent of the reaction rate. Therefore, if insufficient information is available to derive upper limit atmospherically relevant rate constants for a compound, then kinetic reactivities of unity can be used for upper limit estimation purposes.

The *mechanistic reactivity* is the number of molecules of ozone formed for each molecule of VOC that reacts. It reflects both the nature of the VOCs reaction mechanism and also the efficiency of ozone formation from the reactions of VOCs in the particular scenario. Although the mechanistic reactivity factor can be given in other units besides molecules of ozone per molecule VOC, molecular

units are more meaningful chemically and therefore are more straightforward to use for estimation purposes. Upper limits for mechanistic reactivities can be estimated based on the range of mechanistic reactivities of compounds with known mechanisms or ozone impacts, as discussed below. In some cases, structural information and knowledge of the general features of atmospheric chemistry may permit limiting the range of possible mechanisms and products, allowing for lower upper limit estimates for mechanistic reactivities for certain types of compounds.

The product of the kinetic and mechanistic reactivities is incremental reactivities in units of molecules of ozone formed per molecule of VOC emitted. Since emissions of VOCs are quantified and regulated on a mass basis, the appropriate incremental reactivity units for regulatory applications is ozone formed per unit mass of VOC emitted. Therefore, a *mass conversion factor* is applied to place the incremental reactivities on a mass VOC basis. It is inversely proportional to the VOC's molecular weight.

b. Environmental Conditions

Both kinetic and mechanistic reactivities depend on the conditions of the environment where the VOC reacts. For example, the OH radical levels in the environment determine the fraction reacted for a VOC which reacts primarily with OH radicals, and the NO_x levels significantly affect the efficiency for O_3 formation once a VOC reacts, which determines its mechanistic reactivity (see, for example, Carter and Atkinson, 1989). However, if the VOCs with known reactivities are to be regulated according to their MIR's, then we need only be concerned with estimates of kinetic and mechanistic reactivities for MIR conditions. Therefore, in this work we are concerned only with a single set of environmental conditions, which is that used to derive the MIR scale.

MIR conditions consist of scenarios where the NO_x inputs have been adjusted so that the peak ozone levels are the most sensitive to changes in total reactive VOC emissions. The MIR scale developed by Carter (1994a) is based on averages of incremental reactivities calculated for 39 different single-day EKMA model scenarios (Baugues, 1990) where NO_x inputs have been adjusted in this way. However, it was also found that incremental reactivities calculated using a single "Averaged Conditions" MIR scenario were essentially the same, to within a few percent for all positively reactive VOCs, as average reactivities calculated from the 39 MIR scenarios. Therefore, for the purpose of estimating approximate upper limit kinetic and mechanistic reactivities for upper limit MIR determinations, it is sufficient to limit our consideration to the Averaged Conditions MIR scenario. The detailed input data and derivation of this scenario are given elsewhere (Carter, 1994a,b).

2. Upper Limit Kinetic Reactivities for MIR

a. Information Required

Most VOCs react in the atmosphere with OH radicals, and many also react to non-negligible extents with O_3, NO_3 radicals, or by photolysis. If insufficient information is available concerning the rate constants for these processes (or their upper limits) under atmospheric conditions, then an upper limit kinetic reactivity of unity should used when deriving upper limit MIR values. However, for many if not most VOCs, sufficient information is available to permit more precise kinetic reactivity estimates. The minimum information for making kinetic reactivity estimates is summarized in the following section.

OH Radical Rate Constant. Because VOCs react in the atmosphere with OH radicals, the rate constant for this reaction, or its upper limit, must be determined, or its upper limit must be estimated. Some VOCs can be concluded not to react significantly with OH radicals based on the lack of modes for which OH to react, such as a lack of abstractable hydrogens or double bonds. Only if a VOC contains only functional groups which have been shown in other molecules not to react with OH radicals, or if there are no thermodynamically feasible means for OH radicals to react with the compound, it is safe to conclude that it does not react with OH radicals without the benefit of carrying out a direct experimental measurement. (Because of possible interactions, functional groups that are immediately adjacent to another functional group should be considered to be different from those that are isolated. This is applicable for all reactions discussed here.) Available information concerning OH + VOC rate constants is summarized by Atkinson (1989, 1994).

Methods exist for estimating OH radical rate constants for many compounds that are usually accurate to within a factor of 2 or better (Kwok and Atkinson, 1995). Therefore, if no measurements are available concerning the OH radical rate constant of the compound, but the rate constant can be measured using the methods of Kwok and Atkinson (1995), then a rate constant which is two times the estimated value can be used for the purpose of making upper limit kinetic reactivity estimates. The factor of two increase is necessary to take into account the uncertainty of the estimation methods when making upper limit determinations.

Ozone Rate Constant. Some VOCs, usually (but not always) those with C=C double bonds, can react with ozone at significant rates, and these reactions often have a net positive effect on ozone because of the subsequent reactions of the radicals formed. Only if a VOC contains only functional groups that have been shown in other molecules not to react with ozone, or if there are no thermodynamically feasible means for such a reaction to occur, is it safe to conclude that the reaction with ozone will be negligible in the absence of direct experimental measurement. Available information concerning ozone + VOC rate constants is given by Atkinson and Carter (1984), and is updated by Atkinson (1994).

Although Atkinson and Carter (1984) discuss possible approaches for estimating O_3 rate constants, no comprehensive approach has been developed which performs very reliably for estimation purposes. Therefore, if the compound contains groups which might possibly react with O_3 (e.g. C=C, C=N, or N-N bonds), and its O_3 rate constant has not been measured or its upper limit determined, then a kinetic reactivity of unity must be assumed when making upper limit reactivity estimates.

NO_3 Radical Rate Constant. Some VOCs, usually (but not always) those with C=C double bonds, can react with NO_3 radicals at sufficiently high rates to affect their ozone impact. Only if a VOC contains only functional groups which have been shown in other molecules not to react with NO_3 radicals, or if there are no thermodynamically feasible means for such a reaction to occur, is it safe to conclude that this reaction with ozone will be negligible in the absence of direct experimental measurement. Available information concerning NO_3 + VOC rate constants is given by Atkinson (1991, 1994). Atkinson (1991, 1994) also gives methods for estimating these rate constants. As with the OH radical rate constant, if the rate constant has to be estimated, then the estimate should be increased by a factor of two for upper limit reactivity estimates.

Photolysis Rates. Some VOCs can react in the atmosphere by direct photolysis, and if photodecomposition is sufficiently rapid and involves radical formation, then their reactions can result in

high ozone impacts. Upper limit atmospheric photolysis rates can be estimated given the compound's UV-visible absorption spectrum for wavelengths $\approx$ 290 nm, and the actinic fluxes for direct overhead sunlight for clear-sky conditions, assuming unit quantum yields. The actinic fluxes given by Peterson (1976) should be sufficient for this purpose. Only if the VOC contains only functional groups which have no absorption at $\lambda \approx 290$ nm, or has no decomposition pathway with a heat of reaction of less than the energy of a 290 nm photon, is it safe to conclude that the compound will not photolyze in the absence of absorption cross section data. If the compound has non-negligible absorption cross sections in the $\lambda \approx$ 290 nm region, then unit quantum yields should be assumed for making upper limit photolysis rate estimates, unless there is information justifying the use of lower quantum yields for this purpose. Information concerning absorption cross sections and quantum yields for photolyses of smaller molecules of atmospheric significance are given in the most recent NASA (1994) and IUPAC (Atkinson et al, 1997, 1999) evaluations, though for higher molecular weight VOCs, and organics in general, there does not appear to be a more current or comprehensive review of absorption cross section data than that of Calvert and Pitts (1966).

b. Estimation of MIR Kinetic Reactivities from Rate Constants

Most VOCs react significantly only with OH radicals. In this case, the fraction reacted in given scenario can be estimated by

$$\text{Kinetic Reactivity} \approx (1 - e^{-kOH \cdot EffIntOH}) \qquad \text{(II)}$$

or

$$\text{Kinetic Reactivity} \approx kOH \cdot EffIntOH \qquad \text{(III)}$$

(if kOH · IntOH <<1). Here, kOH is the VOC's OH radical rate constant, and EffIntOH is a scenario-dependent "Effective Integrated OH" parameter which is related to, but is not exactly the same as, the integrated OH radical levels (Carter and Atkinson, 1989). Note that for slowly reacting compounds, Equation (III) predicts that the kinetic reactivities are approximately proportional to the integrated reaction rates, while for rapidly reacting compounds the kinetic reactivity approaches the upper limit value of unity. For the Averaged Conditions MIR scenario, a value of

$$EffIntOH^{MIR} = 1.8 \times 10^{11} \text{ molec cm}^3 \text{ s}$$

is appropriate for use in upper limit kinetic reactivity estimates. This gives good fits to kinetic reactivities for VOCs with $kOH < 5 \times 10^{-12}$ cm^3 $molec^{-1}$ s^{-1}, while slightly overestimating (by no more than ~5%) kinetic reactivities for faster reacting compounds.

Equation (II) obviously will not work if the VOC reacts significantly with O_3 or NO_3 radicals or undergoes photolysis. For the purpose of estimating kinetic reactivities for such compounds, we assume that Equation (II) can be generalized to

$$\text{Kinetic Reactivity} \approx (1 - e^{-\text{Integrated Reaction Rate}}) \qquad \text{(IV)}$$

where

$$\text{Integrated Reaction Rate} \approx kOH^{VOC} \cdot IntOH + kO_3^{VOC} \cdot IntO_3 + kNO_3^{VOC} \cdot IntNO_3 + \int kPhot^{VOC} dt \qquad \text{(V)}$$

and IntOH, $IntO_3$, and $IntNO_3$ are the integrated levels of OH radicals, O_3, and NO_3 radicals, respectively, and $\int kPhot^{VOC}dt$ is the integrated photolysis rate. (Note that IntOH, the actual integrated OH radical levels, is not the same as EffIntOH, which depends on the when the VOC is emitted in the scenario as well as the integrated OH radical levels.) For the Averaged Conditions MIR scenario, the integrated OH, O_3, and NO_3 are

$$IntOH^{MIR} = 1.8 \times 10^{11} \text{ molec cm}^{-3} \text{ s}$$

$$IntO_3^{MIR} = 8.0 \times 10^{16} \text{ molec cm}^{-3} \text{ s},$$

and

$$IntNO_3^{MIR} = 8.5 \times 10^{11} \text{ molec cm}^{-3} \text{ s}.$$

An estimate of the upper limit $\int kPhot^{VOC}dt$ can be obtained using the measured cross sections, the measured or upper limit quantum yields, and the clear-sky, direct overhead sun actinic flux data (such as those given by Peterson, 1976) to calculate the maximum photolysis rate, kPhot. If there is no information available concerning the quantum yield for the photodecomposition of the compound (as usually is the case), then unit quantum yields at all wavelengths should be assumed. For the Averaged Conditions MIR scenario, the integrated photolysis rate can then be approximated from kPhot using:

$$\int kPhot^{VOC}dt \approx 3.6 \times 10^4 \text{ s} \cdot 0.7 \cdot kPhot \approx 2.5\text{x}10^4 \text{ sec} \cdot kPhot \qquad \text{(VI)}$$

where 3.6×10^4 seconds is the length of time in the scenario [10 hours for all EKMA scenarios used by Carter (1994a,b)], and the 0.7 factor is the ratio of the average to the maximum photolysis rate, and was derived for the photolysis of NO_2 in the Averaged Conditions MIR scenario. Most photolysis reactions are more sensitive to shorter wavelength UV than is NO_2 photolysis, and would have a lower average-to-maximum ratio because their photolysis rates would vary more with solar zenith angle. Therefore, the 0.7 factor is considered appropriate for upper limit estimates. To be consistent with the units shown above, the units of kPhot should be s^{-1}.

Equations (IV) and (V) can be combined to yield

$$\text{Kinetic Reactivity} \approx (1 - e^{-\text{Effective kOH} \cdot \text{EffIntOH}}) \qquad \text{(VII)}$$

where

$$\text{Effective } k_{OH} = kOH^{VOC} + \frac{IntO_3}{IntOH} kO_3^{VOC} + \frac{IntNO_3}{IntOH} kNO_3^{VOC} + \frac{3.0\text{x}10^4}{IntOH} kPhot_{max}^{VOC} \qquad \text{(VIII)}$$

Using the IntOH, $IntO_3$, $IntNO_3$, and $\int kPhot^{VOC}dt/kPhot$ for the Averaged Conditions MIR scenario (see above), we then obtain

$$\text{Effective } kOH^{VOC} \approx kOH^{VOC} + 4.4\text{x}10^5\, kO_3^{VOC} + 4.6\, kNO_3^{VOC} + 1.3\text{x}10^{-7}\, kPhot. \qquad \text{(IX)}$$

where the units of the bimolecular rate constants are cm^3 $molec^{-1}$ s^{-1}, and the units of kPhot is s^{-1}. This in effect amounts to a correction to the OH radical rate constant for the other reaction pathways for the purpose of estimating kinetic reactivities.

3. Estimation of Upper Limit MIR Maximum Mechanistic Reactivities

Upper limit estimates for mechanistic reactivities can be obtained from examining the mechanistic reactivities for a sufficiently wide variety of VOCs under MIR conditions. Incremental reactivities calculated using the SAPRC-99 mechanism (Carter, 2000) were used for this purpose. This mechanism contains separate representations for the atmospheric reactions of approximately 400 different types of VOCs, though only a fraction of these have been experimentally evaluated. Although some of these mechanisms are uncertain, they can be considered to represent a sufficiently wide variety of ways that VOCs can react for the purpose of establishing upper limit mechanistic reactivity estimates.

Figure C-1 and Figure C-2 show the mechanistic reactivities for the Averaged Conditions MIR scenario calculated for a variety of VOCs. Note that the mechanistic reactivities shown will be different than those calculated by Carter (1994a), who used the SAPRC-90 (Carter, 1990) mechanism. Figure C-1 shows the mechanistic reactivities in units of moles O_3 per mole VOC reacted, and Figure C-2 shows the values as moles O_3 per mole carbon reacted. The highest molar MIR mechanistic reactivities is in the ~30-40 range, which are calculated for methyl methacrolate, 1,3,5- and 1,2,3-trimethyl benzene, and biacetyl. The highest per-carbon MIR mechanistic reactivities are for biacetyl, methyl glyoxal and glyoxal, which are in the range of ~8-10. However, if photoreactive compounds are excluded, then no compound has per-carbon MIR mechanistic reactivities which are significantly greater than ~7, with values in the 4-5 range being observed for methane and a variety of olefins and aromatics.

These data suggest that the upper limit per molecule MIR mechanistic reactivities can be estimated by

$$\text{Mechanistic Reactivity} \approx \text{MIN}\,(7 \cdot n_C,\ 35) \qquad \text{(X)}$$

for compounds which are known to be non-photoreactive, and by

$$\text{Mechanistic Reactivity} \approx \text{MIN}\,(10 \cdot n_C,\ 40) \qquad \text{(XI)}$$

for photoreactive compounds or compounds for which photodecomposition cannot be ruled out. The units are moles of ozone per mole carbon VOC that reacts, and n_C is the number of carbons in the molecule.

For some compounds, specifically saturated hydrocarbons or non-photoreactive compounds containing only alcohol, ether, or ester groups, our knowledge of atmospheric reaction mechanisms, and how various types of reactions affects reactivity, can permit somewhat lower upper limit estimates to be made. Compounds such as these will react significantly only with OH radicals, would probably convert no more than 3-4 molecules of NO to NO_2, and the most reactive products they are likely to form are higher aldehydes or, in the case of esters, possibly some α-dicarbonyls such as methyl glyoxal (Carter, 2000). Probably the most reactive reasonable mechanism for such compounds would be:

$$\text{OH + compound} \rightarrow HO_2 + -3\ \text{NO} + 3\ NO_2 + \text{Formaldehyde + Other Aldehyde + Other Carbonyl} \quad \text{(Mechanism A)}$$

if the compound did not have a carbonyl group (i.e., not an ester), or

$$\text{OH + compound} \rightarrow HO_2 + -3\ \text{NO} + 3\ NO_2 + \text{Formaldehyde + Other Aldehyde + Other Carbonyl + 0.5 Methyl Glyoxal} \quad \text{(Mechanism B)}$$

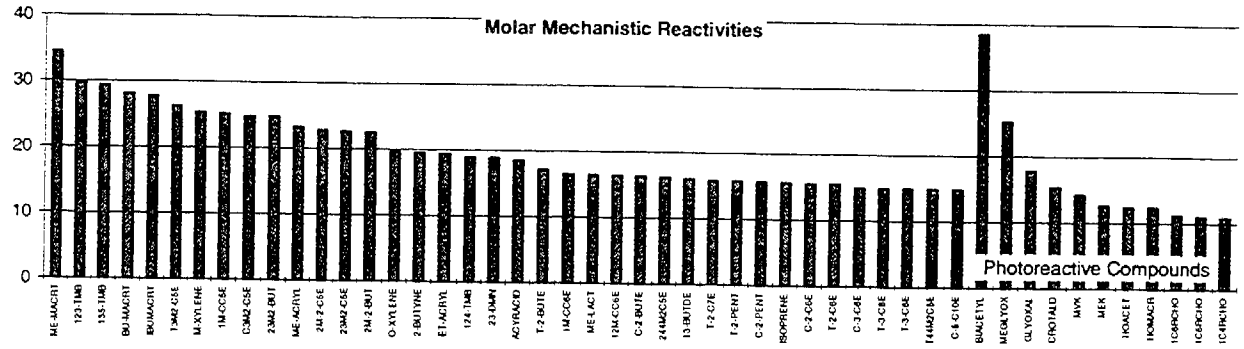


Figure D-1. Plots of calculated mechanistic reactivities, in units of moles ozone formed per mole VOC reacted, for selected compounds in the averaged conditions MIR scenario.

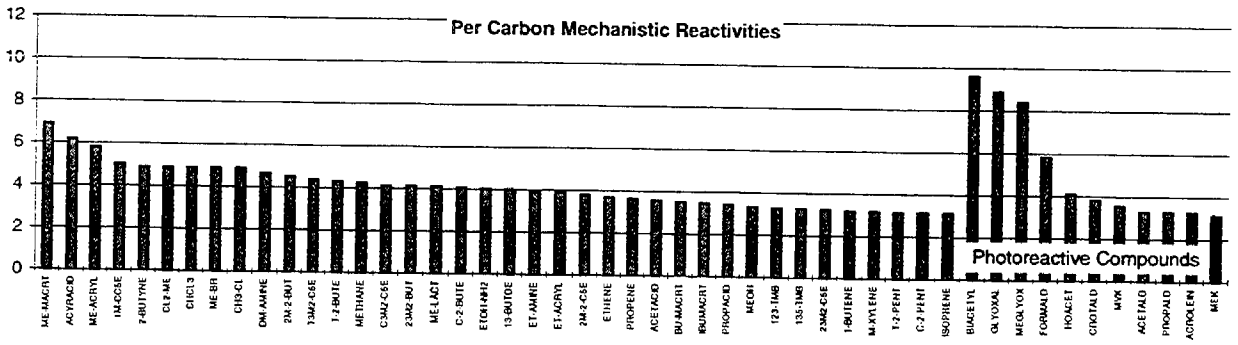


Figure D-2. Plots of calculated mechanistic reactivities, in units of moles ozone formed per mole carbon VOC reacted, for selected compounds in the averaged conditions MIR scenario.

otherwise. These are based on the observations that mechanisms with more than three NO to NO_2 conversions have not been observed for such compounds, that aldehydes are the most reactive products expected to be formed from compounds not containing carbonyl groups but formation of more than two moles of aldehydes rarely occurs, and that although some carbonyl-containing compounds may form α-dicarbonyls (e.g., see Carter et al, 1997d), it is probably not the dominant reaction route since carbonyl substitution tends to deactivate OH reaction at groups next to it (Kwok and Atkinson, 1995).

As discussed by Carter and Atkinson (1989), mechanistic reactivities of compounds that react only with OH radicals can be expressed in terms of sums of mechanistic reactivities of "pure mechanism species", which reflect specific aspects of the VOC's mechanism, such as the numbers of NO to NO_2 conversions, and yields of various types of reactive products. Table D-1 gives MIR mechanistic reactivities calculated for the major pure mechanism species likely to be involved in atmospheric reaction mechanisms of saturated hydrocarbons, alcohols, ethers or esters, and the corresponding mechanistic reactivities calculated for Mechanisms A and B, above. Note that the high mechanistic reactivities of the α-dicarbonyls make it appropriate to consider upper-limit reactivity mechanisms of carbonyl-containing compounds, whose reactions might result in formation of α-dicarbonyls, separately from upper limit mechanisms for compounds where these products cannot be formed.

Table D-1. Mechanistic reactivities of the major pure mechanism species affecting reactivities of non-photoreactive saturated hydrocarbons or oxygenates, and mechanistic reactivities of the mechanisms used for upper limit reactivity estimates for such compounds.

Pure Mechanism	Yields in Upper Limit Mechanisms A	B	MIR Mechanisitc Reactivity (Mol O_3 / Mol Pure Mechanism Species)		
OH Rate Constant (cm^3 $molec^{-1}$ s^{-1})			2.0e-12	2.0e-11	6.8e-11
Methyl Glyoxal Formation		0.5	9.7	14.9	20.3
Higher Aldehyde Formation	1.0	1.0	3.7	6.1	8.4
Acetaldehyde Formation			2.6	4.2	5.6
Formaldehyde Formation	1.0	1.0	2.3	3.5	4.8
Higher Ketone Formation	1.0	1.0	2.6	4.1	5.6
Acetone Formation			0.2	0.3	0.4
Organic Nitrates (radical termination)			-2.8	-3.8	-5.6
HO_2 Radicals (radical propigation)	1.0	1.0	1.0	1.2	1.4
Extra NO to NO_2 Conversions	3.0	3.0	1.1	1.3	1.4
Mechanism A Upper Limit Mechanistic Reactivities (no carbonyl group)			13.0	18.8	24.3
Mechanism B Upper Limit Mechanistic Reactivities (with carbonyl group)			17.8	26.3	34.4

Table D-1 shows that mechanistic reactivities of some of the pure model species, and thus of the upper limit mechanisms A and B, are not independent of the OH radical rate constant, particularly at higher rate constants. In particular, although the mechanistic reactivity contribution of NO to NO_2 conversions is relatively unaffected by the reaction rate, the mechanistic reactivity contribution of reactive products tends to increase as the rate constant increases. For Mechanisms A and B, the Averaged Conditions MIR mechanistic reactivities shown on Table D-1 can be fit by the following empirical equations:

$$\text{MIR Mechanistic Reactivity A} = 25.4 - 13.2 \exp(-3.3 \times 10^{10} \cdot \text{kOH}) \qquad \text{(XII)}$$

$$\text{MIR Mechanistic Reactivity B} = 36.3 - 19.5 \exp(-3.2 \times 10^{10} \cdot \text{kOH}) \qquad \text{(XIII)}$$

where the units of the mechanistic reactivities are mole O_3 per mole VOC, and the kOH is the OH radical rate constants in units of cm^3 $molec^{-1}$ s^{-1}.

Based on these considerations, we conclude that for alkanes or saturated compounds containing no groups other than alcohols and ethers, and no atoms other than H, C, or O, then the upper limit mechanistic reactivity can be given by either Equation (X) or (XII), whichever gives the lower value. Likewise, if the compound contains a carbonyl group but no other groups besides alcohol or ether and no atoms other than N, C, or O, then the upper limit mechanistic reactivity can be given by either Equation

(XI) or (XIII), whichever is lower. For any other compound, only Equations (X) or (XI) can be used, depending on whether the compound is or may be photoreactive.

4. Upper Limit MIR Estimates

The upper limit kinetic and mechanistic reactivities derived as discussed above can then be combined, according to Equation (I1) to obtain an estimate of the *incremental reactivity* in the MIR scale, which is the quantity of interest. The incremental reactivities obtained by multiplying the kinetic and mechanistic reactivities derived as discussed above will be in units of moles of ozone formed per mole VOC emitted, but for regulatory applications the appropriate units are grams of O_3 per gram VOC. This conversion is done by multiplying by the ratio of the molecular weight of O_3 to the molecular weight of the VOC. Therefore,

$$\begin{matrix}\text{Upper Limit MIR} \\ (\text{gm } O_3 / \text{gm VOC})\end{matrix} = \begin{matrix}\text{Upper Limit} \\ \text{Kinetic Reactivity}\end{matrix} \cdot \begin{matrix}\text{Upper Limit Mech. React'y} \\ (\text{mol } O_3 / \text{mol VOC})\end{matrix} \cdot \frac{48\,(\text{gm } O_3 / \text{gm VOC})}{\text{Mwt}^{\text{VOC}}\,(\text{gm/mol})} \qquad \text{(XIV)}$$

D. Results and Discussion

1. Kinetic Reactivities

Table D-2 gives the rate constants and the corresponding estimated MIR kinetic reactivities for all the VOCs that can be separately represented in the SAPRC-99 mechanism (Carter, 2000). The table also indicates which rate constants were estimated and which are based on measurement data. Note that a factor of 2 uncertainty factor was applied to all estimated rate constants, but measured rate constants (no matter how uncertain) were used without any uncertainty adjustments. The $kPhot^{MAX}$ values were calculated using the absorption cross sections in the mechanism, but assuming unit quantum yields. This is based on the assumption that quantum yields are not known for most photoreactive VOCs for which upper limit reactivity estimates have to be made, and thus upper limit quantum yields of unity would have to be used.

2. Mechanistic Reactivities

Table D-2 gives the both the directly calculated ("best estimate") and the upper limit MIR mechanistic reactivities for all the compounds in the current mechanism. The "MR Tp." column on the table shows how the compounds were classified for the purpose of estimating upper limit mechanistic reactivities, and shows how the upper limit values were obtained. The upper limits are close to the directly calculated values for the most mechanistically reactive compounds such as methane some of the alkyl benzenes, but are up to a factor of ~5-10 for compounds with low mechanistic reactivity. The latter include compounds such as naphthalenes or high molecular weight esters, where the relatively low upper limit mechanism A cannot be used. On the average, the upper limit mechanistic reactivities are higher than the directly calculated values a factor of ~3. Given the large variability and many factors that affect mechanistic reactivities, this is probably as close an estimate that can reasonably be obtained.

3. Upper Limit MIR's

The upper limit MIR's for all the for all the separately represented VOCs in the mechanism are shown on Table D-2, where they can be compared with their directly calculated ("best estimate") values. The table also shows the ratio of the upper limit to the directly calculated MIRs, which is in effect the margin of error involved in making the upper limit estimates. For most compounds, whose rate constants have been measured or which react sufficiently rapidly that the kinetic reactivity is not highly sensitive to the rate constant, the difference between upper limit and best estimate MIRs reflect primarily the differences for the mechanistic reactivities. Obviously the differences between upper limit and best estimate would be greater if the rate constants were unknown or significantly uncertain, and unit kinetic reactivities had to be used.

4. Discussion

The recommendations for estimating upper limit reactivities were developed to assist the application of reactivity-based regulations to compounds of uncertain reactivity. The objective to derive upper limit MIR estimates for compounds of uncertain reactivity such that it is unlikely that the actual ozone impacts of the compounds would be higher than the upper limit, but which are as low as possible given our limited knowledge. It is also important that the procedure be as objective and straightforward as possible, so that it can be applied to the full variety of compounds which might be subject to reactivity based regulations. The procedures discussed above should adequately address these objectives.

The recommendations given in this work are based on reactivity calculations for a wide variety of compounds. However, it should be pointed out that the upper limit mechanistic reactivities for compounds with unknown mechanisms are driven primarily by calculated reactivities for aromatic hydrocarbons, methyl glyoxal, and methane. The other classes of compounds which were considered were primarily alkanes, olefins, and various relatively low molecular weight oxygenates (see Carter, 2000). If a compound is expected to possibly have a significantly different mechanism than any compound in this group, then the possibility that the ozone impacts may actually be higher than estimated using these procedures cannot be totally ruled out. In this case, the upper limit estimates would need to be modified accordingly. However, given our current knowledge of atmospheric chemistry and the variety of compounds studied, we think that the probability of any given compound having a greater ozone impact the upper limit estimate is relatively low.

It is important to recognize the limitations of this work. The procedure is intended only for estimating upper limits for Maximum Incremental Reactivities calculated using the approach and one-day EKMA model airshed scenarios employed by Carter (1990), and using the SAPRC-99 mechanisms as described by Carter (2000). The upper limit mechanistic reactivities are particularly sensitive to the type of scenario employed, and are also subject to change as the chemical mechanism is updated. Therefore, these upper limit estimates should not be considered as independent of the reactivity scale upon which it is based, but rather as an extension of it, which would be updated and modified as the scale is updated in the process of ongoing research.

In particular, the upper limits given here are *not* to be compared with MIR values used in the current CARB vehicle regulations (CARB, 1993), or those given by Carter (1994a), since they were calculated using an earlier chemical mechanism, which generally gives lower MIR values. The upper

limit MIRs given on Table D-2 should be compared *only* with the best estimate MIRs given on the same table [or by Carter (2000)], and not with those given in any previously published or distributed tabulation, or with any updated scale that may be developed in the future. However, the general approach discussed here can be used to update the upper limit estimates if any changes are made to the chemical mechanism or scenarios used to derive the underlying reactivity scale upon which this is based.

It is also important to recognize that the general procedures discussed here are only applicable to regulatory or other applications where, by their nature, the ozone impacts must be quantified using a single scale. Examples would include the CARB clean-fuel/low emissions vehicle regulations (CARB, 1993), or the reactivity adjustments to VOC content limits being considered for CARB consumer product regulations. This procedure is *not* applicable to applications such as deciding whether to exempt a VOC from regulation on the basis of having negligible ozone impact, which can be based on a VOC's impact under a full variety of atmospheric conditions. A set of procedures considered more appropriate for upper limit reactivity estimates for making VOC exemption decisions is described in a separate document (Carter, 1997).

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Table D-2. Summary of upper limit MIR estimates for the SAPRC-99 mechanism, and comparison with directly calculated MIRs.

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1}) (* = Estimated k)				(s^{-1})							
CO	Carbon Monoxide	1	28.0	2.1e-13	2.1e-13				0.04	A	7	0.45	1	0.06	7.8
METHANE	Methane	1	16.0	6.6e-15	6.6e-15				0.00	A	7	0.03	1	0.01	1.8
ETHANE	Ethane	2	30.1	2.6e-13	2.6e-13				0.05	A	12	0.92	1	0.31	3.0
PROPANE	Propane	3	44.1	1.1e-12	1.1e-12				0.19	A	13	2.61	1	0.56	4.7
N-C4	n-Butane	4	58.1	2.5e-12	2.5e-12				0.36	A	13	3.99	1	1.33	3.0
N-C5	n-Pentane	5	72.2	4.0e-12	4.0e-12				0.52	A	14	4.83	1	1.54	3.1
N-C6	n-Hexane	6	86.2	5.5e-12	5.5e-12				0.63	A	14	5.09	2	1.45	3.5
N-C7	n-Heptane	7	100.2	7.0e-12	7.0e-12				0.73	A	15	5.20	2	1.28	4.1
N-C8	n-Octane	8	114.2	8.8e-12	8.8e-12				0.80	A	16	5.22	2	1.11	4.7
N-C9	n-Nonane	9	128.3	1.0e-11	1.0e-11				0.84	A	16	5.02	3	0.95	5.3
N-C10	n-Decane	10	142.3	1.1e-11	1.1e-11				0.87	A	16	4.81	3	0.83	5.8
N-C11	n-Undecane	11	156.3	1.3e-11	1.3e-11				0.91	A	17	4.68	3	0.74	6.3
N-C12	n-Dodecane	12	170.3	1.4e-11	1.4e-11				0.92	A	17	4.44	3	0.66	6.8
N-C13	n-Tridecane	13	184.4	1.6e-11	1.6e-11				0.95	A	18	4.35	3	0.62	7.0
N-C14	n-Tetradecane	14	198.4	1.8e-11	1.8e-11				0.96	A	18	4.23	3	0.58	7.3
N-C15	n-Pentadecane	15	212.4	2.1e-11	2.1e-11				0.98	A	19	4.17	3	0.56	7.5
N-C16	n-C16	16	226.5	2.3e-11	2.3e-11				0.99	A	19	4.02	3	0.52	7.7
2-ME-C3	Isobutane	4	58.1	2.2e-12	2.2e-12				0.33	A	13	3.62	1	1.35	2.7
2-ME-C4	Iso-Pentane	5	72.2	3.7e-12	3.7e-12				0.49	A	14	4.51	2	1.68	2.7
22-DM-C3	Neopentane	5	72.2	8.6e-13	8.6e-13				0.15	A	13	1.23	2	0.69	1.8
22-DM-C4	2,2-Dimethyl Butane	6	86.2	2.4e-12	2.4e-12				0.35	A	13	2.61	2	1.33	2.0
23-DM-C4	2,3-Dimethyl Butane	6	86.2	5.8e-12	5.8e-12				0.65	A	15	5.30	2	1.14	4.7
2-ME-C5	2-Methyl Pentane	6	86.2	5.3e-12	5.3e-12				0.62	A	14	4.97	2	1.80	2.8
3-ME-C5	3-Methylpentane	6	86.2	5.4e-12	5.4e-12				0.63	A	14	5.04	2	2.07	2.4
223TM-C4	2,2,3-Trimethyl Butane	7	100.2	4.3e-12	4.3e-12				0.54	A	14	3.62	2	1.32	2.7
22-DM-C5	2,2-Dimethyl Pentane	7	100.2	3.4e-12	3.4e-12				0.46	A	14	3.03	2	1.22	2.5
23-DM-C5	2,3-Dimethyl Pentane	7	100.2	1.4e-11	7.2e-12	*			0.93	A	17	7.64	2	1.55	4.9
24-DM-C5	2,4-Dimethyl Pentane	7	100.2	5.0e-12	5.0e-12				0.60	A	14	4.10	2	1.65	2.5
2-ME-C6	2-Methyl Hexane	7	100.2	1.4e-11	6.9e-12	*			0.92	A	17	7.52	2	1.37	5.5
33-DM-C5	3,3-Dimethyl Pentane	7	100.2	6.0e-12	3.0e-12	*			0.67	A	15	4.67	2	1.32	3.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
3-ME-C6	3-Methyl Hexane	7	100.2	1.4e-11	7.2e-12	*			0.93	A	17	7.65	2	1.86	4.1
2233M-C4	2,2,3,3-Tetramethyl Butane	8	114.2	1.1e-12	1.1e-12				0.18	A	13	0.94	3	0.44	2.1
224TM-C5	2,2,4-Trimethyl Pentane	8	114.2	3.6e-12	3.6e-12				0.48	A	14	2.78	2	1.44	1.9
22-DM-C6	2,2-Dimethyl Hexane	8	114.2	4.8e-12	4.8e-12				0.59	A	14	3.49	3	1.13	3.1
234TM-C5	2,3,4-Trimethyl Pentane	8	114.2	7.1e-12	7.1e-12				0.73	A	15	4.59	3	1.23	3.7
23-DM-C6	2,3-Dimethyl Hexane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.34	5.4
24-DM-C6	2,4-Dimethyl Hexane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.80	4.0
25-DM-C6	2,5-Dimethyl Hexane	8	114.2	1.7e-11	8.3e-12	*			0.95	A	18	7.12	3	1.68	4.2
2-ME-C7	2-Methyl Heptane	8	114.2	1.7e-11	8.3e-12	*			0.95	A	18	7.13	3	1.20	5.9
3-ME-C7	3-Methyl Heptane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.35	5.4
4-ME-C7	4-Methyl Heptane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.48	4.9
225TM-C6	2,2,5-Trimethyl Hexane	9	128.3	1.2e-11	6.1e-12	*			0.89	A	17	5.55	3	1.33	4.2
235TM-C6	2,3,5-Trimethyl Hexane	9	128.3	7.9e-12	7.9e-12				0.77	A	15	4.37	3	1.33	3.3
24-DM-C7	2,4-Dimethyl Heptane	9	128.3	2.0e-11	1.0e-11	*			0.97	A	19	6.79	3	1.48	4.6
2-ME-C8	2-Methyl Octane	9	128.3	1.0e-11	1.0e-11				0.84	A	16	5.04	3	0.96	5.3
33-DE-C5	3,3-Diethyl Pentane	9	128.3	4.9e-12	4.9e-12				0.59	A	14	3.15	3	1.35	2.3
35-DM-C7	3,5-Dimethyl Heptane	9	128.3	2.1e-11	1.0e-11	*			0.98	A	19	6.86	3	1.63	4.2
4-ET-C7	4-Ethyl Heptane	9	128.3	2.1e-11	1.0e-11	*			0.98	A	19	6.88	3	1.44	4.8
4-ME-C8	4-Methyl Octane	9	128.3	9.7e-12	9.7e-12				0.83	A	16	4.93	3	1.08	4.6
24-DM-C8	2,4-Dimethyl Octane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	1.09	5.8
26DM-C8	2,6-Dimethyl Octane	10	142.3	1.3e-11	1.3e-11				0.91	A	17	5.15	3	1.27	4.1
2-ME-C9	2-Methyl Nonane	10	142.3	1.3e-11	1.3e-11				0.90	A	17	5.12	3	0.86	6.0
34-DE-C6	3,4-Diethyl Hexane	10	142.3	7.4e-12	7.4e-12				0.74	A	15	3.78	3	1.20	3.2
3-ME-C9	3-Methyl Nonane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	0.89	7.2
4-ME-C9	4-Methyl Nonane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	0.99	6.5
4-PR-C7	4-Propyl Heptane	10	142.3	2.4e-11	1.2e-11	*			0.99	A	19	6.45	3	1.24	5.2
26DM-C9	2,6-Dimethyl Nonane	11	156.3	2.6e-11	1.3e-11	*			0.99	A	20	6.02	3	0.95	6.3
35-DE-C7	3,5-Diethyl Heptane	11	156.3	2.8e-11	1.4e-11	*			0.99	A	20	6.16	3	1.21	5.1
3-ME-C10	3-Methyl Decane	11	156.3	2.6e-11	1.3e-11	*			0.99	A	20	6.03	3	0.77	7.9

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH		kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. /
										KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	Direct
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)			(s^{-1})							
4-ME-C10	4-Methyl Decane	11	156.3	2.6e-11	1.3e-11	*				0.99	A	20	6.03	3	0.80	7.5
36-DE-C8	2,6-Diethyl Octane	12	170.3	3.1e-11	1.5e-11	*				1.00	A	21	5.79	3	1.09	5.3
36DM-C10	3,6-Dimethyl Decane	12	170.3	2.9e-11	1.5e-11	*				1.00	A	20	5.71	3	0.88	6.5
3-ME-C11	3-Methyl Undecane	12	170.3	2.9e-11	1.4e-11	*				0.99	A	20	5.69	3	0.70	8.1
5-ME-C11	5-Methyl Undecane	12	170.3	2.9e-11	1.4e-11	*				0.99	A	20	5.69	3	0.72	7.9
36DM-C11	3,6-Dimethyl Undecane	13	184.4	3.2e-11	1.6e-11	*				1.00	A	21	5.41	3	0.82	6.6
37-DE-C9	3,7-Diethyl Nonane	13	184.4	3.4e-11	1.7e-11	*				1.00	A	21	5.48	3	1.08	5.1
3-ME-C12	3-Methyl Dodecane	13	184.4	3.1e-11	1.6e-11	*				1.00	A	21	5.39	3	0.64	8.4
5-ME-C12	5-Methyl Dodecane	13	184.4	3.1e-11	1.6e-11	*				1.00	A	21	5.39	3	0.64	8.4
37DM-C12	3,7-Dimethyl Dodecane	14	198.4	3.5e-11	1.7e-11	*				1.00	A	21	5.13	3	0.74	6.9
38DE-C10	3,8-Diethyl Decane	14	198.4	3.6e-11	1.8e-11	*				1.00	A	21	5.19	3	0.68	7.6
3-ME-C13	3-Methyl Tridecane	14	198.4	3.4e-11	1.7e-11	*				1.00	A	21	5.11	3	0.57	9.0
6-ME-C13	6-Methyl Tridecane	14	198.4	3.4e-11	1.7e-11	*				1.00	A	21	5.11	3	0.62	8.3
37DM-C13	3,7-Dimethyl Tridecane	15	212.4	3.8e-11	1.9e-11	*				1.00	A	22	4.88	3	0.64	7.6
39DE-C11	3,9-Diethyl Undecane	15	212.4	3.9e-11	2.0e-11	*				1.00	A	22	4.93	3	0.62	7.9
3-ME-C14	3-Methyl Tetradecane	15	212.4	3.7e-11	1.9e-11	*				1.00	A	22	4.86	3	0.53	9.1
6-ME-C14	6-Methyl Tetradecane	15	212.4	3.7e-11	1.9e-11	*				1.00	A	22	4.86	3	0.57	8.5
3-ME-C15	3-Methyl Pentadecane	16	226.5	4.0e-11	2.0e-11	*				1.00	A	22	4.64	3	0.50	9.2
48DM-C14	4,8-Dimethyl Tetradecane	16	226.5	4.0e-11	2.0e-11	*				1.00	A	22	4.65	3	0.58	8.1
7-ME-C15	7-Methyl Pentadecane	16	226.5	4.0e-11	2.0e-11	*				1.00	A	22	4.64	3	0.51	9.0
CYCC3	Cyclopropane	3	42.1	8.4e-14	8.4e-14					0.02	A	12	0.21	3	0.10	2.1
CYCC4	Cyclobutane	4	56.1	1.5e-12	1.5e-12					0.24	A	13	2.65	3	1.05	2.5
CYCC5	Cyclopentane	5	70.1	5.1e-12	5.1e-12					0.61	A	14	5.91	2	2.69	2.2
CYCC6	Cyclohexane	6	84.2	7.3e-12	7.3e-12					0.74	A	15	6.32	2	1.46	4.3
IPR-CC3	Isopropyl Cyclopropane	6	84.2	2.7e-12	2.7e-12					0.39	A	13	2.98	3	1.52	2.0
ME-CYCC5	Methylcyclopentane	6	84.2	1.1e-11	5.7e-12	*				0.88	A	16	8.17	3	2.42	3.4
13DMCYC5	1,3-Dimeth. Cyclopentane	7	98.2	1.4e-11	6.8e-12	*				0.92	A	17	7.64	3	2.15	3.6
CYCC7	Cycloheptane	7	98.2	1.3e-11	1.3e-11					0.91	A	17	7.48	3	2.26	3.3
ET-CYCC5	Ethyl Cyclopentane	7	98.2	1.5e-11	7.3e-12	*				0.93	A	17	7.86	3	2.27	3.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. /
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	Direct
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
ME-CYCC6	Methylcyclohexane	7	98.2	1.0e-11	1.0e-11				0.84	A	16	6.55	3	1.99	3.3
13DMCYC6	1,3-Dimethyl Cyclohexane	8	112.2	2.4e-11	1.2e-11	*			0.99	A	19	8.20	3	1.72	4.8
CYCC8	Cyclooctane	8	112.2	1.4e-11	1.4e-11				0.92	A	17	6.76	3	1.73	3.9
ET-CYCC6	Ethylcyclohexane	8	112.2	2.4e-11	1.2e-11	*			0.99	A	19	8.22	3	1.75	4.7
PR-CYCC5	Propyl Cyclopentane	8	112.2	1.7e-11	8.7e-12	*			0.96	A	18	7.38	3	1.91	3.9
113MCYC6	1,1,3-Trimethyl Cyclohex.	9	126.2	8.7e-12	8.7e-12				0.80	A	16	4.71	3	1.37	3.4
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	9	126.2	2.7e-11	1.4e-11	*			0.99	A	20	7.59	3	1.62	4.7
C3-CYCC6	Propyl Cyclohexane	9	126.2	2.7e-11	1.3e-11	*			0.99	A	20	7.55	3	1.47	5.1
13DECYC6	1,3-Diethyl-Cyclohexane	10	140.3	3.1e-11	1.6e-11	*			1.00	A	21	7.06	3	1.34	5.3
14DECYC6	1,4-Diethyl-Cyclohexane	10	140.3	3.1e-11	1.6e-11	*			1.00	A	21	7.06	3	1.49	4.7
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	10	140.3	3.0e-11	1.5e-11	*			1.00	A	21	7.01	3	1.26	5.6
C4-CYCC6	Butyl Cyclohexane	10	140.3	3.0e-11	1.5e-11	*			1.00	A	21	6.99	3	1.07	6.5
13E5MCC6	13-Dieth-5-Me. Cyclohex.	11	154.3	3.4e-11	1.7e-11	*			1.00	A	21	6.58	3	1.11	5.9
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	11	154.3	3.4e-11	1.7e-11	*			1.00	A	21	6.56	3	0.95	6.9
C5-CYCC6	Pentyl Cyclohexane	11	154.3	3.3e-11	1.6e-11	*			1.00	A	21	6.50	3	0.91	7.1
135ECYC6	1,3,5-Triethyl Cyclohex.	12	168.3	3.8e-11	1.9e-11	*			1.00	A	22	6.17	3	1.06	5.8
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	12	168.3	3.6e-11	1.8e-11	*			1.00	A	21	6.10	3	0.81	7.6
C6-CYCC6	Hexyl Cyclohexane	12	168.3	1.8e-11	1.8e-11				0.96	A	18	4.97	2	0.75	6.6
13E5PCC6	13-Dieth-5-Pent Cyclohx.	13	182.4	4.1e-11	2.1e-11	*			1.00	A	22	5.80	3	0.99	5.8
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	13	182.4	3.9e-11	1.9e-11	*			1.00	A	22	5.73	3	0.70	8.2
C7-CYCC6	Heptyl Cyclohexane	13	182.4	3.8e-11	1.9e-11	*			1.00	A	22	5.71	3	0.66	8.6
13P5ECC6	13-Diprop-5-Eth Cyclohx.	14	196.4	4.4e-11	2.2e-11	*			1.00	A	22	5.46	3	0.94	5.8
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	14	196.4	4.2e-11	2.1e-11	*			1.00	A	22	5.40	3	0.58	9.3
C8-CYCC6	Octyl Cyclohexane	14	196.4	4.1e-11	2.1e-11	*			1.00	A	22	5.38	2	0.60	8.9
135PCYC6	135-Tripropyl Cyclohex.	15	210.4	4.7e-11	2.3e-11	*			1.00	A	23	5.16	3	0.90	5.7
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	15	210.4	4.4e-11	2.2e-11	*			1.00	A	22	5.11	3	0.60	8.5
C9-CYCC6	Nonyl Cyclohexane	15	210.4	4.4e-11	2.2e-11	*			1.00	A	22	5.10	3	0.54	9.4
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	16	224.4	4.9e-11	2.5e-11	*			1.00	A	23	4.89	3	0.77	6.3
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	16	224.4	4.7e-11	2.4e-11	*			1.00	A	23	4.85	3	0.55	8.8

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH		kO3		kNO3		kPhot Max (s^{-1})	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})			(* = Estimated k)											
C10CYCC6	Decyl Cyclohexane	16	224.4	4.7e-11	2.3e-11	*						1.00	A	23	4.84	3	0.50	9.6
ETHENE	Ethene	2	28.1	9.2e-12	8.4e-12		1.7e-18		2.2e-16			0.81	NP	14	19.51	1	9.08	2.1
PROPENE	Propene	3	42.1	3.1e-11	2.6e-11		1.1e-17		9.7e-15			1.00	NP	21	23.87	1	11.58	2.1
1-BUTENE	1-Butene	4	56.1	3.6e-11	3.1e-11		1.0e-17		1.4e-14			1.00	NP	28	23.92	2	10.29	2.3
1-PENTEN	1-Pentene	5	70.1	3.6e-11	3.1e-11		1.0e-17		1.4e-14	*		1.00	NP	35	23.92	2	7.79	3.1
3M-1-BUT	3-Methyl-1-Butene	5	70.1	3.7e-11	3.1e-11		1.1e-17		1.4e-14	*		1.00	NP	35	23.92	3	6.99	3.4
1-HEXENE	1-Hexene	6	84.2	4.2e-11	3.7e-11		1.1e-17		1.4e-14	*		1.00	NP	35	19.95	2	6.17	3.2
33M1-BUT	3,3-Dimethyl-1-Butene	6	84.2	3.0e-11	2.8e-11		5.4e-18		1.4e-14	*		1.00	NP	35	19.88	3	6.06	3.3
3M1-C5E	3-Methyl-1-Pentene	6	84.2	6.6e-11	3.2e-11	*	5.1e-18		1.4e-14	*		1.00	NP	35	19.96	3	6.22	3.2
4M1-C5E	4-Methyl-1-Pentene	6	84.2	6.8e-11	3.2e-11	*	9.6e-18		1.4e-14	*		1.00	NP	35	19.96	3	6.26	3.2
1-HEPTEN	1-Heptene	7	98.2	4.5e-11	4.0e-11		1.2e-17		1.4e-14	*		1.00	NP	35	17.11	3	4.56	3.8
1-OCTENE	1-Octene	8	112.2	7.0e-11	3.2e-11	*	1.5e-17		1.4e-14	*		1.00	NP	35	14.97	4	3.45	4.3
1-C9E	1-Nonene	9	126.2	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	13.31	4	2.76	4.8
1-C10E	1-Decene	10	140.3	6.8e-11	3.2e-11	*	9.7e-18		1.4e-14	*		1.00	NP	35	11.98	4	2.28	5.2
1-C11E	1-Undecene	11	154.3	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	10.89	4	1.95	5.6
1-C12E	1-Dodecene	12	168.3	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	9.98	4	1.72	5.8
1-C13E	1-Tridecene	13	182.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	9.21	4	1.55	6.0
1-C14E	1-Tetradecene	14	196.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	8.55	4	1.48	5.8
1-C15E	1-Pentadecene	15	210.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*		1.00	NP	35	7.98	4	1.30	6.2
ISOBUTEN	Isobutene	4	56.1	5.8e-11	5.1e-11		1.2e-17		3.3e-13			1.00	NP	28	23.95	1	6.35	3.8
2M-1-BUT	2-Methyl-1-Butene	5	70.1	7.1e-11	6.0e-11		1.7e-17		3.3e-13	*		1.00	NP	35	23.95	3	6.51	3.7
23M1-BUT	23-Dimethyl-1-Butene	6	84.2	1.2e-10	5.8e-11	*	1.3e-17		3.3e-13	*		1.00	NP	35	19.96	3	4.77	4.2
2E1-BUT	2-Ethyl-1-Butene	6	84.2	1.2e-10	5.8e-11	*	1.3e-17		3.3e-13	*		1.00	NP	35	19.96	3	5.04	4.0
2M1-C5E	2-Methyl-1-Pentene	6	84.2	7.2e-11	6.2e-11		1.6e-17		3.3e-13	*		1.00	NP	35	19.96	3	5.18	3.9
233M1BUT	2,3,3-trimethyl-1-Butene	7	98.2	1.2e-10	5.8e-11	*	8.6e-18		3.3e-13	*		1.00	NP	35	17.11	3	4.62	3.7
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	8	112.2	1.2e-10	5.8e-11	*	3.5e-18		3.3e-13	*		1.00	NP	35	14.97	4	3.29	4.6
C-2-BUTE	cis-2-Butene	4	56.1	1.1e-10	5.6e-11		1.3e-16		3.5e-13			1.00	NP	28	23.95	2	13.22	1.8
T-2-BUTE	trans-2-Butene	4	56.1	1.5e-10	6.3e-11		1.9e-16		3.9e-13			1.00	NP	28	23.95	1	13.91	1.7

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})	(* = Estimated k)			(s^{-1})							
2M-2-BUT	2-Methyl-2-Butene	5	70.1	3.1e-10	8.6e-11	4.1e-16	9.4e-12		1.00	NP	35	23.95	3	14.45	1.7
C-2-PENT	cis-2-Pentene	5	70.1	1.7e-10	6.4e-11	1.2e-16 *	3.7e-13 *		1.00	NP	35	23.95	3	10.24	2.3
T-2-PENT	trans-2-Pentene	5	70.1	1.7e-10	6.6e-11	1.2e-16 *	3.7e-13 *		1.00	NP	35	23.95	3	10.23	2.3
23M2-BUT	2,3-Dimethyl-2-Butene	6	84.2	8.7e-10	1.1e-10	1.1e-15	5.7e-11		1.00	NP	35	19.96	3	13.32	1.5
2M-2-C5E	2-Methyl-2-Pentene	6	84.2	4.8e-10	8.8e-11	3.5e-16 *	9.4e-12 *		1.00	NP	35	19.96	3	12.28	1.6
C-2-C6E	Cis-2-Hexene	6	84.2	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	19.96	3	8.44	2.4
C-3-C6E	Cis-3-Hexene	6	84.2	2.0e-10	6.3e-11 *	1.5e-16	3.7e-13 *		1.00	NP	35	19.96	3	8.22	2.4
C3M2-C5E	Cis-3-Methyl-2-Hexene	6	84.2	4.6e-10	8.7e-11 *	4.6e-16	9.4e-12 *		1.00	NP	35	19.96	3	13.38	1.5
T3M2-C5E	Trans 3-Methyl-2-Hexene	6	84.2	5.1e-10	8.7e-11 *	5.7e-16	9.4e-12 *		1.00	NP	35	19.96	3	14.17	1.4
T4M2-C5E	Trans 4-Methyl-2-Hexene	6	84.2	1.6e-10	6.0e-11	1.2e-16 *	3.7e-13 *		1.00	NP	35	19.96	3	7.88	2.5
T-2-C6E	Trans-2-Hexene	6	84.2	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	19.96	3	8.44	2.4
T-3-C6E	Trans-3-Hexene	6	84.2	2.1e-10	6.3e-11 *	1.7e-16	3.7e-13 *		1.00	NP	35	19.96	3	8.16	2.4
23M2-C5E	2,3-Dimethyl-2-Hexene	7	98.2	1.2e-9	1.0e-10	6.7e-16 *	5.7e-11 *		1.00	NP	35	17.11	4	10.41	1.6
C-3-C7E	Cis-3-Heptene	7	98.2	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	17.11	4	6.96	2.5
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	7	98.2	1.6e-10	5.4e-11	1.2e-16 *	3.7e-13 *		1.00	NP	35	17.11	4	6.99	2.4
T-2-C7E	Trans-2-Heptene	7	98.2	1.7e-10	6.7e-11	1.2e-16 *	3.7e-13 *		1.00	NP	35	17.11	4	7.33	2.3
T-3-C7E	Trans-3-Heptene	7	98.2	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	17.11	4	6.96	2.5
C-4-C8E	Cis-4-Octene	8	112.2	1.7e-10	6.3e-11 *	9.7e-17	3.7e-13 *		1.00	NP	35	14.97	4	5.94	2.5
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	8	112.2	1.5e-10	6.3e-11 *	4.3e-17	3.7e-13 *		1.00	NP	35	14.97	4	5.97	2.5
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	8	112.2	1.5e-10	6.3e-11 *	4.2e-17	3.7e-13 *		1.00	NP	35	14.97	4	5.44	2.8
T-3-C8E	Trans-3-Octene	8	112.2	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	14.97	4	6.13	2.4
T-4-C8E	Trans-4-Octene	8	112.2	1.3e-10	6.8e-11	1.4e-16	3.7e-13 *		1.00	NP	35	14.97	4	5.90	2.5
244M2C5E	2,4,4-trimethyl-2-Pentene	8	126.2	3.2e-10	8.7e-11 *	1.4e-16	9.4e-12 *		1.00	NP	35	13.31	4	5.85	2.3
T-4-C9E	Trans-4-Nonene	9	128.3	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	13.10	4	5.23	2.5
34E2-C6E	3,4-Diethyl-2-Hexene	10	140.3	2.6e-10	8.7e-11 *	4.4e-18	9.4e-12 *		1.00	NP	35	11.98	4	3.95	3.0
C-5-C10E	Cis-5-Decene	10	140.3	1.8e-10	6.3e-11 *	1.2e-16	3.7e-13 *		1.00	NP	35	11.98	4	4.89	2.5
T-4-C10E	Trans-4-Decene	10	140.3	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	11.98	4	4.50	2.7
T-5-C11E	Trans-5-Undecene	11	154.3	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	10.89	4	4.23	2.6
T-5-C12E	Trans-5-Dodecene	12	168.3	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	9.98	4	3.74	2.7

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max (s^{-1})	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})	(* = Estimated k)										
T-5-C13E	Trans-5-Tridecene	13	182.4	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	9.21	4	3.38	2.7
T-5-C14E	Trans-5-Tetradecene	14	196.4	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	8.55	4	3.08	2.8
T-5-C15E	Trans-5-Pentadecene	15	210.4	2.3e-10	6.3e-11 *	1.2e-16 *	3.7e-13 *		1.00	NP	35	7.98	4	2.82	2.8
CYC-PNTE	Cyclopentene	5	68.1	3.1e-10	6.6e-11	5.6e-16	5.3e-13		1.00	NP	35	24.66	4	7.38	3.3
1M-CC5E	1-Methyl cyclopentene	5	82.2	5.6e-10	8.7e-11 *	6.8e-16	9.4e-12 *		1.00	NP	35	20.45	4	13.95	1.5
CYC-HEXE	Cyclohexene	6	82.2	1.1e-10	6.7e-11	8.3e-17	5.9e-13		1.00	NP	35	20.45	4	5.45	3.8
1M-CC6E	1-Methyl Cyclohexene	7	96.2	3.3e-10	8.7e-11 *	1.7e-16	9.4e-12 *		1.00	NP	35	17.47	4	7.81	2.2
4M-CC6E	4-Methyl Cyclohexene	7	96.2	1.7e-10	6.3e-11 *	8.4e-17	3.7e-13 *		1.00	NP	35	17.47	4	4.48	3.9
12M-CC6E	1,2-Dimethyl Cyclohexene	8	110.2	8.3e-10	1.1e-10 *	2.1e-16	5.7e-11 *		1.00	NP	35	15.25	4	6.77	2.3
13-BUTDE	1,3-Butadiene	4	54.1	6.9e-11	6.6e-11	6.6e-18	1.0e-13		1.00	NP	28	24.85	3	13.58	1.8
ISOPRENE	Isoprene	5	68.1	1.1e-10	1.0e-10	1.3e-17	6.9e-13		1.00	NP	35	24.66	1	10.69	2.3
3-CARENE	3-Carene	10	136.2	1.5e-10	8.7e-11	3.8e-17	9.1e-12		1.00	NP	35	12.33	2	3.21	3.8
A-PINENE	a-Pinene	10	136.2	1.2e-10	5.3e-11	8.8e-17	6.1e-12		1.00	NP	35	12.33	2	4.29	2.9
B-PINENE	b-Pinene	10	136.2	9.7e-11	7.8e-11	1.5e-17	2.5e-12		1.00	NP	35	12.33	3	3.28	3.8
D-LIMONE	d-Limonene	10	136.2	3.1e-10	1.7e-10	2.0e-16	1.2e-11		1.00	NP	35	12.33	2	3.99	3.1
SABINENE	Sabinene	10	136.2	2.0e-10	1.2e-10	8.7e-17	1.0e-11		1.00	NP	35	12.33	2	3.67	3.4
STYRENE	Styrene	8	104.2	6.6e-11	5.8e-11	1.7e-17	1.5e-13		1.00	NP	35	16.13	2	1.95	8.3
BENZENE	Benzene	6	78.1	1.2e-12	1.2e-12				0.20	NP	35	4.38	3	0.81	5.4
TOLUENE	Toluene	7	92.1	5.9e-12	5.9e-12				0.66	NP	35	12.07	2	3.97	3.0
C2-BENZ	Ethyl Benzene	8	106.2	7.1e-12	7.1e-12				0.73	NP	35	11.53	2	2.79	4.1
I-C3-BEN	Isopropyl Benzene (cumene)	9	120.2	6.5e-12	6.5e-12				0.70	NP	35	9.74	3	2.32	4.2
N-C3-BEN	n-Propyl Benzene	9	120.2	6.0e-12	6.0e-12				0.67	NP	35	9.33	3	2.20	4.2
S-C4-BEN	s-Butyl Benzene	10	134.2	6.0e-12	6.0e-12				0.67	NP	35	8.36	3	1.97	4.2
M-XYLENE	m-Xylene	8	106.2	2.4e-11	2.4e-11				0.99	NP	35	15.62	2	10.61	1.5
O-XYLENE	o-Xylene	8	106.2	1.4e-11	1.4e-11				0.92	NP	35	14.55	2	7.49	1.9
P-XYLENE	p-Xylene	8	106.2	1.4e-11	1.4e-11				0.93	NP	35	14.68	2	4.25	3.5
123-TMB	1,2,3-Trimethyl Benzene	9	120.2	3.3e-11	3.3e-11				1.00	NP	35	13.94	2	11.26	1.2
124-TMB	1,2,4-Trimethyl Benzene	9	120.2	3.3e-11	3.3e-11				1.00	NP	35	13.94	2	7.18	1.9
135-TMB	1,3,5-Trimethyl Benzene	9	120.2	5.8e-11	5.8e-11				1.00	NP	35	13.98	2	11.22	1.2

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
NAPHTHAL	Naphthalene	10	128.2	2.1e-11	2.1e-11				0.98	NP	35	12.84	3	3.26	3.9
TETRALIN	Tetralin	10	132.2	3.4e-11	3.4e-11				1.00	NP	35	12.68	3	2.83	4.5
ME-NAPH	Methyl Naphthalenes	11	142.2	5.2e-11	5.2e-11				1.00	NP	35	11.81	3	4.61	2.6
23-DMN	2,3-Dimethyl Naphth.	12	156.2	7.7e-11	7.7e-11				1.00	NP	35	10.75	3	5.54	1.9
ACETYLEN	Acetylene	2	26.0	9.2e-13	9.1e-13	8.6e-21			0.15	NP	14	3.99	2	1.25	3.2
ME-ACTYL	Methyl Acetylene	3	40.1	5.9e-12	5.9e-12	1.6e-20			0.66	NP	21	16.65	4	6.45	2.6
2-BUTYNE	2-Butyne	4	54.1	2.7e-11	2.7e-11	2.1e-20			0.99	NP	28	24.68	4	16.33	1.5
ET-ACTYL	Ethyl Acetylene	4	54.1	8.0e-12	8.0e-12	2.1e-20			0.77	NP	28	19.14	4	6.20	3.1
MEOH	Methanol	1	32.0	9.3e-13	9.3e-13				0.16	A	7	1.65	1	0.71	2.3
ETOH	Ethanol	2	46.1	3.3e-12	3.3e-12				0.45	A	14	6.39	1	1.69	3.8
I-C3-OH	Isopropyl Alcohol	3	60.1	5.3e-12	5.3e-12				0.62	A	14	7.14	1	0.71	10.0
N-C3-OH	n-Propyl Alcohol	3	60.1	5.5e-12	5.5e-12				0.64	A	14	7.35	2	2.74	2.7
I-C4-OH	Isobutyl Alcohol	4	74.1	1.4e-11	6.9e-12	*			0.92	A	17	10.18	3	2.24	4.5
N-C4-OH	n-Butyl Alcohol	4	74.1	8.6e-12	8.6e-12				0.79	A	15	7.95	3	3.34	2.4
S-C4-OH	s-Butyl Alcohol	4	74.1	2.0e-11	1.0e-11	*			0.97	A	19	11.73	3	1.60	7.4
T-C4-OH	t-Butyl Alcohol	4	74.1	1.1e-12	1.1e-12				0.19	A	13	1.54	3	0.45	3.4
CC5-OH	Cyclopentanol	5	86.1	1.1e-11	1.1e-11				0.86	A	16	7.74	3	1.96	4.0
2-C5OH	2-Pentanol	5	88.2	1.2e-11	1.2e-11				0.89	A	16	7.95	3	1.74	4.6
3-C5OH	3-Pentanol	5	88.2	1.2e-11	1.2e-11				0.89	A	17	8.08	3	1.73	4.7
C5OH	Pentyl Alcohol	5	88.2	1.1e-11	1.1e-11				0.87	A	16	7.71	3	3.35	2.3
CC6-OH	Cyclohexanol	6	100.2	3.5e-11	1.7e-11	*			1.00	A	21	10.17	3	2.25	4.5
1-C6OH	1-Hexanol	6	102.2	1.3e-11	1.3e-11				0.90	A	17	7.05	3	2.74	2.6
2-C6OH	2-Hexanol	6	102.2	1.2e-11	1.2e-11				0.89	A	17	6.94	3	2.46	2.8
1-C7OH	1-Heptanol	7	116.2	1.4e-11	1.4e-11				0.92	A	17	6.47	3	2.21	2.9
1-C8-OH	1-Octanol	8	130.2	2.0e-11	2.0e-11				0.98	A	19	6.71	2	2.01	3.3
2-ETC6OH	2-Ethyl-1-Hexanol	8	130.2	2.7e-11	1.3e-11	*			0.99	A	20	7.30	3	2.20	3.3
2-C8-OH	2-Octanol	8	130.2	2.5e-11	2.5e-11				0.99	A	20	7.19	2	2.16	3.3
3-C8-OH	3-Octanol	8	130.2	3.1e-11	3.1e-11				1.00	A	21	7.63	2	2.57	3.0
4-C8-OH	4-Octanol	8	130.2	2.9e-11	2.9e-11				0.99	A	20	7.45	3	3.07	2.4

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max (s^{-1})	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1}) (* = Estimated k)											
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	10	158.3	3.1e-11	1.5e-11 *				1.00	A	21	6.24	3	1.18	5.3
ET-GLYCL	Ethylene Glycol	2	62.1	1.5e-11	1.5e-11				0.93	A	14	10.10	2	3.36	3.0
PR-GLYCL	Propylene Glycol	3	76.1	2.2e-11	2.2e-11				0.98	A	19	11.72	1	2.75	4.3
12-C4OH2	1,2-Butandiol	4	90.1	3.2e-11	1.6e-11 *				1.00	A	21	11.06	2	2.21	5.0
GLYCERL	Glycerol	3	92.1	3.7e-11	1.9e-11 *				1.00	A	21	10.93	2	3.27	3.3
C6-GLYCL	1,2-Dihydroxy Hexane	6	118.2	3.7e-11	1.9e-11 *				1.00	A	22	8.76	3	2.75	3.2
2M24C5OH	2-Methyl-2,4-Pentanediol	6	118.2	1.1e-11	1.1e-11				0.86	A	16	5.62	3	1.04	5.4
ME-O-ME	Dimethyl Ether	2	46.1	3.0e-12	3.0e-12				0.42	A	13	5.96	1	0.93	6.4
TME-OX	Trimethylene Oxide	3	58.1	1.0e-11	1.0e-11				0.85	A	16	11.25	3	5.22	2.2
THF	Tetrahydrofuran	4	72.1	1.6e-11	1.6e-11				0.95	A	18	11.16	3	4.95	2.3
ET-O-ET	Diethyl Ether	4	74.1	1.3e-11	1.3e-11				0.91	A	17	9.92	2	4.01	2.5
METHYLAL	Dimethoxy methane	3	76.1	4.9e-12	4.9e-12				0.59	A	14	5.31	1	1.04	5.1
AM-THF	Alpha-Methyltetrahydrofuran	5	86.1	2.2e-11	2.2e-11				0.98	A	19	10.43	3	4.62	2.3
THP	Tetrahydropyran	5	86.1	1.4e-11	1.4e-11				0.92	A	17	8.76	3	3.81	2.3
ET-O-IPR	Ethyl Isopropyl Ether	5	88.2	4.9e-11	2.4e-11 *				1.00	A	23	12.41	3	3.86	3.2
MNBE	Methyl n-Butyl Ether	5	88.2	1.5e-11	1.5e-11				0.93	A	17	8.82	3	3.66	2.4
MTBE	Methyl t-Butyl Ether	5	88.2	2.9e-12	2.9e-12				0.42	A	13	3.06	1	0.78	3.9
PR-O-PR	Di n-Propyl Ether	6	102.2	1.8e-11	1.8e-11				0.97	A	18	8.29	3	3.24	2.6
ENBE	Ethyl n-Butyl Ether	6	102.2	2.1e-11	2.1e-11				0.98	A	19	8.70	3	3.86	2.3
ETBE	Ethyl t-Butyl Ether	6	102.2	8.8e-12	8.8e-12				0.80	A	16	5.87	3	2.11	2.8
MTAE	Methyl t-Amyl Ether	6	102.2	7.9e-12	7.9e-12				0.77	A	15	5.49	3	2.14	2.6
2BU-THF	2-Butyl Tetrahydrofuran	8	128.2	5.5e-11	2.8e-11 *				1.00	A	23	8.72	3	2.53	3.5
IBU2-O	Di-Isobutyl Ether	8	130.2	2.6e-11	2.6e-11				0.99	A	20	7.25	3	1.29	5.6
BU-O-BU	Di-n-butyl Ether	8	130.2	2.9e-11	2.9e-11				0.99	A	20	7.46	3	3.17	2.4
C5-O-C5	Di-n-Pentyl Ether	10	158.3	3.5e-11	3.5e-11				1.00	A	21	6.43	3	2.64	2.4
MEO-ETOH	2-Methoxyethanol	3	76.1	1.3e-11	1.3e-11				0.91	A	17	9.75	3	2.98	3.3
MEOC3OH	1-Methoxy-2-Propanol	4	90.1	2.0e-11	2.0e-11				0.97	A	19	9.66	1	2.62	3.7
ETO-ETOH	2-Ethoxyethanol	4	90.1	1.9e-11	1.9e-11				0.97	A	18	9.44	2	3.78	2.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH		kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
										KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)			(s^{-1})							
2MEOC3OH	2-Methoxy-1-Propanol	4	90.1	5.1e-11	2.5e-11	*				1.00	A	23	12.22	3	3.01	4.1
ETOC3OH	1-Ethoxy-2-Propanol	5	104.2	5.2e-11	2.6e-11	*				1.00	A	23	10.64	3	3.25	3.3
2PROETOH	2-Propoxyethanol	5	104.2	4.9e-11	2.5e-11	*				1.00	A	23	10.53	3	3.52	3.0
3ETOC3OH	3-Ethoxy-1-Propanol	5	104.2	2.2e-11	2.2e-11					0.98	A	19	8.63	3	4.24	2.0
3MEOC4OH	3-Methoxy-1-Butanol	5	104.2	2.4e-11	2.4e-11					0.99	A	19	8.82	3	0.97	9.1
DET-GLCL	Diethylene Glycol	4	106.1	5.5e-11	2.8e-11	*				1.00	A	23	10.53	3	3.55	3.0
PROXC3OH	1-Propoxy-2-Propanol	6	118.2	2.9e-11	2.9e-11					1.00	A	20	8.24	3	2.86	2.9
BUO-ETOH	2-Butoxyethanol	6	118.2	2.6e-11	2.6e-11					0.99	A	20	7.96	1	2.90	2.7
3MOMC4OH	3 methoxy -3 methyl-Butanol	6	118.2	1.4e-11	7.1e-12	*				0.93	A	17	6.46	3	1.74	3.7
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	5	120.2	6.8e-11	3.4e-11	*				1.00	A	24	9.60	3	2.90	3.3
PG-1TB-E	1-tert-Butoxy-2-Propanol	7	132.2	3.7e-11	1.9e-11	*				1.00	A	22	7.83	3	1.71	4.6
PG-2TB-E	2-tert-Butoxy-1-Propanol	7	132.2	4.9e-11	2.5e-11	*				1.00	A	23	8.29	3	1.81	4.6
BUOC3OH	n-Butoxy-2-Propanol	7	132.2	6.1e-11	3.1e-11	*				1.00	A	24	8.59	3	2.70	3.2
CARBITOL	2-(2-Ethoxyethoxy) EtOH	6	134.2	5.1e-11	5.1e-11					1.00	A	23	8.22	2	3.19	2.6
DPR-GLCL	Dipropylene Glycol	6	134.2	7.3e-11	3.6e-11	*				1.00	A	24	8.67	3	2.48	3.5
EGHE	2-Hexyloxyethanol	8	146.2	5.8e-11	2.9e-11	*				1.00	A	23	7.71	3	2.45	3.1
DGPE	2-(2-Propoxyethoxy) ethanol	7	148.2	8.8e-11	4.4e-11	*				1.00	A	25	8.00	3	3.00	2.7
DPRGOME	Dipropylene Glycol Methyl Ether	7	148.2	9.8e-11	4.9e-11	*				1.00	A	25	8.06	3	2.21	3.7
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	8	162.2	9.0e-11	4.5e-11	*				1.00	A	25	7.32	3	2.70	2.7
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	7	164.2	1.1e-10	5.3e-11	*				1.00	A	25	7.32	3	2.62	2.8
EGEHE	2-(2-Ethylhexyloxy) ethanol	10	174.3	6.5e-11	3.2e-11	*				1.00	A	24	6.58	3	1.71	3.8
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	8	178.2	1.2e-10	6.0e-11	*				1.00	A	25	6.78	3	2.66	2.5
DGHE	2-(2-Hexyloxyethoxy) ethanol	10	190.3	9.6e-11	4.8e-11	*				1.00	A	25	6.27	3	2.03	3.1
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	9	192.3	1.3e-10	6.3e-11	*				1.00	A	25	6.29	3	2.46	2.6

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max (s^{-1})	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)									
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	10	206.3	1.3e-10	6.4e-11	*			1.00	A	25	5.87	3	2.24	2.6
TPRGOME	Tripropylene Glycol Monomethyl Ether	10	206.3	1.6e-10	7.8e-11	*			1.00	A	25	5.90	3	1.90	3.1
TETRAGME	2,5,8,11-Tetraoxatridecan-13-ol	9	208.3	1.4e-10	7.2e-11	*			1.00	A	25	5.83	3	2.15	2.7
TETRAGBE	3,6,9,12-Tetraoxahexadecan-1-ol	12	250.3	1.7e-10	8.4e-11	*			1.00	A	25	4.86	3	1.90	2.6
ME-FORM	Methyl Formate	2	60.1	2.3e-13	2.3e-13				0.04	B	14	0.46	3	0.07	6.9
ET-FORM	Ethyl Formate	3	74.1	1.0e-12	1.0e-12				0.17	B	17	1.93	3	0.52	3.7
ME-ACET	Methyl Acetate	3	74.1	3.5e-13	3.5e-13				0.06	B	17	0.68	1	0.07	9.4
ET-ACET	Ethyl Acetate	4	88.1	1.6e-12	1.6e-12				0.25	B	18	2.46	1	0.64	3.8
ME-PRAT	Methyl Propionate	4	88.1	1.0e-12	1.0e-12				0.17	B	17	1.63	3	0.71	2.3
C3-FORM	n-Propyl Formate	4	88.1	2.4e-12	2.4e-12				0.35	B	18	3.51	3	0.93	3.8
ET-PRAT	Ethyl Propionate	5	102.1	2.1e-12	2.1e-12				0.32	B	18	2.76	3	0.79	3.5
IPR-ACET	Isopropyl Acetate	5	102.1	3.4e-12	3.4e-12				0.46	B	19	4.10	2	1.24	3.3
ME-BUAT	Methyl Butyrate	5	102.1	3.0e-12	3.0e-12				0.43	B	19	3.73	3	1.18	3.2
ME-IBUAT	Methyl Isobutyrate	5	102.1	1.7e-12	1.7e-12				0.27	B	18	2.28	2	0.70	3.2
C4-FORM	n-Butyl Formate	5	102.1	3.1e-12	3.1e-12				0.44	B	19	3.82	3	0.95	4.0
PR-ACET	Propyl Acetate	5	102.1	3.4e-12	3.4e-12				0.46	B	19	4.10	3	0.87	4.7
ET-BUAT	Ethyl Butyrate	6	116.2	4.9e-12	4.9e-12				0.60	B	20	4.83	3	1.25	3.9
IBU-ACET	Isobutyl Acetate	6	116.2	9.2e-12	4.6e-12	*			0.82	B	22	7.33	3	0.67	10.9
ME-PVAT	Methyl Pivalate	6	116.2	1.3e-12	1.3e-12				0.21	B	18	1.51	2	0.41	3.7
BU-ACET	n-Butyl Acetate	6	116.2	4.2e-12	4.2e-12				0.54	B	19	4.27	2	0.89	4.8
PR-PRAT	n-Propyl Propionate	6	116.2	4.0e-12	4.0e-12				0.52	B	19	4.12	3	0.93	4.4
SBU-ACET	s-Butyl Acetate	6	116.2	5.5e-12	5.5e-12				0.64	B	20	5.23	3	1.43	3.6
TBU-ACET	t-Butyl Acetate	6	116.2	4.3e-13	4.3e-13				0.08	B	17	0.53	2	0.22	2.4
BU-PRAT	Butyl Propionate	7	130.2	1.0e-11	5.1e-12	*			0.84	B	22	6.89	3	0.89	7.8
AM-ACET	Amyl Acetate	7	130.2	1.2e-11	6.1e-12	*			0.89	B	23	7.56	3	0.96	7.9

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})	(* = Estimated k)			(s^{-1})							
PR-BUAT	n-Propyl Butyrate	7	130.2	7.4e-12	7.4e-12				0.74	B	21	5.72	3	1.17	4.9
23MC4ACT	2,3-Dimethylbutyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.96	3	0.84	13.1
2MC5-ACT	2-Methylpentyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.97	3	1.11	9.9
3MC5-ACT	3-Methylpentyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.97	3	1.31	8.4
4MC5-ACT	4-Methylpentyl Acetate	8	144.2	1.5e-11	7.5e-12	*			0.94	NP	35	10.89	3	0.92	11.9
IBU-IBTR	Isobutyl Isobutyrate	8	144.2	1.1e-11	5.5e-12	*			0.87	B	23	6.51	3	0.64	10.2
BU-BUAT	n-Butyl Butyrate	8	144.2	1.1e-11	1.1e-11				0.86	B	22	6.38	3	1.12	5.7
NC6-ACET	n-Hexyl Acetate	8	144.2	1.5e-11	7.5e-12	*			0.94	NP	35	10.90	3	0.87	12.5
E3EOC3OH	Ethyl 3-Ethoxy Propionate	7	146.2	3.9e-11	2.0e-11	*			1.00	B	31	10.06	3	3.61	2.8
24MC5ACT	2,4-Dimethylpentyl Acetate	9	158.2	1.8e-11	9.1e-12	*			0.97	NP	35	10.25	3	0.98	10.5
2MC6-ACT	2-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	0.89	11.5
3EC5-ACT	3-Ethylpentyl Acetate	9	158.2	1.9e-11	9.6e-12	*			0.97	NP	35	10.30	3	1.24	8.3
3MC6-ACT	3-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	1.01	10.2
4MC6-ACT	4-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	0.91	11.3
5MC6-ACT	5-Methylhexyl Acetate	9	158.2	1.8e-11	8.9e-12	*			0.96	NP	35	10.21	3	0.79	12.9
IC5IBUAT	Isoamyl Isobutyrate	9	158.2	1.4e-11	6.9e-12	*			0.92	B	24	6.63	3	0.89	7.4
NC7-ACET	n-Heptyl Acetate	9	158.2	1.8e-11	8.9e-12	*			0.96	NP	35	10.21	3	0.73	14.0
24MC6ACT	2,4-Dimethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.57	3	0.93	10.3
2ETHXACT	2-Ethyl-Hexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	B	27	7.28	3	0.79	9.3
34MC6ACT	3,4-Dimethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.57	3	1.16	8.2
35MC6ACT	3,5-Dimethylhexyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	1.09	8.8
3EC6-ACT	3-Ethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.58	3	1.03	9.3
3MC7-ACT	3-Methylheptyl Aceate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.76	12.6
45MC6ACT	4,5-Dimethylhexyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.86	11.1
4MC7-ACT	4-Methylheptyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.72	13.2
5MC7-ACT	5-Methylheptyl Aceate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.73	13.1
NC8-ACET	n-Octyl Acetate	10	172.3	2.1e-11	1.0e-11	*			0.98	NP	35	9.53	3	0.64	14.8
235M6ACT	2,3,5-Teimethylhexyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.86	10.3
23MC7ACT	2,3-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.84	10.6

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
24MC7ACT	2,4-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.88	10.2
25MC7ACT	2,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.86	10.3
2MC8-ACT	2-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.63	14.2
35MC7ACT	3,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	1.01	8.8
36MC7ACT	3,6-Dimethylheptyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.87	10.2
3EC7-ACT	3-Ethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.71	12.6
45MC7ACT	4,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.96	9.3
46MC7ACT	4,6-Dimethylheptyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.83	10.7
4MC8-ACT	4-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.68	13.1
5MC8-ACT	5-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.67	13.3
NC9-ACET	n-Nonyl Acetate	11	186.3	2.3e-11	1.2e-11	*			0.99	NP	35	8.89	3	0.58	15.3
36MC8ACT	3,6-Dimethyloctyl Acetate	12	200.3	2.7e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.88	9.5
3IPC7ACT	3-Isopropylheptyl Acetate	12	200.3	2.8e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.71	11.7
46MC8ACT	4,6-Dimethyloctyl Acetate	12	200.3	2.7e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.85	9.8
357M8ACT	3,5,7-Trimethyloctyl Acetate	13	214.4	3.0e-11	1.5e-11	*			1.00	NP	35	7.81	3	0.83	9.4
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	13	214.4	3.1e-11	1.6e-11	*			1.00	NP	35	7.81	3	0.80	9.8
47MC9ACT	4,7-Dimethylnonyl Acetate	13	214.4	3.0e-11	1.5e-11	*			1.00	NP	35	7.81	3	0.64	12.3
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	14	228.4	3.4e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.74	10.0
357M9ACT	3,5,7-Trimethylnonyl Acetate	14	228.4	3.4e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.76	9.7
368M9ACT	3,6,8-Trimethylnonyl Acetate	14	228.4	3.3e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.72	10.2
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	15	242.4	3.6e-11	1.8e-11	*			1.00	NP	35	6.92	3	0.63	11.1
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	15	242.4	3.7e-11	1.9e-11	*			1.00	NP	35	6.92	3	0.76	9.1
479M10AC	4,7,9-Trimethyldecyl Acetate	15	242.4	3.6e-11	1.8e-11	*			1.00	NP	35	6.92	3	0.55	12.6
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	16	256.4	4.0e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.74	8.8

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	16	256.4	3.9e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.58	11.2
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	16	256.4	4.0e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.77	8.5
DMC	Dimethyl Carbonate	3	90.1	3.3e-13	3.3e-13				0.06	B	17	0.53	2	0.06	9.0
PC	Propylene Carbonate	4	102.1	6.9e-13	6.9e-13				0.12	B	17	0.96	2	0.25	3.8
ME-LACT	Methyl Lactate	4	104.1	2.8e-12	2.8e-12				0.40	B	18	3.37	3	2.75	1.2
MCSVACET	2-Methoxyethyl Acetate	5	118.1	2.5e-11	1.3e-11	*			0.99	B	28	11.07	3	1.18	9.4
ET-LACT	Ethyl Lactate	5	118.1	3.9e-12	3.9e-12				0.51	B	19	3.97	3	2.71	1.5
MIPR-CB	Methyl Isopropyl Carbonate	5	118.1	2.6e-12	2.6e-12				0.37	B	18	2.78	2	0.69	4.0
PGME-ACT	1-Methoxy-2-Propyl Acetate	6	132.2	1.4e-11	1.4e-11				0.93	B	24	8.08	2	1.71	4.7
CSV-ACET	2-Ethoxyethyl Acetate	6	132.2	3.9e-11	1.9e-11	*			1.00	B	31	11.10	3	1.90	5.8
2PGMEACT	2-Methyoxy-1-propyl Acetate	6	132.2	4.6e-11	2.3e-11	*			1.00	B	32	11.53	3	1.12	10.3
DBE-4	Dimethyl Succinate	6	146.1	1.5e-12	1.5e-12				0.24	B	18	1.40	3	0.25	5.6
ETGLDACT	Ethylene Glycol Diacetate	6	146.1	7.6e-12	3.8e-12	*			0.75	B	21	5.16	3	0.72	7.2
DIPR-CB	Diisopropyl Carbonate	7	146.2	1.4e-11	6.9e-12	*			0.92	B	24	7.15	3	1.04	6.9
DBE-5	Dimethyl Glutarate	7	160.2	3.5e-12	3.5e-12				0.47	B	19	2.67	3	0.49	5.4
2BUETACT	2-Butoxyethyl Acetate	8	160.2	4.8e-11	2.4e-11	*			1.00	B	32	9.58	3	1.67	5.7
DBE-6	Dimethyl Adipate	8	174.2	8.8e-12	8.8e-12				0.80	B	22	4.75	3	1.95	2.4
DGEEA	2-(2-Ethoxyethoxy) ethyl acetate	8	176.2	7.7e-11	3.9e-11	*			1.00	B	35	9.42	3	1.50	6.3
DGBEA	2-(2-Butoxyethoxy) ethyl acetate	10	204.3	8.6e-11	4.3e-11	*			1.00	B	35	8.22	3	1.38	6.0
TEXANOL2	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	12	216.3	2.6e-11	1.3e-11	*			0.99	B	28	6.09	3	0.92	6.6
TEXANOL1	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	12	216.3	3.2e-11	1.6e-11	*			1.00	B	29	6.49	3	0.88	7.4
ETOX	Ethylene Oxide	2	44.1	7.6e-14	7.6e-14				0.01	A	12	0.18	3	0.05	4.1

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max (s^{-1})	Upper Limit Est. (U.L.) KR	MR Tp.	MR Max	MIR (g/g)	Direct Calc Unc	MIR (g/g)	U.L. / Direct
				(cm^3 $molec^{-1}$ s^{-1})	(* = Estimated k)										
PROX	Propylene Oxide	3	58.1	5.2e-13	5.2e-13				0.09	A	12	0.94	3	0.32	2.9
12BUOX	1,2-Epoxybutane	4	72.1	1.9e-12	1.9e-12				0.30	A	13	2.56	3	1.02	2.5
FORMACID	Formic Acid	1	46.0	4.5e-13	4.5e-13				0.08	A	7	0.58	3	0.08	7.6
ACETACID	Acetic Acid	2	60.1	8.0e-13	8.0e-13				0.14	A	13	1.37	3	0.71	1.9
ACYRACID	Acrylic Acid	3	72.1	3.7e-11	2.8e-11	1.0e-17 *	2.8e-18 *		1.00	NP	21	13.97	5	11.66	1.2
PROPACID	Propionic Acid	3	74.1	1.2e-12	1.2e-12				0.19	A	13	1.58	3	1.16	1.4
ME-ACRYL	Methyl Acrylate	4	86.1	6.6e-11	2.8e-11 *	1.0e-17 *	2.8e-18 *		1.00	NP	28	15.61	5	12.24	1.3
VIN-ACET	Vinyl Acetate	4	86.1	7.2e-11	3.2e-11 *	1.0e-17 *	1.4e-14 *		1.00	NP	28	15.61	5	3.26	4.8
MBUTENOL	2-Methyl-2-Butene-3-ol	4	86.1	6.7e-11	6.3e-11	9.3e-18	1.2e-14		1.00	NP	28	15.60	3	4.12	3.8
ET-ACRYL	Ethyl Acrylate	5	100.1	6.6e-11	2.8e-11 *	1.0e-17 *	2.8e-18 *		1.00	NP	35	16.78	5	8.78	1.9
ME-MACRT	Methyl Methacrylate	5	100.1	6.2e-11	5.2e-11	1.2e-17 *	6.6e-17 *		1.00	NP	35	16.78	5	15.84	1.1
BU-MACRT	Butyl Methacrylate	8	142.2	6.2e-11	5.2e-11	1.2e-17 *	6.6e-17 *		1.00	NP	35	11.81	5	9.09	1.3
IBUMACRT	Isobutyl Methacrylate	8	142.2	6.2e-11	5.2e-11	1.2e-17 *	6.6e-17 *		1.00	NP	35	11.81	5	8.99	1.3
FORMALD	Formaldehyde	1	30.0	2.5e-11	9.2e-12			1.2e-4	0.99	P	10	15.81	2	8.97	1.8
ACETALD	Acetaldehyde	2	44.1	2.1e-11	1.6e-11		2.8e-15	4.3e-5	0.98	P	20	21.36	1	6.84	3.1
PROPALD	Propionaldehyde	3	58.1	2.8e-11	2.0e-11		3.8e-15 *	5.8e-5	0.99	P	30	24.64	2	7.89	3.1
2MEC3AL	2-Methylpropanal	4	72.1	3.4e-11	2.6e-11		3.8e-15 *	5.8e-5	1.00	P	40	26.57	3	5.87	4.5
1C4RCHO	Butanal	4	72.1	3.1e-11	2.3e-11		3.8e-15 *	5.8e-5	1.00	P	40	26.53	3	6.74	3.9
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	5	86.1	3.4e-11	2.6e-11		3.8e-15 *	5.8e-5	1.00	P	40	22.25	3	5.40	4.1
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	5	86.1	3.5e-11	2.7e-11		3.8e-15 *	5.8e-5	1.00	P	40	22.26	3	5.52	4.0
1C5RCHO	Pentanal (Valeraldehyde)	5	86.1	3.6e-11	2.8e-11		3.8e-15 *	5.8e-5	1.00	P	40	22.26	3	5.76	3.9
GLTRALD	Glutaraldehyde	5	100.1	9.1e-11	4.2e-11 *		7.6e-15 *	5.8e-5	1.00	P	40	19.18	3	4.79	4.0
1C6RCHO	Hexanal	6	100.2	5.6e-11	2.4e-11 *		3.8e-15 *	5.8e-5	1.00	P	40	19.17	3	4.98	3.8
1C7RCHO	Heptanal	7	114.2	5.9e-11	2.6e-11 *		3.8e-15 *	5.8e-5	1.00	P	40	16.81	3	4.23	4.0
1C8RCHO	Octanal	8	128.2	6.2e-11	2.7e-11 *		3.8e-15 *	5.8e-5	1.00	P	40	14.97	3	3.65	4.1
GLYOXAL	Glyoxal	2	58.0	4.0e-10	1.1e-11			3.0e-3	1.00	P	20	16.54	3	14.22	1.2
MEGLYOX	Methyl Glyoxal	3	72.1	1.8e-10	1.5e-11			1.3e-3	1.00	P	30	19.98	3	16.21	1.2

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
ACROLEIN	Acrolein	3	56.1	9.2e-11	2.0e-11	3.1e-19	9.7e-17 *	5.5e-4	1.00	P	30	25.69	3	7.60	3.4
CROTALD	Crotonaldehyde	4	70.1	1.1e-10	3.6e-11	9.0e-19	5.1e-15	5.5e-4	1.00	P	40	27.39	3	10.07	2.7
METHACRO	Methacrolein	4	70.1	1.1e-10	3.3e-11	1.2e-18	4.8e-15	5.5e-4	1.00	P	40	27.39	1	6.23	4.4
HOMACR	Hydroxy Methacrolein	4	86.1	1.2e-10	4.3e-11	1.2e-18	4.8e-15	5.5e-4	1.00	P	40	22.30	3	6.61	3.4
BENZALD	Benzaldehyde	7	106.1	1.5e-10	1.3e-11			1.0e-3	1.00	P	40	18.09	2	-0.61	-29.7
ACETONE	Acetone	3	58.1	2.2e-12	2.2e-13			1.5e-5	0.33	P	30	8.28	1	0.43	19.4
CC4-KET	Cyclobutanone	4	70.1	2.9e-12	8.7e-13			1.6e-5	0.42	P	40	11.39	4	0.68	16.7
MEK	Methyl Ethyl Ketone	4	72.1	3.3e-12	1.2e-12			1.6e-5	0.45	P	40	11.97	1	1.49	8.0
CC5-KET	Cyclopentanone	5	84.1	5.0e-12	2.9e-12			1.6e-5	0.60	P	40	13.70	4	1.43	9.6
MPK	2-Pentanone	5	86.1	6.6e-12	4.6e-12			1.6e-5	0.70	P	40	15.68	2	3.07	5.1
DEK	3-Pentanone	5	86.1	4.1e-12	2.0e-12			1.6e-5	0.53	P	40	11.71	3	1.45	8.1
CC6-KET	Cyclohexanone	6	98.2	8.4e-12	6.4e-12			1.6e-5	0.79	P	40	15.41	3	1.61	9.6
MIBK	4-Methyl-2-Pentanone	6	100.2	1.6e-11	1.4e-11			1.6e-5	0.95	P	40	18.18	2	4.31	4.2
MNBK	Methyl n-Butyl Ketone	6	100.2	1.1e-11	9.1e-12			1.6e-5	0.87	P	40	16.70	3	3.55	4.7
MTBK	Methyl t-Butyl Ketone	6	100.2	3.3e-12	1.2e-12			1.6e-5	0.45	P	40	8.65	3	0.78	11.0
C7-KET-2	2-Heptanone	7	114.2	1.4e-11	1.2e-11			1.6e-5	0.92	P	40	15.47	2	2.80	5.5
2M-3-HXO	2-Methyl-3-Hexanone	7	114.2	1.6e-11	7.2e-12 *			1.6e-5	0.95	P	40	16.00	3	1.79	9.0
DIPK	Di-Isopropyl Ketone	7	114.2	7.4e-12	5.4e-12			1.6e-5	0.74	P	40	12.52	3	1.63	7.7
C8-KET-2	2-Octanone	8	128.2	1.3e-11	1.1e-11			1.6e-5	0.91	P	40	13.61	3	1.66	8.2
C9-KET-2	2-Nonanone	9	142.2	1.4e-11	1.2e-11			1.6e-5	0.93	P	40	12.51	3	1.30	9.6
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	9	142.2	3.0e-11	2.8e-11			1.6e-5	1.00	P	40	13.44	3	2.94	4.6
C10-K-2	2-Decanone	10	156.3	1.5e-11	1.3e-11			1.6e-5	0.94	P	40	11.54	3	1.06	10.9
BIACETYL	Biacetyl	4	86.1	2.8e-10				2.2e-3	1.00	P	40	22.30	3	20.73	1.1
MVK	Methylvinyl ketone	4	70.1	9.3e-11	1.9e-11	4.7e-18		5.5e-4	1.00	P	40	27.39	1	8.73	3.1
HOACET	Hydroxy Acetone	3	74.1	5.1e-12	3.0e-12			1.6e-5	0.61	P	30	11.78	3	3.08	3.8
MEOACET	Methoxy Acetone	4	88.1	8.8e-12	6.8e-12			1.6e-5	0.80	P	40	17.48	3	2.14	8.2
DIACTALC	Diacetone Alcohol	6	116.2	5.0e-12	1.5e-12 *			1.6e-5	0.60	P	40	9.97	3	0.68	14.6
PHENOL	Phenol	6	94.1	2.6e-11	2.6e-11				0.99	NP	35	17.71	4	1.82	9.7

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
O-CRESOL	o-Cresol	7	108.1	4.2e-11	4.2e-11				1.00	NP	35	15.53	3	2.34	6.6
NO2-BENZ	Nitrobenzene	6	123.1	1.5e-13	1.5e-13				0.03	NP	35	0.37	6	0.07	5.5
P-TI	Para Toluene Isocyanate	7	134.2	5.9e-12	5.9e-12				0.66	NP	35	8.29	2	0.93	8.9
TDI	Toluene Diisocyanate	9	174.2	7.4e-12	7.4e-12				0.74	NP	35	7.17	2	-0.13	-54.3
MDI	Methylene Diphenylene Diisocyanate	15	250.3	1.2e-11	1.2e-11				0.89	NP	35	5.94	3	0.79	7.5
DM-AMINE	Dimethyl Amine	2	45.1	6.6e-11	6.6e-11				1.00	NP	14	14.91	6	9.37	1.6
ET-AMINE	Ethyl Amine	2	45.1	2.8e-11	2.8e-11				0.99	NP	14	14.81	6	7.80	1.9
TM-AMINE	Trimethyl Amine	3	59.1	6.1e-11	6.1e-11				1.00	NP	21	17.05	6	7.06	2.4
ETOH-NH2	Ethanolamine	2	61.1	3.2e-11	3.2e-11				1.00	NP	14	10.97	6	5.97	1.8
DMAE	Dimethylaminoethanol	4	89.1	9.0e-11	9.0e-11				1.00	A	25	13.33	6	4.76	2.8
ETOH2-NH	Diethanol Amine	4	105.1	9.4e-11	9.4e-11				1.00	NP	28	12.78	6	4.05	3.2
ETOH3-N	Triethanolamine	6	149.2	1.2e-10	1.2e-10				1.00	NP	35	11.26	6	2.76	4.1
NMP	N-Methyl-2-Pyrrolidone	5	99.1	2.2e-11	2.2e-11		1.3e-13		0.98	NP	35	16.65	2	2.56	6.5
CH3-CL	Methyl Chloride	1	50.5	4.5e-14	4.5e-14				0.01	NP	7	0.05	6	0.03	1.6
CL-ETHE	Vinyl Chloride	2	62.5	6.9e-12	6.9e-12				0.72	NP	14	7.72	6	2.92	2.6
C2-CL	Ethyl Chloride	2	64.5	4.2e-13	4.2e-13				0.07	NP	14	0.77	6	0.25	3.1
CL2-ME	Dichloromethane	1	84.9	1.5e-13	1.5e-13				0.03	NP	7	0.10	6	0.07	1.6
ME-BR	Methyl Bromide	1	95.0	4.1e-14	4.1e-14				0.01	NP	7	0.03	6	0.02	1.6
11CL2-C2	1,1-Dichloroethane	2	99.0	2.6e-13	2.6e-13				0.05	NP	14	0.32	6	0.10	3.1
12CL2-C2	1,2-Dichloroethane	2	99.0	2.5e-13	2.5e-13				0.05	NP	14	0.31	6	0.10	3.1
C2-BR	Ethyl Bromide	2	109.0	3.1e-13	3.1e-13				0.06	NP	14	0.34	6	0.11	3.1
CHCL3	Chloroform	1	119.4	1.1e-13	1.1e-13				0.02	NP	7	0.05	6	0.03	1.6
C3-BR	n-Propyl Bromide	3	123.0	1.2e-12	1.2e-12				0.19	NP	21	1.60	6	0.35	4.6
111-TCE	1,1,1-Trichloroethane	2	133.4	1.2e-14	1.2e-14				0.00	NP	14	0.01	6	0.00	3.2
112CL3C2	1,1,2-Trichloroethane	2	133.4	2.0e-13	2.0e-13				0.04	NP	14	0.18	6	0.06	3.1
C4-BR	n-Butyl Bromide	4	137.0	2.5e-12	2.5e-12				0.36	NP	28	3.57	6	0.60	5.9
11BR2-C2	1,2-Dibromoethane	2	187.9	2.3e-13	2.3e-13				0.04	NP	14	0.15	6	0.05	3.1
T-12-DCE	Trans-1,2-Dichloroethene	2	97.0	2.3e-12	2.3e-12				0.35	NP	14	2.41	6	0.81	3.0

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH	kOH	kO3	kNO3	kPhot Max	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
				(cm^3 $molec^{-1}$ s^{-1})		(* = Estimated k)		(s^{-1})							
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	4	125.0	3.2e-11	3.2e-11	3.9e-19	1.0e-15		1.00	NP	28	10.72	6	1.13	9.5
CL3-ETHE	Trichloroethylene	2	131.4	2.3e-12	2.3e-12				0.35	NP	14	1.78	6	0.60	3.0
CL4-ETHE	Perchloroethylene	2	165.9	1.7e-13	1.7e-13				0.03	NP	14	0.13	6	0.04	3.2
CL-BEN	Monochlorobenzene	6	112.6	7.7e-13	7.7e-13				0.13	NP	35	1.97	6	0.36	5.4
CF3-BEN	Benzotrifluoride	7	146.1	4.6e-13	4.6e-13				0.08	NP	35	0.93	6	0.26	3.5
CL2-BEN	p-Dichlorobenzene	6	147.0	5.6e-13	5.6e-13				0.10	NP	35	1.11	6	0.20	5.5
PCBTF	p-Trifluoromethyl-Cl-Benzene	7	180.6	2.4e-13	2.4e-13				0.04	NP	35	0.40	6	0.11	3.5