IV. THE ROLE OF AROMATIC HYDROCARBONS IN POLLUTED URBAN ATMOSPHERES: DEVELOPMENT AND VALIDATION OF MECHANISMS OF PHOTOOXIDATION

Aromatic hydrocarbons are recognized to be an important constituent of anthropogenic emissions in polluted urban atmospheres (Lonneman et al., 1974). In order to develop chemical kinetic computer models of photochemical air pollution as an integral part of urban airshed models for the formulation of emission control strategies, the chemistry involved in the photooxidation of these aromatic hydrocarbons under atmospheric conditions must be reasonably well understood (Finlayson-Pitts and Pitts, 1977). As a first step, such computer kinetic models must, as far as possible, be validated against accurate smog chamber data, even though it is recognized that there are significant wall effects associated with smog chambers (Carter et al., 1979). At the present time, while reasonably validated detailed chemical kinetic computer models exist for the n-butane (a representative short chain [$\leq C_4$] alkane) and propene (a representative alkene)-NO_x-air systems (Carter et al., 1979; Hendry et al., 1978), the chemistry occurring in the NO_x photooxidations of the aromatic hydrocarbons is still incompletely understood (Atkinson et al., 1979).

In recent years laboratory studies have shown that under atmospheric conditions the major initial reaction of the aromatics is with the hydroxyl radical and data are now available concerning both the overall OH radical rate constants (Atkinson et al., 1979, and references contained therein; Hendry, 1979) and the relative amounts of OH radical addition and H atom abstraction (Atkinson et al., 1979; Hendry, 1979) for many of these compounds. Additionally, the reactions of ozone with the aromatic hydrocarbons, leading to the production of α-dicarbonyls have been shown to be negligible under atmospheric conditions (Pate et al., 1976a; Bufalini and Altshuller, 1965; Stedman and Niki, 1973).

Several product studies of irradiated NO_x-aromatic-air systems (mainly of the NO_x-toluene-air system) have been carried out (Altshuller et al., 1970; Spicer and Jones, 1977; Grosjean et al., 1978; Akimoto et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b). Quantitative measurements of a large variety of products and of the reactants under carefully controlled experimental conditions have not been available.

Products which retain the aromatic ring have been observed, including benzaldehyde, benzyl nitrate, cresols, nitrotoluene and nitrocresols in the gas phase (Altshuller et al., 1970; Spicer and Jones, 1977; Grosjean et al., 1978; Akimoto et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b) and dihydroxynitrotoluenes in the aerosol phase (Grosjean et al., 1978). The formation of large yields of products such as PAN, CO, and HCHO in the toluene-NO_x irradiations (Grosjean et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b) and the recent observation of significant yields (18 $\pm$ 4% of the total reaction) of biacetyl in irradiated NO_x-o-xylene-air mixtures (Darnall et al., 1979) indicate the importance of ring cleavage.

Recently Hendry and co-workers (1978) have formulated a detailed chemical computer model for the NO_x photooxidation of toluene involving aromatic ring cleavage only <u>after</u> cresol formation, i.e., OH radical addition to toluene yields mainly o-cresol, with the o-cresol reacting further with OH radical to yield a variety of ring cleavage products. However, it has been shown (Darnall et al., 1979) that the rate determining step for the formation of the ring cleavage product biacetyl from the reaction of OH radicals with o-xylene was that for the initial reaction of OH radicals with o-xylene, and that its production from the reaction of OH radicals (or ozone) with a hydroxyxylene would have led to an incorrect biacetyl concentration-time profile.

In this section product studies of toluene-NO_x-air, toluene-benzaldehyde-NO_x-air, and cresol-NO_x-air mixtures irradiated under controlled conditions in an environmental chamber are presented, and a reaction scheme which employs the available kinetic and mechanistic information and is based in part upon a previously-developed chemical computer model for the n-butane-propene-NO_x-air system (Carter et al., 1979) is formulated. Some of the detailed chemistry is, by necessity, speculative, but this reaction scheme fits the data reasonably well over a significant range of initial reactant levels.

<u>Experimental</u>. The apparatus and general techniques used have been described previously (Pitts et al., 1979b; Pitts, et al., 1977; Darnall et al., 1979). Irradiations were carried out in the 5800-liter evacuable, Teflon-lined, thermostatted environmental chamber (Winer et al., 1980)

using a 25 KW solar simulator. Prior to each run the chamber was evacuated to pressures of ~10^{-5} torr, and was then filled with purified matrix air (Doyle et al., 1977) humidified to ~50% relative humidity (RH) at 303 $\pm$ 1 K. Toluene or the cresols, and NO and NO_2 were injected into the chamber using precision bore syringes, while benzaldehyde was expanded into the evacuated chamber from known benzaldehyde-N_2-mixtures prepared in a 5.5-liter bulb. All reactants were allowed to mix for at least 30 minutes before t = 0. During a run the temperature of the irradiated mixture was maintained at the desired value by means of the chamber refrigeration or heating system.

The parameters monitored and the methods employed were: O_3 by UV absorbance (Dasibi Model 1212); NO, NO_2, and NO_x by chemiluminescence (Winer et al., 1974; NO_2 and NO_x values are corrected for response to PAN and alkyl nitrates) (Thermo Electron Model 14B); CO by gas chromatography (Beckman 6800); RH by a thin film, bulk effect humidity sensor (Brady Array); light intensity and spectral distribution by a photodiode and an absolute radiometer (EG&G), and by a double monochromator-photomultiplier combination, respectively (Pitts et al., 1979b); and HCHO using an improved chromotropic acid method (Pitts et al., 1979b; Darnall et al., 1979; Smith et al., 1970). The absolute light intensity was determined periodically using the rate of photolysis of NO_2 in N_2 to determine k_1 (Holmes et al., 1973).

Benzaldehyde, benzyl nitrate, cresols, nitrotoluenes, and hydroxynitrotoluenes were monitored by gas chromatography (GC) with flame ionization detection (FID) (Pitts et al., 1979b) using either (a) a 10′ x 1/4" (2mm i.d.) borosilicate glass column packed with 60/80 mesh Tenax GC, temperature programmed from 373 to 523 K at 20 K per minute, or (b) a 6′ x 1/4" 0.1% SP 1000/Carbopack C (Supelco) column, temperature programmed from 423 K to 523 K at 20 K per minute. In both cases 10.8- or 3.6-liter gas samples from the chamber were drawn through a 1/4" x 3 1/4" borosilicate glass trap packed with 1 1/2" Tenax GC 60/80 mesh. The sample was then transferred by the carrier gas at 528 K from this trap to the column head which was at 373 or 423 K, followed by the temperature programming of the columns as noted above.

Peroxyacetyl nitrate (PAN) and methyl nitrate were monitored by GC using an 18" x 1/8" Teflon column of 5% Carbowax 400 on Chromosorb G (80/100 mesh) operated at 301 K with electron capture detection (ECD) (Darley et al., 1963; Stephens and Price, 1973). Toluene and the oxygenates were monitored employing a 10′ x 1/8" stainless steel (SS) column of 10% Carbowax 600 on C-22 firebrick (100/20 mesh) (Pitts et al., 1979b; Darnall et al., 1979; Stephens, 1973). In later runs, toluene and benzaldehyde were monitored employing a 5′ x 1/8" SS column of 5% Carbowax 600 on C-22 firebrick (100/115 mesh) for which the sampling trap and injection valve was heated to 368-373 K (Pitts et al., 1979b). Acetylene and background alkanes and alkenes were monitored on Porapak N or 2,4-dimethylsulfolane columns as described previously (Pitts et al., 1979b; Darnall et al., 1979; Stephens, 1973).

The reliability of the reactant and product analyses employing these techniques is estimated (Pitts et al., 1979b; Darnall et al., 1979) to be as follows: O_3 and NO, $\pm$5%; NO_2, at best $\pm$5% but more uncertain due to uncertainties in the measurements of interfering compounds (Winer et al., 1974) and the possibility of interferences from unmonitored compounds; CO, $\pm$10%; toluene, $\pm$10%; aromatic products monitored on the SP-1000 or the Tenax GC system, at best $\pm$25%; benzaldehyde on the 5′ Carbowax 600 system, $\pm$10%; PAN $\pm$20%; formaldehyde, +10 to -30%; and methyl nitrate, $\pm$50%.

In addition, qualitative analyses of the aromatic products (benzaldehyde, benzyl nitrate, cresols, nitrotoluenes, and hydroxynitrotoluenes) were carried out using a Finnigan 3100-combined gas chromatograph-mass spectrometer (GC-MS), with a 6100 data system (Glangetas, 1978). A 26-meter x 0.29-mm i.d. glass capillary column coated with Ucon-50-HB-5100 polypropylene glycol, temperature programmed from 313 K to 492 K at 8 K min^{-1} was employed for these analyses.

Product assignments were made by comparison of the retention times (FID and ECD) and/or mass spectra (GC-MS) (Glangetas, 1978) with authentic samples, wherever possible.

Most calculations were carried out at Riverside as discussed previously (Carter et al., 1979). Input parameters consisted of the initial concentrations of the reactants, a reaction mechanism consisting of a list

of reactions and their rate constants, or photolysis rates, which is given in Appendix A together with the relevant notes and references, and the dilution rate. The set of differential equations resulting from this reaction mechanism were integrated using the Gear algorithm (Gear, 1971; Hindmarsh, 1972). Initial exploratory calculations were carried out on a Univac 1108 computer at Shell Research Ltd., Thornton Research Centre, Chester, UK, using an implicit one-step method with single precision to solve stiff ordinary differential equations (Prothero and Robinson, 1974).

The reaction scheme used in our model calculations, along with associated references and notes, is given in Appendix A. The inorganic reactions (reactions 1-34) are essentially identical to those used recently by Carter et al. (1979) for the NO_x-n-butane-propene-air system, apart from a minor updating of rate constants. Hence, the inorganic reaction scheme will not be discussed in any detail here; Appendix A should be consulted for further details. Analogous to this previous (Carter et al., 1979) and the other recent (Hendry et al., 1978) modeling studies, a constant (for a given run) chamber radical source was found necessary in order to match the calculated and the experimental time-concentration profiles; and as before (Carter et al., 1979), these radicals were presumed to be OH radicals (see note 8 of Appendix A).

The organic reaction scheme is given in Appendix A as reactions 35-166; reactions 46-53 and 70-77 represent overall processes whose detailed reactions are given for aromatic systems in general in Appendix B. The general reactions listed in Appendix B were applied to both the toluene-NO_x-air and the o-cresol-NO_x-air mechanisms, and are intended to be applicable to the NO_x-air photooxidations of all substituted benzenes (see notes 14-19, 26 and 27 of Appendix A and the discussion below). A number of possible alternative mechanisms, discussed below, were examined, and the appendices list all reactions considered, including those which were subsequently found to give unacceptable fits to the data. Throughout the discussion, unprimed reaction numbers (e.g., 35, 36, etc.) will refer to those in Appendix A, while primed reaction numbers (e.g., 1′, 2′, etc.) will refer to specific examples of the general reactions in Appendix B.

Experimental Results. Initial conditions and selected reactivity

parameters for the experiments reported here are given in Table 11. In order to check reproducibility several duplicate irradiations were carried out. In those cases, very similar reactivity parameters were observed (especially for runs carried out with the same solar simulator lamp [Pitts et al., 1979b; Darnall et al., 1979], which was changed between runs 290 and 327), and product yields agreed to within their stated uncertainty limits (compare runs 264-266 and 327 and 340).

The products observed in the toluene-NO_x-air runs for which quantitative results were obtained (in approximate order of yield) were CO, formaldehyde, PAN, benzaldehyde, o-cresol, m-nitrotoluene, acetylene, and methyl nitrate. Also detected (Glangetas, 1978) were small amounts of m- and p-cresol, o- and p-nitrotoluene, benzyl nitrate, and 2,3-, 2,5-, 3,2-, 3,4-, and 4,3-hydroxynitrotoluenes. In the cresol-NO_x-air runs, the products detected were CO, PAN, and 2,3- and 2,5-hydroxynitrotoluenes from o-cresol; CO, PAN and 3,2- and 3,4-hydroxynitrotoluenes from m-cresol, and CO, PAN and 4,3-hydroxynitrotoluene from p-cresol. The organic product yields in the cresol runs were very low and the PAN yields were much lower than those observed in the toluene runs. The maximum yields of the major organic products observed in the toluene-NO_x-air and toluene-benzaldehyde-NO_x-air irradiations are given in Table 12.

Figure 36 compares the concentration-time profiles observed for O_3, NO, NO_2, PAN and the reactant cresol in the o-, m-, and p-cresol-NO_x-air runs. (The nonzero initial ozone values observed are believed to be due to a cresol interference on the UV absorbance O_3 monitor.) In addition, concentration-time profiles for selected species observed in the o-cresol and in selected toluene and toluene-benzaldehyde runs are plotted in Figures 37 - 42, along with results of model calculations (discussed below). In general, it can be seen that the cresol runs and the added benzaldehyde runs have a lower overall reactivity than comparable toluene runs, and that m-cresol is by far the most reactive of the cresol isomers. These results can be rationalized in terms of the mechanism which is discussed below.

Detailed data tabulations, giving concentrations of all organic and inorganic species monitored, and values of measured physical parameters as a function of time, including the spectral distribution of the photolyz-

Table 11

Initial conditions and selected reactivity parameters for the irradiated toluene-NO_x-air, toluene-benzaldehyde-NO_x-air and cresol-NO_x-air mixtures

Run	EC-264	EC-265	EC-266	EC-269	EC-271	EC-273	EC-281	EC-289	EC-290	EC-327	EC-337	EC-339	EC-340
Reactants (ppm)													
Toluene	1.156	1.070	1.196	0.566	1.146	0.587				0.573	0.959	0.536	0.537
o-Cresol							0.394						
m-Cresol								0.297					
p-Cresol									0.364				
Benzaldehyde											0.172	0.187	
NO	0.420	0.435	0.432	0.398	0.186	0.096	0.458	0.404	0.413	0.357	0.322	0.341	0.333
NO_2	0.056	0.048	0.059	0.074	0.029	0.014	0.020	0.045	0.067	0.096	0.124	0.102	0.096
NO_x	0.470	0.482	0.494	0.472	0.215	0.110	0.480	0.449	0.481	0.448	0.448	0.445	0.430
Physical Parameters													
k_1 (min^{-1})	0.35	0.35	0.35	0.35	0.37	0.37	0.35	0.39	0.39	0.40	0.39	0.39	0.39
Ave. Temp. (K)	304.5	302.6	302.8	302.9	303.0	303.6	302.9	303.0	303.1	303.4	303.0	303.4	303.1
Ave. RH (%)	42.0	54.0	47.5	46.5	49.5	49.5	48.0	56.5	52.4	~60	65.6	64.0	63.2
Reactivity Parameters													
Max. O_3 (ppm)	0.419	0.393	0.403	>0.298*	0.296	0.215	>0.064*	0.137	≥0.068*	0.376	0.325	>0.225*	0.346
Time O_3 max. (min.)	210	210	215	>360	90	80	>360	210	≥360	~360	255	>360	360

* 6-hour value given.

Table 12

Observed and Calculated[a] Maximum Product Yields in the Toluene and Toluene-Benzaldehyde-NO_x-Air Runs

Run	EC-266[b]		EC-269		EC-271		EC-273		EC-337		EC-339		EC-340[b]	
Products (ppb)	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.
Aromatic														
Benzaldehyde	22[c]	23	9[d]	12	17[d]	18	16[d]	10	(e)		(e)		8.4	11
o-Cresol	9[c]	18	7	10	13	14	3	8	11	12	5	8	12	9
m-Cresol	2[c]	NC[f]	1[c]	NC	--	NC	0.2	NC	--	NC	--	NC	--	NC
p-Cresol	2[c]	NC	0.7[c]	NC	--	NC	≲0.6	NC	--	NC	--	NC	--	NC
o-Nitrotoluene	0[c]	NC	1[c]	NC	0.1	NC	0.6	NC	--	NC	--	NC	--	NC
m-Nitrotoluene	3[c]	0.2	1[c]	0.1	--	<0.1	0.3	0.3	2	0.2	0.7	0.1	1	0.1
p-Nitrotoluene	4[c]	NC	0.9[c]	NC	--	NC	0.3	NC	--	NC	--	NC	--	NC
Σ Hydroxynitrotoluenes	--	NC	6.7[c]	NC	--	NC	--	NC	--	NC	--	NC	--	NC
Benzyl nitrate[g]	--	14	0.8[c]	10	--	8	--	4	--	10	--	7	--	9
PBzN	--	9	--	9	--	3	--	2	--	39	--	35	--	8
Other Organic Nitrates[g,h]	--	60	--	48	--	35	--	21	--	45	--	33	--	44
Fragmentation														
PAN	75	91	50	52	53	60	31	32	47	61	24	32	42	47
Other peroxy nitrates[i]	--	67	--	56	--	29	--	17	--	46	--	32	--	51
Glyoxyl	--	18	--	19	--	7	--	5	--	15	--	14	--	16
Methyl glyoxyl	--	21	--	10	--	21	--	12	--	8	--	4	--	8
2-Butene-1,4-dial	--	75	--	39	--	64	--	36	--	57	--	33	--	36
Formaldehyde	75	31	40	26	42	17	17	11	65	26	48	19	48	23
Methyl nitrate[g]	1	0.6	1	0.6	--	0.1	--	<0.1	0.6	0.5	--	0.4	0.5	0.5
CO[j]	500	202	~300	211	(e)		(e)		(e)		(e)		(e)	
Acetylene[j]	--	NC	--	NC	--	NC	--	NC	2.4	NC	1.0	NC	1.7	NC

Table 12 (continued)

Notes

[a]Calculated using model A. Yields given are maximum calculated at the time of complete NO_2 consumption, or at 6 hours, whichever came first.

[b]Duplicate runs done gave either less well characterized product data, or data which was consistent with results given here.

[c]Only semi-quantitative GC/MS data [47] is available.

[d]Chromatographic column employed could not separate benzaldehyde and benzyl nitrate, so reported data is benzaldehyde + benzyl nitrate.

[e]Present as a reactant in this run.

[f]NC = Not calculated. Assumed to be negligible in the model.

[g]Reactions consuming this product were not included in the model, so the actual calculated yields should be smaller.

[h]Primarily C_7ONO_2 formed in Reactions 46-53.

[i]Primarily $HCOCH{=}CHCO_3NO_2$ formed in Reaction 112.

[j]Background levels subtracted.

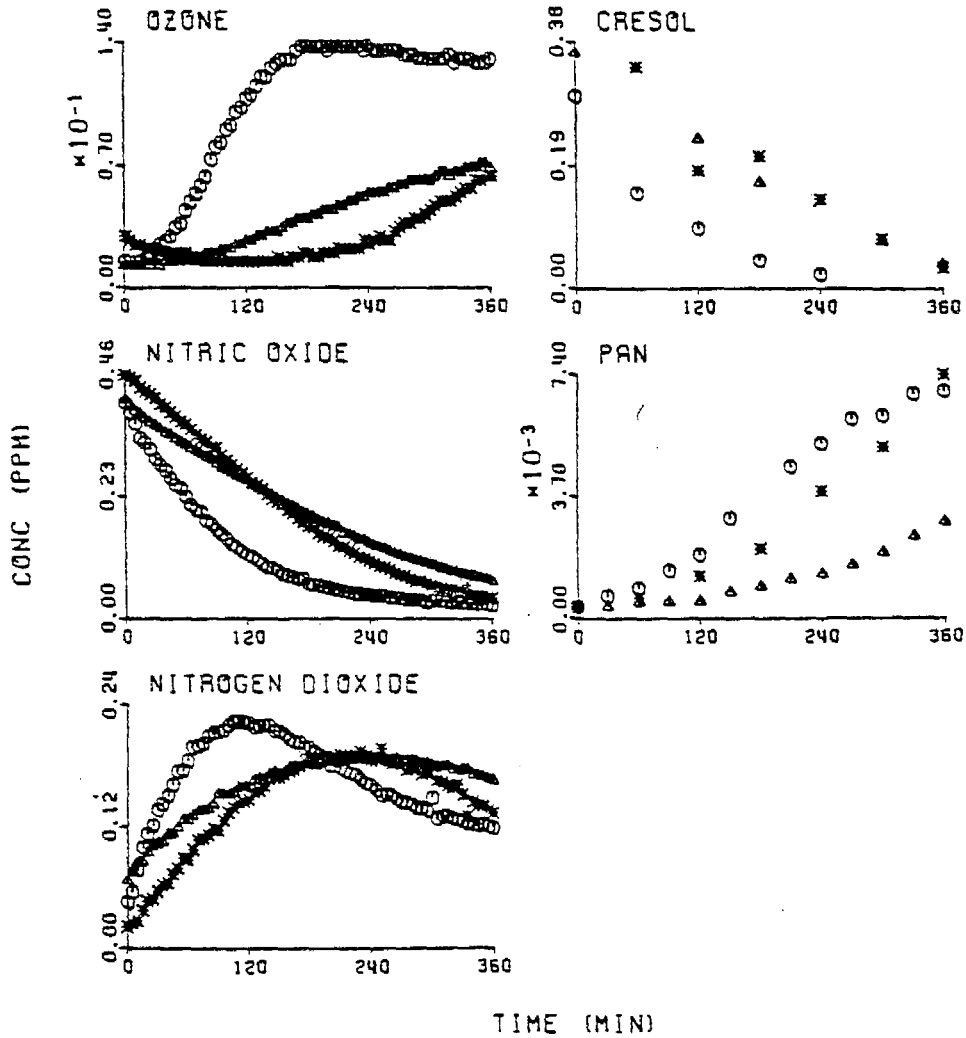


Figure 36. Concentration-Time Profiles Observed in Cresol-NO-NO_x Air Runs.

* = o-Cresol, EC-281
⊙ = m-Cresol, EC-289
△ = p-Cresol, EC-290

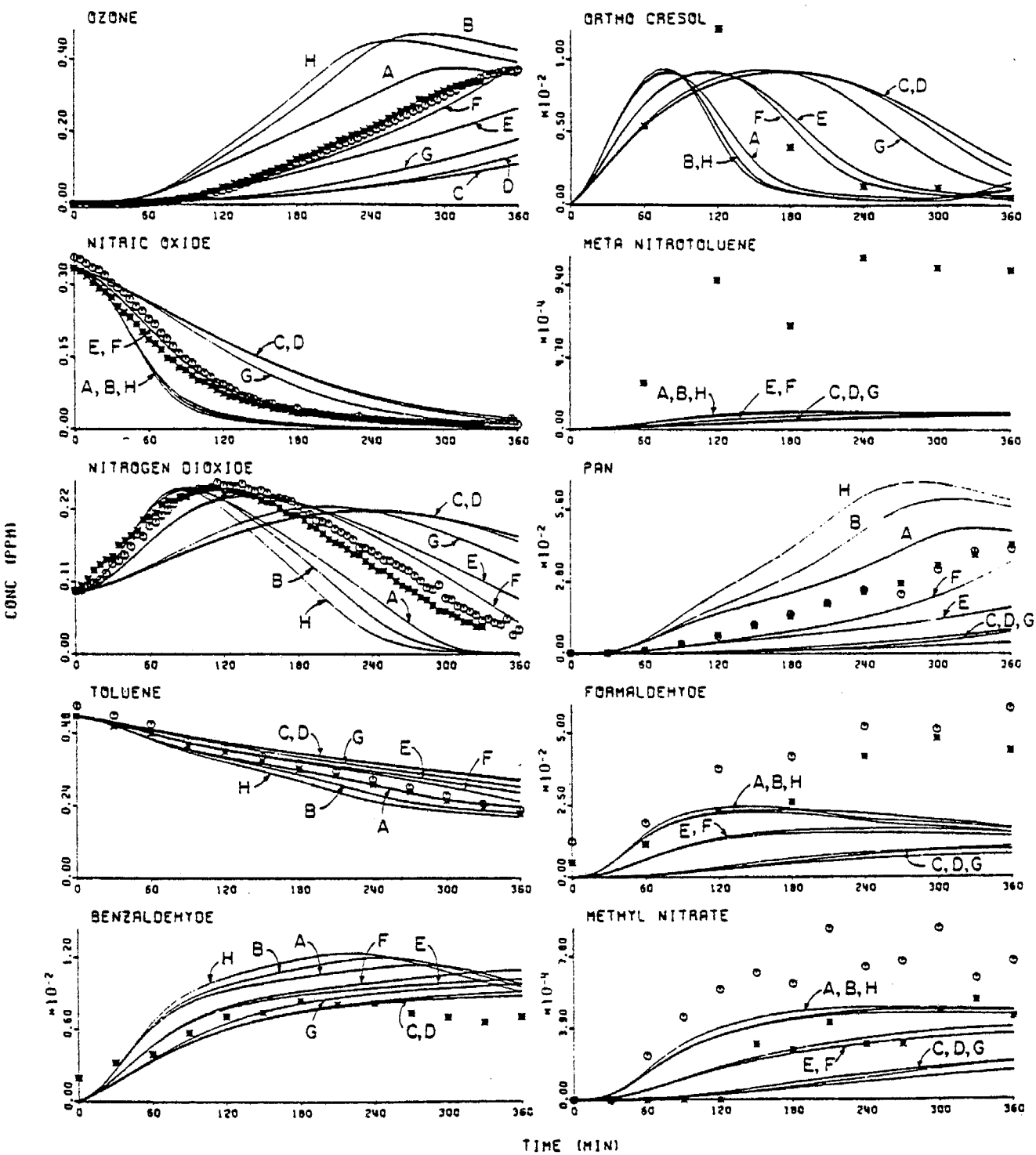


Figure 37. Experimental and Calculated Concentration-Time Profiles for Reactants and Products in Toluene-NO_x Runs EC-327 and EC-340. Effect of Alternate Mechanisms for OH-Aromatic Adduct Fragmentations. ⊙ = Experimental Data, Run EC-327; * = Experimental Data Run EC-340; —— = Calculated, using Mechanisms A-H.

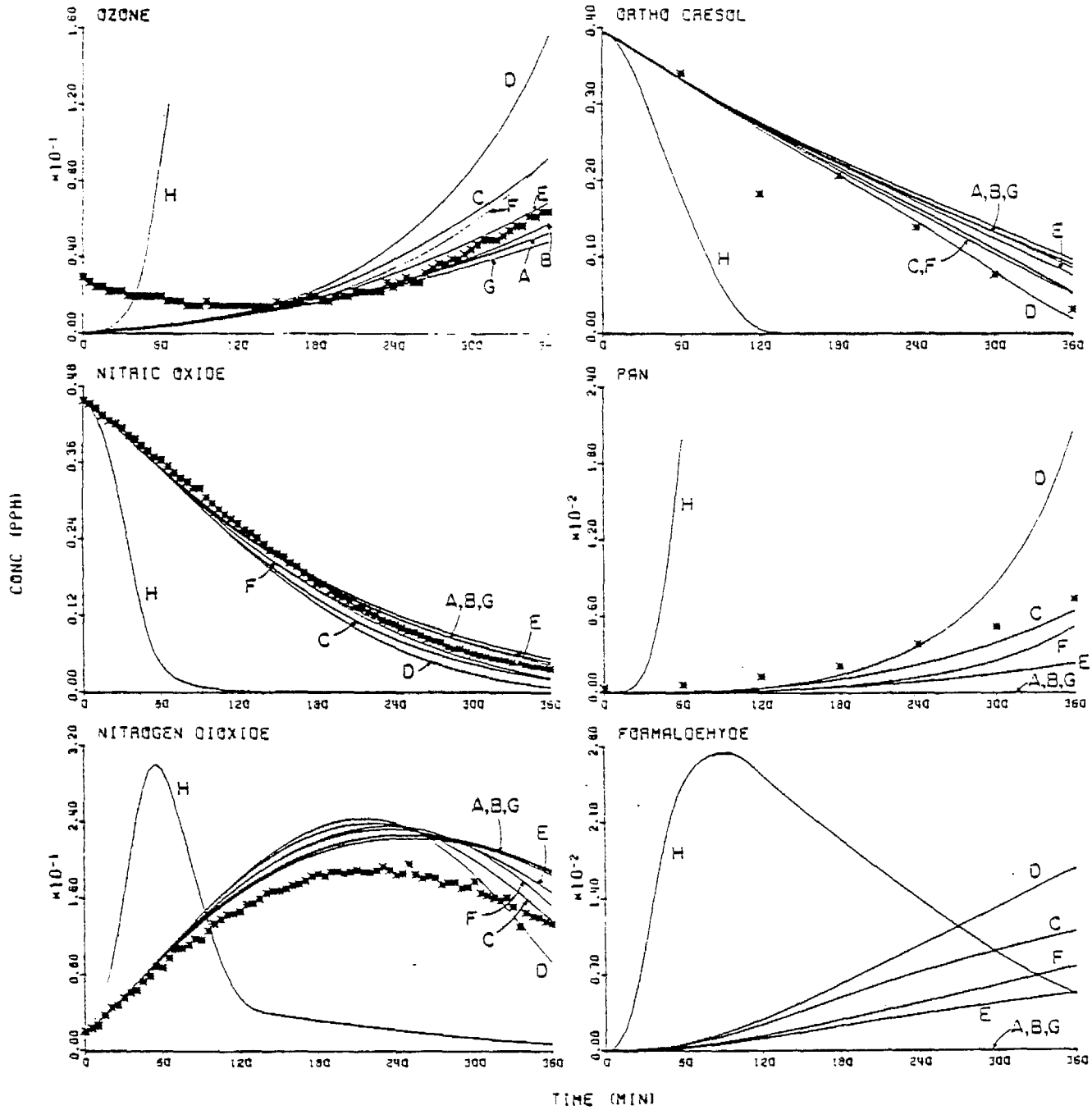


Figure 38. Experimental and Calculated Concentration-Time Profiles for Reactants and Products in o-Cresol-NO_x Run EC-281. Effect of Alternate Mechanisms for OH-Aromatic Adduct Fragmentations. * = Experimental Data; —— = Calculated using Mechanisms A-H.

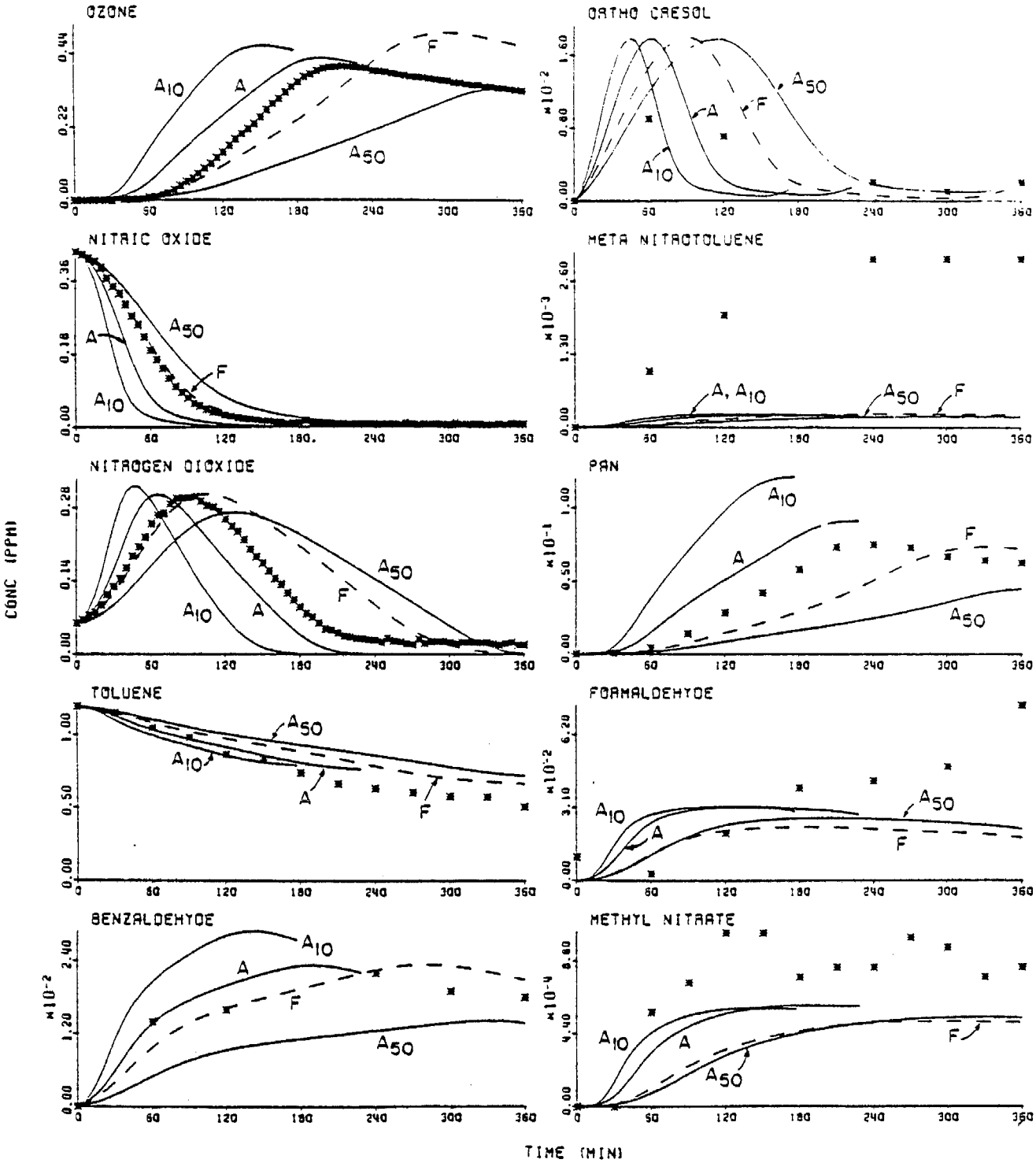


Figure 39. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene-NO_x Run EC-266. Effect of Varying the Efficiency of Alkyl Nitrate Formation from RO_2 + NO_2 from 10% (A_{10}) to 50% (A_{50}). * = Experimental Data; ——, --- = Calculated.

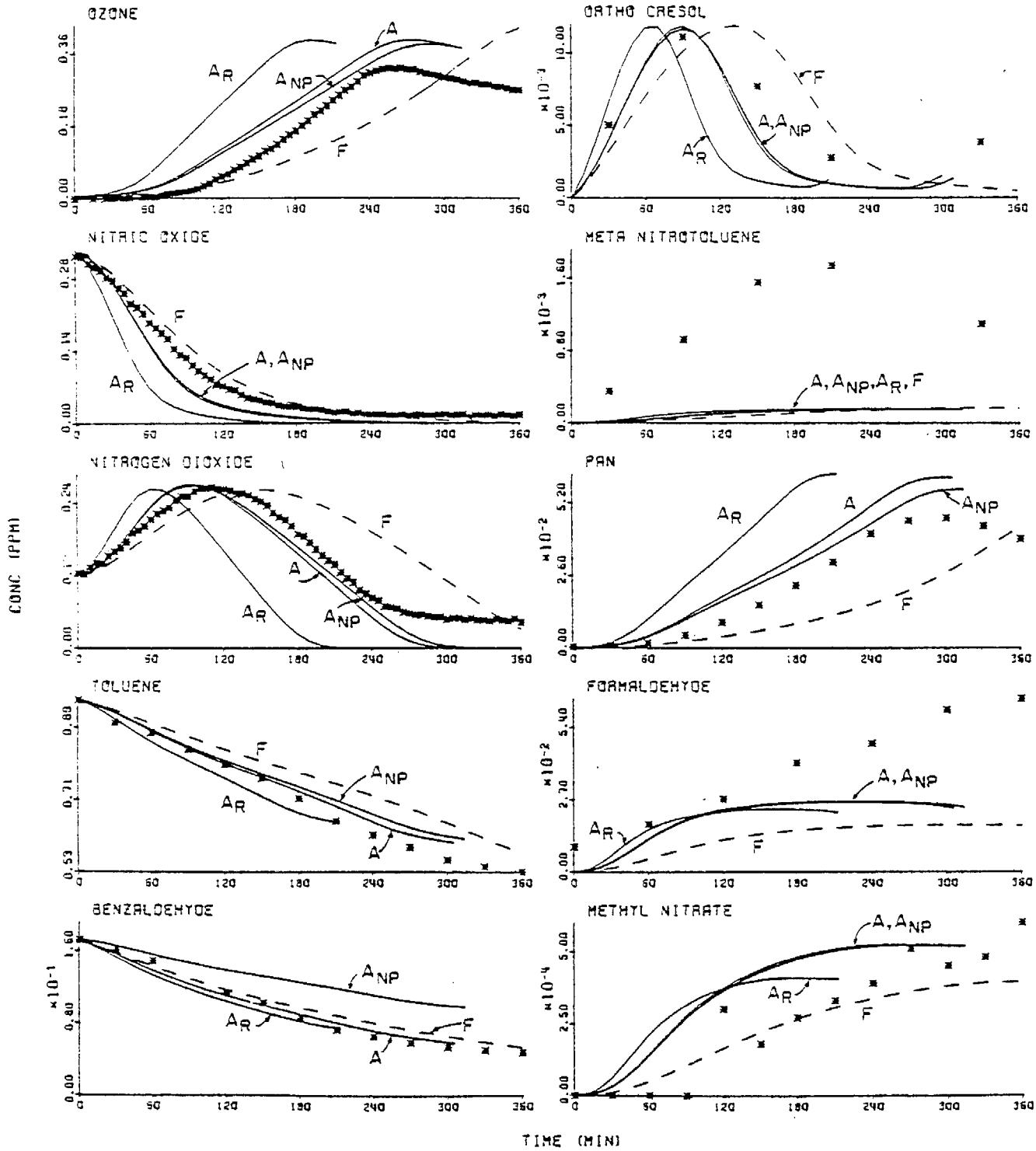


Figure 40. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene-Benzaldehyde-NO_x Run EC-337. Effect of Assuming 100% Efficiency of Radical Production in Benzaldehyde Photolysis (A_R), and Effect of Neglecting Benzaldehyde Photolysis (A_{NP}). * = Experimental Data; ——, --- = Calculated.

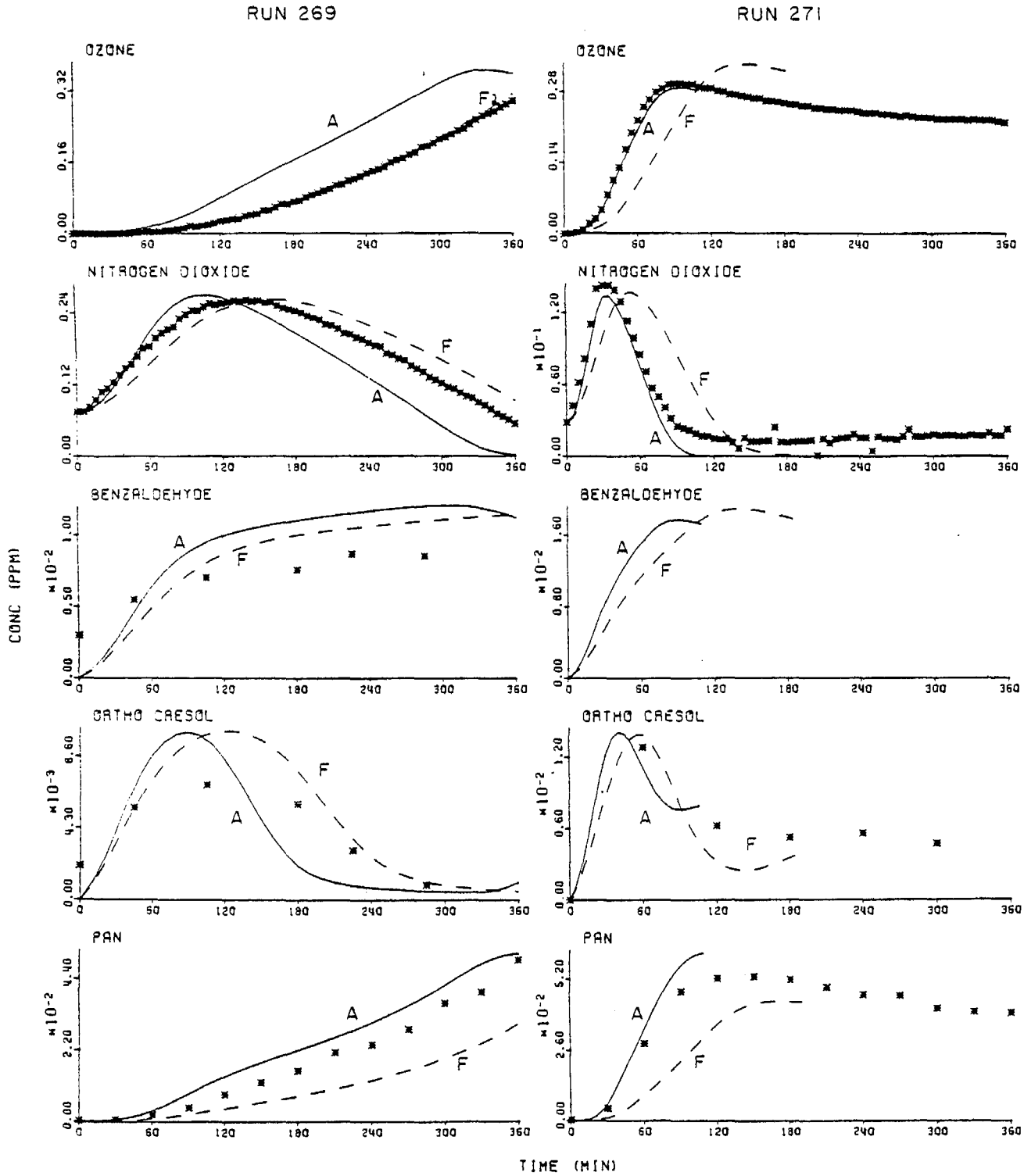


Figure 41. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene-NO_x Runs EC-269 and EC-271. * = Experimental Data; ——, --- = Calculated.

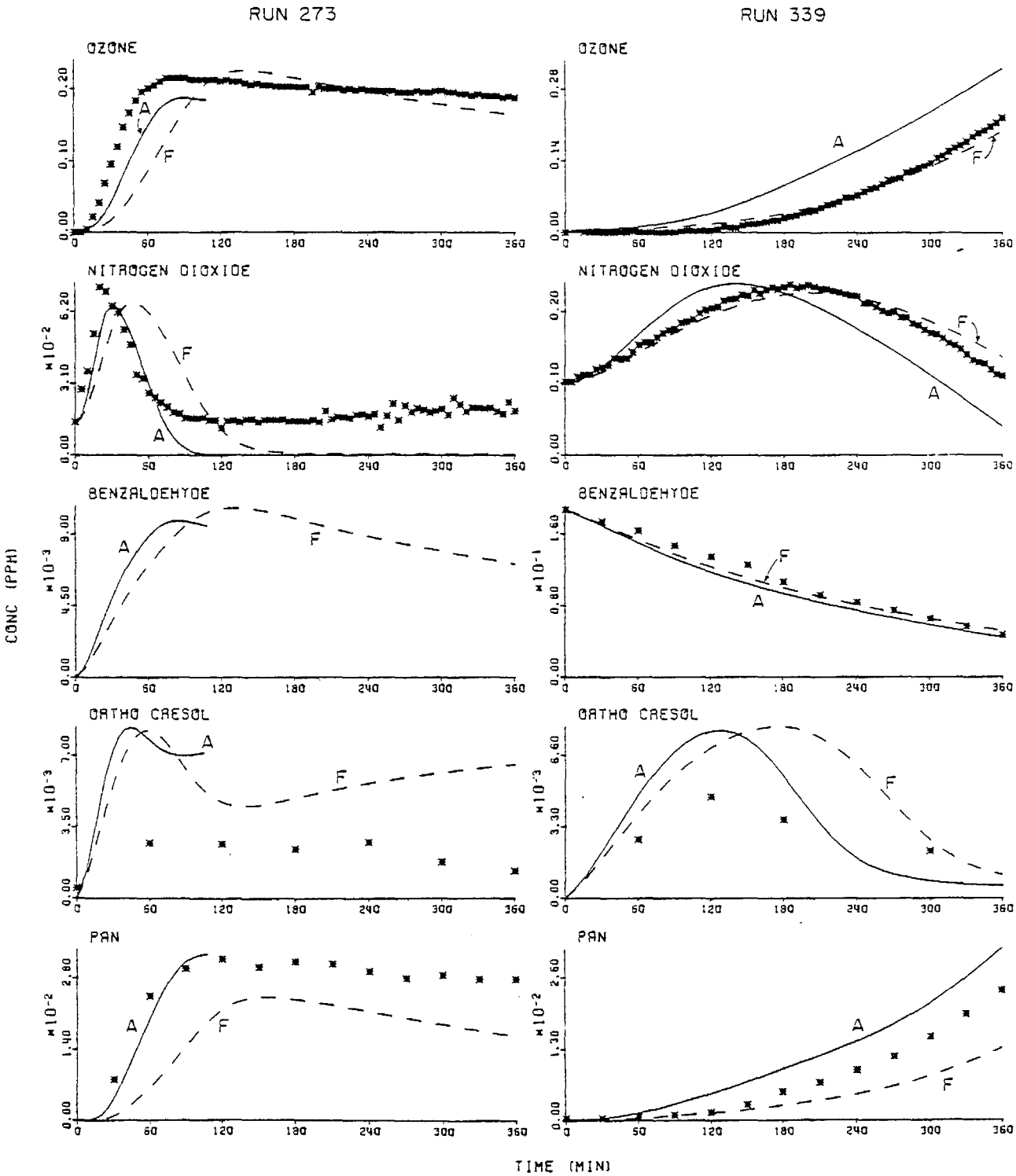


Figure 42. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene-NO_x Run EC-273 and in Toluene-Benzaldehyde-NO_x Run EC-339.
* = Experimental Data; ——, --- = Calculated.

ing light, are available from the Statewide Air Pollution Research Center upon request.

Results of Model Calculations. Calculations were carried out with varying mechanistic pathways and rate constant ratios. The various mechanistic options, which are described in more detail in the discussion, concern (a) the reactions of the species formed by the addition of hydroxyl radicals and then O_2 to the aromatic ring, (b) the reactions of the predicted conjugated γ-dicarbonyl products, (c) the relative importance of the chain-terminating formation of organic nitrates from the RO_2 + NO reaction (e.g., reaction 38 and 4′), (d) the photolysis of benzaldehyde, and (e) the reaction of o-cresol with NO_3 radicals. The varying assumptions made concerning these options, and the designation given the calculations using the different sets of assumptions, are given in Table 13.

Figure 37 and 38 show the effect of using different alternate mechanisms concerning the reactions of the OH-aromatic-O_2 adduct and the reactions of the γ-dicarbonyl products, compared with the experimental data for a representative toluene run and the o-cresol run; and Figure 39 shows the effect of varying the relative importance of the formation of nitrate from the RO_2 + NO reaction. From these figures, it can be seen that best fits are obtained if it is assumed that the aromatic-OH-O_2 adducts undergo cyclization but not re-cyclization (see discussion), and that the C_7 bicyclic peroxy radicals formed in the toluene and cresol photooxidations react with NO ~25% of the time to give nitrates. Both calculations A (assuming exclusively 3-addition of O_2 to the aromatic-OH adduct, [2.2.2] cyclization of this aromatic-OH-O_2 adduct, and no cyclization of the $RCH{=}CHCO_3$ radicals formed from the γ-dicarbonyl products) and calculations F ([3.2.1] cyclization of either the 1-O_2- or 3-O_2-aromatic-OH adduct, and rapid cyclization of $RCH{=}CHCO_3$) fit the data reasonably well, and the predictions of these two mechanisms are compared with the data from other toluene and toluene-benzaldehyde runs in Figures 39 - 42. In general, calculations A predict an initial reactivity which is slightly high, while calculations F predict a slightly low initial reactivity, although in both cases the calculated initial reactivity can be made to fit experimental results by respectively reducing or increasing the adjustable radical input rate from chamber sources (Carter et al., 1979)

Table 13

Sets of Mechanistic Options Examined in Model Calculations and Their Designation Symbols

Designation Symbol	Mechanistic Options							
	Arom-OH-O_2 Adduct Formed	Arom-OH-O_2 Cyclization	Recyclization	RCOCH=CHCO$_3$ Cyclization	Tricyclic Radical Decomposition Mechanism	$\frac{k(C_7O_2+NO \rightarrow C_7ONO_2)}{k(C_7O_2+NO)}$	C_6H_5CHO Photolysis Mechanism	$k(NO_3+\text{cresol})$ (cc-molecule^{-1} sec^{-1})
A	3-adduct[a]	[2.2.2][b]	No[c]	No[d]	NA[e]	0.25	Non-Radical	1.5×10^{-11}
B	3-adduct	[2.2.2]	No	Yes	NA	0.25	Non-Radical	1.5×10^{-11}
C	1-adduct	[2.2.2]	No	No	NA	0.25	Non-Radical	1.5×10^{-11}
D	1-adduct	[2.2.2]	No	Yes	NA	0.25	Non-Radical	1.5×10^{-11}
E	NE[f]	[3.2.1]	No	No	NA	0.25	Non-Radical	1.5×10^{-11}
F	NE	[3.2.1]	No	Yes	NA	0.25	Non-Radical	1.5×10^{-11}
G	NE	NE	Yes	NA	$k'_{31} \gg k'_{33}$	0.25	Non-Radical	1.5×10^{-11}
H	NE	NE	Yes	NA	$k'_{33} \gg k'_{31}$	0.25	Non-Radical	1.5×10^{-11}
A_{10}	----------Same as A----------					0.1	Non-Radical	1.5×10^{-11}
A_{50}	----------Same as A----------					0.5	Non-Radical	1.5×10^{-11}
A_R	----------Same as A----------					0.25	Radical	1.5×10^{-11}
A_{NP}	----------Same as A----------					0.25	No Photolysis	1.5×10^{-11}
A_{NN}	----------Same as A----------					0.25	Non-Radical	0

[a] 3-adduct: $k_{45} \gg k_{44}$ (toluene system); $k_{69} \gg k_{68}$ (cresol system); 1 adduct: $k_{44} \gg k_{45}$, $k_{68} \gg k_{69}$.

[b] Refers to structure of bicyclic ring system. [2.2.2]: $k'_1 \gg k'_7$; [3.2.1]: $k'_7 \gg k'_1$.

[c] Yes: $k'_{16} \gg k'_3[NO]$ or $k'_{17} \gg k'_9[NO]$ or $k'_{18} \gg k'_{11}[NO]$; No: k'_{16}, k'_{17}, k'_{18} negligible.

[d] Yes: $k_{108} \gg (k_{110}[NO] + k_{112}[NO_2])$ and $k_{109} \gg (k_{111}[NO] + k_{113}[NO_2])$; No: k_{108}, k_{109} negligible

[e] NA = Not applicable. Intermediates involved not formed in this set of options.

[f] NE = No effect. The same intermediates or products are formed regardless of the assumptions made.

(see note 8 of Appendix A).

Figure 40 shows the effect on model calculations of varying assumptions concerning benzaldehyde photolysis for a toluene-benzaldehyde run. It can be seen that in order to fit the benzaldehyde concentration-time profiles and the overall reactivity, it is necessary to assume that benzaldehyde undergoes photolyses at a signficant rate, but that it forms non-radical products.

Figure 43 shows the effect that a reaction of NO_3 with o-cresol has on the O_3, NO_2 and o-cresol concentration-time profiles in the o-cresol run and in a toluene-benzaldehyde run. Predicted concentration-time profiles of other monitored reactants and products are less affected by this reaction. It can be seen that the data are much better fit by assuming that the reaction occurs with a rate constant on the order of (1-2) x 10^{-11} cm^3 $molecule^{-1}$ sec^{-1} than by assuming it is negligible.

Table 12 lists the experimental and calculated (using model A) yields of the major products monitored, and gives the maximum calculated yields of major products predicted by the model which were not experimentally monitored. Among the products monitored the major discrepancy appears to be that the observed nitrotoluene yields are higher by a factor of ~10 than those calculated, despite the fact that the calculations generally fit the cresol data and used the experimentally determined ratio (k_{42}/k_{43}) for cresol vs. nitrotoluene formation obtained by Kenley et al. (1978). In addition, the predicted formaldehyde yields are slightly low, relative to the experimental data. This may be due to the neglect of glyoxal photolysis in our mechanism (see note 29). For the other major products, the fits of calculated to experimental yields can be considered to be within the range of the experimental uncertainties. Although the model predicts the formation of products which were not experimentally observed (mainly C_7 organic nitrates, α-dicarbonyls, 2-butene-1,4-dial, peroxybenzoyl nitrate (PBzN) and nitrophenols), we have no evidence that these species are <u>not</u> formed in the yields predicted. Indeed, the low carbon balance observed for these systems suggests a significant formation of unmonitored products, and thus, except for the nitrotoluene yields (a very minor product) our model simulations can be considered to be generally consistent with the experimental data reported here.

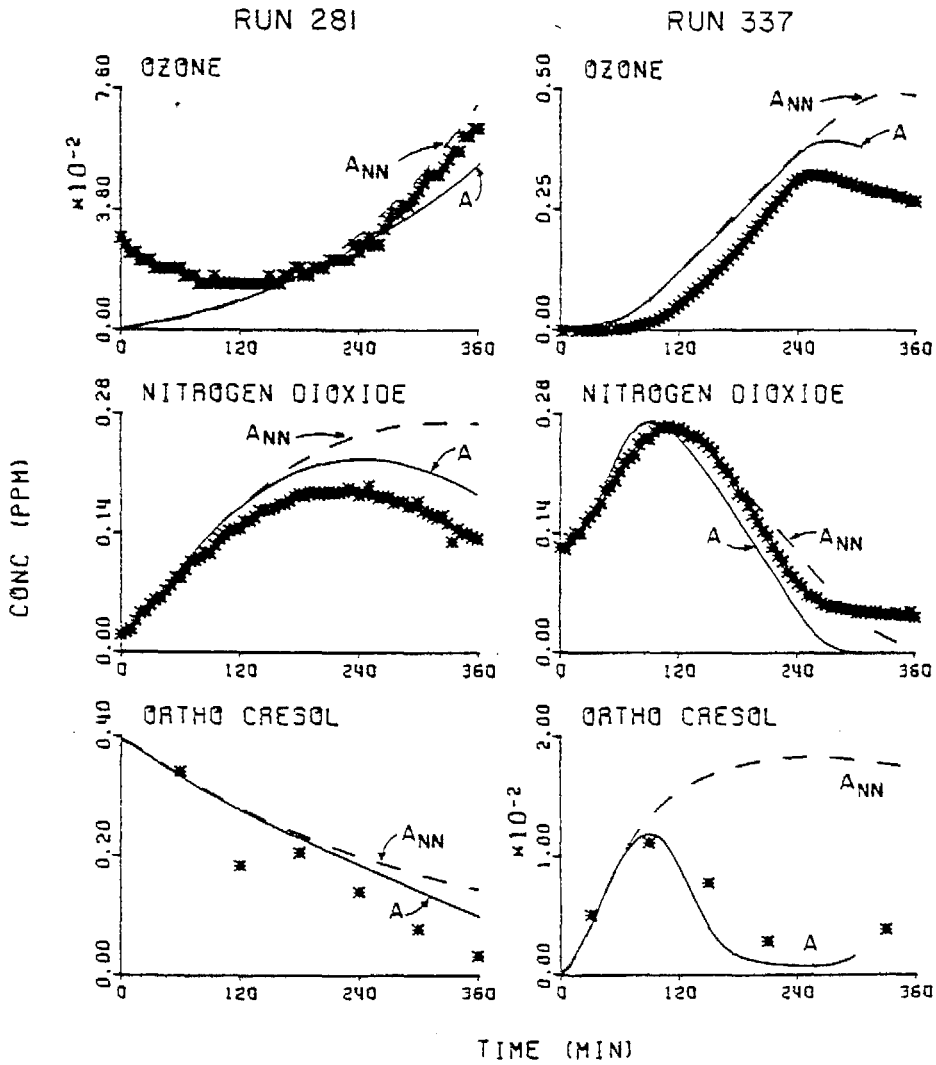
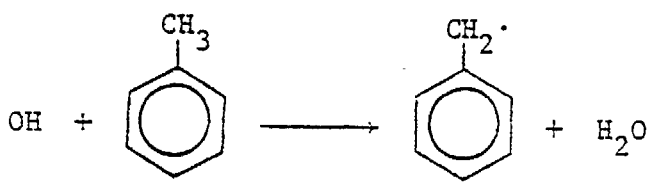


Figure 43. Experimental and Calculated Concentration-Time Profiles for O_3, NO_2, and o-Cresol in o-Cresol-NO_x Run EC-281 and in Toluene-Benzaldehyde-NO_x Run EC-337. Effect of Neglecting the NO_3 + o-Cresol Reaction (A_{NN}). * = Experimental Data; ——, --- = Calculated.

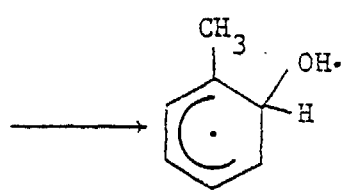
Discussion.

1. Initial Toluene Reactions. The only significant chemical loss process of toluene under simulated polluted atmospheric conditions is now known to be by reaction with the OH radical (Hendry et al., 1978; Atkinson et al., 1979; Doyle et al., 1975; Davis et al., 1975; Hansen et al., 1975; Lloyd et al., 1976; Perry et al., 1977a; Ravishankara et al., 1978; Kenley et al., 1978; Hendry, 1979; Pate et al., 1976a).

This reaction proceeds via two pathways: H atom abstraction from the substituent methyl group (reaction 35), and OH radical addition to the ring (reaction 41) (Hendry et al., 1978; Atkinson et al., 1979; Davis et al., 1975; Perry et al., 1977a; Ravishankara et al., 1978; Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Spicer and Jones, 1977; Hoshino et al., 1978; Grosjean et al., 1978; O'Brien et al., 1979; Akimoto et al., 1978),



(35)

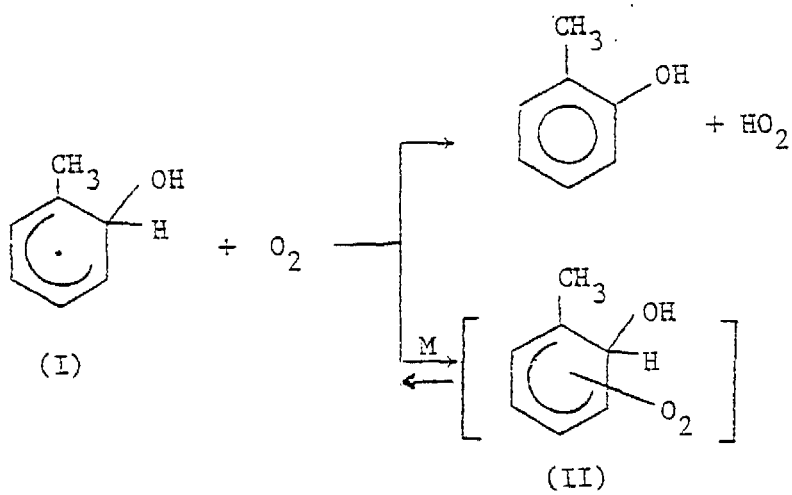


(41)

with $k_{35}/(k_{35} + k_{41}) \cong 0.15$ (Atkinson, et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979) and $(k_{35} + k_{41}) \cong 6 \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1} (Atkinson et al., 1979; Davis et al., 1975; Hansen et al., 1975; Perry et al., 1977a) at room temperature. Under atmospheric conditions the benzyl radical will react to form benzaldehyde and benzyl nitrate (reactions 36-40), as has been discussed previously (Hendry et al., 1978; Atkinson et al., 1979; Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Spicer and Jones, 1977; Hoshino et al., 1978; Grosjean et al., 1978;

O'Brien et al., 1979). The reasonably good fits of the model calculations to the experimental benzaldehyde yields (see Table 12) indicate that our data is consistent with the reported ratios (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979) for OH abstraction of hydrogen vs. OH radical addition to the aromatic ring.

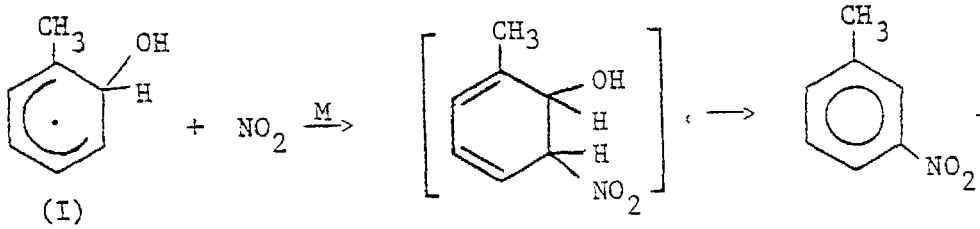
OH Radical Addition Pathway: Formation of Cresols and Nitrotoluene. The major pathway (~85%) for reaction of OH radicals with toluene is via the initial formation of an OH-toluene adduct (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979). By analogy with the position of $O(^3P)$ atom addition to toluene (Jones and Cvetanovic, 1961; Grovenstein and Mosher, 1970; Gaffney et al., 1976) and based on the available experimental product data (Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Hoshino et al., 1978; Grosjean et al., 1978; O'Brien et al., 1979; Akimoto et al., 1978), the OH radical is presumed to add primarily at the ortho position. The thermalized adduct (I) can react under atmospheric conditions with O_2 via two pathways (Atkinson et al., 1979): H atom abstraction to form the cresol (reaction 42), or reversible addition to form the peroxy radical (II) (reaction 44, 45):



(42)

(44,45)

or it can react with NO_2 to form the nitrotoluene:



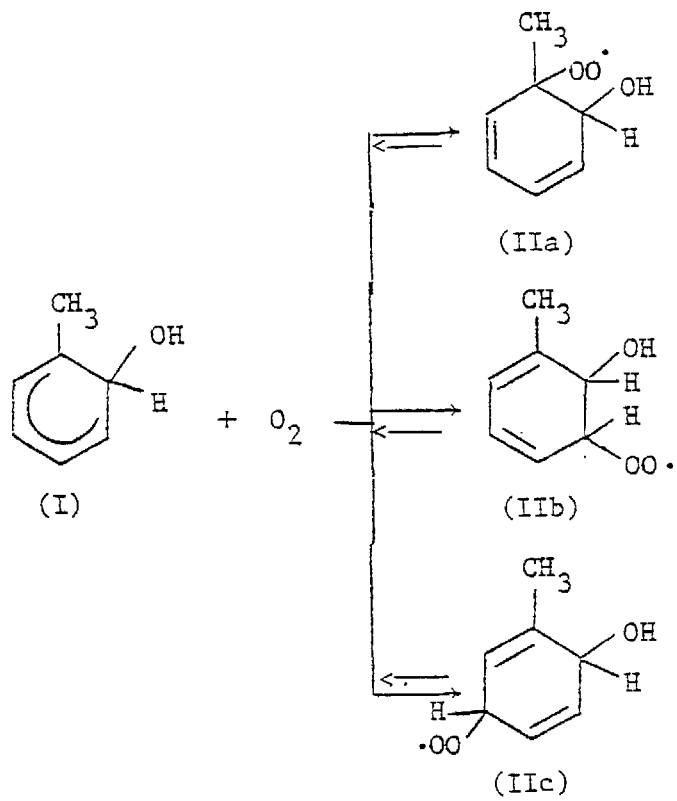
(43)

Hendry and co-workers (Kenley et al., 1978; Hendry, 1979) concluded from their discharge flow study of the reaction of OH radicals with toluene that the cresol isomers and m-nitrotoluene (i.e., reaction 42 and 43) are the sole initial products of the OH radical addition pathway, and that $k_{43}/k_{42} = (4.4 \pm 0.5) \times 10^3$. If the discharge-flow results (Kenley et al., 1978; Hendry, 1979) are applicable to the present experimental study, the only significant initial products of toluene photooxidation would be benzaldehyde and the cresols, with the latter being formed ~85% of the time. Because the cresols are consumed more rapidly in the NO_x-air irradiations than toluene, due to their higher rate constant for reaction with the OH radical (Atkinson et al., 1979; Perry et al., 1977b; Atkinson et al., 1978b) this would mean that the chemistry of the toluene-NO_x system would be dominated by that of the cresol-NO_x system. However, the present smog chamber results indicate that in terms of ozone and PAN formation and NO to NO_2 conversion rates, the cresol-NO_x-air systems are far less reactive than the toluene system. The excess reactivity of the toluene system cannot be attributed to benzaldehyde reactions, since, as is discussed below, benzaldehyde acts as an inhibitor (Gitchell et al., 1974; Niki et al., 1978; Niki et al., 1979). Thus the initial formation of products other than these is necessary to account for the relatively high reactivity of toluene runs, and for the high yields of products such as PAN, as well as for the observation of biacetyl as an initial product in o-xylene-NO_x-air irradiations (Darnall et al., 1979). We find the o-cresol data is best fit by assuming it is formed to the extent of only ~20% of the total OH + toluene reaction, with products other than cresol, benzaldehyde, benzyl nitrate and nitrotoluenes being formed ~65% of the time.

The apparent inconsistency in terms of predicted cresol and nitrotoluene yields between the results of the discharge flow studies (Kenley et al., 1978) and our smog chamber studies may be due to the fact that the former was carried out at a total pressure of ~6-15 torr of (Ar + O_2) (Kenley et al., 1978) against a total pressure of 1 atm of air in the smog chamber studies. O_2 addition to (I) to form (II) and the reaction of (I) with NO_2 to form nitrotoluenes both may have not been in the limiting high pressure second order kinetic regime under the conditions of the discharge-flow study (Kenley et al., 1978), and thus could be significantly

faster at 1 atm total pressure. This is indeed assumed to be the case for the addition reaction of (I) with O_2, but the model still uses the low pressure-derived value for the (I) + NO_2 addition reaction (reaction 43). However, the fact that the model significantly underpredicts nitrotoluene yields suggests that k_{43} is pressure dependent as well.

Stucture and Reactions of the OH-Aromatic-O_2 Adducts. The structure of the radical (II) is not known; addition of O_2 to (I) may be at the 1-, 3-, or 5-position:



(44)

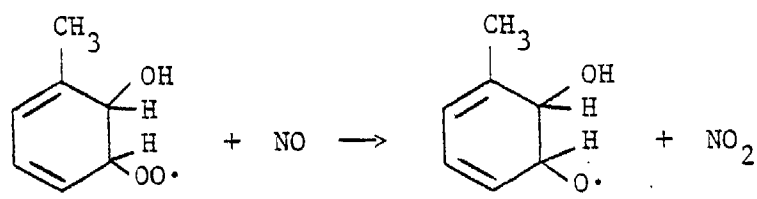
(45)

O_2 addition at the 5-position should be the least thermodynamically favored, since the double bonds are nonconjugated. Addition at the 1-position (reaction 44) is estimated (Benson, 1976) to be slightly more favored thermodynamically over addition to the 3-position (reaction 45), although the resulting radical (IIa) will also have the most steric hindrance. In the calculations, the consequences of assuming exclusively 1-addition or exclusively 3-addition are both considered.

Based on thermochemical estimates (Perry et al., 1977a; Benson, 1976), O_2 addition to radical I is expected to be only ~10 kcal $mole^{-1}$ exothermic. This means that significant back-decomposition of radicals II to radical I may be occurring, which could account for the relatively low effective rate constant for O_2 addition to radical I required to fit the cresol data (see note 13, Appendix A).

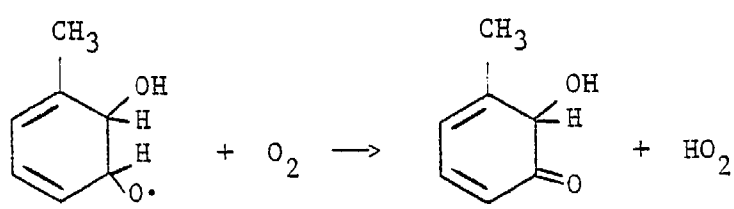
At the present time little is known about the other reaction pathways of the OH-aromatic-O_2 adducts. There are a number of possible alternative pathways, and these are listed for a general aromatic adduct in Appendix B and are discussed below for the case of adduct IIb (substituent 6 in Appendix B = CH_3, substituents 1-5 = H). Reactions of the other adducts are assumed to be analogous.

If the OH-aromatic-O_2 adducts react in a manner analogous to other peroxy radicals, the following scheme would appear to be the most reasonable:

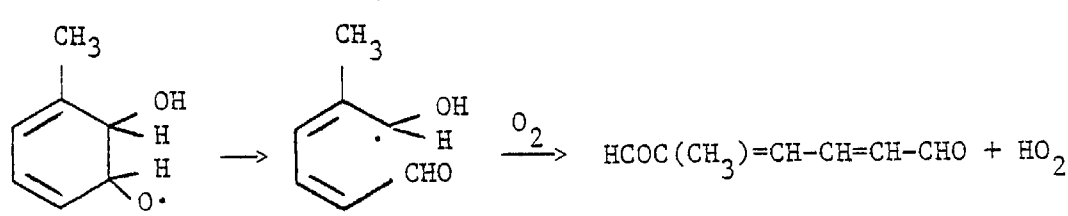


(IIb)

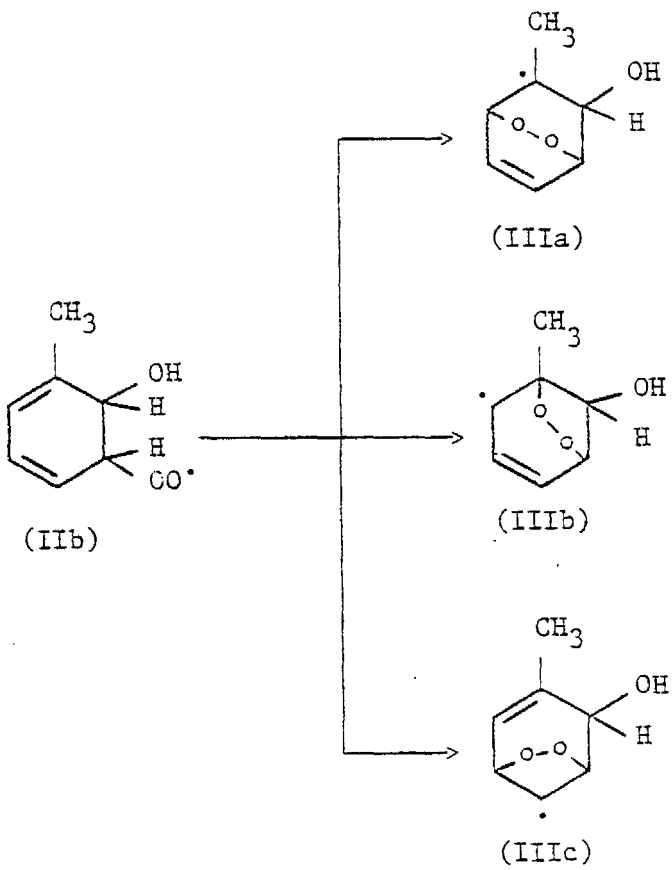
followed by either reaction with O_2



or ring opening



However, this scheme is inconsistent with the observation of biacetyl as a primary product in the NO_x-o-xylene-air system (Darnall et al., 1979), and no reasonable mechanism accounting for that observation (Darnall et al., 1979) could be derived without assuming formation of bicyclic radicals. It is thus assumed that the OH-aromatic-O_2 adduct primarily undergoes cyclization reations such as those shown below:



(1')

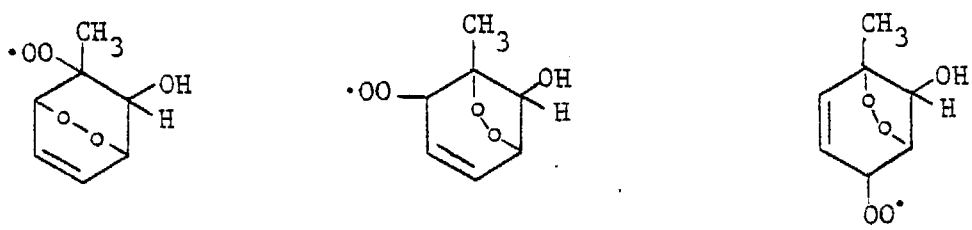
(7')

In addition to accounting for the ring cleavage products observed, these reactions are expected to dominate on the basis of thermochemical and kinetic estimates. If we assume that the rate constant for the reaction of the peroxy radical IIb with NO is ~8 x 10^{-12} cm^3 $molecule^{-1}$ sec^{-1} (see note 9 of Appendix A), then under realistic atmospheric conditions [[NO] < 1 ppm (2 x 10^{13} molecule cm^{-3})] cyclization should dominate if its rate constant is >160 sec^{-1}. If we further assume that (1) the A factors for the cyclization reactions are at a minimum ~10^{10} sec^{-1} (Benson, 1976), (2) that the

activation energy for cyclization is [$\lesssim$9 kcal mole^{-1} (based on the activation energies of bimolecular radical + double bond addition reactions [Kerr and Parsonage, 1972]) + the reaction endothermicity (if any)] and (3) that ΔH (cyclization) $\cong$ (ring strain-14) kcal mole^{-1}, based on thermochemical calculations using group additivity principles (Benson, 1976), then cyclization should dominate if the ring strain of the bicyclic radicals is less than ~16 kcal mole^{-1}. Although such ring strains are not known, this would appear to be likely (Benson, 1976).

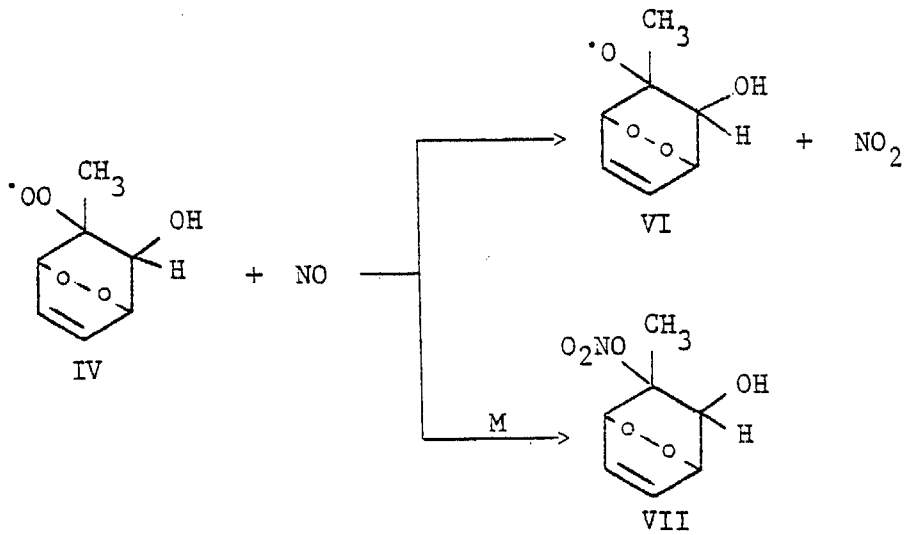
Of the radicals IIIa-c, IIIa will probably have the least ring strain, while IIIb will have some resonance stabilization energy by virtue of its allylic character. Since we cannot determine, a priori, which of these structures is favored, it is again necessary to consider both options in the model calculations, i.e. IIIa or IIIb.

These cyclized aromatic-OH-O_2 adducts are then expected to add O_2 to form radicals of the type



IV Va Vb

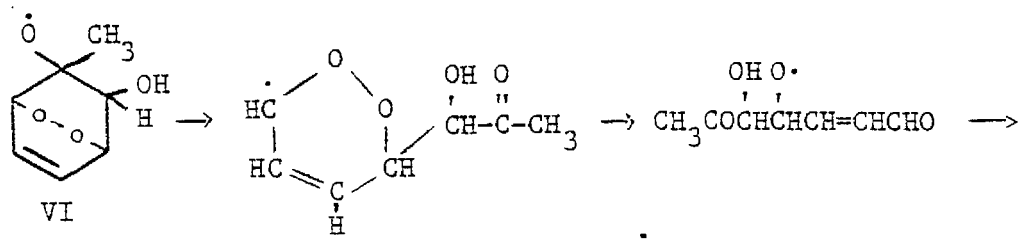
which could react with NO either to form an alkoxy radical or yield a stable nitrate (analogous to the $\geq C_4$ alkylperoxy cases [Carter et al., 1979]), for example:



(3')

(4')

The reactions of the bicyclic peroxy organic nitrates such as (VII) are unknown; they may undergo molecular decomposition to form HNO_3 or other organic nitrates. In our model we assume their reactions, if any, have a negligible effect on the overall mechanism and are thus ignored. The bicyclic peroxy alkoxy radicals such as (VI) are expected to undergo a series of highly favorable β-scission fragmentations, resulting in the formation of α-dicarbonyl and conjugated γ-dicarbonyl products. For example, (VI) is assumed to decompose as shown, with the other isomers, resulting from the reaction of NO with Va and Vb, reacting analogously:

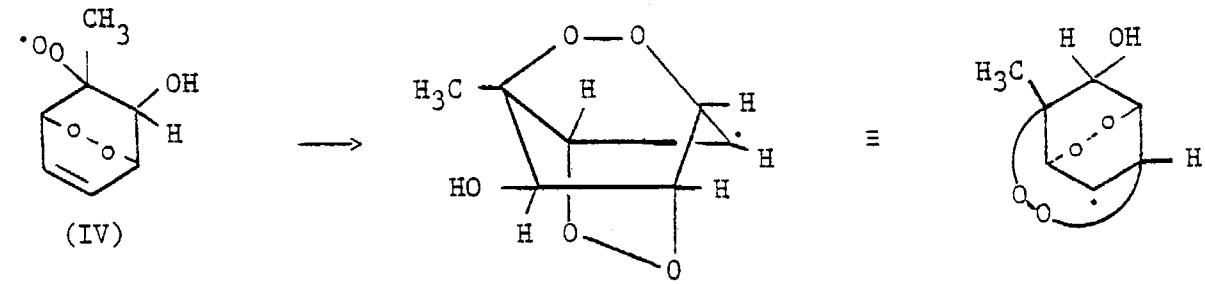


$$CH_3COCHOH + HCOCH{=}CHCHO \qquad (5')$$

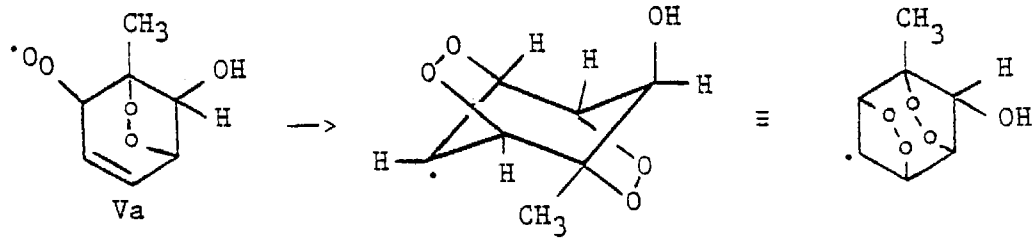
$$\xrightarrow{O_2} CH_3COCHO + HO_2 \qquad (6')$$

The relative importance assumed for nitrate formation vs. alkoxy radical formation has an important effect on model simulations, since the former process is radical terminating and is an effective nitrogen sink, while the latter is radical propagating. This effect is shown in Figure 39, where $k_{4'}/(k_{3'} + k_{4'})$ (and also the analogous rate constant ratios in the cresol system and for the benzyl peroxy radical) is varied from 0.1 to 0.5. It can be seen that toluene-NO_x-air data is best fit by assuming nitrate formation occurs ~25% of the time; this is true for the toluene-benzaldehyde-NO_x-air and the cresol-NO_x-air system as well. Assuming nitrate formation is negligible results in a significant overproduction at ozone maxima regardless of the other mechanistic options used.

A possibility which must also be considered is that the bicyclic peroxy radicals may further cyclize, such as shown below (for radical (IV) and the O_2 adduct to radical (IIIb)):

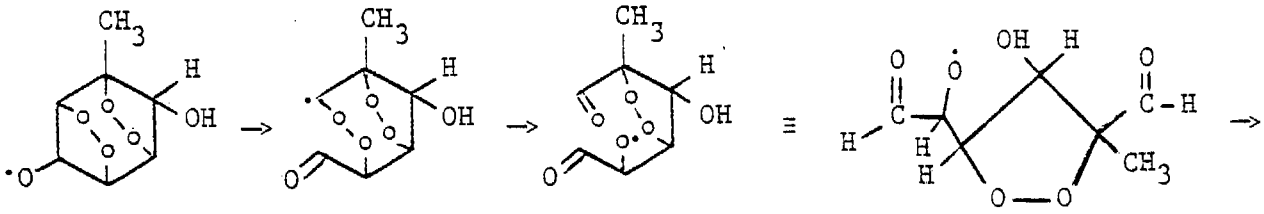


(IV) (16')

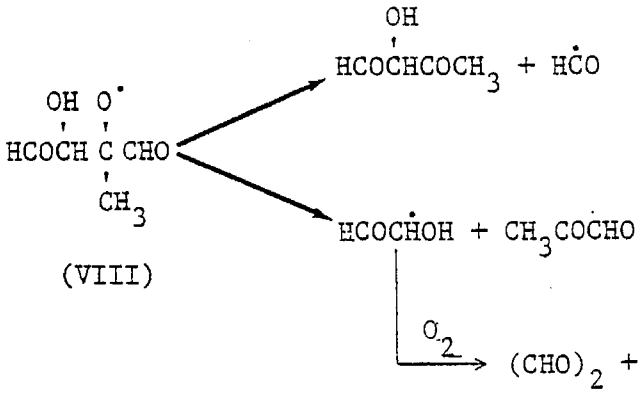


Va (17')

If formed, these double cyclized radicals should react with O_2 and then NO forming alkoxy radicals or alkyl nitates by reactions analogous to those shown above for (IV). The tricyclic bridged-peroxy alkoxy radicals are also expected to rapidly fragment via consecutive β-scissions:



$$(CHO)_2 + HCOCH(OH)\dot{C}(O\cdot)CHO(CH_3) \qquad (27',29')$$



(VIII)

$$HCOCH(OH)COCH_3 + H\dot{C}O \qquad (31')$$

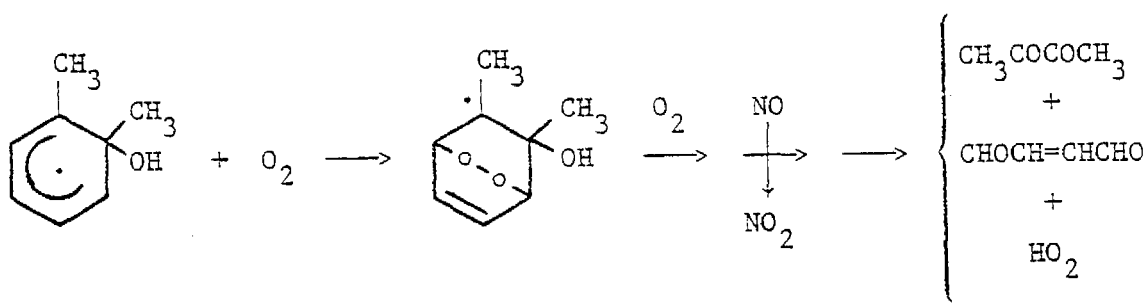
$$HCO\dot{C}HOH + CH_3COCHO \qquad (33')$$

$$\xrightarrow{O_2} (CHO)_2 + HO_2 \qquad (14')$$

The relative importance of the two possible modes of decomposition (e.g., reaction 31′ and 33′) of species such as (VIII) is not known so both possibilities are considered.

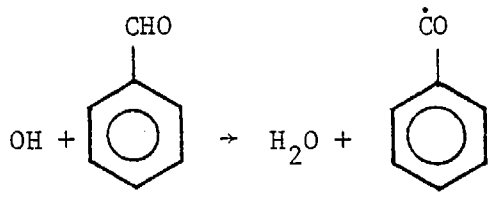
As can be seen from Figures 37 and 38, the data do not clearly indicate which aromatic-OH-O_2 adduct is formed or whether it undergoes [2.2.2] or [3.2.1] cyclization, but do indicate that recyclization probably is negligible. If recyclization occurs, the assumption made concerning the fragmentation of radical (VIII) is important (assuming reaction 33′ dominates results in over-prediction of reactivity in the toluene and the o-cresol systems, while assuming reaction 31′ dominates results in the reactivity in the toluene system being underpredicted, but gives reasonably good fits to the o-cresol system); but it is clear that no adjustment of the $k_{31'}/k_{33'}$ ratio would allow both the toluene-NO_x data and the o-cresol-NO_x data to be fit by models assuming recyclization. Model (A) assumes [2.2.2] cyclization and predominant addition of O_2 to the 1-position of the OH-aromatic adduct, although 3-addition should not be completely negligible. If [3.2.1] cyclization occurs, as assumed in the other model which gives reasonable fits to the data (F), formation of the 1-adduct or the 3-adduct is immaterial, since each cyclize to form the same intermediate (i.e., radical IIIb).

The aromatic ring-opening mechanisms which best fit the toluene and o-cresol data, when applied to the o-xylene system, yield biacetyl after OH radical addition at the 1- or 2-position, for example:



This is, as noted previously, in accord with the recent observation of significant yields (18 ± 4%) of biacetyl from irradiated NO_x-o-cresol-air systems (Darnall et al., 1979) and the magnitude of the biacetyl yield is then consistent with the mode of $O(^3P)$ atom addition to o-xylene (Grovenstein and Mosher, 1970).

Benzaldehyde Reactions. The reaction of benzaldehyde with OH radicals must, because of the magnitude of the OH radical rate constant (Niki et al., 1978), proceed predominately via H atom abstraction from the substituent CHO group (Hendry et al., 1978; Atkinson et al., 1979; Hendry, 1979) to form the benzoyl radical:



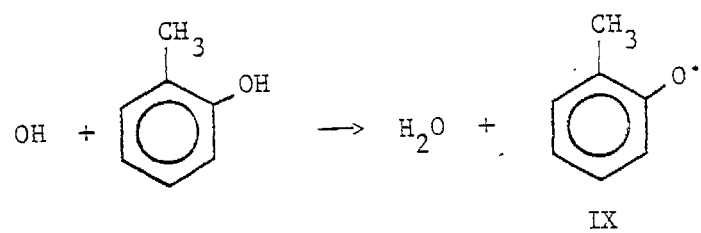
(54)

This C_6H_5CO radical is then expected to add O_2 (reaction 56) to form the peroxybenzoyl radical which can react with NO or NO_2. Reaction with NO_2 (reaction 57) will lead to the formation of peroxybenzoylnitrate (PBzN), which was not observed, but which may have been formed and not detected. PBzN thermally decomposes (Hendry and Kenley, 1979) with an analogous mechanism to PAN (Pate et al., 1976b; Hendry and Kenley, 1977; Cox and Roffey, 1977) to lead to the ultimate formation of, among other products, o- and p-nitrophenols (reactions 58-65) (Niki et al., 1979). Note that in each case the ultimate result of the OH-benzaldehyde reaction is radical termination, which is consistent with these and previously reported observations (Gitchell et al., 1974; Niki et al., 1978; Niki et al., 1979).

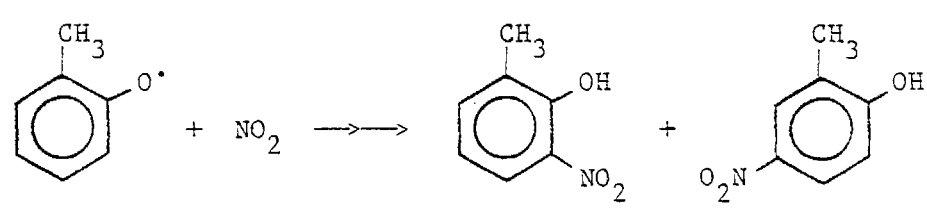
While little is known about benzaldehyde photolysis under atmospheric conditions, its photolysis at rates approximately 5 times greater than that used for the aliphatic aldehydes (Carter et al., 1979) is included in the mechanism to account for the observed benzaldehyde loss rates in the toluene-benzaldehyde runs (see note 20 of Appendix A). As noted previously (see Figure 40), the data are best fit by assuming that benzaldehyde photolysis results in the formation of nonradical products. The most likely pathway would thus appear to be formation of benzene + CO, but although small yields of benzene (~0.5-1 ppb) are indeed observed in the toluene-benzaldehyde runs, the yields are far less than the amounts predicted (50-60 ppb) if it were the major product of benzaldehyde photolysis.

Cresol Reactions. The cresols, represented in this model by o-cresol alone (substantiated to a large extent by the smog chamber data reproduced here), are known to react rapidly with OH radicals (Atkinson et al., 1979; Perry et al., 1977b; Atkinson et al., 1978b), with this reaction being a major cresol loss process under simulated atmospheric conditions (Atkinson et al., 1978b). The slow reaction with O_3 (Atkinson et al., 1978b; Hendry, 1979) has been neglected in the present model since it will contribute $\leq$5-10% of the total cresol loss rate under the experimental conditions employed in the NO_x-toluene-air and NO_x-o-cresol-air irradiations. The irradiated NO_x-o-cresol-air data yields little evidence as to the reaction mechanisms--very little PAN is formed and the major organic products observed are hydroxynitrotoluenes in low (< 5%) yields. The reaction of OH radicals with o-cresol can proceed via OH radical addition to the ring or by H atom abstraction (Atkinson et al., 1979; Perry et al., 1977b).

The abstraction pathway, which accounts for ~8% of the total OH radical reaction (Atkinson et al., 1979), probably proceeds mainly via H atom abstraction from the substituent-OH group, since the abstraction rate constant for o-cresol is a factor of ~4 higher at 400 K than that for toluene (Perry et al., 1977a; 1977b).

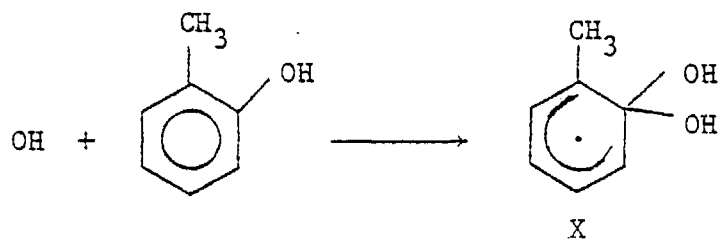


Reactions of NO_2 with radical IX can, by analogy to the phenoxy radical reaction 64 (Niki et al., 1979), lead to formation of the observed hydroxynitrotoluene isomers. This minor H atom abstraction pathway has been



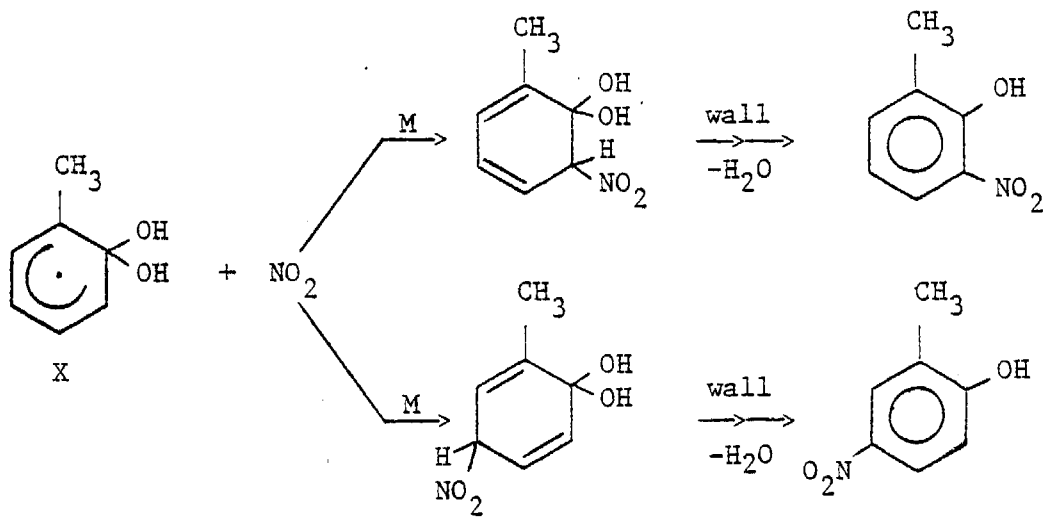
neglected in the model calculations since its inclusion would have an insignificant effect on the calculated time-concentration profiles of the major species.

The major OH radical reaction pathway is in addition to the aromatic ring (Atkinson et al., 1979), and thermochemical calculations (Benson, 1976) show that radical X is the most thermochemically favorable adduct. Its formation is thus assumed to be the sole pathway.

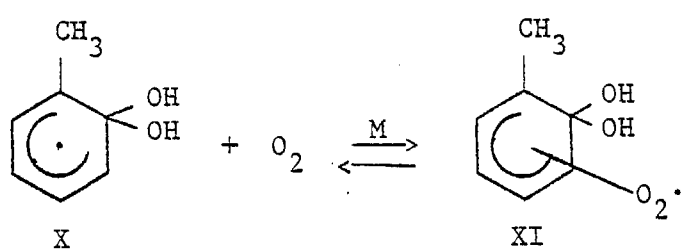


(65)

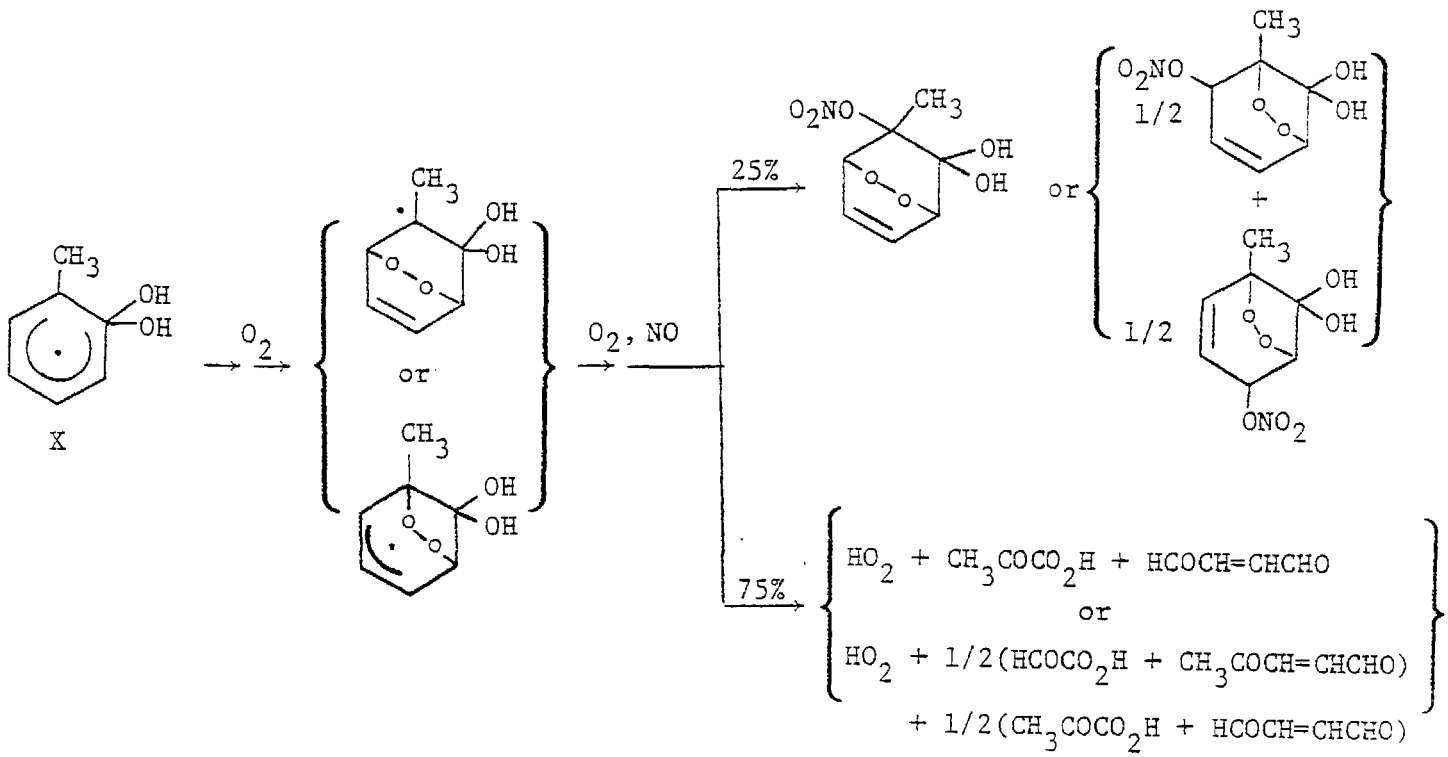
Species such as X can also react with NO_2 to give rise to the observed hydroxynitrotoluene isomers.



However, the dominant reaction of X is expected to be with O_2:



The subsequent reactions of radicals XI are assumed to be analogous to those of radical II formed in the toluene system. The various possible detailed reactions for these species are listed in Appendix B (substituent 1 = OH, 2 = CH_3 for the 1 adduct; substituent 1 = OH, 6 = CH_3 for the 3 adduct), and the overall processes are given in Appendix A as reactions 70-77. The best fit models predict that the major overall processes are as shown below:

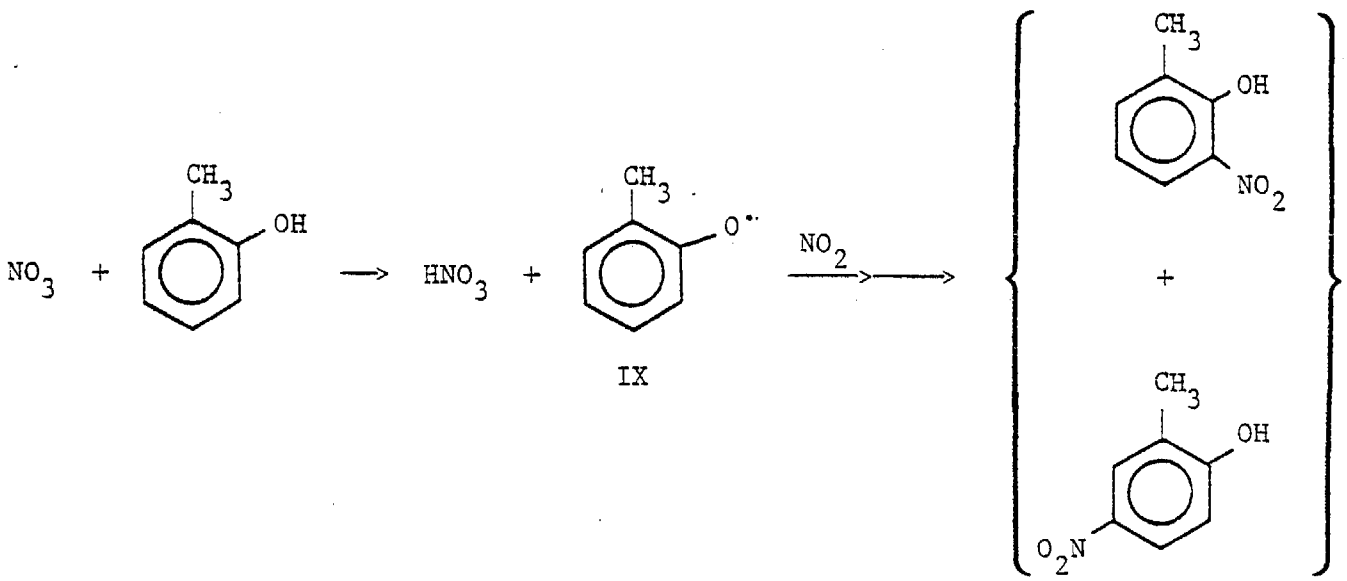


There is evidence that there is an additional significant loss process for cresols in NO_x-air systems. It has been independently observed by O'Brien (1979) and in our laboratories (Carter et al., 1980) that although the cresols do not react at significant rates with either O_3 (Atkinson et al., 1978b; Hendry, 1979; O'Brien, 1979) or NO_2 (O'Brien, 1979; Carter et al., 1980), they do appear to rapidly disappear in chambers dosed with NO_2 and O_3 together. Since O_3 and NO_2 react rapidly to form NO_3 and N_2O_5 (Graham and Johnston, 1978)

$$O_3 + NO_2 \rightarrow NO_3 + O_2 \qquad (5)$$

(10) $$NO_3 + NO_2 \overset{M}{\rightleftarrows} N_2O_5 \qquad (9)$$

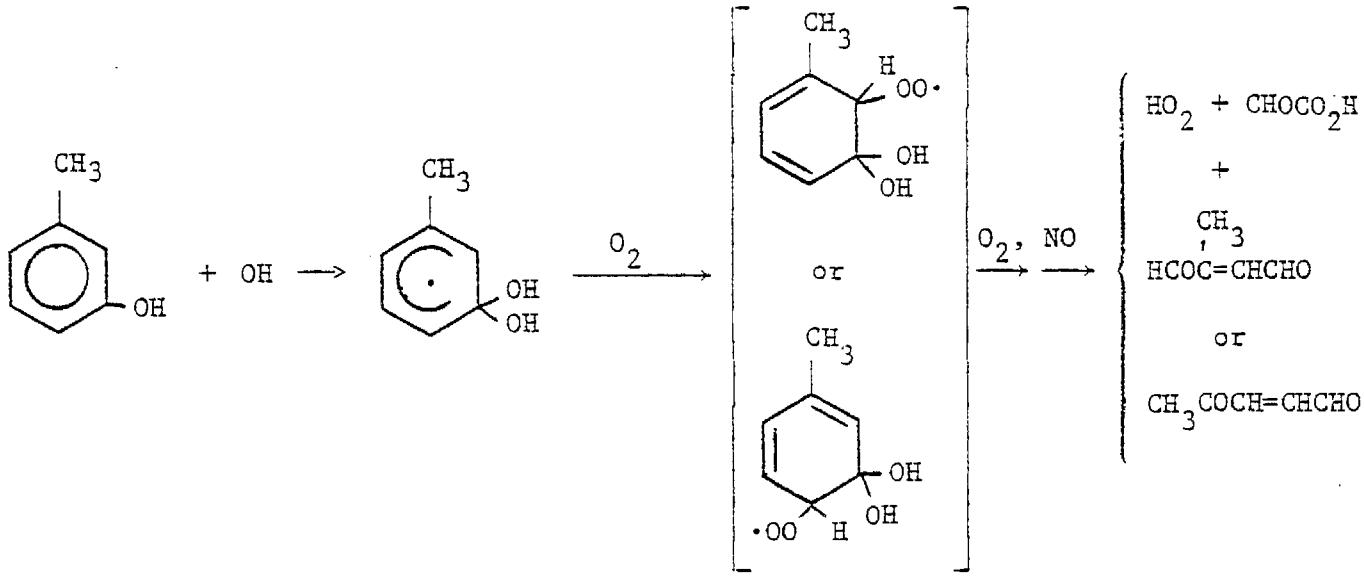
these observations can be attributed to rapid reaction of cresols with either NO_3 or N_2O_5. Since NO_3 is known to react with alkenes (Japar and Niki, 1975), it is probable that it is also NO_3 which is reacting with the cresols. We have recently obtained, using a relative rate technique, a rate constant for the reaction of NO_3 radicals with o-cresol of ~1.5 x 10^{-11} cm^3 $molecule^{-1}$ sec^{-1} (Carter et al., 1980). As can be seen in Figure 43, this rate constant is sufficiently high that reaction with NO_3 becomes a significant sink for o-cresol after O_3 formation begins, and accounts for the rapid decrease in the o-cresol concentrations observed after their initial rise in the toluene-NO_x-air runs. The observation that NO_3 radicals react rapidly with phenol and the cresols, but only very slowly with toluene and methoxybenzene indicates that the reaction with phenol and the cresols proceeds via H atom abstraction from the substituent-OH group to form radical IX (Carter et al., 1980):

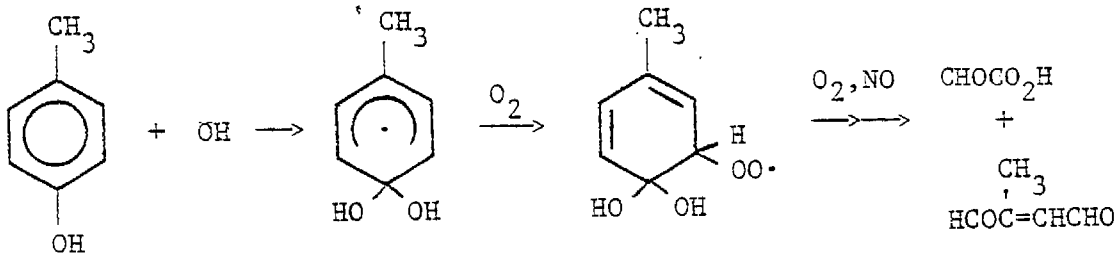


Hence this reaction is another explanation for the formation of the hydroxynitrotoluene isomers observed.

As noted previously, the order of the overall reactivity of the cresol isomers in NO_x-air systems is meta >> para > ortho (see Figure 36). This effect is larger than can be attributed to the relatively small differences in the OH + cresol rate constants (Atkinson et al., 1979; Atkinson et al., 1978b) (meta/ortho = 1.4; para/ortho = 1.1), but it can

readily be rationalized in terms of the mechanism. On the basis of the mechanisms which best fit the toluene-NO_x and the o-cresol-NO_x data, m- and p-cresol are expected to react as shown:





$CHOCO_2H$ formed in the m- and p-cresol systems is expected to be more reactive towards OH radicals than the CH_3COCO_2H formed in the o-cresol system, since it has the labile -CHO group. In addition, both 2-methyl-2-butene-1,4-dial and 2-pentene-1,4-dial are expected to give rise to methylglyoxal, a powerful photoinitiator, in their photooxidation mechanism (see Appendix A, reactions 100-141), which is not formed from the 2-butene-1,4-dial predicted in the o-cresol mechanism (the latter instead forming glyoxal, which is believed to have far lower quantum yields for photodecomposition (see Note 29, Appendix A)). Furthermore, in the m-cresol system, the OH radical may add to a significant extent at the 2-position, since the radical formed is stabilized by both the OH and the $-CH_3$ groups,

unlike analogous adducts for the other cresol isomers. Applying our mechanism this adduct is expected to give rise to methylglyoxal directly, which may explain the far greater reactivity of m-cresol relative to the o- and p-isomers.

Subsequent Reactions of Ring-Opening Products. The subsequent reactions of the ring cleavage products formed in the toluene and the cresol photooxidations are given in Appendix A. In many cases the mechanisms are uncertain and rate constants have had to be estimated; these are discussed in the associated notes. The following points concerning the reactions of these products should be noted:

a) In order for the model to fit the smog chamber data, it must include the formation of radical initiator(s) in the toluene photooxidation mechanism which are not formed in the o-cresol system. The major initiator appears to be methylglyoxal, whose photolysis is also primarily responsible for the observed production of PAN, HCHO, and CH_3ONO_2. No other product predicted by our mechanism is believed to photodecompose to give radicals as rapidly as methylglyoxal (see Notes 20, 29 and 33 in Appendix A for brief discussions of benzaldehyde, glyoxal, and conjugated γ-dicarbonyl photolyses, respectively).

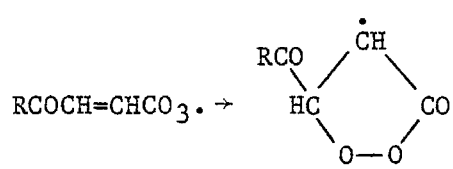
b) There is a significant uncertainty in the photooxidation mechanism of the conjugated γ-dicarbonyls which are predicted to be formed as major products. These products are expected to react predominately with OH radicals, giving rise to unsaturated α-carbonyl peroxy radicals

$$OH + RCOCH{=}CHCHO \rightarrow H_2O + RCHOCH{=}CH\dot{C}O$$

$$RCOCH{=}CH\dot{C}O + O_2 \xrightarrow{M} RCOCH{=}CHCO_3\cdot$$

(XII)

These radicals could react with NO and NO_2 (e.g., reactions 110-113), in a manner analogous to the reactions of acyl peroxy radicals, forming unsaturated PAN analogues such as $HCOCH{=}CHCO_3NO_2$. However, these unsaturated peroxy radicals may also undergo cyclization,



(XII)

resulting in the ultimate formation of glyoxal (R=H) or PAN + methylglyoxal ($R=CH_3$) (see Appendix A). It is not known at the present time whether this cyclization is rapid enough to compete with reaction of (XII) with NO or NO_2. The recent observation of methylvinylketone and methacrolein formation during the early stages (before significant ozone formation) of the NO_x photooxidation of isoprene (Arnts and Gay, 1979) indicates that in the case of the unsaturated alkyl peroxy radicals, (XIII) cyclization is negligible compared to reaction with NO.

$$CH_2{=}CR{-}\overset{OO\cdot}{\overset{|}{C}}R'{-}CH_2OH \qquad (R = H \text{ or } CH_3;\ R' = CH_3 \text{ or } H)$$

(XIII)

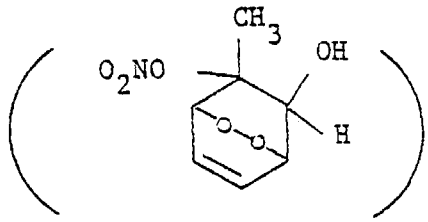
However, it is not clear that the unsaturated acylperoxy radicals such as (XII) formed in this sytem will react analogously, and hence it is necessary to consider both mechanistic options.

As can be seen in Figures 37 and 38, where results of the calculations assuming cyclization of (XII) is rapid, are compared with those assuming it is negligible, (compare Model A with B, C with D, or E with F) the uncertainty concerning the rate of this cyclization has a significant impact on model predictions concerning both the toluene and the cresol systems. It is this uncertainty which does not allow us to distinguish unambiguously whether these data are best fit by assuming [2.2.2] cyclization and predominant 3-addition of O_2 to the OH-aromatic adduct (calculations A), or by assuming [3.2.1] cyclization dominates (calculations F), since the former assumes that cyclization of XII is negligible while the latter assumes it dominates. If the rate of this cyclization were known, one of these mechanisms could probably be eliminated.

Conclusions. The chemical kinetic computer models for irradiated toluene-benzaldehyde-o-cresol-NO_x-air mixtures, which are discussed above and are consistent with available basic kinetic and mechanistic data and with reasonable thermochemical and kinetic estimates, have been shown to be capable of giving predictions of reactant and major and minor product concentration-time profiles which are in reasonably good agreement with results of well-characterized smog chamber irradiations performed with a variety of initial reactant concentrations. However, with the

information available to date, it is not possible to choose between various optional sets of equally reasonable reaction sequences. For example, the experimental data appear to be reasonably well fit by the two sets of mechanistic options discussed above. In addition, in our initial studies it was found that most of the concentration-time profiles, except for those of o-cresol, could be equally well fit by a model giving the same products as A, but assuming that organic nitrate formation from RO_2 + NO occurs ~40% of the time instead of ~25%, providing that fragmentation is increased by decreasing the formation of o-cresol from ~20% to ~8% of the overall reaction, and that the resulting increased production of PAN is compensated by changing the ratio $k(CH_3CO_3 + NO)/k(CH_3CO_3 + NO_2)$ from 1.5 to 2.0, which is within its range of uncertainty (Carter et al., 1979).

These chemical kinetic models predict the formation of products and reactive intermediates in aromatic-NO_x-air photooxidations which have not yet been detected in such systems, and whose atmospheric chemistry is at best poorly characterized. Such products predicted in the toluene system include the α-dicarbonyls glyoxal and methylglyoxal, and the γ-unsaturated dicarbonyls RCOCH=CHCHO (R=H, CH_3) and possibly the corresponding peroxyacyl nitrates $RCOCH{=}CHCO_3NO_2$, together with the alicyclic nitrate which is proposed to be formed from the OH-toluene-O_2 adduct and NO; for example



Furthermore, quantitative rate and mechanistic information is required for: the photolysis of benzaldehyde and the α-carbonyl carboxylic acids, the fraction of the alkyl nitrate from the peroxy radical intermediates in the aromatic photooxidation mechanism, and the general atmospheric chemistry of α-dicarbonyls and γ-unsaturated dicarbonyls.

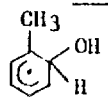
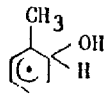
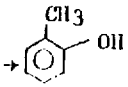
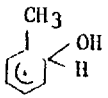
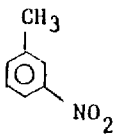
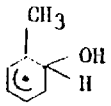
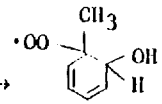
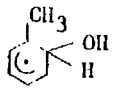
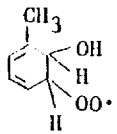
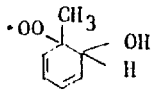
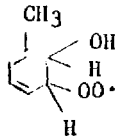
APPENDIX A. Reactions and Rate Constants Used in the NO_x-Toluene-Air Model

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
	I. Inorganic Reactions			
1	$NO_2 + h\nu \rightarrow NO + O(^3P)$	6.6×10^{-3}	1	
2	$O(^3P) + O_2 + M \rightarrow O_3 + M$	5.7×10^{-34}		Hampson & Garvin (1978)
3	$O(^3P) + NO_2 \rightarrow NO + O_2$	9.1×10^{-12}		Hampson & Garvin (1978)
4	$O_3 + NO \rightarrow NO_2 + O_2$	1.8×10^{-14}		Hampson & Garvin (1978)
5	$O_3 + NO_2 \rightarrow NO_3 + O_2$	3.7×10^{-17}		Hampson & Garvin (1978)
6	$NO + NO_3 \rightarrow 2NO_2$	1.9×10^{-11}		Graham & Johnston (1978)
7	$NO_2 + NO_3 \rightarrow NO + NO_2 + O_2$	4.3×10^{-16}		Graham & Johnston (1978)
8	$NO + NO + O_2 \rightarrow 2NO_2$	1.9×10^{-38}		Hampson & Garvin (1978)
9	$NO_2 + NO_3 \rightarrow N_2O_5$	1.9×10^{-12}	2	Graham & Johnston (1978)
10	$N_2O_5 \rightarrow NO_2 + NO_3$	0.15	2,3	Connell & Johnston (1979)
11	$N_2O_5 + H_2O \rightarrow 2HNO_3$	3×10^{-21}	Estimated 4,5	
12	$NO_3 + h\nu \rightarrow NO + O_2$	2.8×10^{-2}	1	Graham & Johnston (1978)
13	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	7.4×10^{-2}	1	Graham & Johnston (1978)
14	$O_3 + h\nu \rightarrow O_2 + O(^3P)$	(2.4×10^{-4})	1	Hampson & Garvin (1978)
15	$O_3 + h\nu \rightarrow O_2 + O(^1D)$	9.8×10^{-6}	1	Hampson & Garvin (1978)
16	$O(^1D) + M \rightarrow O(^3P) + M$	3.0×10^{-11}		Hampson & Garvin (1978) Streit et al. (1976)
17	$O(^1D) + H_2O \rightarrow 2OH$	2.3×10^{-10}		Hampson & Garvin (1978) Streit et al. (1976)
18	$OH + NO \rightarrow HONO$	6.8×10^{-12}	2	Anastasi & Smith (1978) Overend et al. (1976)
19	$OH + NO_2 \rightarrow HNO_3$	1.1×10^{-11}	2	Hampson & Garvin (1978)
20	$HONO + h\nu \rightarrow OH + NO$	1.1×10^{-3}	1	Stockwell & Calvert (1978)
21	$OH + O_3 \rightarrow HO_2 + O_2$	8.5×10^{-14}		Ravishankara et al. (1979)

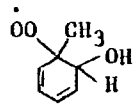
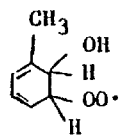
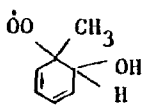
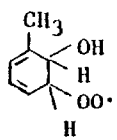
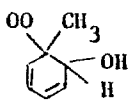
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
22	$HO_2 + O_3 \rightarrow OH + 2O_2$	2.1×10^{-15}		Zahniser & Howard (1978)
23	$HO_2 + NO \rightarrow OH + NO_2$	8.1×10^{-12}		Howard & Evenson (1977) Hampson & Garvin (1978)
24	$HO_2 + NO_2 \rightarrow HO_2NO_2$	1.2×10^{-12}	2	Graham et al. (1977)
25	$HO_2NO_2 \rightarrow HO_2 + NO_2$	0.15	2	Graham et al. (1977)
26	$HO_2 + NO_3 \rightarrow HNO_3 + O_2$	3×10^{-12}	Estimated 6	
27	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	2.5×10^{-12}		Hampson & Garvin (1978) Hamilton & Lii (1977)
28	$HO_2 + HO_2 + H_2O \rightarrow H_2O_2 + O_2 + H_2O$	6.5×10^{-30}	7	Hamilton & Lii (1977)
29	$H_2O_2 + h\nu \rightarrow 2OH$	4.7×10^{-6}	1	
30	$OH + CO \rightarrow CO_2 + H$	3.0×10^{-13}	2	Hampson & Garvin (1978)
31	$H + O_2 + M \rightarrow HO_2 + M$	Fast		
32	$O_3 \longrightarrow$ wall	2.8×10^{-5}	5	Pitts et al. (1977)
33	$H_2O_2 \longrightarrow$ wall	7.0×10^{-5}	5	Pitts et al. (1977)
34	$? + h\nu \longrightarrow OH$	$(6\text{-}24) \times 10^{7}$	5,8	Carter et al. (1979)
	II. <u>Toluene Photooxidation Reactions</u>			
	A. <u>Abstraction</u>			
35	$OH + \text{toluene} \rightarrow C_6H_5\dot{C}H_2 + H_2O$	1.0×10^{-12}		Perry et al. (1977a) Kenley et al. (1978)
36	$C_6H_5\dot{C}H_2 + O_2 \rightarrow C_6H_5CH_2\dot{O}_2$	Fast		
37	$C_6H_5CH_2\dot{O}_2 + NO \rightarrow C_6H_5CH_2\dot{O} + NO_2$	6×10^{-12}	Ratio adjusted 9	
38	$C_6H_5CH_2\dot{O}_2 + NO \xrightarrow{M} C_6H_5CH_2ONO_2$	2×10^{-12}		
39	$C_6H_5CH_2\dot{O} + O_2 \rightarrow C_6H_5CHO + HO_2$	1.2×10^{-15}	6	
40	$C_6H_5CH_2\dot{O} + NO_2 \xrightarrow{M} C_6H_5ONO_2$	1.6×10^{-11}	6	

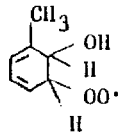
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
	B. Addition			
41	OH + toluene → 	5.4×10^{-12}	10	Perry et al. (1977a) Kenley et al. (1978)
42	 + O_2 →  + HO_2	1.2×10^{-15}	11	
43	 + NO_2 →  + H_2O	5.2×10^{-12}	12	Kenley et al. (1978)
44	 + O_2 $\xrightarrow{M}$ 	(Slow) Mech. A,B only 3.5×10^{-15} (Mech. C,D; (adjusted))	2,13	
45	 + O_2 $\xrightarrow{M}$ 	3.5×10^{-15} (Mech. A,B; (adjusted)) (Slow) Mech. C,D only	2,13	
46[c]	 $\xrightarrow{NO}$ $\xrightarrow{O_2}$ $0.75(HO_2 + (CHO)_2 + CH_3COCH{=}CHCHO + NO_2)$ + $0.25\ C_7ONO_2$	(Slow) Mech. A,B,E-H Fast Mech. C,D	14,15	
47[c]	 $\xrightarrow{NO}$ $\xrightarrow{O_2}$ $0.75(HO_2 + CH_3COCHO + HCOCH{=}CHCHO + NO_2)$ + $0.25\ C_7ONO_2$	Fast Mech. A,B (Slow) Mech. C-H	15,16	

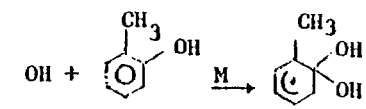
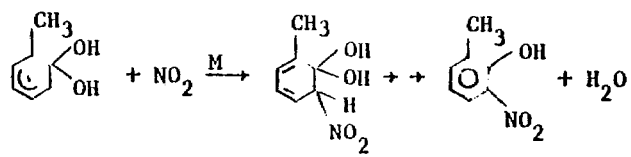
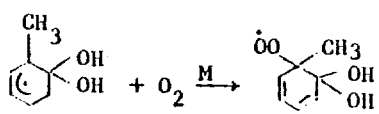
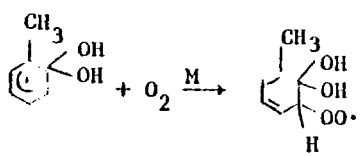
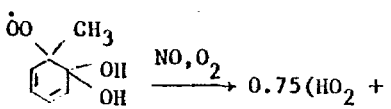
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
48[c]	 $\xrightarrow{NO,O_2}$ 0.75(HO_2 + 1/2$(CHO)_2$ + 1/2 CH_3COCHO + 1/2 HCOCH=CHCHO + 1/2 CH_3COCH=CHCHO + NO_2) + 0.25 C_7ONO_2	(Slow) Mech. A-E,G,H Fast Mech. E,F	14,17	
49[c]	 $\xrightarrow{NO,O_2}$ 0.75(HO_2 + 1/2$(CHO)_2$ + 1/2 CH_3COCHO + 1/2 HCOCH=CHCHO + 1/2 CH_3COCH=CHCHO + NO_2) + 0.25 C_7ONO_2	(Slow) Mech. A-E,G,H Fast Mech. E,F	16,17	
50[c]	 $\xrightarrow{NO,O_2}$ 0.75(HCO + $(CHO)_2$ + $CH_3COCHOHCHO$ + NO_2) + 0.25 C_7ONO_2	(Slow) Mech. A-F,H Fast Mech. G	14,18	
51[c]	 $\xrightarrow{NO,O_2}$ 0.75(HCO + $(CHO)_2$ + $CH_3COCHOHCHO$ + NO_2) + 0.25 C_7ONO_2	(Slow) Mech. A-F,H Fast Mech. G	16,18	
52[c]	 $\xrightarrow{NO,O_2}$ 0.75(HO_2 + 2$(CHO)_2$ + CH_3COCHO + NO_2) + 0.25 C_7ONO_2	(Slow) Mech. A-G Fast Mech. H	14,19	

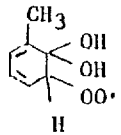
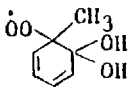
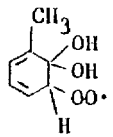
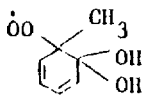
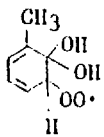
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]		Notes	References
53[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + 2(CHO)_2 + CH_3COCHO + NO_2)$ + $0.25\ C_7ONO_2$	(Slow) Fast	Mech. A-G Mech. H	14,19	
	III. Organic Product Photooxidations				
	A. Benzaldehyde				
54	$OH + C_6H_5CHO \rightarrow H_2O + C_6H_5CO$	1.3×10^{-11}			Niki et al. (1978) Atkinson et al. (1979)
55	$C_6H_5CHO + h\nu \rightarrow$ Products	3×10^{-5}	Adjusted	20	
56	$C_6H_5\dot{C}O + O_2 \rightarrow C_6H_5C\dot{O}_3$	Fast			
57	$C_6H_5C\dot{O}_3 + NO_2 \xrightarrow{M} C_6H_5CO_3NO_2$	5×10^{-12}		21	
58	$C_6H_5CO_3NO_2 \rightarrow C_6H_5C\dot{O}_3 + NO_2$	3.3×10^{-4}			Hendry & Kenley (1979)
59	$C_6H_5C\dot{O}_3 + NO \rightarrow C_6H_5C\dot{O}_2 + NO_2$	8×10^{-12}		21	
60	$C_6H_5C\dot{O}_2 \rightarrow C_6H_5^{\cdot} + CO_2$	Fast		6	
61	$C_6H_5^{\cdot} + O_2 \xrightarrow{M} C_6H_5\dot{O}_2$	Fast			
62	$C_6H_5\dot{O}_2 + NO \rightarrow C_6H_5\dot{O} + NO_2$	6×10^{-12}	Ratio adjusted	9	
63	$C_6H_5\dot{O}_2 + NO \xrightarrow{M} C_6H_5ONO_2$	2×10^{-12}			

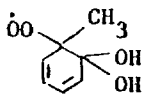
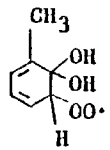
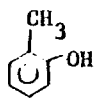
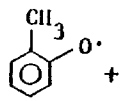
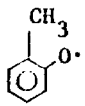
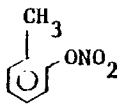
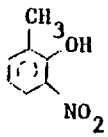
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
64	$C_6H_5O\cdot + NO_2 \xrightarrow{M} C_6H_5(OH)NO_2$ (o- and p-)	1.6×10^{-11}	6	Niki et al. (1979)
65	$C_6H_5O\cdot + HO_2 \rightarrow C_6H_5OH + O_2$	3×10^{-12}	22	
	B. <u>O-Cresol</u>			
66		4.7×10^{-11}	23	Atkinson et al. (1978b)
67		5.2×10^{-12}	24	
68		(Slow) Mech. A,B only; 3.5×10^{-15} Mech. C,D; (adjusted)	2,25	
69		3.5×10^{-15} Mech. A,B; (adjusted); (Slow) Mech. C,D only	2,25	
70[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + HOCOCHO + CH_3COCH{=}CHCHO + NO_2)$ $+ 0.25\ C_7ONO_2$	(Slow) Mech. A,B,E-H; Fast Mech. C,D	15,26	

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
71[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + HOCOCOCH_3 + HCOCH{=}CHCHO + NO_2) + 0.25\ C_7ONO_2$	(Fast Mech. A,B; (Slow) Mech. C-H)	15,27	
72[2]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + 1/2\ HOCOCHO + 1/2\ HOCOCOCH_3 + 1/2\ HCOCH{=}CHCHO + 1/2\ CH_3COCH{=}CHCHO + NO_2) + 0.25\ C_7ONO_2$	((Slow) Mech. A-E,G,H; Fast Mech. E,F)	17,26	
73[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + 1/2\ HOCOCHO + 1/2\ HOCOCOCH_3 + 1/2\ HOCOCH{=}CHCHO + 1/2\ CH_3COCH{=}CHCHO + NO_2) + 0.25\ C_7ONO_2$	((Slow) Mech. A-E,G,H; Fast Mech. E,F)	17,27	
74[c]	 $\xrightarrow{NO,O_2}$ $0.75(H\dot{C}O + (CHO)_2 + CH_3COC(OH)_2CHO + NO_2) + 0.25\ C_7ONO_2$	((Slow) Mech. A-F,H; Fast Mech. G)	18,26	
75[c]	 $\xrightarrow{NO,O_2}$ $0.75(H\dot{C}O + (CHO)_2 + CH_3COC(OH)_2CHO + NO_2) + 0.25\ C_7ONO_2$	((Slow) Mech. A-F,H; Fast Mech. G)	18,27	

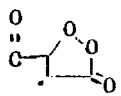
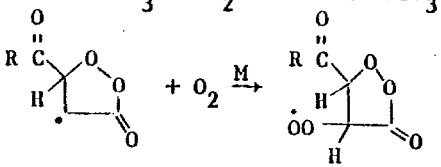
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
76[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + 3/2(CHO)_2 + 1/2\ CH_3COCHO + 1/2\ HOCO\ CHO + 1/2\ HOCOCOCH_3 + NO_2) + 0.25\ C_7ONO_2$	(Slow) Mech. A-G Fast Mech. H	19,26	
77[c]	 $\xrightarrow{NO,O_2}$ $0.75(HO_2 + 3/2(CHO)_2 + 1/2\ CH_3COCHO + 1/2\ HOCOCHO + 1/2\ HOCOCOCH_3 + NO_2) + 0.25\ C_7ONO_2$	(Slow) Mech. A-G Fast Mech. H	19,27	
78	NO_3 +  $\rightarrow$  + HNO_3	1.5×10^{-11}	28	Carter et al. (1979)
79	 + NO_2 $\xrightarrow{M}$  or 	1.6×10^{-11}	6	
	C. Glyoxal			
80	$(CHO)_2 + h\nu \rightarrow$ Products	(Slow)	29	
81	$OH + (CHO)_2 \rightarrow H_2O + HCO\dot{C}O$	2×10^{-11}	30	
82	$HCOCO \rightarrow H\dot{C}O + CO$	Fast		

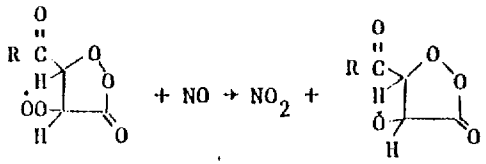
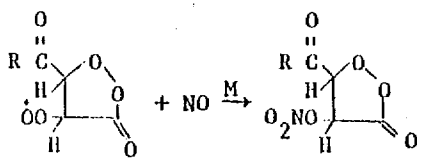
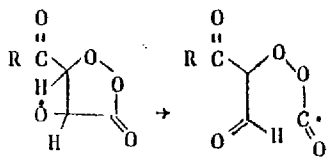
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
83	$HCO + O_2 \rightarrow HO_2 + CO$	5.6×10^{-12}		Washida et al. (1974) Shibuya et al. (1977)
	D. Methyl Glyoxal (And its Products)			
84	$CH_3COCHO + h\nu \rightarrow CH_3\dot{C}O + HCO$	1.0×10^{-3}	1,6	
85	$OH + CH_3COCHO \rightarrow H_2O + CH_3CO\dot{C}O$	1.6×10^{-11}	30	
86	$CH_3CO\dot{C}O \rightarrow CH_3\dot{C}O + CO$	Fast	6	
87	$CH_3\dot{C}O + O_2 \rightarrow CH_3C\dot{O}_3$	Fast	6	
88	$CH_3C\dot{O}_3 + NO \rightarrow CH_3C\dot{O}_2 + NO_2$	8×10^{-12}	21	
89	$CH_3C\dot{O}_3 + NO_2 \rightarrow CH_3CO_3NO_2$	5×10^{-12}	21	
90	$CH_3CO_3NO_2 \rightarrow CH_3C\dot{O}_3 + NO_2$	8.0×10^{-4}		Hendry & Kenley (1977) Cox & Roffey (1977)
91	$CH_3C\dot{O}_2 \rightarrow CH_3^{\bullet} + CO_2$	Fast	6	
92	$CH_3^{\bullet} + O_2 \rightarrow CH_3\dot{O}_2$	Fast		
93	$CH_3\dot{O}_2 + NO \rightarrow CH_3\dot{O} + NO_2$	8×10^{-12}	9	
94	$CH_3\dot{O} + NO_2 \rightarrow CH_3ONO_2$	1.3×10^{-11}	6	
95	$CH_3\dot{O} + NO_2 \rightarrow HCHO + HONO$	2.1×10^{-12}	6	

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
96	$CH_3\dot{O} + O_2 \rightarrow HCHO + HO_2$	1.2×10^{-15}	6	
97	$HCHO + h\nu \rightarrow H + HCO$	1.5×10^{-5}	1	Horowitz & Calvert (1978)
98	$HCHO + h\nu \rightarrow H_2 + CO$	4.1×10^{-5}		
99	$OH + HCHO \rightarrow H_2O + \dot{H}CO$	9.4×10^{-12}		Atkinson & Pitts (1978)
	E. Conjugated α-Dicarbonyls			
100	$OH + HCHO{=}CHCHO \rightarrow H_2O + HCOCH{=}CH\dot{C}O$	3×10^{-11}	30,31	
101	$OH + CH_3COCH{=}CHCHO \rightarrow H_2O + CH_3COCH{=}CH\dot{C}O$	1.6×10^{-11}	30,31	
102,103[d]	$O_3 + RCOCH{=}CHCHO \rightarrow$ Products	(Slow)	32	
104,105[d]	$RCOCH{=}CHCHO + h\nu \rightarrow$ Products	(Slow)	33	
106,107[d]	$RCOCH{=}CH\dot{C}O + O_2 \xrightarrow{M} RCOCH{=}CH\dot{C}O_3$	Fast		
108,109[d]	$RCOCH{=}CH\dot{C}O_3 \rightarrow$ 	(Slow) Mech. A,C,E Fast Mech. B,D,F	34	
110,111[d]	$RCOCH{=}CH\dot{C}O_3 + NO \rightarrow NO_2 + RCOCH{=}CH\dot{C}O_2$	8×10^{-12}	21	
112,113[d]	$RCOCH{=}CH\dot{C}O_3 + NO_2 \xrightarrow{M} RCOCH{=}CHCO_3NO_2$	5×10^{-12}	21	
114,115[d]		Fast		

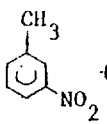
APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
116,117[d]		7×10^{-12}	9,35	
118,119[d]		8×10^{-13}		
120,121[d]	 $\rightarrow$ RCOCH(O·)CHO + CO_2	Fast		
122	HCOCH(O·)CHO $\rightarrow$ H$\dot{C}$O + $(CHO)_2$	Fast	6	
123	CH_3COCH(O·)CHO $\rightarrow$ 1/2($CH_3\dot{C}O$ + $(CHO)_2$) + 1/2 (CH_3COCHO + H$\dot{C}$O)	Fast	6	
124,125[d]	RCOCH=CH$\dot{O}_2$ $\rightarrow$ RCOCH=$\dot{C}$H + CO_2	Fast	6	
126,127[d]	RCOCH=$\dot{C}$H + O_2 $\xrightarrow{M}$ RCOCH=CHO_2·	Fast		
128,129[d]	RCOCH=CH$\dot{O}_2$ + NO $\rightarrow$ NO_2 + RCOCH=CHO· $\leftrightarrow$ RCO$\dot{C}$HCHO	7×10^{-12}	9,35	
130,131[d]	RCOCH=CHO_2· + NO $\xrightarrow{M}$ RCOCH=CHONO_2	8×10^{-13}		
132,133[d]	RCO$\dot{C}$HCHO + O_2 $\xrightarrow{M}$ RCOCH(O_2·)CHO	Fast		

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
134,135[d]	$RCOCH(O_2\cdot)CHO + NO \rightarrow RCOCH(O\cdot)CHO + NO_2$	7×10^{-12}	9,35	
136,137[d]	$RCOCH(O_2\cdot)CHO + NO \xrightarrow{M} RCOCH(ONO_2)CHO$	8×10^{-13}		
138	$HCOCH(O\cdot)CHO \rightarrow (CHO)_2 + H\dot{C}O$	Fast	6	
139	$CH_3COCH(O\cdot)CHO \rightarrow 1/2(CH_3\dot{C}O + (CHO)_2)$ $+ 1/2\ (HCO + CH_3COCHO)$	Fast	6	
140,141[d]	$RCOCH{=}CHCO_3NO_2 \rightarrow RCOCH{=}CHCO_3 + NO_2$	8.0×10^{-4}	36	
	F. <u>β-Hydroxy-β-Dicarbonyls</u>			
142	$CH_3COCH(OH)CHO + OH \rightarrow CH_3CO\dot{C}(OH)CHO + H_2O$	6×10^{-12}	37	
143	$CH_3CO\dot{C}(OH)CHO + O_2 \rightarrow HO_2 + CH_3COCOCHO$	Fast	38	
144	$CH_3COCOCHO \rightarrow CH_3COCHO + CO$	Fast		
145,146[e]	$CH_3COCX(OH)CHO + OH \rightarrow CH_3COCX(OH)\dot{C}O$	1.6×10^{-11}	30	
147,148[e]	$CH_3COCX(OH)\dot{C}O + O_2 \xrightarrow{M} CH_3COCX(OH)C\dot{O}_3$	Fast		
149,150[e]	$CH_3COCX(OH)C\dot{O}_3 + NO \rightarrow CH_3COCX(OH)C\dot{O}_2$	8×10^{-12}	21	
151,152[e]	$CH_3COCX(OH)CO_3 + NO_2 \rightarrow CH_3COCX(OH)CO_3NO_2$	5×10^{-12}	21	
153,154[e]	$CH_3COCX(OH)C\dot{O}_2 \rightarrow CH_3CO\dot{C}XOH + CO_2$	Fast	6	
155,156[e]	$CH_3CO\dot{C}XOH + O_2 \rightarrow HO_2 + CH_3COCOX$	Fast	38	
157,158[e]	$CH_3COCX(OH)CO_3NO_2 \rightarrow CH_3COCX(OH)C\dot{O}_3 + NO_2$	8.0×10^{-4}	36	

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes	References
	G. α-Carbonyl Acids			
159	$HOCOCHO + OH \rightarrow HOCO\dot{C}O + H_2O$	1.6×10^{-11}	30	
160	$HOCO\dot{C}O \rightarrow HO\dot{C}O + CO$	Fast		
161	$HO\dot{C}O + O_2 \rightarrow HO_2 + CO_2$	Fast		
162,163[d]	$HOCOCOR + h\nu \rightarrow$ Products	(Slow)	39	
164	 $+ OH \rightarrow$ Products $+ HO_2$	$\sim 6 \times 10^{-12}$	40	
	IV. Hydroperoxides			
165	$RO_2{}^f + HO_2 \rightarrow RO_2H + O_2$	3×10^{-12}	6	
166	$RO_2H^f + h\nu \rightarrow OH + HO_2 +$ Products	5×10^{-6}	6	

[a]Rate constants are given for the conditions of the smog chamber runs listed in Table 1 (303 K, 735 torr, M=air). Photolysis rate constants are given for the light intensity and spectral distributions associated with runs 327-340 (Pitts et al., 1979b); photolysis rates for runs 266-281 are somewhat lower.

[b]First order reaction: sec^{-1}; 2nd order reaction: cm^3 $molecule^{-1}$ sec^{-1}; 3rd order reaction: cm^6 $molecule^{-2}$ sec^{-1}. Zero order reaction (reaction 34 only) molecule cm^{-3} sec^{-1}. "Fast" means that the reaction is the sole pathway for that particular species; the predictions are insensitive for the actual rate constant. "(Slow)", or rate constants given in parentheses mean that the reaction is assumed to be negligible or that the reaction has a negligible effect on the predictions of the model for the concentration regimes studied here.

[c]The reaction as written represents an overall process for which the detailed reactions involved are given in Appendix B.

[d]Reaction numbers refer to R = -H or $-CH_3$, respectively.

[e]Reaction numbers refer to X = -H or X = -OH, respectively.

[f]"RO_2" refers to all radicals of the form RO_2 or RCO_3 in the mechanism. RO_2H is treated as a single species.

Notes

1. k_1 was determined from the photolysis of NO_2 in N_2 (Pitts et al., 1979b; Darnall et al., 1979; Holmes et al., 1973). All other photolysis rate constants were derived as described previously (Carter et al., 1979) from the absorption coefficients of the photolyzing species, the quantum yields, and the relative spectral distribution of the photolysis light (Pitts et al., 1979b).
2. The rate constant is pressure dependent and is given for 1 atmosphere of air.
3. k_9 was derived from the equilibrium constant of Graham and Johnston (1978) combined with the N_2O_5 decomposition rate constant, k_{10}, derived by interpolating the data of Connell and Johnston (1979), which was reported at various N_2 number densities, to 760 torr of N_2.
4. Value consistent with that required for the NO_x-n-butane-propene-air system (Carter et al., 1979), and is also consistent with the gas phase upper limit of $k_{11} \leq 1.3 \times 10^{-20}$ cm^3 $molecule^{-1}$ sec^{-1} obtained by Morris and Niki (1973).
5. Value given is specific for the SAPRC evacuable chamber.
6. Based on the assignment or estimate of Carter et al. (1979) for the same or for analogous reactions.
7. Pseudo-third order reaction added to account for the observed effects of humidity on this reaction (Hamilton and Lii, 1977). k_{28} was calculated to be consistent with the data of Hamilton and Lii (1977) and the $HO_2 \cdot H_2O$ equilibrium constant calcuated by Hamilton and Naleway (1976).
8. Reaction 34 is required in the model to account for the excess radical initiation associated with all of our smog chamber experiments (Carter et al., 1979; Hendry et al., 1978). In modeling our NO_x-propene and/or n-butane-air chamber runs (Carter et al., 1979), we found that the values of k_{34} required for calculations to fit the data generally depended on initial NO, NO_2, and humidity values. Based on these correlations (Carter et al., 1979; Carter, 1977-1978) the following values of k_{34} have been assigned: $k_{34} \cong 0.2$ ppb min^{-1} for run 273; 0.3 ppb min^{-1} for runs 271 and 281; and 0.4 ppb min^{-1} for runs 266, 269, 293, 339, and 340.

9. The total RO_2 + NO rate constant used was assumed to be equal to that for the CH_3O_2 + NO rate constant k_{93}. Recently, Plumb et al. (1979) obtained a value of $k_{93} = (8 \pm 2) \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1} at room temperature, Adachi and Basco (1979) obtained $k_{93} = (3.0 \pm 0.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1} and Cox and Tyndall (1979) obtained $(6.5 \pm 2.0) \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1}. Since Adachi and Basco (1979) may have had problems with the product CH_3ONO in their u.v. absorption system, and since HO_2 formed from HCO + O_2 may have caused problems in the study of Plumb et al. (1979), the data to date are ambiguous. We have used a value of k_{93} of 8×10^{-12} cm^3 $molecule^{-1}$ sec^{-1}, identical to that for the reaction of HO_2 radicals with NO, and consistent with the above-mentioned rate constant studies. The relative rates of alkoxy formation vs. alkyl nitrate formation are unknown for these systems, but based on the results of Darnall et al. (1976), alkyl nitrate formation probably occurs at least 10% of the time in C_{5+} systems. For these calculations the efficiency of alkyl nitrate formation was assumed to be the same for all C_6 and C_7 peroxy radicals, and the best fits to the data are obtained when ~25% alkyl nitrate formation is assumed. These reactions have also been discussed by Hoshino et al. (1978).

10. Ortho addition is assumed to predominate, based on experimental product data (Kenley et al., 1978; Hoshino et al., 1978; Grosjean et al., 1978), and results of the analogous addition of $O(^3P)$ atoms to toluene (Jones and Cvetanovic, 1961; Grovenstein and Mosher, 1970; Gaffney et al., 1976).

11. Reaction 42 is assumed to have the same rate constant as RCH_2O + O_2 RCHO + HO_2 (e.g., reaction 96) since they have similar exothermicities (Benson, 1976) and probably have similar transition states.

12. Derived from k_{42} and the k_{42}/k_{43} ratio of Kenley et al., (1978). However, the nitrotoluene yields would be better fit if $k_{43}/(k_{42} + k_{43} + k_{44} + k_{45})$ is a factor of ~10 higher.

13. The total rate constant of O_2 addition to the toluene-OH adduct was the same for all mechanisms considered, and was adjusted to fit the observed maximum cresol yields in the runs modeled. Since the OH-aromatic-O_2 adduct can back-decompose to the O_2 + the OH-aromatic

adduct (Atkinson et al., 1979) or cyclize, this rate constant is a composite of k(O_2 + OH-aromatic-adduct) x k(cyclization)/k(back-decomposition). Since k(O_2 + OH-aromatic-adduct) is expected, by analogy with other alkyl radicals, to be ~10^{-12} cm^3 $molecule^{-1}$ sec^{-1} (Hampson and Garvin, 1978), this implies that the ratio of dissociation/cyclization for the OH-aromatic-O_2 adduct is ~300. This means that the OH-aromatic adduct and the OH-aromatic-O_2 adduct are probably essentially in equilibrium under atmospheric conditions.

14. Detailed reactions shown in Appendix B for substituent 2 = CH_3, 1,3-6 = H.
15. The overall reaction occurs as shown if [2.2.2] cyclization predominates and re-cyclization is negligible (reactions 1′-6′ in Appendix B). $k_3'/(k_3' + k_4')$ is assumed to be 0.75.
16. Detailed reactions shown in Appendix B for substituent 6 = CH_3, 1-4 = H.
17. The reaction occurs as shown if [3.2.1] cyclization predominates and re-cyclization is negligible (reactions 7′-15′, 6′ in Appendix B). $k_9'/(k_9' + k_{10}') = k_{11}'/(k_{11}' + k_{12}')$ is assumed to be 0.75.
18. The reaction occurs as shown if re-cyclization predominates and if β-scission of α-carbonyl, β-hydroxy alkoxy radicals results primarily in formation of carbonyl radicals. The same products are formed regardless of whether [3.2.1] or [2.2.2] cyclization predominates (reactions 1′, 2′, 7′, 8′, 16′-32′). $k_{21}'/(k_{21}' + k_{22}') = k_{23}'/(k_{23}' + k_{24}')$ is assumed to be 0.75.
19. The reaction occurs as shown if re-cyclization predominates and if β-scission of α-carbonyl, β-hydroxy alkoxy radicals results primarily in formation of α-hydroxy radicals. The same products are formed regardless of whether [3.2.1] or [2.2.2] cyclization predominates (reactions 1′, 2′, 7′, 8′, 16′-30′, 33′, 34′, 6′, 14′). $k_{21}'/(k_{21}' + k_{22}') = k_{23}'/(k_{23}' + k_{24}')$ is assumed to be 0.75.
20. Estimated from the observed disappearance rates of benzaldehyde in runs 337 and 339, after correcting for reaction of benzaldehyde with OH (Atkinson et al., 1979; Niki et al., 1978) and for benzaldehyde formation from OH + toluene (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978). The hydroxyl radical concentrations were estimated using the toluene disappearance rates, and the OH + toluene rate constant (Atkinson et al., 1979; Perry et al., 1977a).

It is necessary to assume formation of nonradical products, or the overall reactivities of runs 337 and 339 are overpredicted.

21. RCO_3 is assumed to react with NO with the same rate constant as CH_3O_2 (see note 9). The $k(RCO_3 + NO)/k(RCO_3 + NO_2)$ ratio assigned by Carter et al. (1979) was used.

22. Assumed to occur with the same rate constant as that assigned for RO_2 + HO_2 and $NO_3 + HO_2$ (Carter et al., 1979).

23. OH addition as shown is estimated (Benson, 1976) to be at least 3-7 kcal $mole^{-1}$ more thermochemically favorable than addition at any other position, and is therefore assumed to predominate. Additionally, OH radical addition at this position yields the hydroxy nitrotoluene isomers observed for the different cresol isomers.

24. Assumed to have same rate constant as assigned for reaction 43 (see note 12).

25. Assumed to be analogous to O_3 addition to the OH-toluene adduct, i.e., $k_{68} = k_{44}$ and $k_{69} = k_{45}$ (see note 13).

26. Detailed reaction shown in Appendix B for substituent 1 = OH, 2 = CH_3, 3, 4, and 6 = H.

27. Detailed reactions shown in Appendix B for substituent 1 = OH, 6 = CH_3, 2-5 = H.

28. Included in the mechanism to account for the observed rapid disappearance of cresols in the presence of $O_3 + NO_2$ (O'Brien, 1979; Carter et al., 1980), and the loss of cresol formed in NO_x-toluene-air runs following NO consumption. The rate constant was derived from subsidiary experiments (Carter et al., 1980). The mechanism is speculative, but its major feature is that net radical formation does not occur, since mechanisms which assume that NO_3 + cresol gives radicals result in significant overprediction of reactivity in NO_x-cresol-air runs.

29. Although glyoxal has large absorption coefficients in the 340-460 nm wavelength region (Calvert and Pitts, 1966) where the intensity of the photolyzing light is high, it appears to have low photodecomposition quantum yields at atmospheric pressure (Calvert and Pitts, 1966).

30. Assumed to react with a similar rate constant as other aldehydes (Atkinson et al., 1979).

31. This mechanism is assumed to be primarily H abstraction as shown

since OH radical addition to the double bond would be anticipated, by analogy with the reaction of $O(^3P)$ atom with acrolein and crotonaldehyde (Gaffney et al., 1975) [when compared to $O(^3P)$ and OH + ethene (Atkinson et al., 1979; Hampson and Garvin, 1978)] to have a rate constant of $<5 \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1}.

32. O_3 addition to the double bond is anticipated to be slow, by analogy with the reaction of $O(^3P)$ atoms with acrolein and crotonaldehyde (Gaffney et al., 1975) when compared to ethene (Atkinson et al., 1979; Hampson and Garvin, 1978).

33. The photochemistry of these species assumed to be analogous to that of acrolein and crotonaldehyde (Calvert and Pitts, 1966) which are believed to be photochemically stable under atmospheric conditions.

34. These initial additions to the double bond are estimated to be exothermic by ~3 kcal $mole^{-1}$. If the estimates of Demerjian et al. (1974) (assuming an A factor of $10^{11.5}$ sec^{-1} and an activation energy of 11 kcal $mole^{-1}$) are correct, these reactions should dominate over competing processes. However, if their activation energy estimate is low by ≥ 5 kcal $mole^{-1}$, which is within the uncertainty range of their estimation, the reaction would be expected to be unimportant.

35. Nitrate formation is arbitrarily assumed to occur ~10% of the time, based on results for C_4 and C_5 alkyl radicals (Darnall et al., 1976).

36. Assumed to decompose with the same rate constant as peroxyacetylnitrate (PAN) (Hendry and Kenley, 1977; Cox and Roffey, 1977).

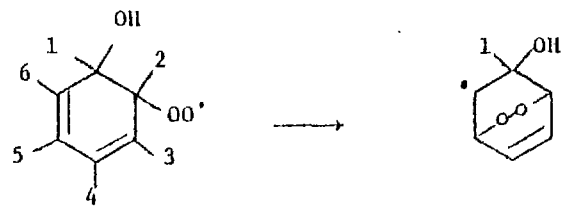
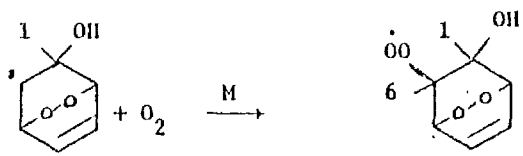
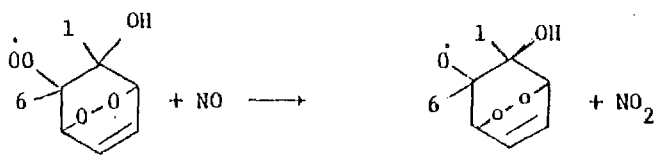
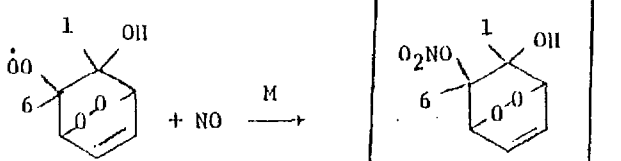
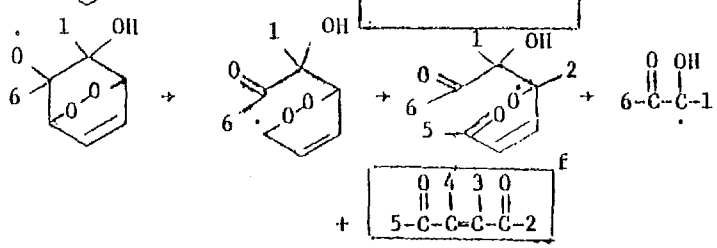
37. Assumed to occur with the same rate constant as OH + isopropanol (Atkinson et al., 1979).

38. Reaction with O_2 forming HO_2 and carbonyls has been shown to be the primary fate of α-hydroxy radicals in air [Carter et al., J. Phys. Chem. 83, 2305 (1979)].

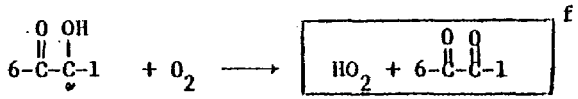
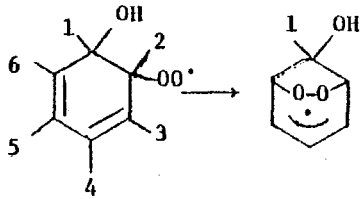
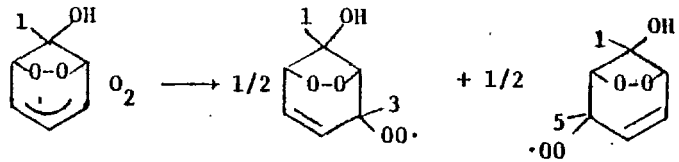
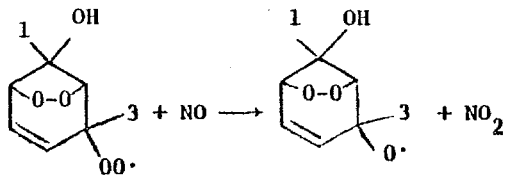
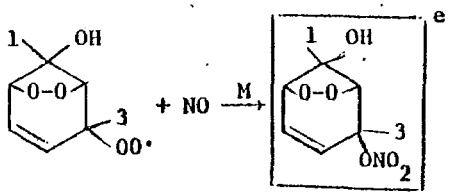
39. The rates of photolysis for these acids are unknown. However, if it is assumed that they photolyze to form radicals rapidly (analogously to methylglyoxal), model calculations greatly overpredict the reactivity of the o-cresol-NO_x system, regardless of which mechanistic option is used.

40. Assumed to react with the same rate constant as OH + toluene. This reaction is only significant in affecting primary nitrotoluene yields.

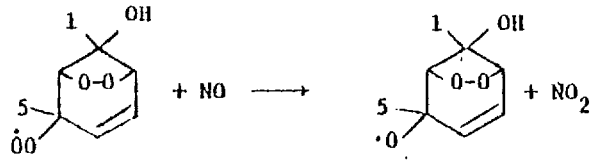
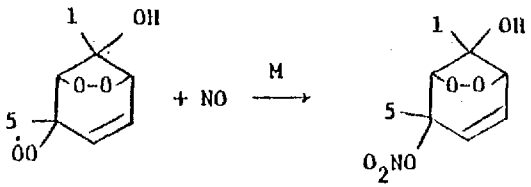
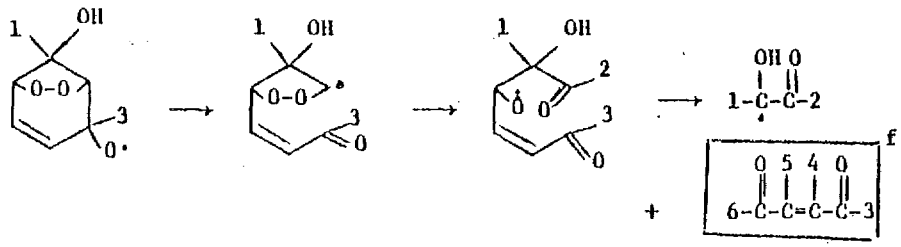
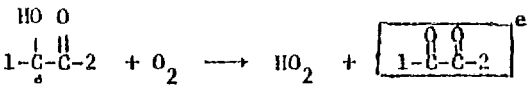
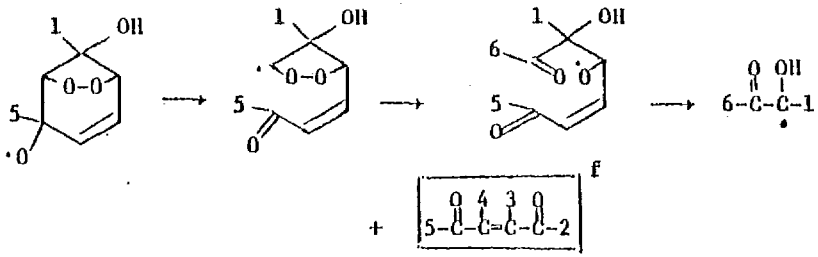
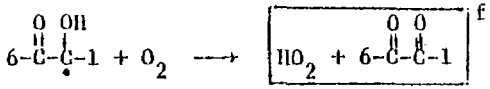
Appendix B. Reactions and Rate Constants for the General Aromatic-OH-O_2 Adduct System

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
	[2.2.2] Cyclization		
1'		Fast Mech. A-D, (G,H)[d] (Slow) Mech. E,F	
2'		Fast	
	[2.2.2] Cyclization, No Re-cyclization		
3'		6×10^{-12}	
4'	 e	2×10^{-12}	Ratio adjusted 9
5'	 f	Fast	

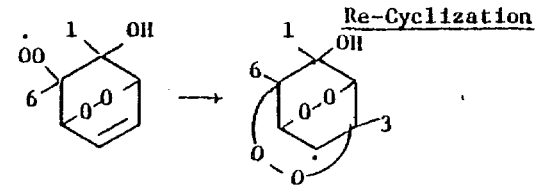
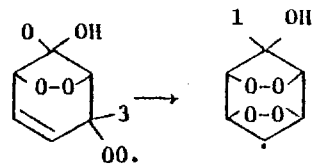
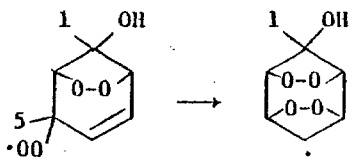
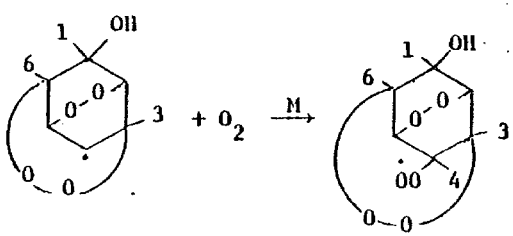
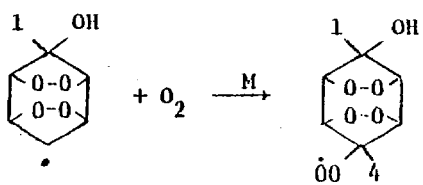
Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
6'		Fast	38
	[3.2.1] Cyclization		
7'		(Slow) Mech. A-D Fast Mech. E,F,(G,H)[d]	
8'		Fast	
	[3.2.1] Cyclization, No Re-cyclization		
9'		6×10^{-12}	
		Ratio adjusted	9
10'		2×10^{-12}	

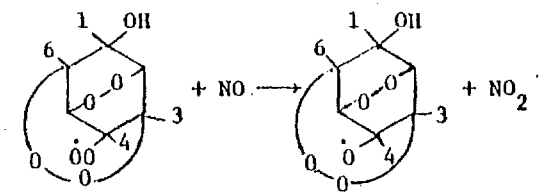
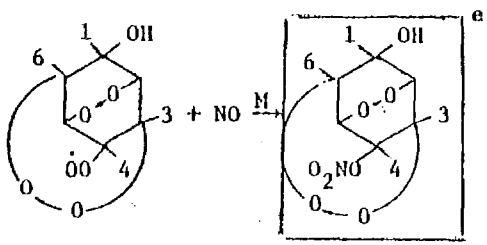
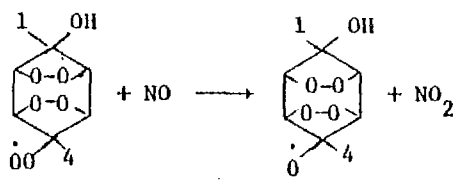
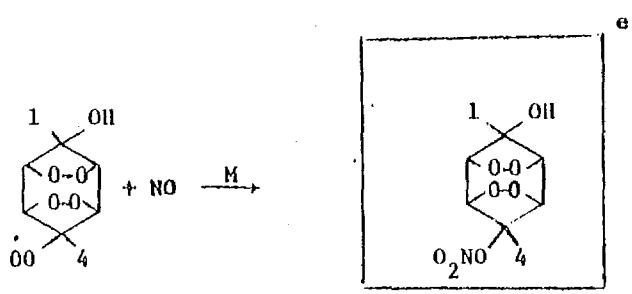
Appendix B. (cont.)

	Reaction	Rate Constant cm molecule sec units[a,b]	Notes[c]
11'		6×10^{-12}	Ratio adjusted 9
12'		2×10^{-12}	
13'		Fast	
14'		Fast	38
15'		Fast	
		Fast (Reaction 6')	

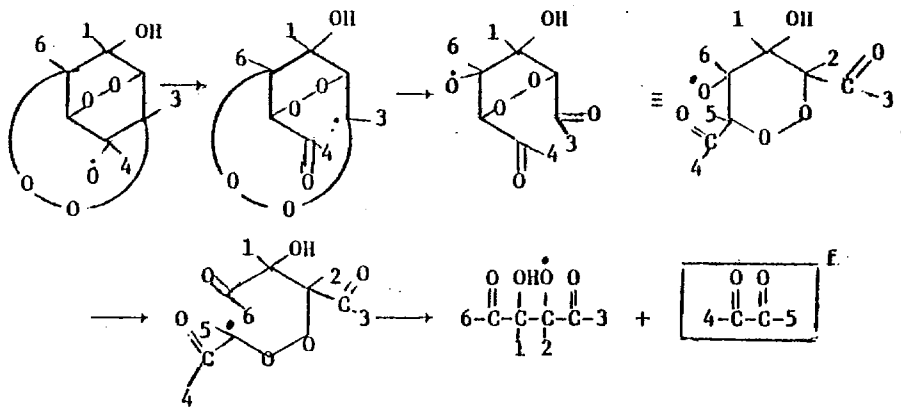
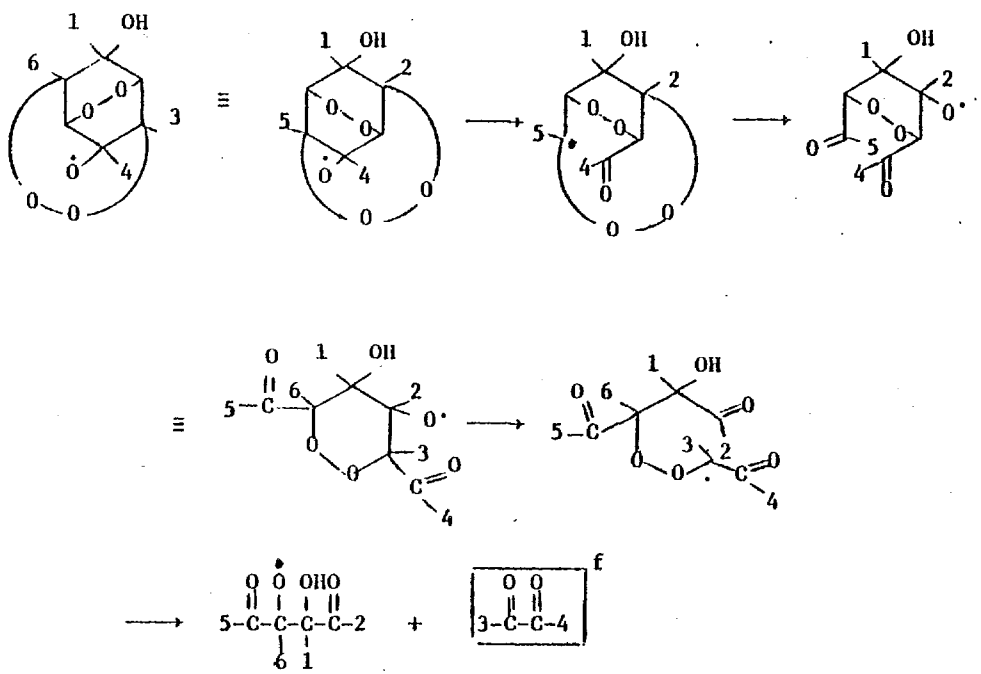
Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
16'		(Slow) Mech. A-F Fast Mech. G,H	
17'		(Slow) Mech. A-F Fast Mech. G,H	
18'		(Slow) Mech. A-F Fast Mech. G,H	
19'		Fast	
20'		Fast	

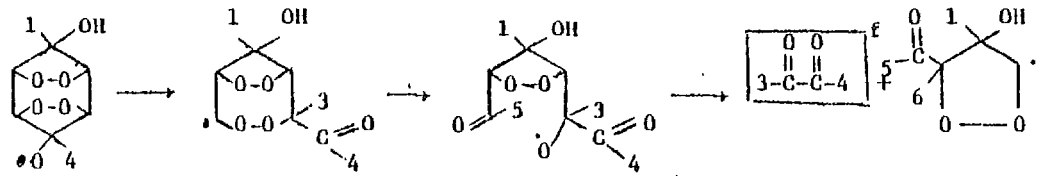
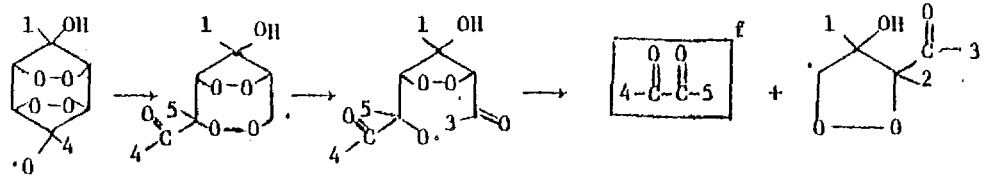
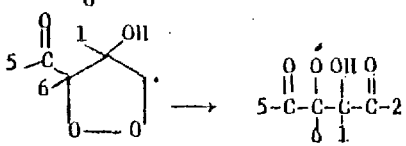
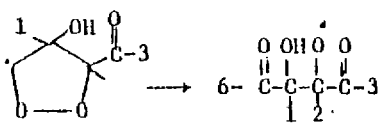
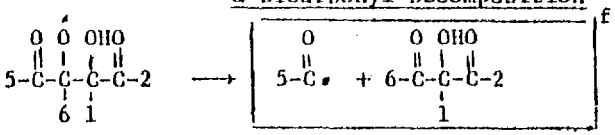
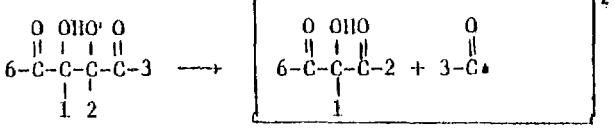
Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
21'		6×10^{-12}	Ratio adjusted 9
22'		2×10^{-12}	
23'		6×10^{12}	Ratio adjusted 9
24'		2×10^{12}	

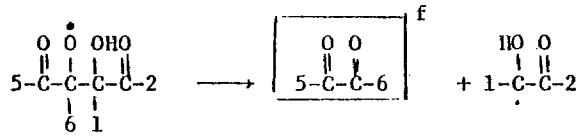
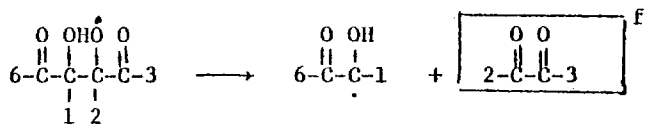
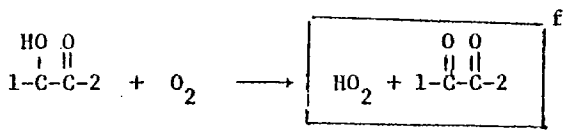
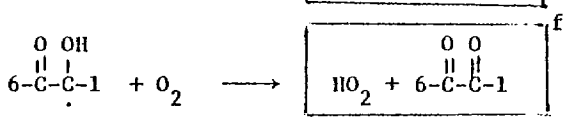
Appendix B. (cont.)

	Reaction	Rate Constant cm molecule sec units[a,b]	Notes[c]
25'		Fast	$k_{25'} = k_{26'}$
26'			

Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
27'		Fast $k_{27'}=k_{28'}$	
28'			
29'		Fast	
30'		Fast	
	α-Dicarbonyl Decomposition		
31'		Fast Mech. G (Slow) Mech. H	
32'		Fast Mech. G (Slow) Mech. H	

Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec units[a,b]	Notes[c]
	β-Hydroxy Decomposition		
33'		(Slow) Mech. G Fast Mech. H	
34'		(Slow) Mech. G Fast Mech. H	
		Fast	(Reaction 14')
		Fast	(Reaction 6')

[a] Rate constants are given for the conditions of the smog chamber runs listed in Appendix A (T = 303 K, 735 torr, M = air). Photolysis rate constants are given for the light intensity and spectral distributions associated with runs 327-340 (Pitts et al., 1979b); photolyses rate for runs 266-281 are somewhat lower.

[b] First order reaction: sec^{-1}; 2nd order reaction: cm^3 $molecule^{-1}$ sec^{-1}; "Fast" means that the reaction is the sole pathway for that particular species; the predictions are insensitive for the actual rate constant. "(Slow)" means that the reaction is assumed to be negligible, or that the reaction has a negligible effect on the predictions of the model for the concentration regimes studied here.

[c] Footnotes are those of Appendix A.

[d] Mechanisms G and H predict formation of same products regardless of whether [2.2.2] or [3.2.2] cyclization occurs.

[e] Subsequent reactions of this product are ignored.

[f] Subsequent reactions of these species or intermediates are shown in Appendix A.

V. INVESTIGATION OF THE EFFECT OF TEMPERATURE ON PHOTOCHEMICAL SMOG FORMATION

The formation of photochemical smog is influenced by a number of meteorological factors whose natural fluctuations contribute to the observed variations in frequency and intensity of episodes at different locations and times of year. Among the most important factors from a fundamental gas phase chemical kinetic standpoint is temperature. Although there has recently been considerable progress in understanding the temperature dependencies of the many individual elementary processes occurring in photochemical smog mechanisms, there has been very limited data available for the purpose of testing the temperature-dependent aspects of these kinetic mechanisms in their entirety. Analysis of air quality data is not particularly useful in this regard because conditions of lower temperature are usually also associated with conditions of reduced light intensity or duration, both of which are known to significantly affect photochemical smog formation. Smog chamber studies are potentially more useful for elucidating temperature effects, but the amount of smog chamber data obtained at varying temperatures has been highly limited, and the impact of chamber effects on temperature dependencies observed in such experiments has not been adequately characterized.

In order to satisfy the need for well characterized smog chamber data suitable for the validation of models of the effect of temperature on photochemical smog formation, a series of variable temperature chamber experiments has been performed employing the SAPRC evacuable chamber-solar simulator facility. This included the irradiation of surrogate hydrocarbon-NO_x-air mixtures at average temperatures of 8^oC, 30^oC and 51^oC, and, for control purposes, alkane-NO_x-air mixtures at the same temperatures. The alkane system is chosen as a control because its chemistry is reasonably well understood (Carter et al., 1979). Efforts have been made to assure that these experiments are well characterized, with experimental variables unrelated to temperature effects, such as light intensity and characteristics, reactant injections, moisture content, etc. held constant. A description of the experimental design and procedures, and the results of the 14 surrogate and the 10 control irradiations are given below.

Experimental Design. The composition of the surrogate hydrocarbon mixture employed in this study is given in Table 14. It is based on the mixture previously employed in SAPRC-ARB chamber experiments (Pitts et al., 1975; 1976a; 1979a) which was designed to represent the ambient air pollutant burden from all sources in the South Coast Air Basin. The hydrocarbon mixture was modified to include n-hexane as a representative of the longer chain alkanes, which are missing in the previous surrogate mixture. (Recent results have shown that because of the possibility of a rapid, 1,5-H shift isomerization of sufficiently long alkoxy radicals, the reactions of the longer alkanes in photochemical smog conditions are not analogous to those of, for example, n-butane or 2,3-dimethylbutane.) The relative concentrations of n-hexane and the other alkanes in the modified surrogate were chosen so that (1) the total ppmC of alkane relative to the other types of hydrocarbons was the same as in the previous SAPRC-ARB surrogate mixture, and (2) the ratios of the different types of labile C-H bonds was the same as those for the alkanes listed by Calvert for an 8:30 a.m. LARPP Los Angeles sample (Calvert, 1976). (Primary, secondary, tertiary, and C-H bonds that can, after reacting with OH, O_2 and NO, form alkoxy radicals which undergo the rapid 1,5-H shift isomerization, were counted as separate types.) An additional modification of the hydrocarbon mixture was that the oxygenates were represented entirely by acetaldehyde rather than primarily by formaldehyde; this was done to simplify and make more reproducible the hydrocarbon reactant injections.

Another modification of the reactant mixtures relative to the previous surrogate programs was that in the initial NO_x mixture, NO_2 was increased from 10% to 25%. This makes the NO_2:NO ratio more consistent with early morning monitoring data, and is what is assumed in the EPA EKMA model (Dodge, 1977b).

The composition of the control alkane-NO_x runs consisted of equal amounts of n-butane and neopentane as the reactant hydrocarbons, with the initial NO_x approximately 25% NO_2. n-Butane was chosen because its mechanism has been reasonably well validated (Hendry et al., 1978; Carter et al., 1979), with its major uncertainties being attributed to chamber effects. A dual rather than a single alkane system is preferred because

Table 14. Composition of Surrogate Hydrocarbon Mixture Used in Temperature Effects Study

Hydrocarbon	Mole %	% Carbon
Alkanes -- Total	64.0	65.3
Ethane	13.0	6.5
Propane	5.8	4.4
n-Butane	27.6	27.8
2,3-Dimethylbutane	9.3	14.1
n-Hexane	8.3	12.5
Olefins -- Total	13.3	10.1
Ethene	6.8	3.4
Propene	1.9	1.4
cis-2-Butene	2.4	2.4
2-Methyl-2-butene	2.2	2.8
Aromatics -- Total	9.2	17.9
Toluene	2.7	4.8
m-Xylene	6.5	13.1
Alkynes		
Acetylene	8.2	4.1
Oxygenates		
Acetaldehyde	5.2	2.6

the change in the ratios of the two alkanes with time gives a good technique to estimate hydroxyl radical concentrations without the necessity to correct for dilution. Neopentane was chosen as the second alkane because it is the least reactive alkane which can reliably be analyzed on the same chromatographic column as n-butane, allowing changes in their ratio to be determined with maximum precision. Neopentane reactions account for less than 24% of the hydrocarbon consumed, and its mechanism is expected to be analogous to that of n-butane and other alkanes; therefore its presence should introduce no major uncertainties.

The blocks of surrogate-NO_x-air and control n-butane/neopentane-NO_x-air runs were done at varying hydrocarbon and NO_x levels, with each experiment performed at both high (51°C) and low (8°C) temperatures. In addition, representative surrogate and n-butane/neopentane runs were done at 30°C. The experimental protocol was such that surrogate and n-butane/neopentane and runs, and runs with different initial hydrocarbon and NO_x levels were dispersed so that chamber memory effects, if any, should not have a systematic impact on the data.

Experimental Procedures. All experiments in this program were performed in the SAPRC 6800-liter, thermostatted evacuable smog chamber. The evacuable chamber, the solar simulator light source, and the pure air system employed have been described previously (Beauchene et al., 1973; Doyle et al., 1977; Winer et al., 1980). In these experiments, continuous monitoring was done using a Dasibi O_3 analyzer, and using simultaneously a TECO 14B and a newly acquired TECO 14B/E chemiluminescent NO-NO_x analyzer. Chromatographic samples were taken at 15-45 minute intervals for analysis of reactant hydrocarbons, PAN and oxygenated products; samples for analysis of formaldehyde using the chromotropic acid technique were taken hourly. The intensity of the photolyzing light was monitored by periodic NO_2 actinometry experiments, and its relative spectral distribution was determined for each experiment by a spectrometer-photomultiplier system. The experimental and analytical procedures and techniques used in these experiments were those generally employed in our evacuable chamber programs reported elsewhere (Pitts et al., 1979a,b), except as noted below.

For all runs temperature control was maintained to within ±1°C and

k_1 for NO_2 photolysis was held constant at 0.39 min^{-1}. The spectral distribution of the photolyzing light did not change significantly throughout the program. Regardless of the temperature of the run, purified air was humidified to ~15% RH at ambient temperature (~30°C) prior to entering the chamber; this corresponds to ~5% RH at 51°C and ~60% RH at 8°C.

Efforts were made to minimize the introduction of nitrous acid (HONO) into the chamber during injection of NO_x by removing moisture HONO and other impurities from the NO and NO_2 used, and by not allowing high concentrations of NO or NO_2 to be exposed to each other or to water vapor prior to and during the injection procedure. Because of the potential of initially present HONO, due to its rapid photolysis, to affect the results of the irradiation, the NO_x purification and injection procedures are described in detail and were used for all runs in this study.

NO was purified by passing it through a trap containing Linde Molecular Sieve 13X cooled to -98°C with a methanol slush. The contents of the trap were previously dried by being flushed with dry N_2 at 300°C. NO_2 was prepared by reaction of ~100 torr of the purified NO with ~1 atm of excess O_2 overnight, followed by trapping the NO_2 formed by pumping the reaction mixture through a liquid N_2-cooled trap. The O_2 used to make the NO_2 was previously dried by being passed through a Linde Molecular Sieve 13X-filled trap cooled with liquid Ar. Both the purified NO and the synthesized NO_2 were stored in bulbs (darkened for NO_2) attached to a conventional high vacuum rack interfaced directly to the evacuable chamber.

NO and NO_2 were introduced into the evacuated chamber prior to the fill of the chamber with humidified air, as follows. On the day prior to the experiment, the desired pressures of NO and NO_2 were placed in separate ~5 liter bulbs of accurately known volumes attached both to the chamber and the vacuum rack. The chamber was evacuated to $<10^{-5}$ torr and pumped overnight. On the day of the run, the chamber was filled to $\sim 10^{-20}$ torr with dry N_2, followed by flushing the NO into the chamber with N_2. After the NO was completely injected, the NO_2 was injected through a separate port into the chamber.

Similar high vacuum techniques were also used in introducing surrogate hydrocarbon mixture into the chamber in order to obtain greater reproducibility in hydrocarbon injection. All hydrocarbon reactants in the surrogate

mixture except the liquids 2-methyl-2-butene and m-xylene were pre-mixed and stored in the gas phase in a Pyrex bulb. Appropriate pressures in accurately known volumes of this "gas surrogate" mixture and the m-xylene and 2-methyl-2-butene were mixed the day before the experiment and stored in a liquid N_2 cooled trap prior to being flushed into the chamber with N_2. Surrogate injection was done after NO_x injection but prior to the pure air fill. For the alkane runs, neopentane and n-butane were injected using syringes after the pure air fill.

Results. The initial reactant concentrations, temperature, and humidity for the experiments are summarized in Table 15 for the surrogate runs and in Table 16 for the alkane control runs. Table 17 summarizes the levels of reproducibility, average values and standard deviations of initial reactant concentrations, temperatures, and humidity in runs where duplicate values were desired.

The 6-hr ozone values and the estimated average hydroxyl (OH) radical concentrations obtained in these runs are shown in Tables 18 and 19. Both the 6-hr ozone value and the estimated average OH levels increase significantly with increasing temperature. For both the surrogate and the control runs, the average OH levels increase by factors of 3 to 4 with increase in temperature from 8°C to 50°C. The OH levels observed for 30°C are approximately the geometrical mean of the corresponding runs ~22°C warmer or cooler.

Detailed tabulations of the reactant and product data, and of the physical parameters monitored during these runs are given in Appendix D. In order to facilitate the utilization of these data in model validations, they will be made available on magnetic tape in computer readable format upon request. A description of the organization of the tape and associated computer usage will be provided with the tape.

Discussion. Since the primary purpose of this study is to provide data suitable for model validation, a full discussion of the implications of the results presented here of the effects of temperature on photochemical smog formation must await the results of model calculations simulating these runs. However, several observations can be made without the benefit of such calculations.

Table 15. Initial Reactant Concentration, Average Temperature, Humidity and Water Content of Surrogate Hydrocarbon-NO_x-Air Evacuable Chamber Runs

Run No.	Avg. Temp. (°C)	H_2O[a] (10^3 ppm)	Humidity[b] (%)	Initial Concentrations NO[c] (ppm)	NO_2[c] (ppm)	NO_x[c] (ppm)	NMHC[d] (ppmC)	CO (ppm)
362	29.6	4.3	20	0.082	0.029	0.111	0.67	0.6
365	7.9	6.7	63	0.072	0.027	0.099	0.68	2.4
366	51.7	5.2	5	0.078	0.034	0.111	0.71	0.4
367	49.3	6.3	5	0.097	0.021	0.118	0.46	0.4
368	8.7	1.7	29	0.068	0.033	0.102	0.44[e]	0.3
371	8.9	5.2	34	0.033	0.025	0.058	2.00[e]	1.4
372	51.6	6.1	5	0.040	0.023	0.063	1.96	0.2
375	8.2	5.0	38	0.210	0.079	0.289	1.94	–[f]
376	51.1	6.6	5	0.248	0.091	0.339	2.37	0.7
379	7.9	5.2	49	0.067	0.027	0.094	2.17	–
380	52.3	6.2	5	0.076	0.034	0.110	2.40	–
381	51.5	5.2	5	0.035	0.020	0.055	0.50	–
382	7.8	3.3	32	0.029	0.020	0.046	0.43	–
387	28.9	6.1	17	0.073	0.034	0.107	0.79	0.7

[a]Calculated from the wet and dry bulb temperature at the time of the pure air fill.

[b]Calculated from the average temperature and the initial H_2O temperature using H_2O vapor pressures.

[c]Average of readings from TECO 14B/1 and 14B/E chemiluminescent NO-NO_x monitors.

[d]Calculations based on the measured initial concentrations of the injected ethane, propane, n-butane, 2,3-dimethylbutane, n-hexane, ethene, propene, cis-2-butene, 2-methyl-2-butene, toluene, m-xylene, acetylene, and acetaldehyde.

[e]Data values for acetaldehyde missing. NMHC calculated using intended initial acetaldehyde concentrations.

[f]– No data taken.

Table 16. Initial Reactant Concentration, Average Temperature, Humidity and Water Content of Alkane-NO_x-Air Evacuable Chamber Runs

Run No.	Avg. Temp. (°C)	H_2O[a] (10^3 ppm)	Humidity[b] (%)	Initial Concentrations					
				NO[c] (ppm)	NO_2[c] (ppm)	NO_x[c] (ppm)	n-Butane (ppmC)	Neo-pentane (ppm)	CO (ppm)
360	7.5	5.7	51	0.368	0.123	0.495	2.75	2.81	–[e]
361	51.9	6.1	5	0.392	0.132	0.524	2.83	2.81	1.1
363	25.9	5.2	20	0.153	0.060	0.213	1.49	1.50	0.3
369	7.5	4.3	33	0.138	0.052	0.190	1.42	1.39	0.8
370	51.2	5.5	5	0.157	0.062	0.219	1.55	1.55	0.8
373	7.6	4.4	31	0.350	0.125	0.475	1.40	1.40	0.7
374	50.8	5.6	5	0.391	0.137	0.528	1.55	1.57	–
383	9.5	6.3	41	0.030	0.022	0.052	1.39	1.39	0.3
384	50.2	6.9	5	0.037	0.019	0.056	1.64	1.64	0.6
386	29.6	5.2	14	0.147	0.058	0.204	1.54	1.53	0.4

[a]Calculated from the wet and dry bulb temperature at the time of the pure air fill.

[b]Calculated from the average temperature and the initial H_2O temperature using H_2O vapor pressures.

[c]Average of readings from TECO 14B/1 and 14B/E chemiluminescent NO-NO_x monitors.

[d]Calculations based on the measured initial concentrations of the injected ethane, propane, n-butane, 2,3-dimethylbutane, n-hexane, ethene, propene, cis-2-butene, 2-methyl-2-butene, toluene, m-xylene, acetylene, and acetaldehyde.

[e]– No data taken.

Table 17. Intended and Observed Average Values and Observed Standard Deviations of Initial Reactant and Water Concentrations and Temperature Measurements in Comparable Evacuable Chamber Runs

Quantity Measured	Desired Value	Observed Value	No. Runs	Desired Value	Observed Value	No. Runs	Desired Value	Observed Value	No. Runs
Temperature (°C)	8°C	8.2 ± 0.7	10	30°C	28.5 ± 1.8	4	51°C	51.2 ± 0.9	10
$H_2O(10^3$ ppm)[a]	~6	5.3 ± 1.2	24	-	-	-	-	-	-
RH (%)	~60	44 ± 13	10	~15	14 ± 4	4	~5	4.6 ± 0.6	10
Initial Concentrations									
NO (ppm)[b]	0.038	0.034 ± 0.006	6	0.075	0.077 ± 0.020	8	0.150	0.149 ± 0.012	4
NO_2 (ppm)	0.013	0.021 ± 0.004	6	0.025	0.030 ± 0.009	8	0.050	0.058 ± 0.004	4
NO_x (ppm)	0.050	0.055 ± 0.009	6	0.100	0.107 ± 0.014	8	0.200	0.207 ± 0.017	4
NO (ppm)	0.225	0.23 ± 0.03	2	0.375	0.38 ± 0.02	4			
NO_2 (ppm)	0.075	0.08 ± 0.01	2	0.125	0.129 ± 0.01	4			
NO_x (ppm)	0.300	0.31 ± 0.03	2	0.500	0.51 ± 0.02	4			
n-Butane (ppm)[c]	1.5	1.59 ± 0.09	8	3.0	2.79 ± 0.05	2			
Neopentane (ppm)[c]	1.5	1.49 ± 0.09	8	3.0	2.808 ± 0.002	2			
Total Surrogate (ppmC)[d]	0.45	0.46 ± 0.03	4	0.70	0.73 ± 0.06	4	2.2	2.1 ± 0.2	6
Surrogate Components (ppb)[d]									
Ethane	14.6	16.7 ± 1.0	4	22.8	25.8 ± 1.3	3	71.5	68 ± 10	6
Propane	6.6	8.4 ± 0.6	4	10.3	12.1 ± 0.6	4	32.3	36 ± 2	6
n-Butane	31.3	32.9 ± 2.7	4	48.7	50.6 ± 2.5	4	152.9	162 ± 11	6
2,3-Dimethylbutane	10.6	10.7 ± 0.8	4	16.5	16.9 ± 1.4	4	51.7	54 ± 4	6
n-Hexane	9.4	9.5 ± 0.5	4	14.6	14.4 ± 0.8	4	45.8	47 ± 4	6
Ethene	7.7	5.6 ± 1.1	4	11.9	12.9 ± 1.2	3	37.4	31 ± 6	6
Propene	2.1	2.3 ± 0.2	4	3.3	3.5 ± 0.2	4	10.3	11.3 ± 1.0	6
cis-2-Butene	2.7	2.5 ± 0.2	4	4.2	4.0 ± 0.3	4	13.2	13 ± 2	6
2-Methyl-2-butene[e]	2.5	2.3 ± 0.3	4	3.9	3.5 ± 0.3	4	12.3	11.6 ± 2	6
Toluene	3.1	3.1 ± 0.8	4	4.8	5.0 ± 1.1	4	15.1	14.3 ± 1.0	6
m-Xylene[e]	7.4	6.9 ± 0.4	4	11.5	10.8 ± 1.0	4	36.0	34 ± 8	5
Acetylene	9.2	11.5 ± 0.7	4	14.4	16.8 ± 0.5	3	45.1	47 ± 7	6
Acetaldehyde	5.9	4.9 ± 1.1	2	9.1	12.3 ± 3.1	3	28.6	18 ± 5	5

[a]Calculated from the wet and dry bulb temperature at the time of the pure air fill.

[b]Average of readings from TECO 14B/1 and TECO 14B/E chemiluminescent NO-NO_x monitors.

[c]Alkane runs only.

[d]Surrogate runs only.

[e]Injected separately from other components of the mixture, so greater variability relative to the other components expected.

Table 18. Six-Hour Ozone and Estimated Hydroxyl Levels Observed in Surrogate-NO_x-Air Evacuable Chamber Experiments

Nominal Initial Concentrations[a]		T = 8°C			T = 30°C			T = 51°C		
NMHC (ppmC)	NO_x (ppm)	Run No.	6-hr O_3 (ppm)	Est. [OH][b] (molec cm^{-3})	Run No.	6-hr O_3 (ppm)	Est. [OH][b] (molec cm^{-3})	Run No.	6-hr O_3 (ppm)	Est. [OH][b] (molec cm^{-3})
0.45	0.05	382	0.068	4.4×10^6				381	0.237	1.3×10^7
0.45	0.1	368	0.039	2.3×10^6				367	0.237	9.5×10^6
0.7	0.1	365	0.056	3.1×10^6	362 387	0.176 0.167	5.8×10^6 5.6×10^6	366	0.327	1.2×10^7
2.2	0.05	371	0.085[c]	3.1×10^6				372	0.359	6.0×10^6
2.2	0.1	379	0.176[c]	1.4×10^6				380	0.477	7.8×10^6
2.2	0.3	375	0.044	2.1×10^6				376	0.576	7.6×10^6

[a]Concentrations given are desired initial concentrations. Actual initial concentrations may be slightly different.

[b]Calculated from the relative decay rates of n-butane and 2,3-dimethylbutane using k(OH + n-butane) = 2.8×10^{-12} cm^3 $molecule^{-1}$ sec^{-1} and k(OH + 2,3-DMB) = 5.7×10^{-12} cm^3 $molecule^{-1}$ sec^{-1}.

[c]Maximum O_3 observed prior to 6 hours.

Table 19. Six-Hour Ozone and Estimated Hydroxyl Levels Observed in Alkane-NO_x-Air Evacuable Chamber Experiments

Nominal Initial Concentrations[a]		T = 8°C			T = 30°C			T = 51°C		
Alkane (ppm)[b]	NO_x (ppm)	Run No.	6-hr O_3 (ppm)	Est. [OH][c] (molec cm^{-3})	Run No.	6-hr O_3 (ppm)	Est. [OH][c] (molec cm^{-3})	Run No.	6-hr O_3 (ppm)	Est. [OH][c] (molec cm^{-3})
3	0.05	383	0.098	7×10^5				384	0.391	1.8×10^6
3	0.2	369	0.042	6×10^5	363 386	>0.076[d] 0.196	1.1×10^6 1.3×10^6	370	0.696	3.0×10^6
3	0.5	373	0.010	5×10^5				374	0.332	2.0×10^6
6	0.5	360	0.027	6×10^5				361	0.989	2.3×10^6

[a]Concentrations given are initial concentrations desired. Actual initial concentrations may be slightly different.

[b]Given as concentration of neopentane + n-butane (ppm). Equal quantities of each used.

[c]Calculated from the relative decay rates of n-butane and neopentane using k(OH + n-butane) = 2.8×10^{-12} cm^3 $molecule^{-1}$ sec^{-1}, and k(OH + neopentane) = 8.7×10^{-13} cm^3 $molecule^{-1}$ sec^{-1}.

[d]4-hour value. Compare with 4-hour O_3 value of 0.098 ppm for EC-386.

The data in Tables 18 and 19 indicate that temperature strongly affects radical levels in both the surrogate-NO_x and the alkane-NO_x runs. Much, if not all, of the effect of temperature on ozone formation can be attributed to this increase of radical levels with temperature, since it is the radical propagation reactions converting NO to NO_2 which are responsible for O_3 build-up. Therefore, an understanding of the cause of the strong effect of temperature on radical levels is important to understanding the effect of temperature on photochemical smog formation.

The increase in radical levels with temperature could be due to increasing rates of radical initiation reactions, or to decreasing rates of radical termination processes, or to a combination of both. Prior to the consumption of NO_x, the major termination reactions are radical + NO_2 reactions forming nitrates or peroxynitrates. In the alkane system the major known radical initiation processes are ozone and aldehyde photolysis (Demerjian et al., 1974; Hendry et al., 1978; Carter et al., 1979). In the surrogate system, reactions of ozone with olefins and photolysis of the α-dicarbonyls will also contribute to initiation, and the higher radical levels observed in surrogate runs can be rationalized on the basis of these reactions. Although the radical levels in the surrogate runs are on the average over four times higher than those of alkane runs at the same temperature, the <u>relative</u> increase in OH concentration with temperature increase from 8°C to 30°C and from 30°C to 51°C is the same in both systems. This suggests that the cause of the strong effect of temperature on radical levels is in some aspect of the mechanism common to both systems.

In the alkane-NO_x system, where the major organic photooxidation products can be monitored, it is possible to estimate the total extent of initiation or termination from the known processes. Estimates are made using (1) observed yields of termination products (e.g., alkyl nitrates and PAN), (2) estimations of average OH + NO_2 rates using average measured NO_2 values and estimated OH levels, and (3) integrated O_3 and oxygenate yields and calculated photolysis rate constants for the photolysis conditions. Such estimates are given in Table 20 for three representative alkane-NO_x runs with similar initial reactant concentrations at the three temperatures studied. At all three temperatures the total amount of

Table 20. Estimated Integrated Initiation and Termination Rates from Known Processes in Representative Alkane-NO_x-Air Chamber Runs

Temperature (°C)	8	30	51	Notes
EC Run No.	369	386	370	
	6-hr Integrated Rates (ppb radicals)			
Initiation - Total	9	15	50	
$O_3 + h\nu \overset{H_2O}{\rightarrow} 2\ OH + O_2$	0.4	2	10	a,b
$HCHO + h\nu \rightarrow$ Radicals	4	5	19	b,c
$CH_3CHO + h\nu \rightarrow$ Radicals	1	2	8	b,c
$CH_3CH_2COCH_3 + h\nu \rightarrow$ Radicals	3	3	5	b,c
$CH_3COCH_3 + h\nu \rightarrow$ Radicals	1	3	8	b,c
Termination - Total	17	56	241	
$OH + NO_2 \overset{M}{\rightarrow} HNO_3$	11	36	205	d
$CH_3CO_3 + NO_2 \overset{M}{\rightarrow} PAN$	1	12	26	e
Radicals + $NO_x \rightarrow RONO_2$	5	8	10	e
Excess Initiation				
6-hr Integrated Rate (ppb)	8	41	191	
Avg. Rate (ppb min^{-1})	0.02	0.1	0.5	

a) Estimated from the measured 6-hr O_3 dose, the calculated rate of O_3 photolysis to O^1D, and the O^1D rate constants (Hampson & Garvin, 1978) as shown below:

$$\int_0^{360} (\text{rate OH input})dt = 2 \left[\int_0^{360} [O_3]\ dt\right] k\ (O_3 \overset{h\nu}{\rightarrow} O^1D) \frac{k(O^1D + H_2O)}{k(O^1D + H_2O + k(O^1D + M)}$$

b) These estimates used photolysis rate constants for O_3 (to O^1D) for formaldehyde, acetaldehyde, and ketone respectively of 2×10^{-3}, 9×10^{-4}, 2×10^{-4}, and 4×10^{-4} sec^{-1}. These were calculated from the appropriate absorption coefficients, quantum yields, measured intensities, and spectral distribution of the photolyzing light in these runs. Absorption coefficients and quantum yields for O_3 and formaldehyde used are those recommended by

Table 20. (Continued)

Hampson & Garvin (1978) and Horowitz & Calvert (1978), respectively. Acetaldehyde and ketone absorption coefficients and quantum yields were those of Calvert & Pitts (1966); acetaldehyde quantum yields were those of Weaver et al. (1977); and ketone photolysis to radicals was assumed to be 100% efficient.

c) Estimated from the measured integrated aldehyde yield and the appropriate photolysis rate constant as shown

$$\int_0^{360} (\text{rate, radical input})dt = 2 \left[\int_0^{360} [RCHO]\, dt \right] k(RCHO + h\nu \rightarrow \text{radical})$$

d) Estimated from the measured average $[NO_2]$, the estimated average [OH] (Table 19) and the $OH + NO_2$ rate constant (Hampson & Garvin, 1978) as shown

$$\int_0^{360} \text{rate } (OH + NO_2)dt \cong k\ (OH + NO_2)\ [OH]_{avg} \int_0^{360} [NO_2]\ dt$$

e) Integrated rate identified with the observed yields of the appropriate product(s). "$RONO_2$" includes primarily methyl and butyl nitrates.

termination is significantly greater than the total amount of initiation from known processes, with the discrepancy increasing strongly with temperature. Since initiation and termination must balance, there is an unknown radical source which becomes greater with increasing temperature.

The existence of unknown radical sources in smog chamber systems is now generally recognized (Bufalini et al., 1977; Falls and Seinfeld, 1978; Hendry et al., 1978; Whitten et al., 1979; Carter et al., 1979) and is a serious problem in modeling such systems. It is frequently attributed to photolysis of HONO formed during the injection of NO_x through the interaction of NO and NO_2 with water vapor (Chan et al., 1976); but, as discussed above, NO_x injection in this study was done in such a way as to minimize HONO formation. In any case, it is unclear how HONO photolysis could be the cause of the observed increase of the unknown radical source with temperature. In order for the concentration of HONO to be sufficient to affect the system, it must be fairly close to equilibrium with NO, NO_2 and H_2O, but the equilibrium HONO actually <u>decreases</u> with temperature (Benson, 1976). Thus, the nature of the temperature-dependent radical source is unknown, though it appears likely that it is due to offgassing of some highly photoreactive contaminant from the chamber walls. It is reasonable to expect such offgassing to increase with increasing temperature.

Additional evidence for the increased importance of contaminant offgassing at higher temperatures comes from the fact that in the 51°C runs, the total NO_x consumption is considerably less than what would be expected on the basis of estimated rates of the OH + NO_2 reaction. Decreased NO_x consumption could be attributed in part to increased HNO_3 interferences on the chemiluminescent NO_x monitor (Winer et al., 1974) due to less efficient adsorption of HNO_3 vapor on the walls of the sampling tubes at higher temperature, but in a number of 51°C runs the total monitored NO_x actually increased. Because of the uncertainties in the NO_x measurements introduced by the possibility of a semi-quantitative HNO_3 interference, the exact magnitude of the offgassing cannot be determined from these data. It is quite possible that the unknown radical source and the evidence for NO_x offgassing at high temperatures are related, since offgassing of a highly photoreactive nitrogen-containing species such as

HONO or alkyl nitrites could account for both effects.

Conclusions and Future Research. There is a major effect of temperature on photochemical smog simulations in smog chamber systems, but current evidence suggests that most of this could be an artifact introduced by chamber effects. Until chamber effects relating to radical initiation are more completely understood, it will not be possible to unambiguously validate photochemical models concerning temperature effects using smog chamber data. More chamber characterization experiments are required, particularly those with more quantitative data concerning offgassing at higher temperatures.

We are conducting studies in the ongoing SAPRC-ARB chamber program on the effect of temperature on photochemical smog formation in which relative humidity will be varied. Because the data reported here suggest that chamber effects may play a dominant role in these experiments, additional chamber characterization and control experiments will be incorporated into the program. Contaminant offgassing will be studied as a function of temperature and humidity both in the dark and during irradiation. It is hoped that these additional experiments will increase the level of characterization, and thus the utility, of the experiments reported here.

VI. STUDIES OF THE RELATIONSHIPS BETWEEN AMBIENT AMMONIA AND NITRIC ACID AND PARTICULATE NITRATE: IMPLICATIONS FOR NITRATE ARTIFACT FORMATION

The need to reliably establish ambient levels of ammonium nitrate particulates in ambient air (National Academy of Sciences, 1978) and the evidence for "artifact effects" (Witz and MacPhee, 1977; Spicer and Schumacher, 1977; Spicer, 1977; Spicer and Schumacher, 1978; Appel et al., 1979; Meserole, 1978) in widely used sampling methods for particulate nitrate have led to recent interest in the roles that the precursors ammonia and nitric acid play in the formation of ammonium nitrate in the atmosphere and on filters. Unfortunately, direct and simultaneous measurements of ammonia and nitric acid in ambient air have previously been unavailable. Indeed, the only data of a related nature are the pairs of 1-hr maxima for NH_3 and HNO_3 concentrations in West Covina reported by Spicer (1974), who employed microcoulometric and modified chromatropic acid (colorimetric) techniques for HNO_3 and dual-catalyst chemiluminescence detection for NH_3.

Stelson, Friedlander, and Seinfeld (1979) recently utilized these data (Spicer, 1974) in an analysis of the applicability of the equilibrium relationship in Equation 1 to the atmosphere. We wish to extend this

$$NH_4NO_3(s) \rightleftarrows NH_3(g) + HNO_3(g) \qquad (1)$$

analysis using simultaneous, absolute concentrations of NH_3 and HNO_3 in ambient air, which we measured with short (<6 min) integration times in Riverside, California, in 1977 using a kilometer path-length Fourier transform infrared (FT-IR) spectrometer (Tuazon et al., 1978; Tuazon et al., 1980).

Experimental. High-resolution FT-IR spectra of ambient air have been obtained during air pollution episodes in the California South Coast Air Basin at a downwind site (Riverside) during 1976 and 1977 (Pitts et al., 1979a) using a long-path FT-IR system and experimental methods that have been previously described (Tuazon et al., 1978; Tuazon et al., 1980). The system consists of a Digilab Model 196 interferometer (0.5 cm^{-1} maximum resolution) interfaced to an eight-mirror long-path cell with a 22.5-m base path and capable of achieving kilometer path lengths. The cell optics are

gold-coated for maximum reflectivity in the infrared, and a HgCdTe liquid-N_2 cooled detector was employed for the 700-2000 cm^{-1} region. The detection limits for NH_3 and HNO_3 afforded by this facility for a 5-min scanning interval are 4 and 6 ppb, respectively, and the average uncertainty in each quantity is approximately one-half of the detection limit. From 249 spectra, 54 instances were found where the concentrations of both ammonia and nitric acid were above the detection limits. These cases were found among spectra taken at half-hour intervals between late morning and early evening during air pollution episodes in the months of July to October, 1977. Temperature and relative humidity data were obtained from instruments operating in the ACHEX laboratory (Appel et al., 1978) immediately adjacent to the kilometer path-length FT-IR facility. During selected episodes, 24-hr high-volume particulate samples were also collected on washed Gelman AE glass fiber filters and were subsequently analyzed for ammonium, nitrate, and sulfate ions by the indophenol blue (Weatherburn, 1967), cadmium reduction-diazotization, and turbidimetric methods, respectively.

Results. The data employed in the present analysis are given in Table 21 and plotted in Figure 44. These data met two conditions: (1) concentrations of both NH_3 and HNO_3 exceeded the detection limits, and (2) measurements were made during high oxidant episodes (i.e., $O_3 \geq 100$ ppb). Relative humidity never exceeded 50% during these observations and did not correlate significantly with concentration data. Temperatures given in Table 21 are interpolated to the times of the spectral observations from readings recorded at 10-min intervals.

The mass concentrations determined for the NH_4^+, NO_3^-, and $SO_4^=$ ions from particulate data are given in Table 22. Multiple linear regressions using these data and a much larger data block obtained at the same sampling site during the previous two years (Pitts and Grosjean, 1978) suggest that the mixture consists of ammonium nitrate and two sulfates of ammonia. A recent field study of high-volume sampling artifacts for particulate inorganics (Mischke, 1979) indicates small positive errors for nitrate ($\lesssim$15%) and a probable negative error for ammonium for 24-hr samples obtained from highly polluted air at Riverside on Gelman AE filters.

Table 21. Ambient Concentrations of Ammonia and Nitric Acid from Kilometer Path-Length FT-IR Spectroscopic Measurements

1977 (Date)	Time (PST)	NH_3 (ppb)	HNO_3 (ppb)	Temp. (°C)
7/21	1434	24	10	36.2
	1452	19	7	35.5
	1510	13	9	35.0
	1532	11	10	34.2
	1611	6	10	33.0
	1718	9	12	32.4
7/25	1523	18	20	37.6
	1542	19	17	37.3
	1604	13	15	36.4
	1622	14	12	36.3
	1655	13	14	35.5
8/11	1057	13	8	31.3
	1400	37	8	36.0
	1435	21	13	35.4
	1454	14	10	34.6
	1516	16	10	34.2
	1535	13	9	34.2
	1553	10	11	33.5
	1616	9	9	32.9
8/12	1132	15	16	33.2
	1202	33	11	34.0
	1230	38	9	34.4
	1300	46	9	35.0
	1400	29	9	35.8
	1430	32	9	35.5
	1459	22	9	34.5
	1529	20	10	34.0
	1603	13	11	33.0
	1612	9	10	32.2
	1640	4	8	31.5
9/9	1113	17	9	33.5
	1132	13	8	33.1
	1200	16	8	34.7
	1235	47	6	35.3
10/3	1300	25	10	33.6
	1405	54	9	33.7
10/4	1500	37	8	33.5
	1530	28	9	31.9

Table 21. (continued)

1977 (Date)	Time (PST)	NH_3 (ppb)	HNO_3 (ppb)	Temp. (°C)
10/11	1224	6	12	30.1
	1244	5	9	30.9
	1333	59	8	32.9
10/14	1230	23	9	35.2
	1330	102	7	35.7
	1400	93	8	34.7
	1424	55	8	33.8
	1444	46	8	33.7
10/17	1202	15	9	29.6
	1231	20	11	29.6
	1300	27	9	30.5
10/18	1411	16	6	27.3
10/26	1130	5	10	27.3
	1202	6	8	28.2
	1231	9	8	31.3
	1300	24	8	30.5

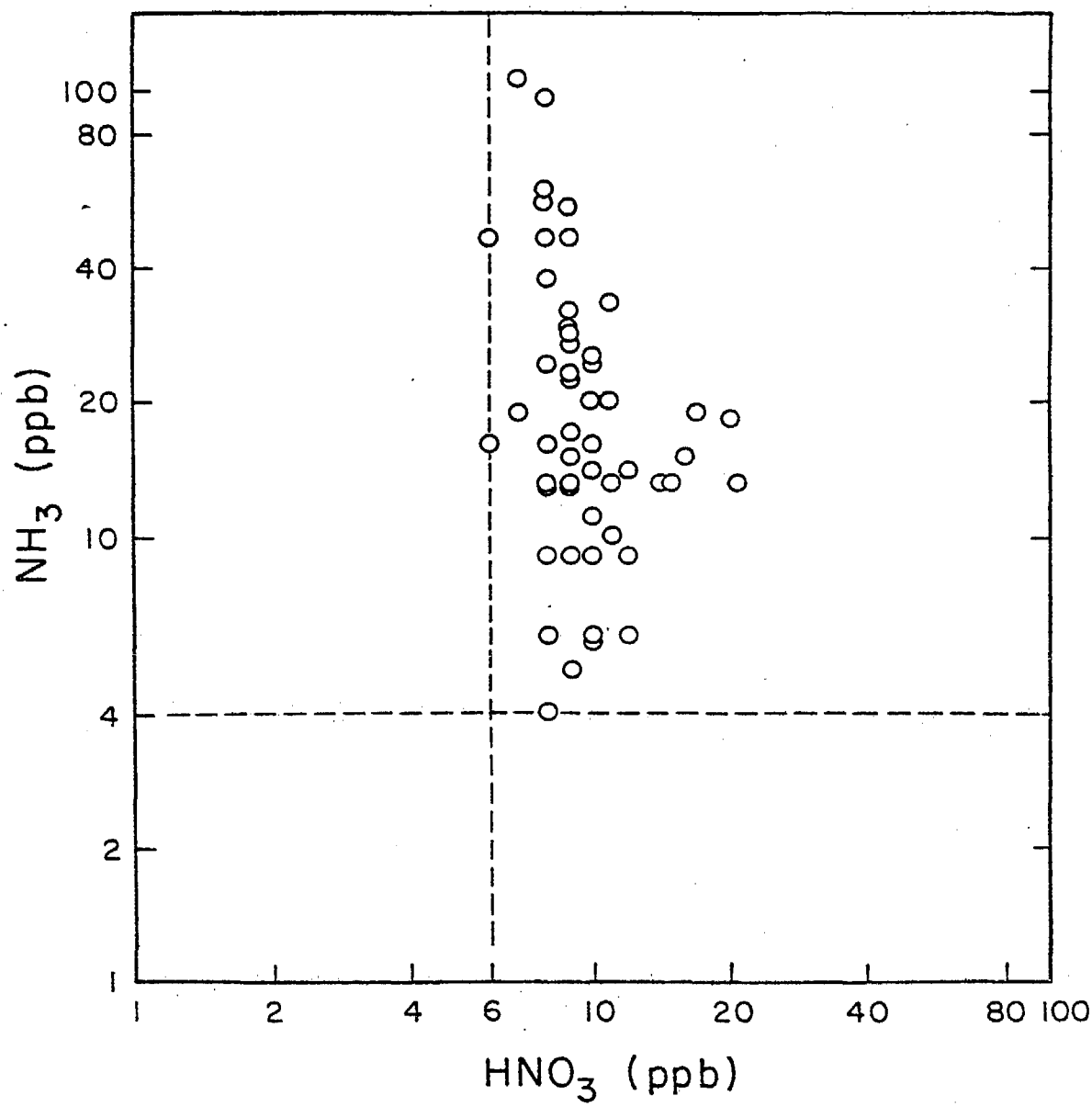


Figure 44. Distribution of Simultaneous Observations of Ammonia and Nitric Acid Concentrations: (---) Detection Threshold.

Table 22. Particulate Analyses of 24-hr Samples

Date (1977)	Mass Concentration $\mu g\ m^{-3}$			
	NH_4^+	NO_3^-	$SO_4^=$	NH_4NO_3[a]
7/21	13	42	12	54
7/25	4	18	13	29
8/11	17	60	25	77
8/12	14	50	20	64
9/09	2	21	NI[b]	27
10/03	18	67	18	86
10/04	NI	NI	NI	NI
10/11	20	65	6	84
10/14	16	50	21	64
10/17	27	74	26	96
10/18	33	86	31	111
10/26	20	64	16	83

[a]Ammonium nitrate equivalent to nitrate ion data.

[b]NI means no information available.

Consequently, the best estimates of ammonium nitrate concentrations can be calculated from the nitrate data and are given in the fifth column of Table 22. A more extensive analysis of data for particulate samples at this site is given by Pitts and Grosjean (1978). Although the data in Table 22 are averages for 24-hr periods, the presence of particulate ammoninum nitrate seems probable during many, if not all, periods when FT-IR spectra were obtained.

A small negative correlation (-0.31 with a 95% confidence level for the range -0.53 to -0.05) between the NH_3 and HNO_3 concentrations in Table 21 indicates qualitatively that these concentrations are being affected by chemical reaction or an equilibrium relationship (i.e., Equation 1), since the concentrations of two noninteracting pollutants are usually positively correlated as a result of common meteorological influences. Strict adherence to the equilibrium of Equation 1 would give a hyperbolic

relationship between the NH_3 and HNO_3 concentrations and a correlation coefficient between -1.0 and 0.0. In this case the values of the coefficient depends on the variance of the independent variable, and approaches zero for very large variances. The logarithm of the NH_3-HNO_3 concentration product has a significant positive correlation with temperature (e.g., +0.55 with a 95% confidence level for the range +0.33 to 0.71), as expected for the NH_4NO_3 equilibrium. The data are insufficient, however, to resolve any dependence of the logarithm of the concentration production on humidity.

The effect of temperature on the logarithmic concentration products at these low to moderate humidities is well represented by a regression coefficient of about 0.2 deg^{-1}. This is consistent with the concentration product representing an equilibrium constant for solid particulate, which is the probable state of ammonium nitrate containing particles at these temperatures and humidities (i.e., RH < 55%) (Dingemans, 1941). The temperature dependence of the equilibrium relationship of Equation 1 from thermochemical data is compared to our experimental data in the scatter diagram shown in Figure 45. The means of the concentration product and temperature data and their least-squares regression coefficients are given in Table 23 as changes in the free energy and enthalpy for Reaction 1; the same quantities, as estimated from compilations of thermochemical data, are also given in Table 23 for comparison.

It should be noted that temperatures were not measured directly in the FT-IR multiple reflection cell but were inferred from adjacent ambient air measurements. Deviation of up to $1^{o}C$ were possible, which can have significant effects when the enthalpy change is ~44 kcal.

Discussion. Much of the difference between the enthalpy change calculated from the regression slope of our experimental data and the enthalpy change from thermochemical data (see Table 23) may be due to deviations from ambient temperature in the outdoor FT-IR cell. Since temperature deviations are affected by diurnal variations of such factors as radiation intensity and wind speed, they may not be completely random and can result in a bias. The regression coefficient estimate is quite sensitive to bias in the independent variable (in this case temperature), and thus the enthalpy change calculated from our data could contain a systematic error.

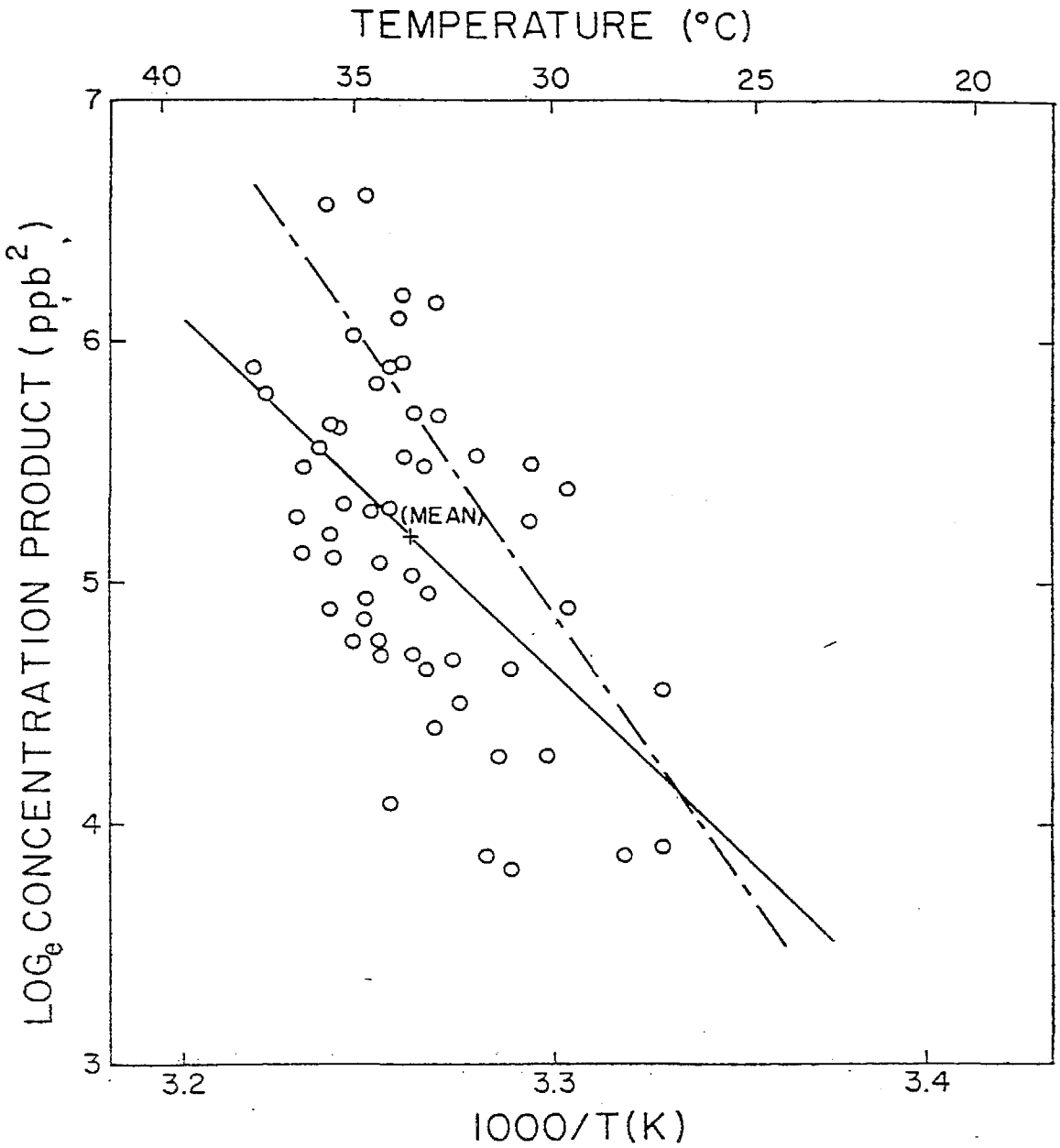


Figure 45. Logarithm of the NH_3-HNO_3 Concentration Product vs. the Reciprocal Absolute Ambient Temperature: (——) Regression Line Calculated from Unweighted Experimental Data (54 Observations); (---) Regression Line Calculated from Thermodynamic Data.

Table 23. Thermodynamic Data for the NH_4NO_3 Equilibrium at 306.6 K[a]

	Derived from Experimental Data[b]	Calculated from Thermodynamic Data[c]
Free-energy Change, kcal/mol	22.08 (±0.12)	21.78
Enthalpy Change, kcal/mol	30 (±12)	43.79

[a]Average of all temperatures in these experiments.

[b]The temperature and free-energy change are the means of the 54 observations. Enthalpy is calculated from the slope of the unweighted regression line. The uncertainties in parentheses are 95% confidence intervals.

[c]Calculated at 306.6 K from heat of formation data given by JANAF Tables (Stull and Prophet, 1971) and by Wagman et al. (1968) using gas heat capacities from Benson (1968) and solid heat capacities from Wagman et al. (1968). The small heat of transition contribution for NH_4NO_3 at 305.4 K was included (ΔH = 0.410 kcal/mol).

The free-energy change is calculated from the mean of all our observations, and this quantity is thus both much more precise than the enthalpy change and less sensitive to systematic temperature errors. The very good agreement (see Table 23) between the free-energy change calculated from our NH_3 and HNO_3 data and that from tabulated thermodynamic data may be somewhat fortuitous; the presence of possible bias due to several factors such as lack of ammonium nitrate saturation for some air samples or errors in temperature measurements cannot be ruled out. Surface effects would tend to lower the experimental free-energy change, but the characteristic particle size of nitrate in the eastern end of the South Coast Air Basin is fairly large (e.g., ~0.5 m) and particle destabilization due to the free energy of the surface should be negligible (i.e., <0.02 kcal/mol). Moreover, most ammonium nitrate containing particles in a polluted atmosphere are probably impure, and the adsorption of impurities and water vapor tends to reduce thermodynamic surface effects.

Stelson et al. (1979) compared the NH_4NO_3 equilibrium constant calculated from thermodynamic data to some gas-phase HNO_3 and NH_3 data collected at West Covina by Spicer (1974). Although no equilibrium constant was calculated from the experimental data, a plot showed reasonable agreement with the equilibrium constant from thermodynamic data (Stelson et al., 1979)

and with NH_4NO_3 dissociation pressure measurements by Brandner et al. (1962). Since experimental data presented here were obtained at a mean temperature of 306.6 K, a small heat of transition for a NH_4NO_3 phase change at 305.4 K was included in the calculations using thermodynamic data (see Table 23). The experimental data and thermodynamics calculations presented here are in good agreement with the conclusions of Stelson et al. (1979) and support the hypothesis that gaseous ammonia and nitric acid are in equilibrium with solid ammonium nitrate in the atmosphere.

The probable existence of this equilibrium in a polluted atmosphere has direct utility for the calculation of particulate nitrate concentrations from chemical models. However, its implications for nitrate-sampling artifacts are unclear. Transfer of ammonium nitrate to and from a filter sample via the precursors involves a fairly complex mass transfer process at the interface; the rate of this process seems quite sensitive to surface conditions. In a few experiments it was found that impure nitrate in atmospheric filter samples volatilized into a simulated sampling flow of precursor-free air much more slowly than pure ammonium nitrate on a filter (Meserole, 1978; Mischke, 1979). Inhibition of volatilization implies inhibition of condensation, and thus further investigation into nitrate sampling artifacts is needed.

Conclusion. Although subject to uncertainties in temperature and in particulate composition for individual air samples, our observations support the hypothesis that particulate ammonium nitrate is in equilibrium with its precursors, ammonia and nitric acid. Atmospheric measurements under more carefully controlled conditions and a precise, direct determination of the thermodynamic data for Reaction 1 would be required for complete confirmation. Nonetheless, the ammonium nitrate equilibrium constant derived from tabulated thermochemical data is consistent with our atmospheric measurements of NH_3 and HNO_3 and is of direct utility in atmospheric models for calculating particle nitrate concentrations.

VII. REFERENCES

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APPENDIX C

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BAG-101
DUAL OUTDOOR BAG DMAE SURROGATE RUN #1
1979 APR 4

TIME (PDT)
0600-0820 BAG # 11 (WITH NO DIVIDING BAR) FILLED WITH CHAMBER PURE AIR.
BAG VOLUME IS APPROXIMATELY 48 CUBIC METERS
0800 BAG COVERED
0930,1015,&1107 200 MICROLITERS (U-L) DMAE INJECTED
(3.1 PPM IN BAG, CALCULATED)
1310 16 ML NO INJECTED
1312 4 ML NO2 INJECTED
1516 BAG UNCOVERED
1723-1746 HI VOL (FREE FLOW) USED TO EMPTY CONTENTS (APP 40 CUBIC METERS)
1130 RH IS 34% AT 32.5 DEG C (OUTDOOR TEMPERATURE)

GC-MS SAMPLES TAKEN:
1004-1014 #1 (5.0 L)
1453-1504 #2 & #3 (BACKUP) (5.9 L)
1540-1600 #4 & #4' (BACKUP) (4.6 L)
1711-1741 #5 & #5' (BACKUP) (5.5 L)
DASIBI 1790 AND BENDIX USED

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1200 PDT

TS	DEG K	AVERAGE	300.3
UV		AVERAGE	0.004

* ASSIGNED INITIAL CONDITION

BAG-101
DUAL OUTDOOR BAG CMAE SURROGATE RUN #1
1979 APR 4

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DASIBI	OZONE PPM BENDIX	NO PPM	NO2-CORR PPM	NOX-CORR PPM
842	-198.	0.018	0.003	0.0	0.002	0.007
855	-185.	******	******	******	******	******
920	-160.	******	******	******	******	******
949	-131.	0.037	0.003	0.0	0.003	0.0
955	-125.	******	******	******	******	******
1035	-85.	0.011	0.001	0.0	0.0	0.003
1055	-65.	******	******	******	******	******
1124	-36.	0.028	0.001	0.0	0.0	0.0
1130	-30.	******	******	******	******	******
1155	-5.	******	******	******	******	******
1215	15.	******	******	******	******	******
1230	30.	******	******	******	******	******
1255	55.	******	******	******	******	******
1325	85.	0.005	0.002	0.322	0.078	0.384
1350	110.	******	******	******	******	******
1400	120.	0.004	0.005	0.278	0.076	0.340
1415	135.	******	******	******	******	******
1430	150.	0.011	0.004	0.249	0.078	0.318
1500	180.	0.015	0.001	******	******	******
1530	210.	0.028	0.003	0.246	0.086	0.321
1600	240.	******	******	******	******	******
1605	245.	0.047	0.004	******	******	******
1630	270.	0.047	0.004	0.247	0.111	0.345
1645	285.	******	******	******	******	******
1700	300.	0.041	0.005	0.257	0.120	0.357
1734	334.	0.040	0.002	0.315	0.120	0.413

BAG-101
DUAL OUTDOOR BAG DMAE SURROGATE RUN #1
1979 APR 4

CLOCK TIME	ELAPSED T(MIN)	DMAE PPM	ACETALD PPM	PROPALD PPM	ACETONE PPM	MEK PPM	METHANE PPM	ETHANE PPM	ETHENE PPM	ACETYLEN PPM PN	ACETYLEN PPM DMS	PROPANE PPM	PROPENE PPM	I-C4 PPM
842	-198.	******	******	******	******	******	******	******	******	******	******	******	******	******
855	-185.	******	0.007	0.0003	0.0013	0.0005	1.42	0.0047	0.0094	0.0017	0.0014	0.0018	0.001	0.0004
920	-160.	0.0005	******	******	******	******	******	******	******	******	******	******	******	******
949	-131.	******	******	******	******	******	******	******	******	******	******	******	******	******
955	-125.	0.0008	******	******	******	******	******	******	******	******	******	******	******	******
1035	-85.	0.0074	******	******	******	******	******	******	******	******	******	******	******	******
1055	-65.	0.0473	******	******	******	******	******	******	******	******	******	******	******	******
1124	-36.	******	******	******	******	******	******	******	******	******	******	******	******	******
1130	-30.	0.2898	******	******	******	******	******	******	******	******	******	******	******	******
1155	-5.	0.6444	******	******	******	******	******	******	******	******	******	******	******	******
1215	15.	0.7495	******	******	******	******	******	******	******	******	******	******	******	******
1230	30.	0.7615	******	******	******	******	******	******	******	******	******	******	******	******
1255	55.	0.7987	******	******	******	******	******	******	******	******	******	******	******	******
1325	85.	0.8049	******	******	******	******	******	******	******	******	******	******	******	******
1350	110.	0.7881	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	******	******	******	******	******	******	******	******	******	******	******	******
1415	135.	0.7975	******	******	******	******	******	******	******	******	******	******	******	******
1430	150.	0.7721	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	0.005	******	0.0011	0.0003	1.41	0.0038	0.0184	0.0011	0.0010	0.0015	0.000	0.0002
1530	210.	0.7938	******	******	******	******	******	******	******	******	******	******	******	******
1600	240.	0.6847	******	******	******	******	******	******	******	******	******	******	******	******
1605	245.	******	******	******	******	******	******	******	******	******	******	******	******	******
1630	270.	0.7636	******	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	0.007	0.0003	0.0015	0.0005	1.47	0.0057	0.0058	0.0021	0.0020	0.0036	0.000	0.0009
1700	300.	******	******	******	******	******	******	******	******	******	******	******	******	******
1734	334.	******	******	******	******	******	******	******	******	******	******	******	******	******

BAG-101
DUAL OUTDOOR BAG DMAE SURROGATE RUN #1
1979 APR 4

CLOCK TIME	ELAPSED T(MIN)	N-C4 PPM	1-C4= PPM	I-C5 PPM	BENZENE PPM	TOLUENE PPM
842	-198.	******	******	******	******	******
855	-185.	0.001	0.0002	0.0013	0.0004	0.001
920	-160.	******	******	******	******	******
949	-131.	******	******	******	******	******
955	-125.	******	******	******	******	******
1035	-85.	******	******	******	******	******
1055	-65.	******	******	******	******	******
1124	-36.	******	******	******	******	******
1130	-30.	******	******	******	******	******
1155	-5.	******	******	******	******	******
1215	15.	******	******	******	******	******
1230	30.	******	******	******	******	******
1255	55.	******	******	******	******	******
1325	85.	******	******	******	******	******
1350	110.	******	******	******	******	******
1400	120.	******	******	******	******	******
1415	135.	******	******	******	******	******
1430	150.	******	******	******	******	******
1500	180.	0.000	0.0002	0.0003	0.0002	0.000
1530	210.	******	******	******	******	******
1600	240.	******	******	******	******	******
1605	245.	******	******	******	******	******
1630	270.	******	******	******	******	******
1645	285.	0.002	0.0	0.0019	0.0004	0.001
1700	300.	******	******	******	******	******
1734	334.	******	******	******	******	******

BAG-101
DUAL OUTDOOR BAG DMAE SUPROGATE RUN #1
1979 APR 4

CLOCK TIME	ELAPSED T(MIN)	B-SCAT *	CONDENS. *	AEROSL N *	AEROSL S *	AEROSL V *	TS DEG F	UV *
842	-198.	0.40	0.0	2.47	0.54	2.10	71.5	******
855	-185.	******	******	******	******	******	******	******
920	-160.	******	******	******	******	******	******	******
949	-131.	0.30	3.00	9.09	0.99	1.73	77.1	******
955	-125.	******	******	******	******	******	******	******
1035	-85.	0.30	3.90	9.37	2.38	5.79	81.4	******
1055	-65.	******	******	******	******	******	******	******
1124	-36.	0.30	3.40	9.03	2.85	8.03	81.9	******
1130	-30.	******	******	******	******	******	******	******
1155	-5.	******	******	******	******	******	******	******
1215	15.	******	******	******	******	******	******	******
1230	30.	******	******	******	******	******	******	******
1255	55.	******	******	******	******	******	******	******
1325	85.	0.70	11.00	24.10	8.78	27.10	83.9	******
1350	110.	******	******	******	******	******	******	******
1400	120.	0.55	8.50	22.10	7.93	26.00	83.6	******
1415	135.	******	******	******	******	******	******	******
1430	150.	0.80	8.00	19.50	8.26	28.60	84.3	******
1500	180.	0.85	8.00	19.90	8.47	31.30	83.0	.00610
1530	210.	4.00	8.50	20.90	23.00	138.00	82.1	.00510
1600	240.	******	******	******	******	******	******	******
1605	245.	13.00	8.00	19.40	28.90	208.00	80.7	.00400
1630	270.	18.00	7.50	15.90	32.20	244.00	78.3	.00280
1645	285.	******	******	******	******	******	******	******
1700	300.	20.00	6.80	17.20	30.80	238.00	77.1	.00130
1734	334.	21.00	5.50	12.20	28.60	218.00	74.9	.00190

BAG-102
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2
1979 APR 19

0600-0800 BAG # 11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM
BAG VOLUME APPROXIMATELY 44 CUBIC METERS
0745 BAG COVERED
0822 RH IS 14% AT 20 DEG C
0925-0940 400 MICROLITERS (U-L) DMAE INJECTED AND MIXED
(2.2 PPM IN BAG, CALCULATED)
1138 11.0 ML NO2 INJECTED AND MIXED
1142 11.0 ML NO INJECTED AND MIXED
1344 BAG UNCOVERED
1715-1731 BAG EMPTIED WITH A HIGH VOL RUNNING FREE (APP 65 CFM)
1150-1700 GAS PHASE DIRECT EXPOSURE TO MUTAGEN TESTING PLATES (1.6 LPM)
TENAX GC-MS SAMPLES TAKEN
0855-0905 (0.67 L)
1210-1220 (0.99 L)
1325-1337 (0.59 L)
1410-1420 (1.04 L)
1508-1518 (1.06 L)
1527-1557 (4.5 L)
1608-1618 (0.87 L)
1624-1649 (5.0 L)

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1200 PDT

TS	DEG K	AVERAGE	300.2
UV		AVERAGE	0.004

* ASSIGNED INITIAL CONDITION

BAG-102
DUAL OUTDOOR BAG CMAE SURROGATE RUN#2
1979 APR 19

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM	OZONE PPM BENDIX	NO PPM	NO2-CORR PPM	NOX-CORR PPM
820	-220.	******	******	******	******	******
825	-215.	0.007	0.011	0.0	0.0	0.0
1025	-95.	******	******	******	******	******
1040	-80.	0.016	0.002	0.0	0.0	0.0
1050	-70.	******	******	******	******	******
1110	-50.	******	******	******	******	******
1150	-10.	******	******	******	******	******
1200	0.	0.015	0.002	0.300	0.270	0.543
1220	20.	******	******	******	******	******
1230	30.	0.005	0.003	0.269	0.243	0.491
1250	50.	******	******	******	******	******
1305	65.	0.015	0.003	0.280	0.264	0.510
1320	80.	******	******	******	******	******
1335	95.	0.0	0.003	0.282	0.251	0.508
1400	120.	******	0.006	0.281	0.233	0.500
1430	150.	******	0.005	0.261	0.210	0.455
1500	180.	0.002	0.006	0.231	0.200	0.415
1505	185.	******	******	******	******	******
1535	215.	0.005	0.006	0.196	0.191	0.369
1600	240.	0.005	0.008	0.180	0.200	0.360
1630	270.	0.002	0.007	0.175	0.229	0.383
1700	300.	******	******	******	******	******
1701	301.	0.007	0.004	0.195	0.272	0.448

BAG-102
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2
1979 APR 19

CLOCK TIME	ELAPSED T(MIN)	DMAE PPM	ACETALD PPM	ACETONE PPM	MEK PPM	METHANE PPM	ETHANE PPM	ETHENE PPM	ACETYLEN PPM PN	ACETYLEN PPM DMS	PROPANE PPM	PROPENE PPM	I-C4 PPM	N-C4 PPM
820	-220.	0.0022	0.005	0.0025	0.0018	1.46	0.0040	0.0046	0.0025	0.0017	0.0022	0.000	0.0004	0.001
825	-215.	******	******	******	******	******	******	******	******	******	******	******	******	******
1025	-95.	0.2882	******	******	******	******	******	******	******	******	******	******	******	******
1040	-80.	******	******	******	******	******	******	******	******	******	******	******	******	******
1050	-70.	0.4961	******	******	******	******	******	******	******	******	******	******	******	******
1110	-50.	0.5579	******	******	******	******	******	******	******	******	******	******	******	******
1150	-10.	0.4846	******	******	******	******	******	******	******	******	******	******	******	******
1200	0.	******	******	******	******	******	******	******	******	******	******	******	******	******
1220	20.	0.5136	******	******	******	******	******	******	******	******	******	******	******	******
1230	30.	******	******	******	******	******	******	******	******	******	******	******	******	******
1250	50.	0.5319	******	******	******	******	******	******	******	******	******	******	******	******
1305	65.	******	******	******	******	******	******	******	******	******	******	******	******	******
1320	80.	0.5683	******	******	******	******	******	******	******	******	******	******	******	******
1335	95.	******	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	0.5314	******	******	******	******	******	******	******	******	******	******	******	******
1430	150.	0.5080	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	******	******	******	******	******	******	******	******	******	******	******	******
1505	185.	0.4555	******	******	******	******	******	******	******	******	******	******	******	******
1535	215.	0.4555	******	******	******	******	******	******	******	******	******	******	******	******
1600	240.	0.4358	******	******	******	******	******	******	******	******	******	******	******	******
1630	270.	0.4166	******	******	******	******	******	******	******	******	******	******	******	******
1700	300.	0.3943	0.012	0.0041	******	1.48	0.0045	0.0049	0.0023	0.0017	******	0.000	0.0007	0.001
1701	301.	******	******	******	******	******	******	******	******	******	******	******	******	******

BAG-102
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2
1979 APR 19

CLOCK TIME	ELAPSED T(MIN)	1-C4= PPM	I-C4= PPM	I-C5 PPM	N-C5 PPM	BENZENE PPM
820	-220.	0.0002	0.0001	0.0011	0.0003	0.0004
825	-215.	******	******	******	******	******
1025	-95.	******	******	******	******	******
1040	-80.	******	******	******	******	******
1050	-70.	******	******	******	******	******
1110	-50.	******	******	******	******	******
1150	-10.	******	******	******	******	******
1200	0.	******	******	******	******	******
1220	20.	******	******	******	******	******
1230	30.	******	******	******	******	******
1250	50.	******	******	******	******	******
1305	65.	******	******	******	******	******
1320	80.	******	******	******	******	******
1335	95.	******	******	******	******	******
1400	120.	******	******	******	******	******
1430	150.	******	******	******	******	******
1500	180.	******	******	******	******	******
1505	185.	******	******	******	******	******
1535	215.	******	******	******	******	******
1600	240.	******	******	******	******	******
1630	270.	******	******	******	******	******
1700	300.	0.0	0.0002	0.0012	0.0003	0.0007
1701	301.	******	******	******	******	******

BAG-102
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2
1979 APR 19

CLOCK TIME	ELAPSED T(MIN)	B-SCAT *	CONDENS. *	AEROSL N *	AEROSL S *	AEROSL V *	TS DEG F	UV *
820	-220.	******	******	******	******	******	******	******
825	-215.	0.30	0.15	2.84	0.66	2.66	67.7	******
1025	-95.	******	******	******	******	******	******	******
1040	-80.	0.40	19.50	44.00	10.30	26.60	******	******
1050	-70.	******	******	******	******	******	******	******
1110	-50.	******	******	******	******	******	******	******
1150	-10.	******	******	******	******	******	******	******
1200	0.	1.40	40.00	91.40	34.00	111.40	81.2	******
1220	20.	******	******	******	******	******	******	******
1230	30.	1.50	31.00	85.00	31.00	100.20	85.7	******
1250	50.	******	******	******	******	******	******	******
1305	65.	1.60	27.00	66.20	28.90	101.00	82.1	******
1320	80.	******	******	******	******	******	******	******
1335	95.	1.60	23.00	60.40	28.30	100.00	******	******
1400	120.	10.50	23.00	52.40	73.40	408.00	82.1	.00460
1430	150.	24.00	20.00	42.90	100.70	780.00	******	.00420
1500	180.	37.50	19.00	40.60	95.00	688.00	83.0	.00410
1505	185.	******	******	******	******	******	******	******
1535	215.	48.00	19.00	32.80	93.10	706.00	******	.00380
1600	240.	51.00	18.00	31.10	89.50	698.00	81.2	.00420
1630	270.	55.00	13.00	25.40	79.70	632.00	******	.00270
1700	300.	******	******	******	******	******	******	******
1701	301.	55.00	16.00	23.90	72.60	589.00	69.5	.00230

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    BAG-103
    DUAL OUTDOOR DAG DMAE SURROGATE RUN #3
    1979 OCT 16

TIMES (PDT)
0600-0750 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM
                BAG VOLUME IS APPROXIMATELY 44 CUBIC METERS
0800      BAG COVERED
0832      RH IS 30% AT 19 DEG C
0905      5.5 ML NO INJECTED AND MIXED
0908      2.0 ML NO2 INJECTED AND MIXED
0915      17.5 MICROLITERS(U-L) 2.3DMB INJECTED
0922      540 ML SURROGATE J INJECTED
0927      2.3 U-L TOLUENE, 2.0 U-L 2MEC4-2, 6.7 U-L M-XYLENE INJECTED
0935      BAG MIXED THOROUGHLY AND DIVIDED
1000      12.24 U-L DMAE INJECTED INTO SIDE 1 AND MIXED
     (0.14 PPM IN BAG, CALCULATED)
1156      BAG UNCOVERED
1648-1652 SIDE 1 EMPTIED WITH FREE-RUNNING HI-VOL SAMPLER TIGF (WASHED) FILTER
TENAX GC-MS SAMPLES:
BAG UNDIVIDED:          0949-1014 (15.0 L)
SIDE 1                  1125-1142 (15.0 L)
                        1412-1435 (15.0 L)
                        1608-1633 (15.0 L)
SIDE 2                  1106-1121 (15.0 L)
                        1437-1501 (15.1 L)
                        1634-1654 (15.0 L)

*MEASUREMENTS SC MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:
  B-SCAT                (METERS-1)                    X E+4
  CONDENSATION NUCLEI   (PART/CUBIC CM)               X E-3
  AEROSOL NUMBER        (PART/CUBIC CM)               X E-3
  AEROSOL SURFACE       (U-METERS2/CUBIC CM)          X E-2
  AEROSOL VOLUME        (CUBIC U-METERS/CUBIC CM)     X 1
  UV                    (CAL/CM2-MIN)                 X 1

T=0 AT 1200 PDT


   TS      DEG K    AVERAGE          300.1
   UV               AVERAGE          0.003

   *   ASSIGNED INITIAL CONDITION
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BAG-103
DUAL OUTDOOR BAG DMAE SUPROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM SIDE 1	NOX-CORR PPM SIDE 2
830	-210.	******	******	******	******	******	******	******	******	******	******
832	-208.	******	0.0	******	0.0	******	0.003	******	0.005	******	0.010
850	-190.	******	******	******	******	******	******	******	******	******	******
936	-144.	******	0.0	******	0.0	******	0.131	******	0.069	******	0.192
945	-135.	******	******	******	******	******	******	******	******	******	******
952	-128.	0.007	******	0.0	******	0.134	******	0.068	******	0.193	******
1015	-105.	******	0.012	******	0.0	******	0.130	******	0.066	******	0.189
1028	-92.	0.019	******	0.0	******	0.131	******	0.071	******	0.193	******
1045	-75.	******	0.001	******	0.001	******	0.129	******	0.067	******	0.188
1051	-69.	******	******	******	******	******	******	******	******	******	******
1056	-64.	0.006	******	0.0	******	0.130	******	0.070	******	0.191	******
1110	-50.	******	******	******	******	******	******	******	******	******	******
1115	-45.	******	0.003	******	0.001	******	0.127	******	0.068	******	0.187
1118	-42.	******	******	******	******	******	******	******	******	******	******
1126	-34.	0.014	******	0.001	******	0.128	******	0.069	******	0.189	******
1139	-21.	******	******	******	******	******	******	******	******	******	******
1145	-15.	******	******	******	******	******	******	******	******	******	******
1200	0.	******	0.022	******	0.008	******	0.121	******	0.071	******	0.184
1214	14.	0.012	******	0.008	******	0.105	******	0.088	******	0.185	******
1230	30.	******	0.016	******	0.011	******	0.091	******	0.096	******	0.182
1237	37.	0.032	******	0.016	******	0.081	******	0.107	******	0.170	******
1300	60.	******	0.030	******	0.022	******	0.058	******	0.121	******	0.173
1306	66.	******	******	******	******	******	******	******	******	******	******
1314	74.	0.036	******	0.040	******	0.034	******	0.139	******	0.165	******
1315	75.	******	******	******	******	******	******	******	******	******	******
1321	81.	******	******	******	******	******	******	******	******	******	******
1330	90.	******	0.036	******	0.037	******	0.043	******	0.135	******	0.165
1340	100.	0.101	******	0.082	******	0.015	******	0.129	******	0.140	******
1345	105.	******	******	******	******	******	******	******	******	******	******
1400	120.	******	0.055	******	0.052	******	0.020	******	0.141	******	0.159
1413	133.	******	******	******	******	******	******	******	******	******	******
1414	134.	0.122	******	0.126	******	0.010	******	0.099	******	0.109	******
1430	150.	******	0.075	******	0.087	******	0.020	******	0.130	******	0.152
1438	158.	******	******	******	******	******	******	******	******	******	******
1500	180.	0.197	******	0.210	******	0.007	******	0.065	******	0.080	******
1502	182.	******	******	******	******	******	******	******	******	******	******
1507	187.	******	******	******	******	******	******	******	******	******	******
1514	194.	******	0.099	******	0.104	******	0.012	******	0.128	******	0.145
1524	204.	0.225	******	0.231	******	0.007	******	0.048	******	0.072	******
1535	215.	******	0.109	******	0.113	******	0.010	******	0.139	******	0.144
1539	219.	******	******	******	******	******	******	******	******	******	******
1545	225.	******	******	******	******	******	******	******	******	******	******
1546	226.	0.232	******	0.243	******	0.007	******	0.042	******	0.067	******
1600	240.	******	0.119	******	0.213	******	0.009	******	0.126	******	0.139
1602	242.	******	******	******	******	******	******	******	******	******	******
1609	249.	0.238	******	0.250	******	0.007	******	0.034	******	0.061	******
1615	255.	******	******	******	******	******	******	******	******	******	******
1635	275.	******	0.111	******	0.128	******	0.009	******	0.122	******	0.135
1639	279.	******	******	******	******	******	******	******	******	******	******
1645	285.	******	******	******	******	******	******	******	******	******	******
1702	302.	******	******	******	******	******	******	******	******	******	******

BAG-103
DUAL OUTDOOR DAG DMAE SURROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	DMAE PPM SIDE 1	DMAE PPM SIDE 2	PAN PPM SIDE 1	PAN PPM SIDE 2	ACETALD PPM SIDE 1	ACETALD PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	MEK PPM SIDE 1	MEK PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2
830	-210.	******	******	******	******	0.002	0.002	0.0004	0.0004	0.0007	0.0007	1.57	1.57
832	-208.	******	******	******	0.0	******	******	******	******	******	******	******	******
850	-190.	******	******	******	******	******	******	******	******	******	******	******	******
936	-144.	******	******	******	0.0	******	******	******	******	******	******	******	******
945	-135.	******	******	******	******	******	******	0.0021	0.0021	******	******	1.76	1.76
952	-128.	******	******	0.0	******	******	******	******	******	******	******	******	******
1015	-105.	******	******	******	0.0	******	******	******	******	******	******	******	******
1028	-92.	******	******	0.0	******	******	******	******	******	******	******	******	******
1045	-75.	******	******	******	0.0	******	******	******	******	******	******	******	******
1051	-69.	******	0.0	******	******	******	******	******	******	******	******	******	******
1056	-64.	0.0726	******	0.0	******	******	******	******	******	******	******	******	******
1110	-50.	******	******	******	******	******	******	******	0.0043	******	******	******	1.75
1115	-45.	******	******	******	0.0	******	******	******	******	******	******	******	******
1118	-42.	0.0764	******	******	******	******	******	******	******	******	******	******	******
1126	-34.	******	******	0.0	******	******	******	******	******	******	******	******	******
1139	-21.	0.0826	******	******	******	******	******	******	******	******	******	******	******
1145	-15.	******	******	******	******	******	******	0.0062	******	0.0004	******	1.76	******
1200	0.	******	******	******	0.0	******	******	******	******	******	******	******	******
1214	14.	******	******	0.0	******	******	******	******	******	******	******	******	******
1230	30.	******	******	******	0.0	******	******	******	0.0096	******	0.0011	******	1.75
1237	37.	******	******	0.0	******	******	******	******	******	******	******	******	******
1300	60.	******	******	******	0.000	******	******	******	******	******	******	******	******
1306	66.	******	0.0	******	******	******	******	******	******	******	******	******	******
1314	74.	******	******	0.000	******	******	******	******	******	******	******	******	******
1315	75.	******	******	******	******	******	******	0.0111	******	0.0013	******	******	******
1321	81.	0.0298	******	******	******	******	******	******	******	******	******	******	******
1330	90.	******	******	******	0.001	******	******	******	******	******	******	******	******
1340	100.	******	******	0.001	******	******	******	******	******	******	******	******	******
1345	105.	0.0226	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	******	******	0.001	******	******	******	0.0170	******	0.0028	******	******
1413	133.	0.0157	******	******	******	******	******	******	******	******	******	******	******
1414	134.	******	******	0.002	******	******	******	******	******	******	******	******	******
1430	150.	******	******	******	0.002	******	******	******	******	******	******	******	******
1438	158.	0.0116	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	******	0.003	******	******	******	******	******	******	******	******	******
1502	182.	******	******	******	******	******	******	******	******	******	******	******	******
1507	187.	******	******	******	******	0.770	******	0.0339	******	0.0062	******	******	******
1514	194.	******	******	******	0.003	******	******	******	******	******	******	******	******
1524	204.	******	******	0.006	******	******	******	******	******	******	******	******	******
1535	215.	******	******	******	0.003	******	******	******	******	******	******	******	******
1539	219.	0.0065	******	******	******	******	******	******	******	******	******	******	******
1545	225.	******	******	******	******	******	0.720	******	0.0227	******	0.0048	******	******
1546	226.	******	******	0.006	******	******	******	******	******	******	******	******	******
1600	240.	******	******	******	0.003	******	******	******	******	******	******	******	******
1602	242.	0.0047	******	******	******	******	******	******	******	******	******	******	******
1609	249.	******	******	0.006	******	******	******	******	******	******	******	******	******
1615	255.	******	******	******	******	0.703	******	0.0225	******	0.0036	******	1.71	******
1635	275.	******	******	******	0.003	******	******	******	******	******	******	******	******
1639	279.	0.0015	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	******	******	******	******	0.697	******	0.0278	******	0.0060	******	1.73
1702	302.	******	0.0	******	******	******	******	******	******	******	******	******	******

BAG-103
DUAL OUTDOOR BAG CMAE SURROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2	ACETYLEN PPM PN-1	ACETYLEN PPM PN-2	ACETYLEN PPM DMS-1	ACETYLEN PPM DMS-2	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2
830	-210.	******	******	0.0038	0.0038	0.0028	0.0028	0.0033	0.0033	0.0272	0.0272	0.001	0.001
832	-208.	******	******	******	******	******	******	******	******	******	******	******	******
850	-190.	0.0579	0.0579	******	******	******	******	******	******	******	******	******	******
936	-144.	******	******	******	******	******	******	******	******	******	******	******	******
945	-135.	0.1338	0.1338	0.0399	0.0399	0.0383	0.0383	0.0430	0.0430	0.0397	0.0397	0.013	0.013
952	-128.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-105.	******	******	******	******	******	******	******	******	******	******	******	******
1028	-92.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1051	-69.	******	******	******	******	******	******	******	******	******	******	******	******
1056	-64.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-50.	******	0.1385	******	0.0317	******	0.0466	******	0.0447	******	0.0410	******	0.013
1115	-45.	******	******	******	******	******	******	******	******	******	******	******	******
1118	-42.	******	******	******	******	******	******	******	******	******	******	******	******
1126	-34.	******	******	******	******	******	******	******	******	******	******	******	******
1139	-21.	******	******	******	******	******	******	******	******	******	******	******	******
1145	-15.	0.1356	******	0.0430	******	0.0460	******	0.0452	******	0.0410	******	0.013	******
1200	0.	******	******	******	******	******	******	******	******	******	******	******	******
1214	14.	******	******	******	******	******	******	******	******	******	******	******	******
1230	30.	******	0.1360	******	0.0418	******	0.0453	******	0.0439	******	0.0406	******	0.012
1237	37.	******	******	******	******	******	******	******	******	******	******	******	******
1300	60.	******	******	******	******	******	******	******	******	******	******	******	******
1306	66.	******	******	******	******	******	******	******	******	******	******	******	******
1314	74.	******	******	******	******	******	******	******	******	******	******	******	******
1315	75.	0.1352	******	0.0416	******	0.0442	******	0.0443	******	0.0408	******	0.011	******
1321	81.	******	******	******	******	******	******	******	******	******	******	******	******
1330	90.	******	******	******	******	******	******	******	******	******	******	******	******
1340	100.	******	******	******	******	******	******	******	******	******	******	******	******
1345	105.	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	0.1327	******	0.0374	******	0.0438	******	0.0430	******	0.0397	******	0.008
1413	133.	******	******	******	******	******	******	******	******	******	******	******	******
1414	134.	******	******	******	******	******	******	******	******	******	******	******	******
1430	150.	******	******	******	******	******	******	******	******	******	******	******	******
1438	158.	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	******	******	******	******	******	******	******	******	******	******	******
1502	182.	******	******	******	******	******	******	******	******	******	******	******	******
1507	187.	******	******	******	******	******	******	0.0421	******	0.0368	******	0.005	******
1514	194.	******	******	******	******	******	******	******	******	******	******	******	******
1524	204.	******	******	******	******	******	******	******	******	******	******	******	******
1535	215.	******	******	******	******	******	******	******	******	******	******	******	******
1539	219.	******	******	******	******	******	******	******	******	******	******	******	******
1545	225.	******	0.1290	******	0.0331	******	0.0430	******	0.0426	******	0.0385	******	0.005
1546	226.	******	******	******	******	******	******	******	******	******	******	******	******
1600	240.	******	******	******	******	******	******	******	******	******	******	******	******
1602	242.	******	******	******	******	******	******	******	******	******	******	******	******
1609	249.	******	******	******	******	******	******	******	******	******	******	******	******
1615	255.	0.1323	******	0.0299	******	0.0442	******	0.0421	******	0.0393	******	0.003	******
1635	275.	******	******	******	******	******	******	******	******	******	******	******	******
1639	279.	******	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	0.1329	******	0.0400	******	0.0434	******	0.0400	******	0.0333	******	0.004
1702	302.	******	******	******	******	******	******	******	******	******	******	******	******

BAG-103
DUAL OUTDOOR DAG DMAE SURROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 1	N-C4 PPM SIDE 2	1-C4= PPM SIDE 1	1-C4= PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	T2-C4= PPM SIDE 1	T2-C4= PPM SIDE 2	I-C5 PPM SIDE 1	I-C5 PPM SIDE 2
830	-210.	0.0016	0.0016	0.001	0.001	0.0001	0.0001	0.0001	0.0001	******	******	0.0008	0.0008
832	-208.	******	******	******	******	******	******	******	******	******	******	******	******
850	-190.	******	******	******	******	******	******	******	******	******	******	******	******
936	-144.	******	******	******	******	******	******	******	******	******	******	******	******
945	-135.	0.0017	0.0017	0.197	0.197	0.0003	0.0003	0.0001	0.0001	0.0007	0.0007	0.0008	0.0008
952	-128.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-105.	******	******	******	******	******	******	******	******	******	******	******	******
1028	-92.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1051	-69.	******	******	******	******	******	******	******	******	******	******	******	******
1056	-64.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-50.	******	0.0017	******	0.200	******	0.0002	******	0.0002	******	0.0007	******	0.0005
1115	-45.	******	******	******	******	******	******	******	******	******	******	******	******
1118	-42.	******	******	******	******	******	******	******	******	******	******	******	******
1126	-34.	******	******	******	******	******	******	******	******	******	******	******	******
1139	-21.	******	******	******	******	******	******	******	******	******	******	******	******
1145	-15.	0.0017	******	0.202	******	0.0002	******	0.0002	******	0.0005	******	0.0005	******
1200	0.	******	******	******	******	******	******	******	******	******	******	******	******
1214	14.	******	******	******	******	******	******	******	******	******	******	******	******
1230	30.	******	0.0017	******	0.197	******	0.0001	******	0.0001	******	0.0005	******	0.0008
1237	37.	******	******	******	******	******	******	******	******	******	******	******	******
1300	60.	******	******	******	******	******	******	******	******	******	******	******	******
1306	66.	******	******	******	******	******	******	******	******	******	******	******	******
1314	74.	******	******	******	******	******	******	******	******	******	******	******	******
1315	75.	0.0017	******	0.199	******	0.0002	******	0.0001	******	0.0004	******	0.0005	******
1321	81.	******	******	******	******	******	******	******	******	******	******	******	******
1330	90.	******	******	******	******	******	******	******	******	******	******	******	******
1340	100.	******	******	******	******	******	******	******	******	******	******	******	******
1345	105.	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	0.0016	******	0.191	******	******	******	0.0001	******	0.0002	******	0.0006
1413	133.	******	******	******	******	******	******	******	******	******	******	******	******
1414	134.	******	******	******	******	******	******	******	******	******	******	******	******
1430	150.	******	******	******	******	******	******	******	******	******	******	******	******
1438	158.	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	******	******	******	******	******	******	******	******	******	******	******
1502	182.	******	******	******	******	******	******	******	******	******	******	******	******
1507	187.	0.0015	******	0.184	******	0.0002	******	0.0002	******	0.0001	******	0.0004	******
1514	194.	******	******	******	******	******	******	******	******	******	******	******	******
1524	204.	******	******	******	******	******	******	******	******	******	******	******	******
1535	215.	******	******	******	******	******	******	******	******	******	******	******	******
1539	219.	******	******	******	******	******	******	******	******	******	******	******	******
1545	225.	******	0.0016	******	0.183	******	0.0001	******	0.0001	******	0.0	******	0.0004
1546	226.	******	******	******	******	******	******	******	******	******	******	******	******
1600	240.	******	******	******	******	******	******	******	******	******	******	******	******
1602	242.	******	******	******	******	******	******	******	******	******	******	******	******
1609	249.	******	******	******	******	******	******	******	******	******	******	******	******
1615	255.	0.0017	******	0.182	******	0.0001	******	0.0002	******	0.0	******	0.0004	******
1635	275.	******	******	******	******	******	******	******	******	******	******	******	******
1639	279.	******	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	0.0016	******	0.176	******	0.0001	******	0.0001	******	0.0	******	0.0007
1702	302.	******	******	******	******	******	******	******	******	******	******	******	******

BAG-103
DUAL OUTDOOR BAG DMAE SURROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	CIS2-C4= PPM SIDE 1	CIS2-C4= PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2	2ME-C4=2 PPM SIDE 1	2ME-C4=2 PPM SIDE 2	2,3-DMB PPM SIDE 1	2,3-DMB PPM SIDE 2	TOLUENE PPM SIDE 1	TOLUENE PPM SIDE 2	M-XYL PPM SIDE 1	M-XYL PPM SIDE 2
830	-210.	******	******	0.0003	0.0028	******	******	******	******	0.000	0.000	0.0	0.0
832	-208.	******	******	******	******	******	******	******	******	******	******	******	******
850	-190.	******	******	******	******	******	******	******	******	******	******	******	******
936	-144.	******	******	******	******	******	******	******	******	******	******	******	******
945	-135.	0.0150	0.0150	0.0005	0.0005	0.0108	0.0108	0.0902	0.0902	0.015	0.015	0.0378	0.0378
952	-128.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-105.	******	******	******	******	******	******	******	******	******	******	******	******
1028	-92.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1051	-69.	******	******	******	******	******	******	******	******	******	******	******	******
1056	-64.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-50.	******	0.0148	******	0.0003	******	0.0099	******	0.0939	******	0.015	******	0.0376
1115	-45.	******	******	******	******	******	******	******	******	******	******	******	******
1118	-42.	******	******	******	******	******	******	******	******	******	******	******	******
1126	-34.	******	******	******	******	******	******	******	******	******	******	******	******
1139	-21.	******	******	******	******	******	******	******	******	******	******	******	******
1145	-15.	0.0149	******	0.0002	******	0.0099	******	0.0942	******	0.015	******	0.0382	******
1200	0.	******	******	******	******	******	******	******	******	******	******	******	******
1214	14.	******	******	******	******	******	******	******	******	******	******	******	******
1230	30.	******	0.0116	******	0.0003	******	0.0064	******	0.0911	******	0.015	******	0.0340
1237	37.	******	******	******	******	******	******	******	******	******	******	******	******
1300	60.	******	******	******	******	******	******	******	******	******	******	******	******
1306	66.	******	******	******	******	******	******	******	******	******	******	******	******
1314	74.	******	******	******	******	******	******	******	******	******	******	******	******
1315	75.	0.0088	******	0.0002	******	0.0025	******	0.0912	******	0.015	******	0.0340	******
1321	81.	******	******	******	******	******	******	******	******	******	******	******	******
1330	90.	******	******	******	******	******	******	******	******	******	******	******	******
1340	100.	******	******	******	******	******	******	******	******	******	******	******	******
1345	105.	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	0.0036	******	0.0002	******	0.0003	******	0.0850	******	0.014	******	0.0258
1413	133.	******	******	******	******	******	******	******	******	******	******	******	******
1414	134.	******	******	******	******	******	******	******	******	******	******	******	******
1430	150.	******	******	******	******	******	******	******	******	******	******	******	******
1438	158.	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	******	******	******	******	******	******	******	******	******	******	******	******
1502	182.	******	******	******	******	******	******	******	******	******	******	******	******
1507	187.	0.0002	******	0.0002	******	******	******	0.0807	******	0.013	******	0.0203	******
1514	194.	******	******	******	******	******	******	******	******	******	******	******	******
1524	204.	******	******	******	******	******	******	******	******	******	******	******	******
1535	215.	******	******	******	******	******	******	******	******	******	******	******	******
1539	219.	******	******	******	******	******	******	******	******	******	******	******	******
1545	225.	******	0.0003	******	0.0002	******	******	******	0.0793	******	0.011	******	0.0191
1546	226.	******	******	******	******	******	******	******	******	******	******	******	******
1600	240.	******	******	******	******	******	******	******	******	******	******	******	******
1602	242.	******	******	******	******	******	******	******	******	******	******	******	******
1609	249.	******	******	******	******	******	******	******	******	******	******	******	******
1615	255.	0.0	******	0.0001	******	******	******	0.0775	******	0.012	******	0.0159	******
1635	275.	******	******	******	******	******	******	******	******	******	******	******	******
1639	279.	******	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	0.0	******	0.0002	******	******	******	0.0786	******	0.012	******	0.0177
1702	302.	******	******	******	******	******	******	******	******	******	******	******	******

BAG-103
DUAL OUTDOOR BAG DMAE SURROGATE RUN #3
1979 OCT 16

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2	UV *
830	-210.	******	******	******	******	******	******	******	******	******	******	******	******	******
832	-208.	******	0.50	******	0.0	******	1.36	******	0.50	******	0.94	******	65.9	******
850	-190.	******	******	******	******	******	******	******	******	******	******	******	******	******
936	-144.	******	0.50	******	0.20	******	0.95	******	0.49	******	2.21	******	******	******
945	-135.	******	******	******	******	******	******	******	******	******	******	******	******	******
952	-128.	0.50	******	0.20	******	1.23	******	0.47	******	1.66	******	******	******	******
1015	-105.	******	0.60	******	0.40	******	1.38	******	0.42	******	1.97	******	71.3	******
1028	-92.	0.60	******	0.50	******	1.58	******	0.47	******	1.70	******	78.5	******	******
1045	-75.	******	0.60	******	0.60	******	1.78	******	0.55	******	2.18	******	74.9	******
1051	-69.	******	******	******	******	******	******	******	******	******	******	******	******	******
1056	-64.	0.50	******	0.50	******	2.06	******	1.02	******	8.58	******	78.5	******	******
1110	-50.	******	******	******	******	******	******	******	******	******	******	******	******	******
1115	-45.	******	0.60	******	0.60	******	1.74	******	0.96	******	3.77	******	80.3	******
1118	-42.	******	******	******	******	******	******	******	******	******	******	******	******	******
1126	-34.	0.60	******	0.50	******	1.87	******	0.46	******	1.89	******	83.9	******	******
1139	-21.	******	******	******	******	******	******	******	******	******	******	******	******	******
1145	-15.	******	******	******	******	******	******	******	******	******	******	******	******	******
1200	0.	******	0.70	******	0.60	******	1.85	******	0.46	******	1.86	******	74.9	.00370
1214	14.	0.70	******	38.00	******	90.09	******	15.70	******	34.70	******	80.3	******	******
1230	30.	******	0.70	******	0.20	******	2.13	******	0.57	******	2.52	******	82.1	.00390
1237	37.	1.00	******	34.00	******	82.70	******	27.70	******	72.00	******	78.5	******	******
1300	60.	******	0.60	******	0.80	******	0.99	******	0.54	******	2.54	******	78.5	.00410
1306	66.	******	******	******	******	******	******	******	******	******	******	******	******	******
1314	74.	2.60	******	30.00	******	72.60	******	50.60	******	188.00	******	82.1	******	******
1315	75.	******	******	******	******	******	******	******	******	******	******	******	******	******
1321	81.	******	******	******	******	******	******	******	******	******	******	******	******	******
1330	90.	******	0.60	******	1.00	******	1.42	******	0.48	******	2.15	******	78.5	.00350
1340	100.	7.10	******	26.00	******	68.30	******	73.00	******	343.00	******	78.5	******	******
1345	105.	******	******	******	******	******	******	******	******	******	******	******	******	******
1400	120.	******	0.70	******	0.90	******	1.52	******	0.59	******	3.24	******	78.5	.00380
1413	133.	******	******	******	******	******	******	******	******	******	******	******	******	******
1414	134.	15.70	******	23.00	******	59.10	******	90.40	******	506.00	******	80.3	******	******
1430	150.	******	0.70	******	1.60	******	0.95	******	0.51	******	2.53	******	80.3	.00330
1438	158.	******	******	******	******	******	******	******	******	******	******	******	******	******
1500	180.	15.40	******	19.00	******	34.70	******	80.90	******	484.00	******	83.9	******	.00300
1502	182.	******	******	******	******	******	******	******	******	******	******	******	******	******
1507	187.	******	******	******	******	******	******	******	******	******	******	******	******	******
1514	194.	******	0.80	******	0.60	******	0.71	******	0.67	******	4.23	******	83.9	******
1524	204.	13.00	******	17.70	******	38.00	******	64.60	******	383.00	******	82.1	******	******
1535	215.	******	0.60	******	1.10	******	1.12	******	0.55	******	2.38	******	80.3	.00260
1539	219.	******	******	******	******	******	******	******	******	******	******	******	******	******
1545	225.	******	******	******	******	******	******	******	******	******	******	******	******	******
1546	226.	11.00	******	16.00	******	34.10	******	56.80	******	336.00	******	78.5	******	******
1600	240.	******	0.60	******	1.10	******	2.19	******	0.76	******	3.12	******	78.5	.00180
1602	242.	******	******	******	******	******	******	******	******	******	******	******	******	******
1609	249.	9.00	******	13.20	******	29.60	******	47.80	******	277.00	******	80.3	******	******
1615	255.	******	******	******	******	******	******	******	******	******	******	******	******	******
1635	275.	******	0.60	******	1.40	******	1.61	******	0.77	******	3.44	******	76.7	.00140
1639	279.	******	******	******	******	******	******	******	******	******	******	******	******	******
1645	285.	******	******	******	******	******	******	******	******	******	******	******	******	******
1702	302.	******	******	******	******	******	******	******	******	******	******	******	******	******

BAG-104
OMAE SURROGATE RUN #4
1977 OCT 23

TIME (PDT)
0600-0738 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM
BAG VOLUME IS APPROXIMATELY 33 CUBIC METERS
0800 BAG COVERED
0830 RH IS 25% AT T=19 DEG C
0841 2.6 ML NO2 INJECTED AND MIXED
0843 7.3 ML NO INJECTED AND MIXED
0845 500 ML SURROGATE J INJECTED
0900 13.1 MICROLITERS(UL) 2,3DMB, 1.7 U-L TOLUENE, 1.5 U-L 2MEC4-2,
5.0 U-L M-XYLENE INJECTED
0910 BAG MIXED THOROUGHLY AND DIVIDED
0925 3.5 U-L OMAE INJECTED INTO SIDE 1
(0.05 PPM IN BAG, CALCULATED)
1140 BAG UNCOVERED
1703-1706 SIDE ONE EMPTIED WITH FREE RUNNING HI VOL SAMPLER
USED SOLVENT-WASHED TIGF FILTER #174
UPPER LIMIT OF HNO3 IS 0.010 PPM (USING NOX ANALYZER WITH
AND WITHOUT NYLON SCRUBBER)

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1140 PDT

TS	DEG K	AVERAGE	297.6
UV		AVERAGE	0.003

* ASSIGNED INITIAL CONDITION

BAG-104
DMAE SURROGATE RUN #4
1979 OCT 23

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM SIDE 1	NOX-CORR PPM SIDE 2
818	-202.	0.003	******	0.0	******	0.010	******	0.001	******	0.011	******
820	-200.	******	******	******	******	******	******	******	******	******	******
835	-185.	******	******	******	******	******	******	******	******	******	******
912	-148.	0.003	******	0.0	******	0.168	******	0.094	******	0.260	******
924	-136.	******	0.003	******	0.0	******	0.169	******	0.093	******	0.260
930	-130.	******	******	******	******	******	******	******	******	******	******
949	-111.	0.004	******	0.0	******	0.164	******	0.092	******	0.253	******
951	-109.	******	******	******	******	******	******	******	******	******	******
958	-102.	******	0.004	******	0.0	******	0.161	******	0.093	******	0.255
1010	-90.	******	******	******	******	******	******	******	******	******	******
1011	-89.	******	******	******	******	******	******	******	******	******	******
1012	-88.	******	******	******	******	******	******	******	******	******	******
1015	-85.	0.003	******	0.0	******	0.161	******	0.094	******	0.251	******
1025	-75.	******	0.004	******	0.0	******	0.161	******	0.095	******	0.250
1030	-70.	******	******	******	******	******	******	******	******	******	******
1045	-55.	0.002	******	0.0	******	0.167	******	0.095	******	0.257	******
1050	-50.	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	******	******	******	******	******	******	******	******	******
1057	-43.	******	******	******	******	******	******	******	******	******	******
1115	-25.	0.0	******	0.0	******	0.165	******	0.097	******	0.258	******
1116	-24.	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	0.004	******	0.0	******	0.163	******	0.098	******	0.255
1140	0.	******	******	******	******	******	******	******	******	******	******
1145	5.	0.010	******	0.008	******	0.008	******	0.099	******	0.251	******
1155	15.	******	0.011	******	0.010	******	0.150	******	0.102	******	0.249
1215	35.	0.010	******	0.001	******	0.001	******	0.126	******	0.243	******
1216	36.	******	******	******	******	******	******	******	******	******	******
1229	49.	******	0.010	******	0.010	******	0.120	******	0.130	******	0.243
1244	64.	******	******	******	******	******	******	******	******	******	******
1246	66.	0.013	******	0.010	******	0.010	******	0.146	******	0.240	******
1300	80.	******	0.013	******	0.009	******	0.092	******	0.150	******	0.230
1315	95.	0.026	******	0.012	******	0.012	******	0.160	******	0.234	******
1330	110.	******	0.016	******	0.016	******	0.082	******	0.156	******	0.232
1345	125.	0.024	******	0.024	******	0.024	******	0.167	******	0.226	******
1356	136.	******	0.024	******	0.016	******	0.061	******	0.170	******	0.229
1415	155.	0.025	******	0.024	******	0.043	******	0.188	******	0.220	******
1426	166.	******	0.020	******	0.015	******	0.048	******	0.173	******	0.219
1430	170.	******	******	******	******	******	******	******	******	******	******
1432	172.	******	******	******	******	******	******	******	******	******	******
1445	185.	0.032	******	0.024	******	0.035	******	0.186	******	0.206	******
1455	195.	******	0.015	******	0.018	******	0.041	******	0.185	******	0.218
1500	200.	******	******	******	******	******	******	******	******	******	******
1515	215.	0.040	******	0.036	******	0.036	******	0.180	******	0.209	******
1527	227.	******	0.030	******	0.032	******	0.041	******	0.182	******	0.212
1529	229.	******	******	******	******	******	******	******	******	******	******
1545	245.	0.038	******	0.040	******	0.021	******	0.186	******	0.197	******
1600	260.	******	0.026	******	0.028	******	0.031	******	0.189	******	0.208
1615	275.	0.045	******	0.049	******	0.021	******	0.178	******	0.193	******
1631	291.	******	0.030	******	0.031	******	0.025	******	0.183	******	0.199
1644	304.	0.046	******	0.048	******	0.018	******	0.187	******	0.193	******
1645	305.	******	******	******	******	******	******	******	******	******	******
1650	310.	******	0.029	******	0.029	******	0.021	******	0.145	******	0.158

BAG-104
DMAE SURROGATE RUN #4
1979 OCT 23

CLOCK TIME	ELAPSED T(MIN)	DMAE PPM SIDE 1	DMAE PPM SIDE 2	PAN PPM SIDE 1	PAN PPM SIDE 2	ACETALD PPM SIDE 1	ACETALD PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	MEK PPM SIDE 1	MEK PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2
918	-202.	******	******	0.0	******	******	******	******	******	******	******	******	******
820	-200.	******	******	******	******	0.003	0.003	0.0003	0.0003	******	******	1.33	1.33
835	-185.	0.0	0.0	******	******	******	******	******	******	******	******	******	******
912	-148.	******	******	0.0	******	******	******	******	******	******	******	******	******
924	-136.	******	******	******	0.0	******	******	******	******	******	******	******	******
930	-130.	******	******	******	******	******	******	******	0.0058	******	******	******	1.30
949	-111.	******	******	0.0	******	******	******	******	******	******	******	******	******
951	-109.	0.0109	******	******	******	******	******	******	******	******	******	******	******
958	-102.	******	******	******	0.0	******	******	******	******	******	******	******	******
1010	-90.	******	******	******	******	******	******	0.0068	******	******	******	1.33	******
1011	-89.	******	******	******	******	******	******	******	******	******	******	******	******
1012	-88.	0.0125	******	******	******	******	******	******	******	******	******	******	******
1015	-85.	******	******	0.0	******	******	******	******	******	******	******	******	******
1025	-75.	******	******	******	0.0	******	******	******	******	******	******	******	******
1030	-70.	0.0131	******	******	******	******	******	******	******	******	******	******	******
1045	-55.	******	******	0.0	******	******	******	******	******	******	******	******	******
1050	-50.	0.0160	******	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	******	******	******	******	******	******	0.0053	******	******	******	1.36
1057	-43.	******	******	******	******	******	******	******	******	******	******	******	******
1115	-25.	******	******	0.0	******	******	******	******	******	******	******	******	******
1116	-24.	0.0111	******	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	******	******	0.0	******	******	******	******	******	******	******	******
1140	0.	******	******	******	******	******	******	******	******	******	******	******	******
1145	5.	******	******	0.0	******	******	******	******	******	******	******	******	******
1155	15.	******	******	******	0.0	******	******	******	******	******	******	******	******
1215	35.	******	******	0.0	******	******	******	0.0080	******	******	******	1.30	******
1216	36.	0.0047	******	******	******	******	******	******	******	******	******	******	******
1229	49.	******	******	******	0.0	******	******	******	******	******	******	******	******
1244	64.	0.0055	******	******	******	******	******	******	******	******	******	******	******
1246	66.	******	******	0.0	******	******	******	******	******	******	******	******	******
1300	80.	******	******	******	0.0	******	******	******	0.0109	******	0.0015	******	1.30
1315	95.	0.0042	******	0.0	******	******	******	******	******	******	******	******	******
1330	110.	0.0038	******	******	0.0	******	******	******	******	******	******	******	******
1345	125.	0.0018	******	0.0	******	******	******	0.0119	******	0.0019	******	******	******
1356	136.	******	******	******	0.0	******	******	******	******	******	******	******	******
1415	155.	0.0026	******	0.000	******	******	******	******	******	******	******	******	******
1426	166.	******	******	******	0.000	******	******	******	******	******	******	******	******
1430	170.	******	******	******	******	******	******	******	0.0146	******	0.0025	******	******
1432	172.	0.0008	******	******	******	******	******	******	******	******	******	******	******
1445	185.	******	******	0.0	******	******	******	******	******	******	******	******	******
1455	195.	******	******	******	0.000	******	******	******	******	******	******	******	******
1500	200.	0.0011	******	******	******	******	******	******	******	******	******	******	******
1515	215.	******	******	0.0	******	******	******	0.0170	******	0.0027	******	******	******
1527	227.	******	******	******	0.000	******	******	******	******	******	******	******	******
1529	229.	0.0002	******	******	******	******	******	******	******	******	******	******	******
1545	245.	******	******	0.000	******	******	******	******	******	******	******	******	******
1600	260.	0.0003	******	******	0.000	******	******	******	0.0177	******	0.0036	******	1.30
1615	275.	******	******	0.001	******	******	******	******	******	******	******	******	******
1631	291.	******	******	******	0.000	******	******	******	******	******	******	******	******
1644	304.	******	******	0.001	******	******	******	******	******	******	******	******	******
1645	305.	******	0.0001	******	******	******	******	0.0175	******	0.0039	******	1.30	******
1650	310.	******	******	******	0.000	******	******	******	******	******	******	******	******

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DMAE SURROGATE RUN #4
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CLOCK TIME	ELAPSED T(MIN)	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2	ACETYLEN PPM PN-1	ACETYLEN PPM PN-2	ACETYLEN PPM DMS-1	ACETYLEN PPM DMS-2	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2
818	-202.	******	******	******	******	******	******	******	******	******	******	******	******
820	-200.	0.0106	0.0106	0.0066	0.0066	0.0024	0.0024	0.0025	0.0025	0.0230	0.0230	0.001	0.001
835	-185.	******	******	******	******	******	******	******	******	******	******	******	******
912	-148.	******	******	******	******	******	******	******	******	******	******	******	******
924	-136.	******	******	******	******	******	******	******	******	******	******	******	******
930	-130.	******	0.0812	******	0.0429	******	0.0419	******	0.0391	******	0.0330	******	0.011
949	-111.	******	******	******	******	******	******	******	******	******	******	******	******
951	-109.	******	******	******	******	******	******	******	******	******	******	******	******
958	-102.	******	******	******	******	******	******	******	******	******	******	******	******
1010	-90.	0.0836	******	0.0454	******	0.0405	******	0.0400	******	0.0344	******	0.012	******
1011	-89.	******	******	******	******	******	******	******	******	******	******	******	******
1012	-88.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-85.	******	******	******	******	******	******	******	******	******	******	******	******
1025	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1030	-70.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-55.	******	******	******	******	******	******	******	******	******	******	******	******
1050	-50.	******	******	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	0.0809	******	0.0415	******	0.0419	******	0.0409	******	0.0346	******	0.012
1057	-43.	******	******	******	******	******	******	******	******	******	******	******	******
1115	-25.	******	******	******	******	******	******	******	******	******	******	******	******
1116	-24.	******	******	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	******	******	******	******	******	******	******	******	******	******	******
1140	0.	******	******	******	******	******	******	******	******	******	******	******	******
1145	5.	******	******	******	******	******	******	******	******	******	******	******	******
1155	15.	******	******	******	******	******	******	******	******	******	******	******	******
1215	35.	0.0816	******	0.0408	******	0.0416	******	0.0396	******	0.0343	******	0.011	******
1216	36.	******	******	******	******	******	******	******	******	******	******	******	******
1229	49.	******	******	******	******	******	******	******	******	******	******	******	******
1244	64.	******	******	******	******	******	******	******	******	******	******	******	******
1246	66.	******	******	******	******	******	******	******	******	******	******	******	******
1300	80.	******	0.0804	******	0.0389	******	0.0404	******	0.0396	******	0.0344	******	0.009
1315	95.	******	******	******	******	******	******	******	******	******	******	******	******
1330	110.	******	******	******	******	******	******	******	******	******	******	******	******
1345	125.	0.0809	******	0.0387	******	0.0407	******	0.0396	******	0.0341	******	0.009	******
1356	136.	******	******	******	******	******	******	******	******	******	******	******	******
1415	155.	******	******	******	******	******	******	******	******	******	******	******	******
1426	166.	******	******	******	******	******	******	******	******	******	******	******	******
1430	170.	******	0.0802	******	0.0384	******	0.0397	******	0.0396	******	0.0344	******	0.008
1432	172.	******	******	******	******	******	******	******	******	******	******	******	******
1445	185.	******	******	******	******	******	******	******	******	******	******	******	******
1455	195.	******	******	******	******	******	******	******	******	******	******	******	******
1500	200.	******	******	******	******	******	******	******	******	******	******	******	******
1515	215.	0.0802	******	0.0369	******	0.0406	******	0.0409	******	0.0344	******	0.007	******
1527	227.	******	******	******	******	******	******	******	******	******	******	******	******
1529	229.	******	******	******	******	******	******	******	******	******	******	******	******
1545	245.	******	******	******	******	******	******	******	******	******	******	******	******
1600	260.	******	0.0799	******	0.0350	******	0.0394	******	0.0396	******	0.0343	******	0.007
1615	275.	******	******	******	******	******	******	******	******	******	******	******	******
1631	291.	******	******	******	******	******	******	******	******	******	******	******	******
1644	304.	******	******	******	******	******	******	******	******	******	******	******	******
1645	305.	0.0792	******	0.0330	******	0.0395	******	0.0396	******	0.0341	******	0.006	******
1650	310.	******	******	******	******	******	******	******	******	******	******	******	******

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DMAE SURROGATE RUN #4
1979 OCT 23

CLOCK TIME	ELAPSED T(MIN)	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 1	N-C4 PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	T2-C4= PPM SIDE 1	T2-C4= PPM SIDE 2	I-C5 PPM SIDE 1	I-C5 PPM SIDE 2
818	-202.	******	******	******	******	******	******	******	******	******	******	******	******
820	-200.	0.0013	0.0013	0.001	0.001	0.0001	0.0001	0.0001	0.0001	0.0	0.0	0.0003	0.0003
835	-185.	******	******	******	******	******	******	******	******	******	******	******	******
912	-148.	******	******	******	******	******	******	******	******	******	******	******	******
924	-136.	******	******	******	******	******	******	******	******	******	******	******	******
930	-130.	******	0.0012	******	0.179	******	******	******	******	******	******	******	******
949	-111.	******	******	******	******	******	******	******	******	******	******	******	******
951	-109.	******	******	******	******	******	******	******	******	******	******	******	******
958	-102.	******	******	******	******	******	******	******	******	******	******	******	******
1010	-90.	0.0014	******	0.183	******	******	******	******	******	0.0006	******	0.0003	******
1011	-89.	******	******	******	******	******	******	******	******	******	******	******	******
1012	-88.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-85.	******	******	******	******	******	******	******	******	******	******	******	******
1025	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1030	-70.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-55.	******	******	******	******	******	******	******	******	******	******	******	******
1050	-50.	******	******	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	0.0013	******	0.183	******	0.0002	******	0.0001	******	0.0007	******	0.0003
1057	-43.	******	******	******	******	******	******	******	******	******	******	******	******
1115	-25.	******	******	******	******	******	******	******	******	******	******	******	******
1116	-24.	******	******	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	******	******	******	******	******	******	******	******	******	******	******
1140	0.	******	******	******	******	******	******	******	******	******	******	******	******
1145	5.	******	******	******	******	******	******	******	******	******	******	******	******
1155	15.	******	******	******	******	******	******	******	******	******	******	******	******
1215	35.	0.0013	******	0.181	******	0.0002	******	0.0001	******	0.0005	******	0.0002	******
1216	36.	******	******	******	******	******	******	******	******	******	******	******	******
1229	49.	******	******	******	******	******	******	******	******	******	******	******	******
1244	64.	******	******	******	******	******	******	******	******	******	******	******	******
1246	66.	******	******	******	******	******	******	******	******	******	******	******	******
1300	80.	******	0.0013	******	0.179	******	******	******	******	******	0.0004	******	0.0003
1315	95.	******	******	******	******	******	******	******	******	******	******	******	******
1330	110.	******	******	******	******	******	******	******	******	******	******	******	******
1345	125.	0.0013	******	0.178	******	0.0002	******	0.0001	******	0.0002	******	0.0003	******
1356	136.	******	******	******	******	******	******	******	******	******	******	******	******
1415	155.	******	******	******	******	******	******	******	******	******	******	******	******
1426	166.	******	******	******	******	******	******	******	******	******	******	******	******
1430	170.	******	0.0013	******	0.177	******	******	******	******	******	0.0002	******	0.0004
1432	172.	******	******	******	******	******	******	******	******	******	******	******	******
1445	185.	******	******	******	******	******	******	******	******	******	******	******	******
1455	195.	******	******	******	******	******	******	******	******	******	******	******	******
1500	200.	******	******	******	******	******	******	******	******	******	******	******	******
1515	215.	0.0013	******	0.178	******	******	******	******	******	0.0001	******	0.0004	******
1527	227.	******	******	******	******	******	******	******	******	******	******	******	******
1529	229.	******	******	******	******	******	******	******	******	******	******	******	******
1545	245.	******	******	******	******	******	******	******	******	******	******	******	******
1600	260.	******	0.0013	******	0.175	******	0.0001	******	0.0001	******	0.0001	******	0.0002
1615	275.	******	******	******	******	******	******	******	******	******	******	******	******
1631	291.	******	******	******	******	******	******	******	******	******	******	******	******
1644	304.	******	******	******	******	******	******	******	******	******	******	******	******
1645	305.	0.0013	******	0.176	******	******	******	******	******	******	******	0.0002	******
1650	310.	******	******	******	******	******	******	******	******	******	******	******	******

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DMAE SURROGATE RUN #4
1979 OCT 23

CLOCK TIME	ELAPSED T(MIN)	CIS2-C4= PPM SIDE 1	CIS2-C4= PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2	2ME-C4=2 PPM SIDE 1	2ME-C4=2 PPM SIDE 2	2,3-DMB PPM SIDE 1	2,3-DMB PPM SIDE 2	TOLUENE PPM SIDE 1	TOLUENE PPM SIDE 2	M-XYL PPM SIDE 1	M-XYL PPM SIDE 2
818	-202.	******	******	******	******	******	******	******	******	******	******	******	******
820	-200.	0.0	0.0	0.0	0.0	******	******	******	******	0.000	0.000	******	******
835	-185.	******	******	******	******	******	******	******	******	******	******	******	******
912	-148.	******	******	******	******	******	******	******	******	******	******	******	******
924	-136.	******	******	******	******	******	******	******	******	******	******	******	******
930	-130.	******	0.0133	******	0.0	******	0.0102	******	0.0732	******	0.012	******	0.0314
949	-111.	******	******	******	******	******	******	******	******	******	******	******	******
951	-109.	******	******	******	******	******	******	******	******	******	******	******	******
958	-102.	******	******	******	******	******	******	******	******	******	******	******	******
1010	-90.	0.0140	******	0.0	******	0.0103	******	0.0741	******	0.012	******	0.0314	******
1011	-89.	******	******	******	******	******	******	******	******	******	******	******	******
1012	-88.	******	******	******	******	******	******	******	******	******	******	******	******
1015	-85.	******	******	******	******	******	******	******	******	******	******	******	******
1025	-75.	******	******	******	******	******	******	******	******	******	******	******	******
1030	-70.	******	******	******	******	******	******	******	******	******	******	******	******
1045	-55.	******	******	******	******	******	******	******	******	******	******	******	******
1050	-50.	******	******	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	0.0137	******	0.0	******	0.0100	******	0.0746	******	0.012	******	0.0316
1057	-43.	******	******	******	******	******	******	******	******	******	******	******	******
1115	-25.	******	******	******	******	******	******	******	******	******	******	******	******
1116	-24.	******	******	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	******	******	******	******	******	******	******	******	******	******	******
1140	0.	******	******	******	******	******	******	******	******	******	******	******	******
1145	5.	******	******	******	******	******	******	******	******	******	******	******	******
1155	15.	******	******	******	******	******	******	******	******	******	******	******	******
1215	35.	0.0106	******	0.0001	******	0.0062	******	0.0722	******	0.012	******	0.0286	******
1216	36.	******	******	******	******	******	******	******	******	******	******	******	******
1229	49.	******	******	******	******	******	******	******	******	******	******	******	******
1244	64.	******	******	******	******	******	******	******	******	******	******	******	******
1246	66.	******	******	******	******	******	******	******	******	******	******	******	******
1300	80.	******	0.0074	******	0.0	******	0.0023	******	0.0704	******	0.011	******	0.0251
1315	95.	******	******	******	******	******	******	******	******	******	******	******	******
1330	110.	******	******	******	******	******	******	******	******	******	******	******	******
1345	125.	0.0057	******	0.0000	******	0.0014	******	0.0696	******	0.011	******	0.0244	******
1356	136.	******	******	******	******	******	******	******	******	******	******	******	******
1415	155.	******	******	******	******	******	******	******	******	******	******	******	******
1426	166.	******	******	******	******	******	******	******	******	******	******	******	******
1430	170.	******	0.0040	******	0.0	******	0.0006	******	0.0685	******	0.011	******	0.0221
1432	172.	******	******	******	******	******	******	******	******	******	******	******	******
1445	185.	******	******	******	******	******	******	******	******	******	******	******	******
1455	195.	******	******	******	******	******	******	******	******	******	******	******	******
1500	200.	******	******	******	******	******	******	******	******	******	******	******	******
1515	215.	0.0028	******	0.0001	******	******	******	0.0671	******	0.011	******	0.0216	******
1527	227.	******	******	******	******	******	******	******	******	******	******	******	******
1529	229.	******	******	******	******	******	******	******	******	******	******	******	******
1545	245.	******	******	******	******	******	******	******	******	******	******	******	******
1600	260.	******	0.0018	******	0.0001	******	0.0	******	0.0665	******	0.011	******	0.0198
1615	275.	******	******	******	******	******	******	******	******	******	******	******	******
1631	291.	******	******	******	******	******	******	******	******	******	******	******	******
1644	304.	******	******	******	******	******	******	******	******	******	******	******	******
1645	305.	0.0008	******	0.0001	******	0.0002	******	0.0656	******	0.011	******	0.0189	******
1650	310.	******	******	******	******	******	******	******	******	******	******	******	******

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DMAE SURROGATE RUN #4
1979 OCT 23

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2	UV *
818	-202.	0.20	******	0.03	******	0.53	******	0.04	******	0.06	******	65.9	******	******
820	-200.	******	******	******	******	******	******	******	******	******	******	******	******	******
835	-185.	******	******	******	******	******	******	******	******	******	******	******	******	******
912	-148.	0.20	******	0.20	******	0.55	******	0.06	******	0.14	******	69.5	******	******
924	-136.	******	0.20	******	0.20	******	0.41	******	0.05	******	0.05	******	71.3	******
930	-130.	******	******	******	******	******	******	******	******	******	******	******	******	******
949	-111.	0.20	******	0.20	******	0.34	******	0.06	******	0.14	******	69.5	******	******
951	-109.	******	******	******	******	******	******	******	******	******	******	******	******	******
958	-102.	******	0.20	******	0.10	******	0.77	******	0.27	******	2.46	******	71.3	******
1010	-90.	******	******	******	******	******	******	******	******	******	******	******	******	******
1011	-89.	******	******	******	******	******	******	******	******	******	******	******	******	******
1012	-88.	******	******	******	******	******	******	******	******	******	******	******	******	******
1015	-85.	0.20	******	0.20	******	0.11	******	0.07	******	0.37	******	76.7	******	******
1025	-75.	******	0.20	******	0.10	******	0.42	******	0.02	******	0.02	******	78.5	******
1030	-70.	******	******	******	******	******	******	******	******	******	******	******	******	******
1045	-55.	0.20	******	0.10	******	0.76	******	0.11	******	1.17	******	69.5	******	******
1050	-50.	******	******	******	******	******	******	******	******	******	******	******	******	******
1055	-45.	******	******	******	******	******	******	******	******	******	******	******	******	******
1057	-43.	******	******	******	******	******	******	******	******	******	******	******	******	******
1115	-25.	0.30	******	0.01	******	0.60	******	0.06	******	0.09	******	71.3	******	******
1116	-24.	******	******	******	******	******	******	******	******	******	******	******	******	******
1122	-18.	******	0.20	******	0.10	******	0.27	******	0.27	******	0.35	******	73.1	******
1140	0.	******	******	******	******	******	******	******	******	******	******	******	******	******
1145	5.	0.20	******	21.00	******	21.40	******	1.40	******	2.71	******	76.7	******	******
1155	15.	******	0.20	******	0.10	******	0.35	******	0.35	******	0.34	******	76.7	0.0041
1215	35.	0.50	******	22.00	******	56.10	******	16.00	******	40.60	******	76.7	******	******
1216	36.	******	******	******	******	******	******	******	******	******	******	******	******	******
1229	49.	******	0.30	******	0.20	******	0.49	******	0.49	******	1.15	******	78.5	0.0034
1244	64.	******	******	******	******	******	******	******	******	******	******	******	******	******
1246	66.	0.70	******	19.00	******	49.50	******	22.30	******	67.90	******	80.3	******	******
1300	80.	******	0.30	******	0.10	******	0.53	******	0.53	******	0.16	******	78.5	0.0037
1315	95.	1.00	******	17.00	******	44.10	******	24.40	******	82.10	******	80.3	******	******
1330	110.	******	0.30	******	0.10	******	0.61	******	0.61	******	1.92	******	80.3	0.0031
1345	125.	1.30	******	15.00	******	40.30	******	24.70	******	90.00	******	80.3	******	******
1356	136.	******	0.30	******	0.10	******	0.46	******	0.20	******	1.21	******	80.3	0.0037
1415	155.	1.20	******	13.00	******	37.70	******	21.20	******	76.50	******	80.3	******	******
1426	166.	******	0.30	******	0.10	******	3.44	******	0.70	******	3.55	******	78.5	0.0021
1430	170.	******	******	******	******	******	******	******	******	******	******	******	******	******
1432	172.	******	******	******	******	******	******	******	******	******	******	******	******	******
1445	185.	1.00	******	11.00	******	29.20	******	17.80	******	63.90	******	78.5	******	******
1455	195.	******	0.30	******	0.10	******	0.24	******	0.26	******	2.42	******	78.5	0.0022
1500	200.	******	******	******	******	******	******	******	******	******	******	******	******	******
1515	215.	0.70	******	9.00	******	25.50	******	13.60	******	46.20	******	82.1	******	******
1527	227.	******	0.30	******	0.10	******	0.56	******	0.29	******	2.88	******	82.1	0.0028
1529	229.	******	******	******	******	******	******	******	******	******	******	******	******	******
1545	245.	0.50	******	8.00	******	22.30	******	9.18	******	26.70	******	78.5	******	******
1600	260.	******	0.30	******	0.10	******	0.34	******	0.11	******	0.29	******	78.5	0.0025
1615	275.	0.40	******	7.00	******	18.40	******	6.93	******	19.90	******	78.5	******	******
1631	291.	******	0.40	******	0.90	******	1.21	******	0.39	******	1.75	******	78.5	0.0022
1644	304.	0.40	******	6.40	******	16.70	******	5.83	******	14.50	******	78.5	******	******
1645	305.	******	******	******	******	******	******	******	******	******	******	******	******	******
1650	310.	******	0.30	******	0.10	******	0.13	******	0.03	******	0.02	******	74.9	0.0012

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

0630-0800 BAG FILLED WITH PURE AIR FROM CHAMBER SYSTEM
BAG VOLUME APPROXIMATELY 31 CUBIC METERS
BAG TURNED END FOR END TO VERIFY THAT ENHANCED RATE
NOT DUE TO DIFFERENCES FROM SIDE TO SIDE (LIGHT INTENSITY,ETC.)
0830 BAG COVERED
0900 RH IS 14% AT 21 DEG C
0901 2.6 ML NO2 INJECTED AND MIXED
0903 7.3 ML NO INJECTED AND MIXED
0906 500 ML SURROGATE J INJECTED AND MIXED
0910 14.0 MICROLITERS (U-L) 2,3DMB, 1.9 U-L TOLUENE,
1.6 U-L 2ME-2-C4=, 5.4 U-L M-XYLENE INJECTED AND MIXED
0915 BAG DIVIDED
0940 7.2 U-L DMAE INJECTED INTO SIDE 2
(0.11 PPM, CALCULATED)
1015 BAG UNCOVERED

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1015 PST

TS	DEG K	AVERAGE	299.0
UV		AVERAGE	0.004

* ASSIGNED INITIAL CONDITION

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM SIDE 1	NOx-CORR PPM SIDE 2
850	-85.	******	0.010	******	0.0	******	0.0	******	0.0	******	0.0
920	-55.	******	0.008	******	0.001	******	0.150	******	0.083	******	0.231
950	-25.	******	0.008	******	0.001	******	0.150	******	0.086	******	0.229
955	-20.	0.0	******	0.0	******	0.153	******	0.086	******	0.232	******
1000	-15.	******	******	******	******	******	******	******	******	******	******
1009	-6.	******	******	******	******	******	******	******	******	******	******
1030	15.	0.010	******	0.009	******	0.142	******	0.093	******	0.230	******
1039	24.	******	0.010	******	0.011	******	0.129	******	0.099	******	0.221
1050	35.	******	******	******	******	******	******	******	******	******	******
1100	45.	0.013	******	0.013	******	0.112	******	0.110	******	0.227	******
1109	54.	******	0.017	******	0.014	******	0.100	******	0.121	******	0.216
1111	56.	******	******	******	******	******	******	******	******	******	******
1115	60.	******	******	******	******	******	******	******	******	******	******
1130	75.	0.022	******	0.021	******	0.081	******	0.139	******	0.212	******
1131	76.	******	******	******	******	******	******	******	******	******	******
1139	84.	******	0.030	******	0.024	******	0.071	******	0.139	******	0.201
1146	91.	******	******	******	******	******	******	******	******	******	******
1200	105.	0.031	******	0.033	******	0.059	******	0.157	******	0.208	******
1209	114.	******	0.044	******	0.037	******	0.049	******	0.155	******	0.195
1215	120.	******	******	******	******	******	******	******	******	******	******
1230	135.	0.045	******	0.044	******	0.040	******	0.166	******	0.198	******
1238	143.	******	0.066	******	0.053	******	0.029	******	0.156	******	0.178
1245	150.	******	******	******	******	******	******	******	******	******	******
1300	165.	0.055	******	0.058	******	0.029	******	0.173	******	0.190	******
1307	172.	******	0.079	******	0.071	******	0.019	******	0.158	******	0.168
1315	180.	******	******	******	******	******	******	******	******	******	******
1330	195.	0.067	******	0.071	******	0.020	******	0.175	******	0.186	******
1340	205.	******	0.097	******	0.089	******	0.011	******	0.150	******	0.153
1345	210.	******	******	******	******	******	******	******	******	******	******
1400	225.	0.076	******	0.082	******	0.015	******	0.171	******	0.177	******
1409	234.	******	0.110	******	0.104	******	0.010	******	0.144	******	0.146
1415	240.	******	******	******	******	******	******	******	******	******	******
1430	255.	0.083	******	0.089	******	0.011	******	0.171	******	0.173	******
1439	264.	******	0.117	******	0.120	******	0.002	******	0.139	******	0.137
1454	279.	******	******	******	******	******	******	******	******	******	******
1500	285.	0.098	******	0.100	******	0.008	******	0.175	******	0.175	******
1508	293.	******	0.120	******	0.126	******	0.002	******	0.132	******	0.130

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	DMAE PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	MEK PPM SIDE 1	MEK PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2
850	-85.	******	******	******	******	******	******	******	******	******	******	******
920	-55.	******	0.0044	0.0044	******	******	1.40	1.40	0.0728	0.0728	0.0448	0.0448
950	-25.	******	******	******	******	******	******	******	******	******	******	******
955	-20.	******	******	******	******	******	******	******	******	******	******	******
1000	-15.	6.5000	******	******	******	******	******	******	******	******	******	******
1009	-6.	4.6000	******	******	******	******	******	******	******	******	******	******
1030	15.	3.3000	0.0076	******	******	******	1.38	******	0.0768	******	0.0433	******
1039	24.	******	******	******	******	******	******	******	******	******	******	******
1050	35.	0.0	******	******	******	******	******	******	******	******	******	******
1100	45.	******	******	******	******	******	******	******	******	******	******	******
1109	54.	******	******	******	******	******	******	******	******	******	******	******
1111	56.	0.0	******	******	******	******	******	******	******	******	******	******
1115	60.	******	******	0.0099	******	0.0016	******	1.40	******	0.0718	******	0.0393
1130	75.	******	******	******	******	******	******	******	******	******	******	******
1131	76.	0.0	******	******	******	******	******	******	******	******	******	******
1139	84.	******	******	******	******	******	******	******	******	******	******	******
1146	91.	0.0	******	******	******	******	******	******	******	******	******	******
1200	105.	******	0.0171	******	0.0028	******	******	******	0.0738	******	0.0374	******
1209	114.	******	******	******	******	******	******	******	******	******	******	******
1215	120.	0.0	******	******	******	******	******	******	******	******	******	******
1230	135.	******	******	******	******	******	******	******	******	******	******	******
1238	143.	******	******	******	******	******	******	******	******	******	******	******
1245	150.	0.0	******	0.0169	******	0.0026	******	******	******	0.0718	******	0.0367
1300	165.	******	******	******	******	******	******	******	******	******	******	******
1307	172.	******	******	******	******	******	******	******	******	******	******	******
1315	180.	0.0	******	******	******	******	******	******	******	******	******	******
1330	195.	******	0.0219	******	0.0044	******	1.34	******	0.0728	******	0.0334	******
1340	205.	******	******	******	******	******	******	******	******	******	******	******
1345	210.	******	******	******	******	******	******	******	******	******	******	******
1400	225.	******	******	******	******	******	******	******	******	******	******	******
1409	234.	******	******	******	******	******	******	******	******	******	******	******
1415	240.	******	******	0.0195	******	0.0040	******	1.38	******	0.0714	******	0.0332
1430	255.	******	******	******	******	******	******	******	******	******	******	******
1439	264.	******	******	******	******	******	******	******	******	******	******	******
1454	279.	******	******	******	******	******	******	******	******	******	******	******
1500	285.	******	******	******	******	******	******	******	******	******	******	******
1508	293.	******	******	******	******	******	******	******	******	******	******	******

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	ACETYLEN PPM (PN-1)	ACETYLEN PPM (PN-2)	ACETYLEN PPM (DMS-1)	ACETYLEN PPM (DMS-2)	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 2	1-C4= PPM SIDE 1	1-C4= PPM SIDE 2
850	-85.	******	******	******	******	******	******	******	******	******	******	******	******	******
920	-55.	0.0482	0.0475	0.0482	0.0482	0.0317	0.0317	0.013	0.011	0.0012	0.0012	0.171	0.0001	0.0001
950	-25.	******	******	******	******	******	******	******	******	******	******	******	******	******
955	-20.	******	******	******	******	******	******	******	******	******	******	******	******	******
1000	-15.	******	******	******	******	******	******	******	******	******	******	******	******	******
1009	-6.	******	******	******	******	******	******	******	******	******	******	******	******	******
1030	15.	0.0499	******	0.0495	******	0.0322	******	0.011	******	0.0011	******	******	0.0001	******
1039	24.	******	******	******	******	******	******	******	******	******	******	******	******	******
1050	35.	******	******	******	******	******	******	******	******	******	******	******	******	******
1100	45.	******	******	******	******	******	******	******	******	******	******	******	******	******
1109	54.	******	******	******	******	******	******	******	******	******	******	******	******	******
1111	56.	******	******	******	******	******	******	******	******	******	******	******	******	******
1115	60.	******	0.0471	******	0.0473	******	0.0312	******	0.010	******	0.0013	0.165	******	******
1130	75.	******	******	******	******	******	******	******	******	******	******	******	******	******
1131	76.	******	******	******	******	******	******	******	******	******	******	******	******	******
1139	84.	******	******	******	******	******	******	******	******	******	******	******	******	******
1146	91.	******	******	******	******	******	******	******	******	******	******	******	******	******
1200	105.	0.0483	******	0.0477	******	0.0317	******	0.008	******	0.0011	******	******	0.0002	******
1209	114.	******	******	******	******	******	******	******	******	******	******	******	******	******
1215	120.	******	******	******	******	******	******	******	******	******	******	******	******	******
1230	135.	******	******	******	******	******	******	******	******	******	******	******	******	******
1238	143.	******	******	******	******	******	******	******	******	******	******	******	******	******
1245	150.	******	0.0466	******	0.0469	******	0.0309	******	0.008	******	0.0011	0.162	******	******
1300	165.	******	******	******	******	******	******	******	******	******	******	******	******	******
1307	172.	******	******	******	******	******	******	******	******	******	******	******	******	******
1315	180.	******	******	******	******	******	******	******	******	******	******	******	******	******
1330	195.	0.0475	******	0.0473	******	0.0310	******	0.005	******	0.0011	******	******	0.0001	******
1340	205.	******	******	******	******	******	******	******	******	******	******	******	******	******
1345	210.	******	******	******	******	******	******	******	******	******	******	******	******	******
1400	225.	******	******	******	******	******	******	******	******	******	******	******	******	******
1409	234.	******	******	******	******	******	******	******	******	******	******	******	******	******
1415	240.	******	0.0463	******	0.0456	******	0.0299	******	0.005	******	0.0010	0.157	******	0.0001
1430	255.	******	******	******	******	******	******	******	******	******	******	******	******	******
1439	264.	******	******	******	******	******	******	******	******	******	******	******	******	******
1454	279.	******	******	******	******	******	******	******	******	******	******	******	******	******
1500	285.	******	******	******	******	******	******	******	******	******	******	******	******	******
1508	293.	******	******	******	******	******	******	******	******	******	******	******	******	******

BAG-105
DMAE SUPROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	T2-C4= PPM SIDE 1	T2-C4= PPM SIDE 2	I-C5 PPM SIDE 1	I-C5 PPM SIDE 2	CIS2-C4= PPM SIDE 1	CIS2-C4= PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2	2MF-C4=2 PPM SIDE 1	2MF-C4=2 PPM SIDE 2
850	-85.	******	******	******	******	******	******	******	******	******	******	******	******
920	-55.	0.0001	0.0001	0.0006	0.0006	0.0003	0.0005	0.0129	0.0129	0.0002	0.0002	0.0220	0.0220
950	-25.	******	******	******	******	******	******	******	******	******	******	******	******
955	-20.	******	******	******	******	******	******	******	******	******	******	******	******
1000	-15.	******	******	******	******	******	******	******	******	******	******	******	******
1009	-6.	******	******	******	******	******	******	******	******	******	******	******	******
1030	15.	0.0001	******	0.0005	******	0.0002	******	0.0116	******	0.0002	******	0.0090	******
1039	24.	******	******	******	******	******	******	******	******	******	******	******	******
1050	35.	******	******	******	******	******	******	******	******	******	******	******	******
1100	45.	******	******	******	******	******	******	******	******	******	******	******	******
1109	54.	******	******	******	******	******	******	******	******	******	******	******	******
1111	56.	******	******	******	******	******	******	******	******	******	******	******	******
1115	60.	******	0.0001	******	0.0004	******	0.0008	******	0.0087	******	0.0003	******	0.0046
1130	75.	******	******	******	******	******	******	******	******	******	******	******	******
1131	76.	******	******	******	******	******	******	******	******	******	******	******	******
1139	84.	******	******	******	******	******	******	******	******	******	******	******	******
1146	91.	******	******	******	******	******	******	******	******	******	******	******	******
1200	105.	0.0001	******	0.0002	******	0.0002	******	0.0041	******	0.0001	******	0.0007	******
1209	114.	******	******	******	******	******	******	******	******	******	******	******	******
1215	120.	******	******	******	******	******	******	******	******	******	******	******	******
1230	135.	******	******	******	******	******	******	******	******	******	******	******	******
1238	143.	******	******	******	******	******	******	******	******	******	******	******	******
1245	150.	******	******	******	0.0001	******	0.0006	******	0.0030	******	0.0004	******	0.0002
1300	165.	******	******	******	******	******	******	******	******	******	******	******	******
1307	172.	******	******	******	******	******	******	******	******	******	******	******	******
1315	180.	******	******	******	******	******	******	******	******	******	******	******	******
1330	195.	0.0000	******	******	******	0.0002	******	0.0009	******	0.0001	******	******	******
1340	205.	******	******	******	******	******	******	******	******	******	******	******	******
1345	210.	******	******	******	******	******	******	******	******	******	******	******	******
1400	225.	******	******	******	******	******	******	******	******	******	******	******	******
1409	234.	******	******	******	******	******	******	******	******	******	******	******	******
1415	240.	******	0.0001	******	******	******	0.0003	******	0.0003	******	0.0001	******	0.0001
1430	255.	******	******	******	******	******	******	******	******	******	******	******	******
1439	264.	******	******	******	******	******	******	******	******	******	******	******	******
1454	279.	******	******	******	******	******	******	******	******	******	******	******	******
1500	285.	******	******	******	******	******	******	******	******	******	******	******	******
1508	293.	******	******	******	******	******	******	******	******	******	******	******	******

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	2,3-DMB PPM SIDE 1	2,3-DMB PPM SIDE 2	TOLUENE PPM SIDE 1	TOLUENE PPM SIDE 2	M-XYL PPM SIDE 1	M-XYL PPM SIDE 2
850	-85.	******	******	******	******	******	******
920	-55.	0.0761	0.0761	0.014	0.014	0.0329	0.0329
950	-25.	******	******	******	******	******	******
955	-20.	******	******	******	******	******	******
1000	-15.	******	******	******	******	******	******
1009	-6.	******	******	******	******	******	******
1030	15.	0.0774	******	0.014	******	0.0331	******
1039	24.	******	******	******	******	******	******
1050	35.	******	******	******	******	******	******
1100	45.	******	******	******	******	******	******
1109	54.	******	******	******	******	******	******
1111	56.	******	******	******	******	******	******
1115	60.	******	0.0731	******	0.013	******	0.0304
1130	75.	******	******	******	******	******	******
1131	76.	******	******	******	******	******	******
1139	84.	******	******	******	******	******	******
1146	91.	******	******	******	******	******	******
1200	105.	0.0710	******	0.012	******	0.0244	******
1209	114.	******	******	******	******	******	******
1215	120.	******	******	******	******	******	******
1230	135.	******	******	******	******	******	******
1238	143.	******	******	******	******	******	******
1245	150.	******	0.0692	******	0.012	******	0.0240
1300	165.	******	******	******	******	******	******
1307	172.	******	******	******	******	******	******
1315	180.	******	******	******	******	******	******
1330	195.	0.0666	******	0.011	******	0.0190	******
1340	205.	******	******	******	******	******	******
1345	210.	******	******	******	******	******	******
1400	225.	******	******	******	******	******	******
1409	234.	******	******	******	******	******	******
1415	240.	******	0.0651	******	0.011	******	0.0192
1430	255.	******	******	******	******	******	******
1439	264.	******	******	******	******	******	******
1454	279.	******	******	******	******	******	******
1500	285.	******	******	******	******	******	******
1508	293.	******	******	******	******	******	******

BAG-105
DMAE SURROGATE RUN #5
1979 OCT 31

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2	UV *
850	-85.	******	0.40	******	1.30	******	1.73	******	0.69	******	3.92	******	69.5	******
920	-55.	******	0.40	******	1.10	******	1.77	******	0.53	******	2.58	******	******	******
950	-25.	******	0.40	******	1.60	******	3.18	******	0.74	******	2.98	******	******	******
955	-20.	0.30	******	0.80	******	1.72	******	0.26	******	0.77	******	******	******	******
1000	-15.	******	******	******	******	******	******	******	******	******	******	******	******	******
1009	-6.	******	******	******	******	******	******	******	******	******	******	******	******	******
1030	15.	0.30	******	0.20	******	1.67	******	0.33	******	1.59	******	74.9	******	0.0037
1039	24.	******	0.40	******	43.00	******	119.00	******	18.90	******	39.90	******	80.3	******
1050	35.	******	******	******	******	******	******	******	******	******	******	******	******	******
1100	45.	0.40	******	1.30	******	2.00	******	0.38	******	1.26	******	74.9	******	0.0042
1109	54.	******	0.70	******	40.00	******	99.50	******	31.30	******	78.10	******	80.3	******
1111	56.	******	******	******	******	******	******	******	******	******	******	******	******	******
1115	60.	******	******	******	******	******	******	******	******	******	******	******	******	******
1130	75.	0.30	******	0.20	******	1.47	******	0.46	******	2.04	******	76.7	******	0.0034
1131	76.	******	******	******	******	******	******	******	******	******	******	******	******	******
1139	84.	******	1.40	******	36.00	******	70.20	******	48.10	******	149.00	******	******	******
1146	91.	******	******	******	******	******	******	******	******	******	******	******	******	******
1200	105.	0.30	******	0.10	******	1.09	******	0.17	******	0.55	******	80.3	******	0.0043
1209	114.	******	2.50	******	30.00	******	82.60	******	51.30	******	178.00	******	82.1	******
1215	120.	******	******	******	******	******	******	******	******	******	******	******	******	******
1230	135.	0.30	******	0.20	******	1.37	******	0.25	******	0.75	******	76.7	******	0.0044
1238	143.	******	4.30	******	26.00	******	71.30	******	58.40	******	231.00	******	78.5	******
1245	150.	******	******	******	******	******	******	******	******	******	******	******	******	******
1300	165.	0.30	******	0.30	******	1.14	******	0.22	******	0.53	******	78.5	******	0.0036
1307	172.	******	5.90	******	24.00	******	64.00	******	60.70	******	264.00	******	80.3	******
1315	180.	******	******	******	******	******	******	******	******	******	******	******	******	******
1330	195.	0.30	******	0.10	******	0.98	******	0.32	******	1.67	******	80.3	******	0.0039
1340	205.	******	6.50	******	21.00	******	53.40	******	56.30	******	258.00	******	78.5	******
1345	210.	******	******	******	******	******	******	******	******	******	******	******	******	******
1400	225.	0.30	******	0.30	******	1.06	******	0.23	******	0.75	******	80.3	******	0.0037
1409	234.	******	6.00	******	19.00	******	48.70	******	49.50	******	226.00	******	80.3	******
1415	240.	******	******	******	******	******	******	******	******	******	******	******	******	******
1430	255.	0.30	******	0.20	******	0.77	******	0.50	******	3.79	******	82.1	******	0.0031
1439	264.	******	4.90	******	16.00	******	40.00	******	42.10	******	195.00	******	80.3	******
1454	279.	******	******	******	******	******	******	******	******	******	******	******	******	******
1500	285.	0.30	******	0.40	******	1.14	******	0.28	******	1.48	******	80.3	******	0.0027
1508	293.	******	3.80	******	13.00	******	35.70	******	33.60	******	149.00	******	82.1	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

TIME (PDT)
0930-1100 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM, DRY
0940 BAG COVERED
1119 2.6 ML NO2 INJECTED AND MIXED
1132 500 ML SURROGATE J INJECTED
1137 1.6 MICROLITERS (U-L) 2MEC4=, 1.9 U-L TOLUENE, 5.4 U-L M-XYLENE
14 U-L 2,3DMB INJECTED
1144 RH LESS THAN 10% (PURE AIR ON DRY BY MISTAKE)
1150 BAG MIXED THOROUGHLY AND DIVIDED
1221 BAG UNCOVERED
1332 DUE TO LEAK IN SIDE 2, BAG WAS UNDIVIDED, ADJUSTED FOR EQUAL
VOLUMES AND REDIVIDED (SIDE 1 ALMOST EMPTY AT TIME)

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1220 PST

TS	DEG K	AVERAGE	300.4
UV		AVERAGE	0.004

* ASSIGNED INITIAL CONDITION

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM SIDE 1	NOX-CORR PPM SIDE 2
1109	-71.	0.0	******	0.001	******	0.0	******	0.0	******	0.0	******
1110	-70.	******	******	******	******	******	******	******	******	******	******
1150	-30.	******	******	******	******	******	******	******	******	******	******
1200	-20.	******	0.001	******	0.001	******	0.168	******	0.111	******	0.280
1208	-12.	0.004	******	0.001	******	0.171	******	0.115	******	0.281	******
1230	10.	0.007	******	0.010	******	0.162	******	0.117	******	0.277	******
1239	19.	******	0.009	******	0.008	******	0.155	******	0.122	******	0.275
1300	40.	0.012	******	0.014	******	0.119	******	0.148	******	0.269	******
1310	50.	******	0.010	******	0.010	******	0.124	******	0.143	******	0.266
1315	55.	******	******	******	******	******	******	******	******	******	******
1330	70.	0.018	******	0.020	******	0.088	******	0.173	******	0.259	******
1337	77.	******	0.016	******	0.020	******	0.079	******	0.178	******	0.255
1400	100.	0.027	******	0.031	******	0.059	******	0.196	******	0.249	******
1414	114.	******	0.025	******	0.027	******	0.050	******	0.196	******	0.243
1430	130.	0.040	******	0.040	******	0.039	******	0.203	******	0.238	******
1442	142.	******	0.031	******	0.033	******	0.040	******	0.206	******	0.239
1445	145.	******	******	******	******	******	******	******	******	******	******
1500	160.	0.043	******	0.051	******	0.027	******	0.208	******	0.231	******
1514	174.	******	0.035	******	0.038	******	0.029	******	0.216	******	0.237
1530	190.	0.052	******	0.057	******	0.019	******	0.217	******	0.229	******
1544	204.	******	0.037	******	0.041	******	0.020	******	0.217	******	0.229
1600	220.	0.052	******	0.060	******	0.011	******	0.217	******	0.221	******
1613	233.	******	0.037	******	0.042	******	0.011	******	0.218	******	0.224
1615	235.	******	******	******	******	******	******	******	******	******	******
1632	252.	0.052	******	0.059	******	0.005	******	0.219	******	0.217	******
1645	265.	******	0.038	******	0.040	******	0.007	******	0.221	******	0.220
1700	280.	******	******	******	******	******	******	******	******	******	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	PAN PPM SIDE 1	PAN PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	MEK PPM SIDE 1	MEK PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2
1109	-71.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-70.	******	******	0.0015	0.0015	******	******	1.56	1.56	0.0079	0.0079	0.0408	0.0408
1150	-30.	******	******	0.0067	0.0067	0.0004	0.0004	1.55	1.55	0.0779	0.0779	0.0478	0.0478
1200	-20.	******	0.0	******	******	******	******	******	******	******	******	******	******
1208	-12.	******	******	******	******	******	******	******	******	******	******	******	******
1230	10.	******	******	0.0087	******	0.0007	******	1.55	******	0.0772	******	0.0477	******
1239	19.	******	0.0	******	******	******	******	******	******	******	******	******	******
1300	40.	******	******	******	******	******	******	******	******	******	******	******	******
1310	50.	******	0.001	******	******	******	******	******	******	******	******	******	******
1315	55.	******	******	******	0.0120	******	0.0013	******	1.57	******	0.0773	******	0.0462
1330	70.	******	******	******	******	******	******	******	******	******	******	******	******
1337	77.	******	0.001	******	******	******	******	******	******	******	******	******	******
1400	100.	******	******	0.0191	******	0.0027	******	1.54	******	0.0777	******	0.0438	******
1414	114.	******	0.002	******	******	******	******	******	******	******	******	******	******
1430	130.	******	******	******	******	******	******	******	******	******	******	******	******
1442	142.	******	0.002	******	******	******	******	******	******	******	******	******	******
1445	145.	******	******	******	0.0192	******	0.0030	******	1.55	******	0.0772	******	0.0418
1500	160.	******	******	******	******	******	******	******	******	******	******	******	******
1514	174.	******	0.003	******	******	******	******	******	******	******	******	******	******
1530	190.	******	******	0.0253	******	0.0042	******	1.55	******	0.0771	******	0.0390	******
1544	204.	******	0.004	******	******	******	******	******	******	******	******	******	******
1600	220.	******	******	******	******	******	******	******	******	******	******	******	******
1613	233.	******	0.004	******	******	******	******	******	******	******	******	******	******
1615	235.	******	******	******	0.0221	******	0.0039	******	1.56	******	0.0776	******	0.0395
1632	252.	0.0	******	******	******	******	******	******	******	******	******	******	******
1645	265.	******	0.004	******	******	******	******	******	******	******	******	******	******
1700	280.	******	******	******	******	0.0049	******	1.56	******	0.0773	******	0.0378	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	ACETYLEN PPM PN-1	ACETYLEN PPM PN-2	ACETYLEN PPM DMS-1	ACETYLEN PPM DMS-2	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 1	N-C4 PPM SIDE 2
1109	-71.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-70.	0.0038	0.0038	0.0036	0.0036	0.0247	0.0247	0.001	0.001	0.0013	0.0013	0.001	0.001
1150	-30.	0.0417	0.0417	0.0400	0.0400	0.0358	0.0358	0.012	0.012	0.0014	0.0014	0.178	0.178
1200	-20.	******	******	******	******	******	******	******	******	******	******	******	******
1208	-12.	******	******	******	******	******	******	******	******	******	******	******	******
1230	10.	0.0455	******	0.0409	******	0.0359	******	0.011	******	0.0013	******	0.179	******
1239	19.	******	******	******	******	******	******	******	******	******	******	******	******
1300	40.	******	******	******	******	******	******	******	******	******	******	******	******
1310	50.	******	******	******	******	******	******	******	******	******	******	******	******
1315	55.	******	0.0417	******	0.0404	******	0.0355	******	0.010	******	0.0013	******	0.176
1330	70.	******	******	******	******	******	******	******	******	******	******	******	******
1337	77.	******	******	******	******	******	******	******	******	******	******	******	******
1400	100.	0.0409	******	0.0398	******	0.0349	******	0.008	******	0.0013	******	******	******
1414	114.	******	******	******	******	******	******	******	******	******	******	******	******
1430	130.	******	******	******	******	******	******	******	******	******	******	******	******
1442	142.	******	******	******	******	******	******	******	******	******	******	******	******
1445	145.	******	0.0414	******	0.0396	******	0.0335	******	0.007	******	0.0013	******	0.167
1500	160.	******	******	******	******	******	******	******	******	******	******	******	******
1514	174.	******	******	******	******	******	******	******	******	******	******	******	******
1530	190.	0.0402	******	0.0396	******	0.0342	******	0.006	******	0.0013	******	0.166	******
1544	204.	******	******	******	******	******	******	******	******	******	******	******	******
1600	220.	******	******	******	******	******	******	******	******	******	******	******	******
1613	233.	******	******	******	******	******	******	******	******	******	******	******	******
1615	235.	******	0.0415	******	0.0387	******	0.0344	******	0.006	******	0.0014	******	0.166
1632	252.	******	******	******	******	******	******	******	******	******	******	******	******
1645	265.	******	******	******	******	******	******	******	******	******	******	******	******
1700	280.	0.0410	******	0.0387	******	0.0342	******	0.005	******	0.0014	******	******	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	1-C4= PPM SIDE 1	1-C4= PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	T2-C4= PPM SIDE 1	T2-C4= PPM SIDE 2	1-C5 PPM SIDE 1	I-C5 PPM SIDE 2	CIS2-C4= PPM SIDE 1	CIS2-C4= PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2
1109	-71.	******	******	******	******	******	******	******	******	******	******	******	******
1110	-70.	0.0002	0.0002	0.0001	0.0001	0.0	0.0	0.0002	0.0002	0.0	0.0	******	******
1150	-30.	0.0001	0.0001	0.0001	0.0001	0.0	0.0	0.0002	0.0002	0.0134	0.0134	0.0001	0.0001
1200	-20.	******	******	******	******	******	******	******	******	******	******	******	******
1208	-12.	******	******	******	******	******	******	******	******	******	******	******	******
1230	10.	******	******	******	******	0.0011	******	0.0002	******	0.0122	******	******	******
1239	19.	******	******	******	******	******	******	******	******	******	******	******	******
1300	40.	******	******	******	******	******	******	******	******	******	******	******	******
1310	50.	******	******	******	******	******	******	******	******	******	******	******	******
1315	55.	******	0.0002	******	0.0001	******	0.0005	******	0.0001	******	0.0091	******	0.0
1330	70.	******	******	******	******	******	******	******	******	******	******	******	******
1337	77.	******	******	******	******	******	******	******	******	******	******	******	******
1400	100.	0.0003	******	0.0002	******	0.0002	******	0.0001	******	0.0084	******	0.0002	******
1414	114.	******	******	******	******	******	******	******	******	******	******	******	******
1430	130.	******	******	******	******	******	******	******	******	******	******	******	******
1442	142.	******	******	******	******	******	******	******	******	******	******	******	******
1445	145.	******	0.0001	******	0.0002	******	******	******	******	******	0.0025	******	0.0
1500	160.	******	******	******	******	******	******	******	******	******	******	******	******
1514	174.	******	******	******	******	******	******	******	******	******	******	******	******
1530	190.	0.0001	******	0.0001	******	0.0000	******	0.0001	******	0.0010	******	0.0001	******
1544	204.	******	******	******	******	******	******	******	******	******	******	******	******
1600	220.	******	******	******	******	******	******	******	******	******	******	******	******
1613	233.	******	******	******	******	******	******	******	******	******	******	******	******
1615	235.	******	0.0001	******	0.0000	******	******	******	0.0002	******	0.0010	******	0.0001
1632	252.	******	******	******	******	******	******	******	******	******	******	******	******
1645	265.	******	******	******	******	******	******	******	******	******	******	******	******
1700	280.	0.0001	******	0.0001	******	0.0	******	0.0002	******	0.0002	******	0.0002	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	2ME-C4=2 PPM SIDE 1	2ME-C4=2 PPM SIDE 2	2,3-DMB PPM SIDE 1	2,3-DMB PPM SIDE 2	TOLUENE PPM SIDE 1	TOLUENE PPM SIDE 2	M-XYL PPM SIDE 1	M-XYL PPM SIDE 2
1109	-71.	******	******	******	******	******	******	******	******
1110	-70.	0.0	0.0	0.0	0.0	******	******	0.0	0.0
1150	-30.	0.0112	0.0112	0.0817	0.0817	0.014	0.014	0.0355	0.0355
1200	-20.	******	******	******	******	******	******	******	******
1208	-12.	******	******	******	******	******	******	******	******
1230	10.	0.0092	******	0.0807	******	0.014	******	0.0344	******
1239	19.	******	******	******	******	******	******	******	******
1300	40.	******	******	******	******	******	******	******	******
1310	50.	******	******	******	******	******	******	******	******
1315	55.	******	0.0046	******	0.0780	******	0.013	******	0.0306
1330	70.	******	******	******	******	******	******	******	******
1337	77.	******	******	******	******	******	******	******	******
1400	100.	0.0009	******	0.0741	******	0.013	******	0.0252	******
1414	114.	******	******	******	******	******	******	******	******
1430	130.	******	******	******	******	******	******	******	******
1442	142.	******	******	******	******	******	******	******	******
1445	145.	******	0.0007	******	0.0720	******	0.012	******	0.0233
1500	160.	******	******	******	******	******	******	******	******
1514	174.	******	******	******	******	******	******	******	******
1530	190.	0.0	******	0.0704	******	0.012	******	0.0205	******
1544	204.	******	******	******	******	******	******	******	******
1600	220.	******	******	******	******	******	******	******	******
1613	233.	******	******	******	******	******	******	******	******
1615	235.	******	******	******	0.0702	******	0.012	******	0.0212
1632	252.	******	******	******	******	******	******	******	******
1645	265.	******	******	******	******	******	******	******	******
1700	280.	0.0	******	0.0689	******	0.012	******	0.0193	******

BAG-201
SURROGATE CONTROL #1
1979 OCT 24

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2	UV *
1109	-71.	0.30	******	0.30	******	0.35	******	0.09	******	0.22	******	85.7	******	******
1110	-70.	******	******	******	******	******	******	******	******	******	******	******	******	******
1150	-30.	******	******	******	******	******	******	******	******	******	******	******	******	******
1200	-20.	******	0.40	******	0.10	******	0.37	******	0.14	******	0.87	******	83.9	******
1208	-12.	0.40	******	0.10	******	0.19	******	0.08	******	0.80	******	87.5	******	******
1230	10.	0.30	******	0.20	******	0.44	******	0.04	******	0.10	******	91.1	******	.00390
1239	19.	******	0.40	******	0.10	******	0.27	******	0.08	******	0.33	******	83.9	******
1300	40.	0.40	******	0.50	******	0.09	******	0.05	******	0.27	******	78.5	******	.00420
1310	50.	******	0.30	******	0.20	******	0.11	******	0.28	******	1.27	******	82.1	******
1315	55.	******	******	******	******	******	******	******	******	******	******	******	******	******
1330	70.	0.30	******	0.30	******	0.16	******	0.26	******	0.88	******	82.1	******	.00400
1337	77.	******	0.40	******	0.00	******	0.25	******	0.56	******	5.07	******	83.9	******
1400	100.	0.40	******	3.00	******	0.00	******	0.09	******	0.01	******	82.1	******	.00370
1414	114.	******	0.40	******	0.10	******	0.19	******	0.11	******	0.81	******	80.3	******
1430	130.	0.40	******	2.00	******	0.38	******	0.14	******	0.80	******	80.3	******	.00390
1442	142.	******	0.40	******	0.10	******	0.24	******	0.07	******	0.31	******	80.3	******
1445	145.	******	******	******	******	******	******	******	******	******	******	******	******	******
1500	160.	0.40	******	1.50	******	0.69	******	0.06	******	0.04	******	82.1	******	.00360
1514	174.	******	0.40	******	0.10	******	0.24	******	0.09	******	0.31	******	82.1	******
1530	190.	0.40	******	1.00	******	0.62	******	0.07	******	0.13	******	80.3	******	.00350
1544	204.	******	0.30	******	0.10	******	0.15	******	0.10	******	0.87	******	78.5	******
1600	220.	0.30	******	0.60	******	0.55	******	0.07	******	0.28	******	78.5	******	.00250
1613	233.	******	0.30	******	0.10	******	0.29	******	0.18	******	1.33	******	76.7	******
1615	235.	******	******	******	******	******	******	******	******	******	******	******	******	******
1632	252.	0.30	******	0.40	******	0.93	******	0.20	******	1.62	******	74.9	******	.00240
1645	265.	******	0.40	******	0.10	******	0.57	******	0.22	******	1.49	******	74.9	******
1700	280.	******	******	******	******	******	******	******	******	******	******	******	******	******

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

TIME (PDT)
0913-1048 BAG#11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM
BAG VOLUME APPROXIMATELY 32 CUBIC METERS

0920	BAG COVERED
1121	RH=30% AT T=30 DEG C
1123	2.6 ML NO2 INJECTED AND MIXED
1125	7.3 ML NO INJECTED AND MIXED
1132	14.0 ML N-BUTANE INJECTED
1132	4.9 ML PROPYLENE INJECTED AND MIXED
1155	BAG MIXED THOROUGHLY AND DIVIDED (AIR LET OUT TO DIVIDE BAG)
1217	BAG UNCOVERED
1650	SIDE 2 PARTIALLY SHADED

*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1217 PST

TS	DEG K	AVERAGE	300.7
UV		AVERAGE	0.003

* ASSIGNED INITIAL CONDITION

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM SIDE 1	NOX-CORR PPM SIDE 2
1100	-77.	******	******	******	******	******	******	******	******	******	******
1101	-76.	0.0	******	0.0	******	0.0	******	0.0	******	0.0	******
1115	-62.	******	******	******	******	******	******	******	******	******	******
1141	-36.	0.003	******	0.002	******	0.141	******	0.071	******	0.205	******
1145	-32.	******	******	******	******	******	******	******	******	******	******
1158	-19.	0.003	******	0.003	******	0.141	******	0.070	******	0.203	******
1206	-11.	******	0.003	******	0.004	******	0.139	******	0.071	******	0.200
1230	13.	0.004	******	0.009	******	0.131	******	0.079	******	0.206	******
1242	25.	******	0.013	******	0.012	******	0.122	******	0.083	******	0.200
1300	43.	0.005	******	0.013	******	0.118	******	0.091	******	0.200	******
1313	56.	******	0.019	******	0.015	******	0.107	******	0.099	******	0.199
1330	73.	0.014	******	0.016	******	0.098	******	0.102	******	0.197	******
1341	84.	******	0.013	******	0.018	******	0.092	******	0.108	******	0.195
1400	103.	0.015	******	0.016	******	0.083	******	0.121	******	0.196	******
1415	118.	******	0.019	******	0.019	******	0.078	******	0.120	******	0.191
1430	133.	0.013	******	0.017	******	0.074	******	0.124	******	0.191	******
1442	145.	******	0.009	******	0.019	******	0.069	******	0.131	******	0.191
1500	163.	0.017	******	0.018	******	0.064	******	0.131	******	0.190	******
1510	173.	******	0.012	******	0.019	******	0.059	******	0.139	******	0.189
1530	193.	0.012	******	0.017	******	0.057	******	0.140	******	0.190	******
1538	201.	******	0.023	******	0.018	******	0.052	******	0.145	******	0.189
1600	223.	0.020	******	0.016	******	0.050	******	0.147	******	0.189	******
1611	234.	******	0.017	******	0.017	******	0.046	******	0.150	******	0.189
1630	253.	0.023	******	0.013	******	0.047	******	0.155	******	0.192	******
1638	261.	******	0.011	******	0.015	******	0.040	******	0.152	******	0.182
1700	283.	0.013	******	0.010	******	0.039	******	0.155	******	0.188	******
1710	293.	******	0.022	******	0.011	******	0.033	******	0.159	******	0.185

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

CLOCK TIME	ELAPSED T(MIN)	PAN PPM SIDE 1	PAN PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2
1100	-77.	******	******	0.0012	0.0012	1.72	1.72	******	******	******	******
1101	-76.	0.0	******	******	******	******	******	******	******	******	******
1115	-62.	******	******	******	******	******	******	0.0076	0.0076	0.0002	0.0047
1141	-36.	0.0	******	******	******	******	******	******	******	******	******
1145	-32.	******	******	0.0016	0.0016	1.68	1.68	0.0080	0.0080	0.0044	0.0044
1158	-19.	0.0	******	******	******	******	******	******	******	******	******
1206	-11.	******	0.0	******	******	******	******	******	******	******	******
1230	13.	0.0	******	******	******	******	******	******	******	******	******
1242	25.	******	0.0	******	******	******	******	******	******	******	******
1300	43.	0.0	******	******	******	******	******	******	******	******	******
1313	56.	******	0.0	******	******	******	******	******	******	******	******
1330	73.	0.001	******	******	******	******	******	******	******	******	******
1341	84.	******	0.001	******	******	******	******	******	******	******	******
1400	103.	0.0	******	******	******	******	******	******	******	******	******
1415	118.	******	0.001	******	******	******	******	******	******	******	******
1430	133.	0.001	******	******	******	******	******	******	******	******	******
1442	145.	******	0.0	******	******	******	******	******	******	******	******
1500	163.	0.001	******	******	******	******	******	******	******	******	******
1510	173.	******	0.0	******	******	******	******	******	******	******	******
1530	193.	0.001	******	******	******	******	******	******	******	******	******
1538	201.	******	0.0	******	******	******	******	******	******	******	******
1600	223.	0.0	******	******	******	******	******	******	******	******	******
1611	234.	******	0.001	******	******	******	******	******	******	******	******
1630	253.	0.0	******	0.0012	******	1.69	******	0.0087	******	0.0042	******
1638	261.	******	0.0	******	******	******	******	******	******	******	******
1700	283.	0.001	******	******	0.0013	******	1.69	******	0.0081	******	0.0045
1710	293.	******	0.001	******	******	******	******	******	******	******	******

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

CLOCK TIME	ELAPSED T(MIN)	ACETYLEN PPM PN-1	ACETYLEN PPM PN-2	ACETYLEN PPM DMS-1	ACETYLEN PPM DMS-2	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 1	N-C4 PPM SIDE 2
1100	-77.	******	******	0.0010	0.0010	0.0239	0.0239	0.001	0.001	0.0015	0.0015	0.001	0.001
1101	-76.	******	******	******	******	******	******	******	******	******	******	******	******
1115	-62.	0.0187	0.0182	******	******	******	******	******	******	******	******	******	******
1141	-36.	******	******	******	******	******	******	******	******	******	******	******	******
1145	-32.	0.0111	0.0107	0.0138	0.0138	0.0253	0.0253	0.134	0.134	0.0017	0.0017	0.377	0.377
1158	-19.	******	******	******	******	******	******	******	******	******	******	******	******
1206	-11.	******	******	******	******	******	******	******	******	******	******	******	******
1230	13.	******	******	0.0155	******	0.0249	******	0.123	******	0.0017	******	0.366	******
1242	25.	******	******	******	******	******	******	******	******	******	******	******	******
1300	43.	******	******	******	0.0138	******	0.0249	******	0.112	******	0.0017	******	0.355
1313	56.	******	******	******	******	******	******	******	******	******	******	******	******
1330	73.	******	******	0.0138	******	0.0247	******	0.107	******	0.0016	******	0.363	******
1341	84.	******	******	******	******	******	******	******	******	******	******	******	******
1400	103.	******	******	******	0.0138	******	0.0246	******	0.097	******	0.0017	******	0.349
1415	118.	******	******	******	******	******	******	******	******	******	******	******	******
1430	133.	******	******	0.0138	******	0.0249	******	0.097	******	0.0017	******	0.358	******
1442	145.	******	******	******	******	******	******	******	******	******	******	******	******
1500	163.	******	******	******	0.0117	******	0.0247	******	0.089	******	0.0017	******	0.349
1510	173.	******	******	******	******	******	******	******	******	******	******	******	******
1530	193.	******	******	0.0129	******	0.0247	******	0.089	******	0.0017	******	0.357	******
1538	201.	******	******	******	******	******	******	******	******	******	******	******	******
1600	223.	******	******	******	0.0117	******	0.0247	******	0.082	******	0.0017	******	0.346
1611	234.	******	******	******	******	******	******	******	******	******	******	******	******
1630	253.	0.0121	******	0.0129	******	0.0249	******	0.086	******	0.0017	******	0.356	******
1638	261.	******	******	******	******	******	******	******	******	******	******	******	******
1700	283.	******	0.0104	******	0.0146	******	0.0248	******	0.080	******	0.0018	******	0.346
1710	293.	******	******	******	******	******	******	******	******	******	******	******	******

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

CLOCK TIME	ELAPSED T(MIN)	1-C4= PPM SIDE 1	1-C4= PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	I-C5 PPM SIDE 1	I-C5 PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2
1100	-77.	0.0002	0.0002	0.0003	0.0003	0.0009	0.0009	0.0005	0.0005
1101	-76.	******	******	******	******	******	******	******	******
1115	-62.	******	******	******	******	******	******	******	******
1141	-36.	******	******	******	******	******	******	******	******
1145	-32.	******	******	******	******	******	******	******	******
1158	-19.	******	******	******	******	******	******	******	******
1206	-11.	******	******	******	******	******	******	******	******
1230	13.	******	******	******	******	******	******	******	******
1242	25.	******	******	******	******	******	******	******	******
1300	43.	******	******	******	******	******	******	******	******
1313	56.	******	******	******	******	******	******	******	******
1330	73.	******	******	******	******	******	******	******	******
1341	84.	******	******	******	******	******	******	******	******
1400	103.	******	******	******	******	******	******	******	******
1415	118.	******	******	******	******	******	******	******	******
1430	133.	******	******	******	******	******	******	******	******
1442	145.	******	******	******	******	******	******	******	******
1500	163.	******	******	******	******	******	******	******	******
1510	173.	******	******	******	******	******	******	******	******
1530	193.	******	******	******	******	******	******	******	******
1538	201.	******	******	******	******	******	******	******	******
1600	223.	******	******	******	******	******	******	******	******
1611	234.	******	******	******	******	******	******	******	******
1630	253.	******	******	******	******	******	******	******	******
1638	261.	******	******	******	******	******	******	******	******
1700	283.	******	******	******	******	******	******	******	******
1710	293.	******	******	******	******	******	******	******	******

BAG-202
SURROGATE CONTROL #2
1979 OCT 25

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2	UV *
1100	-77.	******	******	******	******	******	******	******	******	******	******	******	******	******
1101	-76.	0.50	******	0.30	******	******	******	0.28	******	1.64	******	85.7	******	******
1115	-62.	******	******	******	******	******	******	******	******	******	******	******	******	******
1141	-36.	0.50	******	0.60	******	******	******	0.33	******	1.37	******	85.7	******	******
1145	-32.	******	******	******	******	******	******	******	******	******	******	******	******	******
1158	-19.	0.60	******	0.40	******	******	******	0.47	******	1.93	******	******	******	0.0035
1206	-11.	******	0.70	******	0.80	******	1.91	******	0.66	******	2.95	******	******	******
1230	13.	0.60	******	0.60	******	******	******	0.40	******	2.06	******	74.9	******	0.0039
1242	25.	******	0.70	******	0.50	******	0.88	******	0.60	******	3.34	******	76.7	******
1300	43.	0.60	******	0.30	******	******	******	0.29	******	1.55	******	87.5	******	0.0037
1313	56.	******	0.60	******	0.90	******	1.65	******	0.52	******	1.72	******	83.9	******
1330	73.	0.50	******	0.10	******	******	******	0.36	******	1.95	******	89.3	******	0.0043
1341	84.	******	0.70	******	1.70	******	1.03	******	0.53	******	2.27	******	87.5	******
1400	103.	0.60	******	0.10	******	******	******	0.32	******	1.70	******	87.5	******	0.0035
1415	118.	******	0.70	******	2.90	******	1.28	******	0.68	******	2.89	******	83.9	******
1430	133.	0.60	******	0.20	******	******	******	0.48	******	2.49	******	89.3	******	0.0031
1442	145.	******	0.60	******	0.20	******	0.84	******	0.37	******	1.35	******	85.7	******
1500	163.	0.60	******	0.20	******	******	******	0.37	******	1.35	******	82.1	******	0.0032
1510	173.	******	0.80	******	2.80	******	1.40	******	0.78	******	4.01	******	82.1	******
1530	193.	0.70	******	0.40	******	******	******	0.60	******	2.75	******	82.1	******	0.0027
1538	201.	******	0.70	******	2.20	******	1.67	******	0.67	******	2.84	******	82.1	******
1600	223.	******	******	1.00	******	0.0	******	0.41	******	1.14	******	78.5	******	0.0020
1611	234.	******	0.50	******	2.70	******	2.70	******	2.37	******	15.00	******	82.1	******
1630	253.	******	******	0.80	******	******	******	0.46	******	2.10	******	74.9	******	0.0025
1638	261.	******	0.60	******	2.20	******	2.30	******	0.68	******	2.60	******	76.7	******
1700	283.	******	******	1.10	******	******	******	0.48	******	1.82	******	69.5	******	0.0014
1710	293.	******	0.50	******	2.20	******	******	******	0.63	******	2.49	******	69.5	******

BAG-203
SURROGATE CONTROL #3
1979 NOV 2

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0630-0800 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM
          BAG VOLUME APPROXIMATELY 33 CUBIC METERS
0845      BAG COVERED
0847      RH IS 20% AT 19 DEG C
0904      2.6 ML NO2 INJECTED AND MIXED
0906      7.3 ML NO INJECTED AND MIXED
0911      500 ML SURROGATE J INJECTED AND MIXED
0915      14.0 MICROLITERS (U-L) 2,3-DMB, 1.9 U-L TOLUENE,
               1.6 U-L 2-ME-2-C4=, AND 5.4 U-L M-XYLENE INJECTED AND MIXED
0920      BAG DIVIDED
1012      BAG UNCOVERED
          NO2 AND NOX WERE NOT CORRECTED FOR PAN DUE TO INSTRUMENT
               MALFUNCTION DURING MOST OF EXPERIMENT. MAXIMUM OF 8 PPB
               OBSERVED AT END OF EXPERIMENT
1245      TSI WHITBY OBSERVED TO BE DISCONNECTED FROM SAMPLING LINE.
               SOME READINGS FROM OTHER INSTRUMENTS MAY BE AFFECTED
          SIDE 1 AND SIDE 2 POSSIBLY RECEIVING DIFFERING AMOUNTS OF SUNLIGHT
          DASIBI 1770 AND BENDIX O3 ANALYZERS, TSI 3030 (WHITBY),
               CLIMET OPTICAL COUNTER USED
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*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS2/CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM2-MIN)	X 1

T=0 AT 1012 PST

TS	DEG K	AVERAGE	301.5
UV		AVERAGE	0.004

* ASSIGNED INITIAL CONDITION

BAG-203
SURROGATE CONTROL #2
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	OZONE PPM DAS-1	OZONE PPM DAS-2	OZONE PPM BNX-1	OZONE PPM BNX-2	NO PPM SIDE 1	NO PPM SIDE 2	NO2-CORR PPM SIDE 1	NO2-CORR PPM SIDE 2	NOX-CORR PPM	NOX-CORR PPM SIDE 2
829	-103.	0.005	******	0.005	******	0.001	******	0.009	******	0.010	******
930	-42.	******	******	******	******	******	******	******	******	******	******
932	-40.	0.008	******	0.003	******	0.159	******	0.084	******	0.235	******
941	-31.	******	0.005	******	0.003	******	0.153	******	0.081	******	0.228
1005	-7.	******	******	******	******	******	******	******	******	******	******
1015	3.	******	******	******	******	******	******	******	******	******	******
1016	4.	0.007	******	0.009	******	0.159	******	0.082	******	0.233	******
1023	11.	******	0.004	******	0.010	******	0.145	******	0.087	******	0.221
1045	33.	0.010	******	0.013	******	0.129	******	0.107	******	0.225	******
1051	39.	******	0.011	******	0.013	******	0.119	******	0.108	******	0.216
1100	48.	******	******	******	******	******	******	******	******	******	******
1115	63.	0.033	******	0.017	******	0.092	******	0.139	******	0.223	******
1122	70.	******	0.028	******	0.019	******	0.086	******	0.132	******	0.209
1145	93.	0.031	******	0.028	******	0.064	******	0.159	******	0.213	******
1152	100.	******	0.034	******	0.029	******	0.061	******	0.150	******	0.200
1215	123.	******	0.040	******	0.038	******	0.043	******	0.165	******	0.195
1221	129.	0.045	******	0.045	******	0.039	******	0.175	******	0.199	******
1230	138.	******	******	******	******	******	******	******	******	******	******
1245	153.	0.064	******	0.065	******	0.031	******	0.188	******	0.204	******
1249	157.	******	0.055	******	0.059	******	0.028	******	0.171	******	0.191
1315	183.	0.086	******	0.084	******	0.021	******	0.189	******	0.197	******
1322	190.	******	0.068	******	0.078	******	0.019	******	0.171	******	0.181
1345	213.	0.101	******	0.103	******	0.017	******	0.183	******	0.188	******
1352	220.	******	0.080	******	0.086	******	0.017	******	0.173	******	0.178
1400	228.	******	******	******	******	******	******	******	******	******	******
1415	243.	0.106	******	0.120	******	0.012	******	0.185	******	0.180	******
1422	250.	******	0.095	******	0.099	******	0.010	******	0.171	******	0.171
1445	273.	0.115	******	0.132	******	0.009	******	0.180	******	0.174	******
1455	283.	******	0.098	******	0.109	******	0.005	******	0.171	******	0.167
1516	304.	0.120	******	0.138	******	0.008	******	0.179	******	0.173	******
1525	313.	******	0.094	******	0.119	******	0.002	******	0.170	******	0.165
1530	318.	******	******	******	******	******	******	******	******	******	******

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	PAN PPM SIDE 1	PAN PPM SIDE 2	ACETONE PPM SIDE 1	ACETONE PPM SIDE 2	MEK PPM SIDE 1	MEK PPM SIDE 2	METHANE PPM SIDE 1	METHANE PPM SIDE 2	ETHANE PPM SIDE 1	ETHANE PPM SIDE 2	ETHENE PPM SIDE 1	ETHENE PPM SIDE 2
829	-103.	******	******	******	******	******	******	******	******	******	******	******	******
930	-42.	******	******	0.0040	0.0040	******	******	******	******	******	******	******	******
932	-40.	******	******	******	******	******	******	******	******	******	******	******	******
941	-31.	******	******	******	******	******	******	******	******	******	******	******	******
1005	-7.	******	******	******	******	******	******	1.12	1.12	0.0636	0.0636	0.0374	0.0374
1015	3.	******	******	0.0065	******	******	******	1.12	******	0.0667	******	0.0384	******
1016	4.	******	******	******	******	******	******	******	******	******	******	******	******
1023	11.	******	******	******	******	******	******	******	******	******	******	******	******
1045	33.	******	******	******	******	******	******	******	******	******	******	******	******
1051	39.	******	******	******	******	******	******	******	******	******	******	******	******
1100	48.	******	******	******	0.0118	******	******	******	1.19	******	0.0671	******	0.0426
1115	63.	******	******	******	******	******	******	******	******	******	******	******	******
1122	70.	******	******	******	******	******	******	******	******	******	******	******	******
1145	93.	******	******	0.0178	******	******	******	******	******	0.0708	******	0.0362	******
1152	100.	******	******	******	******	******	******	******	******	******	******	******	******
1215	123.	******	******	******	******	******	******	******	******	******	******	******	******
1221	129.	******	******	******	******	******	******	******	******	******	******	******	******
1230	138.	******	******	******	0.0179	******	******	******	******	******	0.0631	******	0.0363
1245	153.	******	******	******	******	******	******	******	******	******	******	******	******
1249	157.	******	******	******	******	******	******	******	******	******	******	******	******
1315	183.	******	******	0.0233	******	0.0047	******	******	******	0.0726	******	0.0328	******
1322	190.	******	******	******	******	******	******	******	******	******	******	******	******
1345	213.	******	******	******	******	******	******	******	******	******	******	******	******
1352	220.	******	******	******	******	******	******	******	******	******	******	******	******
1400	228.	******	******	******	0.0247	******	0.0049	******	******	******	0.0668	******	0.0337
1415	243.	******	******	******	******	******	******	******	******	******	******	******	******
1422	250.	******	******	******	******	******	******	******	******	******	******	******	******
1445	273.	******	******	0.0267	******	0.0059	******	1.17	******	0.0719	******	0.0297	******
1455	283.	******	******	******	******	******	******	******	******	******	******	******	******
1516	304.	0.002	******	******	******	******	******	******	******	******	******	******	******
1525	313.	******	0.002	******	******	******	******	******	******	******	******	******	******
1530	318.	******	******	******	0.0266	******	0.0060	******	1.19	******	0.0672	******	0.0314

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	ACETYLEN PPM PN-2	ACETYLEN PPM PN-1	ACETYLEN PPM DMS-2	ACETYLEN PPM DMS-1	PROPANE PPM SIDE 1	PROPANE PPM SIDE 2	PROPENE PPM SIDE 1	PROPENE PPM SIDE 2	I-C4 PPM SIDE 1	I-C4 PPM SIDE 2	N-C4 PPM SIDE 1	N-C4 PPM SIDE 2
829	-103.	******	******	******	******	******	******	******	******	******	******	******	******
930	-42.	******	******	0.0486	0.0486	0.0337	0.0337	0.012	0.012	0.0011	0.0011	0.184	0.184
932	-40.	******	******	******	******	******	******	******	******	******	******	******	******
941	-31.	******	******	******	******	******	******	******	******	******	******	******	******
1005	-7.	0.0384	0.0384	******	******	******	******	******	******	******	******	******	******
1015	3.	******	0.0406	******	0.0477	0.0337	******	0.012	******	0.0012	******	0.182	******
1016	4.	******	******	******	******	******	******	******	******	******	******	******	******
1023	11.	******	******	******	******	******	******	******	******	******	******	******	******
1045	33.	******	******	******	******	******	******	******	******	******	******	******	******
1051	39.	******	******	******	******	******	******	******	******	******	******	******	******
1100	43.	0.0399	******	0.0452	******	******	0.0319	******	0.010	******	0.0011	******	0.171
1115	63.	******	******	******	******	******	******	******	******	******	******	******	******
1122	70.	******	******	******	******	******	******	******	******	******	******	******	******
1145	93.	******	0.0418	******	0.0473	0.0329	******	0.008	******	0.0011	******	0.175	******
1152	100.	******	******	******	******	******	******	******	******	******	******	******	******
1215	123.	******	******	******	******	******	******	******	******	******	******	******	******
1221	129.	******	******	******	******	******	******	******	******	******	******	******	******
1230	138.	0.0405	******	0.0473	******	******	0.0306	******	0.006	******	0.0012	******	0.162
1245	153.	******	******	******	******	******	******	******	******	******	******	******	******
1249	157.	******	******	******	******	******	******	******	******	******	******	******	******
1315	183.	******	0.0429	******	0.0464	0.0319	******	0.005	******	0.0011	******	0.167	******
1322	190.	******	******	******	******	******	******	******	******	******	******	******	******
1345	213.	******	******	******	******	******	******	******	******	******	******	******	******
1352	220.	******	******	******	******	******	******	******	******	******	******	******	******
1400	228.	0.0392	******	0.0439	******	******	0.0306	******	0.004	******	0.0012	******	0.158
1415	243.	******	******	******	******	******	******	******	******	******	******	******	******
1422	250.	******	******	******	******	******	******	******	******	******	******	******	******
1445	273.	******	0.0421	******	0.0469	0.0330	******	0.004	******	0.0012	******	0.168	******
1455	283.	******	******	******	******	******	******	******	******	******	******	******	******
1516	304.	******	******	******	******	******	******	******	******	******	******	******	******
1525	313.	******	******	******	******	******	******	******	******	******	******	******	******
1530	318.	0.0398	******	0.0439	******	******	0.0305	******	0.003	******	0.0012	******	0.155

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	I-C4= PPM SIDE 1	I-C4= PPM SIDE 2	T2-C4= PPM SIDE 1	T2-C4= PPM SIDE 2	I-C5 PPM SIDE 1	I-C5 PPM SIDE 2	CIS2-C4= PPM SIDE 1	CIS2-C4= PPM SIDE 2	N-C5 PPM SIDE 1	N-C5 PPM SIDE 2
829	-103.	******	******	******	******	******	******	******	******	******	******	******	******
930	-42.	0.0001	0.0001	0.0002	0.0002	0.0007	0.0007	0.0005	0.0005	0.0155	0.0155	0.0018	0.0018
932	-40.	******	******	******	******	******	******	******	******	******	******	******	******
941	-31.	******	******	******	******	******	******	******	******	******	******	******	******
1005	-7.	******	******	******	******	******	******	******	******	******	******	******	******
1015	3.	******	******	******	******	0.0007	******	0.0002	******	0.0187	******	0.0001	******
1016	4.	******	******	******	******	******	******	******	******	******	******	******	******
1023	11.	******	******	******	******	******	******	******	******	******	******	******	******
1045	33.	******	******	******	******	******	******	******	******	******	******	******	******
1051	39.	******	******	******	******	******	******	******	******	******	******	******	******
1100	48.	******	0.0002	******	0.0001	******	0.0003	******	0.0005	******	0.0087	******	0.0002
1115	63.	******	******	******	******	******	******	******	******	******	******	******	******
1122	70.	******	******	******	******	******	******	******	******	******	******	******	******
1145	93.	******	******	******	******	0.0003	******	0.0003	******	0.0048	******	0.0002	******
1152	100.	******	******	******	******	******	******	******	******	******	******	******	******
1215	123.	******	******	******	******	******	******	******	******	******	******	******	******
1221	129.	******	******	******	******	******	******	******	******	******	******	******	******
1230	138.	******	0.0001	******	0.0001	******	0.0001	******	0.0006	******	0.0023	******	0.0002
1245	153.	******	******	******	******	******	******	******	******	******	******	******	******
1249	157.	******	******	******	******	******	******	******	******	******	******	******	******
1315	183.	******	******	******	******	0.0001	******	0.0003	******	0.0008	******	0.0001	******
1322	190.	******	******	******	******	******	******	******	******	******	******	******	******
1345	213.	******	******	******	******	******	******	******	******	******	******	******	******
1352	220.	******	******	******	******	******	******	******	******	******	******	******	******
1400	228.	******	******	******	******	******	0.0001	******	0.0006	******	0.0006	******	0.0004
1415	243.	******	******	******	******	******	******	******	******	******	******	******	******
1422	250.	******	******	******	******	******	******	******	******	******	******	******	******
1445	273.	******	******	******	******	******	******	0.0004	******	0.0002	******	0.0	******
1455	283.	******	******	******	******	******	******	******	******	******	******	******	******
1516	304.	******	******	******	******	******	******	******	******	******	******	******	******
1525	313.	******	******	******	******	******	******	******	******	******	******	******	******
1530	318.	******	0.0002	******	0.0001	******	******	******	0.0007	******	0.0001	******	0.0003

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	2ME-C4=2 PPM SIDE 1	2ME-C4=2 PPM SIDE 2	2,3-DMB PPM SIDE 1	2,3-DMB PPM SIDE 2	TOLUENE PPM SIDE 1	TOLUENE PPM SIDE 2	M-XYL PPM SIDE 1	M-XYL PPM SIDE 2
829	-103.	******	******	******	******	******	******	******	******
930	-42.	0.0115	0.0115	0.0822	0.0822	0.014	0.014	0.0353	0.0353
932	-40.	******	******	******	******	******	******	******	******
941	-31.	******	******	******	******	******	******	******	******
1005	-7.	******	******	******	******	******	******	******	******
1015	3.	0.0076	******	0.0815	******	0.014	******	0.0350	******
1016	4.	******	******	******	******	******	******	******	******
1023	11.	******	******	******	******	******	******	******	******
1045	33.	******	******	******	******	******	******	******	******
1051	39.	******	******	******	******	******	******	******	******
1100	48.	******	0.0046	******	0.0746	******	0.013	******	0.0298
1115	63.	******	******	******	******	******	******	******	******
1122	70.	******	******	******	******	******	******	******	******
1145	93.	0.0014	******	0.0747	******	0.013	******	0.0256	******
1152	100.	******	******	******	******	******	******	******	******
1215	123.	******	******	******	******	******	******	******	******
1221	129.	******	******	******	******	******	******	******	******
1230	138.	******	0.0002	******	0.0681	******	0.012	******	0.0211
1245	153.	******	******	******	******	******	******	******	******
1249	157.	******	******	******	******	******	******	******	******
1315	183.	******	******	0.0686	******	0.012	******	0.0193	******
1322	190.	******	******	******	******	******	******	******	******
1345	213.	******	******	******	******	******	******	******	******
1352	220.	******	******	******	******	******	******	******	******
1400	228.	******	0.0002	******	0.0629	******	0.011	******	0.0169
1415	243.	******	******	******	******	******	******	******	******
1422	250.	******	******	******	******	******	******	******	******
1445	273.	0.0001	******	0.0658	******	0.011	******	0.0161	******
1455	283.	******	******	******	******	******	******	******	******
1516	304.	******	******	******	******	******	******	******	******
1525	313.	******	******	******	******	******	******	******	******
1530	318.	******	0.0	******	0.0614	******	0.011	******	0.0149

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	B-SCAT SIDE 1*	B-SCAT SIDE 2*	CONDENS. SIDE 1*	CONDENS. SIDE 2*	AEROSL N SIDE 1*	AEROSL N SIDE 2*	AEROSL S SIDE 1*	AEROSL S SIDE 2*	AEROSL V SIDE 1*	AEROSL V SIDE 2*	TS DEG F SIDE 1	TS DEG F SIDE 2
829	-103.	0.40	******	******	******	0.0	******	0.0	******	0.0	******	65.9	******
930	-42.	******	******	******	******	******	******	******	******	******	******	******	******
932	-40.	0.40	******	******	******	0.0	******	0.0	******	0.0	******	******	******
941	-31.	******	0.40	******	******	******	0.0	******	0.0	******	0.0	******	******
1005	-7.	******	******	******	******	******	******	******	******	******	******	******	******
1015	3.	******	******	******	******	******	******	******	******	******	******	******	******
1016	4.	0.30	******	******	******	0.0	******	0.0	******	0.0	******	80.3	******
1023	11.	******	0.30	******	******	******	0.0	******	0.0	******	0.0	******	83.9
1045	33.	0.30	******	******	******	0.0	******	0.0	******	0.0	******	80.3	******
1051	39.	******	0.30	******	******	******	0.0	******	0.0	******	0.0	******	87.5
1100	48.	******	******	******	******	******	******	******	******	******	******	******	******
1115	63.	0.30	******	******	******	0.0	******	0.0	******	0.0	******	82.1	******
1122	70.	******	0.30	******	******	******	0.0	******	0.0	******	0.0	******	87.5
1145	93.	0.30	******	******	******	0.0	******	0.0	******	0.0	******	83.9	******
1152	100.	******	0.30	******	******	******	0.0	******	0.0	******	0.0	******	89.3
1215	123.	******	0.30	******	******	******	0.0	******	0.0	******	0.0	******	85.7
1221	129.	0.30	******	******	******	0.0	******	0.0	******	0.0	******	80.3	******
1230	138.	******	******	******	******	******	******	******	******	******	******	******	******
1245	153.	0.30	******	0.10	******	0.85	******	0.07	******	0.09	******	85.7	******
1249	157.	******	0.30	******	3.70	******	1.55	******	0.21	******	0.30	******	83.9
1315	183.	0.30	******	0.70	******	1.14	******	0.14	******	0.92	******	83.9	******
1322	190.	******	0.30	******	5.00	******	2.07	******	0.29	******	1.25	******	87.5
1345	213.	0.30	******	0.10	******	0.82	******	0.10	******	0.38	******	85.7	******
1352	220.	******	0.30	******	4.40	******	2.59	******	0.21	******	0.28	******	83.9
1400	228.	******	******	******	******	******	******	******	******	******	******	******	******
1415	243.	0.30	******	0.60	******	1.26	******	0.13	******	0.91	******	85.7	******
1422	250.	******	0.20	******	4.30	******	3.40	******	0.27	******	0.58	******	87.5
1445	273.	0.30	******	0.40	******	1.11	******	0.20	******	1.27	******	83.9	******
1455	283.	******	0.30	******	3.90	******	6.12	******	0.53	******	1.84	******	83.9
1516	304.	0.30	******	0.70	******	1.11	******	0.16	******	0.36	******	80.3	******
1525	313.	******	0.30	******	4.10	******	3.96	******	0.44	******	1.09	******	80.3
1530	318.	******	******	******	******	******	******	******	******	******	******	******	******

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SURROGATE CONTROL #3
1979 NOV 2

CLOCK TIME	ELAPSED T(MIN)	UV SIDE 1*	UV SIDE 2*
829	-103.	******	******
930	-42.	******	******
932	-40.	0.0037	******
941	-31.	******	0.0036
1005	-7.	******	******
1015	3.	******	******
1016	4.	0.0039	******
1023	11.	******	******
1045	33.	0.0040	******
1051	39.	******	******
1100	48.	******	******
1115	63.	0.0044	******
1122	70.	******	******
1145	93.	0.0040	******
1152	100.	******	******
1215	123.	******	0.0036
1221	129.	******	******
1230	138.	******	******
1245	153.	0.0037	******
1249	157.	******	******
1315	183.	0.0034	******
1322	190.	******	******
1345	213.	0.0036	******
1352	220.	******	******
1400	228.	******	******
1415	243.	0.0034	******
1422	250.	******	******
1445	273.	0.0028	******
1455	283.	******	******
1516	304.	0.0026	******
1525	313.	******	******
1530	318.	******	******