IMPLEMENTATION OF THE SAPRC-99 CHEMICAL MECHANISM INTO THE MODELS-3 FRAMEWORK

Report to the United States Environmental Protection Agency

By

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ABSTRACT

This report documents the files, software and procedures needed to implement the SAPRC-99 detailed chemical mechanism into the Models-3 software framework. The SAPRC-99 mechanism is a detailed mechanism for the gas-phase atmospheric reactions of volatile organic compounds (VOCs) and oxides of nitrogen (NO_x) in urban and regional atmospheres, and represents the state-of-the-art as of mid-1999. It is a completely updated and expanded version of the earlier SAPRC mechanisms, and is comprehensively documented in a report to the California Air Resources Board (Carter, 1999). It has the capability of separately representing the atmospheric reactions of ~400 types of VOCs, and can be used to estimate reactivities for ~550 VOC categories. Condensed versions of this mechanism have been developed for use in regional models, using a more limited number of lumped VOC classes whose mechanistic parameters depend on the mixture of compounds they represent. Different versions can be used depending on which VOC mixture is used to derive the mechanisms and parameters for these lumped VOC classes. This report describes the implementation of two condensed versions of SAPRC-99 into the Models-3 framework, one where the lumped VOC classes are derived from VOCs measured in ambient air, and one where the lumped VOC classes are derived from VOCs present in a recent EPA emissions inventory. Methods for deriving versions of the mechanism representing other mixtures or emissions inventories, and for explicitly representing selected VOCs for reactivity assessment and other purposes, are discussed. The procedures for obtaining, installing, and using the software and files needed to implement this mechanism are described.

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The major work in developing the SAPRC-99 chemical mechanism was funded by the California Air Resources Board (CARB) through CARB Contract 92-329 and in part through Contract 95-308. The work on the CARB contracts is documented in a separate report, and this report has not been reviewed by that agency and no official endorsement by the CARB should be inferred. This report focuses on the development of the mechanism for airshed models, which was funded by the U.S. Environmental Protection Agency through a consulting agreement.

The opinions and conclusions in this report are entirely those of the author. Mention of trade names and commercial products does not constitute endorsement or recommendation for use. This report has not been reviewed by the Environmental Protection Agency, and no official endorsement should be inferred.

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I. INTRODUCTION

Airshed models are essential for the development of effective control strategies for reducing photochemical air pollution because they provide the only available scientific basis for making quantitative estimates of changes in air quality resulting from changes in emissions. The chemical mechanism is the portion of the model that represents the processes by which emitted primary pollutants, such as volatile organic compounds (VOCs) and oxides of nitrogen (NO_x), interact in the gas phase to form secondary pollutants such as ozone (O_3) and other oxidants. This is an important component of airshed models because if the mechanism is incorrect or incomplete in significant respects, then the model's predictions of secondary pollutant formation may also be incorrect, and its use might result in implementation of inappropriate or even counter-productive air pollution control strategies.

Over the years, a number of chemical mechanisms have been developed for use in urban and regional airshed models. The mechanisms used in the urban and regional models currently employed in the United States for regulatory and research purposes include the Carbon Bond 4 (Gery et al, 1998), RADM-2 (Stockwell et al, 1990), and various versions of the SAPRC mechanisms (Carter, 1990, Carter et al, 1997a). However, the chemical processes that these mechanisms are highly complex and have many uncertainties, and research into these uncertainties, and in developing better representing the highly complex chemical processes in useable models, has continued since these mechanism were developed. For example, Stockwell and co-workers have recently developed the "RACM" mechanism a complete update to RADM-2 (Stockwell et al, 1997), and Carter (1999) recently completed a complete update of the SAPRC mechanism, designated SAPRC-99. Both these mechanisms represent the current state of the art in atmospheric chemistry, though RACM was developed primarily for urban and regional modeling applications, while SAPRC-99 was developed with the additional capability of representing reactions of a wide variety of individual VOCs. The latter capability allows the development of condensed versions of the mechanism for urban and regional models that can incorporate our knowledge of the composition and chemistry of the specific mixtures of VOCs that are being represented.

An advanced third-generation air quality modeling system is currently being developed by the Atmospheric Modeling Division of the U.S. EPA (EPA 1997, 1999a). The air quality simulation model at the heart of the system is known as the Community Multiscale Air Quality (CMAQ) Model. It is comprehensive in scope and allows for the simulation of ozone and photochemical oxidants, acid deposition, and fine and coarse particles at spatial scales ranging from urban to regional. The model is contained within a computational framework, Models-3 (for 3 generation), that enables users to interact with the modeling system through a high-level graphical user interface and also facilitates data transmission among the components of the system and provides for analysis, graphics, and visualization capabilities for model simulation results. The modeling system is available from the U.S. EPA[1] and is currently being evaluated for photochemical oxidants and fine particles using field study databases from the eastern United States from 1990 and 1995.

The Models-3 framework has a relatively flexible chemical mechanism interface that permits use of different chemical mechanisms in CMAQ simulations. However, the initial versions only implement the Carbon Bond 4 (Gery et al, 1988) and the RADM-2 (Stockwell et al, 1990) mechanisms, which, as indicted above, are somewhat out of date. Until this work, no version of the SAPRC mechanisms were

[1] The current version of Models-3 is available at www.epa.gov/asmdnerl/models3.

implemented into the Models-3 framework, despite the widespread use of various versions of the SAPRC mechanism for VOC reactivity and various research applications.

Because of a desire to implement an alternative mechanism into the Models-3/CMAQ framework that represents the current state-of-the-art, the EPA contracted with the author to provide the files, documentation, and software needed to implement the latest SAPRC mechanism into Models-3. This report describes the files and software and provides the documentation needed to implement the SAPRC-99 mechanism (Carter, 1999) into Models-3/CMAQ.

II. MECHANISM DESCRIPTION

The SAPRC-99 mechanism was developed under funding from the California Air Resources Board (CARB) and is comprehensively documented by Carter (1999)[2]. The CARB also funded William Stockwell, the principal developer of the RADM-2 (Stockwell et al, 1990) and RACM (Stockwell et al, 1997) mechanisms, to conduct a peer review of this mechanism, and the results of this review, and the authors response to this review (Stockwell, 1999) are also available[2]. The report of Carter (1999) should be consulted for details, and only a brief summary of the mechanism is given here.

The major components of the SAPRC mechanisms are the base mechanism, the assignments and/or estimation procedures used to estimate the reactions of the represented VOCs that are not in the base mechanism, and the lumping procedures used to represent complex mixtures or VOCs for which assignments or estimates are not available. The base mechanism is the portion of the mechanism that represents the reactions of the inorganic species, the common organic products, the intermediate radicals leading to these products, including those formed from the initial reactions of the represented VOCs not in the base mechanism. Most of the VOCs that can be separately represented are not in the base mechanism, but can be added to the mechanism, either as explicit reactions for individual VOCs or as lumped model species whose parameters are derived from the mixture of detailed model species they represent, as needed in the model application.

Airshed model applications require simulations of highly complex mixtures of large numbers of VOCs, and in most cases it is not necessary or practical to represent each of them separately. For such applications, models with lumped model species that represent reactions of a large number of species with similar reaction rates and mechanisms, are generally employed. Even for VOC reactivity assessment it is only really necessary to separately represent the VOC whose reactivity is being assessed, the reactions of most of the other VOCs present in the ambient simulation can be represented using appropriate lumped model species. This was the approach that was employed in our previous reactivity studies (e.g., Carter and Atkinson, 1989, Carter, 1994a), and continues to be the approach used in this work.

As with the previous versions of the SAPRC mechanism (Carter, 1988), two different approaches, referred to as lumped molecule and variable lumped parameter condensation, can be employed to represent VOCs in complex mixtures using this mechanism. The lumped molecule approach involves representing the VOC by a model species in the base mechanism, on a molecule-for-molecule basis. The variable lumped parameter approach representing a group of VOCs that react with similar rate constants with model species whose kinetic and product yield parameters are weighted averages of the mixture of VOCs they are being used to represent. A third approach, referred to here as fixed parameter condensation is used in condensed models such as the LCC (Lurmann et al, 1987), RADM-2 (Stockwell et al, 1990), and RACM (Stockwell et al, 1997) can also be employed, and may be appropriate or necessary in some applications. A fourth approach, referred to as lumped structure is employed in the widely-used Carbon Bond mechanism (Gery et al, 1988) and was used to represent hydroperoxides in the previous SAPRC mechanism (Carter, 1990), though it is not used in the current mechanism. These approaches, and their advantages and disadvantages, are discussed in more detail by Carter (1999).

The optimum lumping approach in terms of minimizing the number of model species without introducing nonnegligible approximations depends on the model application and type of scenario

[2] This report and associated documentation and files is available at http://cert.ucr.edu/~carter/reactdat.htm

employed. The use of the variable parameter approach permits a high degree of lumping with very little approximation in single box or EKMA model scenarios, which involve only a single day simulation with all the VOCs being introduced together (Carter, 1988). However, the requirements of multi-cell and multi-day regional models are more demanding. This is because different compositions of VOCs can be emitted at different times and locations, so no single parameterization may represent the emissions profile in all locations at all times. In addition, representing slowly reacting VOCs with more rapidly reacting model species using reactivity weighting such as employed for RADM-2 (Middleton et al, 1990) may not appropriately represent these VOCs in multi-day simulations, since they would persist longer than the model species used to represent them. More lumped classes are therefore needed to minimize the time and space variation of the reactivity characteristics of the VOCs represented by any given lumped species, and to permit the slowly reacting species to be more appropriately represented in multi-day scenarios.

The approach adopted in this work is to recommend a lumping approach that addresses the requirements of regional, multi-cell, multi-day model applications. Since that is the most demanding requirement, this will then give a mechanism that should be appropriate for most applications, albeit with more species than may be necessary for some applications such as EKMA. This permits use of a consistent mechanism and degree of condensation, regardless of the application.

In this work we present fixed parameter versions of this mechanism that can be used to permit implementation of this mechanism in modeling systems that do not support the emissions processing needed for automatically implementing the variable parameter approach. This is because the mechanism implementation software presently used in the Models-3/CMAQ framework does not support use of variable product yield parameters. However, since different fixed parameter mechanisms can be derived to represent various VOC emissions profiles or assumed compositions of complex mixtures that are represented, in principle the variable parameter approach can be employed in fixed parameter implementations such as the current version of Models-3. Two examples of such mechanisms are given in this report, and methods to derive mechanisms representing different mixtures are discussed in Section III.B.

A. Mechanism Listing

The model species used in the condensed version of the mechanism recommended for urban or regional model applications are given in Table 1. As indicated there, these include the inorganic and common organic product species in the base mechanism that are included in all versions of the mechanism regardless of the application, the model species for the few primary emitted VOCs we recommend be represented explicitly, and the model species representing complex mixtures whose parameters depend on the mixtures being represented. Note that many of the model species used to represent common organic product can also represent primary emitted VOCs, based on the “lumped molecule” approach. The specific assignments of which model species are used to represent each individual VOC are given in Section II.B.1.

Table 1. List of model species in the SAPRC-99 mechanism as implemented for the Models-3 format.

Type and Name	Description
Species used in Base Mechanism	
Constant Species.	
O2	Oxygen
M	Air
H2O	Water
H2	Hydrogen Molecules
Active Inorganic Species.	
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HNO3	Nitric Acid
HNO4	Peroxynitric Acid
HO2H	Hydrogen Peroxide
CO	Carbon Monoxide
SO2	Sulfur Dioxide
Active Radical Species and Operators.	
HO	Hydroxyl Radicals
HO2	Hydroperoxide Radicals
C_O2	Methyl Peroxy Radicals
RO2_R	Peroxy Radical Operator representing NO to NO2 conversion with HO2 formation.
R2O2	Peroxy Radical Operator representing NO to NO2 conversion without HO2 formation.
RO2_N	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
CCO_O2	Acetyl Peroxy Radicals
RCO_O2	Peroxy Propionyl and higher peroxy acyl Radicals
BZCO_O2	Peroxyacyl radical formed from Aromatic Aldehydes
MA_RCO3	Peroxyacyl radicals formed from methacrolein and other acroleins.
Steady State Radical Species	
O3P	Ground State Oxygen Atoms
O1D2	Excited Oxygen Atoms
TBU_O	t-Butoxy Radicals
BZ_O	Phenoxy Radicals
BZ(NO2)_O	Nitro-substituted Phenoxy Radical
HOCOO	Radical formed when Formaldehyde reacts with HO2
PAN and PAN Analogues	
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues

Table 1 (continued)

Type and Name	Description
PBZN	PAN analogues formed from Aromatic Aldehydes
MA_PAN	PAN analogue formed from Methacrolein
Explicit and Lumped Molecule Reactive Organic Product Species	
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals slower than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
MEOH	Methanol
COOH	Methyl Hydroperoxide
ROOH	Lumped higher organic hydroperoxides
GLY	Glyoxal
MGLY	Methyl Glyoxal
BACL	Biacetyl
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
BALD	Aromatic aldehydes (e.g., benzaldehyde)
METHACRO	Methacrolein
MVK	Methyl Vinyl Ketone
ISOPROD	Lumped isoprene product species
Lumped Parameter Products	
PROD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
RNO3	Lumped Organic Nitrates
Uncharacterized Reactive Aromatic Ring Fragmentation Products	
DCB1	Reactive Aromatic Fragmentation Products that do not undergo signficant photodecomposition to radicals.
DCB2	Reactive Aromatic Fragmentation Products which photolyze with alpha-dicarbonyl-like action spectrum.
DCB3	Reactive Aromatic Fragmentation Products which photolyze with acrolein action spectrum.
Non-Reacting Species and Low Reactivity Compounds or Unknown Products Represented as Unreactive	
SULF	Sulfates (SO_3 or H_2SO_4)
HCOOH	Formic Acid
CCO_OH	Acetic Acid
RCO_OH	Higher organic acids
CCO_OOH	Peroxy Acetic Acid
RCO_OOH	Higher organic peroxy acids

Table 1 (continued)

Type and Name	Description
Species used in Lumped Mechanisms for Base Case and Ambient Simulations	
Primary Organics Represented explicitly	
CH4	Methane
ETHENE	Ethene
ISOPRENE	Isoprene
Lumped Parameter Species	
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH < 5 x 10^2 ppm-1 min-1. (Primarily ethane)
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm-1 min-1. (Primarily propane and acetylene)
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm-1 min-1.
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^3 and 1 x 10^4 ppm-1 min-1.
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1 x 10^4 ppm-1 min-1.
ARO1	Aromatics with kOH < 2x10^4 ppm-1 min-1.
ARO2	Aromatics with kOH > 2x10^4 ppm-1 min-1.
OLE1	Alkenes (other than ethene) with kOH < 7x10^4 ppm-1 min-1.
OLE2	Alkenes with kOH > 7x10^4 ppm-1 min-1.
TRP1	Terpenes
others	Model species to represent reactions of explicitly represented VOCs whose mechanisms have been derived for SAPRC-99, if needed.

Table 2. Listing of reactions used in the SAPRC-99 mechanism to represent the reactions of the inorganics and the common organic products. Reactions of primary emitted VOCs that are represented explicitly in urban and regional model applications are also shown. Reactions of lumped parameter species whose mechanisms depend on the mixture of VOCs being represented are shown in separate tables.

Label	Reaction	Kinetic Parameters [a]
1	NO2 = NO + O3P	# 1.0 / <NO2>
2	O3P + O2 + M = O3	# 5.68e-34 ^ -2.80
3	O3P + O3 =	# 8.00e-12 @ 2060
4	O3P + NO + M = NO2	# 1.00e-31 ^ -1.60
5	O3P + NO2 = NO	# 6.50e-12 @ -120
6	O3P + NO2 = NO3	# 9.00e-32 ^ -2.00 & 2.20e-11 & 0.80 & 1.0
8	O3 + NO = NO2	# 1.80e-12 @ 1370
9	O3 + NO2 = NO3	# 1.40e-13 @ 2470
10	NO + NO3 = 2*NO2	# 1.80e-11 @ -110
11	NO + NO + O2 = 2*NO2	# 3.30e-39 @ -530
12	NO2 + NO3 = N2O5	# 2.80e-30 ^ -3.50 & 2.00e-12 ^ 0.20 & 0.45 & 1.0
13	N2O5 = NO2 + NO3	# 1.00e-03 ^ -3.50 @ 11000 & 9.70e+14 ^ 0.10 @ 11080 & 0.45 & 1.0
14	N2O5 + H2O = 2*HNO3	# 2.60e-22
17	NO2 + NO3 = NO + NO2	# 4.50e-14 @ 1260
18	NO3 = NO	# 1.0 / <NO3NO>
19	NO3 = NO2 + O3P	# 1.0 / <NO3NO2>
20	O3 = O3P	# 1.0 / <O3O3P>
21	O3 = O1D2	# 1.0 / <O3O1D>
22	O1D2 + H2O = 2*HO	# 2.20e-10
23	O1D2 + M = O3P	# 2.09e-11 @ -95
24	HO + NO = HONO	# 7.00e-31 ^ -2.60 & 3.60e-11 ^ -0.10 & 0.60 & 1.0
25	HONO = HO + NO	# 1.0 / <HONO-NO>
26	HONO = HO2 + NO2	# 1.0 / <HONO-NO2>
27	HO + HONO = NO2	# 2.70e-12 @ -260
28	HO + NO2 = HNO3	# 2.43e-30 ^ -3.10 & 1.67e-11 ^ -2.10 & 0.60 & 1.0
29	HO + NO3 = HO2 + NO2	# 2.00e-11
30	HO + HNO3 = NO3	%2 # 7.20e-15 @ -785 & 4.10e-16 @ -1440 & 1.90e-33 @ -725
31	HNO3 = HO + NO2	# 1.0 / <HNO3>
32	HO + CO = HO2	%3 # 1.30e-13 & 3.19e-33
33	HO + O3 = HO2	# 1.90e-12 @ 1000

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
34	HO2 + NO = HO + NO2	# 3.40e-12 @ -270
35	HO2 + NO2 = HNO4	# 1.80e-31 ^ -3.20 & 4.70e-12 & 0.60 & 1.0
36	HNO4 = HO2 + NO2	# 4.10e-05 @ 10650 & 5.70e+15 @ 11170 & 0.50 & 1.0
37	HNO4 = 0.61*HO2 + 0.61*NO2 + 0.39*HO + 0.39*NO3	# 1.0 / <HO2NO2>
38	HNO4 + HO = NO2	# 1.50e-12 @ -360
39	HO2 + O3 = HO	# 1.40e-14 @ 600
40A	HO2 + HO2 = HO2H	%3 # 2.20e-13 @ -600 & 1.85e-33 @ -980
40B	HO2 + HO2 + H2O = HO2H	%3 # 3.08e-34 @ -2800 & 2.59e-54 @ -3180
41	NO3 + HO2 = 0.8*HO + 0.8*NO2 + 0.2*HNO3	# 4.00e-12
42	NO3 + NO3 = 2*NO2	# 8.50e-13 @ 2450
43	HO2H = 2*HO	# 1.0 / <H2O2>
44	HO2H + HO = HO2	# 2.90e-12 @ 160
45	HO + HO2 =	# 4.80e-11 @ -250
S2OH	HO + SO2 = HO2 + SULF	# 4.00e-31 ^ -3.30 & 2.00e-12 & 0.45 & 1.0
H2OH	HO + H2 = HO2	# 7.70e-12 @ 2100
MER1	C_O2 + NO = NO2 + HCHO + HO2	# 2.80e-12 @ -285
MER4	C_O2 + HO2 = COOH	# 3.80e-13 @ -780
MEN3	C_O2 + NO3 = HCHO + HO2 + NO2	# 1.30e-12
MER5	C_O2 + C_O2 = MEOH + HCHO	# 2.45e-14 @ -710
MER6	C_O2 + C_O2 = 2*HCHO + 2*HO2	# 5.90e-13 @ 509
RRNO	RO2_R + NO = NO2 + HO2	# 2.70e-12 @ -360
RRH2	RO2_R + HO2 = ROOH	# 1.90e-13 @ -1300
RRN3	RO2_R + NO3 = NO2 + HO2	# 2.30e-12
RRME	RO2_R + C_O2 = HO2 + 0.75*HCHO + 0.25*MEOH	# 2.00e-13
RRR2	RO2_R + RO2_R = HO2	# 3.50e-14
R2NO	R2O2 + NO = NO2	# 1.0 * <KRRNO>
R2H2	R2O2 + HO2 = HO2	# 1.0 * <KRRH2>
R2N3	R2O2 + NO3 = NO2	# 1.0 * <KRRN3>
R2ME	R2O2 + C_O2 = C_O2	# 1.0 * <KRRME>
R2RR	R2O2 + RO2_R = RO2_R	# 1.0 * <KRRR2>
R2R3	R2O2 + R2O2 =	# 1.0 * <KRRR2>
RNNO	RO2_N + NO = RNO3	# 1.0 * <KRRNO>
RNH2	RO2_N + HO2 = ROOH	# 1.0 * <KRRH2>
RNME	RO2_N + C_O2 = HO2 + 0.25*MEOH + 0.5*MEK + 0.5*PROD2 + 0.75*HCHO	# 1.0 * <KRRME>

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
RNN3	RO2_N + NO3 = NO2 + HO2 + MEK	# 1.0 * <KRRN3>
RNRR	RO2_N + RO2_R = HO2 + 0.5*MEK + 0.5*PROD2	# 1.0 * <KRRR2>
RNR2	RO2_N + R2O2 = RO2_N	# 1.0 * <KRRR2>
RNRN	RO2_N + RO2_N = MEK + HO2 + PROD2	# 1.0 * <KRRR2>
APN2	CCO_O2 + NO2 = PAN	# 2.70e-28 ^ -7.10 & 1.20e-11 ^ -0.90 & 0.30 & 1.0
DPAN	PAN = CCO_O2 + NO2	# 4.90e-03 @ 12100 & 4.00e+16 @ 13600 & 0.30 & 1.0
APNO	CCO_O2 + NO = C_O2 + NO2	# 7.80e-12 @ -300
APH2	CCO_O2 + HO2 = 0.75*CCO_OOH + 0.25*CCO_OH + 0.25*O3	# 4.30e-13 @ -1040
APN3	CCO_O2 + NO3 = C_O2 + NO2	# 4.00e-12
APME	CCO_O2 + C_O2 = CCO_OH + HCHO	# 1.80e-12 @ -500
APRR	CCO_O2 + RO2_R = CCO_OH	# 7.50e-12
2-Apr	CCO_O2 + R2O2 = CCO_O2	# 1.0 * <KAPRR>
APRN	CCO_O2 + RO2_N = CCO_OH + PROD2	# 1.0 * <KAPRR>
APAP	CCO_O2 + CCO_O2 = 2*C_O2	# 2.90e-12 @ -500
PPN2	RCO_O2 + NO2 = PAN2	# 1.20e-11 ^ -0.90
PAN2	PAN2 = RCO_O2 + NO2	# 2.00e+15 @ 12800
PPNO	RCO_O2 + NO = NO2 + CCHO + RO2_R	# 1.25e-11 @ -240
PPH2	RCO_O2 + HO2 = 0.75*RCO_OOH + 0.25*RCO_OH + 0.25*O3	# 1.0 * <KAPH2>
PPN3	RCO_O2 + NO3 = NO2 + CCHO + RO2_R	# 1.0 * <KAPN3>
PPME	RCO_O2 + C_O2 = RCO_OH + HCHO	# 1.0 * <KAPME>
PPRR	RCO_O2 + RO2_R = RCO_OH	# 1.0 * <KAPRR>
PPR2	RCO_O2 + R2O2 = RCO_O2	# 1.0 * <KAPRR>
PPRN	RCO_O2 + RO2_N = RCO_OH + PROD2	# 1.0 * <KAPRR>
PPAP	RCO_O2 + CCO_O2 = C_O2 + CCHO + RO2_R	# 1.0 * <KAPAP>
PPPP	RCO_O2 + RCO_O2 = 2*CCHO + 2*RO2_R	# 1.0 * <KAPAP>
BPN2	BZCO_O2 + NO2 = PBZN	# 1.37e-11
BPAN	PBZN = BZCO_O2 + NO2	# 7.90e+16 @ 14000
BPNO	BZCO_O2 + NO = NO2 + BZ_O + R2O2	# 1.0 * <KPPNO>
BPH2	BZCO_O2 + HO2 = 0.75*RCO_OOH + 0.25*RCO_OH + 0.25*O3	# 1.0 * <KAPH2>
BPN3	BZCO_O2 + NO3 = NO2 + BZ_O + R2O2	# 1.0 * <KAPN3>
BPME	BZCO_O2 + C_O2 = RCO_OH + HCHO	# 1.0 * <KAPME>
BPRR	BZCO_O2 + RO2_R = RCO_OH	# 1.0 * <KAPRR>
BPR2	BZCO_O2 + R2O2 = BZCO_O2	# 1.0 * <KAPRR>
BPRN	BZCO_O2 + RO2_N = RCO_OH + PROD2	# 1.0 * <KAPRR>
BPAP	BZCO_O2 + CCO_O2 = C_O2 + BZ_O + R2O2	# 1.0 * <KAPAP>
BPPP	BZCO_O2 + RCO_O2 = CCHO + RO2_R + BZ_O + R2O2	# 1.0 * <KAPAP>
BPBP	BZCO_O2 + BZCO_O2 = 2*BZ_O + 2*R2O2	# 1.0 * <KAPAP>

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
MPN2	MA_RCO3 + NO2 = MA_PAN	# 1.0 * <KPPN2>
MPPN	MA_PAN = MA_RCO3 + NO2	# 1.60e+16 @ 13486
MPNO	MA_RCO3 + NO = NO2 + HCHO + CCO_O2	# 1.0 * <KPPNO>
MPH2	MA_RCO3 + HO2 = 0.75*RCO_OOH + 0.25*RCO_OH + 0.25*O3	# 1.0 * <KAPH2>
MPN3	MA_RCO3 + NO3 = NO2 + HCHO + CCO_O2	# 1.0 * <KAPN3>
MPME	MA_RCO3 + C_O2 = RCO_OH + HCHO	# 1.0 * <KAPME>
MPRR	MA_RCO3 + RO2_R = RCO_OH	# 1.0 * <KAPRR>
MPR2	MA_RCO3 + R2O2 = MA_RCO3	# 1.0 * <KAPRR>
MPRN	MA_RCO3 + RO2_N = 2*RCO_OH	# 1.0 * <KAPRR>
MPAP	MA_RCO3 + CCO_O2 = C_O2 + HCHO + CCO_O2	# 1.0 * <KAPAP>
MPPP	MA_RCO3 + RCO_O2 = HCHO + CCO_O2 + CCHO + RO2_R	# 1.0 * <KAPAP>
MPBP	MA_RCO3 + BZCO_O2 = HCHO + CCO_O2 + BZ_O + R2O2	# 1.0 * <KAPAP>
MPMP	MA_RCO3 + MA_RCO3 = 2*HCHO + 2*CCO_O2	# 1.0 * <KAPAP>
TBON	TBU_O + NO2 = RNO3	# 2.40e-11
TBOD	TBU_O = ACET + C_O2	# 7.50e+14 @ 8152
BRN2	BZ_O + NO2 = NPHE	# 2.30e-11 @ -150
BRH2	BZ_O + HO2 = PHEN	# 1.0 * <KRRH2>
BRXX	BZ_O = PHEN	# 1.00e-3
BNN2	BZ(NO2)_O + NO2 =	# 1.0 * <KBRN2>
BNH2	BZ(NO2)_O + HO2 = NPHE	# 1.0 * <KRRH2>
BNXX	BZ(NO2)_O = NPHE	# 1.0 * <KBRXX>
FAHV	HCHO = 2*HO2 + CO	# 1.0 / <HCHO_R>
FAVS	HCHO = CO	# 1.0 / <HCHO_M>
FAOH	HCHO + HO = HO2 + CO	# 8.60e-12 @ -20
FAH2	HCHO + HO2 = HOCOO	# 9.70e-15 @ -625
FAHR	HOCOO = HO2 + HCHO	# 2.40e+12 @ 7000
FAHN	HOCOO + NO = HCOOH + NO2 + HO2	# 1.0 * <KMER1>
FAN3	HCHO + NO3 = HNO3 + HO2 + CO	# 2.00e-12 @ 2431
AAOH	CCHO + HO = CCO_O2	# 5.60e-12 @ -310
AAHV	CCHO = CO + HO2 + C_O2	# 1.0 / <CCHO_R>
AAN3	CCHO + NO3 = HNO3 + CCO_O2	# 1.40e-12 @ 1860
PAOH	RCHO + HO = 0.034*RO2_R + 0.001*RO2_N + 0.965*RCO_O2 + 0.034*CO + 0.034*CCHO	# 2.00e-11
PAHV	RCHO = CCHO + RO2_R + CO + HO2	# 1.0 / <C2CHO>
PAN3	RCHO + NO3 = HNO3 + RCO_O2	# 1.40e-12 @ 1771
K3OH	ACET + HO = HCHO + CCO_O2 + R2O2	# 1.10e-12 @ 520
K3HV	ACET = CCO_O2 + C_O2	# 1.0 / <ACETONE>
K4OH	MEK + HO = 0.37*RO2_R + 0.042*RO2_N + 0.616*R2O2 + 0.492*CCO_O2 + 0.096*RCO_O2 + 0.115*HCHO + 0.482*CCHO + 0.37*RCHO	# 1.30e-12 ^ 2.00 @ 25

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
K4HV	MEK = CCO_O2 + CCHO + RO2_R	# 1.50e-1 / <KETONE>
MeOH	MEOH + HO = HCHO + HO2	# 3.10e-12 ^ 2.00 @ 360
MER9	COOH + HO = 0.35*HCHO + 0.35*HO + 0.65*C_O2	# 2.90e-12 @ -190
MERA	COOH = HCHO + HO2 + HO	# 1.0 / <COOH>
LPR9	ROOH + HO = RCHO + 0.34*RO2_R + 0.66*HO	# 1.10e-11
LPRA	ROOH = RCHO + HO2 + HO	# 1.0 / <COOH>
GLHV	GLY = 2*CO + 2*HO2	# 1.0 / <GLY_R>
GLVM	GLY = HCHO + CO	# 6.00e-3 / <GLY_ABS>
GLOH	GLY + HO = 0.63*HO2 + 1.26*CO + 0.37*RCO_O2	# 1.10e-11
GLN3	GLY + NO3 = HNO3 + 0.63*HO2 + 1.26*CO + 0.37*RCO_O2	# 2.80e-12 @ 2376
MGHV	MGLY = HO2 + CO + CCO_O2	# 1.0 / <MGLY_ADJ>
MGOH	MGLY + HO = CO + CCO_O2	# 1.50e-11
MGN3	MGLY + NO3 = HNO3 + CO + CCO_O2	# 1.40e-12 @ 1895
BAHV	BACL = 2*CCO_O2	# 1.0 / <BACL_ADJ>
PHOH	PHEN + HO = 0.24*BZ_O + 0.76*RO2_R + 0.23*GLY	# 2.63e-11
PHN3	PHEN + NO3 = HNO3 + BZ_O	# 3.78e-12
CROH	CRES + HO = 0.24*BZ_O + 0.76*RO2_R + 0.23*MGLY	# 4.20e-11
CRN3	CRES + NO3 = HNO3 + BZ_O	# 1.37e-11
NPN3	NPHE + NO3 = HNO3 + BZ(NO2)_O	# 1.0 * <KPHN3>
BZOH	BALD + HO = BZCO_O2	# 1.29e-11
BZHV	BALD =	# 5.00e-2 / <BZCHO>
BZNT	BALD + NO3 = HNO3 + BZCO_O2	# 1.40e-12 @ 1872
MAOH	METHACRO + HO = 0.5*RO2_R + 0.416*CO + 0.084*HCHO + 0.416*MEK + 0.084*MGLY + 0.5*MA_RCO3	# 1.86e-11 @ -176
MAO3	METHACRO + O3 = 0.008*HO2 + 0.1*RO2_R + 0.208*HO + 0.1*RCO_O2 + 0.45*CO + 0.2*HCHO + 0.9*MGLY + 0.333*HCOOH	# 1.36e-15 @ 2114
MAN3	METHACRO + NO3 = 0.5*HNO3 + 0.5*RO2_R + 0.5*CO + 0.5*MA_RCO3	# 1.50e-12 @ 1726
MAOP	METHACRO + O3P = RCHO	# 6.34e-12
MAHV	METHACRO = 0.34*HO2 + 0.33*RO2_R + 0.33*HO + 0.67*CCO_O2 + 0.67*CO + 0.67*HCHO + 0.33*MA_RCO3	# 4.10e-3 / <ACROLEIN>
MVOH	MVK + HO = 0.3*RO2_R + 0.025*RO2_N + 0.675*R2O2 + 0.675*CCO_O2 + 0.3*HCHO + 0.675*RCHO + 0.3*MGLY	# 4.14e-12 @ -453
MVO3	MVK + O3 = 0.064*HO2 + 0.05*RO2_R + 0.164*HO + 0.05*RCO_O2 + 0.475*CO + 0.1*HCHO + 0.95*MGLY + 0.351*HCOOH	# 7.51e-16 @ 1520
MVOP	MVK + O3P = 0.45*RCHO + 0.55*MEK	# 4.32e-12
MVHV	MVK = 0.3*C_O2 + 0.7*CO + 0.7*PROD2 + 0.3*MA_RCO3	# 2.10e-3 / <ACROLEIN>
IPOH	ISOPROD + HO = 0.67*RO2_R + 0.041*RO2_N + 0.289*MA_RCO3 + 0.336*CO + 0.055*HCHO + 0.129*CCHO + 0.013*RCHO + 0.15*MEK + 0.332*PROD2 + 0.15*GLY + 0.174*MGLY	# 6.19e-11

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
IPO3	ISOPROD + O3 = 0.4*HO2 + 0.048*RO2_R + 0.048*RCO_O2 + 0.285*HO + 0.498*CO + 0.125*HCHO + 0.047*CCHO + 0.21*MEK + 0.023*GLY + 0.742*MGLY + 0.1*HCOOH + 0.372*RCO_OH	# 4.18e-18
IPN3	ISOPROD + NO3 = 0.799*RO2_R + 0.051*RO2_N + 0.15*MA_RCO3 + 0.572*CO + 0.15*HNO3 + 0.227*HCHO + 0.218*RCHO + 0.008*MGLY + 0.572*RNO3	# 1.00e-13
IPHV	ISOPROD = 1.233*HO2 + 0.467*CCO_O2 + 0.3*RCO_O2 + 1.233*CO + 0.3*HCHO + 0.467*CCHO + 0.233*MEK	# 4.10e-3 / <ACROLEIN>
K6OH	PROD2 + HO = 0.379*HO2 + 0.473*RO2_R + 0.07*RO2_N + 0.029*CCO_O2 + 0.049*RCO_O2 + 0.213*HCHO + 0.084*CCHO + 0.558*RCHO + 0.115*MEK + 0.329*PROD2	# 1.50e-11
K6HV	PROD2 = 0.96*RO2_R + 0.04*RO2_N + 0.515*R2O2 + 0.667*CCO_O2 + 0.333*RCO_O2 + 0.506*HCHO + 0.246*CCHO + 0.71*RCHO	# 2.00e-2 / <KETONE>
RNOH	RNO3 + HO = 0.338*NO2 + 0.113*HO2 + 0.376*RO2_R + 0.173*RO2_N + 0.596*R2O2 + 0.01*HCHO + 0.439*CCHO + 0.213*RCHO + 0.006*ACET + 0.177*MEK + 0.048*PROD2 + 0.31*RNO3	# 7.80e-12
RNHV	RNO3 = NO2 + 0.341*HO2 + 0.564*RO2_R + 0.095*RO2_N + 0.152*R2O2 + 0.134*HCHO + 0.431*CCHO + 0.147*RCHO + 0.02*ACET + 0.243*MEK + 0.435*PROD2	# 1.0 / <IC3ONO2>
D1OH	DCB1 + HO = RCHO + RO2_R + CO	# 5.00e-11
D1O3	DCB1 + O3 = 1.5*HO2 + 0.5*HO + 1.5*CO + GLY	# 2.00e-18
D2OH	DCB2 + HO = R2O2 + RCHO + CCO_O2	# 5.00e-11
D2HV	DCB2 = RO2_R + 0.5*CCO_O2 + 0.5*HO2 + CO + R2O2 + 0.5*GLY + 0.5*MGLY	# 3.65e-1 / <MGLY_ABS>
D3OH	DCB3 + HO = R2O2 + RCHO + CCO_O2	# 5.00e-11
D3HV	DCB3 = RO2_R + 0.5*CCO_O2 + 0.5*HO2 + CO + R2O2 + 0.5*GLY + 0.5*MGLY	# 7.28e+0 / <ACROLEIN>
c1OH	CH4 + HO = C_O2	# 2.15e-12 @ 1735
etOH	ETHENE + HO = RO2_R + 1.61*HCHO + 0.195*CCHO	# 1.96e-12 @ -438
etO3	ETHENE + O3 = 0.12*HO + 0.12*HO2 + 0.5*CO + HCHO + 0.37*HCOOH	# 9.14e-15 @ 2580
etN3	ETHENE + NO3 = RO2_R + RCHO	# 4.39e-13 ^ 2.00 @ 2282
etOA	ETHENE + O3P = 0.5*HO2 + 0.2*RO2_R + 0.3*C_O2 + 0.491*CO + 0.191*HCHO + 0.25*CCHO + 0.009*GLY	# 1.04e-11 @ 792
isOH	ISOPRENE + HO = 0.907*RO2_R + 0.093*RO2_N + 0.079*R2O2 + 0.624*HCHO + 0.23*METHACRO + 0.32*MVK + 0.357*ISOPROD	# 2.50e-11 @ -408
isO3	ISOPRENE + O3 = 0.266*HO + 0.066*RO2_R + 0.008*RO2_N + 0.126*R2O2 + 0.192*MA_RCO3 + 0.275*CO + 0.592*HCHO + 0.1*PROD2 + 0.39*METHACRO + 0.16*MVK + 0.204*HCOOH + 0.15*RCO_OH	# 7.86e-15 @ 1912
isN3	ISOPRENE + NO3 = 0.187*NO2 + 0.749*RO2_R + 0.064*RO2_N + 0.187*R2O2 + 0.936*ISOPROD	# 3.03e-12 @ 448
isOP	ISOPRENE + O3P = 0.01*RO2_N + 0.24*R2O2 + 0.25*C_O2 + 0.24*MA_RCO3 + 0.24*HCHO + 0.75*PROD2	# 3.60e-11

Table 2 (continued)

Label	Reaction	Kinetic Parameters [a]
t1OH	TRP1 + HO = 0.75*RO2_R + 0.25*RO2_N + 0.5*R2O2 + 0.276*HCHO + 0.474*RCHO + 0.276*PROD2	# 1.83e-11 @ -449
t1O3	TRP1 + O3 = 0.567*HO + 0.033*HO2 + 0.031*RO2_R + 0.18*RO2_N + 0.729*R2O2 + 0.123*CCO_O2 + 0.201*RCO_O2 + 0.157*CO + 0.235*HCHO + 0.205*RCHO + 0.13*ACET + 0.276*PROD2 + 0.001*GLY + 0.031*BACL + 0.103*HCOOH + 0.189*RCO_OH	# 1.08e-15 @ 821
t1N3	TRP1 + NO3 = 0.474*NO2 + 0.276*RO2_R + 0.25*RO2_N + 0.75*R2O2 + 0.474*RCHO + 0.276*RNO3	# 3.66e-12 @ -175
t1OP	TRP1 + O3P = 0.147*RCHO + 0.853*PROD2	# 3.27e-11

[a] See Models-3 documentation (EPA, 1998) for format of mechanistic parameters. Units of rate constants and A factors are cm^3 $molec^{-1}$ s^{-1}. Units of activation energies are degrees Kelvin. See Table A-2 for absorption cross sections and quantum yields used to calculate photolysis reactions (indicated by "/ <photname>", where "phothame" is the name of the absorption cross-section and quantum yield set as used on Table A-2.

Table 3. Reactions of lumped parameter species in the condensed mechanism, with parameters derived based on the ambient mixture used in the reactivity simulations of Carter (1994a, 1999).

Label	Reaction	Kinetic Parameters [a]
A1OH	ALK1 + HO = RO2_R + CCHO	# 1.37e-12 ^ 2.00 @ 498
A2OH	ALK2 + HO = 0.246*HO + 0.121*HO2 + 0.612*RO2_R + 0.021*RO2_N + 0.16*CO + 0.039*HCHO + 0.155*RCHO + 0.417*ACET + 0.248*GLY + 0.121*HCOOH	# 9.87e-12@671
A3OH	ALK3 + HO = 0.695*RO2_R + 0.07*RO2_N + 0.559*R2O2 + 0.236*TBU_O + 0.026*HCHO + 0.445*CCHO + 0.122*RCHO + 0.024*ACET + 0.332*MEK	# 1.02e-11@434
A4OH	ALK4 + HO = 0.835*RO2_R + 0.143*RO2_N + 0.936*R2O2 + 0.011*C_O2 + 0.011*CCO_O2 + 0.002*CO + 0.024*HCHO + 0.455*CCHO + 0.244*RCHO + 0.452*ACET + 0.11*MEK + 0.125*PROD2	# 5.95e-12@91
A5OH	ALK5 + HO = 0.653*RO2_R + 0.347*RO2_N + 0.948*R2O2 + 0.026*HCHO + 0.099*CCHO + 0.204*RCHO + 0.072*ACET + 0.089*MEK + 0.417*PROD2	# 1.11e-11@52
B1OH	ARO1 + HO = 0.224*HO2 + 0.765*RO2_R + 0.011*RO2_N + 0.055*PROD2 + 0.118*GLY + 0.119*MGLY + 0.017*PHEN + 0.207*CRES + 0.059*BALD + 0.491*DCB1 + 0.108*DCB2 + 0.051*DCB3	# 1.81e-12@-355
B2OH	ARO2 + HO = 0.187*HO2 + 0.804*RO2_R + 0.009*RO2_N + 0.097*GLY + 0.287*MGLY + 0.087*BACL + 0.187*CRES + 0.05*BALD + 0.561*DCB1 + 0.099*DCB2 + 0.093*DCB3	# 2.64E-11
O1OH	OLE1 + HO = 0.91*RO2_R + 0.09*RO2_N + 0.205*R2O2 + 0.732*HCHO + 0.294*CCHO + 0.497*RCHO + 0.005*ACET + 0.119*PROD2	# 7.10e-12@-451
O1O3	OLE1 + O3 = 0.155*HO + 0.056*HO2 + 0.022*RO2_R + 0.001*RO2_N + 0.076*C_O2 + 0.345*CO + 0.5*HCHO + 0.154*CCHO + 0.363*RCHO + 0.001*ACET + 0.215*PROD2 + 0.185*HCOOH + 0.05*CCO_OH + 0.119*RCO_OH	# 2.62e-15@1640
O1N3	OLE1 + NO3 = 0.824*RO2_R + 0.176*RO2_N + 0.488*R2O2 + 0.009*CCHO + 0.037*RCHO + 0.024*ACET + 0.511*RNO3	# 4.45e-14@376
O1OP	OLE1 + O3P = 0.45*RCHO + 0.437*MEK + 0.113*PROD2	# 1.07e-11@234
O2OH	OLE2 + HO = 0.918*RO2_R + 0.082*RO2_N + 0.001*R2O2 + 0.244*HCHO + 0.732*CCHO + 0.511*RCHO + 0.127*ACET + 0.072*MEK + 0.061*BALD + 0.025*METHACRO + 0.025*ISOPROD	# 1.74e-11@-384
O2O3	OLE2 + O3 = 0.378*HO + 0.003*HO2 + 0.033*RO2_R + 0.002*RO2_N + 0.137*R2O2 + 0.197*C_O2 + 0.137*CCO_O2 + 0.006*RCO_O2 + 0.265*CO + 0.269*HCHO + 0.456*CCHO + 0.305*RCHO + 0.045*ACET + 0.026*MEK + 0.006*PROD2 + 0.042*BALD + 0.026*METHACRO + 0.073*HCOOH + 0.129*CCO_OH + 0.303*RCO_OH	# 5.02e-16@461
O2N3	OLE2 + NO3 = 0.391*NO2 + 0.442*RO2_R + 0.136*RO2_N + 0.711*R2O2 + 0.03*C_O2 + 0.079*HCHO + 0.507*CCHO + 0.151*RCHO + 0.102*ACET + 0.001*MEK + 0.015*BALD + 0.048*MVK + 0.321*RNO3	# 7.26E-13
O2OP	OLE2 + O3P = 0.013*HO2 + 0.012*RO2_R + 0.001*RO2_N + 0.012*CO + 0.069*RCHO + 0.659*MEK + 0.259*PROD2 + 0.012*METHACRO	# 2.09E-11

[a] See Footnote [a] on Table 2.

Table 4. Reactions of the lumped parameter species used in the condensed mechanism, derived using a Models-3 emissions profile supplied by the EPA (EPA, 1999b).

Label	Reaction	Kinetic Parameters [a]
A1OH	ALK1 + HO = RO2_R + 0.012*CO + 0.145*HCHO + 0.685*CCHO + 0.142*RCHO + 0.012*HCOOH	# 8.148E-12@1061.
A2OH	ALK2 + HO = 0.195*HO + 0.096*HO2 + 0.616*RO2_R + 0.021*RO2_N + 0.108*R2O2 + 0.066*CCO_O2 + 0.006*TBU_O + 0.168*CO + 0.069*HCHO + 0.001*CCHO + 0.134*RCHO + 0.324*ACET + 0.197*GLY + 0.001*MGLY + 0.107*HCOOH + 0.095*CCO_OH	# 6.083E-12@542.
A3OH	ALK3 + HO = 0.488*HO2 + 0.351*RO2_R + 0.029*RO2_N + 0.25*R2O2 + 0.025*C_O2 + 0.002*CCO_O2 + 0.01*RCO_O2 + 0.096*TBU_O + 0.064*HCHO + 0.644*CCHO + 0.051*RCHO + 0.015*ACET + 0.124*MEK + 0.004*MGLY + 0.012*CCO_OH	# 1.701E-12@-166.
A4OH	ALK4 + HO = 0.001*HO + 0.372*HO2 + 0.528*RO2_R + 0.078*RO2_N + 0.464*R2O2 + 0.005*C_O2 + 0.004*CCO_O2 + 0.01*RCO_O2 + 0.001*TBU_O + 0.001*CO + 0.038*HCHO + 0.217*CCHO + 0.108*RCHO + 0.594*ACET + 0.054*MEK + 0.152*PROD2 + 0.001*MGLY + 0.01*CCO_OH + 0.001*RCO_OH	# 2.372E-12@-215.
A5OH	ALK5 + HO = 0.001*HO + 0.199*HO2 + 0.575*RO2_R + 0.186*RO2_N + 0.507*R2O2 + 0.038*C_O2 + 0.001*RCO_O2 + 0.003*CO + 0.154*HCHO + 0.078*CCHO + 0.301*RCHO + 0.025*ACET + 0.129*MEK + 0.345*PROD2 + 0.001*MGLY + 0.004*CCO_OH	# 1.419E-11@-6.
B1OH	ARO1 + HO = 0.228*HO2 + 0.763*RO2_R + 0.009*RO2_N + 0.035*PROD2 + 0.123*GLY + 0.116*MGLY + 0.026*PHEN + 0.201*CRES + 0.063*BALD + 0.5*DCB1 + 0.115*DCB2 + 0.049*DCB3	# 5.91E-12
B2OH	ARO2 + HO = 0.188*HO2 + 0.785*RO2_R + 0.011*RO2_N + 0.017*RCO_O2 + 0.114*GLY + 0.24*MGLY + 0.061*BACL + 0.009*PHEN + 0.179*CRES + 0.053*BALD + 0.53*DCB1 + 0.108*DCB2 + 0.094*DCB3	# 1.816E-11@-24.
O1OH	OLE1 + HO = 0.933*RO2_R + 0.052*RO2_N + 0.099*R2O2 + 0.015*CCO_O2 + 0.001*RCO_O2 + 0.843*HCHO + 0.432*CCHO + 0.34*RCHO + 0.001*ACET + 0.046*PROD2 + 0.06*MGLY + 0.02*BACL	# 7.901E-12@-392.
O1O3	OLE1 + O3 = 0.19*HO + 0.062*HO2 + 0.015*RO2_R + 0.113*C_O2 + 0.38*CO + 0.5*HCHO + 0.226*CCHO + 0.204*RCHO + 0.053*PROD2 + 0.056*MGLY + 0.185*HCOOH + 0.074*CCO_OH + 0.131*RCO_OH	# 1.289E-15@1438.
O1N3	OLE1 + NO3 = 0.821*RO2_R + 0.102*RO2_N + 0.329*R2O2 + 0.026*CCO_O2 + 0.05*RCO_O2 + 0.002*CO + 0.011*CCHO + 0.026*RCHO + 0.007*ACET + 0.07*BACL + 0.336*RNO3 + 0.049*CCO_OH	# 8.655E-14@630.
O1OA	OLE1 + O3P = 0.45*RCHO + 0.481*MEK + 0.045*PROD2 + 0.024*RCO_OH	# 9.720E-12@227.
O2OH	OLE2 + HO = 0.925*RO2_R + 0.075*RO2_N + 0.398*HCHO + 0.481*CCHO + 0.287*RCHO + 0.032*ACET + 0.041*MEK + 0.056*BACL + 0.206*BALD + 0.094*METHACRO + 0.094*ISOPROD	# 2.065E-11@-333.
O2O3	OLE2 + O3 = 0.253*HO + 0.012*HO2 + 0.033*RO2_R + 0.003*RO2_N + 0.073*R2O2 + 0.129*C_O2 + 0.048*CCO_O2 + 0.029*RCO_O2 + 0.211*CO + 0.312*HCHO + 0.294*CCHO + 0.191*RCHO + 0.01*ACET + 0.014*MEK + 0.034*PROD2 + 0.016*MGLY + 0.02*BACL + 0.142*BALD + 0.098*METHACRO + 0.074*MVK + 0.191*HCOOH + 0.084*CCO_OH + 0.196*RCO_OH	# 4.663E-16@447.

Table 4 (continued)

Label	Reaction	Kinetic Parameters [a]
O2N3	OLE2 + NO3 = 0.317*NO2 + 0.528*RO2_R + 0.114*RO2_N + 0.511*R2O2 + 0.001*C_O2 + 0.039*RCO_O2 + 0.006*CO + 0.054*HCHO + 0.342*CCHO + 0.142*RCHO + 0.032*ACET + 0.001*MEK + 0.005*MGLY + 0.052*BALD + 0.18*MVK + 0.294*RNO3	# 5.403E-13@-3.
O2OA	OLE2 + O3P = 0.049*HO2 + 0.045*RO2_R + 0.004*RO2_N + 0.045*CO + 0.042*RCHO + 0.442*MEK + 0.467*PROD2 + 0.045*METHACRO	# 2.00E-11

[a] See Footnote [a] on Table 2.

The reactions in the two versions of the condensed SAPRC-99 mechanism for urban and regional model applications are given in Table 2 and Table 3 or in Table 2 and Table 4. These reactions are shown in the format used by the Models-3 mechanism implementation software, as described by EPA (1998). Table 2 give the reactions that are used in all versions of the mechanism, which include the reactions of the inorganics, the common organic products, the primary emitted VOCs that are represented explicitly, and the lumped terpenes[3]. Table 3 gives the reactions of the lumped parameter species that represent the other VOCs, whose parameters were derived to represent the ambient VOCs in the base case simulations used to derive the reactivity scales of Carter (1994a, 1999). The composition of this mixture, which is given by Carter (1994b, 1999), was derived from an analysis of hydrocarbons in urban atmospheres in the United States (Jeffries et al, 1989) and from oxygenate measurements in the California South Coast Air Basin (Carter, 1994a,b and references therein). This mixture was also used when deriving parameters for the lumped parameter product species in the base mechanism (Carter, 1999)[4].

Table 4 gives the reactions of the lumped parameter species that were derived to represent the composition of a Models-3 emissions profile provided by the EPA (EPA, 1999b). These reactions, in conjunction with those in Table 2, comprise a version of the mechanism that is optimized to represent this particular emissions mixture. The procedure used to derive these reactions, and to derive reactions corresponding to other emissions profiles, is discussed below in Section III.B.2.

Note that Table 1 also indicates that other model species can be added to the mechanism, if it is desired that certain individual compounds or VOC classes be represented explicitly. This approach is necessary, for example, if it is desired to calculate the reactivities of individual compounds that would otherwise be lumped with other species, or if it is desired to compare model simulations with measurement data for such compounds. The mechanisms used for individual compounds or VOC classes represented in the SAPRC-99 mechanism are given in Table A-1 in Appendix A. These reactions can be added when the model application requires explicit representation of compounds listed on that table.

As indicated on Table 1, there are a number of photolysis reactions in this mechanism, whose rate constants must be calculated from their corresponding absorption cross sections and quantum yields given the spectrum and intensity of the sunlight or other light source in the simulation. The absorption cross sections and quantum yields used are listed in Table A-2 in Appendix A. No recommendation is given as

[3] See Carter (1999) for a discussion of how the mechanism of the lumped terpene model species is derived.

[4] As discussed by Carter (1999), the mechanisms for the RNO3 and PROD2 model species are derived based on the composition of the ambient mixture used to represent ambient VOCs in the reactivity calculations. Presently, there is no provision for changing the mechanisms of these species when different VOC mixtures are represented.

to the actual photolysis rates to use in model simulations, since an analysis of environmental conditions is beyond the scope of this work.

B. VOC Assignments for Emissions Processing

An important component of any mechanism for airshed models is the set of assignments used to determine how individual VOCs are represented in the model. Because emissions inventories include many chemical categories that are poorly defined or are not well represented in the current mechanism, a somewhat different assignment procedure is used when processing emissions data than when compositions are given in terms of SAPRC-99 detailed model species. In addition, biogenic emissions are assigned different model species than biogenic emissions, because of their significantly different spatial and temporal characteristics.

1. Assignments for SAPRC Detailed Model Species

As discussed by Carter (1999), the SAPRC-99 mechanism represents individual VOCs using "detailed model species", that can represent individual compounds or mixtures of compounds for which mechanisms or "lumped molecule" assignments have been derived. Compositions must be given in terms of these species in order to derive lumped parameter mechanisms that best represent the mixtures employed. Compositions should also given in terms of these species when speciating measurement data or other data that do not involve emissions profiles for which assignments have been given.

Although many of the SAPRC detailed model species refer to individual compounds or isomeric mixtures that are represented explicitly or that have specific mechanistic assignments, a number refer to compounds that are represented by other model species, or to mixtures that are represented using more than one model species. Therefore, the model species assignment procedure involves two steps. In the first those detailed model species that are represented by other species or mixtures are removed and replaced by equal molar amounts of the species or mixtures representing them. The revised profile therefore includes only species that are explicitly represented in the mechanism or for which mechanistic parameter assignments have been made. In the second step, the species that are represented explicitly are retained and those that are represented by lumped parameter model species are assigned to their appropriate lumped group, and then optionally used to derive the parameters for those groups.

Table A-3 lists the detailed model species in the current SAPRC mechanism, and shows how each are represented in models using the recommended condensed SAPRC-99 mechanism. As discussed by Carter (1999), most compounds are represented in the model on a mole-for-mole basis with one mole of model species representing one mole of each individual VOC. This is in contrast with the RADM-2 mechanism, where reactivity weighting is extensively used to account for differences in reactivity among VOCs being lumped together (Middleton et al, 1990). In this mechanism, the approach has been to increase the number of lumped classes to minimize the disparity of reactivities of species being lumped together, to permit a more chemically accurate molar representation to be used.

The one exception in this regard is the representation of benzene and a few other low-reactivity aromatics, which have too little of an overall impact on model simulations to justify reserving a separate model species just for them. Instead, they are represented by the ARO1 (e.g., toluene-like) model species a reactivity weighting approach similar to that used for RADM-2. In particular, for aromatics that have an OH radical rate constant lower than 5.9×10^{-12} cm^3 $molec^{-1}$ s^{-1}, i.e., that have lower OH reactivity than toluene, the following reactivity weighting factor is employed.

$$\text{Moles of ARO1 representing one mole of VOC} = \frac{1 - e^{-\text{IntOH} \times \text{kOH}_{\text{VOC}}}}{1 - e^{-\text{IntOH} \times \text{kOH}_{\text{ARO1}}}} \qquad \text{(I)}$$

were kOH_{VOC} is the OH rate constant for the VOC, kOH_{ARO1} is the OH rate constant used for the ARO1 model species, which is 9.91 x 10^{-12} cm^3 $molec^{-1}$ s^{-1} in the recommended mechanism, and IntOH is the "effective integrated OH parameter" relating the OH rate constant with the estimated amount of VOC reacting in the scenario. The IntOH value of 110 ppt-min, which is recommended for use with the RADM-2 mechanism (Middleton et al, 1990), is also recommended for use with this mechanism. Table A-3 shows the weighting factors so derived for these compounds.

The assignments shown on Table A-3 are used when deriving mechanisms for model species whose parameters depend on the mixture of compounds they represent. Each compound is weighed by its mole fraction contribution to the variable parameter model species representing it, with reactivity weighting factors being used where applicable when deriving parameters for the ARO1 class. Therefore, in order to determine the optimum mechanism for representing a particular total emissions profile, it is necessary first to convert this profile into a distribution of SAPRC detailed model species. This is discussed further below.

2. Assignments for Anthropogenic Emissions Processing

Anthropogenic Emissions data bases generally use a much larger number of classes of VOCs than represented by the set of SAPRC-99 detailed model species, and many of these classes are poorly defined in terms of exactly which compound, or mixtures of compounds, they represent. For that reason, use of a two-step emissions processing scheme with this mechanism similar to that developed by Middleton et al (1990) for RADM-2 is recommended. In this approach, each emissions speciation category is aggregated, on a mole-for-mole basis, to an intermediate set of lumped classes or groups, referred to as "emissions groups", which in turn are aggregated into the model species used in the model, using reactivity weighting where applicable. This two-step approach has the advantage of simplifying the assignments for the many types of chemical categories used in the emissions database, yet permitting a greater level of detail to be retained in the processed data, which can optionally be used in models requiring more chemical detail. The two-step process also provides an appropriate and relatively straightforward means to process emissions categories that refer to mixtures, and allows for more flexibility on how the reactivity weighting approach is applied. This procedure also has the advantage that software developed for use with the RADM-2 mechanism can also be used for this mechanism, provided that the software permits changes in the assignments and numbers of emissions groups and model species.

Table 5 lists the emissions groups recommended for use when processing emissions data for the SAPRC-99 mechanism, and shows how each are assigned to lumped species in the recommended condensed mechanism. These groupings are similar to those used by Middleton et al (1990), though a larger number of classes have been added. This larger number of emissions classes is necessary because some of the Middleton et al (1990) classes did not unambiguously correspond to a single SAPRC-99 model species, and because some of the Middleton et al (1990) classes represent compounds with quite different reactivity characteristics. In addition, separate emissions classes were added for compounds, such as perchloroethylene, which are important in the inventories but are not represented in the current mechanisms. A total of 58 emissions classes are used in the current system, compared to 32 used by Middleton et al (1990) for RADM-2. Footnotes to the table indicate those classes that are the same as those used by Middleton et al (1990) and the reasons the additional classes were added.

Table 5. Recommended emissions lumping for the SAPRC-99 mechanism, showing how the lumped emissions groups are assigned to the lumped model species in the mechanism.

Emissions Groups		Model Species.	Factors [a]		Notes
No.	Description		Split	React	[b]
1	Methane	CH4	1.0	1.0	1
2	Ethane	ALK1	1.0	1.0	1
3	Propane	ALK2	1.0	1.0	1
4	Alkanes (<0.25)	ALK2	1.0	1.0	2
5	Alkanes (0.25-0.50)	ALK3	1.0	1.0	1
6	Alkanes (0.50-1.00)	ALK4	1.0	1.0	1
7	Alkanes (1.00-2.00)	ALK5	1.0	1.0	1
8	Alkanes (>2.00)	ALK5	1.00	1.0	1
9	Alkane/Aromatic Mix	ALK5	0.910	1.0	3
		ARO1	0.045	1.0	
		ARO2	0.045	1.0	
10	Ethene	ETHENE	1.000	1.0	1
11	Propene	OLE1	1.0	1.0	4
12	Alkenes (Primary)	OLE1	1.0	1.0	1
13	Alkenes (Internal)	OLE2	1.0	1.0	1
14	Alkenes (Prim/Internal Mix)	OLE1	0.5	1.0	1
		OLE2	0.5	1.0	
15	1,3-Butadiene	OLE2	1.0	1.0	4
16	Isoprene	ISOPRENE	1.0	1.0	5
17	Terpenes	TRP1	1.0	1.0	6
18	Benzene	ARO1	1.0	0.3	4,7
19	Halo and nitrobenzenes	ARO1	1.0	0.3	7,8
20	Aromatics (<2 react)	ARO1	1.0	1.0	1
21	Aromatics (>2 react)	ARO2	1.0	1.0	1
22	Naphthalenes	ARO2	1.0	1.0	2
23	Phenols	PHEN	1.0	1.0	2
24	Cresols	CRES	1.0	1.0	1
25	Styrenes	OLE2	1.0	1.0	9
26	Formaldehyde	HCHO	1.0	1.0	1
27	Acetaldehyde	CCHO	1.0	1.0	10
28	Higher Aldehydes	RCHO	1.0	1.0	10
29	Aromatic Aldehydes	BALD	1.0	1.0	2
30	Acetone	ACET	1.0	1.0	1
31	Ketones (<0.73 react)	MEK	0.6	1.0	11
32	Ketones (>0.73 react)	PROD2	0.4	1.0	11
33	Formic Acid	HCOOH	1.0	1.0	12
34	Acetic Acid	ALK2	1.0	1.0	13
		CCO_OH	1.0	1.0	
35	Higher organic acids	ALK2	1.0	1.0	13
		RCO_OH	1.0	1.0	
36	Acetylene	ALK2	1.0	1.0	1
37	Perchloroethylene	ALK1	0.6	1.0	14

Table 5 (continued)

Emissions Groups		Model Species.	Factors [a]		Notes
No.	Description		Split	React	[b]
38	Other Haloalkenes	ALK3	0.4	1.0	14
39	Others (<0.05 react)	ALK1	1.0	1.0	2
40	Others (0.05-0.25 react)	ALK2	1.0	1.0	1
41	Others (0.25-0.5 react)	ALK3	1.0	1.0	1
42	Others (0.5-1.0 react)	ALK4	1.0	1.0	1
43	Others (1-2 react)	ALK5	1.0	1.0	1
44	Others (>2 react)	ALK5	1.0	1.0	2
45	Methanol	MEOH	1.0	1.0	4
46	Ethanol	ALK3	1.0	1.0	4
47	Inhibitors		(not represented)		15
48	Glyoxal	GLY	1.0	1.0	5
49	Methyl Glyoxal	MGLY	1.0	1.0	5
50	Biacetyl	BACL	1.0	1.0	5
51	Acrolein	MACR	1.0	1.0	16
52	Methacrolein	MACR	1.0	1.0	5
53	Other Unsaturated Aldehydes	IPROD	1.0	1.0	17
54	Unsaturated Ketones	MVK	1.0	1.0	18
55	Other photoreactive	BACL	1.0	1.000	19
97	Unreactive		(not represented)		1
98	Unidentified		(no recommendation)		1
99	Unassigned		(no recommendation)		1

[a] The moles of model species emitted for each mole of lumped class is given by the product of the "split" times the "reactivity" factors. The split factor allocates the emissions group to one or more model species. The reactivity weighting factor is used when the compounds in the emissions group have a much lower reactivity than the model species representing the group. In this mechanism, it is used only when benzene, halobenzenes, and nitrobenzenes are represented by the more reactive "ARO1" species.

[b] Documentation notes and comments are as follows:

1 Same assignments as used for RADM-2 (Middleton et al, 1990)

2 New emissions group added for completeness. Compounds in this group were lumped with compounds with different reactivity characteristics in the RADM-2 emissions processing scheme (Middleton et al, 1990).

3 The alkane / aromatic split is based on that used in the RADM-2 assignments (Middleton et al, 1990). The ARO1 / ARO2 split is based on the composition of the Mineral Spirits "A" mixture from the Safety-Kleen study (Carter et al, 1997b)

4 Individual VOCs that are important in the emissions are split out.

5 Split out because this compound is represented explicitly in the mechanism.

6 Terpenes split out from other higher alkenes because the mechanism has a separate lumped species for them.

7 The lumping of benzene and halobenzene/nitrobenzene compounds into ARO1 is the only case where OH reactivity weighting is used. The weighting factor used is based on the OH rate constants for benzene and ARO1, and an IntOH of 110 ppt-min, as used by Middleton et al (1990).

Table 5 (continued)

8 Nitrobenzene is lumped with the halobenzenes because the OH reactivities tend to be similar, and the estimated mechanism is the same. The reactivity weighting factor of benzene is used on a preliminary basis, but this should be updated based on the actual average OH rate constant for these compounds.

9 Styrene is lumped with the alkenes in the current mechanism. Its mechanism is much better represented by an alkene mechanism than one for aromatics.

10 Acetaldehyde is split out from the higher aldehydes because it is represented explicitly in the mechanism, and also is the most important aldehyde emitted.

11 Higher ketones are not well represented by an MEK-like mechanism. Ketones are split by their OH reactivity to correspond to the MEK and PROD2 model species in the base mechanism.

12 Formic acid is represented explicitly in the mechanism, but by an unreactive model species. Given its relatively low OH rate constant, this probably is not a bad approximation.

13 Acetic acid is split out from the higher organic acids because it is important in the emissions and because there is a separate model species for it. However, since the model species for the acid products are non reactive, acetic acid and the higher organic acids are also lumped with the "others" group according to their OH rate constants, to account for their O3 and OH reactivity effects.

14 Perchloroethylene is split out from the other haloalkenes because it lumped with ALK1, while the others are more reactive and are lumped with ALK3. Also, perchloroethylene is the major compound in this class.

15 This is used for volatile silicone compounds (Carter et al, 1992) and toluene diisocyanate (Carter et al, 1997c), which have been shown to be radical and O3 inhibitors under all conditions. Since there is no separate model species for inhibitors (other than benzaldehyde, which is a much stronger inhibitor and has a different mechanism), it is recommended that they not be represented rather than representing them as if they were positively reactive.

16 A separate emissions group is used for acrolein because of its unique reactivity characteristics. It is considered to be better represented by methacrolein than lumped higher saturated aldehydes (RCHO).

17 Representation of higher unsaturated aldehydes by "ISOPROD" is consistent with the treatment of these compounds in the condensed isoprene mechanism (Carter, 1996).

18 Unsaturated ketones are split out because they are more appropriately represented by the methyl vinyl ketone (MVK) model species than the lumped saturated ketone (MEK or PROD2) model species.

19 This group is used for highly photoreactive species that are not otherwise represented in the mechanism.

The data file EPAEMIT.PRM included with the files distributed with this report (see Section III.A) gives the VOC categories currently used in the EPA emissions data bases and the assignments of each category to the emissions group listed in Table 5. Note that some emissions categories are unassigned, and no recommendation is made concerning how to represent these categories in the model. The table also lists the percentage mass emissions in each group in the emissions profile that was received from the EPA (EPA, 1999b). Note that only a relatively small fraction of the mass emissions in that profile are in the “unassigned” category, which is lower than amount in the “unknown” category.

The file EPAEMIT.PRM also gives the SAPRC-99 detailed model species assignments for those groups for which such assignments have been made. These are used when converting the emissions

profile into a distribution of detailed model species for the purpose of determining the lumped mechanistic parameters that best represents this profile. The emissions profile whose percentage compositions is given in the file EPAEMIT.EMI (see Sections III.A and III.B.2) was used to derive the mechanisms for the adjusted parameter lumped model species shown on Table 4, above. Note that 6.5% of the mass in that profile is not assigned to any detailed model species, and thus is not used when computing the mechanistic parameters.

3. Assignments for Biogenic Emissions

As a general rule, biogenic emissions should not be lumped with anthropogenic emissions in urban or regional model applications because of their significantly different spatial and temporal profiles. Most biogenic emissions are assumed to consist of isoprene and various terpenes, and thus separate model species are used for these compounds. Isoprene is represented explicitly in the SAPRC-99 mechanism, and the model species TRP1 is used to represent all the terpenes. As discussed by Carter (1999), the parameters for the TRP1 model species is derived using an assumed distribution of terpenes which is shown in Table 6. This is based on the U.S. biogenic inventory given by Guenther et al (1999) (see also Carter, 1999). Because this is used to represent primarily biogenic emissions, the parameters for this species should not be dependent on the anthropogenic inventory, and thus it is recommended that they be held fixed in the mechanism. However, parameter for the TRP1 species can be changed if a terpene distribution other than that given in Table 6 is assumed. Procedures for doing this are discussed in Section III.B.3.

Table 6. Distribution of terpenes used to derive the parameters of the TRP1 model species. Data from Guenther et al (1999).

Terpene	Tg-C / Year
α-Pinene	4.3
β-Pinene	3.1
3-Carene	1.9
Sabinene	1.1
d-Limonene	1.0

In the present mechanism, it is recommended that anthropogenic terpenes also be represented using the TRP1 model species. This is not strictly appropriate since the speciation of anthropogenic terpenes may be different from biogenic terpenes, and their temporal and spatial profiles will be different. However, there presently are not enough terpenes in the anthropogenic inventory to make it worthwhile to add a separate lumped anthropogenic terpene model species to the mechanism, and representing them by the biogenic TRP1 model species is less of an approximation than lumping them with the other anthropogenic alkenes in this reactivity range.

Not all biogenic emissions are isoprene or terpenes. However, in the present mechanism their contributions are assumed to be relatively minor, and is recommended that they be represented by using the same model species as would be used if they were in the anthropogenic emissions.

III. MECHANISM IMPLEMENTATION

A. Programs and Files Implementing the Mechanism and Emissions Processing Procedures

Table 7 lists the programs and files implementing the SAPRC-99 mechanism and its associated emissions processing procedures for the Models-3 system. All these files should be copied to a single directory on a PC compatible computer if it is desired to run the example calculations discussed below. As indicated on the table, the various types of files can be categorized as follows:

1. Mechanism Implementation Files

These consist of the minimum set of files necessary for implementation of the mechanism in Models-3 format. The file SAPRC99F.MEC contains the reactions in the default condensed mechanism that are listed on Table 2 and Table 3, and the file PHOTDATA.ZIP contains the absorption cross section and quantum yield files. The data these files are in the format used by the Models-3 mechanism processing system (EPA, 1997).

The files EMITGRP.DAT and EPAEMIT.PRM consist of the minimum set of files needed for processing emissions data for this mechanism. The file EPAEMIT.PRM contains the assignments of EPA SAROAD classes to the emissions classes listed in Table 5. The comments in the file (the records before the record containing only "." in column 1) indicate the format of the data. The fields needed by the emissions processing system are the "SAROAD number" ("no.") class and the "SAPRC-99 Lumped Model Class" ("lmp") fields. The latter are the emissions group numbers as indicated on Table 5. This file also contains assignments of SAROAD classes to detailed model species. These are used when deriving mechanistic parameters for lumped species to represent different emissions profiles (see examples discussed in the following section), but are not needed for processing emissions for the fixed parameter version of the mechanism.

The file EMITGRP.DAT contains the information needed to convert emissions given as emissions groups into the lumped species used in the recommended condensed mechanism. The format of the data in the file is given in the comments in the file, which are records containing a "!" in column 1. The data in that file consist of the assignments given in Table 5, with the "description" filed removed and with a single factor, the number of moles of model species per mole of emissions group, being given. This factor is the product of the corresponding separate "split" and "reactivity" factors shown on Table 5.

Programs that read these files to process emissions data are not provided in this work. However, as indicated above, the programs used to process emissions data for the RADM-2 mechanism should be useable for this purpose, if the number of classes they process can be increased. The files EMITGRP.DAT and EPAEMIT.PRM may need to be modified to be in the format needed by these programs; a discussion of this is beyond the scope of this project.

Note that EPA's SAROAD emissions categorization scheme is not universally used in all emissions processing databases, and thus the assignments in EPAEMIT.PRM are only appropriate for processing emissions data maintained by the EPA. In particular, the California Air Resources Board (CARB) uses a 5-digit "ChemCode" system to represent emissions. These codes are analogous to the SAROAD codes used by the EPA and many numbers refer to the same chemicals or mixtures, but many

other numbers refer to different mixtures than they do in the EPA system, and each system has many classes that are not on the other.

The file ARBEMIT.PRM contains the assignments of the ARB emissions categories to SAPRC-99 emissions group, in a manner exactly analogous to those in EPAEMIT.PRM. This should be used when processing emissions data maintained by the CARB.

2. Mechanism Implementation Test Files

Input and output files implementing a series of test calculations are included with the distributed files for testing the implementation of the mechanism into a chemical solver system. These are discussed in more detail in Section III.C.1.

3. Emissions and Mixture Lumping Programs and Examples

Batch files and programs for deriving emissions dependent parameters from emissions profiles or mixture composition files are also included with the distributed files. The programs are distributed as executable files that can run on PC compatible systems, and have been tested in DOS windows under Windows 3.1, 95, 98, and NT[5]. Source files for these programs are also distributed; these are discussed in Section III.A.5, below. Example input and output files, and example batch files implementing these programs are also included. These are discussed in more detail in Section III.B.

4. Lumping Control and Mechanism Assignment Files

As discussed elsewhere (Carter, 1998, Kumar et al, 1995), the operation of the emissions and mixture lumping programs are controlled by "lumping control files" and various parameter files used by them. These files, which implement the lumping and parameter assignments in the SAPRC-99 mechanism, are included in this distribution. The various files involved are listed and described in Table 7, and the major files and types of files are briefly discussed below.

The lumping control file EMITLUMP.LPC controls the lumping of the anthropogenic emissions input for model applications using the recommended lumped version of the mechanism. This is used to control the lumping for deriving parameters for the ALKn, AROn, and OLEn that represent the anthropogenic emissions with model species whose parameters can be adjusted based on the mixture being represented.

The lumping control file PARMLUMP.LPC controls the lumping for an extended version of the mechanism where the mechanistic parameters for the terpenes, higher aldehydes, ketones, and acroleins can be adjusted based on the mixture they represent. This is not appropriate for emissions lumping in the recommended condensed mechanism. However, use of this lumping control file is necessary for determining best fit parameters for mixtures of terpenes, for model applications where it may be appropriate to derive the parameters for the lumped terpene species, TRP1, using a different terpene mixture than that given in Table 6. This is discussed in Section III.B.3.

[5] These programs have been found to hang the computer when run under raw DOS mode, though this may not occur on all systems. Sometimes these programs fail for no known reason when run under NT; when this happens, simply run the program again and it will probably work.

Table 7. List of programs and files implementing the SAPRC-99 mechanism and its associated emissions processing procedures for the Models-3 system.

File	Description
	Mechanism implementation files in Models-3 format
SAPRC99F.MEC	Mechanism input file in Models-3 format for the fixed parameter condensed mechanism, with the mechanistic parameter for anthropogenic emissions derived using the mixture in ARBROG.CMP, which is the base ROG mixture used in the reactivity simulations (i.e., based on air quality data)
PHOTDATA.ZIP	Compressed file containing photolysis absorption cross section and quantum yield files in Models-3 format. One .PHD file for each .photolysis reaction in the mechanism that has distinct absorption cross sections and quantum yields. PKUNZIP can extract these files.
	Detailed Model Species and Emissions Assignment Files
EMITGRP.DAT	Assignments of emissions group to lumped model species for use in emissions processing. See comments in file for format of data.
EPAEMIT.PRM	Assignments of detailed model species to emissions categories used in the EPA / Models-3 emissions databases.
ARBEMIT.PRM	Assignments of detailed model species to emissions categories used in the CARB emissions databases.
	Parameter file giving options for programs running in this directory.
MODELING.PRM	Default file locations for programs. In this case, gives the location of the composition files and the mechanism files used in the example calculations.
	Input files for mechanism implementation test simulations
MD3TEST.PRP	Preparation input file to prepare version of simulation program for mechanism implementation test simulations.
MD3TEST1.INT	Static multi-day simulation. Anthropogenic VOCs.
MD3TEST2.INT	Static multi-day simulation. Anthropogenic VOCs. Low NOx.
MD3TEST3.INT	Continuous emissions multi-day simulation, anthropogenic VOCs.
MD3TEST4.INT	Continuous emissions multi-day simulation, biogenic VOCs.
MD3TEST4.INT	Same simulation conditions as MD3TEST1, except for T=320K, rather than T=300K.
	Output files for mechanism implementation test simulations
MD3TEST1.CSV	Results of calculation using MD3TEST1.INT as input.
MD3TEST2.CSV	Results of calculation using MD3TEST2.INT as input.
MD3TEST3.CSV	Results of calculation using MD3TEST3.INT as input.
MD3TEST4.CSV	Results of calculation using MD3TEST4.INT as input.
MD3TEST5.CSV	Results of calculation using MD3TEST5.INT as input.
	Files for Photolysis Rate Calculation Verification
STDZA640.JZS	Actinic flux data as a function of zenith angle for a set of standard zenith angles (0, 10, …, 70, 78, 86^{o}) that were used to calculate photolysis rates in the scenarios used for reactivity assessment by Carter (1994a, 1999). These were used to produce the photolysis rates given in the file STDZA640.KZS. The file consists of comment records indicating the units of the data, a set of records giving the standard zenith angles, then sets of records giving the actinic fluxes at those zenith angles.

Table 7 (continued)

File	Description
STDZA640.KZS	Photolysis rates for all the photolysis reactions in the mechanism with distinct absorption cross sections and quantum yields, calculated using the actinic fluxes in STDZA640.JZS and the absorption cross sections and quantum yields in the .PHD files contained in PHOTDATA.ZIP. The file consists of comment records, a set of records giving the zenith angles, then sets of records giving the photolysis rates corresponding to each .PHD file at those zenith angles, in min^{-1} units.
	Emissions Processing and Mechanism Lumping Examples
LUMPCOMP.BAT	Example batch file to derive the reactions of the ALKn, AROn, and OLEn model species to best represent the composition of the distribution of detailed model species in the file BASEROG.CMP The output file produced is LUMPCOMP.MEC. The reactions in that file can be used to replace the reactions of these species that are in the SAPRC99F.MEC file, as appropriate for the model application. The composition of BASEROG.CMP in this example is the same as that used to derive the lumped model species reactions in the default mechanism, so the reactions in of these species in LUMPCOMP.MEC should be the same as those in SAPRC99F.MEC. However, BASEROG.CMP can be replaced or edited as appropriate to represent different compositions.
LUMPEMIT.BAT	Example batch file to derive the reactions of the ALKn, AROn, and OLEn model species to best represent the composition of the emissions profile given in the file EPAEMIT.EMI. The output file produced is LUMPEMIT.MEC. This can be used to replace the reactions of these species that are in the SAPRC99F.MEC file, if it is desired to use a mechanism optimized to represent this emissions inventory rather than a composition based on air quality data. The reactions of these species will be different than those in SAPRC99F.MEC.
LUMPTERP.BAT	Example batch file to derive the reactions of TRP1 in the lumped mechanism, given the compistion of terpenes in the TERPENES.CMP file. The output file produced is LUMPTERP.MEC. This can be used to replace the reactions of TRP1 in the SAPRC99F.MEC file for model applications where the biogenic inventory suggests it is appropriate to use a different terpene composition than employed to derive these reactions in the current mechanism. This example just produces the same TRP1 mechanism as in SAPRC99F.MEC, but the file TERPENES.CMP can be edited as appropriate to represent a different terpene distribution.
RXPTOMEC.EXE	Produces file giving reactions in Models-3 format for all lumped model species whose parameters were derived for a given mixture, and given in an .RXP file such as produced by CMPTORXP.
	Programs used by Emissions Processing and Lumping Example Batch Files
CMPTORXP.EXE	Produces .RXP files giving lumped species mechanistic parameters and amounts given composition (.CMP) files in terms of molar amounts of detailed model species.
EMITOCMP.EXE	Produces .CMP files giving mixture compositions in terms of detailed model species from .EMI files giving mixture compositions in terms of SAROAD classes used in emissions inventories.
GNATOMEC.EXE	Produces file giving reactions in Models-3 format for all model species whose mechanistic parameters are specified in a .GNA file.
RUN386.EXE	DOS extender file needed for the executable programs in this distribution to run. Note that there is a bug in this program that may cause the system to hang if run in raw MS-DOS mode; running in a DOS window under Windows is recommended.
	Input files for emissions processing and mechanism lumping examples.
BASEROG.CMP	Composition of ambient VOCs based on analyses of ambient air data used to derive the mechanisms of the ALKn, AROn, AND OLEn model species in SAPRC99F.MEC. Given in terms of mole emissions of SAPRC-99 detailed model species. Same as ARBROG.CMP, but can be replaced or edited as desired to represent different compositions.

Table 7 (continued)

File	Description
EPAEMIT.EMI	Emissions profile derived by EPA (1999b) to represent regional model input for Models-3. Given as mass emissions for EPA SAROAD classes. This can be replaced or edited as desired to represent different emissions inputs.
TERPENES.CMP	Composition of mixture used to represent biogenic terpenes. Used to derive TRP1 mechanism in the lumped mechanism. This can be replaced or edited as desired to represent different biogenic inventories.
	Output files for emissions processing and mechanism lumping examples.
BASEROG.RXP	Mechanistic parameters of lumped model species corresponding to the mixture of VOCs in BASEROG.CMP. Produced by CMPTORXP using BASEROG.CMP and EMITLUMP.LPC as input. Should be the same as LUMPCOMP.RXP produced by LUMPCOMP.BAT.
BASEROG.MEC	Reactions of lumped model species corresponding to the mixture of VOCs in BASEROG.CMP. Produced by RXPTOMEC using BASEROG.RXP as input. Should be the same as the file LUMPCOMP.MEC produced by LUMPCOMP.BAT.
EPAEMIT.CMP	EPA (1999b) emissions profile in terms of detailed model species. Produced by EMITOCMP using EPAEMIT.EMI and EPAEMIT.PRM as input. Should be the same as the file LUMPEMIT.CMP produced by LUMPEMIT.BAT.
EPAEMIT.RXP	Mechanistic parameters of lumped model species corresponding to the EPA (1999b) emissions profile. Produced by CMPTORXP using EPAEMIT.CMP and EMITLUMP.LPC as input. Should be the same as the file LUMPEMIT.RXP produced by LUMPEMIT.BAT.
EPAEMIT.MEC	Reactions of lumped model species corresponding to the EPA (1999b) emissions profile. Produced by RXPTOMEC using EPAEMIT.RXP as input. Should be the same as the file LUMPEMIT.MEC produced by LUMPEMIT.BAT.
TERPENES.RXP	Mechanistic parameters of the lumped model species corresponding to the mixture of terpenes in TERPENES.CMP. Produced by CMPTORXP using TERPENES.CMP and PARMLUMP.LPC as input. Should be the same as LUMPTERP.RXP produced by LUMPTERP.BAT.
TERPENES.MEC	Reactions of the TRP1 model species corresponding to the mixture of terpenes in TERPENES.CMP. Produced by RXPTOMEC using TERPENES.RXP as input. Should be the same as the file LUMPTERP.MEC produced by LUMPTERP.BAT.
	Lumping control files for emissions processing and mechanism lumping for recommended mechanisms.
EMITLUMP.LPC	Used for lumping anthropogenic emissions input for model applications using the recommended lumped version of the mechanism. Terpenes are represented by the TRP1 model species, which is assumed to have its parameters pre-defined.
PARMLUMP.LPC	Lumping control file for deriving mechanistic parameters to represent species in an extended version of the condensed mechanism. Similar to EMITLUMP.LPC in terms of lumping of alkanes/others, aromatics and ketones, but has separate lumped parameter groups for terpenes, higher aldehydes, ketones, and acroleins. Not appropriate for emissions lumping in condensed mechanism, but can be used for determining best fit parameters for mixtures of terpenes, etc.
	Mechanism parameter files used by the .LPC files.
ALKOTH.GNA	Mechanism parameter file for Alkanes and other non-aromatic VOCs that react only with OH.
ALKENES.GNA	Mechanism parameter file for non-terpene alkenes.
ALDES.GNA	Mechanism parameter file for saturated aldehydes.
KETONES.GNA	Mechanism parameter file for ketones
ACROLS.GNA	Mechanism parameter file for unsaturated aldehydes.
ACETYLS.GNA	Mechanism parameter file for acetylenes.

Table 7 (continued)

File	Description
ACTYL-OH.GNA	Mechanism parameter file for Acetylenes, including only the OH reaction (for lumping with alkanes, etc.).
ETHEISOP.GNA	Mechanism parameter file for Ethene and isoprene (used for simulations where these are represented separately than the explicit ethene and isoprene base model species.)
ASNOTH.GNA	Mechanism parameter file for Miscellaneous compounds that react only with OH that are not processed using the mechanism generation system.
AROMATIC.GNA	Mechanism parameter file for Aromatic hydrocarbons whose parameters were adjusted to fit chamber data.
ASNALKE.GNA	Mechanism parameter file for Alkenes that are not processed using the mechanism generation system.
ASNARO.GNA	Mechanism parameter file for Miscellaneous compounds that are lumped with aromatics.
TERPENES.GNA	Mechanism parameter file for terpenes
	Other mechanistic assignment files used for lumping.
DMS.PRM	Specifications for detailed model species, giving molecular weights, etc.
LUMPMOLE.LPM	Contains standard lumped molecule substitutions.
EMITLUMP.LPM	Contains lumped molecule substitutions for species that are represented using the "lumped molecule" approach when present in mixtures, but which can be represented explicitly when represented separately for calculating their reactivities. This includes primarily terpenes represented by TRP1, aldehydes represented by RCHO, and ketones represened by MEK or PROD2.
MIXES.LPM	Gives association between names used for detailed model species that represent complex mixtures and the .CMP files specifying their compositions.
OLDNAMES.LPM	Contains substitutions to rename obsolete detailed model species names with names currently in use.
	Compisition files used to define several complex mixture detailed model species. Used in several .LPC files
ARBROG.CMP	Mixture used to represent base ROG composition in the reactivity simulations. Also used to derive mechanisms for the reactions of ALKn, AROn, and OLEn in the lumped mechanism, and reactions of RNO3 and PROD2 in the base mechanism. Normalized for 1 ppmC in total mixture.
MS-A.CMP	Composition of Mineral Spirits Sample "A" used in Safety-Kleen study.
MS-B.CMP	Composition of Mineral Spirits Sample "B" used in Safety-Kleen study.
MS-C.CMP	Composition of Mineral Spirits Sample "C" used in Safety-Kleen study.
MS-D.CMP	Composition of Mineral Spirits Sample "D" used in Safety-Kleen study.
	Used for generating reaction strings given mechanistic parameter files (e.g., by RXPTORXN, RXPTOMEC, GNATORXN, etc.)
GENHV.PRM	Gives the photolysis file name associated with each photolysis parameter code.
MODSPE.PRM	Gives the SAPRC and Models-3 species name for reaction product species that are associated with each product yield parameter code.
	Source files for distributed emissions and mixture lumping programs

Table 7 (continued)

File	Description
SOURCE.ZIP	Source files in condensed format, with recommended subdirectory structure saved with the files. To extract, use the command PKUNZIP -d SOURCE path where "path" is the subdirectory where the source files are to be distributed. The files extracted, and the directory structure into which they are extracted, are listed in Table 8.
	Extraction program for *.ZIP files
PKUNZIP.EXE	Program for extracting ZIP files. Runs on PC-compatible computers.

The mechanistic parameter files (*.GNA) and the lumped molecule and mixture substitution files (*.LPM) are referenced in the lumping control files. The .GNA files contain the parameters for the individual detailed model species for which such assignments have been made. Some of these were output by the computerized mechanism estimation and generation system discussed by Carter (1999), and for the rest the parameters were manually assigned based on various mechanistic considerations or adjustments to fit chamber data (Carter, 1999). The lumped molecule substitution are implemented in the LUMPMOLE.LPM file, and the files giving the compositions corresponding to detailed model species that represent complex mixtures are given in MIXES.LPM. The composition (*.CMP) files referenced by MIXES.LPM are also included in the distribution. These are used for the model species representing the base ROG mixture (ARBROG – the same as BASEROG as used in the examples), and those representing various mineral spirits samples (MS-A, etc) studied by Carter et al (1997b).

The file DMS.PRM gives the molecular weight and other information for all the detailed model species in the SAPRC-99 mechanism. This file is required by the emissions processing program regardless of which lumping control file is used, and is also required by the EMITOCMP program that derives the moles of detailed model species that correspond to a mass emissions profile.

5. Source Files for Emissions Processing and Lumping Programs

As indicated on Table 7 and discussed in the following section, several executable programs are distributed to determine lumped parameters and reactions for emissions profiles or mixtures. These programs are compiled and linked to run on PC compatible computers. Although these executable files are all that is needed to implement the mechanism and run the examples discussed here, the source files for the programs are needed if it is desired to run these programs on different computers, or to examine or modify the procedures they employ. Therefore, the source files are also included with this distribution.

The source files are given in condensed form in the file SOURCE.ZIP. To extract these files, one should (1) create an empty subdirectory where it is desired the files go and (2) give the command

PKUNZIP -d SOURCE path

where "path" is the path where the files are to go. The files as extracted using the above PKUNZIP command are listed on Table 8, where the subdirectories indicated there are relative to the directory specified by "path" in the above command. The three subdirectories are (1) SOURCE, containing utility subroutines used by all SAPRC modeling programs (not all of which may be needed by these programs), (2) LMPSUBS, containing subroutines used by SAPRC lumping programs (including others that are not included in this distribution), and (3) LMPPGMS, containing the source code used by these specific programs.

Table 8. Listing of source files for the distributed emissions processing and lumping programs.

Files	Description
Source Files Root Directory	
BLDALL.BAT	Compiles utility subroutines and then compiles and links all lumping programs. Executable files put in source files root directory.
Subdirectory LMPPGMS	
BLDALL.BAT	Compiles all programs in this subdirectory
EMICLNK3.BAT	Links EMITOCMP
CMPRLNK3.BAT	Links CMPTORXP
COMPSUB3.BAT	Compiles a subroutine in \SOURCE\LMPSUBS
LUMPSPEC.FOR	Specifications for data and arrays used by programs in this directory. This can be edited to change array dimensions, if needed.
SARSPEC.FOR	Specifications for data and arrays used by subroutines that process SAROAD data for emissions assignments.
CMPTORXP.FOR	Produces .RXP files giving lumped species mechanistic parameters and amountsgiven composition (.CMP) files in terms of molar amounts of detailed model species.
EMITOCMP.FOR	Produces .CMP files giving mixture compositions in terms of detailed model species from .EMI files giving mixture compositions in terms of SAROAD classes used in emissions inventories.
GNATOMEC.FOR	Produces file giving reactions in Models-3 format for all model species whose mechanistic parameters are specified in a .GNA file.
RXPTOMEC.FOR	Produces file giving reactions in Models-3 format for all lumped model species whose parameters were derived for a given mixture, and given in an .RXP file such as produced by CMPTORXP.
Subdirectory LMPSUBS	
*.FOR	Various subroutines used by VOC lumping programs and LUMPINT.
Subdirectory SUBS	
BLDALL.BAT	Compiles all subroutines using and puts results in INT3.LIB.
ADDSUB3.BAT	Compiles a new subroutine using F77L/EM and puts results in INT3.LIB
COMPSUB3.BAT	Compiles a subroutine using F77L/EM and replaces results in INT3.LIB
*.FOR	Various utility subroutines that are used by many of the programs.

Batch files to compile these programs using F77L/EM are also included[6]. These can be edited as appropriate for other compilers. Note that some modifications to some of the source files may be necessary for the programs to compile using other compilers, but these modifications should be straightforward. BLDALL.BAT in the root directory of the extracted files runs all the batch files needed to compile and link these programs. The executables are created in the root directory of the extracted files.

B. Procedures for Deriving Emissions or Mixture-Dependent Parameters

As discussed in Section II.A and by Carter (1999) the condensed version of the SAPRC-99 mechanism has a number of model species whose rate constants and product yield parameters depend on the mixture of VOCs they are being used to represent. The default fixed parameter mechanism given in Table 2 and Table 3 was derived such that the parameters for the lumped terpene species (TRP1) best represents the terpene mixture based on the biogenic inventory of Guenther et al (1999) and such that the parameters in the model species used to represent VOCs in anthropogenic emissions are based on the mixture of VOCs measured in ambient air (Jeffries et al, 1989). The procedures in this section can be employed should it be desired to modify the mechanism to represent other biogenic or anthropogenic emissions profiles. These are implemented in three batch files to run various example calculations as discussed below. These batch files or procedures can be modified as appropriate for integration into the overall modeling system.

The three batch files are all run without parameters or arguments, and use fixed input and output file names as indicated below. Each distributed batch file produces a major output file and one or more intermediate files that are used in the process. As indicated on Table 7, the distributed files include files that are identical to the intermediate or output files produced by running the batch files using the input files as distributed. These have different names than those produced by the batch file, so they can be compared with the batch file output.

1. Derivation of Anthropogenic Mechanistic Parameters Given a Mixture of SAPRC Detailed Model Species

The batch file LUMPCOMP.BAT can be used to derive the reactions of the ALKn, AROn, and OLEn model species to best represent the composition of the distribution of detailed model species in the file BASEROG.CMP. The output file produced is LUMPCOMP.MEC, which gives the reactions of these species in Models-3 format. These reactions can then replace those in SAPRC99F.MEC for model applications where it is appropriate to base these reactions on a different mixture than that employed when deriving the default fixed parameter mechanism.

The file BASEROG.CMP as distributed contains the exact same composition as that used to derive the reactions already in SAPRC99F.MEC, so the reactions produced in LUMPCOMP.MEC will be essentially the same as those in SAPRC99F.MEC when the batch file is run. The one difference will be the temperature dependence for the reaction of ALK1, which is derived based on that of ethane. SAPRC99F.MEC has the temperature dependence as recommended in the detailed mechanism (Carter,

[6] F77L/EM is available from Lahey Computer Systems, P.O. Box 6091. Incline Village, NV 89450-6091 (FAX 702-831-8123, http://www.lahey.com). These programs were compiled and linked using Version 5.1, and may not be compatible with later versions. Licensed users of later versions of F77L/EM can contact the author of this report at carter@cert.ucr.edu for assistance.

1999) for ethane, while LUMPCOMP.MEC has the temperature dependence derived using the procedures of the lumping programs[7]. The difference is insignificant.

The LUMPCOMP.BAT procedure operates in two steps, and creates one intermediate file. First the EMITORXP program is run to produce a file, LUMPCOMP.RXP, containing the parameters for the lumped species representing the input mixture. The lumping control file EMITLUMP.LPC is used to control the process. This parameter file is then input into the program RXPTOMEC, which converts it into reactions in Models-3 format.

2. Derivation of Anthropogenic Mechanistic Parameters Given an Aggregate Emissions Profile

The batch file LUMPEMIT.BAT can be used to derive the reactions of the ALKn, AROn, and OLEn model species to best represent an aggregate emissions profile derived to represent anthropogenic emissions into the model. These aggregate emissions profiles consist of mass emissions of EPA SAROAD (or ARB ChemCode[8]) classes, with the files consisting of records containing the 5-digit SAROAD code, one or more blanks, and the mass emissions corresponding to that code[9]. Such aggregate profiles can be derived, for example, by summing up all the emissions of each SAROAD class into the total modeling domain, or into the urban portions of the domain. A discussion of how to produce these aggregate profiles from emissions data is beyond the scope of this report.

This batch file can be used if it is desired that the mechanisms for these lumped species represent the profile of emissions into the modeling domain, rather than the ambient mixture used to derive the reactions in the default mechanism. The output file produced is LUMPEMIT.MEC, which contains the reactions of the lumped species in Models-3 format that can replace the corresponding reactions in SAPRC99F.MEC if desired.

The LUMPEMIT batch file as distributed uses as its primary input the emissions profile in the file EPAEMIT.EMI, which contains aggregate emissions in the 1995 U.S. National inventory (EPA, 1999b) using the current EPA SAROAD classification. The output LUMPEMIT.MEC produced using this input file gives the reactions of the lumped species shown on Table 4, above. This emissions profile input file can be replaced by other emissions profiles as appropriate given the model application, and the LUMPEMIT.MEC file produced by running LUMPEMIT.BAT will then have the reactions corresponding to this profile.

The operation of LUMPEMIT.BAT is similar to LUMPCOMP.BAT, except that involves three steps rather than two. In the first step, the EMITOCMP program is run to produce an intermediate output file, LUMPEMIT.CMP, that gives the composition of the mixture EPAEMIT.EMI terms of moles emissions of SAPRC detailed model species. The subsequent two steps are those used by LUMPCOMP.BAT, except that the input file is EPAEMIT.CMP rather than BASEROG.CMP, and the parameter file and reaction output files are LUMPEMIT.RXP and LUMPEMIT.MEC, respectively.

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[7] The lumping program estimates temperature dependences of rate constants for groups representing mixtures by calculating the weighted average rate constants for the mixtures for T=270, 300, and 330^{o}K, and then deriving Arrhenius parameters which best predict the rate constants at these temperatures.

[8] LUMPEMIT.BAT as distributed can be used for EPA emissions profiles only. However, comments in LUMPEMIT.BAT indicate how it can be edited for use in processing CARB emissions profiles.

[9] Note that it is only the relative amounts of the SAROAD classes that are significant to these programs. The total mass in the profiles does not affect the results.

If it is desired to use LUMPEMIT.BAT to process emissions profiles derived from CARB emissions data bases, then LUMPEMIT.BAT needs to be edited so that the EMITOCMP program uses ARBEMIT.PRM rather than EPAEMIT.PRM to derive the correspondence between emissions classes and SAPRC detailed model species. The batch file contains comments indicating what needs to be changed.

3. Derivation of Terpene Mechanistic Parameters Given a Representative Terpene Mixture Composition

The LUMPTERP batch batch file can be used to derive the reactions of TRP1 in the lumped mechanism, given the composition of terpenes in the TERPENES.CMP file. This composition must be specified in terms of mole emissions of SAPRC-99 detailed model species. The output file produced is LUMPTERP.MEC. This can be used to replace the reactions of TRP1 in the SAPRC99F.MEC file for model applications where the biogenic inventory suggests it is appropriate to use a different terpene compisition than employed to derive these reactions in the current mechanism. This example just produces the same TRP1 mechanism as in SAPRC99F.MEC (and Table 2), but the file TERPENES.CMP can be edited as appropriate to represent a different terpene distribution.

The operation of LUMPTERP.BAT is exactly analogous to that of LUMPCOMP.BAT, discussed above, except that it uses PARMLUMP.LPC as the lumping control file rather than EMITLUMP.LPC, and the intermediate and output file names are LUMPTERP.RXP and LUMPTERP.MEC.

C. Implementation Test Calculations

1. Reaction Implementation Tests

Input and output files for five test calculations are provided to test for correct implementation of the mechanism in SAPRC99F.MEC in the mechanism solver software. All the photolysis rates are specified, and are either constant or zero in all four simulations. Three of these calculations are for static conditions, with all pollutants present initially and none emitted, and two were for the emissions emitted at a constant rate throughout the simulations. VOC and NO_x inputs are also varied. Four of the calculations were with constant temperature of 300^{o}K, and one with a constant temperature of 320^{o}K. The conditions of the four test calculations are listed in Table 9, and the photolysis rates used during the simulated light periods in all calculations are given in Table 10.

The output files of the calculations are in the files MD3TESTn.CSV, where n=1,…5. The data in these files can be compared with output of test calculations using the software and solver where the mechanism is being implemented. The files MD3TESTn.INT are the input files used in the simulations using the SAPRC mechanism implementation software that were used to produce the corresponding .CSV files.

2. Data for Photolysis Rate Calculation Implementation Tests

As indicated on Table 7, the distribution includes two files that can be used to test the programs and files used to calculate the photolysis rates in this mechanism. The file STDZA640.JZS contains a set of actinic fluxes at various zenith angles, and the file STDZA640.KZS contains all the photolysis rates in the present mechanism calculated using those actinic fluxes. These were calculated using the absorption cross sections and quantum yields given in Table A-2, which are contained in the .PHD files contained in PHOTDATA.ZIP.

Table 9. Input conditions for mechanism test calculations

File Name	MD3TEST1	MD3TEST2	MD3TEST3	MD3TEST4	MD3TEST5
Conditions					
VOC Types	Urban	Urban	Biogenic	Urban	Urban
NO_x levels	High	High	Low	Low	High
Reactant Input	All Reactions at t=0	Continuous Emissions	Continuous Emissions	All Reactions at t=0	All Reactions at t=0
Temperature	300K	300K	300K	300K	320K
Dilution			0		
Simulation times:					
Period 1: Light			0 - 1440 minutes		
Period 2: Dark			1440 - 1800 minutes		
Period 3: Light			1800 - 2160 minutes		
Constant Reactants (ppm)					
O2			2.09E+05		
M			1.00E+06		
CH4	0.07	1.00	1.00	0.07	0.07
Reactants					
Input units	ppm @ T=0	ppm/min	ppm/min	ppm @ T=0	ppm @ T=0
NO	1.00e-1	6.94e-5	6.94e-6	1.00e-2	1.00e-1
NO2	5.00e-2	3.47e-5	3.47e-6	5.00e-3	5.00e-2
HONO	1.00e-3	6.94e-7	6.94e-8	1.00e-4	1.00e-3
SO2	5.00e-2	3.47e-5		5.00e-2	5.00e-2
XC	2.00e-1			2.00e-1	2.00e-1
ISOPRENE	4.33e-4	3.01e-7	6.94e-5	4.33e-4	4.33e-4
TERP	8.20e-4	5.69e-7	3.47e-5	8.20e-4	8.20e-4
ETHENE	1.89e-2	1.31e-5		1.89e-2	1.89e-2
MEOH	5.89e-3	4.09e-6		5.89e-3	5.89e-3
HCOOH	6.77e-4			6.77e-4	6.77e-4
CCO-OH	1.16e-3			1.16e-3	1.16e-3
RCO-OH	3.92e-4			3.92e-4	3.92e-4
HCHO	1.12e-2	7.79e-6		1.12e-2	1.12e-2
CCHO	2.32e-3	1.61e-6		2.32e-3	2.32e-3
RCHO	1.72e-3	1.20e-6		1.72e-3	1.72e-3
GLY	1.21e-4	8.43e-8		1.21e-4	1.21e-4
MGLY	8.37e-5	5.82e-8		8.37e-5	8.37e-5
METHACRO	1.30e-3	9.01e-7		1.30e-3	1.30e-3
ISO-PROD	8.93e-5	6.20e-8		8.93e-5	8.93e-5
BALD	7.51e-5	5.22e-8		7.51e-5	7.51e-5

Table 9 (continued)

File Name	MD3TEST1	MD3TEST2	MD3TEST3	MD3TEST4	MD3TEST5
ACET	5.07e-3	3.52e-6		5.07e-3	5.07e-3
MEK	3.26e-3	2.27e-6		3.26e-3	3.26e-3
PROD2	1.93e-3	1.34e-6		1.93e-3	1.93e-3
PHEN	6.06e-4	4.21e-7		6.06e-4	6.06e-4
CRES	5.60e-4	3.89e-7		5.60e-4	5.60e-4
ALK1	1.17e-2	8.10e-6		1.17e-2	1.17e-2
ALK2	1.88e-2	1.31e-5		1.88e-2	1.88e-2
ALK3	4.69e-2	3.26e-5		4.69e-2	4.69e-2
ALK4	4.17e-2	2.89e-5		4.17e-2	4.17e-2
ALK5	3.06e-2	2.12e-5		3.06e-2	3.06e-2
ARO1	1.18e-2	8.19e-6		1.18e-2	1.18e-2
ARO2	8.74e-3	6.07e-6		8.74e-3	8.74e-3
OLE1	1.04e-2	7.21e-6		1.04e-2	1.04e-2
OLE2	7.97e-3	5.54e-6		7.97e-3	7.97e-3

Table 10. Photolysis rates used in mechanism test calculations

Phot Set	k (min^{-1})	Phot Set	k (min^{-1})	Phot Set	k (min^{-1})
NO2	6.69e-1	H2O2	5.64e-4	GLY_ABS	1.81e-1
NO3NO	1.59e+0	HCHO_R	2.32e-3	MGLY_ADJ	1.10e-2
NO3NO2	1.50e+1	HCHO_M	3.15e-3	BACL_ADJ	1.90e-2
O3O3P	3.61e-2	CCHO_R	4.16e-4	BZCHO	6.22e-2
O3O1D	3.05e-3	C2CHO	1.40e-3	ACROLEIN	3.32e-2
HONO-NO	1.27e-1	ACETONE	4.16e-5	IC3ONO2	2.35e-4
HONO-NO2	1.60e-2	KETONE	9.49e-4	MGLY_ABS	2.06e-1
HNO3	5.40e-5	COOH	3.94e-4		
HO2NO2	4.69e-4	GLY_R	8.93e-3		

IV. REFERENCES

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APPENDIX A.

TABULATIONS OF DETAILED MODEL SPECIES AND ABSORPTION CROSS SECTION AND QUANTUM YIELD DATA.

Table A-1. Listing of reactions of individual detailed model species that can optionally be explicitly represented in the mechanism.

Compound	Reactions	Kinetic Parameters [a]
Methane	METHANE + HO. = C-O2.	# 2.150e-12 @ 1735.
Ethane	ETHANE + HO. = RO2-R. + CCHO	# 1.370E-12^2.00@498.
Propane	PROPANE + HO. = 0.965*RO2-R. + 0.035*RO2-N. + 0.261*RCHO + 0.704*ACET + -0.104*XC	# 1.400E-12^2.00@61.
n-Butane	N-C4 + HO. = 0.921*RO2-R. + 0.079*RO2-N. + 0.413*R2O2. + 0.632*CCHO + 0.12*RCHO + 0.485*MEK + -0.038*XC	# 1.520E-12^2.00@-145.
n-Pentane	N-C5 + HO. = 0.855*RO2-R. + 0.145*RO2-N. + 0.65*R2O2. + 0.147*CCHO + 0.22*RCHO + 0.238*MEK + 0.397*PROD2 + -0.157*XC	# 2.200E-12^2.00@-183.
n-Hexane	N-C6 + HO. = 0.775*RO2-R. + 0.225*RO2-N. + 0.787*R2O2. + 0.011*CCHO + 0.113*RCHO + 0.688*PROD2 + 0.162*XC	# 1.380E-12^2.00@-414.
n-Heptane	N-C7 + HO. = 0.705*RO2-R. + 0.295*RO2-N. + 0.799*R2O2. + 0.055*RCHO + 0.659*PROD2 + 1.11*XC	# 1.430E-12^2.00@-478.
n-Octane	N-C8 + HO. = 0.646*RO2-R. + 0.354*RO2-N. + 0.786*R2O2. + 0.024*RCHO + 0.622*PROD2 + 2.073*XC	# 2.480E-12^2.00@-378.
n-Nonane	N-C9 + HO. = 0.602*RO2-R. + 0.398*RO2-N. + 0.777*R2O2. + 0.018*RCHO + 0.584*PROD2 + 3.055*XC	# 2.260E-12^2.00@-447.
n-Decane	N-C10 + HO. = 0.572*RO2-R. + 0.428*RO2-N. + 0.772*R2O2. + 0.015*RCHO + 0.557*PROD2 + 4.045*XC	# 2.820E-12^2.00@-416.
n-Undecane	N-C11 + HO. = 0.553*RO2-R. + 0.447*RO2-N. + 0.771*R2O2. + 0.013*RCHO + 0.54*PROD2 + 5.038*XC	# 1.290E-11
n-Dodecane	N-C12 + HO. = 0.542*RO2-R. + 0.458*RO2-N. + 0.768*R2O2. + 0.011*RCHO + 0.53*PROD2 + 6.034*XC	# 1.390E-11
n-Tridecane	N-C13 + HO. = 0.535*RO2-R. + 0.465*RO2-N. + 0.766*R2O2. + 0.01*RCHO + 0.525*PROD2 + 7.03*XC	# 1.600E-11
n-Tetradecane	N-C14 + HO. = 0.53*RO2-R. + 0.47*RO2-N. + 0.765*R2O2. + 0.009*RCHO + 0.521*PROD2 + 8.027*XC	# 1.800E-11
n-Pentadecane	N-C15 + HO. = 0.527*RO2-R. + 0.473*RO2-N. + 0.764*R2O2. + 0.008*RCHO + 0.519*PROD2 + 9.025*XC	# 2.100E-11
n-C16	N-C16 + HO. = 0.525*RO2-R. + 0.475*RO2-N. + 0.763*R2O2. + 0.008*RCHO + 0.517*PROD2 + 10.023*XC	# 2.300E-11
Isobutane	2-ME-C3 + HO. = 0.198*RO2-R. + 0.042*RO2-N. + 0.833*R2O2. + 0.76*TBU-O. + 0.073*HCHO + 0.128*RCHO + 0.07*ACET + 0.8*XC	# 1.040E-12^2.00@-225.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Neopentane	22-DM-C3 + HO. = 0.021*RO2-R. + 0.088*RO2-N. + 1.819*R2O2. + 0.891*TBU-O. + 0.928*HCHO + 0.021*RCHO + 0.809*XC	# 1.620E-12^2.00@189.
Iso-Pentane	2-ME-C4 + HO. = 0.881*RO2-R. + 0.095*RO2-N. + 0.902*R2O2. + 0.024*C-O2. + 0.012*HCHO + 0.78*CCHO + 0.101*RCHO + 0.762*ACET + 0.038*MEK + 0.094*XC	# 3.700E-12
2,2-Dimethyl Butane	22-DM-C4 + HO. = 0.304*RO2-R. + 0.176*RO2-N. + 1.581*R2O2. + 0.009*C-O2. + 0.51*TBU-O. + 0.227*HCHO + 0.73*CCHO + 0.103*RCHO + 0.202*ACET + 0.009*MEK + 0.765*XC	# 3.220E-11@781.
2,3-Dimethyl Butane	23-DM-C4 + HO. = 0.858*RO2-R. + 0.142*RO2-N. + 0.918*R2O2. + 0.028*HCHO + 0.023*CCHO + 0.078*RCHO + 1.569*ACET + 0.001*MEK + 0.132*XC	# 1.120E-12^2.00@-494.
2-Methyl Pentane	2-ME-C5 + HO. = 0.816*RO2-R. + 0.184*RO2-N. + 0.859*R2O2. + 0.004*HCHO + 0.011*CCHO + 0.661*RCHO + 0.346*ACET + 0.006*MEK + 0.153*PROD2 + 0.904*XC	# 5.300E-12
3-Methylpentane	3-ME-C5 + HO. = 0.844*RO2-R. + 0.156*RO2-N. + 0.989*R2O2. + 0.005*HCHO + 0.986*CCHO + 0.069*RCHO + 0.629*MEK + 0.036*PROD2 + 0.151*XC	# 5.400E-12
2,2,3-Trimethyl Butane	223TM-C4 + HO. = 0.183*RO2-R. + 0.192*RO2-N. + 1.631*R2O2. + 0.625*TBU-O. + 0.16*HCHO + 0.022*CCHO + 0.065*RCHO + 0.87*ACET + 0.964*XC	# 7.610E-13^2.00@-516.
2,2-Dimethyl Pentane	22-DM-C5 + HO. = 0.441*RO2-R. + 0.209*RO2-N. + 1.191*R2O2. + 0.35*TBU-O. + 0.056*HCHO + 0.017*CCHO + 0.516*RCHO + 0.014*ACET + 0.017*MEK + 0.257*PROD2 + 1.408*XC	# 3.400E-12
2,3-Dimethyl Pentane	23-DM-C5 + HO. = 0.783*RO2-R. + 0.217*RO2-N. + 1.09*R2O2. + 0.015*HCHO + 0.453*CCHO + 0.061*RCHO + 0.733*ACET + 0.517*MEK + 0.01*PROD2 + 0.269*XC	# 7.153E-12
2,4-Dimethyl Pentane	24-DM-C5 + HO. = 0.796*RO2-R. + 0.204*RO2-N. + 1.323*R2O2. + 0.333*HCHO + 0.016*CCHO + 0.562*RCHO + 0.483*ACET + 0.013*MEK + 0.135*PROD2 + 1.413*XC	# 5.000E-12
2-Methyl Hexane	2-ME-C6 + HO. = 0.731*RO2-R. + 0.269*RO2-N. + 0.906*R2O2. + 0.022*HCHO + 0.048*CCHO + 0.236*RCHO + 0.137*ACET + 0.508*PROD2 + 1.102*XC	# 6.894E-12
3,3-Dimethyl Pentane	33-DM-C5 + HO. = 0.737*RO2-R. + 0.238*RO2-N. + 1.593*R2O2. + 0.025*C-O2. + 0.163*HCHO + 1.328*CCHO + 0.046*RCHO + 0.618*ACET + 0.096*MEK + 0.002*PROD2 + 0.34*XC	# 2.996E-12
3-Methyl Hexane	3-ME-C6 + HO. = 0.75*RO2-R. + 0.25*RO2-N. + 0.924*R2O2. + 0.002*HCHO + 0.208*CCHO + 0.463*RCHO + 0.256*MEK + 0.235*PROD2 + 1.266*XC	# 7.174E-12
2,2,3,3-Tetrame. Butane	2233M-C4 + HO. = 0.067*RO2-R. + 0.316*RO2-N. + 2.106*R2O2. + 0.617*TBU-O. + 0.761*HCHO + 0.059*RCHO + 0.659*ACET + 1.337*XC	# 1.720E-12^2.00@144.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
2,2,4-Trimethyl Pentane	224TM-C5 + HO. = 0.403*RO2-R. + 0.227*RO2-N. + 1.961*R2O2. + 0.37*TBU-O. + 0.717*HCHO + 0.002*CCHO + 0.388*RCHO + 0.38*ACET + 0.133*MEK + 0.027*PROD2 + 1.809*XC	# 1.870E-12^2.00@-196.
2,2-Dimethyl Hexane	22-DM-C6 + HO. = 0.457*RO2-R. + 0.29*RO2-N. + 0.953*R2O2. + 0.253*TBU-O. + 0.035*HCHO + 0.041*CCHO + 0.367*RCHO + 0.001*ACET + 0.013*MEK + 0.341*PROD2 + 2.183*XC	# 4.800E-12
2,3,4-Trimethyl Pentane	234TM-C5 + HO. = 0.717*RO2-R. + 0.283*RO2-N. + 1.284*R2O2. + 0.039*HCHO + 0.447*CCHO + 0.033*RCHO + 1.141*ACET + 0.296*MEK + 0.664*XC	# 7.100E-12
2,3-Dimethyl Hexane	23-DM-C6 + HO. = 0.7*RO2-R. + 0.3*RO2-N. + 1.143*R2O2. + 0.014*HCHO + 0.128*CCHO + 0.184*RCHO + 0.561*ACET + 0.299*MEK + 0.25*PROD2 + XC	# 8.574E-12
2,4-Dimethyl Hexane	24-DM-C6 + HO. = 0.652*RO2-R. + 0.348*RO2-N. + 1.346*R2O2. + 0.159*HCHO + 0.335*CCHO + 0.306*RCHO + 0.096*ACET + 0.156*MEK + 0.293*PROD2 + 1.492*XC	# 8.574E-12
2,5-Dimethyl Hexane	25-DM-C6 + HO. = 0.649*RO2-R. + 0.351*RO2-N. + 1.53*R2O2. + 0.156*HCHO + 0.434*RCHO + 0.569*ACET + 0.225*PROD2 + 1.378*XC	# 8.293E-12
2-Methyl Heptane	2-ME-C7 + HO. = 0.659*RO2-R. + 0.341*RO2-N. + 0.882*R2O2. + 0.016*HCHO + 0.025*CCHO + 0.155*RCHO + 0.024*ACET + 0.546*PROD2 + 2.077*XC	# 8.314E-12
3-Methyl Heptane	3-ME-C7 + HO. = 0.662*RO2-R. + 0.338*RO2-N. + 0.942*R2O2. + 0.001*HCHO + 0.178*CCHO + 0.15*RCHO + 0.062*MEK + 0.521*PROD2 + 1.788*XC	# 8.594E-12
4-Methyl Heptane	4-ME-C7 + HO. = 0.676*RO2-R. + 0.324*RO2-N. + 0.875*R2O2. + 0.002*HCHO + 0.004*CCHO + 0.377*RCHO + 0.115*MEK + 0.376*PROD2 + 2.201*XC	# 8.594E-12
2,2,5-Trimethyl Hexane	225TM-C6 + HO. = 0.475*RO2-R. + 0.33*RO2-N. + 1.307*R2O2. + 0.195*TBU-O. + 0.046*HCHO + 0.002*CCHO + 0.613*RCHO + 0.433*ACET + 0.004*MEK + 0.056*PROD2 + 2.899*XC	# 6.079E-12
2,3,5-Trimethyl Hexane	235TM-C6 + HO. = 0.622*RO2-R. + 0.378*RO2-N. + 1.356*R2O2. + 0.094*HCHO + 0.104*CCHO + 0.178*RCHO + 0.63*ACET + 0.017*MEK + 0.436*PROD2 + 1.327*XC	# 7.900E-12
2,4-Dimethyl Heptane	24-DM-C7 + HO. = 0.598*RO2-R. + 0.402*RO2-N. + 1.176*R2O2. + 0.104*HCHO + 0.013*CCHO + 0.41*RCHO + 0.049*ACET + 0.073*MEK + 0.381*PROD2 + 2.501*XC	# 9.994E-12
2-Methyl Octane	2-ME-C8 + HO. = 0.587*RO2-R. + 0.413*RO2-N. + 0.914*R2O2. + 0.002*HCHO + 0.064*RCHO + 0.014*ACET + 0.536*PROD2 + 3.072*XC	# 1.010E-11
3,3-Diethyl Pentane	33-DE-C5 + HO. = 0.647*RO2-R. + 0.353*RO2-N. + 1.45*R2O2. + 0.053*HCHO + 1.321*CCHO + 0.022*RCHO + 0.607*MEK + 0.018*PROD2 + 1.585*XC	# 4.900E-12
3,5-Dimethyl Heptane	35-DM-C7 + HO. = 0.549*RO2-R. + 0.451*RO2-N. + 1.467*R2O2. + 0.01*HCHO + 0.648*CCHO + 0.155*RCHO + 0.075*MEK + 0.399*PROD2 + 1.83*XC	# 1.027E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
4-Ethyl Heptane	4-ET-C7 + HO. = 0.633*RO2-R. + 0.367*RO2-N. + 0.862*R2O2. + 0.001*HCHO + 0.049*CCHO + 0.328*RCHO + 0.486*PROD2 + 2.799*XC	# 1.042E-11
4-Methyl Octane	4-ME-C8 + HO. = 0.605*RO2-R. + 0.395*RO2-N. + 0.89*R2O2. + 0.001*HCHO + 0.034*CCHO + 0.127*RCHO + 0.006*MEK + 0.562*PROD2 + 2.788*XC	# 9.700E-12
2,4-Dimethyl Octane	24-DM-C8 + HO. = 0.555*RO2-R. + 0.445*RO2-N. + 1.06*R2O2. + 0.041*HCHO + 0.034*CCHO + 0.21*RCHO + 0.024*ACET + 0.007*MEK + 0.49*PROD2 + 3.55*XC	# 1.141E-11
2,6-Dimethyl Octane	26DM-C8 + HO. = 0.567*RO2-R. + 0.433*RO2-N. + 1.096*R2O2. + 0.108*CCHO + 0.308*RCHO + 0.145*ACET + 0.071*MEK + 0.276*PROD2 + 3.887*XC	# 1.290E-11
2-Methyl Nonane	2-ME-C9 + HO. = 0.551*RO2-R. + 0.449*RO2-N. + 0.895*R2O2. + 0.035*RCHO + 0.012*ACET + 0.516*PROD2 + 4.066*XC	# 1.280E-11
3,4-Diethyl Hexane	34-DE-C6 + HO. = 0.619*RO2-R. + 0.381*RO2-N. + 1.105*R2O2. + 0.007*HCHO + 0.337*CCHO + 0.319*RCHO + 0.709*MEK + 0.126*PROD2 + 2.483*XC	# 7.400E-12
3-Methyl Nonane	3-ME-C9 + HO. = 0.551*RO2-R. + 0.449*RO2-N. + 0.928*R2O2. + 0.036*CCHO + 0.063*RCHO + 0.014*MEK + 0.502*PROD2 + 3.977*XC	# 1.143E-11
4-Methyl Nonane	4-ME-C9 + HO. = 0.572*RO2-R. + 0.428*RO2-N. + 0.876*R2O2. + 0.001*HCHO + 0.019*CCHO + 0.14*RCHO + 0.004*MEK + 0.52*PROD2 + 3.831*XC	# 1.143E-11
4-Propyl Heptane	4-PR-C7 + HO. = 0.593*RO2-R. + 0.407*RO2-N. + 0.834*R2O2. + 0.001*HCHO + 0.001*CCHO + 0.296*RCHO + 0.461*PROD2 + 3.899*XC	# 1.184E-11
2,6-Dimethyl Nonane	26DM-C9 + HO. = 0.533*RO2-R. + 0.467*RO2-N. + 1.036*R2O2. + 0.001*CCHO + 0.221*RCHO + 0.12*ACET + 0.006*MEK + 0.376*PROD2 + 4.888*XC	# 1.283E-11
3,5-Diethyl Heptane	35-DE-C7 + HO. = 0.465*RO2-R. + 0.535*RO2-N. + 1.311*R2O2. + 0.002*HCHO + 0.475*CCHO + 0.123*RCHO + 0.044*MEK + 0.371*PROD2 + 4.064*XC	# 1.392E-11
3-Methyl Decane	3-ME-C10 + HO. = 0.526*RO2-R. + 0.474*RO2-N. + 0.917*R2O2. + 0.029*CCHO + 0.038*RCHO + 0.012*MEK + 0.489*PROD2 + 4.998*XC	# 1.285E-11
4-Methyl Decane	4-ME-C10 + HO. = 0.531*RO2-R. + 0.469*RO2-N. + 0.907*R2O2. + 0.001*CCHO + 0.08*RCHO + 0.003*MEK + 0.5*PROD2 + 4.932*XC	# 1.285E-11
2,6-Diethyl Octane	36-DE-C8 + HO. = 0.518*RO2-R. + 0.482*RO2-N. + 1.155*R2O2. + 0.301*CCHO + 0.058*RCHO + 0.108*MEK + 0.473*PROD2 + 5.062*XC	# 1.534E-11
3,6-Dimethyl Decane	36DM-C10 + HO. = 0.494*RO2-R. + 0.506*RO2-N. + 1.079*R2O2. + 0.001*HCHO + 0.088*CCHO + 0.11*RCHO + 0.055*MEK + 0.458*PROD2 + 5.488*XC	# 1.453E-11
3-Methyl Undecane	3-ME-C11 + HO. = 0.516*RO2-R. + 0.484*RO2-N. + 0.896*R2O2. + 0.025*CCHO + 0.033*RCHO + 0.011*MEK + 0.484*PROD2 + 5.997*XC	# 1.427E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
5-Methyl Undecane	5-ME-C11 + HO. = 0.524*RO2-R. + 0.476*RO2-N. + 0.867*R2O2. + 0.01*CCHO + 0.059*RCHO + 0.504*PROD2 + 5.923*XC	# 1.427E-11
3,6-Dimethyl Undecane	36DM-C11 + HO. = 0.488*RO2-R. + 0.512*RO2-N. + 1.046*R2O2. + 0.001*HCHO + 0.07*CCHO + 0.124*RCHO + 0.046*MEK + 0.442*PROD2 + 6.579*XC	# 1.595E-11
3,7-Diethyl Nonane	37-DE-C9 + HO. = 0.5*RO2-R. + 0.5*RO2-N. + 1.107*R2O2. + 0.132*CCHO + 0.293*RCHO + 0.105*MEK + 0.304*PROD2 + 6.607*XC	# 1.676E-11
3-Methyl Dodecane	3-ME-C12 + HO. = 0.51*RO2-R. + 0.49*RO2-N. + 0.88*R2O2. + 0.023*CCHO + 0.03*RCHO + 0.009*MEK + 0.482*PROD2 + 6.997*XC	# 1.569E-11
5-Methyl Dodecane	5-ME-C12 + HO. = 0.514*RO2-R. + 0.486*RO2-N. + 0.863*R2O2. + 0.009*CCHO + 0.044*RCHO + 0.498*PROD2 + 6.942*XC	# 1.569E-11
3,7-Dimethyl Dodecane	37DM-C12 + HO. = 0.496*RO2-R. + 0.504*RO2-N. + 0.98*R2O2. + 0.055*CCHO + 0.11*RCHO + 0.03*MEK + 0.44*PROD2 + 7.772*XC	# 1.737E-11
3,8-Diethyl Decane	38DE-C10 + HO. = 0.471*RO2-R. + 0.529*RO2-N. + 1.03*R2O2. + 0.066*CCHO + 0.057*RCHO + 0.017*MEK + 0.428*PROD2 + 7.885*XC	# 1.818E-11
3-Methyl Tridecane	3-ME-C13 + HO. = 0.506*RO2-R. + 0.494*RO2-N. + 0.871*R2O2. + 0.021*CCHO + 0.015*RCHO + 0.009*MEK + 0.493*PROD2 + 7.958*XC	# 1.711E-11
6-Methyl Tridecane	6-ME-C13 + HO. = 0.512*RO2-R. + 0.488*RO2-N. + 0.852*R2O2. + 0.006*CCHO + 0.041*RCHO + 0.504*PROD2 + 7.909*XC	# 1.711E-11
3,7-Dimethyl Tridecane	37DM-C13 + HO. = 0.487*RO2-R. + 0.513*RO2-N. + 0.98*R2O2. + 0.045*CCHO + 0.087*RCHO + 0.028*MEK + 0.44*PROD2 + 8.82*XC	# 1.879E-11
3,9-Diethyl Undecane	39DE-C11 + HO. = 0.474*RO2-R. + 0.526*RO2-N. + 0.997*R2O2. + 0.058*CCHO + 0.051*RCHO + 0.016*MEK + 0.435*PROD2 + 8.899*XC	# 1.960E-11
3-Methyl Tetradecane	3-ME-C14 + HO. = 0.505*RO2-R. + 0.495*RO2-N. + 0.861*R2O2. + 0.02*CCHO + 0.013*RCHO + 0.008*MEK + 0.493*PROD2 + 8.961*XC	# 1.853E-11
6-Methyl Tetradecane	6-ME-C14 + HO. = 0.51*RO2-R. + 0.49*RO2-N. + 0.843*R2O2. + 0.006*CCHO + 0.037*RCHO + 0.503*PROD2 + 8.918*XC	# 1.853E-11
3-Methyl Pentadecane	3-ME-C15 + HO. = 0.504*RO2-R. + 0.496*RO2-N. + 0.853*R2O2. + 0.018*CCHO + 0.012*RCHO + 0.008*MEK + 0.493*PROD2 + 9.964*XC	# 1.996E-11
4,8-Dimethyl Tetradecane	48DM-C14 + HO. = 0.481*RO2-R. + 0.519*RO2-N. + 0.962*R2O2. + 0.001*CCHO + 0.071*RCHO + 0.003*MEK + 0.473*PROD2 + 9.82*XC	# 2.021E-11
7-Methyl Pentadecane	7-ME-C15 + HO. = 0.503*RO2-R. + 0.497*RO2-N. + 0.853*R2O2. + 0.022*RCHO + 0.5*PROD2 + 9.95*XC	# 1.996E-11
Cyclopropane	CYCC3 + HO. = 0.949*RO2-R. + 0.051*RO2-N. + 0.949*R2O2. + 0.949*RCHO + -0.153*XC	# 8.400E-14
Cyclobutane	CYCC4 + HO. = 0.117*RO2-N. + 1.803*R2O2. + 0.883*RCO-O2. + 0.65*XC	# 1.500E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Cyclopentane	CYCC5 + HO. = 0.776*RO2-R. + 0.224*RO2-N. + 1.661*R2O2. + 0.054*CO + 0.756*RCHO + 0.02*MEK + 1.255*XC	# 2.310E-12^2.00@-235.
Cyclohexane	CYCC6 + HO. = 0.799*RO2-R. + 0.201*RO2-N. + 0.473*R2O2. + 0.203*RCHO + 0.597*PROD2 + 0.608*XC	# 2.590E-12^2.00@-309.
Isopropyl Cyclopropane	IPR-CC3 + HO. = 0.833*RO2-R. + 0.164*RO2-N. + 1.821*R2O2. + 0.002*RCO-O2. + 0.087*HCHO + 0.087*CCHO + 0.835*RCHO + 0.77*ACET + -0.068*XC	# 2.700E-12
Methylcyclopentane	ME-CYCC5 + HO. = 0.453*RO2-R. + 0.306*RO2-N. + 1.847*R2O2. + 0.239*CCO-O2. + 0.003*RCO-O2. + 0.023*CO + 0.017*HCHO + 0.689*RCHO + 0.003*PROD2 + 1.556*XC	# 5.681E-12
1,3-Dimeth. Cyclopentane	13DMCYC5 + HO. = 0.275*RO2-R. + 0.381*RO2-N. + 1.873*R2O2. + 0.344*CCO-O2. + 0.001*RCO-O2. + 0.037*CO + 0.028*HCHO + 0.002*CCHO + 0.584*RCHO + 0.035*PROD2 + 1.999*XC	# 6.818E-12
Cycloheptane	CYCC7 + HO. = 0.509*RO2-R. + 0.39*RO2-N. + 1.578*R2O2. + 0.101*RCO-O2. + 0.492*RCHO + 0.017*PROD2 + 2.778*XC	# 1.300E-11
Ethyl Cyclopentane	ET-CYCC5 + HO. = 0.404*RO2-R. + 0.389*RO2-N. + 1.86*R2O2. + 0.208*RCO-O2. + 0.019*CO + 0.007*HCHO + 0.132*CCHO + 0.59*RCHO + 0.003*MEK + 0.004*PROD2 + 0.01*MGLY + 1.922*XC	# 7.265E-12
Methylcyclohexane	ME-CYCC6 + HO. = 0.66*RO2-R. + 0.34*RO2-N. + 1.146*R2O2. + 0.011*HCHO + 0.002*CCHO + 0.455*RCHO + 0.208*PROD2 + 2.328*XC	# 1.000E-11
1,3-Dimethyl Cyclohexane	13DMCYC6 + HO. = 0.553*RO2-R. + 0.445*RO2-N. + 1.397*R2O2. + 0.001*CCO-O2. + 0.009*CO + 0.02*HCHO + 0.014*CCHO + 0.509*RCHO + 0.001*MEK + 0.059*PROD2 + 3.389*XC	# 1.188E-11
Cyclooctane	CYCC8 + HO. = 0.525*RO2-R. + 0.475*RO2-N. + 1.475*R2O2. + 0.001*CO + 0.525*RCHO + 3.573*XC	# 1.400E-11
Ethylcyclohexane	ET-CYCC6 + HO. = 0.624*RO2-R. + 0.376*RO2-N. + 1.046*R2O2. + 0.002*HCHO + 0.151*CCHO + 0.328*RCHO + 0.299*PROD2 + 2.662*XC	# 1.203E-11
Propyl Cyclopentane	PR-CYCC5 + HO. = 0.39*RO2-R. + 0.458*RO2-N. + 1.739*R2O2. + 0.152*RCO-O2. + 0.013*CO + 0.007*HCHO + 0.001*CCHO + 0.638*RCHO + 0.002*MEK + 0.027*PROD2 + 0.005*MGLY + 2.677*XC	# 8.685E-12
1,1,3-Trimethyl Cyclohex.	113MCYC6 + HO. = 0.484*RO2-R. + 0.512*RO2-N. + 1.581*R2O2. + 0.004*CCO-O2. + 0.073*CO + 0.132*HCHO + 0.107*CCHO + 0.473*RCHO + 0.042*ACET + 0.005*MEK + 0.103*PROD2 + 3.318*XC	# 8.700E-12
1-Eth.-4-Meth. Cyclohex.	1E4MCYC6 + HO. = 0.518*RO2-R. + 0.481*RO2-N. + 1.339*R2O2. + 0.001*CCO-O2. + 0.033*HCHO + 0.142*CCHO + 0.411*RCHO + 0.143*PROD2 + 3.703*XC	# 1.371E-11
Propyl Cyclohexane	C3-CYCC6 + HO. = 0.61*RO2-R. + 0.389*RO2-N. + 0.864*R2O2. + 0.001*RCO-O2. + 0.001*HCHO + 0.363*RCHO + 0.388*PROD2 + 3.242*XC	# 1.345E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
1,3-Diethyl-Cyclohexane	13DECYC6 + HO. = 0.49*RO2-R. + 0.51*RO2-N. + 1.249*R2O2. + 0.004*CO + 0.002*HCHO + 0.176*CCHO + 0.334*RCHO + 0.001*MEK + 0.165*PROD2 + 4.582*XC	# 1.553E-11
1,4-Diethyl-Cyclohexane	14DECYC6 + HO. = 0.508*RO2-R. + 0.49*RO2-N. + 1.229*R2O2. + 0.002*RCO-O2. + 0.021*HCHO + 0.226*CCHO + 0.333*RCHO + 0.209*PROD2 + 4.328*XC	# 1.553E-11
1-Meth.-3-Isopr. Cyclohex.	1M3IPCY6 + HO. = 0.535*RO2-R. + 0.46*RO2-N. + 1.204*R2O2. + 0.004*RCO-O2. + 0.006*CO + 0.008*HCHO + 0.005*CCHO + 0.263*RCHO + 0.339*ACET + 0.293*PROD2 + 3.634*XC	# 1.510E-11
Butyl Cyclohexane	C4-CYCC6 + HO. = 0.576*RO2-R. + 0.423*RO2-N. + 0.827*R2O2. + 0.024*CCHO + 0.179*RCHO + 0.467*PROD2 + 4.07*XC	# 1.487E-11
13-Dieth-5-Me. Cyclohex.	13E5MCC6 + HO. = 0.429*RO2-R. + 0.566*RO2-N. + 1.371*R2O2. + 0.003*CCO-O2. + 0.002*RCO-O2. + 0.006*CO + 0.02*HCHO + 0.168*CCHO + 0.355*RCHO + 0.009*MEK + 0.09*PROD2 + 5.587*XC	# 1.721E-11
1-Ethyl-2-Propyl Cyclohex.	1E2PCYC6 + HO. = 0.461*RO2-R. + 0.539*RO2-N. + 1.199*R2O2. + 0.001*RCO-O2. + 0.007*HCHO + 0.031*CCHO + 0.186*RCHO + 0.349*PROD2 + 5.045*XC	# 1.695E-11
Pentyl Cyclohexane	C5-CYCC6 + HO. = 0.557*RO2-R. + 0.443*RO2-N. + 0.808*R2O2. + 0.016*CCHO + 0.147*RCHO + 0.456*PROD2 + 5.135*XC	# 1.629E-11
1,3,5-Triethyl Cyclohex.	135ECYC6 + HO. = 0.417*RO2-R. + 0.58*RO2-N. + 1.353*R2O2. + 0.003*RCO-O2. + 0.005*CO + 0.014*HCHO + 0.221*CCHO + 0.315*RCHO + 0.008*MEK + 0.116*PROD2 + 6.373*XC	# 1.904E-11
1-Meth.-4-Pentyl Cyclohex.	1M4C5CY6 + HO. = 0.482*RO2-R. + 0.518*RO2-N. + 1.049*R2O2. + 0.001*CCO-O2. + 0.001*HCHO + 0.015*CCHO + 0.21*RCHO + 0.326*PROD2 + 6.274*XC	# 1.797E-11
Hexyl Cyclohexane	C6-CYCC6 + HO. = 0.527*RO2-R. + 0.473*RO2-N. + 0.849*R2O2. + 0.093*RCHO + 0.461*PROD2 + 6.118*XC	# 1.780E-11
13-Dieth-5-Pent Cyclohx.	13E5PCC6 + HO. = 0.433*RO2-R. + 0.564*RO2-N. + 1.237*R2O2. + 0.003*RCO-O2. + 0.002*CO + 0.01*HCHO + 0.132*CCHO + 0.342*RCHO + 0.002*MEK + 0.188*PROD2 + 7.163*XC	# 2.046E-11
1-Meth.-2-Hexyl-Cyclohex.	1M2C6CC6 + HO. = 0.462*RO2-R. + 0.537*RO2-N. + 1.08*R2O2. + 0.001*RCO-O2. + 0.004*HCHO + 0.009*CCHO + 0.128*RCHO + 0.38*PROD2 + 7.092*XC	# 1.939E-11
Heptyl Cyclohexane	C7-CYCC6 + HO. = 0.515*RO2-R. + 0.485*RO2-N. + 0.855*R2O2. + 0.069*RCHO + 0.462*PROD2 + 7.108*XC	# 1.913E-11
13-Diprop-5-Eth Cyclohx.	13P5ECC6 + HO. = 0.445*RO2-R. + 0.553*RO2-N. + 1.158*R2O2. + 0.002*RCO-O2. + 0.001*CO + 0.007*HCHO + 0.06*CCHO + 0.376*RCHO + 0.234*PROD2 + 8.017*XC	# 2.188E-11
1-Meth.-4-Heptyl Cyclohex.	1M4C7CC6 + HO. = 0.455*RO2-R. + 0.544*RO2-N. + 1.059*R2O2. + 0.001*HCHO + 0.131*RCHO + 0.349*PROD2 + 8.242*XC	# 2.081E-11
Octyl Cyclohexane	C8-CYCC6 + HO. = 0.511*RO2-R. + 0.489*RO2-N. + 0.847*R2O2. + 0.063*RCHO + 0.463*PROD2 + 8.099*XC	# 2.055E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
135-Tripropyl Cyclohex.	135PCYC6 + HO. = 0.453*RO2-R. + 0.545*RO2-N. + 1.106*R2O2. + 0.002*RCO-O2. + 0.001*CO + 0.005*HCHO + 0.415*RCHO + 0.258*PROD2 + 8.923*XC	# 2.330E-11
1-Methyl-2-Octyl Cyclohex.	1M2C8CC6 + HO. = 0.462*RO2-R. + 0.538*RO2-N. + 1.035*R2O2. + 0.003*HCHO + 0.008*CCHO + 0.105*RCHO + 0.394*PROD2 + 9.08*XC	# 2.223E-11
Nonyl Cyclohexane	C9-CYCC6 + HO. = 0.509*RO2-R. + 0.49*RO2-N. + 0.838*R2O2. + 0.058*RCHO + 0.465*PROD2 + 9.091*XC	# 2.197E-11
1,3-Prop.-5-Butyl Cyclohex.	13P5BCC6 + HO. = 0.461*RO2-R. + 0.538*RO2-N. + 1.045*R2O2. + 0.001*RCO-O2. + 0.001*CO + 0.003*HCHO + 0.013*CCHO + 0.322*RCHO + 0.318*PROD2 + 9.863*XC	# 2.472E-11
1-Methyl-4-Nonyl Cyclohex.	1M4C9CY6 + HO. = 0.458*RO2-R. + 0.541*RO2-N. + 1.018*R2O2. + 0.001*HCHO + 0.113*RCHO + 0.367*PROD2 + 10.209*XC	# 2.365E-11
Decyl Cyclohexane	C10CYCC6 + HO. = 0.508*RO2-R. + 0.492*RO2-N. + 0.834*R2O2. + 0.055*RCHO + 0.467*PROD2 + 10.085*XC	# 2.339E-11
Ethene	ETHENE + HO. = RO2-R. + 1.611*HCHO + 0.195*CCHO	# 1.960E-12@-438.
	ETHENE + O3 = 0.12*HO. + 0.12*HO2. + 0.5*CO + 0.13*CO2 + HCHO + 0.37*HCOOH	# 9.140E-15@2580.
	ETHENE + NO3 = RO2-R. + RCHO + -1*XC + XN	# 4.390E-13^2.00@2282.
	ETHENE + O3P = 0.5*HO2. + 0.2*RO2-R. + 0.3*C-O2. + 0.491*CO + 0.191*HCHO + 0.25*CCHO + 0.009*GLY + 0.25*INERT + 0.25*XC	# 1.040E-11@792.
Propene	PROPENE + HO. = 0.984*RO2-R. + 0.016*RO2-N. + 0.984*HCHO + 0.984*CCHO + -0.048*XC	# 4.850E-12@-504.
	PROPENE + O3 = 0.32*HO. + 0.06*HO2. + 0.26*C-O2. + 0.51*CO + 0.135*CO2 + 0.5*HCHO + 0.5*CCHO + 0.185*HCOOH + 0.17*CCO-OH + 0.07*INERT + 0.07*XC	# 5.510E-15@1878.
	PROPENE + NO3 = 0.949*RO2-R. + 0.051*RO2-N. + 2.693*XC + XN	# 4.590E-13@1156.
	PROPENE + O3P = 0.45*RCHO + 0.55*MEK + -0.55*XC	# 1.180E-11@324.
1-Butene	1-BUTENE + HO. = 0.975*RO2-R. + 0.025*RO2-N. + 0.006*R2O2. + 0.969*HCHO + 0.975*RCHO + -0.045*XC	# 6.550E-12@-467.
	1-BUTENE + O3 = 0.116*HO. + 0.06*HO2. + 0.057*RO2-R. + 0.306*CO + 0.065*CO2 + 0.5*HCHO + 0.057*CCHO + 0.5*RCHO + 0.185*HCOOH + 0.444*RCO-OH	# 3.360E-15@1744.
	1-BUTENE + NO3 = 0.92*RO2-R. + 0.08*RO2-N. + 0.075*R2O2. + 0.075*CCHO + 0.075*RCHO + 0.844*RNO3 + -1.925*XC + 0.156*XN	# 3.140E-13@938.
	1-BUTENE + O3P = 0.45*RCHO + 0.55*MEK + 0.45*XC	# 1.250E-11@326.
1-Pentene	1-PENTEN + HO. = 0.927*RO2-R. + 0.073*RO2-N. + 0.121*R2O2. + 0.814*HCHO + 0.907*RCHO + 0.021*PROD2 + 0.906*XC	# 5.860E-12@-500.
	1-PENTEN + O3 = 0.101*HO. + 0.06*HO2. + 0.04*RO2-R. + 0.001*RO2-N. + 0.291*CO + 0.065*CO2 + 0.5*HCHO + 0.54*RCHO + 0.185*HCOOH + 0.46*RCO-OH + 0.955*XC	# 3.360E-15@1734.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	1-PENTEN + NO3 = 0.834*RO2-R. + 0.166*RO2-N. + 0.781*R2O2. + 0.033*RCHO + 0.818*RNO3 + -1.001*XC + 0.182*XN	# 1.380E-14
	1-PENTEN + O3P = 0.45*RCHO + 0.55*MEK + 1.45*XC	# 1.480E-11@345.
3-Methyl-1-Butene	3M-1-BUT + HO. = 0.928*RO2-R. + 0.072*RO2-N. + 0.174*R2O2. + 0.749*HCHO + 0.174*CCHO + 0.749*RCHO + 0.167*ACET + 0.012*PROD2 + 0.651*XC	# 5.320E-12@-533.
	3M-1-BUT + O3 = 0.101*HO. + 0.06*HO2. + 0.039*RO2-R. + 0.002*RO2-N. + 0.291*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.039*ACET + 0.185*HCOOH + 0.46*RCO-OH + 0.953*XC	# 3.360E-15@1705.
	3M-1-BUT + NO3 = 0.851*RO2-R. + 0.149*RO2-N. + 0.827*R2O2. + 0.827*RCHO + 0.794*ACET + 0.057*RNO3 + -1.099*XC + 0.943*XN	# 1.380E-14
	3M-1-BUT + O3P = 0.45*RCHO + 0.55*MEK + 1.45*XC	# 1.320E-11@345.
1-Hexene	1-HEXENE + HO. = 0.904*RO2-R. + 0.096*RO2-N. + 0.419*R2O2. + 0.526*HCHO + 0.635*RCHO + 0.269*PROD2 + 1.38*XC	# 6.910E-12@-500.
	1-HEXENE + O3 = 0.085*HO. + 0.041*HO2. + 0.042*RO2-R. + 0.002*RO2-N. + 0.275*CO + 0.065*CO2 + 0.5*HCHO + 0.523*RCHO + 0.475*PROD2 + 0.185*HCOOH + 0.545*XC	# 3.360E-15@1705.
	1-HEXENE + NO3 = 0.763*RO2-R. + 0.237*RO2-N. + 0.845*R2O2. + 0.763*RNO3 + 0.237*XN	# 1.380E-14
	1-HEXENE + O3P = 0.45*RCHO + 0.55*MEK + 2.45*XC	# 1.480E-11@345.
3,3-Dimethyl-1-Butene	33M1-BUT + HO. = 0.372*RO2-R. + 0.119*RO2-N. + 1.044*R2O2. + 0.509*TBU-O. + 0.369*HCHO + 0.53*CCHO + 0.371*RCHO + 0.001*ACET + 1.213*XC	# 5.230E-12@-500.
	33M1-BUT + O3 = 0.085*HO. + 0.036*HO2. + 0.024*RO2-R. + 0.001*RO2-N. + 0.024*TBU-O. + 0.275*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.185*HCOOH + 0.475*RCO-OH + 1.972*XC	# 3.360E-15@1928.
	33M1-BUT + NO3 = 0.188*RO2-N. + 1.658*R2O2. + 0.812*TBU-O. + 0.845*RCHO + -0.1*XC + XN	# 1.380E-14
	33M1-BUT + O3P = 0.45*RCHO + 0.55*MEK + 2.45*XC	# 4.387E-12
3-Methyl-1-Pentene	3M1-C5E + HO. = 0.89*RO2-R. + 0.11*RO2-N. + 0.178*R2O2. + 0.761*HCHO + 0.161*CCHO + 0.785*RCHO + 0.045*MEK + 0.023*PROD2 + 1.581*XC	# 3.160E-11
	3M1-C5E + O3 = 0.085*HO. + 0.051*HO2. + 0.032*RO2-R. + 0.002*RO2-N. + 0.275*CO + 0.065*CO2 + 0.5*HCHO + 0.018*CCHO + 0.5*RCHO + 0.014*MEK + 0.475*PROD2 + 0.185*HCOOH + 0.521*XC	# 3.360E-15@1946.
	3M1-C5E + NO3 = 0.776*RO2-R. + 0.224*RO2-N. + 1.049*R2O2. + 0.454*CCHO + 0.626*RCHO + 0.348*MEK + 0.201*RNO3 + -0.726*XC + 0.799*XN	# 1.380E-14
	3M1-C5E + O3P = 0.45*RCHO + 0.55*PROD2 + 1.35*XC	# 5.604E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
4-Methyl-1-Pentene	4M1-C5E + HO. = 0.884*RO2-R. + 0.116*RO2-N. + 0.189*R2O2. + 0.717*HCHO + 0.001*CCHO + 0.846*RCHO + 0.001*ACET + 0.037*PROD2 + 1.822*XC	# 3.160E-11
	4M1-C5E + O3 = 0.085*HO. + 0.051*HO2. + 0.032*RO2-R. + 0.001*RO2-N. + 0.275*CO + 0.065*CO2 + 0.509*HCHO + 0.515*RCHO + 0.008*ACET + 0.475*PROD2 + 0.185*HCOOH + 0.537*XC	# 3.360E-15@1758.
	4M1-C5E + NO3 = 0.769*RO2-R. + 0.231*RO2-N. + 0.8*R2O2. + 0.006*HCHO + 0.029*RCHO + 0.006*ACET + 0.752*RNO3 + -0.009*XC + 0.248*XN	# 1.380E-14
	4M1-C5E + O3P = 0.45*RCHO + 0.55*MEK + 2.45*XC	# 5.604E-12
1-Heptene	1-HEPTEN + HO. = 0.807*RO2-R. + 0.193*RO2-N. + 0.426*R2O2. + 0.439*HCHO + 0.536*RCHO + 0.271*PROD2 + 2.169*XC	# 7.470E-12@-500.
	1-HEPTEN + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 1.5*XC	# 3.360E-15@1679.
	1-HEPTEN + NO3 = 0.7*RO2-R. + 0.3*RO2-N. + 0.809*R2O2. + 0.7*RNO3 + XC + 0.3*XN	# 1.380E-14
	1-HEPTEN + O3P = 0.45*RCHO + 0.55*PROD2 + 2.35*XC	# 8.525E-12
1-Octene	1-OCTENE + HO. = 0.754*RO2-R. + 0.246*RO2-N. + 0.418*R2O2. + 0.42*HCHO + 0.497*RCHO + 0.257*PROD2 + 3.07*XC	# 3.160E-11
	1-OCTENE + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 2.5*XC	# 3.360E-15@1633.
	1-OCTENE + NO3 = 0.645*RO2-R. + 0.355*RO2-N. + 0.781*R2O2. + 0.645*RNO3 + 2*XC + 0.355*XN	# 1.380E-14
	1-OCTENE + O3P = 0.45*RCHO + 0.55*PROD2 + 3.35*XC	# 5.604E-12
1-Nonene	1-C9E + HO. = 0.708*RO2-R. + 0.292*RO2-N. + 0.417*R2O2. + 0.403*HCHO + 0.471*RCHO + 0.237*PROD2 + 4.009*XC	# 3.160E-11
	1-C9E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 3.5*XC	# 1.010E-17
	1-C9E + NO3 = 0.597*RO2-R. + 0.403*RO2-N. + 0.794*R2O2. + 0.597*RNO3 + 3*XC + 0.403*XN	# 1.380E-14
	1-C9E + O3P = 0.45*RCHO + 0.55*PROD2 + 4.35*XC	# 5.604E-12
1-Decene	1-C10E + HO. = 0.676*RO2-R. + 0.324*RO2-N. + 0.408*R2O2. + 0.391*HCHO + 0.455*RCHO + 0.222*PROD2 + 4.973*XC	# 3.160E-11
	1-C10E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 4.5*XC	# 3.360E-15@1755.
	1-C10E + NO3 = 0.567*RO2-R. + 0.433*RO2-N. + 0.791*R2O2. + 0.567*RNO3 + 4*XC + 0.433*XN	# 1.380E-14
	1-C10E + O3P = 0.45*RCHO + 0.55*PROD2 + 5.35*XC	# 5.604E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
1-Undecene	1-C11E + HO. = 0.657*RO2-R. + 0.343*RO2-N. + 0.399*R2O2. + 0.383*HCHO + 0.444*RCHO + 0.212*PROD2 + 5.949*XC	# 3.160E-11
	1-C11E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 5.5*XC	# 1.010E-17
	1-C11E + NO3 = 0.55*RO2-R. + 0.45*RO2-N. + 0.782*R2O2. + 0.55*RNO3 + 5*XC + 0.45*XN	# 1.380E-14
	1-C11E + O3P = 0.45*RCHO + 0.55*PROD2 + 6.35*XC	# 5.604E-12
1-Dodecene	1-C12E + HO. = 0.644*RO2-R. + 0.356*RO2-N. + 0.395*R2O2. + 0.379*HCHO + 0.438*RCHO + 0.207*PROD2 + 6.935*XC	# 3.160E-11
	1-C12E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 6.5*XC	# 1.010E-17
	1-C12E + NO3 = 0.539*RO2-R. + 0.461*RO2-N. + 0.778*R2O2. + 0.539*RNO3 + 6*XC + 0.461*XN	# 1.380E-14
	1-C12E + O3P = 0.45*RCHO + 0.55*PROD2 + 7.35*XC	# 5.604E-12
1-Tridecene	1-C13E + HO. = 0.637*RO2-R. + 0.363*RO2-N. + 0.392*R2O2. + 0.376*HCHO + 0.434*RCHO + 0.203*PROD2 + 7.926*XC	# 3.160E-11
	1-C13E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 7.5*XC	# 1.010E-17
	1-C13E + NO3 = 0.532*RO2-R. + 0.468*RO2-N. + 0.775*R2O2. + 0.532*RNO3 + 7*XC + 0.468*XN	# 1.380E-14
	1-C13E + O3P = 0.45*RCHO + 0.55*PROD2 + 8.35*XC	# 5.604E-12
1-Tetradecene	1-C14E + HO. = 0.632*RO2-R. + 0.368*RO2-N. + 0.39*R2O2. + 0.374*HCHO + 0.432*RCHO + 0.201*PROD2 + 8.921*XC	# 3.160E-11
	1-C14E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 8.5*XC	# 1.010E-17
	1-C14E + NO3 = 0.528*RO2-R. + 0.472*RO2-N. + 0.773*R2O2. + 0.528*RNO3 + 8*XC + 0.472*XN	# 1.380E-14
	1-C14E + O3P = 0.45*RCHO + 0.55*PROD2 + 9.35*XC	# 5.604E-12
1-Pentadecene	1-C15E + HO. = 0.629*RO2-R. + 0.371*RO2-N. + 0.388*R2O2. + 0.372*HCHO + 0.43*RCHO + 0.2*PROD2 + 9.917*XC	# 3.160E-11
	1-C15E + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*RCHO + 0.5*PROD2 + 0.185*HCOOH + 9.5*XC	# 1.010E-17
	1-C15E + NO3 = 0.525*RO2-R. + 0.475*RO2-N. + 0.771*R2O2. + 0.525*RNO3 + 9*XC + 0.475*XN	# 1.380E-14
	1-C15E + O3P = 0.45*RCHO + 0.55*PROD2 + 10.35*XC	# 5.604E-12
Isobutene	ISOBUTEN + HO. = 0.9*RO2-R. + 0.1*RO2-N. + 0.9*HCHO + 0.9*ACET + -0.2*XC	# 9.470E-12@-504.
	ISOBUTEN + O3 = 0.707*HO. + 0.04*RO2-R. + 0.627*R2O2. + 0.667*CCO-O2. + 0.167*CO + 0.043*CO2 + 1.333*HCHO + 0.333*ACET + 0.123*HCOOH	# 2.700E-15@1632.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	ISOBUTEN + NO3 = 0.644*NO2 + 0.039*RO2-N. + 0.961*R2O2. + 0.316*C-O2. + 0.644*HCHO + 0.644*ACET + 0.87*XC + 0.356*XN	# 3.320E-13
	ISOBUTEN + O3P = 0.4*RCHO + 0.6*MEK + 0.4*XC	# 1.690E-11
2-Methyl-1-Butene	2M-1-BUT + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*HCHO + 0.935*MEK + -0.065*XC	# 1.140E-11@-500.
	2M-1-BUT + O3 = 0.707*HO. + 0.04*RO2-R. + 0.026*RO2-N. + 0.6*R2O2. + 0.558*CCO-O2. + 0.082*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.749*HCHO + 0.558*CCHO + 0.333*MEK + 0.123*HCOOH + -0.053*XC	# 2.700E-15@1528.
	2M-1-BUT + NO3 = 0.019*NO2 + 0.916*RO2-R. + 0.065*RO2-N. + 0.935*R2O2. + 0.019*HCHO + 0.916*CCHO + 0.019*MEK + 2.682*XC + 0.981*XN	# 3.320E-13
	2M-1-BUT + O3P = 0.4*RCHO + 0.6*MEK + 1.4*XC	# 1.875E-11
23-Dimethyl-1-Butene	23M1-BUT + HO. = 0.899*RO2-R. + 0.101*RO2-N. + 0.074*R2O2. + 0.828*HCHO + 0.071*ACET + 0.902*MEK + 0.746*XC	# 5.790E-11
	23M1-BUT + O3 = 0.707*HO. + 0.04*RO2-R. + 0.043*RO2-N. + 0.583*R2O2. + 0.582*CCO-O2. + 0.042*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.708*HCHO + 0.582*ACET + 0.333*MEK + 0.123*HCOOH + 0.332*XC	# 2.700E-15@1590.
	23M1-BUT + NO3 = 0.866*RO2-R. + 0.134*RO2-N. + 0.902*R2O2. + 0.866*ACET + 2.599*XC + XN	# 3.320E-13
	23M1-BUT + O3P = 0.4*RCHO + 0.6*MEK + 2.4*XC	# 1.733E-11
2-Ethyl-1-Butene	2E1-BUT + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*HCHO + 0.902*MEK + 0.902*XC	# 5.790E-11
	2E1-BUT + O3 = 0.707*HO. + 0.04*RO2-R. + 0.043*RO2-N. + 0.583*R2O2. + 0.623*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.667*HCHO + 0.623*CCHO + 0.333*MEK + 0.123*HCOOH + 0.29*XC	# 2.700E-15@1590.
	2E1-BUT + NO3 = 0.009*NO2 + 0.893*RO2-R. + 0.098*RO2-N. + 0.902*R2O2. + 0.009*HCHO + 0.893*CCHO + 0.009*MEK + 0.893*RNO3 + -1.776*XC + 0.098*XN	# 3.320E-13
	2E1-BUT + O3P = 0.4*RCHO + 0.6*MEK + 2.4*XC	# 1.733E-11
2-Methyl-1-Pentene	2M1-C5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*HCHO + 0.902*MEK + 0.902*XC	# 1.180E-11@-500.
	2M1-C5E + O3 = 0.707*HO. + 0.04*RO2-R. + 0.043*RO2-N. + 0.583*R2O2. + 0.556*CCO-O2. + 0.067*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.734*HCHO + 0.556*RCHO + 0.333*MEK + 0.123*HCOOH + 0.357*XC	# 2.700E-15@1547.
	2M1-C5E + NO3 = 0.827*RO2-R. + 0.173*RO2-N. + 0.902*R2O2. + 0.827*RCHO + 2.48*XC + XN	# 3.320E-13
	2M1-C5E + O3P = 0.4*RCHO + 0.6*MEK + 2.4*XC	# 1.999E-11
2,3,3-trimethyl-1-Butene	233M1BUT + HO. = 0.082*RO2-R. + 0.166*RO2-N. + 1.534*R2O2. + 0.752*TBU-O. + 0.082*HCHO + 0.865*MEK + 0.207*XC	# 5.790E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	233M1BUT + O3 = 0.707*HO. + 0.04*RO2-R. + 0.065*RO2-N. + 0.562*R2O2. + 0.602*RCO-O2. + 0.167*CO + 0.043*CO2 + 1.268*HCHO + 0.333*MEK + 0.123*HCOOH + 1.87*XC	# 2.700E-15@1724.
	233M1BUT + NO3 = 0.169*RO2-N. + 1.696*R2O2. + 0.831*TBU-O. + 3.492*XC + XN	# 3.320E-13
	233M1BUT + O3P = 0.4*RCHO + 0.6*MEK + 3.4*XC	# 1.733E-11
3-Methyl-2-Isopropyl-1-Butene	3M2I1C4E + HO. = 0.822*RO2-R. + 0.178*RO2-N. + 0.125*R2O2. + 0.701*HCHO + 0.12*ACET + 0.827*PROD2 + 0.908*XC	# 5.790E-11
	3M2I1C4E + O3 = 0.707*HO. + 0.04*RO2-R. + 0.09*RO2-N. + 0.537*R2O2. + 0.577*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.667*HCHO + 0.577*ACET + 0.333*PROD2 + 0.123*HCOOH + XC	# 2.700E-15@1999.
	3M2I1C4E + NO3 = 0.794*RO2-R. + 0.206*RO2-N. + 0.827*R2O2. + 0.794*ACET + 0.827*RNO3 + -0.579*XC + 0.173*XN	# 3.320E-13
	3M2I1C4E + O3P = 0.4*RCHO + 0.6*PROD2 + 3.2*XC	# 1.733E-11
cis-2-Butene	C-2-BUTE + HO. = 0.965*RO2-R. + 0.035*RO2-N. + 1.93*CCHO + -0.07*XC	# 1.100E-11@-487.
	C-2-BUTE + O3 = 0.52*HO. + 0.52*C-O2. + 0.52*CO + 0.14*CO2 + CCHO + 0.34*CCO-OH + 0.14*INERT + 0.14*XC	# 3.220E-15@968.
	C-2-BUTE + NO3 = 0.705*NO2 + 0.215*RO2-R. + 0.08*RO2-N. + 0.705*R2O2. + 1.41*CCHO + 0.215*RNO3 + -0.59*XC + 0.08*XN	# 1.100E-13@-346.
	C-2-BUTE + O3P = MEK	# 1.760E-11
trans-2-Butene	T-2-BUTE + HO. = 0.965*RO2-R. + 0.035*RO2-N. + 1.93*CCHO + -0.07*XC	# 1.010E-11@-550.
	T-2-BUTE + O3 = 0.52*HO. + 0.52*C-O2. + 0.52*CO + 0.14*CO2 + CCHO + 0.34*CCO-OH + 0.14*INERT + 0.14*XC	# 6.640E-15@1059.
	T-2-BUTE + NO3 = 0.705*NO2 + 0.215*RO2-R. + 0.08*RO2-N. + 0.705*R2O2. + 1.41*CCHO + 0.215*RNO3 + -0.59*XC + 0.08*XN	# 1.100E-13^2.00@-382.
	T-2-BUTE + O3P = MEK	# 2.180E-11
2-Methyl-2-Butene	2M-2-BUT + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*CCHO + 0.935*ACET + -0.065*XC	# 1.920E-11@-450.
	2M-2-BUT + O3 = 0.856*HO. + 0.7*R2O2. + 0.156*C-O2. + 0.7*CCO-O2. + 0.156*CO + 0.042*CO2 + 0.7*HCHO + 0.7*CCHO + 0.3*ACET + 0.102*CCO-OH + 0.042*INERT + 0.042*XC	# 2.870E-15@585.
	2M-2-BUT + NO3 = 0.935*NO2 + 0.065*RO2-N. + 0.935*R2O2. + 0.935*CCHO + 0.935*ACET + -0.065*XC + 0.065*XN	# 9.370E-12
	2M-2-BUT + O3P = MEK + XC	# 5.100E-11
cis-2-Pentene	C-2-PENT + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*CCHO + 0.935*RCHO + -0.065*XC	# 1.210E-11@-500.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	C-2-PENT + O3 = 0.317*HO. + 0.057*RO2-R. + 0.26*C-O2. + 0.317*CO + 0.07*CO2 + 0.556*CCHO + 0.5*RCHO + 0.17*CCO-OH + 0.444*RCO-OH + 0.07*INERT + 0.07*XC	# 1.150E-16
	C-2-PENT + NO3 = 0.471*NO2 + 0.395*RO2-R. + 0.134*RO2-N. + 0.753*R2O2. + 0.481*CCHO + 0.481*RCHO + 0.386*RNO3 + -0.519*XC + 0.143*XN	# 3.700E-13
	C-2-PENT + O3P = MEK + XC	# 1.700E-11
trans-2-Pentene	T-2-PENT + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*CCHO + 0.935*RCHO + -0.065*XC	# 1.250E-11@-500.
	T-2-PENT + O3 = 0.317*HO. + 0.057*RO2-R. + 0.26*C-O2. + 0.317*CO + 0.07*CO2 + 0.556*CCHO + 0.5*RCHO + 0.17*CCO-OH + 0.444*RCO-OH + 0.07*INERT + 0.07*XC	# 1.150E-16
	T-2-PENT + NO3 = 0.471*NO2 + 0.395*RO2-R. + 0.134*RO2-N. + 0.753*R2O2. + 0.481*CCHO + 0.481*RCHO + 0.386*RNO3 + -0.519*XC + 0.143*XN	# 3.700E-13
	T-2-PENT + O3P = MEK + XC	# 2.226E-11
2,3-Dimethyl-2-Butene	23M2-BUT + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 1.805*ACET	# 2.050E-11@-500.
	23M2-BUT + O3 = HO. + R2O2. + CCO-O2. + HCHO + ACET	# 3.030E-15@294.
	23M2-BUT + NO3 = 0.902*NO2 + 0.098*RO2-N. + 0.902*R2O2. + 1.805*ACET + 0.098*XN	# 5.720E-11
	23M2-BUT + O3P = MEK + 2*XC	# 7.640E-11
2-Methyl-2-Pentene	2M-2-C5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*RCHO + 0.902*ACET	# 1.660E-11@-500.
	2M-2-C5E + O3 = 0.734*HO. + 0.034*RO2-R. + 0.7*R2O2. + 0.7*CCO-O2. + 0.034*CO + 0.7*HCHO + 0.034*CCHO + 0.7*RCHO + 0.3*ACET + 0.266*RCO-OH	# 3.480E-16
	2M-2-C5E + NO3 = 0.391*NO2 + 0.46*RO2-R. + 0.149*RO2-N. + 0.92*R2O2. + 0.016*HCHO + 0.845*RCHO + 0.391*ACET + 0.006*RNO3 + 1.346*XC + 0.602*XN	# 9.370E-12
	2M-2-C5E + O3P = MEK + 2*XC	# 3.777E-11
Cis-2-Hexene	C-2-C6E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*CCHO + 0.902*RCHO + 0.902*XC	# 6.340E-11
	C-2-C6E + O3 = 0.301*HO. + 0.04*RO2-R. + 0.001*RO2-N. + 0.26*C-O2. + 0.301*CO + 0.07*CO2 + 0.5*CCHO + 0.54*RCHO + 0.17*CCO-OH + 0.46*RCO-OH + 0.07*INERT + 1.025*XC	# 1.150E-16
	C-2-C6E + NO3 = 0.12*NO2 + 0.659*RO2-R. + 0.221*RO2-N. + 0.807*R2O2. + 0.12*CCHO + 0.134*RCHO + 0.652*RNO3 + 0.12*XC + 0.228*XN	# 3.700E-13
	C-2-C6E + O3P = 0.76*MEK + 0.24*PROD2 + 1.52*XC	# 2.052E-11
Cis-3-Hexene	C-3-C6E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 1.805*RCHO	# 6.340E-11
	C-3-C6E + O3 = 0.113*HO. + 0.113*RO2-R. + 0.113*CO + 0.113*CCHO + RCHO + 0.887*RCO-OH	# 3.220E-15@914.
	C-3-C6E + NO3 = 0.284*NO2 + 0.514*RO2-R. + 0.202*RO2-N. + 0.774*R2O2. + 0.567*RCHO + 0.514*RNO3 + 0.202*XN	# 3.700E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	C-3-C6E + O3P = 0.76*MEK + 0.24*PROD2 + 1.52*XC	# 2.052E-11
Cis-3-Methyl-2-Hexene	C3M2-C5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*CCHO + 0.902*MEK	# 8.710E-11
	C3M2-C5E + O3 = 0.856*HO. + 0.028*RO2-N. + 0.672*R2O2. + 0.156*C-O2. + 0.586*CCO-O2. + 0.087*RCO-O2. + 0.156*CO + 0.042*CO2 + 0.087*HCHO + 1.286*CCHO + 0.3*MEK + 0.102*CCO-OH + 0.042*INERT + -0.013*XC	# 2.870E-15@552.
	C3M2-C5E + NO3 = 0.872*NO2 + 0.03*RO2-R. + 0.098*RO2-N. + 0.902*R2O2. + 0.902*CCHO + 0.872*MEK + 0.03*RNO3 + -0.06*XC + 0.098*XN	# 9.370E-12
	C3M2-C5E + O3P = 0.6*MEK + 0.4*PROD2 + 1.2*XC	# 3.709E-11
Trans-2-Hexene	T-2-C6E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*CCHO + 0.902*RCHO + 0.902*XC	# 6.340E-11
	T-2-C6E + O3 = 0.301*HO. + 0.04*RO2-R. + 0.001*RO2-N. + 0.26*C-O2. + 0.301*CO + 0.07*CO2 + 0.5*CCHO + 0.54*RCHO + 0.17*CCO-OH + 0.46*RCO-OH + 0.07*INERT + 1.025*XC	# 1.150E-16
	T-2-C6E + NO3 = 0.12*NO2 + 0.659*RO2-R. + 0.221*RO2-N. + 0.807*R2O2. + 0.12*CCHO + 0.134*RCHO + 0.652*RNO3 + 0.12*XC + 0.228*XN	# 3.700E-13
	T-2-C6E + O3P = 0.76*MEK + 0.24*PROD2 + 1.52*XC	# 2.052E-11
Trans-3-Hexene	T-3-C6E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 1.805*RCHO	# 6.340E-11
	T-3-C6E + O3 = 0.113*HO. + 0.113*RO2-R. + 0.113*CO + 0.113*CCHO + RCHO + 0.887*RCO-OH	# 6.640E-15@1092.
	T-3-C6E + NO3 = 0.284*NO2 + 0.514*RO2-R. + 0.202*RO2-N. + 0.774*R2O2. + 0.567*RCHO + 0.514*RNO3 + 0.202*XN	# 3.700E-13
	T-3-C6E + O3P = 0.76*MEK + 0.24*PROD2 + 1.52*XC	# 2.052E-11
Trans 3-Methyl-2-Hexene	T3M2-C5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*CCHO + 0.902*MEK	# 8.710E-11
	T3M2-C5E + O3 = 0.856*HO. + 0.028*RO2-N. + 0.672*R2O2. + 0.156*C-O2. + 0.586*CCO-O2. + 0.087*RCO-O2. + 0.156*CO + 0.042*CO2 + 0.087*HCHO + 1.286*CCHO + 0.3*MEK + 0.102*CCO-OH + 0.042*INERT + -0.013*XC	# 2.870E-15@487.
	T3M2-C5E + NO3 = 0.872*NO2 + 0.03*RO2-R. + 0.098*RO2-N. + 0.902*R2O2. + 0.902*CCHO + 0.872*MEK + 0.03*RNO3 + -0.06*XC + 0.098*XN	# 9.370E-12
	T3M2-C5E + O3P = 0.6*MEK + 0.4*PROD2 + 1.2*XC	# 3.709E-11
Trans 4-Methyl-2-Hexene	T4M2-C5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.017*R2O2. + 0.885*CCHO + 0.902*RCHO + 0.016*ACET + 0.883*XC	# 1.140E-11@-500.
	T4M2-C5E + O3 = 0.301*HO. + 0.039*RO2-R. + 0.002*RO2-N. + 0.26*C-O2. + 0.301*CO + 0.07*CO2 + 0.5*CCHO + 0.5*RCHO + 0.039*ACET + 0.17*CCO-OH + 0.46*RCO-OH + 0.07*INERT + 1.023*XC	# 1.150E-16
	T4M2-C5E + NO3 = 0.197*NO2 + 0.611*RO2-R. + 0.192*RO2-N. + 0.807*R2O2. + 0.197*CCHO + 0.585*RCHO + 0.373*ACET + 0.238*RNO3 + 0.151*XC + 0.564*XN	# 3.700E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	T4M2-C5E + O3P = 0.88*MEK + 0.12*PROD2 + 1.76*XC	# 1.875E-11
2,3-Dimethyl-2-Hexene	23M2-C5E + HO. = 0.865*RO2-R. + 0.135*RO2-N. + 0.865*ACET + 0.865*MEK + 0.135*XC	# 1.920E-11@-500.
	23M2-C5E + O3 = HO. + 0.02*RO2-N. + 0.98*R2O2. + 0.918*CCO-O2. + 0.062*RCO-O2. + 0.562*HCHO + 0.418*CCHO + 0.5*ACET + 0.5*MEK + -0.039*XC	# 6.740E-16
	23M2-C5E + NO3 = 0.865*NO2 + 0.135*RO2-N. + 0.865*R2O2. + 0.865*ACET + 0.865*MEK + 0.135*XC + 0.135*XN	# 5.720E-11
	23M2-C5E + O3P = MEK + 3*XC	# 4.953E-11
Cis-3-Heptene	C-3-C7E + HO. = 0.865*RO2-R. + 0.135*RO2-N. + 1.73*RCHO + XC	# 6.340E-11
	C-3-C7E + O3 = 0.098*HO. + 0.097*RO2-R. + 0.001*RO2-N. + 0.098*CO + 0.057*CCHO + 1.04*RCHO + 0.903*RCO-OH + 0.955*XC	# 1.150E-16
	C-3-C7E + NO3 = 0.082*NO2 + 0.632*RO2-R. + 0.286*RO2-N. + 0.787*R2O2. + 0.163*RCHO + 0.632*RNO3 + XC + 0.286*XN	# 3.700E-13
	C-3-C7E + O3P = PROD2 + XC	# 2.052E-11
Trans-2-Heptene	T-2-C7E + HO. = 0.864*RO2-R. + 0.136*RO2-N. + 0.005*R2O2. + 0.859*CCHO + 0.859*RCHO + 0.005*PROD2 + 1.859*XC	# 1.270E-11@-500.
	T-2-C7E + O3 = 0.285*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.26*C-O2. + 0.285*CO + 0.07*CO2 + 0.5*CCHO + 0.523*RCHO + 0.475*PROD2 + 0.17*CCO-OH + 0.07*INERT + 0.615*XC	# 1.150E-16
	T-2-C7E + NO3 = 0.013*NO2 + 0.689*RO2-R. + 0.299*RO2-N. + 0.809*R2O2. + 0.013*CCHO + 0.013*RCHO + 0.689*RNO3 + 1.013*XC + 0.299*XN	# 3.700E-13
	T-2-C7E + O3P = PROD2 + XC	# 2.293E-11
Trans-3-Heptene	T-3-C7E + HO. = 0.865*RO2-R. + 0.135*RO2-N. + 1.73*RCHO + XC	# 6.340E-11
	T-3-C7E + O3 = 0.098*HO. + 0.097*RO2-R. + 0.001*RO2-N. + 0.098*CO + 0.057*CCHO + 1.04*RCHO + 0.903*RCO-OH + 0.955*XC	# 1.150E-16
	T-3-C7E + NO3 = 0.082*NO2 + 0.632*RO2-R. + 0.286*RO2-N. + 0.787*R2O2. + 0.163*RCHO + 0.632*RNO3 + XC + 0.286*XN	# 3.700E-13
	T-3-C7E + O3P = PROD2 + XC	# 2.052E-11
Trans 4,4-dimethyl-2-Pentene	T44M2C5E + HO. = 0.516*RO2-R. + 0.149*RO2-N. + 0.684*R2O2. + 0.335*TBU-O. + 0.516*CCHO + 0.865*RCHO + 1.475*XC	# 1.030E-11@-500.
	T44M2C5E + O3 = 0.285*HO. + 0.001*RO2-N. + 0.024*R2O2. + 0.26*C-O2. + 0.024*TBU-O. + 0.285*CO + 0.07*CO2 + 0.5*CCHO + 0.5*RCHO + 0.17*CCO-OH + 0.475*RCO-OH + 0.07*INERT + 2.042*XC	# 1.150E-16
	T44M2C5E + NO3 = 0.163*NO2 + 0.205*RO2-R. + 0.243*RO2-N. + 1.234*R2O2. + 0.389*TBU-O. + 0.026*HCHO + 0.142*CCHO + 0.569*RCHO + 0.022*ACET + 0.204*RNO3 + 1.07*XC + 0.633*XN	# 3.700E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	T44M2C5E + O3P = MEK + 3*XC	# 1.552E-11
Cis-4-Octene	C-4-C8E + HO. = 0.827*RO2-R. + 0.173*RO2-N. + 1.653*RCHO + 2*XC	# 6.340E-11
	C-4-C8E + O3 = 0.082*HO. + 0.08*RO2-R. + 0.002*RO2-N. + 0.082*CO + 1.08*RCHO + 0.919*RCO-OH + 1.91*XC	# 3.220E-15@1050.
	C-4-C8E + NO3 = 0.014*NO2 + 0.634*RO2-R. + 0.352*RO2-N. + 0.781*R2O2. + 0.028*RCHO + 0.634*RNO3 + 2*XC + 0.352*XN	# 3.700E-13
	C-4-C8E + O3P = PROD2 + 2*XC	# 2.052E-11
Trans 2,2-Dimethyl 3-Hexene	T22M3C6E + HO. = 0.432*RO2-R. + 0.189*RO2-N. + 0.773*R2O2. + 0.379*TBU-O. + 1.259*RCHO + 1.953*XC	# 6.340E-11
	T22M3C6E + O3 = 0.082*HO. + 0.057*RO2-R. + 0.001*RO2-N. + 0.024*R2O2. + 0.024*TBU-O. + 0.082*CO + 0.057*CCHO + RCHO + 0.918*RCO-OH + 1.972*XC	# 6.640E-15@1509.
	T22M3C6E + NO3 = 0.154*NO2 + 0.193*RO2-R. + 0.278*RO2-N. + 1.175*R2O2. + 0.375*TBU-O. + 0.017*HCHO + 0.011*CCHO + 0.706*RCHO + 0.002*ACET + 0.183*RNO3 + 1.948*XC + 0.664*XN	# 3.700E-13
	T22M3C6E + O3P = 0.88*MEK + 0.12*PROD2 + 3.76*XC	# 2.052E-11
Trans 2,5-Dimethyl 3-Hexene	T25M3C6E + HO. = 0.827*RO2-R. + 0.173*RO2-N. + 1.653*RCHO + 2*XC	# 6.340E-11
	T25M3C6E + O3 = 0.082*HO. + 0.079*RO2-R. + 0.003*RO2-N. + 0.082*CO + RCHO + 0.079*ACET + 0.919*RCO-OH + 1.905*XC	# 6.640E-15@1516.
	T25M3C6E + NO3 = 0.168*NO2 + 0.55*RO2-R. + 0.282*RO2-N. + 0.762*R2O2. + 0.636*RCHO + 0.288*ACET + 0.262*RNO3 + 1.964*XC + 0.57*XN	# 3.700E-13
	T25M3C6E + O3P = PROD2 + 2*XC	# 2.052E-11
Trans-3-Octene	T-3-C8E + HO. = 0.826*RO2-R. + 0.174*RO2-N. + 0.004*R2O2. + 1.644*RCHO + 0.004*PROD2 + 2*XC	# 6.340E-11
	T-3-C8E + O3 = 0.082*HO. + 0.08*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.082*CO + 0.057*CCHO + 1.023*RCHO + 0.475*PROD2 + 0.444*RCO-OH + 0.545*XC	# 1.150E-16
	T-3-C8E + NO3 = 0.014*NO2 + 0.634*RO2-R. + 0.352*RO2-N. + 0.781*R2O2. + 0.027*RCHO + 0.634*RNO3 + 2*XC + 0.352*XN	# 3.700E-13
	T-3-C8E + O3P = PROD2 + 2*XC	# 2.052E-11
Trans-4-Octene	T-4-C8E + HO. = 0.827*RO2-R. + 0.173*RO2-N. + 1.653*RCHO + 2*XC	# 1.290E-11@-500.
	T-4-C8E + O3 = 0.082*HO. + 0.08*RO2-R. + 0.002*RO2-N. + 0.082*CO + 1.08*RCHO + 0.919*RCO-OH + 1.91*XC	# 6.640E-15@1150.
	T-4-C8E + NO3 = 0.014*NO2 + 0.634*RO2-R. + 0.352*RO2-N. + 0.781*R2O2. + 0.028*RCHO + 0.634*RNO3 + 2*XC + 0.352*XN	# 3.700E-13
	T-4-C8E + O3P = PROD2 + 2*XC	# 2.360E-11
2,4,4-trimethyl-2-Pentene	244M2C5E + HO. = 0.784*RO2-R. + 0.216*RO2-N. + 0.056*R2O2. + 0.025*CCHO + 0.784*RCHO + 0.784*ACET + 2.95*XC	# 8.710E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	244M2C5E + O3 = 0.7*HO. + 0.7*R2O2. + 0.7*CCO-O2. + 0.7*HCHO + 0.7*RCHO + 0.3*ACET + 0.3*RCO-OH + 3*XC	# 2.870E-15@900.
	244M2C5E + NO3 = 0.524*NO2 + 0.036*RO2-R. + 0.44*RO2-N. + 1.86*R2O2. + 0.077*HCHO + 0.53*CCHO + 0.525*RCHO + 0.492*ACET + 0.032*MEK + 0.035*RNO3 + 1.832*XC + 0.441*XN	# 9.370E-12
	244M2C5E + O3P = 0.6*MEK + 0.4*PROD2 + 4.2*XC	# 3.709E-11
Trans-4-Nonene	T-4-C9E + HO. = 0.793*RO2-R. + 0.207*RO2-N. + 0.005*R2O2. + 1.577*RCHO + 0.004*PROD2 + 3*XC	# 6.340E-11
	T-4-C9E + O3 = 0.066*HO. + 0.063*RO2-R. + 0.003*RO2-N. + 0.019*R2O2. + 0.066*CO + 1.063*RCHO + 0.475*PROD2 + 0.46*RCO-OH + 1.5*XC	# 1.150E-16
	T-4-C9E + NO3 = 0.005*NO2 + 0.6*RO2-R. + 0.395*RO2-N. + 0.761*R2O2. + 0.01*RCHO + 0.6*RNO3 + 3*XC + 0.395*XN	# 3.700E-13
	T-4-C9E + O3P = PROD2 + 3*XC	# 2.052E-11
3,4-Diethyl-2-Hexene	34E2-C6E + HO. = 0.77*RO2-R. + 0.23*RO2-N. + 0.77*CCHO + 0.77*PROD2 + 2.46*XC	# 8.710E-11
	34E2-C6E + O3 = 0.856*HO. + 0.121*RO2-N. + 0.579*R2O2. + 0.156*C-O2. + 0.579*RCO-O2. + 0.156*CO + 0.042*CO2 + 0.841*CCHO + 0.438*MEK + 0.3*PROD2 + 0.102*CCO-OH + 0.042*INERT + 1.745*XC	# 2.870E-15@1944.
	34E2-C6E + NO3 = 0.048*NO2 + 0.629*RO2-R. + 0.323*RO2-N. + 1.057*R2O2. + 0.314*CCHO + 0.274*RCHO + 0.354*MEK + 0.048*PROD2 + 0.699*RNO3 + 0.717*XC + 0.253*XN	# 9.370E-12
	34E2-C6E + O3P = PROD2 + 4*XC	# 3.709E-11
Cis-5-Decene	C-5-C10E + HO. = 0.768*RO2-R. + 0.232*RO2-N. + 0.01*R2O2. + 1.519*RCHO + 0.008*PROD2 + 4*XC	# 6.340E-11
	C-5-C10E + O3 = 0.05*HO. + 0.047*RO2-R. + 0.003*RO2-N. + 0.038*R2O2. + 0.05*CO + 1.047*RCHO + 0.95*PROD2 + 1.09*XC	# 3.220E-15@980.
	C-5-C10E + NO3 = 0.577*RO2-R. + 0.423*RO2-N. + 0.749*R2O2. + 0.577*RNO3 + 4*XC + 0.423*XN	# 3.700E-13
	C-5-C10E + O3P = PROD2 + 4*XC	# 2.052E-11
Trans-4-Decene	T-4-C10E + HO. = 0.768*RO2-R. + 0.232*RO2-N. + 0.01*R2O2. + 1.519*RCHO + 0.008*PROD2 + 4*XC	# 6.340E-11
	T-4-C10E + O3 = 0.041*HO. + 0.04*RO2-R. + 0.001*RO2-N. + 0.041*CO + 1.04*RCHO + 0.5*PROD2 + 0.46*RCO-OH + 2.455*XC	# 1.150E-16
	T-4-C10E + NO3 = 0.005*NO2 + 0.573*RO2-R. + 0.422*RO2-N. + 0.749*R2O2. + 0.01*RCHO + 0.573*RNO3 + 4*XC + 0.422*XN	# 3.700E-13
	T-4-C10E + O3P = PROD2 + 4*XC	# 2.052E-11
Trans-5-Undecene	T-5-C11E + HO. = 0.751*RO2-R. + 0.249*RO2-N. + 0.015*R2O2. + 1.479*RCHO + 0.011*PROD2 + 5*XC	# 6.340E-11
	T-5-C11E + O3 = 0.025*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.025*CO + 1.023*RCHO + 0.975*PROD2 + 2.045*XC	# 1.150E-16

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	T-5-C11E + NO3 = 0.56*RO2-R. + 0.44*RO2-N. + 0.742*R2O2. + 0.56*RNO3 + 5*XC + 0.44*XN	# 3.700E-13
	T-5-C11E + O3P = PROD2 + 5*XC	# 2.052E-11
Trans-5-Dodecene	T-5-C12E + HO. = 0.741*RO2-R. + 0.259*RO2-N. + 0.015*R2O2. + 1.461*RCHO + 0.011*PROD2 + 6*XC	# 6.340E-11
	T-5-C12E + O3 = 0.025*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.025*CO + 1.023*RCHO + 0.975*PROD2 + 3.045*XC	# 1.150E-16
	T-5-C12E + NO3 = 0.547*RO2-R. + 0.453*RO2-N. + 0.746*R2O2. + 0.547*RNO3 + 6*XC + 0.453*XN	# 3.700E-13
	T-5-C12E + O3P = PROD2 + 6*XC	# 2.052E-11
Trans-5-Tridecene	T-5-C13E + HO. = 0.735*RO2-R. + 0.265*RO2-N. + 0.015*R2O2. + 1.449*RCHO + 0.011*PROD2 + 7*XC	# 6.340E-11
	T-5-C13E + O3 = 0.025*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.025*CO + 1.023*RCHO + 0.975*PROD2 + 4.045*XC	# 1.150E-16
	T-5-C13E + NO3 = 0.538*RO2-R. + 0.462*RO2-N. + 0.753*R2O2. + 0.538*RNO3 + 7*XC + 0.462*XN	# 3.700E-13
	T-5-C13E + O3P = PROD2 + 7*XC	# 2.052E-11
Trans-5-Tetradecene	T-5-C14E + HO. = 0.732*RO2-R. + 0.268*RO2-N. + 0.015*R2O2. + 1.442*RCHO + 0.011*PROD2 + 8*XC	# 6.340E-11
	T-5-C14E + O3 = 0.025*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.025*CO + 1.023*RCHO + 0.975*PROD2 + 5.045*XC	# 1.150E-16
	T-5-C14E + NO3 = 0.533*RO2-R. + 0.467*RO2-N. + 0.753*R2O2. + 0.533*RNO3 + 8*XC + 0.467*XN	# 3.700E-13
	T-5-C14E + O3P = PROD2 + 8*XC	# 2.052E-11
Trans-5-Tetradecene	T-5-C15E + HO. = 0.729*RO2-R. + 0.271*RO2-N. + 0.015*R2O2. + 1.437*RCHO + 0.01*PROD2 + 9*XC	# 6.340E-11
	T-5-C15E + O3 = 0.025*HO. + 0.023*RO2-R. + 0.002*RO2-N. + 0.019*R2O2. + 0.025*CO + 1.023*RCHO + 0.975*PROD2 + 6.045*XC	# 1.150E-16
	T-5-C15E + NO3 = 0.53*RO2-R. + 0.47*RO2-N. + 0.752*R2O2. + 0.53*RNO3 + 9*XC + 0.47*XN	# 3.700E-13
	T-5-C15E + O3P = PROD2 + 9*XC	# 2.052E-11
Cyclopentene	CYC-PNTE + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*RCHO + 1.805*XC	# 1.250E-11@-500.
	CYC-PNTE + O3 = 0.05*HO. + 0.002*RO2-N. + 0.048*R2O2. + 0.048*RCO-O2. + 0.05*CO + 0.95*RCHO + 1.944*XC	# 1.800E-15@350.
	CYC-PNTE + NO3 = 0.812*NO2 + 0.064*RO2-R. + 0.125*RO2-N. + 0.949*R2O2. + 0.787*RCHO + 0.077*MGLY + 0.012*RNO3 + 1.59*XC + 0.177*XN	# 5.300E-13
	CYC-PNTE + O3P = 0.24*MEK + 0.76*PROD2 + -0.52*XC	# 2.100E-11
1-Methyl cyclohexene	1M-CC5E + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*RCHO + 2.707*XC	# 8.710E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	1M-CC5E + O3 = 0.7*HO. + 0.068*RO2-N. + 0.632*R2O2. + 0.564*CCO-O2. + 0.068*RCO-O2. + 0.068*HCHO + 0.564*RCHO + 0.3*PROD2 + 0.699*XC	# 2.700E-15@415.
	1M-CC5E + NO3 = 0.837*NO2 + 0.052*RO2-R. + 0.111*RO2-N. + 0.979*R2O2. + 0.812*RCHO + 0.077*BACL + 2.589*XC + 0.163*XN	# 9.370E-12
	1M-CC5E + O3P = PROD2	# 3.709E-11
Cyclohexene	CYC-HEXE + HO. = 0.902*RO2-R. + 0.098*RO2-N. + 0.902*RCHO + 2.707*XC	# 1.260E-11@-500.
	CYC-HEXE + O3 = RCHO + 3*XC	# 2.880E-15@1063.
	CYC-HEXE + NO3 = 0.296*NO2 + 0.539*RO2-R. + 0.165*RO2-N. + 0.401*R2O2. + 0.341*RCHO + 0.494*RNO3 + 1.024*XC + 0.21*XN	# 1.050E-12@174.
	CYC-HEXE + O3P = PROD2	# 2.000E-11
1-Methyl Cyclohexene	1M-CC6E + HO. = 0.865*RO2-R. + 0.135*RO2-N. + 0.865*RCHO + 3.595*XC	# 8.710E-11
	1M-CC6E + O3 = 0.7*HO. + 0.095*RO2-N. + 0.605*R2O2. + 0.54*CCO-O2. + 0.065*RCO-O2. + 0.065*HCHO + 0.54*RCHO + 0.3*PROD2 + 1.67*XC	# 2.870E-15@850.
	1M-CC6E + NO3 = 0.729*NO2 + 0.102*RO2-R. + 0.169*RO2-N. + 0.983*R2O2. + 0.831*RCHO + 3.492*XC + 0.271*XN	# 9.370E-12
	1M-CC6E + O3P = PROD2 + XC	# 9.000E-11
4-Methyl Cyclohexene	4M-CC6E + HO. = 0.865*RO2-R. + 0.135*RO2-N. + 0.865*RCHO + 3.595*XC	# 6.340E-11
	4M-CC6E + O3 = RCHO + 4*XC	# 2.880E-15@1060.
	4M-CC6E + NO3 = 0.264*NO2 + 0.519*RO2-R. + 0.218*RO2-N. + 0.468*R2O2. + 0.003*HCHO + 0.003*CCHO + 0.343*RCHO + 0.003*PROD2 + 0.44*RNO3 + 2*XC + 0.296*XN	# 3.700E-13
	4M-CC6E + O3P = PROD2 + XC	# 2.052E-11
1,2-Dimethyl Cyclohexene	12M-CC6E + HO. = 0.827*RO2-R. + 0.173*RO2-N. + 0.827*PROD2 + 2*XC	# 1.054E-10
	12M-CC6E + O3 = HO. + 0.173*RO2-N. + 0.827*R2O2. + 0.738*CCO-O2. + 0.089*RCO-O2. + 0.089*HCHO + 0.738*RCHO + 2.915*XC	# 3.030E-15@800.
	12M-CC6E + NO3 = 0.827*NO2 + 0.173*RO2-N. + 0.827*R2O2. + 0.827*PROD2 + 2*XC + 0.173*XN	# 5.720E-11
	12M-CC6E + O3P = PROD2 + 2*XC	# 5.292E-11
1,3-Butadiene	13-BUTDE + HO. = 0.961*RO2-R. + 0.039*RO2-N. + 0.48*HCHO + 0.48*METHACRO + 0.48*ISO-PROD + -1.039*XC	# 1.480E-11@-448.
	13-BUTDE + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.19*CO2 + 0.5*HCHO + 0.125*PROD2 + 0.5*METHACRO + 0.375*MVK + 0.185*HCOOH + -1.375*XC	# 1.340E-14@2283.
	13-BUTDE + NO3 = 0.92*RO2-R. + 0.08*RO2-N. + 0.92*MVK + -0.161*XC + XN	# 1.000E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	13-BUTDE + O3P = 0.25*HO2. + 0.23*RO2-R. + 0.02*RO2-N. + 0.23*CO + 0.75*PROD2 + 0.23*METHACRO + -1.77*XC	# 1.980E-11
Isoprene	ISOPRENE + HO. = 0.907*RO2-R. + 0.093*RO2-N. + 0.079*R2O2. + 0.624*HCHO + 0.23*METHACRO + 0.32*MVK + 0.357*ISO-PROD + -0.167*XC	# 2.550E-11@-410.
	ISOPRENE + O3 = 0.266*HO. + 0.066*RO2-R. + 0.008*RO2-N. + 0.126*R2O2. + 0.192*MA-RCO3. + 0.275*CO + 0.122*CO2 + 0.592*HCHO + 0.1*PROD2 + 0.39*METHACRO + 0.16*MVK + 0.15*ISO-PROD + 0.204*HCOOH + -0.558*XC	# 7.860E-15@1913.
	ISOPRENE + NO3 = 0.187*NO2 + 0.748*RO2-R. + 0.065*RO2-N. + 0.187*R2O2. + 0.935*ISO-PROD + -0.065*XC + 0.813*XN	# 3.030E-12@446.
	ISOPRENE + O3P = 0.01*RO2-N. + 0.24*R2O2. + 0.25*C-O2. + 0.24*MA-RCO3. + 0.24*HCHO + 0.75*PROD2 + -1.01*XC	# 3.600E-11
Acetylene	ACETYLEN + HO. = 0.603*HO. + 0.297*HO2. + 0.1*RO2-R. + 0.393*CO + 0.096*HCHO + 0.607*GLY + 0.297*HCOOH	# 9.400E-12@700.
	ACETYLEN + O3 = 0.5*HO. + 1.5*HO2. + 1.5*CO + 0.5*CO2	# 2.000E-14@4398.
Methyl Acetylene	ME-ACTYL + HO. = 0.67*HO. + 0.33*CCO-O2. + 0.67*MGLY + 0.33*HCOOH	# 5.900E-12
	ME-ACTYL + O3 = HO. + R2O2. + RCO-O2. + HCHO + -1*XC	# 1.000E-14@4011.
2-Butyne	2-BUTYNE + HO. = 0.67*HO. + 0.33*CCO-O2. + 0.67*BACL + 0.33*CCO-OH	# 1.000E-11@-300.
	2-BUTYNE + O3 = HO. + 0.039*RO2-N. + 0.961*R2O2. + 0.961*RCO-O2. + 0.961*HCHO + -0.079*XC	# 1.000E-14@3915.
Ethyl Acetylene	ET-ACTYL + HO. = 0.67*HO. + 0.33*RCO-O2. + 0.67*MGLY + 0.33*HCOOH + 0.67*XC	# 8.000E-12
	ET-ACTYL + O3 = HO. + 0.039*RO2-N. + 0.961*R2O2. + 0.961*RCO-O2. + 0.961*CCHO + -1.039*XC	# 1.000E-14@3915.
Methanol	MEOH + HO. = HO2. + HCHO	# 3.100E-12@360.
Ethanol	ETOH + HO. = 0.95*HO2. + 0.05*RO2-R. + 0.081*HCHO + 0.96*CCHO	# 5.560E-13@-532.
Isopropyl Alcohol	I-C3-OH + HO. = 0.953*HO2. + 0.046*RO2-R. + 0.001*RO2-N. + 0.046*HCHO + 0.046*CCHO + 0.953*ACET + -0.003*XC	# 6.490E-13@-631.
n-Propyl Alcohol	N-C3-OH + HO. = 0.759*HO2. + 0.238*RO2-R. + 0.003*RO2-N. + 0.208*HCHO + 0.207*CCHO + 0.79*RCHO + -0.009*XC	# 5.530E-12
Isobutyl Alcohol	I-C4-OH + HO. = 0.56*HO2. + 0.403*RO2-R. + 0.037*RO2-N. + 0.393*HCHO + 0.036*CCHO + 0.607*RCHO + 0.319*ACET + 0.531*XC	# 6.914E-12
n-Butyl Alcohol	N-C4-OH + HO. = 0.517*HO2. + 0.47*RO2-R. + 0.013*RO2-N. + 0.308*HCHO + 0.08*CCHO + 0.827*RCHO + 0.093*PROD2 + 0.414*XC	# 8.570E-12
s-Butyl Alcohol	S-C4-OH + HO. = 0.829*HO2. + 0.165*RO2-R. + 0.006*RO2-N. + 0.016*HCHO + 0.238*CCHO + 0.033*RCHO + 0.843*MEK + 0.005*XC	# 9.950E-12
t-Butyl Alcohol	T-C4-OH + HO. = 0.693*RO2-R. + 0.052*RO2-N. + 0.254*TBU-O. + 0.693*HCHO + 0.693*ACET + 0.15*XC	# 3.860E-13@-322.

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Cyclopentanol	CC5-OH + HO. = 0.399*HO2. + 0.562*RO2-R. + 0.039*RO2-N. + 0.004*CO + 0.101*HCHO + 0.33*RCHO + 0.631*MEK + 1.147*XC	# 1.070E-11
2-Pentanol	2-C5OH + HO. = 0.643*HO2. + 0.335*RO2-R. + 0.022*RO2-N. + 0.034*HCHO + 0.146*CCHO + 0.141*RCHO + 0.73*MEK + 0.093*PROD2 + 0.642*XC	# 1.180E-11
3-Pentanol	3-C5OH + HO. = 0.765*HO2. + 0.22*RO2-R. + 0.015*RO2-N. + 0.174*CCHO + 0.195*RCHO + 0.79*MEK + 0.817*XC	# 1.220E-11
Pentyl Alcohol	C5OH + HO. = 0.375*HO2. + 0.59*RO2-R. + 0.035*RO2-N. + 0.262*HCHO + 0.027*CCHO + 0.881*RCHO + 0.084*PROD2 + 1.326*XC	# 1.110E-11
Cyclohexanol	CC6-OH + HO. = 0.439*HO2. + 0.506*RO2-R. + 0.055*RO2-N. + 0.04*HCHO + 0.246*RCHO + 0.705*PROD2 + 0.664*XC	# 1.744E-11
1-Hexanol	1-C6OH + HO. = 0.108*HO2. + 0.814*RO2-R. + 0.078*RO2-N. + 0.098*HCHO + 0.002*CCHO + 0.675*RCHO + 0.253*PROD2 + 1.885*XC	# 1.250E-11
2-Hexanol	2-C6OH + HO. = 0.543*HO2. + 0.415*RO2-R. + 0.043*RO2-N. + 0.032*HCHO + 0.13*CCHO + 0.15*RCHO + 0.808*PROD2 + 0.155*XC	# 1.210E-11
1-Heptanol	1-C7OH + HO. = 0.862*RO2-R. + 0.138*RO2-N. + 0.025*R2O2. + 0.054*HCHO + 0.547*RCHO + 0.315*PROD2 + 2.587*XC	# 1.370E-11
1-Octanol	1-C8-OH + HO. = 0.771*RO2-R. + 0.229*RO2-N. + 0.32*R2O2. + 0.054*HCHO + 0.387*RCHO + 0.384*PROD2 + 3.108*XC	# 2.020E-11
2-Octanol	2-C8-OH + HO. = 0.062*HO2. + 0.775*RO2-R. + 0.163*RO2-N. + 0.008*HCHO + 0.183*CCHO + 0.198*RCHO + 0.64*PROD2 + 2.219*XC	# 2.520E-11
2-Ethyl-1-Hexanol	2-ETC6OH + HO. = 0.006*HO2. + 0.841*RO2-R. + 0.153*RO2-N. + 0.339*HCHO + 0.04*CCHO + 0.604*RCHO + 0.327*PROD2 + 2.884*XC	# 1.328E-11
3-Octanol	3-C8-OH + HO. = 0.225*HO2. + 0.641*RO2-R. + 0.134*RO2-N. + 0.142*CCHO + 0.355*RCHO + 0.609*PROD2 + 2.19*XC	# 3.140E-11
4-Octanol	4-C8-OH + HO. = 0.161*HO2. + 0.693*RO2-R. + 0.145*RO2-N. + 0.715*RCHO + 0.497*PROD2 + 2.002*XC	# 2.870E-11
Ethylene Glycol	ET-GLYCL + HO. = HO2. + 0.067*HCHO + 0.966*CCHO	# 1.470E-11
Propylene Glycol	PR-GLYCL + HO. = 0.987*HO2. + 0.013*RO2-R. + 0.039*HCHO + 0.039*CCHO + 0.315*RCHO + 0.646*MEK + -0.646*XC	# 2.150E-11
1,2-Butandiol	12-C4OH2 + HO. = 0.916*HO2. + 0.081*RO2-R. + 0.003*RO2-N. + 0.022*HCHO + 0.14*CCHO + 0.285*RCHO + 0.641*MEK + 0.257*XC	# 1.586E-11
Glycerol	GLYCERL + HO. = HO2. + 0.017*HCHO + 0.017*CCHO + 0.435*RCHO + 0.548*PROD2 + -1.645*XC	# 1.872E-11
2-Methyl-2,4-Pentanediol	2M24C5OH + HO. = 0.785*HO2. + 0.195*RO2-R. + 0.02*RO2-N. + 0.046*HCHO + 0.012*CCHO + 0.141*RCHO + 0.133*ACET + 0.785*MEK + 0.042*PROD2 + 1.595*XC	# 1.056E-11
1,2-Dihydroxy Hexane	C6-GLYCL + HO. = 0.779*HO2. + 0.2*RO2-R. + 0.022*RO2-N. + 0.069*CCHO + 0.36*RCHO + 0.618*PROD2 + 0.943*XC	# 1.870E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Dimethyl Ether	ME-O-ME + HO. = RO2-R. + 0.079*HCHO + 0.961*INERT + 0.961*XC	# 1.040E-11@372.
Trimethylene Oxide	TME-OX + HO. = 0.138*RO2-R. + 1.862*R2O2. + 0.862*RCO-O2. + 0.003*CO + 0.006*HCHO + 0.135*RCHO	# 1.030E-11
Tetrahydrofuran	THF + HO. = 0.911*RO2-R. + 0.079*RO2-N. + 1.032*R2O2. + 0.009*RCO-O2. + 0.049*CO + 0.013*HCHO + 0.861*RCHO + 0.05*PROD2 + 0.549*XC	# 1.610E-11
Diethyl Ether	ET-O-ET + HO. = 0.131*RO2-R. + 0.04*RO2-N. + 0.848*R2O2. + 0.829*C-O2. + 0.006*HCHO + 0.168*CCHO + 0.006*RCHO + 0.858*MEK + 0.01*PROD2 + -0.924*XC	# 8.020E-13@-837.
Dimethoxy methane	METHYLAL + HO. = RO2-R. + 0.086*HCHO + 0.639*PROD2 + 0.359*INERT + -1.282*XC	# 4.900E-12
Alpha-Methyltetrahydrofuran	AM-THF + HO. = 0.817*RO2-R. + 0.141*RO2-N. + 1.221*R2O2. + 0.04*C-O2. + 0.003*RCO-O2. + 0.01*CO + 0.025*HCHO + 0.008*CCHO + 0.847*RCHO + 0.007*PROD2 + 1.472*XC	# 2.520E-12@-650.
Tetrahydropyran	THP + HO. = 0.824*RO2-R. + 0.167*RO2-N. + 1.606*R2O2. + 0.009*RCO-O2. + 0.025*CO + 0.026*HCHO + 0.694*RCHO + 0.13*PROD2 + 0.001*GLY + 0.008*HCOOH + 1.046*XC	# 1.380E-11
Ethyl Isopropyl Ether	ET-O-IPR + HO. = 0.246*RO2-R. + 0.066*RO2-N. + 0.701*R2O2. + 0.688*C-O2. + 0.008*HCHO + 0.221*CCHO + 0.002*RCHO + 0.219*ACET + 0.709*MEK + 0.004*PROD2 + -0.052*XC	# 2.439E-11
Methyl n-Butyl Ether	MNBE + HO. = 0.919*RO2-R. + 0.081*RO2-N. + 0.783*R2O2. + 0.006*HCHO + 0.038*CCHO + 0.72*RCHO + 0.068*MEK + 0.131*PROD2 + 0.693*INERT + 0.521*XC	# 1.480E-11
Methyl t-Butyl Ether	MTBE + HO. = 0.743*RO2-R. + 0.078*RO2-N. + 0.381*R2O2. + 0.162*C-O2. + 0.016*TBU-O. + 0.234*HCHO + 0.024*ACET + 0.719*MEK + 0.007*PROD2 + 0.155*INERT + 0.939*XC	# 5.890E-13^2.00@-483.
Ethyl n-Butyl Ether	ENBE + HO. = 0.589*RO2-R. + 0.116*RO2-N. + 0.882*R2O2. + 0.295*C-O2. + 0.011*HCHO + 0.086*CCHO + 0.491*RCHO + 0.721*MEK + 0.104*PROD2 + -0.154*XC	# 2.130E-11
Ethyl t-Butyl Ether	ETBE + HO. = 0.143*RO2-R. + 0.101*RO2-N. + 0.81*R2O2. + 0.644*C-O2. + 0.112*TBU-O. + 0.055*HCHO + 0.127*CCHO + 0.018*RCHO + 0.016*ACET + 0.644*MEK + 0.109*INERT + 1.317*XC	# 8.840E-12
Methyl t-Amyl Ether	MTAE + HO. = 0.535*RO2-R. + 0.13*RO2-N. + 1.076*R2O2. + 0.335*C-O2. + 0.219*HCHO + 0.512*CCHO + 0.028*RCHO + 0.055*ACET + 0.33*MEK + 0.026*PROD2 + 0.001*HCOOH + 0.432*INERT + 1.488*XC	# 7.910E-12
Di n-Propyl Ether	PR-O-PR + HO. = 0.894*RO2-R. + 0.106*RO2-N. + 0.961*R2O2. + 0.873*CCHO + 0.014*RCHO + 0.795*MEK + 0.085*PROD2 + -0.116*XC	# 1.180E-12@-825.
2-Butyl Tetrahydrofuran	2BU-THF + HO. = 0.642*RO2-R. + 0.356*RO2-N. + 1.176*R2O2. + 0.002*RCO-O2. + 0.001*CO + 0.034*HCHO + 0.733*RCHO + 0.001*MEK + 0.003*PROD2 + 0.002*HCOOH + 3.603*XC	# 2.764E-11
Di-n-butyl Ether	BU-O-BU + HO. = 0.788*RO2-R. + 0.212*RO2-N. + 0.903*R2O2. + 0.032*CCHO + 0.737*RCHO + 0.651*MEK + 0.147*PROD2 + 0.969*XC	# 2.880E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Di-Isobutyl Ether	IBU2-O + HO. = 0.767*RO2-R. + 0.233*RO2-N. + 0.961*R2O2. + 0.019*HCHO + 0.006*RCHO + 0.763*ACET + 0.778*MEK + 0.013*PROD2 + 1.083*XC	# 2.600E-11
Di-n-Pentyl Ether	C5-O-C5 + HO. = 0.679*RO2-R. + 0.321*RO2-N. + 1.291*R2O2. + 0.007*CCHO + 0.604*RCHO + 0.704*PROD2 + 2.027*XC	# 3.470E-11
2-Methoxyethanol	MEO-ETOH + HO. = 0.278*HO2. + 0.722*RO2-R. + 0.648*HCHO + 0.307*RCHO + 0.048*PROD2 + 0.642*INERT + 0.497*XC	# 4.500E-12@-325.
2-Methoxy-1-Propanol	2MEOC3OH + HO. = 0.161*HO2. + 0.806*RO2-R. + 0.033*RO2-N. + 0.763*HCHO + 0.001*CCHO + 0.178*RCHO + 0.027*PROD2 + 0.761*INERT + 1.58*XC	# 2.526E-11
2-Ethoxyethanol	ETO-ETOH + HO. = 0.015*HO2. + 0.792*RO2-R. + 0.02*RO2-N. + 0.173*C-O2. + 0.549*HCHO + 0.083*CCHO + 0.268*RCHO + 0.437*MEK + 0.206*PROD2 + -0.793*XC	# 1.870E-11
1-Methoxy-2-Propanol	MEOC3OH + HO. = 0.39*HO2. + 0.6*RO2-R. + 0.01*RO2-N. + 0.001*HCHO + 0.571*CCHO + 0.419*PROD2 + 0.571*INERT + -0.287*XC	# 2.000E-11
2-Propoxyethanol	2PROETOH + HO. = 0.943*RO2-R. + 0.057*RO2-N. + 0.245*R2O2. + 0.406*HCHO + 0.369*CCHO + 0.165*RCHO + 0.368*MEK + 0.41*PROD2 + -0.912*XC	# 2.466E-11
3-Ethoxy-1-Propanol	3ETOC3OH + HO. = 0.706*RO2-R. + 0.055*RO2-N. + 0.475*R2O2. + 0.239*C-O2. + 0.69*HCHO + 0.127*CCHO + 0.28*RCHO + 0.393*MEK + 0.271*PROD2 + -0.551*XC	# 2.200E-11
3-Methoxy-1-Butanol	3MEOC4OH + HO. = 0.933*RO2-R. + 0.055*RO2-N. + 0.582*R2O2. + 0.012*C-O2. + 1.171*HCHO + 0.155*CCHO + 0.19*RCHO + 0.001*MEK + 0.037*PROD2 + 0.714*INERT + 1.664*XC	# 2.360E-12
1-Ethoxy-2-Propanol	ETOC3OH + HO. = 0.163*HO2. + 0.633*RO2-R. + 0.044*RO2-N. + 0.16*C-O2. + 0.033*HCHO + 0.415*CCHO + 0.349*MEK + 0.574*PROD2 + -1.127*XC	# 2.616E-11
Diethylene Glycol	DET-GLCL + HO. = 0.293*HO2. + 0.679*RO2-R. + 0.028*RO2-N. + 0.679*HCHO + 0.293*RCHO + 0.679*PROD2 + -1.802*XC	# 2.753E-11
3 methoxy -3 methyl-Butanol	3MOMC4OH + HO. = 0.127*HO2. + 0.655*RO2-R. + 0.054*RO2-N. + 0.164*C-O2. + 0.11*HCHO + 0.202*CCHO + 0.599*RCHO + 0.026*ACET + 0.141*PROD2 + 0.001*HCOOH + 0.18*INERT + 2.1*XC	# 7.101E-12
2-Butoxyethanol	BUO-ETOH + HO. = 0.888*RO2-R. + 0.112*RO2-N. + 0.133*R2O2. + 0.55*HCHO + 0.013*CCHO + 0.318*RCHO + 0.508*MEK + 0.26*PROD2 + 0.211*XC	# 2.570E-11
1-Propoxy-2-Propanol	PROXC3OH + HO. = 0.927*RO2-R. + 0.073*RO2-N. + 0.047*R2O2. + 0.635*CCHO + 0.302*MEK + 0.625*PROD2 + -0.666*XC	# 2.910E-11
2-(2-Methoxyethoxy) Ethanol	MOEOETOH + HO. = 0.941*RO2-R. + 0.059*RO2-N. + 0.452*R2O2. + 0.307*HCHO + 0.001*CCHO + 0.216*RCHO + 0.019*MEK + 0.717*PROD2 + 0.001*HCOOH + 0.518*INERT + -1.211*XC	# 3.406E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
n-Butoxy-2-Propanol	BUOC3OH + HO. = 0.89*RO2-R. + 0.11*RO2-N. + 0.064*R2O2. + 0.333*CCHO + 0.273*RCHO + 0.276*MEK + 0.618*PROD2 + 0.041*XC	# 3.052E-11
1-tert-Butoxy-2-Propanol	PG-1TB-E + HO. = 0.407*HO2. + 0.497*RO2-R. + 0.077*RO2-N. + 0.019*C-O2. + 0.025*HCHO + 0.452*CCHO + 0.001*ACET + 0.451*MEK + 0.471*PROD2 + 0.956*XC	# 1.871E-11
2-tert-Butoxy-1-Propanol	PG-2TB-E + HO. = 0.132*HO2. + 0.738*RO2-R. + 0.115*RO2-N. + 0.015*C-O2. + 0.722*HCHO + 0.166*RCHO + 0.015*PROD2 + 0.704*INERT + 4.279*XC	# 2.462E-11
2-(2-Ethoxyethoxy) EtOH	CARBITOL + HO. = 0.803*RO2-R. + 0.117*RO2-N. + 0.538*R2O2. + 0.08*C-O2. + 0.249*HCHO + 0.027*CCHO + 0.177*RCHO + 0.405*MEK + 0.757*PROD2 + 0.003*HCOOH + -1.781*XC	# 5.080E-11
Dipropylene Glycol	DPR-GLCL + HO. = 0.464*HO2. + 0.484*RO2-R. + 0.052*RO2-N. + 0.484*CCHO + 0.948*PROD2 + -0.968*XC	# 3.640E-11
Dipropylene Glycol Methyl Ether	DPRGOME + HO. = 0.785*RO2-R. + 0.125*RO2-N. + 0.475*R2O2. + 0.09*C-O2. + 0.047*HCHO + 0.209*CCHO + 0.014*MEK + 0.856*PROD2 + 0.001*HCOOH + 0.511*INERT + -0.01*XC	# 4.885E-11
2-(2-Butoxyethoxy)-EtOH	C8-CELSV + HO. = 0.82*RO2-R. + 0.18*RO2-N. + 0.53*R2O2. + 0.198*HCHO + 0.01*CCHO + 0.345*RCHO + 0.317*MEK + 0.708*PROD2 + 0.149*XC	# 4.523E-11
Tripropylene Glycol Monomethyl Ether	TPRGOME + HO. = 0.572*RO2-R. + 0.26*RO2-N. + 0.993*R2O2. + 0.169*C-O2. + 0.029*HCHO + 0.144*CCHO + 0.098*MEK + 0.946*PROD2 + 0.021*HCOOH + 0.402*INERT + 1.467*XC	# 7.834E-11
Methyl Formate	ME-FORM + HO. = RO2-R. + 0.411*CO + 0.071*CO2 + 0.071*HCHO + 0.411*HCOOH + 0.518*INERT + 0.518*XC	# 2.270E-13
Ethyl Formate	ET-FORM + HO. = 0.098*RO2-R. + 0.902*R2O2. + 0.748*CCO-O2. + 0.154*RCO-O2. + 0.061*CO2 + 0.061*CCHO + 0.014*RCHO + 0.748*HCOOH + 0.023*INERT + 0.047*XC	# 1.020E-12
Methyl Acetate	ME-ACET + HO. = 0.985*RO2-R. + 0.015*RO2-N. + 0.368*CO + 0.368*CCO-OH + 0.617*INERT + 1.188*XC	# 8.300E-13@260.
n-Propyl Formate	C3-FORM + HO. = 0.157*RO2-R. + 0.039*RO2-N. + 0.805*R2O2. + 0.804*RCO-O2. + 0.041*CO2 + 0.001*HCHO + 0.109*RCHO + 0.033*MEK + 0.367*HCOOH + 0.014*INERT + 0.468*XC	# 2.380E-12
Ethyl Acetate	ET-ACET + HO. = 0.148*RO2-R. + 0.04*RO2-N. + 0.818*R2O2. + 0.812*CCO-O2. + 0.096*RCHO + 0.018*MGLY + 0.807*CCO-OH + 0.005*RCO-OH + 0.033*INERT + 0.128*XC	# 1.600E-12
Methyl Propionate	ME-PRAT + HO. = 0.925*RO2-R. + 0.043*RO2-N. + 0.125*R2O2. + 0.032*RCO-O2. + 0.137*CO + 0.032*CCHO + 0.239*RCHO + 0.042*MEK + 0.02*PROD2 + 0.326*BACL + 0.117*RCO-OH + 0.181*INERT + 0.603*XC	# 1.030E-12
n-Butyl Formate	C4-FORM + HO. = 0.334*RO2-R. + 0.073*RO2-N. + 0.831*R2O2. + 0.593*RCO-O2. + 0.014*CO2 + 0.119*CCHO + 0.063*RCHO + 0.199*MEK + 0.072*PROD2 + 0.16*HCOOH + 0.954*XC	# 3.120E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Ethyl Propionate	ET-PRAT + HO. = 0.199*RO2-R. + 0.072*RO2-N. + 0.839*R2O2. + 0.727*CCO-O2. + 0.002*RCO-O2. + 0.002*CCHO + 0.149*RCHO + 0.028*MEK + 0.094*PROD2 + 0.022*BACL + 0.633*RCO-OH + -0.006*XC	# 2.140E-12
Isopropyl Acetate	IPR-ACET + HO. = 0.142*RO2-R. + 0.075*RO2-N. + 0.954*R2O2. + 0.73*C-O2. + 0.053*CCO-O2. + 0.175*CO2 + 0.058*HCHO + 0.034*RCHO + 0.175*ACET + 0.106*MGLY + 0.053*CCO-OH + 0.557*INERT + 1.874*XC	# 3.400E-12
Methyl Butyrate	ME-BUAT + HO. = 0.918*RO2-R. + 0.067*RO2-N. + 0.171*R2O2. + 0.015*RCO-O2. + 0.054*CO + 0.001*HCHO + 0.096*CCHO + 0.099*RCHO + 0.558*MEK + 0.007*PROD2 + 0.08*MGLY + 0.142*BACL + 0.047*RCO-OH + 0.785*XC	# 3.040E-12
Methyl Isobutyrate	ME-IBUAT + HO. = 0.378*RO2-R. + 0.075*RO2-N. + 0.771*R2O2. + 0.547*RCO-O2. + 0.082*CO + 0.106*HCHO + 0.008*CCHO + 0.081*RCHO + 0.539*ACET + 0.135*MEK + 0.005*PROD2 + 0.081*BACL + 0.077*RCO-OH + -0.276*XC	# 1.730E-12
Propyl Acetate	PR-ACET + HO. = 0.433*RO2-R. + 0.066*RO2-N. + 0.552*R2O2. + 0.501*RCO-O2. + 0.007*CO + 0.001*HCHO + 0.038*CCHO + 0.05*RCHO + 0.344*MEK + 0.002*MGLY + 0.499*CCO-OH + 0.01*RCO-OH + 0.031*INERT + 0.43*XC	# 3.400E-12
n-Butyl Acetate	BU-ACET + HO. = 0.675*RO2-R. + 0.12*RO2-N. + 0.516*R2O2. + 0.205*RCO-O2. + 0.006*CO + 0.116*CCHO + 0.172*RCHO + 0.252*MEK + 0.251*PROD2 + 0.211*CCO-OH + 0.024*INERT + 0.95*XC	# 4.200E-12
Ethyl Butyrate	ET-BUAT + HO. = 0.424*RO2-R. + 0.108*RO2-N. + 0.616*R2O2. + 0.466*CCO-O2. + 0.002*RCO-O2. + 0.001*HCHO + 0.053*CCHO + 0.093*RCHO + 0.276*MEK + 0.066*PROD2 + 0.038*MGLY + 0.019*BACL + 0.4*RCO-OH + 1.14*XC	# 4.940E-12
Isobutyl Acetate	IBU-ACET + HO. = 0.811*RO2-R. + 0.12*RO2-N. + 0.89*R2O2. + 0.008*C-O2. + 0.06*RCO-O2. + 0.171*CO + 0.052*HCHO + 0.003*CCHO + 0.015*RCHO + 0.754*ACET + 0.054*MEK + 0.232*CCO-OH + 0.591*INERT + 1.28*XC	# 4.614E-12
Methyl Pivalate	ME-PVAT + HO. = 0.365*RO2-R. + 0.172*RO2-N. + 1.115*R2O2. + 0.463*RCO-O2. + 0.131*CO + 0.576*HCHO + 0.031*RCHO + 0.463*ACET + 0.203*MEK + 0.131*RCO-OH + 0.186*XC	# 1.270E-12
n-Propyl Propionate	PR-PRAT + HO. = 0.421*RO2-R. + 0.105*RO2-N. + 0.574*R2O2. + 0.474*RCO-O2. + 0.006*CO + 0.001*HCHO + 0.034*CCHO + 0.085*RCHO + 0.296*MEK + 0.051*PROD2 + 0.011*BACL + 0.428*RCO-OH + 0.024*INERT + 0.78*XC	# 4.020E-12
s-Butyl Acetate	SBU-ACET + HO. = 0.714*RO2-R. + 0.11*RO2-N. + 1.06*R2O2. + 0.171*CCO-O2. + 0.005*RCO-O2. + 0.006*HCHO + 0.834*CCHO + 0.048*RCHO + 0.011*MEK + 0.176*CCO-OH + 0.655*INERT + 2.115*XC	# 5.500E-12
t-Butyl Acetate	TBU-ACET + HO. = 0.156*RO2-R. + 0.179*RO2-N. + 1.57*R2O2. + 0.666*C-O2. + 0.159*CO2 + 0.811*HCHO + 0.159*ACET + 0.156*MGLY + 0.506*INERT + 1.84*XC	# 4.250E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Butyl Propionate	BU-PRAT + HO. = 0.624*RO2-R. + 0.168*RO2-N. + 0.533*R2O2. + 0.208*RCO-O2. + 0.005*CO + 0.102*CCHO + 0.177*RCHO + 0.222*MEK + 0.243*PROD2 + 0.006*BACL + 0.19*RCO-OH + 0.02*INERT + 1.666*XC	# 5.056E-12
Amyl Acetate	AM-ACET + HO. = 0.762*RO2-R. + 0.222*RO2-N. + 0.741*R2O2. + 0.016*RCO-O2. + 0.019*CCHO + 0.214*RCHO + 0.637*PROD2 + 0.016*CCO-OH + 1.088*XC	# 6.055E-12
n-Propyl Butyrate	PR-BUAT + HO. = 0.482*RO2-R. + 0.148*RO2-N. + 0.517*R2O2. + 0.37*RCO-O2. + 0.004*CO + 0.001*HCHO + 0.06*CCHO + 0.062*RCHO + 0.403*MEK + 0.042*PROD2 + 0.004*MGLY + 0.011*BACL + 0.332*RCO-OH + 1.784*XC	# 7.410E-12
2-Ethoxyethyl Acetate	CSV-ACET + HO. = 0.573*RO2-R. + 0.112*RO2-N. + 0.843*R2O2. + 0.29*C-O2. + 0.026*RCO-O2. + 0.166*CO + 0.004*HCHO + 0.059*CCHO + 0.055*RCHO + 0.746*MEK + 0.064*PROD2 + 0.192*CCO-OH + 0.284*INERT + 0.473*XC	# 1.943E-11
n-Butyl Butyrate	BU-BUAT + HO. = 0.613*RO2-R. + 0.214*RO2-N. + 0.487*R2O2. + 0.173*RCO-O2. + 0.004*CO + 0.104*CCHO + 0.135*RCHO + 0.313*MEK + 0.194*PROD2 + 0.003*MGLY + 0.007*BACL + 0.157*RCO-OH + 2.661*XC	# 1.060E-11
Isobutyl Isobutyrate	IBU-IBTR + HO. = 0.68*RO2-R. + 0.235*RO2-N. + 0.927*R2O2. + 0.006*C-O2. + 0.079*RCO-O2. + 0.12*CO + 0.069*HCHO + 0.002*CCHO + 0.034*RCHO + 0.649*ACET + 0.542*MEK + 0.003*PROD2 + 0.003*BACL + 0.18*RCO-OH + 1.366*XC	# 5.519E-12
Ethyl 3-Ethoxy Propionate	E3EOC3OH + HO. = 0.404*RO2-R. + 0.159*RO2-N. + 0.987*R2O2. + 0.278*C-O2. + 0.159*CCO-O2. + 0.002*HCHO + 0.058*CCHO + 0.056*RCHO + 0.729*MEK + 0.079*PROD2 + 0.315*MGLY + 0.001*BACL + 0.093*RCO-OH + 0.553*XC	# 1.957E-11
Isoamyl Isobutyrate	IC5IBUAT + HO. = 0.58*RO2-R. + 0.294*RO2-N. + 0.843*R2O2. + 0.125*RCO-O2. + 0.028*HCHO + 0.455*RCHO + 0.434*ACET + 0.032*MEK + 0.113*PROD2 + 0.002*BACL + 0.109*RCO-OH + 3.018*XC	# 6.939E-12
2-Ethyl-Hexyl Acetate	2ETHXACT + HO. = 0.581*RO2-R. + 0.415*RO2-N. + 0.933*R2O2. + 0.004*RCO-O2. + 0.002*CO + 0.096*CCHO + 0.127*RCHO + 0.075*MEK + 0.476*PROD2 + 0.006*CCO-OH + 0.064*INERT + 3.692*XC	# 1.098E-11
Dimethyl Carbonate	DMC + HO. = RO2-R. + 0.393*CO + 0.393*RCO-OH + 0.607*INERT + 0.82*XC	# 3.300E-13
Propylene Carbonate	PC + HO. = 0.627*RO2-R. + 0.021*RO2-N. + 1.511*R2O2. + 0.353*CCO-O2. + 0.225*CO + 0.213*HCHO + 0.034*RCHO + 0.577*RCO-OH + 0.368*INERT + 0.53*XC	# 6.900E-13
Methyl Lactate	ME-LACT + HO. = 0.835*HO2. + 0.153*RO2-R. + 0.006*RO2-N. + 0.005*RCO-O2. + 0.023*CO + 0.061*HCHO + 0.005*CCHO + 0.036*MEK + 0.023*PROD2 + 0.061*MGLY + 0.868*BACL + -0.088*XC	# 2.760E-12
Ethyl Lactate	ET-LACT + HO. = 0.175*HO2. + 0.452*RO2-R. + 0.031*RO2-N. + 0.342*CCO-O2. + 0.001*RCO-O2. + 0.039*HCHO + 0.001*CCHO + 0.039*RCHO + 0.013*MEK + 0.342*PROD2 + 0.039*MGLY + 0.536*BACL + -0.391*XC	# 3.910E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Methyl Isopropyl Carbonate	MIPR-CB + HO. = 0.302*RO2-R. + 0.047*RO2-N. + 0.707*R2O2. + 0.599*C-O2. + 0.052*CCO-O2. + 0.023*CO + 0.209*CO2 + 0.265*HCHO + 0.033*RCHO + 0.209*ACET + 0.035*MEK + 0.075*RCO-OH + 0.601*INERT + 1.825*XC	# 2.550E-12
2-Methyoxy-1-propyl Acetate	2PGMEACT + HO. = 0.827*RO2-R. + 0.11*RO2-N. + 0.93*R2O2. + 0.06*C-O2. + 0.003*RCO-O2. + 0.289*CO + 0.011*HCHO + 0.011*CCHO + 0.043*MEK + 0.001*PROD2 + 0.001*HCOOH + 0.291*CCO-OH + 1.404*INERT + 2.785*XC	# 2.296E-11
1-Methoxy-2-Propyl Acetate	PGME-ACT + HO. = 0.324*RO2-R. + 0.127*RO2-N. + 1.4*R2O2. + 0.542*CCO-O2. + 0.006*RCO-O2. + 0.031*HCHO + 0.003*RCHO + 0.049*MEK + 0.05*PROD2 + 0.549*CCO-OH + INERT + 1.499*XC	# 1.440E-11
Dimethyl Succinate	DBE-4 + HO. = 0.899*RO2-R. + 0.085*RO2-N. + 0.07*R2O2. + 0.016*RCO-O2. + 0.31*CO + 0.016*RCHO + 0.516*MEK + 0.002*PROD2 + 0.073*BACL + 0.308*RCO-OH + 1.792*XC	# 1.500E-12
Diisopropyl Carbonate	DIPR-CB + HO. = 0.251*RO2-R. + 0.139*RO2-N. + 0.647*R2O2. + 0.577*C-O2. + 0.033*CCO-O2. + 0.202*CO2 + 0.038*HCHO + 0.048*RCHO + 0.403*ACET + 0.579*MEK + 0.033*RCO-OH + 1.519*XC	# 6.877E-12
Dimethyl Glutarate	DBE-5 + HO. = 0.827*RO2-R. + 0.173*RO2-N. + 0.172*R2O2. + 0.153*CO + 0.601*MEK + 0.153*PROD2 + 0.073*BACL + 2.194*XC	# 3.500E-12
2-Butoxyethyl Acetate	2BUETACT + HO. = 0.779*RO2-R. + 0.206*RO2-N. + 0.899*R2O2. + 0.016*RCO-O2. + 0.142*CO + 0.017*CCHO + 0.369*RCHO + 0.674*MEK + 0.116*PROD2 + 0.157*CCO-OH + 0.239*INERT + 1.488*XC	# 2.378E-11
Dimethyl Adipate	DBE-6 + HO. = 0.782*RO2-R. + 0.218*RO2-N. + 0.623*R2O2. + 0.036*CO + 0.879*RCHO + 0.181*MEK + 0.035*PROD2 + 0.02*MGLY + 0.126*BACL + 0.002*RCO-OH + 2.519*XC	# 8.800E-12
3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	TEXANOL1 + HO. = 0.439*HO2. + 0.43*RO2-R. + 0.126*RO2-N. + 0.004*RCO-O2. + 0.003*CO + 0.034*HCHO + 0.01*CCHO + 0.244*RCHO + 0.218*ACET + 0.12*MEK + 0.628*PROD2 + 0.001*BACL + 0.003*RCO-OH + 5.532*XC	# 1.620E-11
1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	TEXANOL2 + HO. = 0.754*RO2-R. + 0.242*RO2-N. + 0.177*R2O2. + 0.003*RCO-O2. + 0.362*HCHO + 0.001*CCHO + 0.437*RCHO + 0.361*ACET + 0.345*MEK + 0.009*PROD2 + 0.001*RCO-OH + 6.342*XC	# 1.288E-11
Ethylene Oxide	ETOX + HO. = RO2-R. + R2O2. + 0.411*CO + 0.071*CO2 + 0.071*HCHO + 0.411*HCOOH + 0.518*INERT + 0.518*XC	# 7.600E-14
Propylene Oxide	PROX + HO. = 0.765*RO2-R. + 0.008*RO2-N. + 1.441*R2O2. + 0.227*CCO-O2. + 0.282*CO + 0.034*CO2 + 0.235*HCHO + 0.018*CCHO + 0.006*RCHO + 0.317*HCOOH + 0.192*CCO-OH + 0.443*INERT + 0.748*XC	# 5.200E-13
1,2-Epoxybutane	12BUOX + HO. = 0.797*RO2-R. + 0.059*RO2-N. + 1.746*R2O2. + 0.144*RCO-O2. + 0.312*CO + 0.054*CO2 + 0.039*HCHO + 0.554*CCHO + 0.014*RCHO + 0.011*MEK + 0.371*HCOOH + 0.084*RCO-OH + 0.42*INERT + 0.568*XC	# 1.910E-12
Formic Acid	FORMACID + HO. = HO2. + CO2	# 4.500E-13

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Acetic Acid	ACETACID + HO. = 0.491*RO2-R. + 0.509*C-O2. + 0.509*CO2 + 0.491*MGLY + -0.491*XC	# 8.000E-13
Acrylic Acid	ACYRACID + HO. = RO2-R. + 0.015*CO2 + 0.548*HCHO + 0.015*CCHO + 0.208*RCHO + 0.548*MGLY + 0.229*BACL + -0.777*XC	# 2.844E-11
	ACYRACID + O3 = 0.11*HO. + 0.11*HO2. + 0.3*CO + 0.115*CO2 + 0.5*HCHO + 0.5*MGLY + 0.185*HCOOH + 0.45*INERT + -0.05*XC	# 1.010E-17
	ACYRACID + NO3 = RO2-R. + 0.062*CO2 + 0.062*RCHO + 0.938*BACL + -1*XC + XN	# 2.760E-18
	ACYRACID + O3P = 0.45*RCHO + 0.55*RCO-OH	# 4.605E-12
Propionic Acid	PROPACID + HO. = RO2-R. + 0.142*CO2 + 0.142*CCHO + 0.4*RCHO + 0.457*BACL + -0.457*XC	# 1.160E-12
2-Methyl-2-Butene-3-ol	MBUTENOL + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.311*HCHO + 0.624*CCHO + 0.311*RCHO + 0.624*ACET + 0.246*XC	# 8.200E-12@-610.
	MBUTENOL + O3 = 0.099*HO. + 0.099*HO2. + 0.365*CO + 0.091*CO2 + 0.3*HCHO + 0.7*RCHO + 0.015*ACET + 0.259*HCOOH + 0.285*RCO-OH + 0.985*XC	# 9.300E-18
	MBUTENOL + NO3 = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*RCHO + 0.935*ACET + -1*XC + XN	# 4.600E-14@400.
	MBUTENOL + O3P = 0.45*RCHO + 0.55*MEK + 1.45*XC	# 2.005E-11
Methyl Acrylate	ME-ACRYL + HO. = 0.948*RO2-R. + 0.042*RO2-N. + 0.085*R2O2. + 0.01*RCO-O2. + 0.016*CO + 0.681*HCHO + 0.01*CCHO + 0.041*PROD2 + 0.681*MGLY + 0.225*BACL + -0.194*XC	# 2.844E-11
	ME-ACRYL + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*MGLY + 0.185*HCOOH + 1.5*XC	# 1.010E-17
	ME-ACRYL + NO3 = 0.916*RO2-R. + 0.05*RO2-N. + 0.292*R2O2. + 0.034*RCO-O2. + 0.056*CO + 0.034*RCHO + 0.774*BACL + 0.142*RNO3 + -0.507*XC + 0.858*XN	# 2.760E-18
	ME-ACRYL + O3P = 0.45*RCHO + 0.55*MEK + 0.45*XC	# 4.605E-12
Vinyl Acetate	VIN-ACET + HO. = 0.953*RO2-R. + 0.039*RO2-N. + 0.007*R2O2. + 0.007*RCO-O2. + 0.874*HCHO + 0.079*RCHO + 0.007*CCO-OH + 0.874*INERT + 1.74*XC	# 3.160E-11
	VIN-ACET + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.185*HCOOH + 0.5*INERT + 2.5*XC	# 1.010E-17
	VIN-ACET + NO3 = 0.08*RO2-R. + 0.039*RO2-N. + 0.88*R2O2. + 0.88*RCO-O2. + 0.88*CCO-OH + -0.637*XC + XN	# 1.380E-14
	VIN-ACET + O3P = 0.45*RCHO + 0.55*MEK + 0.45*XC	# 5.604E-12
Ethyl Acrylate	ET-ACRYL + HO. = 0.511*RO2-R. + 0.095*RO2-N. + 0.864*R2O2. + 0.394*CCO-O2. + 0.416*HCHO + 0.409*PROD2 + 0.416*MGLY + 0.08*BACL + -0.795*XC	# 2.844E-11

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	ET-ACRYL + O3 = 0.06*HO. + 0.06*HO2. + 0.25*CO + 0.065*CO2 + 0.5*HCHO + 0.5*MGLY + 0.185*HCOOH + 2.5*XC	# 1.010E-17
	ET-ACRYL + NO3 = 0.172*RO2-R. + 0.12*RO2-N. + 1.554*R2O2. + 0.708*CCO-O2. + 0.145*BACL + 0.735*RNO3 + -2.126*XC + 0.265*XN	# 2.760E-18
	ET-ACRYL + O3P = 0.45*RCHO + 0.55*MEK + 1.45*XC	# 4.605E-12
Methyl Methacrylate	ME-MACRT + HO. = 0.935*RO2-R. + 0.065*RO2-N. + 0.935*HCHO + 0.935*BACL + -0.065*XC	# 5.211E-11
	ME-MACRT + O3 = 0.707*HO. + 0.313*RO2-R. + 0.026*RO2-N. + 0.327*R2O2. + 0.367*RCO-O2. + 0.167*CO + 0.043*CO2 + 1.034*HCHO + 0.273*MGLY + 0.333*BACL + 0.123*HCOOH + 0.221*XC	# 1.180E-17
	ME-MACRT + NO3 = 0.256*RO2-R. + 0.083*RO2-N. + 0.935*R2O2. + 0.661*RCO-O2. + 0.101*CO + 0.101*RNO3 + 1.815*XC + 0.899*XN	# 6.640E-17
	ME-MACRT + O3P = 0.4*RCHO + 0.6*MEK + 1.4*XC	# 1.424E-11
Butyl Methacrylate	BU-MACRT + HO. = 0.762*RO2-R. + 0.194*RO2-N. + 0.164*R2O2. + 0.044*RCO-O2. + 0.736*HCHO + 0.003*RCHO + 0.003*MEK + 0.068*PROD2 + 0.736*BACL + 2.6*XC	# 5.211E-11
	BU-MACRT + O3 = 0.707*HO. + 0.286*RO2-R. + 0.09*RO2-N. + 0.291*R2O2. + 0.331*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.997*HCHO + 0.246*MGLY + 0.333*BACL + 0.123*HCOOH + 3.066*XC	# 1.180E-17
	BU-MACRT + NO3 = 0.225*RO2-R. + 0.346*RO2-N. + 1.446*R2O2. + 0.429*RCO-O2. + 0.024*RCHO + 0.575*RNO3 + 1.115*XC + 0.425*XN	# 6.640E-17
	BU-MACRT + O3P = 0.4*RCHO + 0.6*MEK + 4.4*XC	# 1.424E-11
Isobutyl Methacrylate	IBUMACRT + HO. = 0.795*RO2-R. + 0.192*RO2-N. + 0.166*R2O2. + 0.013*RCO-O2. + 0.736*HCHO + 0.059*ACET + 0.062*MEK + 0.013*PROD2 + 0.736*BACL + 2.626*XC	# 5.211E-11
	IBUMACRT + O3 = 0.707*HO. + 0.286*RO2-R. + 0.09*RO2-N. + 0.291*R2O2. + 0.331*RCO-O2. + 0.167*CO + 0.043*CO2 + 0.997*HCHO + 0.246*MGLY + 0.333*BACL + 0.123*HCOOH + 3.066*XC	# 1.180E-17
	IBUMACRT + NO3 = 0.503*RO2-R. + 0.328*RO2-N. + 1.464*R2O2. + 0.169*RCO-O2. + 0.503*ACET + 0.113*RNO3 + 3.337*XC + 0.887*XN	# 6.640E-17
	IBUMACRT + O3P = 0.4*RCHO + 0.6*MEK + 4.4*XC	# 1.424E-11
Acetaldehyde	ACETALD + HO. = CCO-O2.	# 5.600E-12@-310.
	ACETALD + NO3 = CCO-O2. + XN	# 1.400E-12@1860.
	ACETALD = HO2. + C-O2. + CO	# 1.00E+00/<ACETONE>
Propionaldehyde	PROPALD + HO. = 0.034*RO2-R. + 0.002*RO2-N. + 0.965*RCO-O2. + 0.034*CO + 0.034*CCHO + -0.005*XC	# 2.000E-11
	PROPALD + NO3 = RCO-O2. + XN	# 3.800E-15

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	PROPALD = HO2. + RO2-R. + CO + CCHO	# 1.00E+00/<C2CHO>
Butanal	1C4RCHO + HO. = 0.088*RO2-R. + 0.008*RO2-N. + 0.015*R2O2. + 0.905*RCO-O2. + 0.052*CO + 0.014*HCHO + 0.015*CCHO + 0.073*RCHO + 0.001*GLY + 0.924*XC	# 5.260E-12@-446.
	1C4RCHO + NO3 = RCO-O2. + XC + XN	# 3.800E-15
	1C4RCHO = HO2. + 0.98*RO2-R. + 0.02*RO2-N. + CO + 0.98*RCHO + -0.06*XC	# 1.00E+00/<C2CHO>
2-Methylpropanal	2MEC3AL + HO. = 0.082*RO2-R. + 0.004*RO2-N. + 0.011*R2O2. + 0.914*RCO-O2. + 0.078*CO + 0.011*HCHO + 0.011*CCHO + 0.004*RCHO + 0.067*ACET + 0.91*XC	# 6.610E-12@-411.
	2MEC3AL + NO3 = RCO-O2. + XC + XN	# 3.800E-15
	2MEC3AL = HO2. + 0.96*RO2-R. + 0.04*RO2-N. + CO + 0.96*ACET + -0.12*XC	# 1.00E+00/<C2CHO>
Pentanal (Valeraldehyde)	1C5RCHO + HO. = 0.089*RO2-R. + 0.018*RO2-N. + 0.08*R2O2. + 0.893*RCO-O2. + 0.043*CO + 0.011*HCHO + 0.021*CCHO + 0.087*RCHO + 0.002*MGLY + 1.851*XC	# 6.340E-12@-448.
	1C5RCHO + NO3 = RCO-O2. + 2*XC + XN	# 3.800E-15
	1C5RCHO = 0.245*HO2. + 1.686*RO2-R. + 0.069*RO2-N. + CO + 0.931*RCHO + 0.792*XC	# 1.00E+00/<C2CHO>
2,2-Dimethylpropanal (pivaldehyde)	22DMC3AL + HO. = 0.023*RO2-R. + 0.003*RO2-N. + 0.024*R2O2. + 0.974*RCO-O2. + 0.023*CO + 0.024*HCHO + 0.001*RCHO + 0.023*ACET + 1.946*XC	# 6.820E-12@-405.
	22DMC3AL + NO3 = RCO-O2. + 2*XC + XN	# 3.800E-15
	22DMC3AL = 0.039*HO2. + 0.961*RO2-R. + 0.039*RO2-N. + 0.961*TBU-O. + CO + 0.882*XC	# 1.00E+00/<C2CHO>
3-Methylbutanal (Isovaleraldehyde)	3MC4RCHO + HO. = 0.129*RO2-R. + 0.012*RO2-N. + 0.112*R2O2. + 0.002*C-O2. + 0.856*RCO-O2. + 0.125*CO + 0.092*HCHO + 0.036*RCHO + 0.096*ACET + 0.004*GLY + 1.736*XC	# 2.740E-11
	3MC4RCHO + NO3 = RCO-O2. + 2*XC + XN	# 3.800E-15
	3MC4RCHO = 0.652*HO2. + 1.294*RO2-R. + 0.053*RO2-N. + CO + 0.348*HCHO + 0.613*RCHO + 0.334*ACET + 0.492*XC	# 1.00E+00/<C2CHO>
Glutaraldehyde	GLTRALD + HO. = 0.04*RO2-R. + 0.009*RO2-N. + 0.051*R2O2. + 0.951*RCO-O2. + 0.033*CO + 0.023*HCHO + 0.04*RCHO + 0.001*GLY + 1.915*XC	# 4.160E-11
	GLTRALD + NO3 = RCO-O2. + 2*XC + XN	# 7.600E-15
	GLTRALD = 0.039*HO2. + 0.961*RO2-R. + 0.039*RO2-N. + 0.961*RCO-O2. + CO + 0.882*XC	# 1.00E+00/<C2CHO>
Hexanal	1C6RCHO + HO. = 0.112*RO2-R. + 0.04*RO2-N. + 0.154*R2O2. + 0.848*RCO-O2. + 0.014*CO + 0.002*HCHO + 0.103*RCHO + 0.018*MGLY + 2.834*XC	# 2.426E-11
	1C6RCHO + NO3 = RCO-O2. + 3*XC + XN	# 3.800E-15
	1C6RCHO = 0.065*HO2. + 1.809*RO2-R. + 0.126*RO2-N. + CO + 0.874*RCHO + 1.623*XC	# 1.00E+00/<C2CHO>

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Heptanal	1C7RCHO + HO. = 0.136*RO2-R. + 0.067*RO2-N. + 0.191*R2O2. + 0.797*RCO-O2. + 0.009*CO + 0.118*RCHO + 0.017*MGLY + 3.79*XC	# 2.568E-11
	1C7RCHO + NO3 = RCO-O2. + 4*XC + XN	# 3.800E-15
	1C7RCHO = 0.098*HO2. + 1.717*RO2-R. + 0.186*RO2-N. + CO + 0.814*RCHO + 2.443*XC	# 1.00E+00/<C2CHO>
Octanal	1C8RCHO + HO. = 0.164*RO2-R. + 0.096*RO2-N. + 0.219*R2O2. + 0.74*RCO-O2. + 0.008*CO + 0.149*RCHO + 0.015*MGLY + 4.704*XC	# 2.710E-11
	1C8RCHO + NO3 = RCO-O2. + 5*XC + XN	# 3.800E-15
	1C8RCHO = 0.135*HO2. + 1.613*RO2-R. + 0.252*RO2-N. + CO + 0.748*RCHO + 3.244*XC	# 1.00E+00/<C2CHO>
Acrolein	ACROLEIN + HO. = 0.25*RO2-R. + 0.75*MA-RCO3. + 0.167*CO + 0.083*HCHO + 0.167*CCHO + 0.083*GLY + -0.75*XC	# 1.990E-11
	ACROLEIN + O3 = 0.31*HO. + 0.81*HO2. + CO + 0.315*CO2 + 0.5*HCHO + 0.5*GLY + 0.185*HCOOH	# 1.360E-15@2519.
	ACROLEIN + NO3 = 0.031*RO2-R. + 0.002*RO2-N. + 0.967*MA-RCO3. + 0.031*CO + 0.031*RCHO + -1.003*XC + XN	# 2.938E-15
	ACROLEIN + O3P = RCHO	# 2.367E-12
	ACROLEIN = 0.172*HO. + 1.01*HO2. + 0.172*C-O2. + 0.33*MA-RCO3. + 1.182*CO + 0.046*CO2 + 0.34*HCHO + 0.112*CCO-OH + 0.046*INERT + -0.284*XC	# 2.00E-03/<ACROLEIN>
Crotonaldehyde	CROTALD + HO. = 0.528*RO2-R. + 0.022*RO2-N. + 0.45*MA-RCO3. + 0.032*CO + 0.497*CCHO + 0.032*RCHO + 0.497*GLY + -0.043*XC	# 3.640E-11
	CROTALD + O3 = 0.51*HO. + 0.75*HO2. + 0.26*C-O2. + 1.01*CO + 0.32*CO2 + 0.5*CCHO + 0.5*GLY + 0.17*CCO-OH + 0.07*INERT + 0.07*XC	# 9.000E-19
	CROTALD + NO3 = 0.129*NO2 + 0.376*RO2-R. + 0.044*RO2-N. + 0.129*R2O2. + 0.45*MA-RCO3. + 0.253*CO + 0.45*HNO3 + 0.129*CCHO + 0.376*RCHO + 0.129*GLY + 0.035*XC + 0.421*XN	# 5.120E-15
	CROTALD + O3P = 0.88*RCHO + 0.12*MGLY + XC	# 7.294E-12
	CROTALD = 2*HO2. + 2*CO + CCHO	# 4.10E-03/<ACROLEIN>
Methacrolein	METHACRO + HO. = 0.48*RO2-R. + 0.02*RO2-N. + 0.5*MA-RCO3. + 0.396*CO + 0.084*HCHO + 0.396*MEK + 0.084*MGLY + -0.436*XC	# 1.860E-11@-175.
	METHACRO + O3 = 0.208*HO. + 0.008*HO2. + 0.1*RO2-R. + 0.1*RCO-O2. + 0.45*CO + 0.117*CO2 + 0.2*HCHO + 0.9*MGLY + 0.333*HCOOH + -0.1*XC	# 1.360E-15@2114.
	METHACRO + NO3 = 0.48*RO2-R. + 0.02*RO2-N. + 0.5*MA-RCO3. + 0.48*CO + 0.5*HNO3 + 1.401*XC + 0.5*XN	# 1.500E-12@1726.
	METHACRO + O3P = RCHO + XC	# 6.194E-12
	METHACRO = 0.33*HO. + 0.34*HO2. + 0.33*RO2-R. + 0.67*CCO-O2. + 0.33*MA-RCO3. + 0.67*CO + 0.67*HCHO	# 4.10E-03/<ACROLEIN>

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Hydroxy Methacrolein	HOMACR + HO. = 0.596*RO2-R. + 0.024*RO2-N. + 0.38*MA-RCO3. + 0.444*CO + 0.151*HCHO + 0.444*PROD2 + 0.151*MGLY + -1.382*XC	# 4.300E-11
	HOMACR + O3 = 0.208*HO. + 0.208*HO2. + 0.45*CO + 0.117*CO2 + 0.1*HCHO + MGLY + 0.333*HCOOH	# 1.360E-15@2114.
	HOMACR + NO3 = 0.48*RO2-R. + 0.02*RO2-N. + 0.5*MA-RCO3. + 0.452*CO + 0.5*HNO3 + 0.028*HCHO + 0.028*MGLY + 0.452*RNO3 + -1.396*XC + 0.048*XN	# 1.500E-12@1726.
	HOMACR + O3P = RCHO + XC	# 9.951E-12
	HOMACR = HO2. + RCO-O2. + CO + HCHO + -1*XC	# 4.10E-03/<ACROLEIN>
Acetone	ACETONE + HO. = R2O2. + CCO-O2. + HCHO	# 2.800E-12@760.
	ACETONE = C-O2. + CCO-O2.	# 1.00E+00/<CCHO_R>
Cyclobutanone	CC4-KET + HO. = 0.073*RO2-N. + 1.782*R2O2. + 0.927*RCO-O2. + 0.821*HCHO + -0.041*XC	# 8.700E-13
	CC4-KET = 4*XC	# 1.50E-01/<KETONE>
Methyl Ethyl Ketone	MEK + HO. = 0.376*RO2-R. + 0.039*RO2-N. + 0.591*R2O2. + 0.51*CCO-O2. + 0.074*RCO-O2. + 0.088*HCHO + 0.504*CCHO + 0.376*RCHO + 0.297*XC	# 1.300E-12@25.
	MEK = RO2-R. + CCO-O2. + CCHO	# 1.50E-01/<KETONE>
Cyclopentanone	CC5-KET + HO. = 0.624*RO2-R. + 0.118*RO2-N. + 1.072*R2O2. + 0.258*RCO-O2. + 0.077*HCHO + 0.624*RCHO + 0.029*GLY + 1.512*XC	# 2.940E-12
	CC5-KET = 5*XC	# 1.00E-01/<KETONE>
3-Pentanone	DEK + HO. = 0.375*RO2-R. + 0.067*RO2-N. + 0.588*R2O2. + 0.559*RCO-O2. + 0.559*CCHO + 0.375*RCHO + 0.682*XC	# 2.000E-12
	DEK = RO2-R. + RCO-O2. + CCHO	# 1.00E-01/<KETONE>
2-Pentanone	MPK + HO. = 0.154*RO2-R. + 0.065*RO2-N. + 1.373*R2O2. + 0.761*CCO-O2. + 0.02*RCO-O2. + 0.612*HCHO + 0.591*CCHO + 0.203*RCHO + 0.12*MEK + 0.142*XC	# 4.560E-12
	MPK = 0.98*RO2-R. + 0.02*RO2-N. + CCO-O2. + 0.98*RCHO + -0.06*XC	# 1.00E-01/<KETONE>
Cyclohexanone	CC6-KET + HO. = 0.386*RO2-R. + 0.178*RO2-N. + 0.722*R2O2. + 0.436*RCO-O2. + 0.059*HCHO + 0.194*RCHO + 0.197*PROD2 + 1.802*XC	# 6.390E-12
	CC6-KET = 6*XC	# 5.00E-02/<KETONE>
4-Methyl-2-Pentanone	MIBK + HO. = 0.012*RO2-R. + 0.099*RO2-N. + 1.706*R2O2. + 0.878*CCO-O2. + 0.011*RCO-O2. + 0.827*HCHO + 0.021*CCHO + 0.096*RCHO + 0.768*ACET + 0.004*MEK + 0.135*XC	# 1.410E-11
	MIBK = 0.947*RO2-R. + 0.053*RO2-N. + 0.348*R2O2. + CCO-O2. + 0.348*HCHO + 0.613*RCHO + 0.334*ACET + 0.492*XC	# 5.00E-02/<KETONE>
Methyl n-Butyl Ketone	MNBK + HO. = 0.424*RO2-R. + 0.102*RO2-N. + 1.014*R2O2. + 0.459*CCO-O2. + 0.014*RCO-O2. + 0.338*HCHO + 0.195*CCHO + 0.65*RCHO + 0.145*MEK + 0.088*PROD2 + 0.64*XC	# 9.100E-12

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
	MNBK = 0.931*RO2-R. + 0.069*RO2-N. + 0.755*R2O2. + CCO-O2. + 0.931*RCHO + 0.792*XC	# 5.00E-02/<KETONE>
Methyl t-Butyl Ketone	MTBK + HO. = 0.021*RO2-R. + 0.151*RO2-N. + 1.653*R2O2. + 0.772*CCO-O2. + 0.055*RCO-O2. + 0.881*HCHO + 0.021*RCHO + 0.772*ACET + 0.121*XC	# 1.210E-12
	MTBK = 0.039*RO2-N. + 0.961*R2O2. + CCO-O2. + 0.961*TBU-O. + 0.882*XC	# 5.00E-02/<KETONE>
2-Methyl-3-Hexanone	2M-3-HXO + HO. = 0.298*RO2-R. + 0.163*RO2-N. + 0.827*R2O2. + 0.539*RCO-O2. + 0.19*HCHO + 0.187*CCHO + 0.161*RCHO + 0.252*ACET + 0.244*MEK + 1.627*XC	# 7.211E-12
	2M-3-HXO = 0.98*RO2-R. + 0.02*RO2-N. + RCO-O2. + 0.98*RCHO + 0.94*XC	# 2.00E-02/<KETONE>
2-Heptanone	C7-KET-2 + HO. = 0.513*RO2-R. + 0.193*RO2-N. + 0.936*R2O2. + 0.283*CCO-O2. + 0.011*RCO-O2. + 0.099*HCHO + 0.013*CCHO + 0.59*RCHO + 0.347*PROD2 + 1.265*XC	# 1.170E-11
	C7-KET-2 = 0.874*RO2-R. + 0.126*RO2-N. + 0.935*R2O2. + CCO-O2. + 0.874*RCHO + 1.623*XC	# 2.00E-02/<KETONE>
Di-Isopropyl Ketone	DIPK + HO. = 0.095*RO2-R. + 0.162*RO2-N. + 1.015*R2O2. + 0.743*RCO-O2. + 0.259*HCHO + 0.234*CCHO + 0.095*RCHO + 0.509*ACET + 1.259*XC	# 5.380E-12
	DIPK = 0.96*RO2-R. + 0.04*RO2-N. + RCO-O2. + 0.96*ACET + 0.88*XC	# 2.00E-02/<KETONE>
2-Octanone	C8-KET-2 + HO. = 0.515*RO2-R. + 0.296*RO2-N. + 0.914*R2O2. + 0.18*CCO-O2. + 0.009*RCO-O2. + 0.014*HCHO + 0.225*RCHO + 0.487*PROD2 + 2.227*XC	# 1.100E-11
	C8-KET-2 = 0.814*RO2-R. + 0.186*RO2-N. + 0.902*R2O2. + CCO-O2. + 0.814*RCHO + 2.443*XC	# 1.00E-02/<KETONE>
2-Nonanone	C9-KET-2 + HO. = 0.503*RO2-R. + 0.357*RO2-N. + 0.87*R2O2. + 0.14*CCO-O2. + 0.149*RCHO + 0.494*PROD2 + 3.167*XC	# 1.220E-11
Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	DIBK + HO. = 0.019*RO2-R. + 0.282*RO2-N. + 1.401*R2O2. + 0.014*C-O2. + 0.685*RCO-O2. + 0.594*HCHO + 0.005*CCHO + 0.123*RCHO + 0.626*ACET + 0.026*PROD2 + 2.232*XC	# 2.750E-11
2-Decanone	C10-K-2 + HO. = 0.52*RO2-R. + 0.396*RO2-N. + 0.806*R2O2. + 0.083*CCO-O2. + 0.087*RCHO + 0.517*PROD2 + 4.094*XC	# 1.320E-11
Methylvinyl ketone	MVK + HO. = 0.288*RO2-R. + 0.039*RO2-N. + 0.672*R2O2. + 0.672*CCO-O2. + 0.288*HCHO + 0.672*CCHO + 0.288*MGLY + -0.079*XC	# 4.140E-12@-453.
	MVK + O3 = 0.164*HO. + 0.064*HO2. + 0.05*RO2-R. + 0.05*RCO-O2. + 0.475*CO + 0.124*CO2 + 0.1*HCHO + 0.95*MGLY + 0.351*HCOOH + -0.05*XC	# 7.510E-16@1520.
	MVK + O3P = 0.45*RCHO + 0.55*MEK + 0.45*XC	# 2.115E-12
	MVK = 0.3*C-O2. + 0.3*MA-RCO3. + 0.7*CO + 0.7*PROD2 + -2.4*XC	# 2.10E-03/<ACROLEIN>
Hydroxy Acetone	HOACET + HO. = 0.756*HO2. + 0.034*RO2-R. + 0.177*CCO-O2. + 0.034*RCO-O2. + 0.211*HCHO + 0.789*MGLY + -0.034*XC	# 3.020E-12
	HOACET = HO2. + CCO-O2. + HCHO	# 1.50E-01/<KETONE>

Table A-1 (continued)

Compound	Reactions	Kinetic Parameters [a]
Methoxy Acetone	MEOACET + HO. = 0.148*RO2-R. + 0.039*RO2-N. + 0.812*R2O2. + 0.798*CCO-O2. + 0.014*RCO-O2. + 0.028*HCHO + 0.148*MEK + 0.791*INERT + 0.712*XC	# 6.770E-12
	MEOACET = RO2-R. + CCO-O2. + 0.079*HCHO + 0.961*INERT + 0.961*XC	# 1.00E-01/<KETONE>
Diacetone Alcohol	DIACTALC + HO. = 0.233*RO2-R. + 0.086*RO2-N. + 0.681*R2O2. + 0.618*CCO-O2. + 0.063*RCO-O2. + 0.388*HCHO + 0.5*RCHO + 0.143*ACET + 0.207*MEK + 0.026*MGLY + 0.834*XC	# 1.490E-12
	DIACTALC = 0.93*RO2-R. + 0.07*RO2-N. + CCO-O2. + 0.93*HCHO + 0.93*ACET + -0.14*XC	# 2.00E-02/<KETONE>
2-(Cl-methyl)-3-Cl-Propene	CL2IBUTE + HO. = 0.48*RO2-R. + 0.039*RO2-N. + 0.961*R2O2. + 0.48*Cl. + 0.961*HCHO + 0.961*MEK + -1.039*XC	# 3.160E-11
	CL2IBUTE + O3 = 0.707*HO. + 0.04*RO2-R. + 0.627*R2O2. + 0.667*Cl. + 0.167*CO + 0.043*CO2 + 0.667*HCHO + 0.333*MEK + 0.667*MGLY + 0.123*HCOOH + -0.333*XC	# 3.900E-19
	CL2IBUTE + NO3 = 0.039*RO2-N. + 1.921*R2O2. + 0.961*Cl. + 0.961*HCHO + 2.803*XC + XN	# 1.000E-15
	CL2IBUTE + O3P = 0.4*RCHO + 0.6*MEK + 0.4*XC	# 5.604E-12

[a] See Footnote [a] on Table 2

Table A-2. Listing of the absorption cross sections and quantum yields for the photolysis reactions.

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						NO2								
205.0	4.31e-19	1.000	210.0	4.72e-19	1.000	215.0	4.95e-19	1.000	220.0	4.56e-19	1.000	225.0	3.79e-19	1.000
230.0	2.74e-19	1.000	235.0	1.67e-19	1.000	240.0	9.31e-20	1.000	245.0	4.74e-20	1.000	250.0	2.48e-20	1.000
255.0	1.95e-20	1.000	260.0	2.24e-20	1.000	265.0	2.73e-20	1.000	270.0	4.11e-20	1.000	275.0	4.90e-20	1.000
280.0	5.92e-20	1.000	285.0	7.39e-20	1.000	290.0	9.00e-20	1.000	295.0	1.09e-19	1.000	300.0	1.31e-19	1.000
305.0	1.57e-19	1.000	310.0	1.86e-19	1.000	315.0	2.15e-19	0.990	320.0	2.48e-19	0.990	325.0	2.81e-19	0.990
330.0	3.13e-19	0.990	335.0	3.43e-19	0.990	340.0	3.80e-19	0.990	345.0	4.07e-19	0.990	350.0	4.31e-19	0.990
355.0	4.72e-19	0.990	360.0	4.83e-19	0.980	365.0	5.17e-19	0.980	370.0	5.32e-19	0.980	375.0	5.51e-19	0.980
380.0	5.64e-19	0.970	385.0	5.76e-19	0.970	390.0	5.93e-19	0.960	395.0	5.85e-19	0.935	400.0	6.02e-19	0.820
405.0	5.78e-19	0.355	410.0	6.00e-19	0.130	411.0	5.93e-19	0.110	412.0	5.86e-19	0.094	413.0	5.79e-19	0.083
414.0	5.72e-19	0.070	415.0	5.65e-19	0.059	416.0	5.68e-19	0.048	417.0	5.71e-19	0.039	418.0	5.75e-19	0.030
419.0	5.78e-19	0.023	420.0	5.81e-19	0.018	421.0	5.72e-19	0.012	422.0	5.64e-19	0.008	423.0	5.55e-19	0.004
424.0	5.47e-19	0.000												
						NO3NO								
585.0	2.89e-18	0.000	586.0	3.32e-18	0.050	587.0	4.16e-18	0.100	588.0	5.04e-18	0.150	589.0	6.13e-18	0.200
590.0	5.96e-18	0.250	591.0	5.44e-18	0.280	592.0	5.11e-18	0.310	593.0	4.58e-18	0.340	594.0	4.19e-18	0.370
595.0	4.29e-18	0.400	596.0	4.62e-18	0.370	597.0	4.36e-18	0.340	598.0	3.67e-18	0.310	599.0	3.10e-18	0.280
600.0	2.76e-18	0.250	601.0	2.86e-18	0.240	602.0	3.32e-18	0.230	603.0	3.80e-18	0.220	604.0	4.37e-18	0.210
605.0	4.36e-18	0.200	606.0	3.32e-18	0.200	607.0	2.40e-18	0.200	608.0	1.85e-18	0.200	609.0	1.71e-18	0.200
610.0	1.77e-18	0.200	611.0	1.91e-18	0.180	612.0	2.23e-18	0.160	613.0	2.63e-18	0.140	614.0	2.55e-18	0.120
615.0	2.26e-18	0.100	616.0	2.09e-18	0.100	617.0	2.11e-18	0.100	618.0	2.39e-18	0.100	619.0	2.56e-18	0.100
620.0	3.27e-18	0.100	621.0	5.24e-18	0.090	622.0	1.02e-17	0.080	623.0	1.47e-17	0.070	624.0	1.21e-17	0.060
625.0	8.38e-18	0.050	626.0	7.30e-18	0.050	627.0	7.53e-18	0.050	628.0	7.37e-18	0.050	629.0	6.98e-18	0.050
630.0	6.76e-18	0.050	631.0	4.84e-18	0.046	632.0	3.27e-18	0.042	633.0	2.17e-18	0.038	634.0	1.64e-18	0.034
635.0	1.44e-18	0.030	636.0	1.69e-18	0.024	637.0	2.07e-18	0.018	638.0	2.03e-18	0.012	639.0	1.58e-18	0.006
640.0	1.23e-18	0.000												
						NO3NO2								
400.0	0.00e+00	1.000	401.0	0.00e+00	1.000	402.0	0.00e+00	1.000	403.0	2.00e-20	1.000	404.0	0.00e+00	1.000
405.0	3.00e-20	1.000	406.0	2.00e-20	1.000	407.0	1.00e-20	1.000	408.0	3.00e-20	1.000	409.0	0.00e+00	1.000
410.0	1.00e-20	1.000	411.0	2.00e-20	1.000	412.0	5.00e-20	1.000	413.0	5.00e-20	1.000	414.0	2.00e-20	1.000
415.0	6.00e-20	1.000	416.0	6.00e-20	1.000	417.0	7.00e-20	1.000	418.0	5.00e-20	1.000	419.0	8.00e-20	1.000
420.0	8.00e-20	1.000	421.0	8.00e-20	1.000	422.0	9.00e-20	1.000	423.0	1.10e-19	1.000	424.0	9.00e-20	1.000
425.0	7.00e-20	1.000	426.0	1.40e-19	1.000	427.0	1.40e-19	1.000	428.0	1.20e-19	1.000	429.0	1.10e-19	1.000
430.0	1.70e-19	1.000	431.0	1.30e-19	1.000	432.0	1.50e-19	1.000	433.0	1.80e-19	1.000	434.0	1.80e-19	1.000
435.0	1.60e-19	1.000	436.0	1.50e-19	1.000	437.0	1.80e-19	1.000	438.0	2.10e-19	1.000	439.0	2.00e-19	1.000
440.0	1.90e-19	1.000	441.0	1.80e-19	1.000	442.0	2.10e-19	1.000	443.0	1.80e-19	1.000	444.0	1.90e-19	1.000
445.0	2.00e-19	1.000	446.0	2.40e-19	1.000	447.0	2.90e-19	1.000	448.0	2.40e-19	1.000	449.0	2.80e-19	1.000
450.0	2.90e-19	1.000	451.0	3.00e-19	1.000	452.0	3.30e-19	1.000	453.0	3.10e-19	1.000	454.0	3.60e-19	1.000
455.0	3.60e-19	1.000	456.0	3.60e-19	1.000	457.0	4.00e-19	1.000	458.0	3.70e-19	1.000	459.0	4.20e-19	1.000
460.0	4.00e-19	1.000	461.0	3.90e-19	1.000	462.0	4.00e-19	1.000	463.0	4.10e-19	1.000	464.0	4.80e-19	1.000
465.0	5.10e-19	1.000	466.0	5.40e-19	1.000	467.0	5.70e-19	1.000	468.0	5.60e-19	1.000	469.0	5.80e-19	1.000
470.0	5.90e-19	1.000	471.0	6.20e-19	1.000	472.0	6.40e-19	1.000	473.0	6.20e-19	1.000	474.0	6.20e-19	1.000
475.0	6.80e-19	1.000	476.0	7.80e-19	1.000	477.0	7.70e-19	1.000	478.0	7.30e-19	1.000	479.0	7.30e-19	1.000
480.0	7.00e-19	1.000	481.0	7.10e-19	1.000	482.0	7.10e-19	1.000	483.0	7.20e-19	1.000	484.0	7.70e-19	1.000
485.0	8.20e-19	1.000	486.0	9.10e-19	1.000	487.0	9.20e-19	1.000	488.0	9.50e-19	1.000	489.0	9.60e-19	1.000
490.0	1.03e-18	1.000	491.0	9.90e-19	1.000	492.0	9.90e-19	1.000	493.0	1.01e-18	1.000	494.0	1.01e-18	1.000
495.0	1.06e-18	1.000	496.0	1.21e-18	1.000	497.0	1.22e-18	1.000	498.0	1.20e-18	1.000	499.0	1.17e-18	1.000
500.0	1.13e-18	1.000	501.0	1.11e-18	1.000	502.0	1.11e-18	1.000	503.0	1.11e-18	1.000	504.0	1.26e-18	1.000
505.0	1.28e-18	1.000	506.0	1.34e-18	1.000	507.0	1.28e-18	1.000	508.0	1.27e-18	1.000	509.0	1.35e-18	1.000
510.0	1.51e-18	1.000	511.0	1.73e-18	1.000	512.0	1.77e-18	1.000	513.0	1.60e-18	1.000	514.0	1.58e-18	1.000
515.0	1.58e-18	1.000	516.0	1.56e-18	1.000	517.0	1.49e-18	1.000	518.0	1.44e-18	1.000	519.0	1.54e-18	1.000
520.0	1.68e-18	1.000	521.0	1.83e-18	1.000	522.0	1.93e-18	1.000	523.0	1.77e-18	1.000	524.0	1.64e-18	1.000
525.0	1.58e-18	1.000	526.0	1.63e-18	1.000	527.0	1.81e-18	1.000	528.0	2.10e-18	1.000	529.0	2.39e-18	1.000
530.0	2.23e-18	1.000	531.0	2.09e-18	1.000	532.0	2.02e-18	1.000	533.0	1.95e-18	1.000	534.0	2.04e-18	1.000
535.0	2.30e-18	1.000	536.0	2.57e-18	1.000	537.0	2.58e-18	1.000	538.0	2.34e-18	1.000	539.0	2.04e-18	1.000
540.0	2.10e-18	1.000	541.0	2.04e-18	1.000	542.0	1.88e-18	1.000	543.0	1.68e-18	1.000	544.0	1.70e-18	1.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
545.0	1.96e-18	1.000	546.0	2.42e-18	1.000	547.0	2.91e-18	1.000	548.0	2.98e-18	1.000	549.0	2.71e-18	1.000
550.0	2.48e-18	1.000	551.0	2.43e-18	1.000	552.0	2.47e-18	1.000	553.0	2.53e-18	1.000	554.0	2.78e-18	1.000
555.0	3.11e-18	1.000	556.0	3.26e-18	1.000	557.0	3.29e-18	1.000	558.0	3.51e-18	1.000	559.0	3.72e-18	1.000
560.0	3.32e-18	1.000	561.0	2.98e-18	1.000	562.0	2.90e-18	1.000	563.0	2.80e-18	1.000	564.0	2.72e-18	1.000
565.0	2.73e-18	1.000	566.0	2.85e-18	1.000	567.0	2.81e-18	1.000	568.0	2.85e-18	1.000	569.0	2.89e-18	1.000
570.0	2.79e-18	1.000	571.0	2.76e-18	1.000	572.0	2.74e-18	1.000	573.0	2.78e-18	1.000	574.0	2.86e-18	1.000
575.0	3.08e-18	1.000	576.0	3.27e-18	1.000	577.0	3.38e-18	1.000	578.0	3.31e-18	1.000	579.0	3.24e-18	1.000
580.0	3.34e-18	1.000	581.0	3.55e-18	1.000	582.0	3.28e-18	1.000	583.0	2.93e-18	1.000	584.0	2.82e-18	1.000
585.0	2.89e-18	1.000	586.0	3.32e-18	0.950	587.0	4.16e-18	0.900	588.0	5.04e-18	0.850	589.0	6.13e-18	0.800
590.0	5.96e-18	0.750	591.0	5.44e-18	0.720	592.0	5.11e-18	0.690	593.0	4.58e-18	0.660	594.0	4.19e-18	0.630
595.0	4.29e-18	0.600	596.0	4.62e-18	0.590	597.0	4.36e-18	0.580	598.0	3.67e-18	0.570	599.0	3.10e-18	0.560
600.0	2.76e-18	0.550	601.0	2.86e-18	0.540	602.0	3.32e-18	0.530	603.0	3.80e-18	0.520	604.0	4.37e-18	0.510
605.0	4.36e-18	0.400	606.0	3.32e-18	0.380	607.0	2.40e-18	0.360	608.0	1.85e-18	0.340	609.0	1.71e-18	0.320
610.0	1.77e-18	0.300	611.0	1.91e-18	0.290	612.0	2.23e-18	0.280	613.0	2.63e-18	0.270	614.0	2.55e-18	0.260
615.0	2.26e-18	0.250	616.0	2.09e-18	0.240	617.0	2.11e-18	0.230	618.0	2.39e-18	0.220	619.0	2.56e-18	0.210
620.0	3.27e-18	0.200	621.0	5.24e-18	0.190	622.0	1.02e-17	0.180	623.0	1.47e-17	0.170	624.0	1.21e-17	0.160
625.0	8.38e-18	0.150	626.0	7.30e-18	0.130	627.0	7.53e-18	0.110	628.0	7.37e-18	0.090	629.0	6.98e-18	0.070
630.0	6.76e-18	0.050	631.0	4.84e-18	0.040	632.0	3.27e-18	0.030	633.0	2.17e-18	0.020	634.0	1.64e-18	0.010
635.0	1.44e-18	0.000												
							O3O3P							
280.0	3.94e-18	0.095	281.0	3.62e-18	0.093	282.0	3.31e-18	0.090	283.0	2.99e-18	0.088	284.0	2.70e-18	0.086
285.0	2.46e-18	0.084	286.0	2.22e-18	0.082	287.0	1.98e-18	0.079	288.0	1.75e-18	0.077	289.0	1.59e-18	0.075
290.0	1.42e-18	0.073	291.0	1.25e-18	0.070	292.0	1.09e-18	0.068	293.0	9.81e-19	0.066	294.0	8.73e-19	0.064
295.0	7.65e-19	0.061	296.0	6.58e-19	0.059	297.0	5.81e-19	0.057	298.0	5.18e-19	0.055	299.0	4.55e-19	0.052
300.0	3.92e-19	0.050	301.0	3.35e-19	0.035	302.0	3.01e-19	0.025	303.0	2.66e-19	0.015	304.0	2.32e-19	0.010
305.0	1.97e-19	0.020	306.0	1.73e-19	0.050	307.0	1.55e-19	0.123	308.0	1.37e-19	0.227	309.0	1.18e-19	0.333
310.0	9.98e-20	0.400	311.0	8.92e-20	0.612	312.0	7.94e-20	0.697	313.0	6.96e-20	0.738	314.0	5.99e-20	0.762
315.0	5.01e-20	0.765	316.0	4.51e-20	0.779	317.0	4.00e-20	0.791	318.0	3.50e-20	0.806	319.0	2.99e-20	0.822
320.0	2.49e-20	0.852	321.0	2.23e-20	0.879	322.0	1.97e-20	0.903	323.0	1.72e-20	0.908	324.0	1.46e-20	0.920
325.0	1.20e-20	0.930	326.0	1.08e-20	0.934	327.0	9.67e-21	0.938	328.0	8.50e-21	0.942	329.0	7.34e-21	0.946
330.0	6.17e-21	0.950	331.0	5.48e-21	0.950	332.0	4.80e-21	0.950	333.0	4.11e-21	0.950	334.0	3.43e-21	0.950
335.0	2.74e-21	0.950	336.0	2.43e-21	0.960	337.0	2.11e-21	0.970	338.0	1.80e-21	0.980	339.0	1.48e-21	0.990
340.0	1.17e-21	1.000	350.0	0.00e+00	1.000	400.0	0.00e+00	1.000	410.0	1.20e-23	1.000	420.0	2.20e-23	1.000
440.0	1.12e-22	1.000	460.0	3.28e-22	1.000	480.0	6.84e-22	1.000	500.0	1.22e-21	1.000	520.0	1.82e-21	1.000
540.0	2.91e-21	1.000	560.0	3.94e-21	1.000	580.0	4.59e-21	1.000	600.0	5.11e-21	1.000	620.0	4.00e-21	1.000
640.0	2.96e-21	1.000	660.0	2.09e-21	1.000	680.0	1.36e-21	1.000	700.0	9.10e-22	1.000	750.0	3.20e-22	1.000
800.0	1.60e-22	1.000	900.0	0.00e+00	1.000									
							O3O1D							
280.0	3.94e-18	0.905	281.0	3.62e-18	0.907	282.0	3.31e-18	0.910	283.0	2.99e-18	0.912	284.0	2.70e-18	0.914
285.0	2.46e-18	0.916	286.0	2.22e-18	0.918	287.0	1.98e-18	0.921	288.0	1.75e-18	0.923	289.0	1.59e-18	0.925
290.0	1.42e-18	0.927	291.0	1.25e-18	0.930	292.0	1.09e-18	0.932	293.0	9.81e-19	0.934	294.0	8.73e-19	0.936
295.0	7.65e-19	0.939	296.0	6.58e-19	0.941	297.0	5.81e-19	0.943	298.0	5.18e-19	0.945	299.0	4.55e-19	0.948
300.0	3.92e-19	0.950	301.0	3.35e-19	0.965	302.0	3.01e-19	0.975	303.0	2.66e-19	0.985	304.0	2.32e-19	0.990
305.0	1.97e-19	0.980	306.0	1.73e-19	0.950	307.0	1.55e-19	0.877	308.0	1.37e-19	0.773	309.0	1.18e-19	0.667
310.0	9.98e-20	0.600	311.0	8.92e-20	0.388	312.0	7.94e-20	0.303	313.0	6.96e-20	0.262	314.0	5.99e-20	0.238
315.0	5.01e-20	0.235	316.0	4.51e-20	0.221	317.0	4.00e-20	0.209	318.0	3.50e-20	0.194	319.0	2.99e-20	0.178
320.0	2.49e-20	0.148	321.0	2.23e-20	0.121	322.0	1.97e-20	0.097	323.0	1.72e-20	0.092	324.0	1.46e-20	0.080
325.0	1.20e-20	0.070	326.0	1.08e-20	0.066	327.0	9.67e-21	0.062	328.0	8.50e-21	0.058	329.0	7.34e-21	0.054
330.0	6.17e-21	0.050	331.0	5.48e-21	0.050	332.0	4.80e-21	0.050	333.0	4.11e-21	0.050	334.0	3.43e-21	0.050
335.0	2.74e-21	0.050	336.0	2.43e-21	0.040	337.0	2.11e-21	0.030	338.0	1.80e-21	0.020	339.0	1.48e-21	0.010
340.0	1.17e-21	0.000												

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						HONO-NO								
309.0	0.00e+00	0.410	310.0	1.30e-20	0.410	311.0	1.90e-20	0.411	312.0	2.80e-20	0.421	313.0	2.20e-20	0.432
314.0	3.60e-20	0.443	315.0	3.00e-20	0.454	316.0	1.40e-20	0.464	317.0	3.10e-20	0.475	318.0	5.60e-20	0.486
319.0	3.60e-20	0.496	320.0	4.90e-20	0.507	321.0	7.80e-20	0.518	322.0	4.90e-20	0.529	323.0	5.10e-20	0.539
324.0	7.10e-20	0.550	325.0	5.00e-20	0.561	326.0	2.90e-20	0.571	327.0	6.60e-20	0.582	328.0	1.17e-19	0.593
329.0	6.10e-20	0.604	330.0	1.11e-19	0.614	331.0	1.79e-19	0.625	332.0	8.70e-20	0.636	333.0	7.60e-20	0.646
334.0	9.60e-20	0.657	335.0	9.60e-20	0.668	336.0	7.20e-20	0.679	337.0	5.30e-20	0.689	338.0	1.00e-19	0.700
339.0	1.88e-19	0.711	340.0	1.00e-19	0.721	341.0	1.70e-19	0.732	342.0	3.86e-19	0.743	343.0	1.49e-19	0.754
344.0	9.70e-20	0.764	345.0	1.09e-19	0.775	346.0	1.23e-19	0.786	347.0	1.04e-19	0.796	348.0	9.10e-20	0.807
349.0	7.90e-20	0.818	350.0	1.12e-19	0.829	351.0	2.12e-19	0.839	352.0	1.55e-19	0.850	353.0	1.91e-19	0.861
354.0	5.81e-19	0.871	355.0	3.64e-19	0.882	356.0	1.41e-19	0.893	357.0	1.17e-19	0.904	358.0	1.20e-19	0.914
359.0	1.04e-19	0.925	360.0	9.00e-20	0.936	361.0	8.30e-20	0.946	362.0	8.00e-20	0.957	363.0	9.60e-20	0.968
364.0	1.46e-19	0.979	365.0	1.68e-19	0.989	366.0	1.83e-19	1.000	367.0	3.02e-19	1.000	368.0	5.20e-19	1.000
369.0	3.88e-19	1.000	370.0	1.78e-19	1.000	371.0	1.13e-19	1.000	372.0	1.00e-19	1.000	373.0	7.70e-20	1.000
374.0	6.20e-20	1.000	375.0	5.30e-20	1.000	376.0	5.30e-20	1.000	377.0	5.00e-20	1.000	378.0	5.80e-20	1.000
379.0	8.00e-20	1.000	380.0	9.60e-20	1.000	381.0	1.13e-19	1.000	382.0	1.59e-19	1.000	383.0	2.10e-19	1.000
384.0	2.41e-19	1.000	385.0	2.03e-19	1.000	386.0	1.34e-19	1.000	387.0	9.00e-20	1.000	388.0	5.60e-20	1.000
389.0	3.40e-20	1.000	390.0	2.70e-20	1.000	391.0	2.00e-20	1.000	392.0	1.50e-20	1.000	393.0	1.10e-20	1.000
394.0	6.00e-21	1.000	395.0	1.00e-20	1.000	396.0	4.00e-21	1.000	400.0	0.00e+00	1.000			
						HONO-NO2								
309.0	0.00e+00	0.590	310.0	1.30e-20	0.590	311.0	1.90e-20	0.589	312.0	2.80e-20	0.579	313.0	2.20e-20	0.568
314.0	3.60e-20	0.557	315.0	3.00e-20	0.546	316.0	1.40e-20	0.536	317.0	3.10e-20	0.525	318.0	5.60e-20	0.514
319.0	3.60e-20	0.504	320.0	4.90e-20	0.493	321.0	7.80e-20	0.482	322.0	4.90e-20	0.471	323.0	5.10e-20	0.461
324.0	7.10e-20	0.450	325.0	5.00e-20	0.439	326.0	2.90e-20	0.429	327.0	6.60e-20	0.418	328.0	1.17e-19	0.407
329.0	6.10e-20	0.396	330.0	1.11e-19	0.386	331.0	1.79e-19	0.375	332.0	8.70e-20	0.364	333.0	7.60e-20	0.354
334.0	9.60e-20	0.343	335.0	9.60e-20	0.332	336.0	7.20e-20	0.321	337.0	5.30e-20	0.311	338.0	1.00e-19	0.300
339.0	1.88e-19	0.289	340.0	1.00e-19	0.279	341.0	1.70e-19	0.268	342.0	3.86e-19	0.257	343.0	1.49e-19	0.246
344.0	9.70e-20	0.236	345.0	1.09e-19	0.225	346.0	1.23e-19	0.214	347.0	1.04e-19	0.204	348.0	9.10e-20	0.193
349.0	7.90e-20	0.182	350.0	1.12e-19	0.171	351.0	2.12e-19	0.161	352.0	1.55e-19	0.150	353.0	1.91e-19	0.139
354.0	5.81e-19	0.129	355.0	3.64e-19	0.118	356.0	1.41e-19	0.107	357.0	1.17e-19	0.096	358.0	1.20e-19	0.086
359.0	1.04e-19	0.075	360.0	9.00e-20	0.064	361.0	8.30e-20	0.054	362.0	8.00e-20	0.043	363.0	9.60e-20	0.032
364.0	1.46e-19	0.021	365.0	1.68e-19	0.011	366.0	1.83e-19	0.000						
						HNO3								
190.0	1.36e-17	1.000	195.0	1.02e-17	1.000	200.0	5.88e-18	1.000	205.0	2.80e-18	1.000	210.0	1.04e-18	1.000
215.0	3.65e-19	1.000	220.0	1.49e-19	1.000	225.0	8.81e-20	1.000	230.0	5.75e-20	1.000	235.0	3.75e-20	1.000
240.0	2.58e-20	1.000	245.0	2.11e-20	1.000	250.0	1.97e-20	1.000	255.0	1.95e-20	1.000	260.0	1.91e-20	1.000
265.0	1.80e-20	1.000	270.0	1.62e-20	1.000	275.0	1.38e-20	1.000	280.0	1.12e-20	1.000	285.0	8.58e-21	1.000
290.0	6.15e-21	1.000	295.0	4.12e-21	1.000	300.0	2.63e-21	1.000	305.0	1.50e-21	1.000	310.0	8.10e-22	1.000
315.0	4.10e-22	1.000	320.0	2.00e-22	1.000	325.0	9.50e-23	1.000	330.0	4.30e-23	1.000	335.0	2.20e-23	1.000
340.0	1.00e-23	1.000	345.0	6.00e-24	1.000	350.0	4.00e-24	1.000	355.0	0.00e+00	1.000			
						HO2NO2								
190.0	1.01e-17	1.000	195.0	8.16e-18	1.000	200.0	5.63e-18	1.000	205.0	3.67e-18	1.000	210.0	2.39e-18	1.000
215.0	1.61e-18	1.000	220.0	1.18e-18	1.000	225.0	9.32e-19	1.000	230.0	7.88e-19	1.000	235.0	6.80e-19	1.000
240.0	5.79e-19	1.000	245.0	4.97e-19	1.000	250.0	4.11e-19	1.000	255.0	3.49e-19	1.000	260.0	2.84e-19	1.000
265.0	2.29e-19	1.000	270.0	1.80e-19	1.000	275.0	1.33e-19	1.000	280.0	9.30e-20	1.000	285.0	6.20e-20	1.000
290.0	3.90e-20	1.000	295.0	2.40e-20	1.000	300.0	1.40e-20	1.000	305.0	8.50e-21	1.000	310.0	5.30e-21	1.000
315.0	3.90e-21	1.000	320.0	2.40e-21	1.000	325.0	1.50e-21	1.000	330.0	9.00e-22	1.000	335.0	0.00e+00	1.000
						H2O2								
190.0	6.72e-19	1.000	195.0	5.63e-19	1.000	200.0	4.75e-19	1.000	205.0	4.08e-19	1.000	210.0	3.57e-19	1.000
215.0	3.07e-19	1.000	220.0	2.58e-19	1.000	225.0	2.17e-19	1.000	230.0	1.82e-19	1.000	235.0	1.50e-19	1.000
240.0	1.24e-19	1.000	245.0	1.02e-19	1.000	250.0	8.30e-20	1.000	255.0	6.70e-20	1.000	260.0	5.30e-20	1.000
265.0	4.20e-20	1.000	270.0	3.30e-20	1.000	275.0	2.60e-20	1.000	280.0	2.00e-20	1.000	285.0	1.50e-20	1.000
290.0	1.20e-20	1.000	295.0	9.00e-21	1.000	300.0	6.80e-21	1.000	305.0	5.10e-21	1.000	310.0	3.90e-21	1.000
315.0	2.90e-21	1.000	320.0	2.20e-21	1.000	325.0	1.60e-21	1.000	330.0	1.30e-21	1.000	335.0	1.00e-21	1.000
340.0	7.00e-22	1.000	345.0	5.00e-22	1.000	350.0	4.00e-22	1.000	355.0	0.00e+00	1.000			

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						HCHO_R								
240.0	6.40e-22	0.270	241.0	5.60e-22	0.272	242.0	1.05e-21	0.274	243.0	1.15e-21	0.276	244.0	8.20e-22	0.278
245.0	1.03e-21	0.280	246.0	9.80e-22	0.282	247.0	1.35e-21	0.284	248.0	1.91e-21	0.286	249.0	2.82e-21	0.288
250.0	2.05e-21	0.290	251.0	1.70e-21	0.291	252.0	2.88e-21	0.292	253.0	2.55e-21	0.293	254.0	2.55e-21	0.294
255.0	3.60e-21	0.295	256.0	5.09e-21	0.296	257.0	3.39e-21	0.297	258.0	2.26e-21	0.298	259.0	5.04e-21	0.299
260.0	5.05e-21	0.300	261.0	5.49e-21	0.308	262.0	5.20e-21	0.316	263.0	9.33e-21	0.324	264.0	8.23e-21	0.332
265.0	4.30e-21	0.340	266.0	4.95e-21	0.348	267.0	1.24e-20	0.356	268.0	1.11e-20	0.364	269.0	8.78e-21	0.372
270.0	9.36e-21	0.380	271.0	1.79e-20	0.399	272.0	1.23e-20	0.418	273.0	6.45e-21	0.437	274.0	6.56e-21	0.456
275.0	2.23e-20	0.475	276.0	2.42e-20	0.494	277.0	1.40e-20	0.513	278.0	1.05e-20	0.532	279.0	2.55e-20	0.551
280.0	2.08e-20	0.570	281.0	1.48e-20	0.586	282.0	8.81e-21	0.602	283.0	1.07e-20	0.618	284.0	4.49e-20	0.634
285.0	3.59e-20	0.650	286.0	1.96e-20	0.666	287.0	1.30e-20	0.682	288.0	3.36e-20	0.698	289.0	2.84e-20	0.714
290.0	1.30e-20	0.730	291.0	1.75e-20	0.735	292.0	8.32e-21	0.740	293.0	3.73e-20	0.745	294.0	6.54e-20	0.750
295.0	3.95e-20	0.755	296.0	2.33e-20	0.760	297.0	1.51e-20	0.765	298.0	4.04e-20	0.770	299.0	2.87e-20	0.775
300.0	8.71e-21	0.780	301.0	1.72e-20	0.780	302.0	1.06e-20	0.780	303.0	3.20e-20	0.780	304.0	6.90e-20	0.780
305.0	4.91e-20	0.780	306.0	4.63e-20	0.780	307.0	2.10e-20	0.780	308.0	1.49e-20	0.780	309.0	3.41e-20	0.780
310.0	1.95e-20	0.780	311.0	5.21e-21	0.764	312.0	1.12e-20	0.748	313.0	1.12e-20	0.732	314.0	4.75e-20	0.716
315.0	5.25e-20	0.700	316.0	2.90e-20	0.684	317.0	5.37e-20	0.668	318.0	2.98e-20	0.652	319.0	9.18e-21	0.636
320.0	1.26e-20	0.620	321.0	1.53e-20	0.585	322.0	6.69e-21	0.550	323.0	3.45e-21	0.515	324.0	8.16e-21	0.480
325.0	1.85e-20	0.445	326.0	5.95e-20	0.410	327.0	3.49e-20	0.375	328.0	1.09e-20	0.340	329.0	3.35e-20	0.305
330.0	3.32e-20	0.270	331.0	1.07e-20	0.243	332.0	2.89e-21	0.216	333.0	2.15e-21	0.189	334.0	1.71e-21	0.162
335.0	1.43e-21	0.135	336.0	1.94e-21	0.108	337.0	4.17e-21	0.081	338.0	2.36e-20	0.054	339.0	4.71e-20	0.027
340.0	2.48e-20	0.000												
						HCHO_M								
240.0	6.40e-22	0.490	241.0	5.60e-22	0.490	242.0	1.05e-21	0.490	243.0	1.15e-21	0.490	244.0	8.20e-22	0.490
245.0	1.03e-21	0.490	246.0	9.80e-22	0.490	247.0	1.35e-21	0.490	248.0	1.91e-21	0.490	249.0	2.82e-21	0.490
250.0	2.05e-21	0.490	251.0	1.70e-21	0.490	252.0	2.88e-21	0.490	253.0	2.55e-21	0.490	254.0	2.55e-21	0.490
255.0	3.60e-21	0.490	256.0	5.09e-21	0.490	257.0	3.39e-21	0.490	258.0	2.26e-21	0.490	259.0	5.04e-21	0.490
260.0	5.05e-21	0.490	261.0	5.49e-21	0.484	262.0	5.20e-21	0.478	263.0	9.33e-21	0.472	264.0	8.23e-21	0.466
265.0	4.30e-21	0.460	266.0	4.95e-21	0.454	267.0	1.24e-20	0.448	268.0	1.11e-20	0.442	269.0	8.78e-21	0.436
270.0	9.36e-21	0.430	271.0	1.79e-20	0.419	272.0	1.23e-20	0.408	273.0	6.45e-21	0.397	274.0	6.56e-21	0.386
275.0	2.23e-20	0.375	276.0	2.42e-20	0.364	277.0	1.40e-20	0.353	278.0	1.05e-20	0.342	279.0	2.55e-20	0.331
280.0	2.08e-20	0.320	281.0	1.48e-20	0.312	282.0	8.81e-21	0.304	283.0	1.07e-20	0.296	284.0	4.49e-20	0.288
285.0	3.59e-20	0.280	286.0	1.96e-20	0.272	287.0	1.30e-20	0.264	288.0	3.36e-20	0.256	289.0	2.84e-20	0.248
290.0	1.30e-20	0.240	291.0	1.75e-20	0.237	292.0	8.32e-21	0.234	293.0	3.73e-20	0.231	294.0	6.54e-20	0.228
295.0	3.95e-20	0.225	296.0	2.33e-20	0.222	297.0	1.51e-20	0.219	298.0	4.04e-20	0.216	299.0	2.87e-20	0.213
300.0	8.71e-21	0.210	301.0	1.72e-20	0.211	302.0	1.06e-20	0.212	303.0	3.20e-20	0.213	304.0	6.90e-20	0.214
305.0	4.91e-20	0.215	306.0	4.63e-20	0.216	307.0	2.10e-20	0.217	308.0	1.49e-20	0.218	309.0	3.41e-20	0.219
310.0	1.95e-20	0.220	311.0	5.21e-21	0.236	312.0	1.12e-20	0.252	313.0	1.12e-20	0.268	314.0	4.75e-20	0.284
315.0	5.25e-20	0.300	316.0	2.90e-20	0.316	317.0	5.37e-20	0.332	318.0	2.98e-20	0.348	319.0	9.18e-21	0.364
320.0	1.26e-20	0.380	321.0	1.53e-20	0.408	322.0	6.69e-21	0.436	323.0	3.45e-21	0.464	324.0	8.16e-21	0.492
325.0	1.85e-20	0.520	326.0	5.95e-20	0.548	327.0	3.49e-20	0.576	328.0	1.09e-20	0.604	329.0	3.35e-20	0.632
330.0	3.32e-20	0.660	331.0	1.07e-20	0.650	332.0	2.89e-21	0.640	333.0	2.15e-21	0.630	334.0	1.71e-21	0.620
335.0	1.43e-21	0.610	336.0	1.94e-21	0.600	337.0	4.17e-21	0.590	338.0	2.36e-20	0.580	339.0	4.71e-20	0.570
340.0	2.48e-20	0.560	341.0	7.59e-21	0.525	342.0	6.81e-21	0.490	343.0	1.95e-20	0.455	344.0	1.14e-20	0.420
345.0	3.23e-21	0.385	346.0	1.13e-21	0.350	347.0	6.60e-22	0.315	348.0	1.22e-21	0.280	349.0	3.20e-22	0.245
350.0	3.80e-22	0.210	351.0	1.04e-21	0.192	352.0	7.13e-21	0.174	353.0	2.21e-20	0.156	354.0	1.54e-20	0.138
355.0	6.76e-21	0.120	356.0	1.35e-21	0.102	357.0	3.60e-22	0.084	358.0	5.70e-23	0.066	359.0	5.80e-22	0.048
360.0	8.20e-22	0.000												

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						CCHO_R								
262.0	2.44e-20	0.326	266.0	3.05e-20	0.358	270.0	3.42e-20	0.390	274.0	4.03e-20	0.466	278.0	4.19e-20	0.542
280.0	4.50e-20	0.580	281.0	4.69e-20	0.575	282.0	4.72e-20	0.570	283.0	4.75e-20	0.565	284.0	4.61e-20	0.560
285.0	4.49e-20	0.555	286.0	4.44e-20	0.550	287.0	4.59e-20	0.545	288.0	4.72e-20	0.540	289.0	4.77e-20	0.535
290.0	4.89e-20	0.530	291.0	4.78e-20	0.520	292.0	4.68e-20	0.510	293.0	4.53e-20	0.500	294.0	4.33e-20	0.490
295.0	4.27e-20	0.480	296.0	4.24e-20	0.470	297.0	4.38e-20	0.460	298.0	4.41e-20	0.450	299.0	4.26e-20	0.440
300.0	4.16e-20	0.430	301.0	3.99e-20	0.418	302.0	3.86e-20	0.406	303.0	3.72e-20	0.394	304.0	3.48e-20	0.382
305.0	3.42e-20	0.370	306.0	3.42e-20	0.354	307.0	3.36e-20	0.338	308.0	3.33e-20	0.322	309.0	3.14e-20	0.306
310.0	2.93e-20	0.290	311.0	2.76e-20	0.266	312.0	2.53e-20	0.242	313.0	2.47e-20	0.218	314.0	2.44e-20	0.194
315.0	2.20e-20	0.170	316.0	2.04e-20	0.156	317.0	2.07e-20	0.142	318.0	1.98e-20	0.128	319.0	1.87e-20	0.114
320.0	1.72e-20	0.100	321.0	1.48e-20	0.088	322.0	1.40e-20	0.076	323.0	1.24e-20	0.064	324.0	1.09e-20	0.052
325.0	1.14e-20	0.040	326.0	1.07e-20	0.032	327.0	8.58e-21	0.024	328.0	7.47e-21	0.016	329.0	7.07e-21	0.008
						C2CHO								
294.0	5.80e-20	0.890	295.0	5.57e-20	0.885	296.0	5.37e-20	0.880	297.0	5.16e-20	0.875	298.0	5.02e-20	0.870
299.0	5.02e-20	0.865	300.0	5.04e-20	0.860	301.0	5.09e-20	0.855	302.0	5.07e-20	0.850	303.0	4.94e-20	0.818
304.0	4.69e-20	0.786	305.0	4.32e-20	0.755	306.0	4.04e-20	0.723	307.0	3.81e-20	0.691	308.0	3.65e-20	0.659
309.0	3.62e-20	0.627	310.0	3.60e-20	0.596	311.0	3.53e-20	0.564	312.0	3.50e-20	0.532	313.0	3.32e-20	0.500
314.0	3.06e-20	0.480	315.0	2.77e-20	0.460	316.0	2.43e-20	0.440	317.0	2.18e-20	0.420	318.0	2.00e-20	0.400
319.0	1.86e-20	0.380	320.0	1.83e-20	0.360	321.0	1.78e-20	0.340	322.0	1.66e-20	0.320	323.0	1.58e-20	0.300
324.0	1.49e-20	0.280	325.0	1.30e-20	0.260	326.0	1.13e-20	0.248	327.0	9.96e-21	0.236	328.0	8.28e-21	0.223
329.0	6.85e-21	0.211	330.0	5.75e-21	0.199	331.0	4.94e-21	0.187	332.0	4.66e-21	0.174	333.0	4.30e-21	0.162
334.0	3.73e-21	0.150	335.0	3.25e-21	0.133	336.0	2.80e-21	0.117	337.0	2.30e-21	0.100	338.0	1.85e-21	0.083
339.0	1.66e-21	0.067	340.0	1.55e-21	0.050	341.0	1.19e-21	0.033	342.0	7.60e-22	0.017	343.0	4.50e-22	0.000
						KETONE								
198.5	3.95e-19	1.000	199.0	1.61e-19	1.000	199.5	7.75e-20	1.000	200.0	3.76e-20	1.000	200.5	2.51e-20	1.000
201.0	1.83e-20	1.000	201.5	1.36e-20	1.000	202.0	1.16e-20	1.000	202.5	8.97e-21	1.000	203.0	4.62e-21	1.000
203.5	3.18e-21	1.000	204.0	2.42e-21	1.000	204.5	2.01e-21	1.000	205.0	1.77e-21	1.000	205.5	1.64e-21	1.000
206.0	1.54e-21	1.000	206.5	1.52e-21	1.000	207.0	1.54e-21	1.000	207.5	1.62e-21	1.000	208.0	1.64e-21	1.000
208.5	1.60e-21	1.000	209.0	1.57e-21	1.000	209.5	1.49e-21	1.000	210.0	1.47e-21	1.000	210.5	1.52e-21	1.000
211.0	1.50e-21	1.000	211.5	1.62e-21	1.000	212.0	1.81e-21	1.000	212.5	2.10e-21	1.000	213.0	2.23e-21	1.000
213.5	2.06e-21	1.000	214.0	1.69e-21	1.000	214.5	1.49e-21	1.000	215.0	1.42e-21	1.000	215.5	1.42e-21	1.000
216.0	1.42e-21	1.000	216.5	1.48e-21	1.000	217.0	1.48e-21	1.000	217.5	1.53e-21	1.000	218.0	1.56e-21	1.000
218.5	1.67e-21	1.000	219.0	1.68e-21	1.000	219.5	1.78e-21	1.000	220.0	1.85e-21	1.000	220.5	1.92e-21	1.000
221.0	2.01e-21	1.000	221.5	2.11e-21	1.000	222.0	2.23e-21	1.000	222.5	2.33e-21	1.000	223.0	2.48e-21	1.000
223.5	2.60e-21	1.000	224.0	2.74e-21	1.000	224.5	2.85e-21	1.000	225.0	3.04e-21	1.000	225.5	3.15e-21	1.000
226.0	3.33e-21	1.000	226.5	3.55e-21	1.000	227.0	3.73e-21	1.000	227.5	3.93e-21	1.000	228.0	4.11e-21	1.000
228.5	4.34e-21	1.000	229.0	4.56e-21	1.000	229.5	4.75e-21	1.000	230.0	5.01e-21	1.000	230.5	5.27e-21	1.000
231.0	5.53e-21	1.000	231.5	5.83e-21	1.000	232.0	6.15e-21	1.000	232.5	6.45e-21	1.000	233.0	6.73e-21	1.000
233.5	7.02e-21	1.000	234.0	7.42e-21	1.000	234.5	7.83e-21	1.000	235.0	8.11e-21	1.000	235.5	8.45e-21	1.000
236.0	8.82e-21	1.000	236.5	9.21e-21	1.000	237.0	9.65e-21	1.000	237.5	1.00e-20	1.000	238.0	1.05e-20	1.000
238.5	1.10e-20	1.000	239.0	1.15e-20	1.000	239.5	1.20e-20	1.000	240.0	1.23e-20	1.000	240.5	1.28e-20	1.000
241.0	1.32e-20	1.000	241.5	1.38e-20	1.000	242.0	1.44e-20	1.000	242.5	1.50e-20	1.000	243.0	1.57e-20	1.000
243.5	1.63e-20	1.000	244.0	1.68e-20	1.000	244.5	1.75e-20	1.000	245.0	1.81e-20	1.000	245.5	1.88e-20	1.000
246.0	1.96e-20	1.000	246.5	2.03e-20	1.000	247.0	2.11e-20	1.000	247.5	2.19e-20	1.000	248.0	2.25e-20	1.000
248.5	2.33e-20	1.000	249.0	2.40e-20	1.000	249.5	2.48e-20	1.000	250.0	2.56e-20	1.000	250.5	2.64e-20	1.000
251.0	2.73e-20	1.000	251.5	2.81e-20	1.000	252.0	2.88e-20	1.000	252.5	2.98e-20	1.000	253.0	3.07e-20	1.000
253.5	3.16e-20	1.000	254.0	3.25e-20	1.000	254.5	3.34e-20	1.000	255.0	3.43e-20	1.000	255.5	3.51e-20	1.000
256.0	3.59e-20	1.000	256.5	3.67e-20	1.000	257.0	3.75e-20	1.000	257.5	3.84e-20	1.000	258.0	3.94e-20	1.000
258.5	4.03e-20	1.000	259.0	4.13e-20	1.000	259.5	4.22e-20	1.000	260.0	4.28e-20	1.000	260.5	4.33e-20	1.000
261.0	4.41e-20	1.000	261.5	4.49e-20	1.000	262.0	4.57e-20	1.000	262.5	4.65e-20	1.000	263.0	4.72e-20	1.000
263.5	4.78e-20	1.000	264.0	4.85e-20	1.000	264.5	4.92e-20	1.000	265.0	4.99e-20	1.000	265.5	5.04e-20	1.000
266.0	5.12e-20	1.000	266.5	5.22e-20	1.000	267.0	5.28e-20	1.000	267.5	5.34e-20	1.000	268.0	5.41e-20	1.000
268.5	5.46e-20	1.000	269.0	5.51e-20	1.000	269.5	5.55e-20	1.000	270.0	5.59e-20	1.000	270.5	5.63e-20	1.000
271.0	5.66e-20	1.000	271.5	5.70e-20	1.000	272.0	5.74e-20	1.000	272.5	5.78e-20	1.000	273.0	5.81e-20	1.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
273.5	5.86e-20	1.000	274.0	5.90e-20	1.000	274.5	5.93e-20	1.000	275.0	5.96e-20	1.000	275.5	5.97e-20	1.000
276.0	5.98e-20	1.000	276.5	5.98e-20	1.000	277.0	5.99e-20	1.000	277.5	5.99e-20	1.000	278.0	5.98e-20	1.000
278.5	5.96e-20	1.000	279.0	5.96e-20	1.000	279.5	5.95e-20	1.000	280.0	5.94e-20	1.000	280.5	5.92e-20	1.000
281.0	5.90e-20	1.000	281.5	5.88e-20	1.000	282.0	5.86e-20	1.000	282.5	5.83e-20	1.000	283.0	5.79e-20	1.000
283.5	5.75e-20	1.000	284.0	5.71e-20	1.000	284.5	5.67e-20	1.000	285.0	5.61e-20	1.000	285.5	5.56e-20	1.000
286.0	5.51e-20	1.000	286.5	5.45e-20	1.000	287.0	5.41e-20	1.000	287.5	5.37e-20	1.000	288.0	5.33e-20	1.000
288.5	5.27e-20	1.000	289.0	5.21e-20	1.000	289.5	5.15e-20	1.000	290.0	5.08e-20	1.000	290.5	4.99e-20	1.000
291.0	4.89e-20	1.000	291.5	4.82e-20	1.000	292.0	4.73e-20	1.000	292.5	4.62e-20	1.000	293.0	4.53e-20	1.000
293.5	4.41e-20	1.000	294.0	4.32e-20	1.000	294.5	4.23e-20	1.000	295.0	4.15e-20	1.000	295.5	4.11e-20	1.000
296.0	4.01e-20	1.000	296.5	3.94e-20	1.000	297.0	3.88e-20	1.000	297.5	3.77e-20	1.000	298.0	3.69e-20	1.000
298.5	3.63e-20	1.000	299.0	3.54e-20	1.000	299.5	3.46e-20	1.000	300.0	3.36e-20	1.000	300.5	3.24e-20	1.000
301.0	3.16e-20	1.000	301.5	3.06e-20	1.000	302.0	2.95e-20	1.000	302.5	2.82e-20	1.000	303.0	2.70e-20	1.000
303.5	2.59e-20	1.000	304.0	2.49e-20	1.000	304.5	2.42e-20	1.000	305.0	2.34e-20	1.000	305.5	2.28e-20	1.000
306.0	2.19e-20	1.000	306.5	2.11e-20	1.000	307.0	2.04e-20	1.000	307.5	1.93e-20	1.000	308.0	1.88e-20	1.000
308.5	1.80e-20	1.000	309.0	1.73e-20	1.000	309.5	1.66e-20	1.000	310.0	1.58e-20	1.000	310.5	1.48e-20	1.000
311.0	1.42e-20	1.000	311.5	1.34e-20	1.000	312.0	1.26e-20	1.000	312.5	1.17e-20	1.000	313.0	1.13e-20	1.000
313.5	1.08e-20	1.000	314.0	1.04e-20	1.000	314.5	9.69e-21	1.000	315.0	8.91e-21	1.000	315.5	8.61e-21	1.000
316.0	7.88e-21	1.000	316.5	7.25e-21	1.000	317.0	6.92e-21	1.000	317.5	6.43e-21	1.000	318.0	6.07e-21	1.000
318.5	5.64e-21	1.000	319.0	5.19e-21	1.000	319.5	4.66e-21	1.000	320.0	4.36e-21	1.000	320.5	3.95e-21	1.000
321.0	3.64e-21	1.000	321.5	3.38e-21	1.000	322.0	3.17e-21	1.000	322.5	2.80e-21	1.000	323.0	2.62e-21	1.000
323.5	2.29e-21	1.000	324.0	2.13e-21	1.000	324.5	1.93e-21	1.000	325.0	1.70e-21	1.000	325.5	1.58e-21	1.000
326.0	1.48e-21	1.000	326.5	1.24e-21	1.000	327.0	1.20e-21	1.000	327.5	1.04e-21	1.000	328.0	9.51e-22	1.000
328.5	8.44e-22	1.000	329.0	7.26e-22	1.000	329.5	6.70e-22	1.000	330.0	6.08e-22	1.000	330.5	5.15e-22	1.000
331.0	4.56e-22	1.000	331.5	4.13e-22	1.000	332.0	3.56e-22	1.000	332.5	3.30e-22	1.000	333.0	2.97e-22	1.000
333.5	2.67e-22	1.000	334.0	2.46e-22	1.000	334.5	2.21e-22	1.000	335.0	1.93e-22	1.000	335.5	1.56e-22	1.000
336.0	1.47e-22	1.000	336.5	1.37e-22	1.000	337.0	1.27e-22	1.000	337.5	1.19e-22	1.000	338.0	1.09e-22	1.000
338.5	1.01e-22	1.000	339.0	9.09e-23	1.000	339.5	8.22e-23	1.000	340.0	7.66e-23	1.000	340.5	7.43e-23	1.000
341.0	6.83e-23	1.000	341.5	6.72e-23	1.000	342.0	6.04e-23	1.000	342.5	4.78e-23	1.000	343.0	0.00e+00	1.000
COOH														
210.0	3.12e-19	1.000	215.0	2.09e-19	1.000	220.0	1.54e-19	1.000	225.0	1.22e-19	1.000	230.0	9.62e-20	1.000
235.0	7.61e-20	1.000	240.0	6.05e-20	1.000	245.0	4.88e-20	1.000	250.0	3.98e-20	1.000	255.0	3.23e-20	1.000
260.0	2.56e-20	1.000	265.0	2.11e-20	1.000	270.0	1.70e-20	1.000	275.0	1.39e-20	1.000	280.0	1.09e-20	1.000
285.0	8.63e-21	1.000	290.0	6.91e-21	1.000	295.0	5.51e-21	1.000	300.0	4.13e-21	1.000	305.0	3.13e-21	1.000
310.0	2.39e-21	1.000	315.0	1.82e-21	1.000	320.0	1.37e-21	1.000	325.0	1.05e-21	1.000	330.0	7.90e-22	1.000
335.0	6.10e-22	1.000	340.0	4.70e-22	1.000	345.0	3.50e-22	1.000	350.0	2.70e-22	1.000	355.0	2.10e-22	1.000
360.0	1.60e-22	1.000	365.0	1.20e-22	1.000	370.0	0.00e+00	1.000						
GLY_R														
230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
345.0	0.00e+00	1.000	350.0	0.00e+00	1.000	355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000
370.0	8.03e-21	1.000	375.0	1.00e-20	1.000	380.0	1.72e-20	0.972	382.0	1.58e-20	0.855	384.0	1.49e-20	0.737
386.0	1.49e-20	0.619	388.0	2.87e-20	0.502	390.0	3.15e-20	0.384	391.0	3.24e-20	0.326	392.0	3.04e-20	0.267
393.0	2.23e-20	0.208	394.0	2.63e-20	0.149	395.0	3.04e-20	0.090	396.0	2.63e-20	0.032	397.0	2.43e-20	0.000
398.0	3.24e-20	0.000	399.0	3.04e-20	0.000	400.0	2.84e-20	0.000	401.0	3.24e-20	0.000	402.0	4.46e-20	0.000
403.0	5.27e-20	0.000	404.0	4.26e-20	0.000	405.0	3.04e-20	0.000	406.0	3.04e-20	0.000	407.0	2.84e-20	0.000
408.0	2.43e-20	0.000	409.0	2.84e-20	0.000	410.0	6.08e-20	0.000	411.0	5.07e-20	0.000	411.5	6.08e-20	0.000
412.0	4.86e-20	0.000	413.0	8.31e-20	0.000	413.5	6.48e-20	0.000	414.0	7.50e-20	0.000	414.5	8.11e-20	0.000
415.0	8.11e-20	0.000	415.5	6.89e-20	0.000	416.0	4.26e-20	0.000	417.0	4.86e-20	0.000	418.0	5.88e-20	0.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						GLY_ABS								
230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000	370.0	8.03e-21	1.000	375.0	1.00e-20	1.000
380.0	1.72e-20	1.000	382.0	1.58e-20	1.000	384.0	1.49e-20	1.000	386.0	1.49e-20	1.000	388.0	2.87e-20	1.000
390.0	3.15e-20	1.000	391.0	3.24e-20	1.000	392.0	3.04e-20	1.000	393.0	2.23e-20	1.000	394.0	2.63e-20	1.000
395.0	3.04e-20	1.000	396.0	2.63e-20	1.000	397.0	2.43e-20	1.000	398.0	3.24e-20	1.000	399.0	3.04e-20	1.000
400.0	2.84e-20	1.000	401.0	3.24e-20	1.000	402.0	4.46e-20	1.000	403.0	5.27e-20	1.000	404.0	4.26e-20	1.000
405.0	3.04e-20	1.000	406.0	3.04e-20	1.000	407.0	2.84e-20	1.000	408.0	2.43e-20	1.000	409.0	2.84e-20	1.000
410.0	6.08e-20	1.000	411.0	5.07e-20	1.000	411.5	6.08e-20	1.000	412.0	4.86e-20	1.000	413.0	8.31e-20	1.000
413.5	6.48e-20	1.000	414.0	7.50e-20	1.000	414.5	8.11e-20	1.000	415.0	8.11e-20	1.000	415.5	6.89e-20	1.000
416.0	4.26e-20	1.000	417.0	4.86e-20	1.000	418.0	5.88e-20	1.000	419.0	6.69e-20	1.000	420.0	3.85e-20	1.000
421.0	5.67e-20	1.000	421.5	4.46e-20	1.000	422.0	5.27e-20	1.000	422.5	1.05e-19	1.000	423.0	8.51e-20	1.000
424.0	6.08e-20	1.000	425.0	7.29e-20	1.000	426.0	1.18e-19	1.000	426.5	1.30e-19	1.000	427.0	1.07e-19	1.000
428.0	1.66e-19	1.000	429.0	4.05e-20	1.000	430.0	5.07e-20	1.000	431.0	4.86e-20	1.000	432.0	4.05e-20	1.000
433.0	3.65e-20	1.000	434.0	4.05e-20	1.000	434.5	6.08e-20	1.000	435.0	5.07e-20	1.000	436.0	8.11e-20	1.000
436.5	1.13e-19	1.000	437.0	5.27e-20	1.000	438.0	1.01e-19	1.000	438.5	1.38e-19	1.000	439.0	7.70e-20	1.000
440.0	2.47e-19	1.000	441.0	8.11e-20	1.000	442.0	6.08e-20	1.000	443.0	7.50e-20	1.000	444.0	9.32e-20	1.000
445.0	1.13e-19	1.000	446.0	5.27e-20	1.000	447.0	2.43e-20	1.000	448.0	2.84e-20	1.000	449.0	3.85e-20	1.000
450.0	6.08e-20	1.000	451.0	1.09e-19	1.000	451.5	9.32e-20	1.000	452.0	1.22e-19	1.000	453.0	2.39e-19	1.000
454.0	1.70e-19	1.000	455.0	3.40e-19	1.000	455.5	4.05e-19	1.000	456.0	1.01e-19	1.000	457.0	1.62e-20	1.000
458.0	1.22e-20	1.000	458.5	1.42e-20	1.000	459.0	4.05e-21	1.000	460.0	4.05e-21	1.000	460.5	6.08e-21	1.000
461.0	2.03e-21	1.000	462.0	0.00e+00	1.000									
						MGLY_ADJ								
219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	0.992	344.5	2.91e-21	0.984	345.0	2.95e-21	0.976	345.5	3.00e-21	0.968	346.0	3.08e-21	0.960
346.5	3.18e-21	0.953	347.0	3.25e-21	0.945	347.5	3.30e-21	0.937	348.0	3.39e-21	0.929	348.5	3.51e-21	0.921
349.0	3.63e-21	0.913	349.5	3.73e-21	0.905	350.0	3.85e-21	0.897	350.5	3.99e-21	0.889	351.0	4.27e-21	0.881
351.5	4.47e-21	0.873	352.0	4.63e-21	0.865	352.5	4.78e-21	0.858	353.0	4.92e-21	0.850	353.5	5.07e-21	0.842
354.0	5.23e-21	0.834	354.5	5.39e-21	0.826	355.0	5.56e-21	0.818	355.5	5.77e-21	0.810	356.0	5.97e-21	0.802
356.5	6.15e-21	0.794	357.0	6.35e-21	0.786	357.5	6.56e-21	0.778	358.0	6.76e-21	0.770	358.5	6.95e-21	0.763
359.0	7.20e-21	0.755	359.5	7.44e-21	0.747	360.0	7.64e-21	0.739	360.5	7.89e-21	0.731	361.0	8.15e-21	0.723
361.5	8.43e-21	0.715	362.0	8.71e-21	0.707	362.5	9.02e-21	0.699	363.0	9.33e-21	0.691	363.5	9.65e-21	0.683
364.0	1.00e-20	0.675	364.5	1.04e-20	0.668	365.0	1.08e-20	0.660	365.5	1.11e-20	0.652	366.0	1.15e-20	0.644
366.5	1.19e-20	0.636	367.0	1.23e-20	0.628	367.5	1.27e-20	0.620	368.0	1.31e-20	0.612	368.5	1.35e-20	0.604
369.0	1.40e-20	0.596	369.5	1.44e-20	0.588	370.0	1.47e-20	0.580	370.5	1.51e-20	0.573	371.0	1.55e-20	0.565
371.5	1.59e-20	0.557	372.0	1.64e-20	0.549	372.5	1.70e-20	0.541	373.0	1.73e-20	0.533	373.5	1.77e-20	0.525
374.0	1.81e-20	0.517	374.5	1.86e-20	0.509	375.0	1.90e-20	0.501	375.5	1.96e-20	0.493	376.0	2.02e-20	0.486
376.5	2.06e-20	0.478	377.0	2.10e-20	0.470	377.5	2.14e-20	0.462	378.0	2.18e-20	0.454	378.5	2.24e-20	0.446
379.0	2.30e-20	0.438	379.5	2.37e-20	0.430	380.0	2.42e-20	0.422	380.5	2.47e-20	0.414	381.0	2.54e-20	0.406
381.5	2.62e-20	0.398	382.0	2.69e-20	0.391	382.5	2.79e-20	0.383	383.0	2.88e-20	0.375	383.5	2.96e-20	0.367
384.0	3.02e-20	0.359	384.5	3.10e-20	0.351	385.0	3.20e-20	0.343	385.5	3.29e-20	0.335	386.0	3.39e-20	0.327
386.5	3.51e-20	0.319	387.0	3.62e-20	0.311	387.5	3.69e-20	0.303	388.0	3.70e-20	0.296	388.5	3.77e-20	0.288
389.0	3.88e-20	0.280	389.5	3.97e-20	0.272	390.0	4.03e-20	0.264	390.5	4.12e-20	0.256	391.0	4.22e-20	0.248
391.5	4.29e-20	0.240	392.0	4.30e-20	0.232	392.5	4.38e-20	0.224	393.0	4.47e-20	0.216	393.5	4.55e-20	0.208
394.0	4.56e-20	0.201	394.5	4.59e-20	0.193	395.0	4.67e-20	0.185	395.5	4.80e-20	0.177	396.0	4.87e-20	0.169
396.5	4.96e-20	0.161	397.0	5.08e-20	0.153	397.5	5.19e-20	0.145	398.0	5.23e-20	0.137	398.5	5.39e-20	0.129
399.0	5.46e-20	0.121	399.5	5.54e-20	0.113	400.0	5.59e-20	0.106	400.5	5.77e-20	0.098	401.0	5.91e-20	0.090
401.5	5.99e-20	0.082	402.0	6.06e-20	0.074	402.5	6.20e-20	0.066	403.0	6.35e-20	0.058	403.5	6.52e-20	0.050
404.0	6.54e-20	0.042	404.5	6.64e-20	0.034	405.0	6.93e-20	0.026	405.5	7.15e-20	0.018	406.0	7.19e-20	0.011
406.5	7.32e-20	0.003	407.0	7.58e-20	0.000	407.5	7.88e-20	0.000	408.0	7.97e-20	0.000	408.5	7.91e-20	0.000
409.0	8.11e-20	0.000	409.5	8.41e-20	0.000	410.0	8.53e-20	0.000	410.5	8.59e-20	0.000	411.0	8.60e-20	0.000
411.5	8.80e-20	0.000	412.0	9.04e-20	0.000	412.5	9.45e-20	0.000	413.0	9.34e-20	0.000	413.5	9.37e-20	0.000
414.0	9.63e-20	0.000	414.5	9.71e-20	0.000	415.0	9.70e-20	0.000	415.5	9.65e-20	0.000	416.0	9.69e-20	0.000
416.5	9.89e-20	0.000	417.0	1.00e-19	0.000	417.5	1.02e-19	0.000	418.0	1.00e-19	0.000	418.5	1.02e-19	0.000
419.0	1.01e-19	0.000	419.5	1.01e-19	0.000	420.0	1.03e-19	0.000	420.5	1.01e-19	0.000	421.0	1.04e-19	0.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						BACL_ADJ								
230.0	1.30e-20	1.000	232.5	1.46e-20	1.000	235.0	1.68e-20	1.000	237.5	1.84e-20	1.000	240.0	2.16e-20	1.000
242.5	2.49e-20	1.000	245.0	2.65e-20	1.000	247.5	2.71e-20	1.000	250.0	3.03e-20	1.000	252.5	3.46e-20	1.000
255.0	3.46e-20	1.000	257.5	3.57e-20	1.000	260.0	3.95e-20	1.000	262.5	4.17e-20	1.000	265.0	4.17e-20	1.000
267.5	4.22e-20	1.000	270.0	4.60e-20	1.000	272.5	4.54e-20	1.000	275.0	4.33e-20	1.000	277.5	4.22e-20	1.000
280.0	4.44e-20	1.000	282.5	4.33e-20	1.000	285.0	3.90e-20	1.000	287.5	3.57e-20	1.000	290.0	3.25e-20	1.000
292.5	2.92e-20	1.000	295.0	2.60e-20	1.000	297.5	2.16e-20	1.000	300.0	1.79e-20	1.000	302.5	1.73e-20	1.000
305.0	1.46e-20	1.000	307.5	1.08e-20	1.000	310.0	9.20e-21	1.000	312.5	7.03e-21	1.000	315.0	6.49e-21	1.000
317.5	5.41e-21	1.000	320.0	5.41e-21	1.000	322.5	5.41e-21	1.000	325.0	4.33e-21	1.000	327.5	3.25e-21	1.000
330.0	3.79e-21	1.000	332.5	3.79e-21	1.000	335.0	4.33e-21	1.000	337.5	4.87e-21	1.000	340.0	5.41e-21	1.000
342.5	5.95e-21	1.000	345.0	6.49e-21	1.000	347.5	7.03e-21	1.000	350.0	8.12e-21	0.995	352.5	7.57e-21	0.960
355.0	9.20e-21	0.925	357.5	9.74e-21	0.890	360.0	1.08e-20	0.855	362.5	1.19e-20	0.820	365.0	1.41e-20	0.785
367.5	1.51e-20	0.750	370.0	1.79e-20	0.715	372.5	2.00e-20	0.680	375.0	2.11e-20	0.645	377.5	2.33e-20	0.610
380.0	2.60e-20	0.575	382.5	2.81e-20	0.540	385.0	3.14e-20	0.505	387.5	3.46e-20	0.470	390.0	3.90e-20	0.435
392.5	4.11e-20	0.399	395.0	4.33e-20	0.364	397.5	4.38e-20	0.329	400.0	4.65e-20	0.294	402.5	4.81e-20	0.259
405.0	5.19e-20	0.224	407.5	5.84e-20	0.189	410.0	6.06e-20	0.154	412.5	6.49e-20	0.119	415.0	6.92e-20	0.084
417.5	6.87e-20	0.049	420.0	6.82e-20	0.014	422.5	6.71e-20	0.000	425.0	6.49e-20	0.000	427.5	5.95e-20	0.000
430.0	5.73e-20	0.000	432.5	6.28e-20	0.000	435.0	6.01e-20	0.000	437.5	5.84e-20	0.000	440.0	5.95e-20	0.000
442.5	6.49e-20	0.000	445.0	5.95e-20	0.000	447.5	4.98e-20	0.000	450.0	3.79e-20	0.000	452.5	2.81e-20	0.000
455.0	1.73e-20	0.000	457.5	1.08e-20	0.000	460.0	5.41e-21	0.000	462.5	3.79e-21	0.000	465.0	2.16e-21	0.000
467.5	1.08e-21	0.000	470.0	1.08e-21	0.000	472.5	0.00e+00	0.000						
						BZCHO								
299.0	1.78e-19	1.000	304.0	7.40e-20	1.000	306.0	6.91e-20	1.000	309.0	6.41e-20	1.000	313.0	6.91e-20	1.000
314.0	6.91e-20	1.000	318.0	6.41e-20	1.000	325.0	8.39e-20	1.000	332.0	7.65e-20	1.000	338.0	8.88e-20	1.000
342.0	8.88e-20	1.000	346.0	7.89e-20	1.000	349.0	7.89e-20	1.000	354.0	9.13e-20	1.000	355.0	8.14e-20	1.000
364.0	5.67e-20	1.000	368.0	6.66e-20	1.000	369.0	8.39e-20	1.000	370.0	8.39e-20	1.000	372.0	3.45e-20	1.000
374.0	3.21e-20	1.000	376.0	2.47e-20	1.000	377.0	2.47e-20	1.000	380.0	3.58e-20	1.000	382.0	9.90e-21	1.000
386.0	0.00e+00	1.000												
						ACROLEIN								
250.0	1.80e-21	1.000	252.0	2.05e-21	1.000	253.0	2.20e-21	1.000	254.0	2.32e-21	1.000	255.0	2.45e-21	1.000
256.0	2.56e-21	1.000	257.0	2.65e-21	1.000	258.0	2.74e-21	1.000	259.0	2.83e-21	1.000	260.0	2.98e-21	1.000
261.0	3.24e-21	1.000	262.0	3.47e-21	1.000	263.0	3.58e-21	1.000	264.0	3.93e-21	1.000	265.0	4.67e-21	1.000
266.0	5.10e-21	1.000	267.0	5.38e-21	1.000	268.0	5.73e-21	1.000	269.0	6.13e-21	1.000	270.0	6.64e-21	1.000
271.0	7.20e-21	1.000	272.0	7.77e-21	1.000	273.0	8.37e-21	1.000	274.0	8.94e-21	1.000	275.0	9.55e-21	1.000
276.0	1.04e-20	1.000	277.0	1.12e-20	1.000	278.0	1.19e-20	1.000	279.0	1.27e-20	1.000	280.0	1.27e-20	1.000
281.0	1.26e-20	1.000	282.0	1.26e-20	1.000	283.0	1.28e-20	1.000	284.0	1.33e-20	1.000	285.0	1.38e-20	1.000
286.0	1.44e-20	1.000	287.0	1.50e-20	1.000	288.0	1.57e-20	1.000	289.0	1.63e-20	1.000	290.0	1.71e-20	1.000
291.0	1.78e-20	1.000	292.0	1.86e-20	1.000	293.0	1.95e-20	1.000	294.0	2.05e-20	1.000	295.0	2.15e-20	1.000
296.0	2.26e-20	1.000	297.0	2.37e-20	1.000	298.0	2.48e-20	1.000	299.0	2.60e-20	1.000	300.0	2.73e-20	1.000
301.0	2.85e-20	1.000	302.0	2.99e-20	1.000	303.0	3.13e-20	1.000	304.0	3.27e-20	1.000	305.0	3.39e-20	1.000
306.0	3.51e-20	1.000	307.0	3.63e-20	1.000	308.0	3.77e-20	1.000	309.0	3.91e-20	1.000	310.0	4.07e-20	1.000
311.0	4.25e-20	1.000	312.0	4.39e-20	1.000	313.0	4.44e-20	1.000	314.0	4.50e-20	1.000	315.0	4.59e-20	1.000
316.0	4.75e-20	1.000	317.0	4.90e-20	1.000	318.0	5.05e-20	1.000	319.0	5.19e-20	1.000	320.0	5.31e-20	1.000
321.0	5.43e-20	1.000	322.0	5.52e-20	1.000	323.0	5.60e-20	1.000	324.0	5.67e-20	1.000	325.0	5.67e-20	1.000
326.0	5.62e-20	1.000	327.0	5.63e-20	1.000	328.0	5.71e-20	1.000	329.0	5.76e-20	1.000	330.0	5.80e-20	1.000
331.0	5.95e-20	1.000	332.0	6.23e-20	1.000	333.0	6.39e-20	1.000	334.0	6.38e-20	1.000	335.0	6.24e-20	1.000
336.0	6.01e-20	1.000	337.0	5.79e-20	1.000	338.0	5.63e-20	1.000	339.0	5.56e-20	1.000	340.0	5.52e-20	1.000
341.0	5.54e-20	1.000	342.0	5.53e-20	1.000	343.0	5.47e-20	1.000	344.0	5.41e-20	1.000	345.0	5.40e-20	1.000
346.0	5.48e-20	1.000	347.0	5.90e-20	1.000	348.0	6.08e-20	1.000	349.0	6.00e-20	1.000	350.0	5.53e-20	1.000
351.0	5.03e-20	1.000	352.0	4.50e-20	1.000	353.0	4.03e-20	1.000	354.0	3.75e-20	1.000	355.0	3.55e-20	1.000
356.0	3.45e-20	1.000	357.0	3.46e-20	1.000	358.0	3.49e-20	1.000	359.0	3.41e-20	1.000	360.0	3.23e-20	1.000
361.0	2.95e-20	1.000	362.0	2.81e-20	1.000	363.0	2.91e-20	1.000	364.0	3.25e-20	1.000	365.0	3.54e-20	1.000
366.0	3.30e-20	1.000	367.0	2.78e-20	1.000	368.0	2.15e-20	1.000	369.0	1.59e-20	1.000	370.0	1.19e-20	1.000
371.0	8.99e-21	1.000	372.0	7.22e-21	1.000	373.0	5.86e-21	1.000	374.0	4.69e-21	1.000	375.0	3.72e-21	1.000
376.0	3.57e-21	1.000	377.0	3.55e-21	1.000	378.0	2.83e-21	1.000	379.0	1.69e-21	1.000	380.0	8.29e-24	1.000
381.0	0.00e+00	1.000												

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
						IC3ONO2								
185.0	1.79e-17	1.000	188.0	1.81e-17	1.000	190.0	1.79e-17	1.000	195.0	1.61e-17	1.000	200.0	1.26e-17	1.000
205.0	8.67e-18	1.000	210.0	4.98e-18	1.000	215.0	2.47e-18	1.000	220.0	1.17e-18	1.000	225.0	5.80e-19	1.000
230.0	3.10e-19	1.000	235.0	1.80e-19	1.000	240.0	1.10e-19	1.000	245.0	7.00e-20	1.000	250.0	5.70e-20	1.000
255.0	5.20e-20	1.000	260.0	4.90e-20	1.000	265.0	4.60e-20	1.000	270.0	4.10e-20	1.000	275.0	3.60e-20	1.000
280.0	2.90e-20	1.000	285.0	2.30e-20	1.000	290.0	1.70e-20	1.000	295.0	1.20e-20	1.000	300.0	8.10e-21	1.000
305.0	5.20e-21	1.000	310.0	3.20e-21	1.000	315.0	1.90e-21	1.000	320.0	1.10e-21	1.000	325.0	6.10e-22	1.000
330.0	3.70e-22	1.000	335.0	0.00e+00	1.000									
						MGLY_ABS								
219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	1.000	344.5	2.91e-21	1.000	345.0	2.95e-21	1.000	345.5	3.00e-21	1.000	346.0	3.08e-21	1.000
346.5	3.18e-21	1.000	347.0	3.25e-21	1.000	347.5	3.30e-21	1.000	348.0	3.39e-21	1.000	348.5	3.51e-21	1.000
349.0	3.63e-21	1.000	349.5	3.73e-21	1.000	350.0	3.85e-21	1.000	350.5	3.99e-21	1.000	351.0	4.27e-21	1.000
351.5	4.47e-21	1.000	352.0	4.63e-21	1.000	352.5	4.78e-21	1.000	353.0	4.92e-21	1.000	353.5	5.07e-21	1.000
354.0	5.23e-21	1.000	354.5	5.39e-21	1.000	355.0	5.56e-21	1.000	355.5	5.77e-21	1.000	356.0	5.97e-21	1.000
356.5	6.15e-21	1.000	357.0	6.35e-21	1.000	357.5	6.56e-21	1.000	358.0	6.76e-21	1.000	358.5	6.95e-21	1.000
359.0	7.20e-21	1.000	359.5	7.44e-21	1.000	360.0	7.64e-21	1.000	360.5	7.89e-21	1.000	361.0	8.15e-21	1.000
361.5	8.43e-21	1.000	362.0	8.71e-21	1.000	362.5	9.02e-21	1.000	363.0	9.33e-21	1.000	363.5	9.65e-21	1.000
364.0	1.00e-20	1.000	364.5	1.04e-20	1.000	365.0	1.08e-20	1.000	365.5	1.11e-20	1.000	366.0	1.15e-20	1.000
366.5	1.19e-20	1.000	367.0	1.23e-20	1.000	367.5	1.27e-20	1.000	368.0	1.31e-20	1.000	368.5	1.35e-20	1.000
369.0	1.40e-20	1.000	369.5	1.44e-20	1.000	370.0	1.47e-20	1.000	370.5	1.51e-20	1.000	371.0	1.55e-20	1.000
371.5	1.59e-20	1.000	372.0	1.64e-20	1.000	372.5	1.70e-20	1.000	373.0	1.73e-20	1.000	373.5	1.77e-20	1.000
374.0	1.81e-20	1.000	374.5	1.86e-20	1.000	375.0	1.90e-20	1.000	375.5	1.96e-20	1.000	376.0	2.02e-20	1.000
376.5	2.06e-20	1.000	377.0	2.10e-20	1.000	377.5	2.14e-20	1.000	378.0	2.18e-20	1.000	378.5	2.24e-20	1.000
379.0	2.30e-20	1.000	379.5	2.37e-20	1.000	380.0	2.42e-20	1.000	380.5	2.47e-20	1.000	381.0	2.54e-20	1.000
381.5	2.62e-20	1.000	382.0	2.69e-20	1.000	382.5	2.79e-20	1.000	383.0	2.88e-20	1.000	383.5	2.96e-20	1.000
384.0	3.02e-20	1.000	384.5	3.10e-20	1.000	385.0	3.20e-20	1.000	385.5	3.29e-20	1.000	386.0	3.39e-20	1.000
386.5	3.51e-20	1.000	387.0	3.62e-20	1.000	387.5	3.69e-20	1.000	388.0	3.70e-20	1.000	388.5	3.77e-20	1.000
389.0	3.88e-20	1.000	389.5	3.97e-20	1.000	390.0	4.03e-20	1.000	390.5	4.12e-20	1.000	391.0	4.22e-20	1.000
391.5	4.29e-20	1.000	392.0	4.30e-20	1.000	392.5	4.38e-20	1.000	393.0	4.47e-20	1.000	393.5	4.55e-20	1.000
394.0	4.56e-20	1.000	394.5	4.59e-20	1.000	395.0	4.67e-20	1.000	395.5	4.80e-20	1.000	396.0	4.87e-20	1.000
396.5	4.96e-20	1.000	397.0	5.08e-20	1.000	397.5	5.19e-20	1.000	398.0	5.23e-20	1.000	398.5	5.39e-20	1.000
399.0	5.46e-20	1.000	399.5	5.54e-20	1.000	400.0	5.59e-20	1.000	400.5	5.77e-20	1.000	401.0	5.91e-20	1.000
401.5	5.99e-20	1.000	402.0	6.06e-20	1.000	402.5	6.20e-20	1.000	403.0	6.35e-20	1.000	403.5	6.52e-20	1.000
404.0	6.54e-20	1.000	404.5	6.64e-20	1.000	405.0	6.93e-20	1.000	405.5	7.15e-20	1.000	406.0	7.19e-20	1.000
406.5	7.32e-20	1.000	407.0	7.58e-20	1.000	407.5	7.88e-20	1.000	408.0	7.97e-20	1.000	408.5	7.91e-20	1.000
409.0	8.11e-20	1.000	409.5	8.41e-20	1.000	410.0	8.53e-20	1.000	410.5	8.59e-20	1.000	411.0	8.60e-20	1.000
411.5	8.80e-20	1.000	412.0	9.04e-20	1.000	412.5	9.45e-20	1.000	413.0	9.34e-20	1.000	413.5	9.37e-20	1.000
414.0	9.63e-20	1.000	414.5	9.71e-20	1.000	415.0	9.70e-20	1.000	415.5	9.65e-20	1.000	416.0	9.69e-20	1.000
416.5	9.89e-20	1.000	417.0	1.00e-19	1.000	417.5	1.02e-19	1.000	418.0	1.00e-19	1.000	418.5	1.02e-19	1.000
419.0	1.01e-19	1.000	419.5	1.01e-19	1.000	420.0	1.03e-19	1.000	420.5	1.01e-19	1.000	421.0	1.04e-19	1.000
421.5	1.05e-19	1.000	422.0	1.06e-19	1.000	422.5	1.04e-19	1.000	423.0	1.05e-19	1.000	423.5	1.05e-19	1.000
424.0	1.01e-19	1.000	424.5	1.01e-19	1.000	425.0	1.05e-19	1.000	425.5	1.03e-19	1.000	426.0	1.02e-19	1.000
426.5	1.01e-19	1.000	427.0	9.77e-20	1.000	427.5	9.81e-20	1.000	428.0	1.00e-19	1.000	428.5	1.02e-19	1.000
429.0	9.89e-20	1.000	429.5	9.85e-20	1.000	430.0	1.04e-19	1.000	430.5	1.08e-19	1.000	431.0	1.05e-19	1.000
431.5	1.02e-19	1.000	432.0	9.64e-20	1.000	432.5	1.01e-19	1.000	433.0	1.06e-19	1.000	433.5	1.09e-19	1.000
434.0	1.04e-19	1.000	434.5	1.03e-19	1.000	435.0	1.07e-19	1.000	435.5	1.16e-19	1.000	436.0	1.09e-19	1.000
436.5	1.11e-19	1.000	437.0	9.81e-20	1.000	437.5	9.71e-20	1.000	438.0	1.06e-19	1.000	438.5	1.16e-19	1.000
439.0	1.08e-19	1.000	439.5	1.05e-19	1.000	440.0	9.70e-20	1.000	440.5	1.01e-19	1.000	441.0	1.04e-19	1.000
441.5	1.07e-19	1.000	442.0	1.02e-19	1.000	442.5	9.68e-20	1.000	443.0	1.00e-19	1.000	443.5	1.14e-19	1.000
444.0	1.13e-19	1.000	444.5	1.03e-19	1.000	445.0	9.74e-20	1.000	445.5	8.46e-20	1.000	446.0	8.70e-20	1.000
446.5	9.97e-20	1.000	447.0	1.01e-19	1.000	447.5	9.15e-20	1.000	448.0	9.41e-20	1.000	448.5	8.99e-20	1.000
449.0	1.10e-19	1.000	449.5	9.12e-20	1.000	450.0	8.56e-20	1.000	450.5	8.28e-20	1.000	451.0	6.15e-20	1.000
451.5	5.56e-20	1.000	452.0	6.47e-20	1.000	452.5	7.27e-20	1.000	453.0	5.75e-20	1.000	453.5	5.08e-20	1.000
454.0	4.38e-20	1.000	454.5	3.81e-20	1.000	455.0	3.61e-20	1.000	455.5	3.61e-20	1.000	456.0	3.13e-20	1.000
456.5	2.72e-20	1.000	457.0	2.44e-20	1.000	457.5	2.22e-20	1.000	458.0	1.82e-20	1.000	458.5	1.43e-20	1.000
459.0	1.32e-20	1.000	459.5	1.05e-20	1.000	460.0	8.95e-21	1.000	460.5	8.90e-21	1.000	461.0	7.94e-21	1.000
461.5	7.04e-21	1.000	462.0	6.46e-21	1.000	462.5	5.63e-21	1.000	463.0	4.78e-21	1.000	463.5	3.94e-21	1.000
464.0	3.26e-21	1.000	464.5	2.97e-21	1.000	465.0	2.65e-21	1.000	465.5	2.46e-21	1.000	466.0	2.27e-21	1.000
466.5	2.08e-21	1.000	467.0	1.86e-21	1.000	467.5	1.76e-21	1.000	468.0	1.60e-21	1.000	468.5	1.44e-21	1.000
469.0	1.34e-21	1.000	469.5	1.20e-21	1.000	470.0	1.07e-21	1.000	470.5	1.02e-21	1.000	471.0	9.92e-22	1.000

Table A-2 (continued)

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
471.5	9.97e-22	1.000	472.0	8.87e-22	1.000	472.5	8.27e-22	1.000	473.0	7.76e-22	1.000	473.5	7.15e-22	1.000
474.0	6.71e-22	1.000	474.5	6.67e-22	1.000	475.0	6.10e-22	1.000	475.5	6.17e-22	1.000	476.0	5.54e-22	1.000
476.5	5.22e-22	1.000	477.0	5.10e-22	1.000	477.5	5.17e-22	1.000	478.0	4.80e-22	1.000	478.5	4.71e-22	1.000
479.0	4.60e-22	1.000	479.5	4.35e-22	1.000	480.0	3.90e-22	1.000	480.5	3.71e-22	1.000	481.0	3.62e-22	1.000
481.5	3.52e-22	1.000	482.0	3.05e-22	1.000	482.5	3.05e-22	1.000	483.0	2.86e-22	1.000	483.5	2.53e-22	1.000
484.0	2.75e-22	1.000	484.5	2.59e-22	1.000	485.0	2.47e-22	1.000	485.5	2.36e-22	1.000	486.0	2.12e-22	1.000
486.5	1.89e-22	1.000	487.0	1.93e-22	1.000	487.5	1.86e-22	1.000	488.0	1.82e-22	1.000	488.5	1.75e-22	1.000
489.0	1.74e-22	1.000	489.5	1.72e-22	1.000	490.0	1.66e-22	1.000	490.5	1.75e-22	1.000	491.0	1.54e-22	1.000
491.5	1.74e-22	1.000	492.0	1.63e-22	1.000	492.5	1.53e-22	1.000	493.0	1.52e-22	1.000	493.5	5.85e-23	1.000
494.0	0.00e+00	1.000												

Table A-3. List of SAPRC-99 detailed model species, indicating their representation in the model and their emissions group assignments.

Description	Model Name	Emit. Group	Representation
Carbon Monoxide	CO	-	Explicit (CO)
Methane	METHANE	CH4	Explicit (CH4)
Ethane	ETHANE	ETHA	Assigned Parameters (ALK1)
Methane	METHANE	CH4	Assigned parameters (CH4)
Ethane	ETHANE	ETHA	Assigned parameters (ALK1)
Propane	PROPANE	PROP	Assigned parameters (ALK2)
n-Butane	N-C4	ALK3	Assigned parameters (ALK3)
n-Pentane	N-C5	ALK4	Assigned parameters (ALK4)
n-Hexane	N-C6	ALK4	Assigned parameters (ALK4)
n-Heptane	N-C7	ALK5	Assigned parameters (ALK5)
n-Octane	N-C8	ALK5	Assigned parameters (ALK5)
n-Nonane	N-C9	ALK5	Assigned parameters (ALK5)
n-Decane	N-C10	ALK5	Assigned parameters (ALK5)
n-Undecane	N-C11	ALK5	Assigned parameters (ALK5)
n-Dodecane	N-C12	ALK6	Assigned parameters (ALK5)
n-Tridecane	N-C13	ALK6	Assigned parameters (ALK5)
n-Tetradecane	N-C14	ALK6	Assigned parameters (ALK5)
n-Pentadecane	N-C15	ALK6	Assigned parameters (ALK5)
n-C16	N-C16	ALK6	Assigned parameters (ALK5)
n-C17	N-C17	ALK6	Rep'd by N-C16
n-C18	N-C18	ALK6	Rep'd by N-C16
n-C19	N-C19	ALK6	Rep'd by N-C16
n-C20	N-C20	ALK6	Rep'd by N-C16
n-C21	N-C21	ALK6	Rep'd by N-C16
n-C22	N-C22	ALK6	Rep'd by N-C16
Isobutane	2-ME-C3	ALK3	Assigned parameters (ALK3)
Neopentane	22-DM-C3	ALK2	Assigned parameters (ALK2)
Iso-Pentane	2-ME-C4	ALK4	Assigned parameters (ALK4)
Branched C5 Alkanes	BR-C5	ALK4	Rep'd by 2-ME-C4
2,2-Dimethyl Butane	22-DM-C4	ALK3	Assigned parameters (ALK3)
2,3-Dimethyl Butane	23-DM-C4	ALK4	Assigned parameters (ALK4)
2-Methyl Pentane	2-ME-C5	ALK4	Assigned parameters (ALK4)
3-Methylpentane	3-ME-C5	ALK4	Assigned parameters (ALK4)
Branched C6 Alkanes	BR-C6	ALK4	Rep'd by 0.5 23-DM-C4 +0.25 3-ME-C5 +0.25 2-ME-C5
2,2,3-Trimethyl Butane	223TM-C4	ALK4	Assigned parameters (ALK4)
2,2-Dimethyl Pentane	22-DM-C5	ALK3	Assigned parameters (ALK3)
2,3-Dimethyl Pentane	23-DM-C5	ALK5	Assigned parameters (ALK5)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
2,4-Dimethyl Pentane	24-DM-C5	ALK4	Assigned parameters (ALK4)
2-Methyl Hexane	2-ME-C6	ALK5	Assigned parameters (ALK5)
3,3-Dimethyl Pentane	33-DM-C5	ALK3	Assigned parameters (ALK3)
3-Methyl Hexane	3-ME-C6	ALK5	Assigned parameters (ALK5)
Branched C7 Alkanes	BR-C7	ALK4	Rep'd by 0.5 24-DM-C5 +0.25 3-ME-C6 +0.25 2-ME-C6
2,2,3,3-Tetrame. Butane	2233M-C4	ALK2	Assigned parameters (ALK2)
2,2,4-Trimethyl Pentane	224TM-C5	ALK4	Assigned parameters (ALK4)
2,2-Dimethyl Hexane	22-DM-C6	ALK4	Assigned parameters (ALK4)
2,3,4-Trimethyl Pentane	234TM-C5	ALK5	Assigned parameters (ALK5)
2,3-Dimethyl Hexane	23-DM-C6	ALK5	Assigned parameters (ALK5)
2,4-Dimethyl Hexane	24-DM-C6	ALK5	Assigned parameters (ALK5)
2,5-Dimethyl Hexane	25-DM-C6	ALK5	Assigned parameters (ALK5)
2-Methyl Heptane	2-ME-C7	ALK5	Assigned parameters (ALK5)
3-Methyl Heptane	3-ME-C7	ALK5	Assigned parameters (ALK5)
4-Methyl Heptane	4-ME-C7	ALK5	Assigned parameters (ALK5)
Branched C8 Alkanes	BR-C8	ALK5	Rep'd by 0.5 24-DM-C6 +0.25 4-ME-C7 +0.25 2-ME-C7
2,2,5-Trimethyl Hexane	225TM-C6	ALK4	Assigned parameters (ALK4)
2,3,5-Trimethyl Hexane	235TM-C6	ALK5	Assigned parameters (ALK5)
2,4-Dimethyl Heptane	24-DM-C7	ALK5	Assigned parameters (ALK5)
2-Methyl Octane	2-ME-C8	ALK5	Assigned parameters (ALK5)
3,3-Diethyl Pentane	33-DE-C5	ALK4	Assigned parameters (ALK4)
3,5-Dimethyl Heptane	35-DM-C7	ALK5	Assigned parameters (ALK5)
4-Ethyl Heptane	4-ET-C7	ALK5	Assigned parameters (ALK5)
4-Methyl Octane	4-ME-C8	ALK5	Assigned parameters (ALK5)
Branched C9 Alkanes	BR-C9	ALK5	Rep'd by 0.5 24-DM-C7 +0.25 4-ME-C8 +0.25 2-ME-C8
2,4-Dimethyl Octane	24-DM-C8	ALK5	Assigned parameters (ALK5)
2,6-Dimethyl Octane	26DM-C8	ALK5	Assigned parameters (ALK5)
2-Methyl Nonane	2-ME-C9	ALK5	Assigned parameters (ALK5)
3,4-Diethyl Hexane	34-DE-C6	ALK5	Assigned parameters (ALK5)
3-Methyl Nonane	3-ME-C9	ALK5	Assigned parameters (ALK5)
4-Methyl Nonane	4-ME-C9	ALK5	Assigned parameters (ALK5)
4-Propyl Heptane	4-PR-C7	ALK5	Assigned parameters (ALK5)
Branched C10 Alkanes	BR-C10	ALK5	Rep'd by 0.5 26DM-C8 +0.25 4-ME-C9 +0.25 2-ME-C9
2,6-Dimethyl Nonane	26DM-C9	ALK5	Assigned parameters (ALK5)
3,5-Diethyl Heptane	35-DE-C7	ALK6	Assigned parameters (ALK5)
3-Methyl Decane	3-ME-C10	ALK5	Assigned parameters (ALK5)
4-Methyl Decane	4-ME-C10	ALK5	Assigned parameters (ALK5)
Branched C11 alkanes	BR-C11	ALK5	Rep'd by 0.5 26DM-C9 +0.25 4-ME-C10 +0.25 3-ME-C10
2,6-Diethyl Octane	36-DE-C8	ALK6	Assigned parameters (ALK5)
3,6-Dimethyl Decane	36DM-C10	ALK6	Assigned parameters (ALK5)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
3-Methyl Undecane	3-ME-C11	ALK6	Assigned parameters (ALK5)
5-Methyl Undecane	5-ME-C11	ALK6	Assigned parameters (ALK5)
Branched C12 Alkanes	BR-C12	ALK6	Rep'd by 0.5 36DM-C10 +0.25 5-ME-C11 +0.25 3-ME-C11
3,6-Dimethyl Undecane	36DM-C11	ALK6	Assigned parameters (ALK5)
3,7-Diethyl Nonane	37-DE-C9	ALK6	Assigned parameters (ALK5)
3-Methyl Dodecane	3-ME-C12	ALK6	Assigned parameters (ALK5)
5-Methyl Dodecane	5-ME-C12	ALK6	Assigned parameters (ALK5)
Branched C13 Alkanes	BR-C13	ALK6	Rep'd by 0.5 36DM-C11 +0.25 5-ME-C12 +0.25 3-ME-C12
Branched C14 Alkanes	BR-C14	ALK6	Rep'd by 0.5 37DM-C12 +0.25 6-ME-C13 +0.25 3-ME-C13
3,7-Dimethyl Dodecane	37DM-C12	ALK6	Assigned parameters (ALK5)
3,8-Diethyl Decane	38DE-C10	ALK6	Assigned parameters (ALK5)
3-Methyl Tridecane	3-ME-C13	ALK6	Assigned parameters (ALK5)
6-Methyl Tridecane	6-ME-C13	ALK6	Assigned parameters (ALK5)
3,7-Dimethyl Tridecane	37DM-C13	ALK6	Assigned parameters (ALK5)
3,9-Diethyl Undecane	39DE-C11	ALK6	Assigned parameters (ALK5)
3-Methyl Tetradecane	3-ME-C14	ALK6	Assigned parameters (ALK5)
6-Methyl Tetradecane	6-ME-C14	ALK6	Assigned parameters (ALK5)
Branched C15 Alkanes	BR-C15	ALK6	Rep'd by 0.5 37DM-C13 +0.25 6-ME-C14 +0.25 3-ME-C14
Branched C16 Alkanes	BR-C16	ALK6	Rep'd by 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
3-Methyl Pentadecane	3-ME-C15	ALK6	Assigned parameters (ALK5)
4,8-Dimethyl Tetradecane	48DM-C14	ALK6	Assigned parameters (ALK5)
7-Methyl Pentadecane	7-ME-C15	ALK6	Assigned parameters (ALK5)
Branched C17 Alkanes	BR-C17	ALK6	Rep'd by 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
Branched C18 Alkanes	BR-C18	ALK6	Rep'd by 0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
Cyclopropane	CYCC3	INERT	Assigned parameters (ALK2)
Cyclobutane	CYCC4	ALK2	Assigned parameters (ALK2)
Cyclopentane	CYCC5	ALK4	Assigned parameters (ALK4)
Cyclohexane	CYCC6	ALK5	Assigned parameters (ALK5)
C6 Cycloalkanes	CYC-C6	ALK5	Rep'd by CYCC6
Isopropyl Cyclopropane	IPR-CC3	ALK3	Assigned parameters (ALK3)
Methylcyclopentane	ME-CYCC5	ALK4	Assigned parameters (ALK4)
1,3-Dimeth. Cyclopentane	13DMCYC5	ALK5	Assigned parameters (ALK5)
Cycloheptane	CYCC7	ALK5	Assigned parameters (ALK5)
C7 Cycloalkanes	CYC-C7	ALK5	Rep'd by ME-CYCC6
Ethyl Cyclopentane	ET-CYCC5	ALK5	Assigned parameters (ALK5)
Methylcyclohexane	ME-CYCC6	ALK5	Assigned parameters (ALK5)
1,3-Dimethyl Cyclohexane	13DMCYC6	ALK5	Assigned parameters (ALK5)
Cyclooctane	CYCC8	ALK5	Assigned parameters (ALK5)
C8 Cycloalkanes	CYC-C8	ALK5	Rep'd by ET-CYCC6
Ethylcyclohexane	ET-CYCC6	ALK5	Assigned parameters (ALK5)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Propyl Cyclopentane	PR-CYCC5	ALK5	Assigned parameters (ALK5)
C9 Bicycloalkanes	BCYC-C9	ALK5	Rep'd by 0.5 C3-CYCC6 +0.5 1E4MCYC6
1,1,3-Trimethyl Cyclohex.	113MCYC6	ALK5	Assigned parameters (ALK5)
1-Eth.-4-Meth. Cyclohex.	1E4MCYC6	ALK6	Assigned parameters (ALK5)
Propyl Cyclohexane	C3-CYCC6	ALK5	Assigned parameters (ALK5)
C9 Cycloalkanes	CYC-C9	ALK5	Rep'd by 0.5 C3-CYCC6 +0.5 1E4MCYC6
C10 Bicycloalkanes	BCYC-C10	ALK6	Rep'd by 0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
1,3-Diethyl-Cyclohexane	13DECYC6	ALK6	Assigned parameters (ALK5)
1,4-Diethyl-Cyclohexane	14DECYC6	ALK6	Assigned parameters (ALK5)
1-Meth.-3-Isopr. Cyclohex.	1M3IPCY6	ALK6	Assigned parameters (ALK5)
Butyl Cyclohexane	C4-CYCC6	ALK6	Assigned parameters (ALK5)
C10 Cycloalkanes	CYC-C10	ALK6	Rep'd by 0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
C11 Bicycloalkanes	BCYC-C11	ALK6	Rep'd by 0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
13-Dieth-5-Me. Cyclohex.	13E5MCC6	ALK6	Assigned parameters (ALK5)
1-Ethyl-2-Propyl Cyclohex.	1E2PCYC6	ALK6	Assigned parameters (ALK5)
Pentyl Cyclohexane	C5-CYCC6	ALK6	Assigned parameters (ALK5)
C11 Cycloalkanes	CYC-C11	ALK6	Rep'd by 0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
C12 Bicycloalkanes	BCYC-C12	ALK6	Rep'd by 0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
C12 Cycloalkanes	CYC-C12	ALK6	Rep'd by 0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
1,3,5-Triethyl Cyclohex.	135ECYC6	ALK6	Assigned parameters (ALK5)
1-Meth.-4-Pentyl Cyclohex.	1M4C5CY6	ALK6	Assigned parameters (ALK5)
Hexyl Cyclohexane	C6-CYCC6	ALK6	Assigned parameters (ALK5)
C13 Bicycloalkanes	BCYC-C13	ALK6	Rep'd by 0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
13-Dieth-5-Pent Cyclohx.	13E5PCC6	ALK6	Assigned parameters (ALK5)
1-Meth.-2-Hexyl-Cyclohex.	1M2C6CC6	ALK6	Assigned parameters (ALK5)
Heptyl Cyclohexane	C7-CYCC6	ALK6	Assigned parameters (ALK5)
C13 Cycloalkanes	CYC-C13	ALK6	Rep'd by 0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
C14 Bicycloalkanes	BCYC-C14	ALK6	Rep'd by 0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
13-Diprop-5-Eth Cyclohx.	13P5ECC6	ALK6	Assigned parameters (ALK5)
1-Meth.-4-Heptyl Cyclohex.	1M4C7CC6	ALK6	Assigned parameters (ALK5)
Octyl Cyclohexane	C8-CYCC6	ALK6	Assigned parameters (ALK5)
C14 Cycloalkanes	CYC-C14	ALK6	Rep'd by 0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
C15 Bicycloalkanes	BCYC-C15	ALK6	Rep'd by 0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
135-Tripropyl Cyclohex.	135PCYC6	ALK6	Assigned parameters (ALK5)
1-Methyl-2-Octyl Cyclohex.	1M2C8CC6	ALK6	Assigned parameters (ALK5)
Nonyl Cyclohexane	C9-CYCC6	ALK6	Assigned parameters (ALK5)
C15 Cycloalkanes	CYC-C15	ALK6	Rep'd by 0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
1,3-Prop.-5-Butyl Cyclohex.	13P5BCC6	ALK6	Assigned parameters (ALK5)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
1-Methyl-4-Nonyl Cyclohex.	1M4C9CY6	ALK6	Assigned parameters (ALK5)
Decyl Cyclohexane	C10CYCC6	ALK6	Assigned parameters (ALK5)
C16 Cycloalkanes	CYC-C16	ALK6	Rep'd by 0.34 C10CYCC6 +0.33 13P5BCC6 +0.33 1M4C9CY6
Ethene	ETHENE	ETHE	Assigned parameters (ETHENE)
Propene	PROPENE	OLE1	Assigned parameters (OLE1)
1-Butene	1-BUTENE	OLE1	Assigned parameters (OLE1)
1-Pentene	1-PENTEN	OLE1	Assigned parameters (OLE1)
3-Methyl-1-Butene	3M-1-BUT	OLE1	Assigned parameters (OLE1)
1-Hexene	1-HEXENE	OLE1	Assigned parameters (OLE1)
3,3-Dimethyl-1-Butene	33M1-BUT	OLE1	Assigned parameters (OLE1)
3-Methyl-1-Pentene	3M1-C5E	OLE1	Assigned parameters (OLE1)
4-Methyl-1-Pentene	4M1-C5E	OLE1	Assigned parameters (OLE1)
1-Heptene	1-HEPTEN	OLE1	Assigned parameters (OLE1)
1-Octene	1-OCTENE	OLE1	Assigned parameters (OLE1)
1-Nonene	1-C9E	OLE1	Assigned parameters (OLE1)
1-Decene	1-C10E	OLE1	Assigned parameters (OLE1)
1-Undecene	1-C11E	OLE1	Assigned parameters (OLE1)
1-Dodecene	1-C12E	OLE1	Assigned parameters (OLE1)
1-Tridecene	1-C13E	OLE1	Assigned parameters (OLE1)
1-Tetradecene	1-C14E	OLE1	Assigned parameters (OLE1)
1-Pentadecene	1-C15E	OLE1	Assigned parameters (OLE1)
C4 Terminal Alkenes	C4-OLE1	OLE1	Rep'd by 1-BUTENE
Isobutene	ISOBUTEN	OLE2	Assigned parameters (OLE2)
2-Methyl-1-Butene	2M-1-BUT	OLE2	Assigned parameters (OLE2)
C5 Terminal Alkenes	C5-OLE1	OLE1	Rep'd by 1-PENTEN
23-Dimethyl-1-Butene	23M1-BUT	OLE2	Assigned parameters (OLE2)
2-Ethyl-1-Butene	2E1-BUT	OLE2	Assigned parameters (OLE2)
2-Methyl-1-Pentene	2M1-C5E	OLE2	Assigned parameters (OLE2)
C6 Terminal Alkenes	C6-OLE1	OLE1	Rep'd by 1-HEXENE
2,3,3-trimethyl-1-Butene	233M1BUT	OLE2	Assigned parameters (OLE2)
C7 Terminal Alkenes	C7-OLE1	OLE1	Rep'd by 1-HEPTEN
3-Methyl-2-Isopropyl-1-Butene	3M2I1C4E	OLE2	Assigned parameters (OLE2)
C8 Terminal Alkenes	C8-OLE1	OLE1	Rep'd by 1-OCTENE
C9 Terminal Alkenes	C9-OLE1	OLE1	Rep'd by 1-C9E
C10 Terminal Alkenes	C10-OLE1	OLE1	Rep'd by 1-C10E
C11 Terminal Alkenes	C11-OLE1	OLE1	Rep'd by 1-C11E
C12 Terminal Alkenes	C12-OLE1	OLE1	Rep'd by 1-C12E
C13 Terminal Alkenes	C13-OLE1	OLE1	Rep'd by 1-C13E

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
C14 Terminal Alkenes	C14-OLE1	OLE1	Rep'd by 1-C14E
C15 Terminal Alkenes	C15-OLE1	OLE1	Rep'd by 1-C15E
cis-2-Butene	C-2-BUTE	OLE2	Assigned parameters (OLE2)
C4 Alkenes	C4-OLE	OLE	Rep'd by 0.5 1-BUTENE +0.25 T-2-BUTE +0.25 C-2-BUTE
C4 Internal Alkenes	C4-OLE2	OLE2	Rep'd by 0.5 T-2-BUTE +0.5 C-2-BUTE
trans-2-Butene	T-2-BUTE	OLE2	Assigned parameters (OLE2)
2-Pentenes	2-C5-OLE	OLE2	Rep'd by 0.5 C-2-PENT +0.5 T-2-PENT
2-Methyl-2-Butene	2M-2-BUT	OLE2	Assigned parameters (OLE2)
cis-2-Pentene	C-2-PENT	OLE2	Assigned parameters (OLE2)
C5 Alkenes	C5-OLE	OLE	Rep'd by 0.5 1-PENTEN +0.25 C-2-PENT +0.25 T-2-PENT
C5 Internal Alkenes	C5-OLE2	OLE2	Rep'd by 0.5 C-2-PENT +0.5 T-2-PENT
trans-2-Pentene	T-2-PENT	OLE2	Assigned parameters (OLE2)
2,3-Dimethyl-2-Butene	23M2-BUT	OLE2	Assigned parameters (OLE2)
2-Hexenes	2-C6-OLE	OLE2	Rep'd by 0.5 C-2-C6E +0.5 T-2-C6E
2-Methyl-2-Pentene	2M-2-C5E	OLE2	Assigned parameters (OLE2)
Cis-2-Hexene	C-2-C6E	OLE2	Assigned parameters (OLE2)
Cis-3-Hexene	C-3-C6E	OLE2	Assigned parameters (OLE2)
Cis-3-Methyl-2-Hexene	C3M2-C5E	OLE2	Assigned parameters (OLE2)
C6 Alkenes	C6-OLE	OLE	Rep'd by 0.5 1-HEPTEN +0.25 C-2-C6E +0.25 T-2-C6E
C6 Internal Alkenes	C6-OLE2	OLE2	Rep'd by 0.5 C-2-C6E +0.5 T-2-C6E
Trans-2-Hexene	T-2-C6E	OLE2	Assigned parameters (OLE2)
Trans-3-Hexene	T-3-C6E	OLE2	Assigned parameters (OLE2)
Trans 3-Methyl-2-Hexene	T3M2-C5E	OLE2	Assigned parameters (OLE2)
Trans 4-Methyl-2-Hexene	T4M2-C5E	OLE2	Assigned parameters (OLE2)
2,3-Dimethyl-2-Hexene	23M2-C5E	OLE2	Assigned parameters (OLE2)
2-Heptenes	2-C7-OLE	OLE2	Rep'd by 0.5 T-3-C7E +0.5 C-3-C7E
Cis-3-Heptene	C-3-C7E	OLE2	Assigned parameters (OLE2)
C7 Alkenes	C7-OLE	OLE	Rep'd by 0.5 1-HEPTEN +0.5 T-3-C7E
C7 Internal Alkenes	C7-OLE2	OLE2	Rep'd by T-3-C7E
Trans-2-Heptene	T-2-C7E	OLE2	Assigned parameters (OLE2)
Trans-3-Heptene	T-3-C7E	OLE2	Assigned parameters (OLE2)
Trans 4,4-dimethyl-2-Pentene	T44M2C5E	OLE2	Assigned parameters (OLE2)
3-Octenes	3-C8-OLE	OLE2	Rep'd by T-3-C8E
Cis-4-Octene	C-4-C8E	OLE2	Assigned parameters (OLE2)
C8 Alkenes	C8-OLE	OLE	Rep'd by 0.5 1-OCTENE +0.5 T-4-C8E
C8 Internal Alkenes	C8-OLE2	OLE2	Rep'd by T-4-C8E
Trans 2,2-Dimethyl 3-Hexene	T22M3C6E	OLE2	Assigned parameters (OLE2)
Trans 2,5-Dimethyl 3-Hexene	T25M3C6E	OLE2	Assigned parameters (OLE2)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Trans-3-Octene	T-3-C8E	OLE2	Assigned parameters (OLE2)
Trans-4-Octene	T-4-C8E	OLE2	Assigned parameters (OLE2)
2,4,4-trimethyl-2-Pentene	244M2C5E	OLE2	Assigned parameters (OLE2)
3-Nonenes	3-C9-OLE	OLE2	Rep'd by T-4-C9E
C9 Alkenes	C9-OLE	OLE	Rep'd by 0.5 1-C9E +0.5 T-4-C9E
C9 Internal Alkenes	C9-OLE2	OLE2	Rep'd by T-4-C9E
Trans-4-Nonene	T-4-C9E	OLE2	Assigned parameters (OLE2)
3,4-Diethyl-2-Hexene	34E2-C6E	OLE2	Assigned parameters (OLE2)
C10 3-Alkenes	3C10-OLE	OLE2	Rep'd by T-4-C10E
C10 Alkenes	C10-OLE	OLE	Rep'd by 0.5 1-C10E +0.5 T-4-C10E
C10 Internal Alkenes	C10-OLE2	OLE2	Rep'd by T-4-C10E
Cis-5-Decene	C-5-C10E	OLE2	Assigned parameters (OLE2)
Trans-4-Decene	T-4-C10E	OLE2	Assigned parameters (OLE2)
C11 3-Alkenes	3C11-OLE	OLE2	Rep'd by T-5-C11E
C11 Alkenes	C11-OLE	OLE	Rep'd by 0.5 1-C11E +0.5 T-5-C11E
C11 Internal Alkenes	C11-OLE2	OLE2	Rep'd by T-5-C11E
Trans-5-Undecene	T-5-C11E	OLE2	Assigned parameters (OLE2)
C12 2-Alkenes	2C12-OLE	OLE2	Rep'd by T-5-C12E
C12 3-Alkenes	3C12-OLE	OLE2	Rep'd by T-5-C12E
C12 Alkenes	C12-OLE	OLE	Rep'd by 0.5 1-C12E +0.5 T-5-C12E
C12 Internal Alkenes	C12-OLE2	OLE2	Rep'd by T-5-C12E
Trans-5-Dodecene	T-5-C12E	OLE2	Assigned parameters (OLE2)
C13 3-Alkenes	3C13-OLE	OLE2	Rep'd by T-5-C13E
C13 Alkenes	C13-OLE	OLE	Rep'd by 0.5 1-C13E +0.5 T-5-C13E
C13 Internal Alkenes	C13-OLE2	OLE2	Rep'd by T-5-C13E
Trans-5-Tridecene	T-5-C13E	OLE2	Assigned parameters (OLE2)
C14 3-Alkenes	3C14-OLE	OLE2	Rep'd by T-5-C14E
C14 Alkenes	C14-OLE	OLE	Rep'd by 0.5 1-C14E +0.5 T-5-C14E
C14 Internal Alkenes	C14-OLE2	OLE2	Rep'd by T-5-C14E
Trans-5-Tetradecene	T-5-C14E	OLE2	Assigned parameters (OLE2)
C15 3-Alkenes	3C15-OLE	OLE2	Rep'd by T-5-C15E
C15 Alkenes	C15-OLE	OLE	Rep'd by 0.5 1-C15E +0.5 T-5-C15E
C15 Internal Alkenes	C15-OLE2	OLE2	Rep'd by T-5-C15E
Trans-5-Tetradecene	T-5-C15E	OLE2	Assigned parameters (OLE2)
Cyclopentene	CYC-PNTE	OLE2	Assigned parameters (OLE2)
1-Methyl cyclohexene	1M-CC5E	OLE2	Assigned parameters (OLE2)
Cyclohexene	CYC-HEXE	OLE2	Assigned parameters (OLE2)
1-Methyl Cyclohexene	1M-CC6E	OLE2	Assigned parameters (OLE2)
4-Methyl Cyclohexene	4M-CC6E	OLE2	Assigned parameters (OLE2)
1,2-Dimethyl Cyclohexene	12M-CC6E	OLE2	Assigned parameters (OLE2)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
1,3-Butadiene	13-BUTDE	13BDE	Assigned parameters (OLE2)
Isoprene	ISOPRENE	ISOP	Assigned parameters (ISOPRENE)
C6 Cyclic or di-olefins	C6-OL2D	OLE2	Rep'd by 0.5 C-2-C6E +0.5 T-2-C6E
C7 Cyclic or di-olefins	C7-OL2D	OLE2	Rep'd by T-2-C7E
C8 Cyclic or di-olefins	C8-OL2D	OLE2	Rep'd by T-4-C8E
C9 Cyclic or di-olefins	C9-OL2D	OLE2	Rep'd by T-4-C9E
C10 Cyclic or di-olefins	C10-OL2D	OLE2	Rep'd by T-4-C10E
C11 Cyclic or di-olefins	C11-OL2D	OLE2	Rep'd by T-5-C11E
C12 Cyclic or di-olefins	C12-OL2D	OLE2	Rep'd by T-5-C12E
C13 Cyclic or di-olefins	C13-OL2D	OLE2	Rep'd by T-5-C13E
C14 Cyclic or di-olefins	C14-OL2D	OLE2	Rep'd by T-5-C14E
C15 Cyclic or di-olefins	C15-OL2D	OLE2	Rep'd by T-5-C15E
Cyclopentadiene	CYC-PNDE	OLE2	Rep'd by CYC-PNTE
3-Carene	3-CARENE	TERP	Assigned parameters (TERP)
a-Pinene	A-PINENE	TERP	Assigned parameters (TERP)
b-Pinene	B-PINENE	TERP	Assigned parameters (TERP)
d-Limonene	D-LIMONE	TERP	Assigned parameters (TERP)
Sabinene	SABINENE	TERP	Assigned parameters (TERP)
Terpene	TERPENE	TERP	Rep'd by 0.4 A-PINENE +0.25 B-PINENE +0.1 D-LIMONE +0.15 3-CARENE +0.1 SABINENE
Styrene	STYRENE	STYR	Assigned parameters (OLE2)
a-Methyl Styrene	AME-STYR	STYR	Rep'd by STYRENE
C9 Styrenes	C9-STYR	STYR	Rep'd by STYRENE
C10 Styrenes	C10-STYR	STYR	Rep'd by STYRENE
Benzene	BENZENE	BENZ	Assigned parameters with reactivity weighting (0.210 ARO1)
Toluene	TOLUENE	ARO1	Assigned parameters (ARO1)
Ethyl Benzene	C2-BENZ	ARO1	Assigned parameters (ARO1)
C9 Monosub. Benzenes	C9-BEN1	ARO1	Rep'd by N-C3-BEN
Isopropyl Benzene (cumene)	I-C3-BEN	ARO1	Assigned parameters (ARO1)
n-Propyl Benzene	N-C3-BEN	ARO1	Assigned parameters (ARO1)
C10 Monosub. Benzenes	C10-BEN1	ARO1	Rep'd by N-C3-BEN
n-Butyl Benzene	N-C4-BEN	ARO1	Rep'd by N-C3-BEN
s-Butyl Benzene	S-C4-BEN	ARO1	Assigned parameters (ARO1)
C11 Monosub. Benzenes	C11-BEN1	ARO1	Rep'd by N-C3-BEN
C12 Monosub. Benzenes	C12-BEN1	ARO1	Rep'd by N-C3-BEN
C13 Monosub. Benzenes	C13-BEN1	ARO1	Rep'd by N-C3-BEN
C8 Disub. Benzenes	C8-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
m-Xylene	M-XYLENE	ARO2	Assigned parameters (ARO2)
o-Xylene	O-XYLENE	ARO2	Assigned parameters (ARO2)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
p-Xylene	P-XYLENE	ARO2	Assigned parameters (ARO2)
C9 Disub. Benzenes	C9-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C10 Disub. Benzenes	C10-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C11 Disub. Benzenes	C11-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C12 Disub. Benzenes	C12-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C13 Disub. Benzenes	C13-BEN2	ARO2	Rep'd by 0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
Isomers of Ethylbenzene	C8-BEN2	ARO2	Rep'd by 0.17 M-XYLENE +0.17 O-XYLENE+0.17 P-XYLENE +0.49 C2-BENZ
1,2,3-Trimethyl Benzene	123-TMB	ARO2	Assigned parameters (ARO2)
1,2,4-Trimethyl Benzene	124-TMB	ARO2	Assigned parameters (ARO2)
1,3,5-Trimethyl Benzene	135-TMB	ARO2	Assigned parameters (ARO2)
Isomers of Propylbenzene	C9-BEN	ARO2	Rep'd by 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C9 Trisub. Benzenes	C9-BEN3	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
Isomers of Butylbenzene	C10-BEN	ARO2	Rep'd by 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C10 Trisub. Benzenes	C10-BEN3	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C10 Tetrasub. Benzenes	C10-BEN4	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
Isomers of Pentylbenzene	C11-BEN	ARO2	Rep'd by 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C11 Trisub. Benzenes	C11-BEN3	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11 Tetrasub. Benzenes	C11-BEN4	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11 Pentasub. Benzenes	C11-BEN5	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
Isomers of Hexylbenzene	C12-BEN	ARO2	Rep'd by 0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C12 Trisub. Benzenes	C12-BEN3	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12 Tetrasub. Benzenes	C12-BEN4	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11 Pentasub. Benzenes	C12-BEN5	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12 Hexaasub. Benzenes	C12-BEN6	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C13 Trisub. Benzenes	C13-BEN3	ARO2	Rep'd by 0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
Indan	INDAN	NAPT	Rep'd by TETRALIN
Naphthalene	NAPHTHAL	NAPT	Assigned parameters (ARO2)
Tetralin	TETRALIN	NAPT	Assigned parameters (ARO2)
1-Methyl Naphthalene	1ME-NAPH	NAPT	Rep'd by ME-NAPH
2-Methyl Naphthalene	2ME-NAPH	NAPT	Rep'd by ME-NAPH
Methyl Naphthalenes	ME-NAPH	NAPT	Assigned parameters (ARO2)
C11 Tetralin or Indane	C11-TET	NAPT	Rep'd by TETRALIN
2,3-Dimethyl Naphth.	23-DMN	NAPT	Assigned parameters (ARO2)
C12 Monosub. Naphth.	C12-NAP1	NAPT	Rep'd by ME-NAPH
C12 Disub. Naphthalenes	C12-NAP2	NAPT	Rep'd by 23-DMN
Dimethyl Naphthalenes	DM-NAPH	NAPT	Rep'd by 23-DMN

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
C13 Monosub. Naphth.	C13-NAP1	NAPT	Rep'd by ME-NAPH
C13 Disub. Naphthalenes	C13-NAP2	NAPT	Rep'd by 23-DMN
C13 Trisub. Naphthalenes	C13-NAP3	NAPT	Rep'd by 23-DMN
Acetylene	ACETYLEN	ACTYL	Assigned parameters (ALK2)
Methyl Acetylene	ME-ACTYL	OTH4	Assigned parameters (ALK4)
2-Butyne	2-BUTYNE	OTH6	Assigned parameters (ALK5)
Ethyl Acetylene	ET-ACTYL	OTH5	Assigned parameters (ALK5)
Methanol	MEOH	MEOH	Assigned parameters (MEOH)
Ethanol	ETOH	ETOH	Assigned parameters (ALK3)
Isopropyl Alcohol	I-C3-OH	OTH4	Assigned parameters (ALK4)
n-Propyl Alcohol	N-C3-OH	OTH4	Assigned parameters (ALK4)
Isobutyl Alcohol	I-C4-OH	OTH5	Assigned parameters (ALK5)
n-Butyl Alcohol	N-C4-OH	OTH5	Assigned parameters (ALK5)
s-Butyl Alcohol	S-C4-OH	OTH5	Assigned parameters (ALK5)
t-Butyl Alcohol	T-C4-OH	OTH2	Assigned parameters (ALK2)
Cyclopentanol	CC5-OH	OTH5	Assigned parameters (ALK5)
2-Pentanol	2-C5OH	OTH5	Assigned parameters (ALK5)
3-Pentanol	3-C5OH	OTH5	Assigned parameters (ALK5)
Pentyl Alcohol	C5OH	OTH5	Assigned parameters (ALK5)
Cyclohexanol	CC6-OH	OTH6	Assigned parameters (ALK5)
1-Hexanol	1-C6OH	OTH5	Assigned parameters (ALK5)
2-Hexanol	2-C6OH	OTH5	Assigned parameters (ALK5)
1-Heptanol	1-C7OH	OTH6	Assigned parameters (ALK5)
1-Octanol	1-C8-OH	OTH6	Assigned parameters (ALK5)
2-Octanol	2-C8-OH	OTH6	Assigned parameters (ALK5)
2-Ethyl-1-Hexanol	2-ETC6OH	OTH5	Assigned parameters (ALK5)
3-Octanol	3-C8-OH	OTH6	Assigned parameters (ALK5)
4-Octanol	4-C8-OH	OTH6	Assigned parameters (ALK5)
Ethylene Glycol	ET-GLYCL	OTH6	Assigned parameters (ALK5)
Propylene Glycol	PR-GLYCL	OTH6	Assigned parameters (ALK5)
1,2-Butandiol	12-C4OH2	OTH6	Assigned parameters (ALK5)
Glycerol	GLYCERL	OTH6	Assigned parameters (ALK5)
2-Methyl-2,4-Pentanediol	2M24C5OH	OTH5	Assigned parameters (ALK5)
1,2-Dihydroxy Hexane	C6-GLYCL	OTH6	Assigned parameters (ALK5)
Dimethyl Ether	ME-O-ME	OTH3	Assigned parameters (ALK3)
Trimethylene Oxide	TME-OX	OTH5	Assigned parameters (ALK5)
Tetrahydrofuran	THF	OTH6	Assigned parameters (ALK5)
Diethyl Ether	ET-O-ET	OTH5	Assigned parameters (ALK5)
Dimethoxy methane	METHYLAL	OTH4	Assigned parameters (ALK4)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Alpha-Methyl tetrahydrofuran	AM-THF	OTH6	Assigned parameters (ALK5)
Tetrahydropyran	THP	OTH6	Assigned parameters (ALK5)
Ethyl Isopropyl Ether	ET-O-IPR	OTH6	Assigned parameters (ALK5)
Methyl n-Butyl Ether	MNBE	OTH6	Assigned parameters (ALK5)
Methyl t-Butyl Ether	MTBE	OTH3	Assigned parameters (ALK3)
Ethyl n-Butyl Ether	ENBE	OTH6	Assigned parameters (ALK5)
Ethyl t-Butyl Ether	ETBE	OTH5	Assigned parameters (ALK5)
Methyl t-Amyl Ether	MTAE	OTH5	Assigned parameters (ALK5)
Di n-Propyl Ether	PR-O-PR	OTH6	Assigned parameters (ALK5)
2-Butyl Tetrahydrofuran	2BU-THF	OTH6	Assigned parameters (ALK5)
Di-n-butyl Ether	BU-O-BU	OTH6	Assigned parameters (ALK5)
Di-Isobutyl Ether	IBU2-O	OTH6	Assigned parameters (ALK5)
Di-n-Pentyl Ether	C5-O-C5	OTH6	Assigned parameters (ALK5)
2-Methoxyethanol	MEO-ETOH	OTH5	Assigned parameters (ALK5)
2-Methoxy-1-Propanol	2MEOC3OH	OTH6	Assigned parameters (ALK5)
2-Ethoxyethanol	ETO-ETOH	OTH6	Assigned parameters (ALK5)
1-Methoxy-2-Propanol	MEOC3OH	OTH6	Assigned parameters (ALK5)
2-Propoxyethanol	2PROETOH	OTH6	Assigned parameters (ALK5)
3-Ethoxy-1-Propanol	3ETOC3OH	OTH6	Assigned parameters (ALK5)
3-Methoxy-1-Butanol	3MEOC4OH	OTH6	Assigned parameters (ALK3)
1-Ethoxy-2-Propanol	ETOC3OH	OTH6	Assigned parameters (ALK5)
Diethylene Glycol	DET-GLCL	OTH6	Assigned parameters (ALK5)
3 methoxy -3 methyl-Butanol	3MOMC4OH	OTH5	Assigned parameters (ALK5)
2-Butoxyethanol	BUO-ETOH	OTH6	Assigned parameters (ALK5)
1-Propoxy-2-Propanol	PROXC3OH	OTH6	Assigned parameters (ALK5)
2-(2-Methoxyethoxy) Ethanol	MOEOETOH	OTH6	Assigned parameters (ALK5)
n-Butoxy-2-Propanol	BUOC3OH	OTH6	Assigned parameters (ALK5)
1-tert-Butoxy-2-Propanol	PG-1TB-E	OTH6	Assigned parameters (ALK5)
2-tert-Butoxy-1-Propanol	PG-2TB-E	OTH6	Assigned parameters (ALK5)
2-(2-Ethoxyethoxy) EtOH	CARBITOL	OTH6	Assigned parameters (ALK5)
Dipropylene Glycol	DPR-GLCL	OTH6	Assigned parameters (ALK5)
Dipropylene Glycol Methyl Ether	DPRGOME	OTH6	Assigned parameters (ALK5)
2-(2-Butoxyethoxy)-EtOH	C8-CELSV	OTH6	Assigned parameters (ALK5)
Tripropylene Glycol Monomethyl Ether	TPRGOME	OTH6	Assigned parameters (ALK5)
Methyl Formate	ME-FORM	OTH1	Assigned parameters (ALK1)
Ethyl Formate	ET-FORM	OTH2	Assigned parameters (ALK2)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Methyl Acetate	ME-ACET	OTH2	Assigned parameters (ALK2)
n-Propyl Formate	C3-FORM	OTH3	Assigned parameters (ALK3)
Ethyl Acetate	ET-ACET	OTH2	Assigned parameters (ALK2)
Methyl Propionate	ME-PRAT	OTH2	Assigned parameters (ALK2)
n-Butyl Formate	C4-FORM	OTH3	Assigned parameters (ALK3)
Ethyl Propionate	ET-PRAT	OTH3	Assigned parameters (ALK3)
Isopropyl Acetate	IPR-ACET	OTH3	Assigned parameters (ALK3)
Methyl Butyrate	ME-BUAT	OTH3	Assigned parameters (ALK3)
Methyl Isobutyrate	ME-IBUAT	OTH3	Assigned parameters (ALK3)
Propyl Acetate	PR-ACET	OTH3	Assigned parameters (ALK3)
n-Butyl Acetate	BU-ACET	OTH4	Assigned parameters (ALK4)
Ethyl Butyrate	ET-BUAT	OTH4	Assigned parameters (ALK4)
Isobutyl Acetate	IBU-ACET	OTH4	Assigned parameters (ALK4)
Methyl Pivalate	ME-PVAT	OTH2	Assigned parameters (ALK2)
n-Propyl Propionate	PR-PRAT	OTH4	Assigned parameters (ALK4)
s-Butyl Acetate	SBU-ACET	OTH4	Assigned parameters (ALK4)
t-Butyl Acetate	TBU-ACET	OTH2	Assigned parameters (ALK2)
Butyl Propionate	BU-PRAT	OTH4	Assigned parameters (ALK4)
Amyl Acetate	AM-ACET	OTH4	Assigned parameters (ALK4)
n-Propyl Butyrate	PR-BUAT	OTH5	Assigned parameters (ALK5)
2-Ethoxyethyl Acetate	CSV-ACET	OTH6	Assigned parameters (ALK5)
n-Butyl Butyrate	BU-BUAT	OTH5	Assigned parameters (ALK5)
Isobutyl Isobutyrate	IBU-IBTR	OTH4	Assigned parameters (ALK4)
Ethyl 3-Ethoxy Propionate	E3EOC3OH	OTH6	Assigned parameters (ALK5)
Isoamyl Isobutyrate	IC5IBUAT	OTH5	Assigned parameters (ALK5)
2-Ethyl-Hexyl Acetate	2ETHXACT	OTH5	Assigned parameters (ALK5)
Dimethyl Carbonate	DMC	OTH1	Assigned parameters (ALK1)
Propylene Carbonate	PC	OTH2	Assigned parameters (ALK2)
Methyl Lactate	ME-LACT	OTH3	Assigned parameters (ALK3)
Ethyl Lactate	ET-LACT	OTH4	Assigned parameters (ALK4)
Methyl Isopropyl Carbonate	MIPR-CB	OTH3	Assigned parameters (ALK3)
2-Methyoxy-1-propyl Acetate	2PGMEACT	OTH6	Assigned parameters (ALK5)
1-Methoxy-2-Propyl Acetate	PGME-ACT	OTH6	Assigned parameters (ALK5)
Dimethyl Succinate	DBE-4	OTH2	Assigned parameters (ALK2)
Diisopropyl Carbonate	DIPR-CB	OTH5	Assigned parameters (ALK5)
Dimethyl Glutarate	DBE-5	OTH4	Assigned parameters (ALK4)
2-Butoxyethyl Acetate	2BUETACT	OTH6	Assigned parameters (ALK5)
Dimethyl Adipate	DBE-6	OTH5	Assigned parameters (ALK5)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Substituted C7 ester (C12)	SC7ESC12	OTH6	Rep'd by 0.67 TEXANOL1 +0.33 TEXANOL2
Texanol isomers	TEXANOL	OTH6	Rep'd by 0.67 TEXANOL1 +0.33 TEXANOL2
3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	TEXANOL1	OTH6	Assigned parameters (ALK5)
1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	TEXANOL2	OTH5	Assigned parameters (ALK5)
Substituted C9 Ester (C12)	SC9ESC12	OTH6	Rep'd by 0.67 TEXANOL1 +0.33 TEXANOL2
Ethylene Oxide	ETOX	INERT	Assigned parameters (ALK2)
Propylene Oxide	PROX	OTH2	Assigned parameters (ALK2)
1,2-Epoxybutane	12BUOX	OTH3	Assigned parameters (ALK3)
Formic Acid	FORMACID	HCOOH	Assigned parameters (HCOOH)
Acetic Acid	ACETACID	CCOOH	Assigned parameters (CCO-OH)
Acrylic Acid	ACYRACID	OLE1	Assigned parameters (OLE1)
Propionic Acid	PROPACID	RCOOH	Assigned parameters (RCO-OH)
2-Methyl-2-Butene-3-ol	MBUTENOL	OLE1	Assigned parameters (OLE2)
Methyl Acrylate	ME-ACRYL	OLE1	Assigned parameters (OLE1)
Vinyl Acetate	VIN-ACET	OLE1	Assigned parameters (OLE1)
Ethyl Acrylate	ET-ACRYL	OLE1	Assigned parameters (OLE1)
Methyl Methacrylate	ME-MACRT	OLE2	Assigned parameters (OLE2)
Butyl Methacrylate	BU-MACRT	OLE2	Assigned parameters (OLE2)
Isobutyl Methacrylate	IBUMACRT	OLE2	Assigned parameters (OLE2)
Furan	FURAN	ARO2	Rep'd by M-XYLENE
Formaldehyde	FORMALD	HCHO	Explicit (HCHO)
Acetaldehyde	ACETALD	CCHO	Explicit (CCHO)
Propionaldehyde	PROPALD	RCHO	Explicit (RCHO)
Butanal	1C4RCHO	RCHO	Assigned parameters (RCHO)
2-Methylpropanal	2MEC3AL	RCHO	Assigned parameters (RCHO)
C4 aldehydes	C4-RCHO	RCHO	Rep'd by 1C4RCHO
Pentanal (Valeraldehyde)	1C5RCHO	RCHO	Assigned parameters (RCHO)
2,2-Dimethylpropanal (pivaldehyde)	22DMC3AL	RCHO	Assigned parameters (RCHO)
3-Methylbutanal (Isovaleraldehyde)	3MC4RCHO	RCHO	Assigned parameters (RCHO)
C5 Aldehydes	C5-RCHO	RCHO	Rep'd by 1C5RCHO
Glutaraldehyde	GLTRALD	RCHO	Assigned parameters (RCHO)
Hexanal	1C6RCHO	RCHO	Assigned parameters (RCHO)
C6 Aldehydes	C6-RCHO	RCHO	Rep'd by 1C6RCHO
Heptanal	1C7RCHO	RCHO	Assigned parameters (RCHO)
C7 Aldehydes	C7-RCHO	RCHO	Rep'd by 1C7RCHO

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Octanal	1C8RCHO	RCHO	Assigned parameters (RCHO)
C8 Aldehydes	C8-RCHO	RCHO	Rep'd by 1C8RCHO
Glyoxal	GLYOXAL	GLY	Explicit (GLY)
Methyl Glyoxal	MEGLYOX	MGLY	Explicit (MGLY)
Acrolein	ACROLEIN	MACR	Assigned parameters (METHACRO)
Crotonaldehyde	CROTALD	UALD	Assigned parameters (ISO-PROD)
Methacrolein	METHACRO	MACR	Assigned parameters (METHACRO)
Hydroxy Methacrolein	HOMACR	UALD	Assigned parameters (ISO-PROD)
Benzaldehyde	BENZALD	INHIB	Explicit (BALD)
Tolualdehyde	TOLUALD	INHIB	Rep'd by BENZALD
Acetone	ACETONE	ACET	Explicit (ACET)
Cyclobutanone	CC4-KET	KET1	Assigned parameters (MEK)
Methyl Ethyl Ketone	MEK	KET1	Assigned parameters (MEK)
Cyclopentanone	CC5-KET	KET1	Assigned parameters (MEK)
C5 Cyclic Ketones	KET5C	KET2	Rep'd by CC5-KET
3-Pentanone	DEK	KET1	Assigned parameters (MEK)
C5 Ketones	KET5	KET1	Rep'd by MPK
2-Pentanone	MPK	KET1	Assigned parameters (MEK)
Cyclohexanone	CC6-KET	KET2	Assigned parameters (PROD2)
C6 Cyclic Ketones	KET6C	KET2	Rep'd by CC6-KET
C6 Ketones	KET6	KET2	Rep'd by MNBK
4-Methyl-2-Pentanone	MIBK	KET2	Assigned parameters (PROD2)
Methyl n-Butyl Ketone	MNBK	KET2	Assigned parameters (PROD2)
Methyl t-Butyl Ketone	MTBK	KET1	Assigned parameters (MEK)
C7 Cyclic Ketones	KET7C	KET2	Rep'd by CC6-KET
2-Methyl-3-Hexanone	2M-3-HXO	KET2	Assigned parameters (PROD2)
2-Heptanone	C7-KET-2	KET2	Assigned parameters (PROD2)
Di-Isopropyl Ketone	DIPK	KET2	Assigned parameters (PROD2)
C7 Ketones	KET7	KET2	Rep'd by C7-KET-2
C8 Cyclic Ketones	KET8C	KET2	Rep'd by CC6-KET
2-Octanone	C8-KET-2	KET2	Assigned parameters (PROD2)
C8 Ketones	KET8	KET2	Rep'd by C8-KET-2
C9 Cyclic Ketones	KET9C	KET2	Rep'd by CC6-KET
2-Nonanone	C9-KET-2	KET2	Assigned parameters (PROD2)
Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	DIBK	KET2	Assigned parameters (PROD2)
C9 Ketones	KET9	KET2	Rep'd by C9-KET-2
C10 Cyclic Ketones	KET10C	KET2	Rep'd by CC6-KET
2-Decanone	C10-K-2	KET2	Assigned parameters (PROD2)
C10 Ketones	KET10	KET2	Rep'd by C10-K-2

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
Biacetyl	BIACETYL	BACL	Explicit (BACL)
Methylvinyl ketone	MVK	UKET	Assigned parameters (MVK)
Hydroxy Acetone	HOACET	KET1	Assigned parameters (MEK)
Methoxy Acetone	MEOACET	KET2	Assigned parameters (PROD2)
Diacetone Alcohol	DIACTALC	KET1	Assigned parameters (MEK)
Phenol	PHENOL	PHEN	Explicit (PHEN)
Alkyl Phenols	CRESOL	CRES	Rep'd by O-CRESOL
m-Cresol	M-CRESOL	CRES	Rep'd by O-CRESOL
o-Cresol	O-CRESOL	CRES	Explicit (CRES)
p-Cresol	P-CRESOL	CRES	Rep'd by O-CRESOL
Nitrobenzene	NO2-BENZ	HBEN	Assigned parameters with reactivity weighting (0.025 ARO1)
Para Toluene Isocyanate	P-TI	INHIB	Assigned parameters (INERT)
Toluene Diisocyanate	TDI	INHIB	Assigned parameters (INERT)
Methylene Diphenylene Diisocyanate	MDI	INHIB	Assigned parameters (INERT)
Dimethyl Amine	DM-AMINE	OTH6	Assigned parameters (ALK5)
Ethyl Amine	ET-AMINE	OTH6	Assigned parameters (ALK5)
Trimethyl Amine	TM-AMINE	OTH6	Assigned parameters (ALK5)
Methyl Nitrite	ME-NITRT	PHOT	(Not currently represented)
Ethanolamine	ETOH-NH2	OTH6	Assigned parameters (ALK5)
Dimethylaminoethanol	DMAE	OTH6	Assigned parameters (ALK5)
Diethanol Amine	ETOH2-NH	OTH6	Assigned parameters (ALK5)
Triethanolamine	ETOH3-N	OTH6	Assigned parameters (ALK5)
Acrylonitrile	ACRYLNIT	NOASN	(Not currently represented)
N-Methyl-2-Pyrrolidone	NMP	OLE1	Assigned parameters (OLE1)
Methyl Chloride	CH3-CL	INERT	Assigned parameters (INERT)
Vinyl Chloride	CL-ETHE	OTH5	Assigned parameters (ALK5)
Ethyl Chloride	C2-CL	OTH2	Assigned parameters (ALK2)
Dichloromethane	CL2-ME	OTH1	Assigned parameters (ALK1)
1-Chlorobutane	C4-CL	OTH3	(Not currently represented)
Methyl Bromide	ME-BR	INERT	Assigned parameters (INERT)
1,1-Dichloroethane	11CL2-C2	OTH1	Assigned parameters (ALK1)
1,2-Dichloroethane	12CL2-C2	OTH1	Assigned parameters (ALK1)
Ethyl Bromide	C2-BR	OTH1	Assigned parameters (ALK1)
1,2-Dichloropropane	12CL2-C3	OTH2	(Not currently represented)
Chloroform	CHCL3	INERT	Assigned parameters (ALK2)
n-Propyl Bromide	C3-BR	OTH2	Assigned parameters (ALK2)
1,1,1-Trichloroethane	111-TCE	INERT	Assigned parameters (ALK1)
1,1,2-Trichloroethane	112CL3C2	OTH1	Assigned parameters (ALK1)
n-Butyl Bromide	C4-BR	OTH3	Assigned parameters (ALK3)

Table A-3 (continued)

Description	Model Name	Emit. Group	Representation
3-(Chloromethyl)-Heptane	3CLME-C8	OTH4	(Not currently represented)
Carbon Tetrachloride	CCL4	INERT	Not represented (assumed to be inert)
Methylene Bromide	ME-BR2	INERT	Not represented (assumed to be inert)
1,2-Dibromoethane	11BR2-C2	OTH1	Assigned parameters (ALK1)
1,1-Dichloroethene	11CL2ETH	OTH3	(Not currently represented)
Trans-1,2-Dichloroethene	T-12-DCE	OTH3	Assigned parameters (ALK3)
2-(Cl-methyl)-3-Cl-Propene	CL2IBUTE	OLE1	Assigned parameters (OLE1)
Trichloroethylene	CL3-ETHE	OTH3	Assigned parameters (ALK3)
Perchloroethylene	CL4-ETHE	OTH1	Assigned parameters (ALK1)
Monochlorobenzene	CL-BEN	HBEN	Assigned parameters with reactivity weighting (0.130 ARO1)
Benzotrifluoride	CF3-BEN	HBEN	Assigned parameters with reactivity weighting (0.078 ARO1)
p-Dichlorobenzene	CL2-BEN	HBEN	Assigned parameters with reactivity weighting (0.094 ARO1)
p-Trifluoromethyl-Cl-Benzene	PCBTF	INERT	Assigned parameters with reactivity weighting (0.041 ARO1)
Chloropicerin	CCL3NO2	PHOT	(Not currently represented)
Dimethyl Sulfide	DMS	OTH4	(Not currently represented)
Dimethyl Sulfoxide	DMSO	OTH6	(Not currently represented)
Hexamethyldisiloxane	SI2OME6	INHIB	(Not currently represented)
Hydroxymethyldisiloxane	SI2OMEOH	INHIB	(Not currently represented)
D4 Cyclosiloxane	(SIOME)4	INHIB	(Not currently represented)
D5 Cyclosiloxane	(SIOME)5	INHIB	(Not currently represented)