Chapter 8

GAS-PHASE CHEMISTRY

Gerald L. Gipson*
Human Exposure and Atmospheric Sciences Division
National Exposure Research Laboratory
U. S. Environmental Protection Agency
Research Triangle Park, NC 27711, USA

Jeffrey O. Young**
Atmospheric Modeling Division
National Exposure Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711, USA

ABSTRACT

This chapter describes the manner in which gas-phase chemistry is treated in the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. The CMAQ system currently includes two chemical mechanisms -- RADM2 and CB4 -- with plans to incorporate a third -- the SAPRC97 mechanism -- in the near future. Each of these mechanisms is described, and the manner in which the first two are linked to the aqueous chemistry and aerosol formation processes is discussed. Enhanced isoprene chemistry that has been included in the RADM2 mechanism is also described, and procedures for entering new chemical mechanisms in the CMAQ system are addressed. The representation of reaction kinetics in the CMAQ system and the numerical modeling of gas-phase chemistry are also presented. The CMAQ system currently employs two numerical solvers, SMVGEAR and a variant of the QSSA method. The numerical procedures used in each are presented, and the relative computational efficiencies of each on different computing platforms are noted.

*Corresponding author address: Gerald L. Gipson, MD-80, Research Triangle Park, NC 27711. E-mail: ggb@hpcc.epa.gov

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8.0 GAS-PHASE CHEMISTRY

Since atmospheric chemistry plays a major role in many air pollution problems, the representation of chemical interactions among atmospheric constituents is often an essential element of an air quality model. All important chemical transformations relevant to the problem being studied must be included to make accurate predictions of ambient pollutant concentrations. Many atmospheric pollutants or their precursors are emitted as gases and interact primarily in the gaseous phase. However, some important atmospheric processes such as acid deposition and the formation of aerosols involve the interaction of constituents in the gas, liquid, and solid phases, so transformations taking place in all three phases often need to be represented. For computational efficiency, these processes are usually modeled separately. This approach has been adopted in the Chemical Transport Model (CTM) that is part of the Community Multiscale Air Quality (CMAQ) modeling system (hereafter referred to as the CCTM). This section addresses the modeling of gas-phase transformations alone in the CCTM. Descriptions of the linkages of gas-phase constituents with aerosols and with aqueous chemistry are discussed below and in Chapters 10 and 11, respectively. A potential future improvement to the CCTM would involve more closely coupling the chemical interactions taking place in all three phases. Nevertheless, the current formulation still enables the investigation and assessment of environmental problems using a multi-pollutant, one-atmosphere modeling concept.

Interactions in the gas-phase are represented in air quality models by means of chemical mechanisms. The CMAQ system currently includes two base chemical mechanisms that have been developed primarily to address issues associated with urban and regional scale ozone formation and acid deposition -- the CB4 (Gery et al., 1989) and RADM2 (Stockwell et al., 1990) mechanisms. Variants of these two mechanisms have been developed for the CMAQ system to provide the necessary linkages to the aerosol and aqueous chemistry processes. Current plans also call for adding a third mechanism -- the SAPRC-97 mechanism (Carter, 1997). Although these mechanisms should be adequate for many air pollution applications, it may be necessary to modify or even replace these mechanisms to address some issues. To facilitate changing mechanisms and adding new ones, the CMAQ system has been equipped with a generalized chemical mechanism processor. It must be emphasized, however, that supplemental data for other CMAQ processors may be required when one of the predefined mechanisms is modified or replaced. This is addressed in more detail section 8.2.5.

The remainder of this chapter addresses different aspects of the representation of gas-phase chemistry in the CMAQ system. The first section includes background information on chemical mechanisms and provides the rationale for including the predefined chemical mechanisms in the CMAQ system. The subsequent section describes the predefined chemical mechanisms as implemented in the CMAQ system and addresses adding new mechanisms or changing existing ones. This is followed by a description of reaction kinetics as it relates to the CCTM representation, and the final section describes the mathematical procedures used internally in the CCTM to solve the equations that arise from the mathematical representation of gas-phase chemistry.

8.1 Background

A chemical mechanism is a collection of reactions that transforms reactants into products, including all important intermediates. Chemical mechanisms developed for air quality modeling are highly condensed, parameterized representations of a true chemical mechanism. They include artificial species and operators, and many of the mechanism reactions are parameterizations of a large set of true atmospheric reactions. In some cases, mechanism reactions may include elements which have no physical significance (e.g., products with negative stoichiometry). While it would be difficult to design a generalized mechanism processor to handle all possible parameterizations used in various condensed mechanisms, some degree of generalization in the CMAQ system is achieved by using special conventions for entering chemical mechanisms. First, all reactions in the mechanism are treated as if they are elementary, and the stoichiometric coefficients for all reactants must be one. Since all reactions are assumed to be elementary, a reaction can have no more than three reactants. These conventions permit the reaction rate to be derived directly from the stoichiometric equation, thereby simplifying the mathematical representation of the reactions. Other conventions adopted for the CMAQ generalized mechanism processor are included in Section 8.3 and in Chapter 15.

Mechanism species can be divided into two categories: inorganic and organic. The number of important inorganic species is relatively small, and they are almost always represented explicitly in chemical mechanisms. The important inorganic species included in these mechanisms are ozone, nitric oxide, nitrogen dioxide, nitric acid, nitrous acid, hydrogen peroxide, sulfur dioxide, and several radicals formed through their interactions with other species. Although most of the chemical reactions involving these species are common to all mechanisms, some differences do exist. For example, some of the mechanisms omit a few reactions because they are normally minor pathways and thus do not affect modeling results significantly. Also, different rate constants may be used for some reactions, especially those that are photolytic. The representation of organic species usually differs more substantially, however. Some species in the mechanism represent real organic compounds, but others represent a mixture of several different compounds. The manner in which the grouping of organic compounds is carried out typically distinguishes one mechanism from another, and that is described next. In this chapter, the phrase *mechanism species* is used to refer to any species in the gas-phase mechanism, regardless of whether it is an explicit species or not.

Although explicit mechanisms have been developed for many organic compounds, the resultant number of reactions and species needed to represent their atmospheric chemistry is too large to model efficiently in photochemical grid models such as the CCTM. In addition, explicit mechanisms have not yet been developed for most organic compounds, thereby requiring that some reaction pathways be postulated. Thus, both compression and generalization are necessary when depicting organic reactions. Although chemical mechanisms differ in the manner in which organic species are represented, the mechanism developer usually chooses some distinguishable organic property to group similar organics into classes that reduce both the number of mechanism species and reactions. The three most common representations include the lumped structure technique, the surrogate species approach, and the lumped species method. In the lumped

structure approach, organic compounds are apportioned to one or more mechanism species on the basis of chemical bond type associated with individual carbon atoms (Whitten et al., 1980). In the surrogate species method, the chemistry of a single species is used to represent compounds of the same class (e.g., Lurmann et al., 1987). Generalized reactions are then written based on the hypothetical model species. The lumped species method is very similar to the surrogate species approach, but various mechanism parameters associated with a particular surrogate are adjusted to account for variations in the composition of the compounds being represented by the surrogate species (e.g., Carter, 1990, and Stockwell et al., 1990).

The construction of a compact chemical mechanism necessarily introduces varying levels of distortion, generalization, and omission in the representation of atmospheric chemistry (Jeffries, 1995). Although mechanisms are routinely tested using results obtained from environmental chamber experiments, the data are often insufficient to resolve uncertainties associated with some of the chemical representations. For example, Carter (1990) noted that much is unknown about several important reaction types, and that their representations "... continue to be largely speculative or are based on empirical models derived from fits to environmental chamber data." Further, rate constants for some reactions are either unknown completely, or significant disagreement exists as to their accuracy. Several studies have been conducted to compare different chemical mechanisms (e.g., Leone and Seinfeld, 1985; Hough, 1988; and Dodge, 1989). These comparisons revealed that the mechanisms often yield results that are similar for some species. This could indicate that the fundamental atmospheric chemistry is fairly well understood for these species, or that the mechanisms were derived from the same experimental kinetic or mechanistic data, which may or may not be accurate. Larger differences tend to occur for those species for which the atmospheric chemistry is more uncertain. Thus, it is often difficult to assess the relative merits of different mechanisms when applied to any one situation. Therefore, the CMAQ system includes the capability to use more than just one chemical mechanism.

Given the inherent uncertainties in existing chemical mechanisms, alternate approaches for representing gas-phase chemistry are needed. One approach being explored involves decreasing uncertainties associated with the simplifications that are introduced to reduce mechanism size. This approach is based on the concept that much of the information needed for an expanded chemical representation does not necessarily have to be included in the mechanism explicitly, but rather can be maintained in auxiliary variables linked to a relatively small number of core species that are included in the mechanism (Jeffries et al., 1993). Thus, it may be possible to expand chemical representations without greatly increasing the size of the basic mechanism, and this could be a future enhancement to the treatment of gas-phase chemistry in the CMAQ system.

8.2 Chemical Mechanisms in the CMAQ System

This section includes summary descriptions of the two basic chemical mechanisms included in the CMAQ system -- the CB4 (Gery et al., 1989) and the RADM2 (Stockwell et al., 1990). Since the SAPRC-97 mechanism (Carter, 1997) is to be added in the near future, some discussion of it is also included. These mechanisms require that information be supplied to the CCTM in a form that is unique for each mechanism, and this is carried out in several sub-systems incorporated in

the CMAQ system. These include the emissions processing system which generates emissions for key mechanism species; the initial conditions/boundary conditions processor that generates ambient starting and boundary concentrations for mechanism species; and the photolysis rate processor that produces mechanism specific photolysis rates. The reader is referred to the chapters describing those sub-systems for a description of the treatment of mechanistic data, and to the mechanism references for a more detailed description of each chemical mechanism.

In addition the base mechanisms, both the base CB4 and RADM2 mechanisms have been modified in the CMAQ system to provide necessary linkages for aerosol and aqueous chemistry processes, and the RADM2 mechanism has also been modified to create two new mechanism variants that include enhanced isoprene chemistry representations. Note that the existing sub-systems provide all of the necessary information for the extensions to the base mechanism. The modifications to the base mechanisms are discussed below in the section on mechanism extensions. Complete listings of all mechanisms currently available in the CMAQ system are included in Appendix 8A. The last portion of this section briefly discusses changing the base mechanism or their variants or adding new mechanisms to the CMAQ system.

8.2.1 CB4 Mechanism

The CB4 mechanism is a lumped structure type that is the fourth in a series of carbon-bond mechanisms, and differs from its predecessors notably in the detail of the organic compound representation. It has been used in models such as EPA's Empirical Kinetic Modeling Approach (EPA, 1989) and Regional Oxidant Model (Lamb, 1983), and in versions IV and V of the Urban Airshed Model (EPA, 1991 and SAI, 1993). The CMAQ implementation of the basic CB4 mechanism includes 36 species and 93 reactions, including 11 photolytic reactions.

The CB4 uses nine primary organic species (i.e., species emitted directly to the atmosphere as opposed to secondary organic species formed by chemical reaction in the atmosphere). Most of the organic species in the mechanism represent carbon-carbon bond types, but ethene (ETH), isoprene (ISOP) and formaldehyde (FORM) are represented explicitly. The carbon-bond types include carbon atoms that contain only single bonds (PAR), double-bonded carbon atoms (OLE), 7-carbon ring structures represented by toluene (TOL), 8-carbon ring structures represented by xylene (XYL), the carbonyl group and adjacent carbon atom in acetaldehyde and higher molecular weight aldehydes represented by acetaldehyde (ALD2), and non-reactive carbon atoms (NR). Many organic compounds are apportioned to the carbon-bond species based simply on the basis of molecular structure. For example, propane is represented by three PARs since all three carbon atoms have only single bonds, and propene is represented as one OLE (for the one carbon-carbon double bond) and one PAR (for the carbon atom with all single bonds). Some apportionments are based on reactivity considerations, however. For example, olefins with internal double bonds are represented as ALD2s and PARs rather than OLEs and PARs. Further, the reactivity of some compounds may be lowered by apportioning some of the carbon atoms to the non-reactive class NR (e.g., ethane is represented as 0.4 PAR and 1.6 NR). Apportioning rules have been established for hundreds of organic compounds, and are built into

the emissions processing sub-systems to produce the appropriate emission rates for the CB4 mechanism species.

The CB4 mechanism described by Gery et al. (1989) has undergone several changes since its publication. In 1991, the PAN rate constants were changed and a termination reaction between the XO2 operator and the HO2 radical were added. Subsequently, terminal reactions for the XO2N operator were also added. An updated CB4 isoprene chemistry mechanism based on the work of Carter (1996) was developed in 1996. All of these changes have been incorporated in the CMAQ version. It should also be noted that the original CB4 mechanism incorporated simple Arrhenius type rate constant expressions that were derived from more complex expressions for temperature and pressure dependent rate constants. Since the top of the CCTM domain may extend to heights that makes pressure dependencies important, the CMAQ version incorporates the original expressions rather than the derived ones.

8.2.2 RADM2 Mechanism

The RADM2 mechanism is a lumped species type that uses a reactivity based weighting scheme to adjust for lumping (Stockwell et al., 1990). It has evolved from the original RADM1 mechanism (Stockwell, 1986), and is employed in version 2 of the Regional Acid Deposition Model (Chang et al., 1987). The base mechanism as implemented in the CMAQ system contains 57 model species and 158 reactions, of which 21 are photolytic.

In RADM2, the primary organics are represented by 15 mechanism species, five of which are explicit because of their high emission rates or because of special reactivity considerations (methane, ethane, ethene, isoprene, and formaldehyde). The other ten represent groups of organic compounds aggregated on the basis of their reactivity with the hydroxyl radical (HO) and/or their molecular weights. To account for varying reactivities of the different organics that are lumped into a single group, emissions of each organic within a group are weighted by a reactivity factor (F) that is computed as the ratio of the fraction of emitted organic compound that reacts to the fraction of the mechanism species that reacts:

$$F = \frac{1 - \exp(-k_{\mathrm{HO\ Emiss}} \int [\mathrm{HO}]\ \mathrm{d}t)}{1 - \exp(-k_{\mathrm{HO\ Mech}} \int [\mathrm{HO}]\ \mathrm{d}t)} \ . \qquad (8\text{-}1)$$

The integral term is estimated from a daily average integrated HO radical concentration of 110 ppt min that was derived from RADM simulations (Stockwell et al., 1990). Note that F approaches unity if the reactivity of the emitted organic nearly equals that of the mechanism species or if the reactivities of both are very large. As with CB4, the RADM2 lumping and weighting rules have been built into the CMAQ emission processing system.

The implementation of the RADM2 mechanism in the CMAQ system is almost identical to that described by Stockwell et al. (1990), with only two minor modifications. First, the reaction of HO

with cresol (CSL) was reformulated as follows to eliminate negative stoichiometry in the mechanism:

From:	$HO + CSL \rightarrow 0.1\ HO_2 + 0.9\ XO_2 + 0.9\ TCO_3 - 0.9\ HO$	k_{HO+CSL};
To:	$HO + CSL \rightarrow 0.1\ HO_2 + 0.9\ XO_2 + 0.9\ TCO_3$	k_{HO+CSL};
	$HO + CSL \rightarrow CSL$	$0.9\ k_{HO+CSL}$.

(Note that negative stoichiometry is permitted in the CMAQ system, but was removed here for consistency with previous implementations of RADM2.) Second, the concentration of methane in the CCTM is assumed to be constant at $4.5x10^{13}$ molecules/cc. Thus, methane was removed as a reactant in the reaction of OH with methane and the corresponding rate constant changed from second-order to pseudo first-order using the assumed CCTM methane concentration.

8.2.3 SAPRC-97 Mechanism

The SAPRC-97 mechanism (Carter, 1997) employs the lumped surrogate species approach, but offers the capability to incorporate semi-explicit chemistry of selected organics. The SAPRC series of mechanisms evolved from the "ALW" mechanism of Atkinson et al. (1982). SAPRC-97 is similar to its predecessors SAPRC-90 and SAPRC-93, but incorporates improvements to aromatic chemistry and updates to reactions of many individual organic compounds. Although many of the reactions for organic compounds are generalized and incorporate non-explicit species, product yield coefficients and rate constants are tabulated for over 100 individual organic compounds. Thus, each of these organics can be modeled individually by including their semi-explicit chemistry in the mechanism. Due to computational constraints, however, the full set of organic compounds cannot be incorporated in an Eulerian model. For this situation, the mechanism is condensed by lumping individual organic compounds into groups with corresponding rate constants and product yield coefficients that have been weighted by mole fractions of the individual organics. The mole fractions are typically derived from emission inventory data used in the model simulation. Thus, unlike the previous mechanisms, the SAPRC-97 mechanism can potentially change with each application since new rate constants and product yield coefficients can be computed for each application.

The SAPRC-97 mechanism has been developed with supplemental software to facilitate constructing mechanisms of varying levels of condensation. Documentation of the procedures include three distinct levels of detail, differing primarily in the number of organic species that are included in the mechanism (Carter, 1988). Since no decisions have made on the form of the mechanism that will be added to the CMAQ system, listings for this mechanism are not included in Appendix 8A. Documentation will be provided when the CMAQ version is made available however.

8.2.4 Extended Mechanisms

Each gas-phase chemical mechanism has been linked to aqueous chemistry and to aerosol formation processes. Since these linkages required some modifications to the original gas-phase mechanisms, different versions of the same mechanism were created for modeling gas-phase chemistry alone or for modeling gas-phase chemistry with or without aerosols and/or aqueous chemistry. Different versions of the mechanisms are distinguished by means of a special naming convention. Gas-phase mechanisms that have not been modified are referred to by their base name (e.g., CB4, RADM2, and SAPRC when the latter is available). Mechanisms that have been modified to account for aerosol production have their names appended with "_AE", mechanisms modified for aqueous chemistry are appended with "_AQ", and mechanisms modified for both are appended with "_AE_AQ". Thus, CB4_AE_AQ refers to the CB4 gas-phase mechanism that has been modified to include linkages to both aerosols and aqueous chemistry. A second set of RADM2 gas-phase mechanisms that incorporates new isoprene chemistry has also been included in the CMAQ system. These mechanisms include either "_CIS1" or "_CIS4" in their names to denote that the mechanism incorporates enhanced isoprene chemistry. Methods used to develop the extended mechanisms are described below according to the three types of extensions: aerosol, aqueous chemistry, and isoprene chemistry.

8.2.4.1 Aerosol Extensions

A major pathway leading to the formation of aerosols is the oxidation of sulfur dioxide (SO_2) to sulfate, primarily by the gas-phase reaction of SO_2 with the hydroxyl radical (OH). All mechanisms in the CMAQ system incorporate this reaction. Because organics are represented differently in the base mechanisms, however, aerosol formed from the reactions of organic compounds must be handled somewhat differently. In the CCTM, organic aerosol formation is quantified using aerosol yields, i.e., μgm^{-3} of aerosol produced per ppm of organic reacted with OH, ozone or nitrate radical (NO_3). The yields used in the CCTM are those reported by Bowman et al. (1995) that were derived from the work of Pandis et al. (1992). These yields are given in terms of the SAPRC-90 chemical mechanism species, so some adjustments were required to adapt them to the CMAQ mechanisms. In the CMAQ system, aerosol production is assumed to occur from reactions involving five different generic organic groupings. Individual mechanism species are then mapped to these general groupings to obtain the aerosol yields. The five generic groups are defined as: 1) long-chain alkanes; 2) alkyl-substituted benzenes such as toluene and xylene; 3) cresol and phenols; 4) long-chain olefins; and 5) monoterpenes. Note that the aerosol yields vary significantly among these five groups, so it is important to map the organic species in each mechanism to the proper aerosol production group. The remainder of this section describes the mapping that is used for the CMAQ base mechanisms and how the aerosol production rates are determined from the gas-phase reactions. The derivation of the yields used in the CCTM and the manner in which they are used in the aerosol module are described in Chapter 10.

To apply the aerosol yields, the amount of reactant consumed by reaction must be determined for several mechanism species. In the CMAQ system, this is accomplished by using "counter" species that have been added as products to those reactions involving the mechanism species of interest (e.g., Bowman et al., 1995). These counter species are essentially "dummy" species with no physical significance, and are not subjected to any other model process such as advection or

diffusion. Thus, changes in their concentrations reflect the effect of chemical reaction alone. Also, their inclusion in the mechanisms does not affect basic gas-phase chemistry since they do not interact with any of the other species in the mechanism.

Special procedures are used in the CCTM to determine aerosol production from monoterpenes since their aerosol yields are relatively large and they are either lumped with other organic compounds into a single mechanism species or are apportioned among several mechanism species. The approach involves tracking the rate of reaction of monoterpenes separately from the rates of their mechanistic representation. The CMAQ emission processor generates emissions for monoterpenes as a unique species *in addition to* lumping or apportioning the emissions into the appropriate mechanism species. Whenever aerosols are being modeled, the unique monoterpene species is included in the mechanisms and is modeled as a separate species. As with the counter species, however, the monoterpene species is incorporated in the mechanisms such that it does not affect the basic gas-phase chemistry. This is described in more detail below. A potential future modification to the CMAQ system would involve incorporating a more explicit representation of monoterpenes in the base mechanisms that would eliminate the need for this special treatment and would also improve the chemical representation of these species in the gas-phase mechanisms (e.g., Stockwell et al., 1997).

- **RADM2_AE.** Much of the linkage between the RADM2 mechanism and aerosol formation is relatively straightforward. Aerosol production from SO2 and long-chain alkanes is derived from the amount of SO2 and HC8 reacted with OH, respectively. Similarly, aerosol production from alkyl-substituted benzenes is derived from the sum of the TOL and XYL reactions with OH. The production from phenols and cresols is based upon the sum of the CSL reactions with OH and NO_3. Thus, special counter species named SULAER, HC8AER, TOLAER, XYLAER, and CSLAER have been added to track these reactions.

  In the RADM2 mechanism, both monoterpenes and other olefinic compounds are lumped into the mechanism species OLI. As noted above, however, monoterpenes are modeled separately whenever aerosols are modeled. The monoterpenes are represented in the RADM2 mechanism by the species TERP, and the following reactions are added:

  $$TERP + HO \rightarrow TERPAER + HO$$

  $$TERP + NO_3 \rightarrow TERPAER + NO_3$$

  $$TERP + O_3 \rightarrow TERPAER + O_3$$

  These reactions use the same rate constants as the reaction of OLI with these species, and have the TERPAER counter species added to track the throughput of this reaction. Note that concentrations of the reactants OH, NO_3 and ozone are unaffected by these reactions since their production equals their loss.

The final pathway for aerosol production in the RADM2 mechanism is via reaction of long-chain olefins with OH, NO_3 and ozone. The RADM2 mechanism species OLI is used as the surrogate for long-chain olefins, and thus a counter species product named OLIAER is added to each of the reactions of OLI with OH, NO_3 and ozone. Since OLI includes both monoterpenes and other olefins, however, OLIAER tracks the reaction rate of both. The amount of long-chain olefins reacted is determined by subtracting the concentration of the counter species TERPAER from that of OLIAER. The yield of aerosols from long-chain olefins is then applied to this difference to obtain aerosol production by this pathway.

- **CB4_AE.** Since the CB4 gas-phase mechanism is structure-based, individual organic molecules are often disaggregated and assigned to more than one mechanism species. For example, long-chain alkenes are apportioned to both the PAR and OLE mechanism species. Thus, many of the organic mechanism species contain fragments of molecules, and the identity of the original contributing organic compound is lost. As a result, it is not possible to ascertain with certainty the amount of long-chain alkanes and alkenes reacting in the CB4 mechanism, and thus aerosol production via these pathways is omitted. The production of aerosols from the reactions of toluene, xylene, and cresol is included, however, by tracking the amounts of TOL, XYL, and CRES that react using the counter species TOLAER, XYLAER, and CSLAER. The manner in which aerosol production from monoterpenes is modeled is identical to that used in the RADM2 mechanism. Monoterpenes are modeled independently as the mechanism species TERP, with rate constants for the reactions of TERP with OH, O_3, and NO_3 set to the same values as those used in the RADM2 mechanism extension.

8.2.4.2 Isoprene Extensions

Over the past few years, the importance of isoprene in ozone formation has become a major concern. Its representation in the original gas-phase mechanisms was substantially condensed, partially because of computational resource considerations and partially due to significant uncertainties about the pathways of its reaction products. Recent mechanistic and environmental chamber studies have led to a greater understanding of its atmospheric chemistry and thus improved mechanistic representations (Carter and Atkinson, 1996). In the CMAQ system, two different levels of more detailed isoprene chemistry have been included in the RADM2 mechanism, and these are referred to as the one-product and the four-product Carter isoprene mechanisms (Carter, 1996). Both are condensed forms of the more detailed mechanism developed by Carter and Atkinson (1996). Since this detailed mechanism may be too large to use in full-scale Eulerian modeling studies, Carter condensed the detailed mechanism to two levels of detail: one in which isoprene products are represented by four products, and one in which only one product is used. The four-product mechanism is the lesser condensed of the two, and includes the explicit representation of many of the isoprene's unique products (e.g., methacrolein, methyl vinyl ketone, and methacrolein's PAN analogue). The one-product form lumps the major products into a single species, thereby yielding a more compact albeit less explicit mechanism. As noted above, these two mechanisms are named RADM2_CIS4 and

RADM2_CIS1, and both have been linked to aerosols and aqueous chemistry as well. It should also be noted that the isoprene chemistry incorporated in the CMAQ CB4 mechanism corresponds to the Carter 1-product form, but the 4-product form is not available for the CB4 mechanism in the CMAQ system

8.2.4.3 Aqueous Chemistry Extensions

The base RADM2 mechanism does not have to be modified to link it to the aqueous chemistry processes since the aqueous processes in the CMAQ system are similar to those incorporated in the original RADM model. As described in Chapter 15, other aspects of the linkages require a separate mechanism with a unique name. The linkages to aqueous chemistry do require some minor changes to the CB4 mechanism however. These changes were based on a variant of the CB4 mechanism developed for acid deposition modeling by Gery et al. (1987). In this version, the following product species that were omitted in the base CB4 mechanism are included: formic acid, acetic acid, peroxyacetic acid, and methylhydroperoxide (MHP). Since these species are products only, their inclusion in the mechanism does not affect the concentrations of any of the other mechanism species. It should be noted, however, that the concentration of MHP in this modified mechanism represents an upper limit for two reasons. First, known decomposition pathways for it are not included in the mechanism. Second, the production of MHP will be overstated since it is produced by an operator that includes radicals other than the methylperoxy radical (Gery et al., 1987).

8.2.5 Changing or Adding Mechanisms in CMAQ

As noted in the introduction to this chapter, the CMAQ system has been instrumented with a generalized chemical mechanism processor to facilitate making changes to existing mechanisms or adding new mechanisms. The procedures for altering or adding a new mechanism are described in EPA (1998), and will not be repeated here. It should be emphasized, however, that the addition of a new mechanism will likely require modifications to the previously mentioned subsystems that provide key mechanism-specific information, i.e., emissions, initial/boundary condition, and photolytic rate processors. Changes to an existing mechanism would also likely require modifications to these processing subsystems if new organic species are added or if an alternative organic grouping scheme is implemented. If changes are limited such that they affect only the reactions of intermediate and/or product species, however, these subsystems may not need to be changed at all, and the modifications can then be implemented solely within the generalized chemical mechanism processor. For example, the modifications to the base mechanisms to provide linkages to aerosol and aqueous chemistry and to expand isoprene chemistry that were described previously did not require any major changes to the other processors except to add a photolysis rate for acrolein in the photolytic rate processor for the CIS1 and CIS4 versions of RADM2.

Although the CMAQ system provides a convenient tool for making mechanism changes, some caution should be exercised in modifying existing CMAQ mechanisms. The mechanisms currently in the CMAQ system have been evaluated outside of the CMAQ system using

environmental chamber data and/or more detailed chemical mechanism representations. Any proposed changes to reactions or reactions rates that significantly affect model predictions should normally be subjected to similar independent testing before being introduced into the CMAQ system and subsequently used in modeling applications. Thus, it would be expected that the introduction of most changes to a mechanism in the CMAQ system would only be performed by a researcher who is experienced in atmospheric chemistry and is familiar with the base mechanism.. Finally, it should be noted that the existing CMAQ mechanisms are fully specified. In most instances, it will only be necessary for a user to choose one of the existing mechanisms for their application, and it will not be necessary to make any changes to that mechanism.

8.3 Reaction Kinetics

The rates of chemical reaction determine whether a species is formed or destroyed by gas-phase chemistry. Since the CMAQ system treats all reactions as if they are elementary, the laws of reaction kinetics can be used directly to develop mathematical expressions for the rates of each chemical reaction. This section describes the rate expressions and the forms of the rate constants that are used in those expressions, with special emphasis placed on the conventions used in the CMAQ system. The reader may also wish to refer to Chapter 15 and EPA (1998) for details on how mechanism data are entered in the CMAQ system.

8.3.1 Reaction Rates

The rate of a chemical reaction l (r_l) can be expressed as the product of a rate constant (k_l) and a term that is dependent on the concentrations of the reactants:

$$r_l = k_l \, f(\text{concentration}) \; . \tag{8-2}$$

For elementary reactions, the concentration dependent term is simply the product of reactant concentrations, and the rate of reaction takes one of the following forms:

$$r_l = \begin{cases} k_l C_1 & \text{for first-order reactions} \\ k_l C_1 C_2 & \text{for second-order reactions} \\ k_l C_1 C_2 C_3 & \text{for third-order reactions} \end{cases} \tag{8-3}$$

where C_1, C_2,and C_3 refer to the concentration of reactants 1, 2 and 3, respectively. Note that when a species reacts with itself, the concentration dependent term includes the species concentration squared. Thus, the rate for the reaction $NO + NO + O_2 \rightarrow 2NO_2$ is equal to k[NO][NO][O_2] and not k[NO][O_2].

Several important ter-molecular reactions involve O_2 and/or N_2 which mediate those reactions by absorbing energy from exothermic bi-molecular reactions. When either N_2 or O_2 serves this role, the third body is usually referred to as "M", where $M = N_2 + O_2$. Since their concentrations are relatively stable in the atmosphere, some mechanism developers convert second- or third-order

reactions that include these species to a reaction one order lower by multiplying the higher-order rate coefficient by the concentration of M, O_2, or N_2. The CMAQ convention is to include third-body reactants in the reaction rate calculations if they are explicitly shown in the reaction, and to omit them if they are not shown or included only as comments. For example, consider the bimolecular reaction: $O^1D + O_2 \rightarrow O^3P + O_2$. If the reaction is written in this form, the reaction is assumed to be second-order and the CCTM will use the appropriate concentration for O_2 in the rate computation. If the reaction is written as $O^1D \rightarrow O^3P$ (or as $O^1D \{+ O_2\} \rightarrow O^3P$, where here the braces denote a comment), the reaction rate will be assumed to be first-order and the CCTM will *not* include the O_2 concentration in the reaction rate calculation. In the latter case, the mechanism developer must specify a pseudo first-order rate constant for the reaction. The same convention also applies to H_2O.

8.3.2 Rate Constant Expressions

As shown in Equation 8-3, the rate of reaction is related to the concentration term by a constant of proportionality k_l. The rate constant k_l can take many forms depending upon the characteristics of the reaction. One important class of uni-molecular reactions involves the absorption of radiant energy and subsequent dissociation of the reactant into product species. The rate constants for these types of reactions are functions of the incident radiant energy and properties of the absorbing molecule, such as the absorption cross section and the quantum yield. In the CMAQ system, these rate constants are calculated by the photolytic rate processor, and the details of these calculations are described in Chapter 14. The remainder of the reactions are classified as thermal, and their rate constants are typically functions of temperature and sometimes pressure. The calculation of these rate constants is discussed below.

To facilitate incorporating rate constant information for thermal reactions, the CMAQ generalized mechanism processor (discussed in Chapter 15) has been designed to accept the standard rate constant expressions used in NASA (1997). Rate constant information is most often supplied in cms units (i.e., gas concentrations in molecules/cc and time in seconds), but some mechanisms use mixing ratio units (i.e, gas concentrations converted to mixing ratios in parts per million and time in minutes). The CMAQ generalized mechanism reader is designed to accept either, but they must be consistent throughout the mechanism (i.e., the same units must be used for all rate constant forms that can be expressed in either set of units). Some rate constant expressions (e.g., falloff expressions and other special forms discussed below) can be expressed only in cms units, however, and must always be in these units even when mixing ratio units are being used for all other types of rate constants. The CCTM will automatically perform the necessary units conversions during the model simulation. Nevertheless, since the CMAQ domain typically extends through the entire troposphere, cms units are usually preferred because differences in number density differences with height are explicitly accounted for with those units.

Descriptions of the forms of rate constant expressions currently used in the CMAQ system are presented next.

- **Arrhenius Equation**. Many rate constants exhibit a temperature dependence that corresponds to the Arrhenius equation:

$$k = A\ e^{(-E/T)} \tag{8-4}$$

where A is the pre-exponential factor, E is the activation energy divided by the gas constant R, and T is the temperature in degrees Kelvin. For this form of reaction, either cms or mixing ratio units may be used, and only A and E need to be specified.

- **Temperature Dependent A-factors.** For some reactions, the temperature dependence of the pre-exponential factor can become significant, and the Arrhenius equation does not hold. These rate constant expressions can often be put in the following form that is available in the CMAQ system:

$$k = A\ (T/300)^B\ e^{(-E/T)} \tag{8-5}$$

where A, E, and T are defined as above, and B is an empirically derived constant that provides a best fit to the data (Pitts-Finlayson and Pitts, 1986). For this form, either set of units can be used, and only A, E and B need to be specified.

- **Falloff Expressions.** Several ter-molecular reactions exhibit pressure dependencies that can be significant when modeling atmospheric chemistry. These can be especially important when modeling from the troposphere through the stratosphere. In these cases, the rate constant increases with increasing pressure. In effect, the behavior of these reactions approaches second-order at high pressure and third-order at low pressure. Equation 8-6 gives an effective second-order rate constant for the falloff region between these two limits.

$$k = \frac{k_0[\mathrm{M}]}{1 + k_0[\mathrm{M}]/k_\infty}\ F_C^{\{1 + [N^{-1}\log(k_0[\mathrm{M}]/k_\infty)]^2\}^{-1}} \tag{8-6}$$

In Equation 8-6, k_0 and k_∞ are the low- and high-pressure limiting rate constants, respectively, and are calculated using the temperature dependent A-factor form described above. The parameters F_C and N are also reaction specific, but for atmospheric conditions are very often 0.6 and 1.0 respectively (Finlayson-Pitts and Pitts, 1986). For this type of rate constant expression, A, E, and B must be specified for both k_0 and k_∞, and only cms units are allowed. If the parameters N and Fc are not specified, the values listed above will be used.

- **Special Forms.** The following special rate constant forms are also in general use and have been included in the CMAQ system:

$$k = k_1 + k_2[\mathrm{M}] \tag{8-7}$$

$$k = k_0 + \left(\frac{k_3[\mathrm{M}]}{1 + k_3[\mathrm{M}]/k_2} \right) \tag{8-8}$$

$$k = A\,(1.0 + 0.6P) \tag{8-9}$$

Equation 8-7 is used for the rate constants of the reactions forming hydrogen peroxide from hydroperoxy radicals ($HO_2 + HO_2 \rightarrow H_2O_2$ and $HO_2 + HO_2 + H_2O \rightarrow H_2O_2$). Equation 8-8 is used for the reaction of the hydroxyl radical with nitric acid ($HO + HNO_3 \rightarrow NO_3 + H_2O$), and Equation 8-9 is used for the reaction of the hydroxyl radical with carbon monoxide ($HO + CO \rightarrow HO_2 + CO_2$). In these equations, k_0, k_1, k_2, and k_3 are calculated using the Arrhenius equation, and A and E must be specified for each, with A given in cms units. In Equation 8-9, P is the atmospheric pressure in atmospheres and A can be specified in either set of units.

- **Reverse Equilibria Forms.** The CMAQ system also includes a special reverse equilibrium form for first-order decomposition reactions. With these types of reactions, the equilibrium constant is input in a form similar to the Arrhenius equation. Thus, the rate constant can be expressed as follows:

$$k = k_f \,/\, A\mathrm{e}^{(-E/T)} \tag{8-10}$$

In Equation 8-10, k_f is the rate constant for the forward reaction forming a species, and the denominator is an Arrhenius-like form for the equilibrium constant. These reaction rate coefficient types are used, for example, for the decomposition of pernitric acid and nitrogen pentoxide (i.e., $HNO4 \rightarrow HO_2 + NO_2$ and $N_2O_5 \rightarrow NO_2 + NO_3$). In the CMAQ system, A, E, and the corresponding forward reaction must be specified. Either set of units may be used with this form.

8.4 Mathematical Modeling

This section describes the mathematical modeling concepts used in the CCTM to simulate gas-phase chemical reactions. The first sub-section describes the fundamental equations that must be solved and some of the difficulties encountered in obtaining solutions to them. The next two sub-sections describe the two gas-phase chemistry solvers that are currently available in the CCTM. The last sub-section summarizes some of the important solver characteristics.

8.4.1 Governing Equations

As described in Chapter 5, operator splitting allows gas-phase chemistry to be de-coupled from physical processes such as advection, diffusion and deposition, and, as noted in the introduction to this chapter, gas-phase chemistry is modeled separately from aerosol formation and aqueous chemistry. As a consequence, continuity equations for each gas-phase mechanism species can

be formulated and solved independently on a cell-by-cell basis. By using the kinetics laws for elementary reactions and applying a mass balance to each species, the following equation for the rate of change of each species concentration can be derived for a single cell:

$$\frac{dC_i}{dt} = P_i - L_i C_i \tag{8-11}$$

where

$$P_i = \sum_{l=1}^{m_i} \nu_{i,l} r_l \tag{8-12}$$

and

$$L_i C_i = \sum_{l=1}^{n_i} r_l \tag{8-13}$$

In Equations 8-11 through 8-13, C_i is the concentration of species i, $\nu_{i,l}$ is the stoichiometric coefficient for species i in reaction l, and r_l is the rate of reaction l. The sum $l = 1...m_i$ is over all reactions in which species i appears as a product, and the sum $l = 1...n_i$ is over all reactions in which species i appears as a reactant.

Equation 8-11 states that the change in species concentration is equal to the chemical production of that species minus its chemical loss, and it is the fundamental species continuity equation for gas-phase chemistry that is solved in the CCTM. If the concentration of species i is known at some particular time, its concentration can be computed at a later time by solving Equation 8-11. Since the production and loss terms contain references to other species concentrations, however, Equation 8-11 must be solved as part of a coupled set of ordinary differential equations.

It should also be noted that the CCTM contains an option for including emissions in either the vertical diffusion process or in gas-phase chemistry. When emissions are included in gas-phase chemistry, the fundamental form of the Equation 8-11 is not altered since an emission source term is simply a zeroth-order production rate. Thus, for the discussions that follow, the production term P_i is assumed to include an emission source term if species i is emitted and emissions are included in gas-phase chemistry.

The system of non-linear, ordinary differential equations (ODEs) arising from Equation 8-11 for N species can be expressed as follows:

$$\frac{dC_i}{dt} = P_i(\mathbf{c},t) - L_i(\mathbf{c},t) C_i = f_i(\mathbf{c},t) \quad i = 1,2,...,N \tag{8-14a}$$

with the initial conditions:

$$\mathbf{c}(t_0) = \mathbf{c_0} \qquad (8\text{-}14b)$$

where **c** is the vector of species concentrations and N is the total number of species in the chemical mechanism. Numerical "marching" methods are typically employed to obtain approximate solutions for this class of problem. In these methods, the concentrations of all species are given at the starting point and a solution is computed at selected time intervals (i.e., time steps) using the right hand side of Equation 8-14a. Two sources of difficulty arise in obtaining numerical solutions to these equations as they apply to atmospheric chemistry problems. First, the system is nonlinear because the production and loss terms include second- and third-order reactions. Second, the system of equations is "stiff" because of the widely varying time scales of the chemical reactions and complex interactions among species. A stiff system can be described mathematically as one in which all the eigenvalues of the Jacobian matrix of Equation 8-14a are negative, and the ratio of the absolute values of the largest-to-smallest real parts of the eigenvalues is much greater than one. Systems are typically termed stiff if the latter ratio is greater than 10^4. For atmospheric chemistry problems, the ratio is often greater than 10^{10}, making the system very stiff (Gong and Cho, 1993).

The stiffness problem coupled with the fact that these equations must be solved for tens of thousands of cells in a typical modeling application require that special numerical methods be employed. The use of standard explicit methods is often precluded because relatively small time steps are required to maintain numerical stability and obtain accurate solutions. On the other hand, classical implicit methods that are both accurate and stable have not often been used because of high computational demands. As a result, several special techniques have been developed to obtain reasonably accurate solutions in a computationally efficient manner. At present, two solution techniques are available in the CCTM: the implicit Sparse-Matrix Vectorized Gear algorithm (SMVGEAR) and a variant of the explicit Quasi-Steady State Approximation (QSSA) method. Each of these is described in detail below. Although each of these techniques, as well as others that have been used in atmospheric chemistry models, have been designed to be computationally efficient, they still consume 50 to 90% of the total CPU time used in a model simulation. Thus, obtaining a numerical solution to Equation 8-14a,b is normally the most computationally intensive portion of the CCTM.

8.4.2 SMVGEAR

Numerical solvers based on the algorithm developed by Gear (1971b) have traditionally been used to obtain accurate solutions to stiff ODE problems. The technique is implicit in method, does not amplify errors from one step to another and incorporates automatic step size and error control. In fact, solvers based on this method have often been used to evaluate other faster solution methods for accuracy (e.g., Odman et al., 1992; Gong and Cho, 1993; Dabdub and Seinfeld, 1995; and Saylor and Ford, 1995). Past versions of this code have rarely been installed

in Eulerian models, however, because of the high computational cost. Jacobson and Turco (1994) have modified the Gear algorithm to obtain considerable speedups on vector computers. The SMVGEAR algorithm is highly vectorized to improve computational performance on vector computers and it incorporates special sparse matrix techniques to increase computational efficiency. Further enhancements have been obtained by ordering the cells for processing. Each of these are described further below. Since the technique is based on Gear's original algorithm, it is briefly described first. For more details on the Gear method, the reader is referred to Gear (1971a) and Gear (1971b).

8.4.2.1 Standard Gear Algorithm

The Gear algorithm is one of a class of methods referred to as backward differentiation formulae (BDF). The generalized BDF that forms the basis for Gear's method can be expressed as follows:

$$\mathbf{c}_n = h\beta_0 \mathbf{f}(\mathbf{c}_n, t_n) + \sum_{j=1}^{p} \alpha_j \mathbf{c}_{n-j} \tag{8-15}$$

where n refers to the time step, h is the size of the time step, p is the assumed order, β_0 and α_j are scalar quantities that are functions of the order, and $\mathbf{f}(\mathbf{c}_n,t_n)$ is the vector of production and loss terms defined by the right hand side of Equation 8-14a. The method is implicit since concentrations at the desired time step n depend on values of the first derivatives contained in $\mathbf{f}(\mathbf{c}_n,t_n)$ that are functions of the concentrations at the same time. The order of the method corresponds to the number of concentrations at previous time steps that are incorporated in the summation on the right hand side of Equation 8-15.

To facilitate changing step size and estimating errors, the multi-step method in Equation 8-15 is transformed to a multi-value form in which information from only the previous step is retained, but information on higher order derivatives is now used (Gear, 1971b). In this formulation, the solution to Equation 8-14a,b is first approximated by predicting concentrations and higher order derivatives at the end of a time step for each species using the following matrix equation:

$$\mathbf{z}_{i,n,(0)} = \mathbf{B}\,\mathbf{z}_{i,n-1} \tag{8-16}$$

where $\mathbf{z}_i = [c_i, hc'_i, ..., hpc_i^{(p)}/p!]^T$, the subscript n,(0) refers to the prediction at the end of time step n, and the subscript n-1 refers to values obtained at the end of previous time step (or the initial conditions when n = 1). **B** is the Pascal triangle matrix, the columns of which contain the binomial coefficients:

$$\mathbf{B} = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ & 1 & 2 & 3 & \cdots & p-1 & p \\ & & 1 & 3 & \cdots & & \\ & & & 1 & \cdots & & \\ & & & & \ddots & & \\ & 0 & & & & 1 & p \\ & & & & & & 1 \end{bmatrix} \tag{8-17}$$

The prediction obtained from Equation 8-16 is then corrected by solving for $\mathbf{z}_{i,n}$ such that the following relations hold for all species:

$$\mathbf{z}_{i,n} = \mathbf{z}_{i,n,(0)} + \mathbf{r}[hf_i(\mathbf{c}_n, t_n) - hc'_{i,n,(0)}] \tag{8-18}$$

In Equation 8-18, $\mathbf{r}$ is a vector of coefficients that is dependent on the order, but r_2, the element corresponding to the first derivative location in $\mathbf{z}$, is always equal to one. Thus, the correct value of $c_{i,n}$ is obtained when the calculated value of $c'_{i,n}$ equals $f_i(\mathbf{c}_n, t_n)$ in Equation 8-18. An approximate solution for $c_{i,n}$ is obtained by applying Newton's method to the system of equations that correspond to the first equation in 8-18 for all species. This leads to the following corrector iteration equation:

$$\mathbf{c}_{n,(m+1)} = \mathbf{c}_{n,(m)} + [\mathbf{I} - h\beta_0\mathbf{J}]^{-1} r_1[h\mathbf{f}(\mathbf{c}_{n,(m)}, t_n) - h\boldsymbol{\delta}\mathbf{c}_{n,(m)}] \tag{8-19}$$

where m refers to the Newton iteration number, the vector $\mathbf{f}(\mathbf{c}_n, t_n)$ is calculated using concentrations computed for the m-th iteration, $\boldsymbol{\delta}\mathbf{c}$ is a vector containing the most recent estimates of first derivatives, $\mathbf{I}$ is the identity matrix, and $\mathbf{J}$ is the Jacobian matrix whose entries are defined as:

$$J_{ij} = \frac{\partial f_i(\mathbf{c}, t_n)}{\partial c_j} \qquad i, j = 1,2,\ldots N \tag{8-20}$$

At the end of each iteration, the vector containing the first derivatives ($\boldsymbol{\delta}\mathbf{c}$) is updated, but higher order derivatives in $\mathbf{z}$ need not be computed until convergence is achieved.

After convergence is achieved, the local truncation error for each species, e_i, is given by:

$$e_i = \frac{1}{p+2} h^{p+1} c_{i,n}^{(p+1)} + O(h^{p+2}) \tag{8-21}$$

The error is estimated in the algorithm by neglecting the $O(h^{p+2})$ term and approximating $h^{p+1}c_i^{(p+1)}$ from the backward difference of $h^p c_i^{(p)}/p!$ which can be calculated using the last components of

the vectors $\mathbf{z}_{i,n(m)}$ and $\mathbf{z}_{i,n-1}$ defined above. These error estimates are used to control accuracy and to change both the time step size and the order of the method when warranted.

Although several variants of the basic Gear algorithm have been developed, the fundamental computational scheme can be described generically as follows. At the beginning of any integration interval, the order is set to one and the starting time step is either calculated or selected by the user. Each time step is initiated by predicting concentrations at the end of the time step using Equation 8-16. Corrector iterations are then carried out using Equation 8-19 until prescribed convergence criteria are achieved or non-convergence is deemed to have occurred. When convergence is achieved, the error is computed using the approximation for Equation 8-21. If the error is within prescribed limits, the solution for the step is accepted and the step size and order to be used in the next step are estimated. The size of the time step is estimated for the current order, the next lowest order, and the next highest order using error estimates derived from Equation 8-21 for the next step. From these, the largest time-step size and its corresponding order are then selected for use in the next step. If either the convergence or error test fails, the integration is restarted from the beginning of the failed time step after re-evaluating the Jacobian matrix, reducing the size of the time step, and/or lowering the order.

The individual operations described above are normally handled automatically in Gear algorithms. To reduce computational demands, the algorithms also utilize several empirically based rules. For example, the Jacobian matrix is only updated after a prescribed number of successful steps have been completed, if the order changes, or if a convergence or error test failure occurs. In the Newton iterations, progress towards convergence is monitored and the iterations halted if the progress is judged insufficient or if three complete iterations have been performed without convergence being achieved. To maintain numerical stability, changes to the size of the time step and the order are allowed no more than once every p+1 steps for a p-th order method.

8.4.2.2 Vectorized Gear Algorithm

Jacobson and Turco (1994) have modified the Gear algorithm to incorporate additional computational efficiencies that can achieve speedups on the order of 100 on vector computers. About half of the improvement is attributed to enhanced vectorization, and half to improved matrix operations. Because of the improved matrix operations, SMVGEAR also runs faster than traditional Gear solvers on non-vector machines, but the greatest benefit will be obtained with vector machines. The major enhancements incorporated in SMVGEAR are now described in more detail.

In the conventional application of the Gear-type algorithm, the method is applied to each grid cell individually. With this implementation, the length of the innermost loops in most computations corresponds to the number of species, which is typically on the order of 30 to 100. In SMVGEAR, the modeling domain is divided into blocks of cells, and the Gear algorithm is applied to each cell within a block simultaneously. With this structure, the length of the innermost loops for most calculations is equal to the number of cells in a block. Substantial

improvements in vectorization can therefore be obtained if the block size is larger than the number of species. Jacobson and Turco (1994) found that a block size on the order of 500 cells achieves about 90% of the maximum vectorization speed on a Cray C-90 computer. The use of larger block sizes may not substantially increase computational speed and may incur some additional penalties. For example, memory requirements increase with increasing block size. Furthermore, the size of a time step in SMVGEAR is the same for each cell within a block and is based on the time-step estimate for the stiffest cell in the block. Limiting the block size can therefore reduce excess calculations that need to be performed for the less stiff cells. Jacobson (1995) also achieved computational savings by ordering the cells by stiffness before dividing them into blocks. Each block then tends to contain cells of similar stiffness, thereby reducing excess computations for some cells. Jacobson found excess computations were reduced by about a factor of two, and that these reductions more than offset the additional work incurred with calculating and sorting the cells by stiffness.

Much of the computational intensity associated with the Gear method arises from the matrix operations that are needed to perform the Newton iterations in the corrector step. Jacobson and Turco have introduced two techniques to improve the efficiency of these operations. First, all known cases of multiplication by zero in matrix multiplication and decomposition are eliminated. This is particularly beneficial for atmospheric chemistry problems since the Jacobian matrices are almost always sparse (i.e., they contain a large number of zero entries). However, decomposition techniques that are applied to these matrices often result in substantial fill-in, thereby reducing the benefits of employing sparse-matrix techniques. To maintain maximum sparsity after the decomposition operation, SMVGEAR orders the species in the Jacobian such that those with the fewest partial derivative terms are located in the top rows, and those with the most are in the bottom rows. At the very beginning of the program, the ordering is done and a symbolic decomposition is performed to identify multiplies by zero. Since the computations associated with the matrix operations are determined entirely by the structure of the chemical mechanism, it is necessary to do this only once and the results can then be applied to every cell uniformly.

The SMVGEAR algorithm has been implemented in the CCTM with minor changes to the original algorithm but extensive changes to the original computer code. The code changes arose from linking the algorithm to the generalized chemistry processor used in the CMAQ system, and developing a driver routine specific to the CCTM structure. The only significant change to the algorithm involved modifying the code to eliminate the possibility of obtaining negative concentrations. With the standard Gear algorithm, negative concentrations can occur when a species is rapidly depleted, although the magnitudes of these concentrations are extremely small. In the CCTM implementation, a lower bound on allowable concentrations is applied, and the rates of change and the Jacobian matrix are modified to reflect that no changes in concentration are occurring when the lower bound is reached. Comparisons with the standard Gear algorithm show virtually no differences in species concentrations above the lower bound, but a small penalty in computational performance is incurred. Nevertheless, the approach insures a positive-definite solution.

The computational performance of SMVGEAR is also affected by the error tolerances used for the Newton iteration convergence tests and the local truncation error tests. Error control in SMVGEAR is similar to that used in LSODE (Hindmarsh, 1980). Both a relative and an absolute tolerance must be specified. In their discussion of ODE solvers, Byrne and Hindmarsh (1987) relate the relative error tolerance to the number of accurate digits and the absolute error tolerance to the noise level (i.e., the size of the largest concentration that can be neglected). If r is the number of accurate digits required, then Byrne and Hindmarsh suggest setting the relative tolerance to $10^{-(r+1)}$. The absolute error tolerances cannot be specified as generically because particular model applications may require different accuracies for the mechanismn species. In the CCTM implementation of SMVGEAR, the relative tolerance and absolute tolerances have been preset to 10^{-3} and 10^{-9} ppm, respectively. However, these values can be changed by the user relatively easily in the CCTM as described in EPA (1998).

8.4.3 QSSA Solver

The QSSA solver is a low order, explicit solver that exhibits good stability for stiff systems. Although less accurate than the Gear solver, it is still a reasonably accurate, fast solver that is especially suitable for large scale grid models. There are actually many versions of solvers that go by the name "QSSA" (e.g., Mathur et al., 1998). The solver developed for the CCTM is a predictor/corrector version based on the one developed by Lamb and used in the Regional Oxidant Model (Lamb, 1983, and Young et al., 1993).

The QSSA method originates from assuming integration time steps sufficiently small such that in Equation 8-11, the production and loss rate terms P_i and L_i can be considered constant. If the Jacobian is diagonally dominant, this assumption may be valid as $\Delta t \rightarrow 0$, and the time step solution at $t_{n+1} = t_n + \Delta t$ can be written formally as:

$$C_i = C_{i_\infty} + (C_{i_n} - C_{i_\infty}) \, e^{-L_i \Delta t} \tag{8-22}$$

where $C_{i_\infty} = P_i / L_i$ and C_{i_∞} is the solution at t_n.

The CCTM QSSA makes no *a priori* assumptions about reaction time scales. For example, there are no assumed steady states. However, the algorithm separates the numerical computation into either an Euler step, a fully explicit integration, or an asymptotic evaluation based on photochemical lifetimes estimated from an initial, predictor calculation of P_i and L_i. The cut-offs and equations for each predictor step are:

$$\begin{array}{lll} \text{Eulerstep:} & L_i \Delta t \le 0.01 & C_i = C_{i_n} + (P_i + L_i C_{i_n}) \, \Delta t \\ \text{Explicit:} & 0.01 < L_i \Delta t < 10.0 & C_i = C_{i_\infty} + (C_{i_n} - C_{i_\infty}) e^{-L} \\ \text{Asymptotic:} & L_i \Delta t \ge 10.0 & C_i = C_{i_\infty} \end{array} \tag{8-23}$$

The CMAQ QSSA algorithm proceeds in three stages: an optimal time step determination, a

predictor evaluation, and a corrector evaluation. In the first stage, an optimal chemistry time step interval Δt is determined at time t_n based on a tolerance parameter, λ, such that

$$| C_i - C_{i_n} | \leq \lambda C_{i_n} . \tag{8-24}$$

Substituting Equation 8-22 into 8-24 gives:

$$\Delta t \leq -\frac{1}{L_i} \ln\left(1 - \lambda \frac{C_{i_n}}{| C_{i_\infty} - C_{i_n} |} \right) . \tag{8-25}$$

The algorithm attempts to weight the time step determination against species whose concentrations are very small compared to the primary oxidants. These usually include some of the fastest reacting radicals. The following quantity is defined as

$$C_{test} = [NO] + [NO_2] + [O_3] \tag{8-26}$$

Then the following quantity is computed for only those species that satisfy $C_\alpha > \varepsilon C_{test}$ ($\varepsilon = 0.01$):

$$\delta t_\alpha = -\frac{1}{L_\alpha} \ln\left(1 - \lambda \frac{C_{\alpha_n}}{| C_{\alpha_\infty} - C_{\alpha_n} |} \right) \tag{8-27}$$

If $L_\alpha = 0$,

$$\delta t_\alpha = \frac{\lambda C_{\alpha_n}}{P_\alpha} \tag{8-28}$$

The tolerance parameter λ is controlled by the rate at which the key NO species concentrations are changing; if they are changing too rapidly, the tolerance is tightened, otherwise it is relaxed:

$$\lambda = \begin{cases} 0.001, \text{ if } \frac{d[NO]}{dt} / [NO] \geq 0.5\% \text{ per minute} \\ 0.005, \text{ otherwise} \end{cases} \tag{8-29}$$

After determining a time scale for each species α, Δt is set to $\min\{\delta t_\alpha\}$. For computational efficiency, Δt is further constrained to be no less than one second and of course is also constrained to be no greater than the total integration time.

In the predictor step, the species concentrations are updated ($C_i \rightarrow C_i^*$) with the optimal time step using the Euler-step, explicit or asymptotic calculations described above. Once C_i^* is calculated, QSSA computes new production and loss rate coefficients P_i^* and L_i^*, respectively.

In the corrector step, the final production rate is set as the average of the initial and predictor values, $\tilde{P}_i = (P_i^* + P_i)/2$, and the new concentration C_i for time $t_{n+1} = t_n + \Delta t$ is computed using the same cut-offs based on L_i that were determined in the predictor step:

$$\begin{aligned} &\text{Eulerstep:} && C_i = C_{i_n} + (\tilde{P}_i + L_i^* C_{i_n})\,\Delta t \\ &\text{Explicit:} && C_i = \tilde{P}_i / L_i^* + (C_{i_n} - \tilde{P}_i / L_i^*)\, e^{-L_i^* \Delta t} \\ &\text{Asymptotic:} && C_i = \tilde{P}_i / L_i^* \end{aligned} \qquad (8\text{-}30)$$

The algorithm has been optimized for vector computers by moving the grid cell loops into the innermost position (Young et al., 1993) as is done in SMVGEAR described above. To minimize storage requirements, grid cell blocking has been implemented wherein blocks of cells are handed off to the solver in sequence. The CMAQ QSSA has also been optimized for the Cray T3D by utilizing various coding techniques aimed specifically at that architecture. Some of these optimizations are described in Chapter 19.

8.4.4 Summary

Gear type solvers have generally been considered the most accurate for gas chemistry, representing "exact solutions" (provided the controlling numerical tolerances are sufficiently tight). Until the advent of SMVGEAR, however, it has not been feasible to use these solvers in Eulerian models. SMVGEAR is designed to run optimally on high end vector computers such as the Cray C90, but its use on scalar machines may be impractical. Although less accurate, the QSSA solver may be more suitable for those types of computers.

The issue of accuracy versus computational speed is a continuing concern (Mathur et al., 1998), particularly since the availability of high-end machines like the Cray C90 is limited. The CMAQ QSSA solver presents a reasonable, numerically efficient alternative and, although not considered as accurate as a Gear-type solver, may be sufficiently accurate for modeling, taking into consideration the uncertainties of the other numerical modeling components. Accuracy can be somewhat improved by using shorter integration steps in the solver, but then computational work mounts, defeating the purpose. For the CMAQ QSSA, accuracy will be compromised when the ODE system is very stiff and the system Jacobian strays from diagonal dominance.

Nevertheless, the trade-off between solution efficiency and accuracy may still warrant its use in these cases.

Finally, both the SMVGEAR and the QSSA solvers have been incorporated in the CMAQ system with the predefined accuracy controls that were described in the previous two sections. Of course, these error controls can be changed by the user if desired, but that will of course affect both the prediction accuracy and the efficiency of obtaining a solution. Note also, that either solver can be used with any of the CMAQ chemical mechanisms that were described in section 8.2.

8.5 References

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This chapter is taken from *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System,* edited by D. W. Byun and J. K. S. Ching, 1999.

Appendix 8A Chemical Mechanisms Included in the CMAQ System

Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

Notes to Tables 8A-3 through 8A-12:

a) The mechanism listings are divided into two parts. The first lists the reactions and the second lists the rate constant expressions.

b) The parameters for the rate constants are given in cms units. Rate constants calculated in cms units for T=298 °K and P= 1 atm are shown in the rightmost column of these listings.

c) For photolytic reactions, photo table refers to the photolysis rates described in Chapter 14. The rate constant for all photolytic contains a zero entry in these tables, but is calculated in the CCTM as the product of the scale factor and the photolysis rate that is calculated by the CMAQ photolysis rate processor.

d) The falloff rate expression referred to in these tables is Equation 8-6 in Section 8.3.2.

Table 8A-1
CB4 Mechanism Species List

Nitrogen Species	
NO	Nitric oxide
NO2	Nitrogen dioxide
HONO	Nitrous acid
NO3	Nitrogen trioxide
N2O5	Nitrogen pentoxide
HNO3	Nitric acid
PNA	Peroxynitric acid
Oxidants	
O3	Ozone
H2O2	Hydrogen peroxide
Sulfur Species	
SO2	Sulfur dioxide
SULF	Sulfuric acid
Atomic Species	
O	Oxygen atom (triplet)
O1D	Oxygen atom (singlet)
Odd Hydrogen Species	
OH	Hydroxyl radical
HO2	Hydroperoxy radical
Carbon oxides	
CO	Carbon monoxide
Hydrocarbons	
PAR	Paraffin carbon bond (C-C)
ETH	Ethene (CH_2=CH_2)
OLE	Olefinic carbon bond (C=C)
TOL	Toluene (C_6H_4-CH_3)
XYL	Xylene (C_6H_5-$(CH_3)_2$)
ISOP	Isoprene
Carbonyls and phenols	
FORM	Formaldehyde
ALD2	Acetaldehyde and higher aldehydes
MGLY	Methyl glyoxal ($CH_3C(O)C(O)H$)
CRES	Cresol and higher molecular weight phenols
Organic nitrogen	
PAN	Peroxyacyl nitrate ($CH_3C(O)OONO_2$)
NTR	Organic nitrate
Organic Radicals	
C2O3	Peroxyacyl radical ($CH_3C(O)OO\cdot$)
ROR	Secondary organic oxy radical
CRO	Methylphenoxy radical
Operators	
XO2	NO-to-NO_2 Operation
XO2N	NO-to-nitrate operation

Products of organics

TO2	Toluene-hydroxyl radical adduct
OPEN	High molecular weight aromatic oxidation ring fragment
ISPD	Products of isoprene reactions

Species added for aerosols

SULAER	Counter species for H_2SO_4 production
TOLAER	Counter species for toluene reaction
XYLAER	Counter species for xylene reaction
CSLAER	Counter species for cresol reaction
TERPAER	Counter species for terpene reaction
TERP	Monoterpenes

Species added for aqueous chemistry

FACD	Formic acid
AACD	Acetic and higer acids
PACD	Peroxy acetic acid
UMHP	Upper limit of methylhydroperoxide

Table 8A-2
RADM2 Mechanism Species List

Nitrogen Species	
NO	Nitric oxide
NO2	Nitrogen dioxide
HONO	Nitrous acid
NO3	Nitrogen trioxide
N2O5	Nitrogen pentoxide
HNO3	Nitric acid
HNO4	Peroxynitric acid
Oxidants	
O3	Ozone
H2O2	Hydrogen peroxide
Sulfur Species	
SO2	Sulfur dioxide
SULF	Sulfuric acid
Atomic Species	
O3P	Oxygen atom (triplet)
O1D	Oxygen atom (singlet)
Odd Hydrogen Species	
HO	Hydroxyl radical
HO2	Hydroperoxy radical
Carbon oxides	
CO	Carbon monoxide
Alkanes	
ETH	Ethane
HC3	Alkanes w/ $2.7 \times 10^{-13} > k_{OH} < 3.4 \times 10^{-12}$
HC5	Alkanes w/ $3.4 \times 10^{-12} > k_{OH} < 6.8 \times 10^{-12}$
HC8	Alkanes w/ $k_{OH} > 6.8 \times 10^{-12}$
Alkenes	
OL2	Ethene
OLT	Terminal olefins
OLI	Internal olefins
ISO	Isoprene
Aromatics	
TOL	Toluene and less reactive aromatics
XYL	Xylene and more reactive aromatics
CSL	Cresol and other hydroxy substituted aromatics
Carbonyls	
HCHO	Formaldehyde
ALD	Acetaldehyde and higher aldehydes
KET	Ketones
GLY	Glyoxal
MGLY	Methyl glyoxal
DCB	Unsaturated dicarbonyl
Organic nitrogen	
PAN	Peroxyacetyl nitrate and higher PANs
TPAN	$H(CO)CH=CHCO_3NO_2$
ONIT	Organic nitrate
Organic peroxides	
OP1	Methyl hydrogen peroxide
OP2	Higher organic peroxides
PAA	Peroxyacetic acid
Organic acids	
ORA1	Formic acid
ORA2	Acetic and higher acids
Peroxy radicals from alkanes	
MO2	Methyl peroxy radical
ETHP	Peroxy radical formed from ETH
HC3P	Peroxy radical formed from HC3
HC5P	Peroxy radical formed from HC5
HC8P	Peroxy radical formed from HC8
Peroxy radicals from alkenes	
OL2P	Peroxy radical formed from OL2P
OLTP	Peroxy radical formed from OLTP
OLIP	Peroxy radical formed from OLIP
Peroxy radicals from aromatics	
TOLP	Peroxy radical formed from TOL
XYLP	Peroxy radical formed from XYL
Peroxy radicals with carbonyl groups	
ACO3	Acetylperoxy radical
KETP	Peroxy radical formed from KET
TCO3	$H(CO)CH=CHCO_3$
Peroxy radicals involving nitrogen	
XO2	NO-to-NO_2 Operator
XNO2	NO-to-nitrate operator
OLN	NO3-alken adduct
Species added for aerosols	
SULAER	Counter species for H_2SO_4 production
HC8AER	Counter species for HC8 reaction
OLIAER	Counter species for OLI reaction
TOLAER	Counter species for toluene reaction
XYLAER	Counter species for xylene reaction
CSLAER	Counter species for cresol reaction
TERPAER	Counter species for terpene reaction
TERP	Monoterpenes

Table 8A-3. CB4 Mechanism

```
 Reaction List
>-----------------------------------------------------------------------------<
{  1} NO2   + hv            -->         NO    +       O
{  2} O     + [O2]          -->         O3
{  3} O3    + NO            -->         NO2
{  4} O     + NO2           -->         NO
{  5} O     + NO2           -->         NO3
{  6} O     + NO            -->         NO2
{  7} O3    + NO2           -->         NO3
{  8} O3    + hv            -->         O
{  9} O3    + hv            -->         O1D
{ 10} O1D   + [N2]          -->         O
{ 11} O1D   + [O2]          -->         O
{ 12} O1D   + [H2O]         -->   2.000*OH
{ 13} O3    + OH            -->         HO2
{ 14} O3    + HO2           -->         OH
{ 15} NO3   + hv            -->   0.890*NO2   + 0.890*O     + 0.110*NO
{ 16} NO3   + NO            -->   2.000*NO2
{ 17} NO3   + NO2           -->         NO    +       NO2
{ 18} NO3   + NO2           -->         N2O5
{ 19} N2O5  + [H2O]         -->   2.000*HNO3
{ 20} N2O5                  -->         NO3   +       NO2
{ 21} NO    + NO    + [O2]  -->   2.000*NO2
{ 22} NO    + NO2   + [H2O] -->   2.000*HONO
{ 23} OH    + NO            -->         HONO
{ 24} HONO  + hv            -->         OH    +       NO
{ 25} HONO  + OH            -->         NO2
{ 26} HONO  + HONO          -->         NO    +       NO2
{ 27} OH    + NO2           -->         HNO3
{ 28} OH    + HNO3          -->         NO3
{ 29} HO2   + NO            -->         OH    +       NO2
{ 30} HO2   + NO2           -->         PNA
{ 31} PNA                   -->         HO2   +       NO2
{ 32} PNA   + OH            -->         NO2
{ 33} HO2   + HO2           -->         H2O2
{ 34} HO2   + HO2   + [H2O] -->         H2O2
{ 35} H2O2  + hv            -->   2.000*OH
{ 36} H2O2  + OH            -->         HO2
{ 37} CO    + OH            -->         HO2
{ 38} FORM  + OH            -->         HO2   +       CO
{ 39} FORM  + hv            -->   2.000*HO2   +       CO
{ 40} FORM  + hv            -->         CO
{ 41} FORM  + O             -->         OH    +       HO2   +       CO
{ 42} FORM  + NO3           -->         HNO3  +       HO2   +       CO
{ 43} ALD2  + O             -->         C2O3  +       OH
{ 44} ALD2  + OH            -->         C2O3
{ 45} ALD2  + NO3           -->         C2O3  +       HNO3
{ 46} ALD2  + hv            -->         XO2   + 2.000*HO2   +       CO
                              +         FORM
{ 47} C2O3  + NO            -->         NO2   +       XO2   +       FORM
                              +         HO2
{ 48} C2O3  + NO2           -->         PAN
{ 49} PAN                   -->         C2O3  +       NO2
{ 50} C2O3  + C2O3          -->   2.000*XO2   + 2.000*FORM  + 2.000*HO2
{ 51} C2O3  + HO2           -->   0.790*FORM  + 0.790*XO2   + 0.790*HO2
                              + 0.790*OH
{ 52} OH                    -->         XO2   +       FORM  +       HO2
{ 53} PAR   + OH            -->   0.870*XO2   + 0.130*XO2N  + 0.110*HO2
                              + 0.110*ALD2  + 0.760*ROR   - 0.110*PAR


{ 54} ROR                   -->   1.100*ALD2  + 0.960*XO2   + 0.940*HO2
                              - 2.100*PAR   + 0.040*XO2N  + 0.020*ROR
{ 55} ROR                   -->         HO2
{ 56} ROR   + NO2           -->         NTR
{ 57} OLE   + O             -->   0.630*ALD2  + 0.380*HO2   + 0.280*XO2
                              + 0.300*CO    + 0.200*FORM  + 0.020*XO2N
                              + 0.220*PAR   + 0.200*OH
{ 58} OLE   + OH            -->         FORM  +       ALD2  +       XO2
                              +         HO2   -       PAR
{ 59} OLE   + O3            -->   0.500*ALD2  + 0.740*FORM  + 0.330*CO
                              + 0.440*HO2   + 0.220*XO2   + 0.100*OH
                              -         PAR
{ 60} OLE   + NO3           -->   0.910*XO2   + 0.090*XO2N  +       FORM
```

Table 8A-3. CB4 Mechanism

```
                                  +       ALD2  -       PAR   +       NO2
{ 61} ETH   + O             -->           FORM  + 0.700*XO2   +       CO
                                  + 1.700*HO2   + 0.300*OH
{ 62} ETH   + OH            -->           XO2   + 1.560*FORM  +       HO2
                                  + 0.220*ALD2
{ 63} ETH   + O3            -->           FORM  + 0.420*CO    + 0.120*HO2
{ 64} TOL   + OH            -->   0.080*XO2   + 0.360*CRES  + 0.440*HO2
                                  + 0.560*TO2
{ 65} TO2   + NO            -->   0.900*NO2   + 0.900*HO2   + 0.900*OPEN
                                  + 0.100*NTR
{ 66} TO2                   -->           CRES  +       HO2
{ 67} CRES  + OH            -->   0.400*CRO   + 0.600*XO2   + 0.600*HO2
                                  + 0.300*OPEN
{ 68} CRES  + NO3           -->           CRO   +       HNO3
{ 69} CRO   + NO2           -->           NTR
{ 70} XYL   + OH            -->   0.700*HO2   + 0.500*XO2   + 0.200*CRES
                                  + 0.800*MGLY  + 1.100*PAR   + 0.300*TO2
{ 71} OPEN  + OH            -->           XO2   + 2.000*CO    + 2.000*HO2
                                  +       C2O3  +       FORM
{ 72} OPEN  + hv            -->           C2O3  +       HO2   +       CO
{ 73} OPEN  + O3            -->   0.030*ALD2  + 0.620*C2O3  + 0.700*FORM
                                  + 0.030*XO2   + 0.690*CO    + 0.080*OH
                                  + 0.760*HO2   + 0.200*MGLY
{ 74} MGLY  + OH            -->           XO2   +       C2O3
{ 75} MGLY  + hv            -->           C2O3  +       HO2   +       CO
{ 76} ISOP  + O             -->   0.750*ISPD  + 0.500*FORM  + 0.250*XO2
                                  + 0.250*HO2   + 0.250*C2O3  + 0.250*PAR
{ 77} ISOP  + OH            -->   0.912*ISPD  + 0.629*FORM  + 0.991*XO2
                                  + 0.912*HO2   + 0.088*XO2N
{ 78} ISOP  + O3            -->   0.650*ISPD  + 0.600*FORM  + 0.200*XO2
                                  + 0.066*HO2   + 0.266*OH    + 0.200*C2O3
                                  + 0.150*ALD2  + 0.350*PAR   + 0.066*CO
{ 79} ISOP  + NO3           -->   0.200*ISPD  + 0.800*NTR   +       XO2
                                  + 0.800*HO2   + 0.200*NO2   + 0.800*ALD2
                                  + 2.400*PAR
{ 80} XO2   + NO            -->           NO2
{ 81} XO2   + XO2           -->
{ 82} XO2N  + NO            -->           NTR
{ 83} SO2   + OH            -->           SULF  +       HO2
{ 84} SO2                   -->           SULF
{ 85} XO2   + HO2           -->
{ 86} XO2N  + HO2           -->
{ 87} XO2N  + XO2N          -->
{ 88} XO2N  + XO2           -->
{ 89} ISPD  + OH            -->   1.565*PAR   + 0.167*FORM  + 0.713*XO2
                                  + 0.503*HO2   + 0.334*CO    + 0.168*MGLY
                                  + 0.273*ALD2  + 0.498*C2O3
{ 90} ISPD  + O3            -->   0.114*C2O3  + 0.150*FORM  + 0.850*MGLY
                                  + 0.154*HO2   + 0.268*OH    + 0.064*XO2
                                  + 0.020*ALD2  + 0.360*PAR   + 0.225*CO
{ 91} ISPD  + NO3           -->   0.357*ALD2  + 0.282*FORM  + 1.282*PAR
                                  + 0.925*HO2   + 0.643*CO    + 0.850*NTR
                                  + 0.075*C2O3  + 0.075*XO2   + 0.075*HNO3
{ 92} ISPD  + hv            -->   0.333*CO    + 0.067*ALD2  + 0.900*FORM
                                  + 0.832*PAR   + 1.033*HO2   + 0.700*XO2
                                  + 0.967*C2O3
{ 93} ISOP  + NO2           -->   0.200*ISPD  + 0.800*NTR   +       XO2
                                  + 0.800*HO2   + 0.200*NO    + 0.800*ALD2
                                  + 2.400*PAR
>---------------------------------------------------------------------------<

Rate Expression                                                        Rate Constant
=============================================================================
k(  1) uses photo table NO2_CBIV88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) is a falloff expression using:                             {1.37387E-14}
   k0   =  6.0000E-34 * (T/300)**(-2.30)
   kinf =  2.8000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  3) =  1.8000E-12 * exp( -1370.0/T)                            {1.81419E-14}
k(  4) =  9.3000E-12                                              {9.30000E-12}
k(  5) is a falloff expression using:                             {1.57527E-12}
   k0   =  9.0000E-32 * (T/300)**(-2.00)
   kinf =  2.2000E-11 * (T/300)**( 0.00)
```

Table 8A-3. CB4 Mechanism

```
   F =  0.60,  n =  1.00
k(  6) is a falloff expression using:                              {1.66375E-12}
   k0   =  9.0000E-32 * (T/300)**(-1.50)
   kinf =  3.0000E-11 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  7) =  1.2000E-13 * exp( -2450.0/T)                             {3.22581E-17}
k(  8) uses photo table NO2_CBIV88      , scaled by 5.30000E-02    {0.00000E+00}
k(  9) uses photo table O3O1D_CBIV88    , scaled by 1.00000E+00    {0.00000E+00}
k( 10) =  1.8000E-11 * exp(   107.0/T)                             {2.57757E-11}
k( 11) =  3.2000E-11 * exp(    67.0/T)                             {4.00676E-11}
k( 12) =  2.2000E-10                                               {2.20000E-10}
k( 13) =  1.6000E-12 * exp(  -940.0/T)                             {6.82650E-14}
k( 14) =  1.4000E-14 * exp(  -580.0/T)                             {1.99920E-15}
k( 15) uses photo table NO2_CBIV88      , scaled by 3.39000E+01    {0.00000E+00}
k( 16) =  1.3000E-11 * exp(   250.0/T)                             {3.00805E-11}
k( 17) =  2.5000E-14 * exp( -1230.0/T)                             {4.03072E-16}
k( 18) is a falloff expression using:                              {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 19) =  1.3000E-21                                               {1.30000E-21}
k( 20) = k( 18) / Keq,  where Keq =  2.700E-27 * exp( 11000.0/T)   {4.36029E-02}
k( 21) =  3.3000E-39 * exp(   530.0/T)                             {1.95397E-38}
k( 22) =  4.4000E-40                                               {4.39999E-40}
k( 23) is a falloff expression using:                              {6.69701E-12}
   k0   =  6.7000E-31 * (T/300)**(-3.30)
   kinf =  3.0000E-11 * (T/300)**(-1.00)
   F =  0.60,  n =  1.00
k( 24) uses photo table NO2_CBIV88      , scaled by 1.97500E-01    {0.00000E+00}
k( 25) =  6.6000E-12                                               {6.60000E-12}
k( 26) =  1.0000E-20                                               {1.00000E-20}
k( 27) is a falloff expression using:                              {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 28) is a special rate expression of the form:                   {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 29) =  3.7000E-12 * exp(   240.0/T)                             {8.27883E-12}
k( 30) is a falloff expression using:                              {1.48014E-12}
   k0   =  2.3000E-31 * (T/300)**(-4.60)
   kinf =  4.2000E-12 * (T/300)**( 0.20)
   F =  0.60,  n =  1.00
k( 31) = k( 30) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)   {9.17943E-02}
k( 32) =  1.3000E-12 * exp(   380.0/T)                             {4.65309E-12}
k( 33) =  5.9000E-14 * exp(  1150.0/T)                             {2.79783E-12}
k( 34) =  2.2000E-38 * exp(  5800.0/T)                             {6.23927E-30}
k( 35) uses photo table HCHOmol_CBIV88  , scaled by 2.55000E-01    {0.00000E+00}
k( 36) =  3.1000E-12 * exp(  -187.0/T)                             {1.65514E-12}
k( 37) =  1.5000E-13 * (1.0 + 0.6*Pressure)                        {2.40000E-13}
k( 38) =  1.0000E-11                                               {1.00000E-11}
k( 39) uses photo table HCHOrad_CBIV88  , scaled by 1.00000E+00    {0.00000E+00}
k( 40) uses photo table HCHOmol_CBIV88  , scaled by 1.00000E+00    {0.00000E+00}
k( 41) =  3.0000E-11 * exp( -1550.0/T)                             {1.65275E-13}
k( 42) =  6.3000E-16                                               {6.30000E-16}
k( 43) =  1.2000E-11 * exp(  -986.0/T)                             {4.38753E-13}
k( 44) =  7.0000E-12 * exp(   250.0/T)                             {1.61972E-11}
k( 45) =  2.5000E-15                                               {2.50000E-15}
k( 46) uses photo table ALD_CBIV88      , scaled by 1.00000E+00    {0.00000E+00}
k( 47) =  3.4900E-11 * exp(  -180.0/T)                             {1.90766E-11}
k( 48) =  2.6300E-12 * exp(   380.0/T)                             {9.41356E-12}
k( 49) =  2.0000E+16 * exp(-13500.0/T)                             {4.23268E-04}
k( 50) =  2.5000E-12                                               {2.50000E-12}
k( 51) =  6.5000E-12                                               {6.50000E-12}
k( 52) =  1.1000E+02 * exp( -1710.0/T)                             {3.54242E-01}
k( 53) =  8.1000E-13                                               {8.10000E-13}
k( 54) =  1.0000E+15 * exp( -8000.0/T)                             {2.19325E+03}
k( 55) =  1.6000E+03                                               {1.60000E+03}
k( 56) =  1.5000E-11                                               {1.50000E-11}
k( 57) =  1.2000E-11 * exp(  -324.0/T)                             {4.04572E-12}
k( 58) =  5.2000E-12 * exp(   504.0/T)                             {2.82173E-11}
k( 59) =  1.4000E-14 * exp( -2105.0/T)                             {1.19778E-17}
```

Table 8A-3. CB4 Mechanism

```
k( 60) =  7.7000E-15                                                {7.70000E-15}
k( 61) =  1.0000E-11 * exp(  -792.0/T)                              {7.01080E-13}
k( 62) =  2.0000E-12 * exp(   411.0/T)                              {7.94340E-12}
k( 63) =  1.3000E-14 * exp( -2633.0/T)                              {1.89105E-18}
k( 64) =  2.1000E-12 * exp(   322.0/T)                              {6.18715E-12}
k( 65) =  8.1000E-12                                                {8.10000E-12}
k( 66) =  4.2000E+00                                                {4.20000E+00}
k( 67) =  4.1000E-11                                                {4.10000E-11}
k( 68) =  2.2000E-11                                                {2.20000E-11}
k( 69) =  1.4000E-11                                                {1.40000E-11}
k( 70) =  1.7000E-11 * exp(   116.0/T)                              {2.50901E-11}
k( 71) =  3.0000E-11                                                {3.00000E-11}
k( 72) uses photo table HCHOrad_CBIV88  , scaled by 9.04000E+00     {0.00000E+00}
k( 73) =  5.4000E-17 * exp(  -500.0/T)                              {1.00858E-17}
k( 74) =  1.7000E-11                                                {1.70000E-11}
k( 75) uses photo table HCHOrad_CBIV88  , scaled by 9.64000E+00     {0.00000E+00}
k( 76) =  3.6000E-11                                                {3.60000E-11}
k( 77) =  2.5400E-11 * exp(   407.6/T)                              {9.97368E-11}
k( 78) =  7.8600E-15 * exp( -1912.0/T)                              {1.28512E-17}
k( 79) =  3.0300E-12 * exp(  -448.0/T)                              {6.73819E-13}
k( 80) =  8.1000E-12                                                {8.10000E-12}
k( 81) =  1.7000E-14 * exp(  1300.0/T)                              {1.33359E-12}
k( 82) =  8.1000E-12                                                {8.10000E-12}
k( 83) =  4.3900E-13 * exp(   160.0/T)                              {7.51005E-13}
k( 84) =  1.3600E-06                                                {1.36000E-06}
k( 85) =  7.6700E-14 * exp(  1300.0/T)                              {6.01684E-12}
k( 86) =  7.6700E-14 * exp(  1300.0/T)                              {6.01684E-12}
k( 87) =  1.7300E-14 * exp(  1300.0/T)                              {1.35712E-12}
k( 88) =  3.4500E-14 * exp(  1300.0/T)                              {2.70640E-12}
k( 89) =  3.3600E-11                                                {3.36000E-11}
k( 90) =  7.1100E-18                                                {7.11000E-18}
k( 91) =  1.0000E-15                                                {1.00000E-15}
k( 92) uses photo table ACROLEIN        , scaled by 3.60000E-03     {0.00000E+00}
k( 93) =  1.4900E-19                                                {1.49000E-19}
================================================================================
```

Table 8A-4. CB4_AE Mechanism

```
 Reaction List
>-------------------------------------------------------------------------------<
{  1} NO2     + hv                --> NO      +       O
{  2} O       + [O2]              --> O3
{  3} O3      + NO                --> NO2
{  4} O       + NO2               --> NO
{  5} O       + NO2               --> NO3
{  6} O       + NO                --> NO2
{  7} O3      + NO2               --> NO3
{  8} O3      + hv                --> O
{  9} O3      + hv                --> O1D
{ 10} O1D     + [N2]              --> O
{ 11} O1D     + [O2]              --> O
{ 12} O1D     + [H2O]             --> 2.000*OH
{ 13} O3      + OH                --> HO2
{ 14} O3      + HO2               --> OH
{ 15} NO3     + hv                --> 0.890*NO2     + 0.890*O       + 0.110*NO
{ 16} NO3     + NO                --> 2.000*NO2
{ 17} NO3     + NO2               --> NO      +       NO2
{ 18} NO3     + NO2               --> N2O5
{ 19} N2O5    + [H2O]             --> 2.000*HNO3
{ 20} N2O5                        --> NO3     +       NO2
{ 21} NO      + NO      + [O2]    --> 2.000*NO2
{ 22} NO      + NO2     + [H2O]   --> 2.000*HONO
{ 23} OH      + NO                --> HONO
{ 24} HONO    + hv                --> OH      +       NO
{ 25} HONO    + OH                --> NO2
{ 26} HONO    + HONO              --> NO      +       NO2
{ 27} OH      + NO2               --> HNO3
{ 28} OH      + HNO3              --> NO3
{ 29} HO2     + NO                --> OH      +       NO2
{ 30} HO2     + NO2               --> PNA
{ 31} PNA                         --> HO2     +       NO2
{ 32} PNA     + OH                --> NO2
{ 33} HO2     + HO2               --> H2O2
{ 34} HO2     + HO2     + [H2O]   --> H2O2
{ 35} H2O2    + hv                --> 2.000*OH
{ 36} H2O2    + OH                --> HO2
{ 37} CO      + OH                --> HO2
{ 38} FORM    + OH                --> HO2     +       CO
{ 39} FORM    + hv                --> 2.000*HO2     +       CO
{ 40} FORM    + hv                --> CO
{ 41} FORM    + O                 --> OH      +       HO2     +       CO
{ 42} FORM    + NO3               --> HNO3    +       HO2     +       CO
{ 43} ALD2    + O                 --> C2O3    +       OH
{ 44} ALD2    + OH                --> C2O3
{ 45} ALD2    + NO3               --> C2O3    +       HNO3
{ 46} ALD2    + hv                --> XO2     + 2.000*HO2     +       CO
                                    +       FORM
{ 47} C2O3    + NO                --> NO2     +       XO2     +       FORM
                                    +       HO2
{ 48} C2O3    + NO2               --> PAN
{ 49} PAN                         --> C2O3    +       NO2
{ 50} C2O3    + C2O3              --> 2.000*XO2     + 2.000*FORM    + 2.000*HO2
{ 51} C2O3    + HO2               --> 0.790*FORM    + 0.790*XO2     + 0.790*HO2
                                    + 0.790*OH
{ 52} OH                          --> XO2     +       FORM    +       HO2
{ 53} PAR     + OH                --> 0.870*XO2     + 0.130*XO2N    + 0.110*HO2
                                    + 0.110*ALD2    + 0.760*ROR     - 0.110*PAR
{ 54} ROR                         --> 1.100*ALD2    + 0.960*XO2     + 0.940*HO2
                                    - 2.100*PAR     + 0.040*XO2N    + 0.020*ROR
{ 55} ROR                         --> HO2
{ 56} ROR     + NO2               --> NTR
{ 57} OLE     + O                 --> 0.630*ALD2    + 0.380*HO2     + 0.280*XO2
                                    + 0.300*CO      + 0.200*FORM    + 0.020*XO2N
                                    + 0.220*PAR     + 0.200*OH
{ 58} OLE     + OH                --> FORM    +       ALD2    +       XO2
                                    +       HO2     -       PAR
{ 59} OLE     + O3                --> 0.500*ALD2    + 0.740*FORM    + 0.330*CO
                                    + 0.440*HO2     + 0.220*XO2     + 0.100*OH
                                    -       PAR
{ 60} OLE     + NO3               --> 0.910*XO2     + 0.090*XO2N    +       FORM
                                    +       ALD2    -       PAR     +       NO2
{ 61} ETH     + O                 --> FORM    + 0.700*XO2     +       CO
```

Table 8A-4. CB4_AE Mechanism

```
                                    + 1.700*HO2     + 0.300*OH
{ 62} ETH     + OH              -->         XO2     + 1.560*FORM    +       HO2
                                    + 0.220*ALD2
{ 63} ETH     + O3              -->         FORM    + 0.420*CO      + 0.120*HO2
{ 64} TOL     + OH              -->   0.080*XO2     + 0.360*CRES    + 0.440*HO2
                                    + 0.560*TO2     +       TOLAER
{ 65} TO2     + NO              -->   0.900*NO2     + 0.900*HO2     + 0.900*OPEN
                                    + 0.100*NTR
{ 66} TO2                       -->         CRES    +       HO2
{ 67} CRES    + OH              -->   0.400*CRO     + 0.600*XO2     + 0.600*HO2
                                    + 0.300*OPEN    +       CSLAER
{ 68} CRES    + NO3             -->         CRO     +       HNO3    +       CSLAER
{ 69} CRO     + NO2             -->         NTR
{ 70} XYL     + OH              -->   0.700*HO2     + 0.500*XO2     + 0.200*CRES
                                    + 0.800*MGLY    + 1.100*PAR     + 0.300*TO2
                                    +       XYLAER
{ 71} OPEN    + OH              -->         XO2     + 2.000*CO      + 2.000*HO2
                                    +       C2O3    +       FORM
{ 72} OPEN    + hv              -->         C2O3    +       HO2     +       CO
{ 73} OPEN    + O3              -->   0.030*ALD2    + 0.620*C2O3    + 0.700*FORM
                                    + 0.030*XO2     + 0.690*CO      + 0.080*OH
                                    + 0.760*HO2     + 0.200*MGLY
{ 74} MGLY    + OH              -->         XO2     +       C2O3
{ 75} MGLY    + hv              -->         C2O3    +       HO2     +       CO
{ 76} ISOP    + O               -->   0.750*ISPD    + 0.500*FORM    + 0.250*XO2
                                    + 0.250*HO2     + 0.250*C2O3    + 0.250*PAR
{ 77} ISOP    + OH              -->   0.912*ISPD    + 0.629*FORM    + 0.991*XO2
                                    + 0.912*HO2     + 0.088*XO2N
{ 78} ISOP    + O3              -->   0.650*ISPD    + 0.600*FORM    + 0.200*XO2
                                    + 0.066*HO2     + 0.266*OH      + 0.200*C2O3
                                    + 0.150*ALD2    + 0.350*PAR     + 0.066*CO
{ 79} ISOP    + NO3             -->   0.200*ISPD    + 0.800*NTR     +       XO2
                                    + 0.800*HO2     + 0.200*NO2     + 0.800*ALD2
                                    + 2.400*PAR
{ 80} XO2     + NO              -->         NO2
{ 81} XO2     + XO2             -->
{ 82} XO2N    + NO              -->         NTR
{ 83} SO2     + OH              -->         SULF    +       HO2     +       SULAER
{ 84} SO2                       -->         SULF    +       SULAER
{ 85} XO2     + HO2             -->
{ 86} XO2N    + HO2             -->
{ 87} XO2N    + XO2N            -->
{ 88} XO2N    + XO2             -->
{ 89} ISPD    + OH              -->   1.565*PAR     + 0.167*FORM    + 0.713*XO2
                                    + 0.503*HO2     + 0.334*CO      + 0.168*MGLY
                                    + 0.273*ALD2    + 0.498*C2O3
{ 90} ISPD    + O3              -->   0.114*C2O3    + 0.150*FORM    + 0.850*MGLY
                                    + 0.154*HO2     + 0.268*OH      + 0.064*XO2
                                    + 0.020*ALD2    + 0.360*PAR     + 0.225*CO
{ 91} ISPD    + NO3             -->   0.357*ALD2    + 0.282*FORM    + 1.282*PAR
                                    + 0.925*HO2     + 0.643*CO      + 0.850*NTR
                                    + 0.075*C2O3    + 0.075*XO2     + 0.075*HNO3
{ 92} ISPD    + hv              -->   0.333*CO      + 0.067*ALD2    + 0.900*FORM
                                    + 0.832*PAR     + 1.033*HO2     + 0.700*XO2
                                    + 0.967*C2O3
{ 93} ISOP    + NO2             -->   0.200*ISPD    + 0.800*NTR     +       XO2
                                    + 0.800*HO2     + 0.200*NO      + 0.800*ALD2
                                    + 2.400*PAR
{ 94} TERP    + OH              -->         TERPAER +       OH
{ 95} TERP    + NO3             -->         TERPAER +       NO3
{ 96} TERP    + O3              -->         TERPAER +       O3
>-------------------------------------------------------------------------------<

Rate Expression                                                  Rate Constant
 ================================================================================
 k(  1) uses photo table NO2_CBIV88      , scaled by 1.00000E+00   {0.00000E+00}
 k(  2) is a falloff expression using:                             {1.37387E-14}
    k0   =  6.0000E-34 * (T/300)**(-2.30)
    kinf =  2.8000E-12 * (T/300)**( 0.00)
    F =  0.60,  n =  1.00
 k(  3) =  1.8000E-12 * exp( -1370.0/T)                           {1.81419E-14}
 k(  4) =  9.3000E-12                                             {9.30000E-12}
 k(  5) is a falloff expression using:                            {1.57527E-12}
```

Table 8A-4. CB4_AE Mechanism

```
    k0   =  9.0000E-32 * (T/300)**(-2.00)
    kinf =  2.2000E-11 * (T/300)**( 0.00)
    F =  0.60,  n =  1.00
k(  6) is a falloff expression using:                              {1.66375E-12}
    k0   =  9.0000E-32 * (T/300)**(-1.50)
    kinf =  3.0000E-11 * (T/300)**( 0.00)
    F =  0.60,  n =  1.00
k(  7) =  1.2000E-13 * exp( -2450.0/T)                             {3.22581E-17}
k(  8) uses photo table NO2_CBIV88      , scaled by 5.30000E-02    {0.00000E+00}
k(  9) uses photo table O3O1D_CBIV88    , scaled by 1.00000E+00    {0.00000E+00}
k( 10) =  1.8000E-11 * exp(   107.0/T)                             {2.57757E-11}
k( 11) =  3.2000E-11 * exp(    67.0/T)                             {4.00676E-11}
k( 12) =  2.2000E-10                                               {2.20000E-10}
k( 13) =  1.6000E-12 * exp(  -940.0/T)                             {6.82650E-14}
k( 14) =  1.4000E-14 * exp(  -580.0/T)                             {1.99920E-15}
k( 15) uses photo table NO2_CBIV88      , scaled by 3.39000E+01    {0.00000E+00}
k( 16) =  1.3000E-11 * exp(   250.0/T)                             {3.00805E-11}
k( 17) =  2.5000E-14 * exp( -1230.0/T)                             {4.03072E-16}
k( 18) is a falloff expression using:                              {1.26440E-12}
    k0   =  2.2000E-30 * (T/300)**(-4.30)
    kinf =  1.5000E-12 * (T/300)**(-0.50)
    F =  0.60,  n =  1.00
k( 19) =  1.3000E-21                                               {1.30000E-21}
k( 20) = k( 18) / Keq,  where Keq =  2.700E-21 * exp( 11000.0/T)   {4.36029E-08}
k( 21) =  3.3000E-39 * exp(   530.0/T)                             {1.95397E-38}
k( 22) =  4.4000E-40                                               {4.39999E-40}
k( 23) is a falloff expression using:                              {6.69701E-12}
    k0   =  6.7000E-31 * (T/300)**(-3.30)
    kinf =  3.0000E-11 * (T/300)**(-1.00)
    F =  0.60,  n =  1.00
k( 24) uses photo table NO2_CBIV88      , scaled by 1.97500E-01    {0.00000E+00}
k( 25) =  6.6000E-12                                               {6.60000E-12}
k( 26) =  1.0000E-20                                               {1.00000E-20}
k( 27) is a falloff expression using:                              {1.14885E-11}
    k0   =  2.6000E-30 * (T/300)**(-3.20)
    kinf =  2.4000E-11 * (T/300)**(-1.30)
    F =  0.60,  n =  1.00
k( 28) is a special rate expression of the form:                   {1.47236E-13}
    k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
    k0 =  7.2000E-15 * exp(   785.0/T)
    k2 =  4.1000E-16 * exp(  1440.0/T)
    k3 =  1.9000E-33 * exp(   725.0/T)
k( 29) =  3.7000E-12 * exp(   240.0/T)                             {8.27883E-12}
k( 30) is a falloff expression using:                              {1.48014E-12}
    k0   =  2.3000E-31 * (T/300)**(-4.60)
    kinf =  4.2000E-12 * (T/300)**( 0.20)
    F =  0.60,  n =  1.00
k( 31) = k( 30) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)   {9.17943E-02}
k( 32) =  1.3000E-12 * exp(   380.0/T)                             {4.65309E-12}
k( 33) =  5.9000E-14 * exp(  1150.0/T)                             {2.79783E-12}
k( 34) =  2.2000E-38 * exp(  5800.0/T)                             {6.23927E-30}
k( 35) uses photo table HCHOmol_CBIV88  , scaled by 2.55000E-01    {0.00000E+00}
k( 36) =  3.1000E-12 * exp(  -187.0/T)                             {1.65514E-12}
k( 37) =  1.5000E-13 * (1.0 + 0.6*Pressure)                        {2.40000E-13}
k( 38) =  1.0000E-11                                               {1.00000E-11}
k( 39) uses photo table HCHOrad_CBIV88  , scaled by 1.00000E+00    {0.00000E+00}
k( 40) uses photo table HCHOmol_CBIV88  , scaled by 1.00000E+00    {0.00000E+00}
k( 41) =  3.0000E-11 * exp( -1550.0/T)                             {1.65275E-13}
k( 42) =  6.3000E-16                                               {6.30000E-16}
k( 43) =  1.2000E-11 * exp(  -986.0/T)                             {4.38753E-13}
k( 44) =  7.0000E-12 * exp(   250.0/T)                             {1.61972E-11}
k( 45) =  2.5000E-15                                               {2.50000E-15}
k( 46) uses photo table ALD_CBIV88      , scaled by 1.00000E+00    {0.00000E+00}
k( 47) =  3.4900E-11 * exp(  -180.0/T)                             {1.90766E-11}
k( 48) =  2.6300E-12 * exp(   380.0/T)                             {9.41356E-12}
k( 49) =  2.0000E+16 * exp(-13500.0/T)                             {4.23268E-04}
k( 50) =  2.5000E-12                                               {2.50000E-12}
k( 51) =  6.5000E-12                                               {6.50000E-12}
k( 52) =  1.1000E+02 * exp( -1710.0/T)                             {3.54242E-01}
k( 53) =  8.1000E-13                                               {8.10000E-13}
k( 54) =  1.0000E+15 * exp( -8000.0/T)                             {2.19325E+03}
k( 55) =  1.6000E+03                                               {1.60000E+03}
k( 56) =  1.5000E-11                                               {1.50000E-11}
k( 57) =  1.2000E-11 * exp(  -324.0/T)                             {4.04572E-12}
```

Table 8A-4. CB4_AE Mechanism

```
k( 58) =  5.2000E-12 * exp(   504.0/T)                          {2.82173E-11}
k( 59) =  1.4000E-14 * exp( -2105.0/T)                          {1.19778E-17}
k( 60) =  7.7000E-15                                            {7.70000E-15}
k( 61) =  1.0000E-11 * exp(  -792.0/T)                          {7.01080E-13}
k( 62) =  2.0000E-12 * exp(   411.0/T)                          {7.94340E-12}
k( 63) =  1.3000E-14 * exp( -2633.0/T)                          {1.89105E-18}
k( 64) =  2.1000E-12 * exp(   322.0/T)                          {6.18715E-12}
k( 65) =  8.1000E-12                                            {8.10000E-12}
k( 66) =  4.2000E+00                                            {4.20000E+00}
k( 67) =  4.1000E-11                                            {4.10000E-11}
k( 68) =  2.2000E-11                                            {2.20000E-11}
k( 69) =  1.4000E-11                                            {1.40000E-11}
k( 70) =  1.7000E-11 * exp(   116.0/T)                          {2.50901E-11}
k( 71) =  3.0000E-11                                            {3.00000E-11}
k( 72) uses photo table HCHOrad_CBIV88  , scaled by 9.04000E+00   {0.00000E+00}
k( 73) =  5.4000E-17 * exp(  -500.0/T)                          {1.00858E-17}
k( 74) =  1.7000E-11                                            {1.70000E-11}
k( 75) uses photo table HCHOrad_CBIV88  , scaled by 9.64000E+00   {0.00000E+00}
k( 76) =  3.6000E-11                                            {3.60000E-11}
k( 77) =  2.5400E-11 * exp(   407.6/T)                          {9.97368E-11}
k( 78) =  7.8600E-15 * exp( -1912.0/T)                          {1.28512E-17}
k( 79) =  3.0300E-12 * exp(  -448.0/T)                          {6.73819E-13}
k( 80) =  8.1000E-12                                            {8.10000E-12}
k( 81) =  1.7000E-14 * exp(  1300.0/T)                          {1.33359E-12}
k( 82) =  8.1000E-12                                            {8.10000E-12}
k( 83) =  4.3900E-13 * exp(   160.0/T)                          {7.51005E-13}
k( 84) =  1.3600E-06                                            {1.36000E-06}
k( 85) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 86) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 87) =  1.7300E-14 * exp(  1300.0/T)                          {1.35712E-12}
k( 88) =  3.4500E-14 * exp(  1300.0/T)                          {2.70640E-12}
k( 89) =  3.3600E-11                                            {3.36000E-11}
k( 90) =  7.1100E-18                                            {7.11000E-18}
k( 91) =  1.0000E-15                                            {1.00000E-15}
k( 92) uses photo table ACROLEIN        , scaled by 3.60000E-03   {0.00000E+00}
k( 93) =  1.4900E-19                                            {1.49000E-19}
k( 94) =  1.0700E-11 * exp(   549.0/T)                          {6.75269E-11}
k( 95) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k( 96) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
================================================================================
```

Table 8A-5. CB4_AQ Mechanism

```
 Reaction List
>-------------------------------------------------------------------------<
{  1} NO2   + hv            -->         NO    +       O
{  2} O     + [O2]          -->         O3
{  3} O3    + NO            -->         NO2
{  4} O     + NO2           -->         NO
{  5} O     + NO2           -->         NO3
{  6} O     + NO            -->         NO2
{  7} O3    + NO2           -->         NO3
{  8} O3    + hv            -->         O
{  9} O3    + hv            -->         O1D
{ 10} O1D   + [N2]          -->         O
{ 11} O1D   + [O2]          -->         O
{ 12} O1D   + [H2O]         -->   2.000*OH
{ 13} O3    + OH            -->         HO2
{ 14} O3    + HO2           -->         OH
{ 15} NO3   + hv            -->   0.890*NO2   + 0.890*O     + 0.110*NO
{ 16} NO3   + NO            -->   2.000*NO2
{ 17} NO3   + NO2           -->         NO    +       NO2
{ 18} NO3   + NO2           -->         N2O5
{ 19} N2O5  + [H2O]         -->   2.000*HNO3
{ 20} N2O5                  -->         NO3   +       NO2
{ 21} NO    + NO    + [O2]  -->   2.000*NO2
{ 22} NO    + NO2   + [H2O] -->   2.000*HONO
{ 23} OH    + NO            -->         HONO
{ 24} HONO  + hv            -->         OH    +       NO
{ 25} HONO  + OH            -->         NO2
{ 26} HONO  + HONO          -->         NO    +       NO2
{ 27} OH    + NO2           -->         HNO3
{ 28} OH    + HNO3          -->         NO3
{ 29} HO2   + NO            -->         OH    +       NO2
{ 30} HO2   + NO2           -->         PNA
{ 31} PNA                   -->         HO2   +       NO2
{ 32} PNA   + OH            -->         NO2
{ 33} HO2   + HO2           -->         H2O2
{ 34} HO2   + HO2   + [H2O] -->         H2O2
{ 35} H2O2  + hv            -->   2.000*OH
{ 36} H2O2  + OH            -->         HO2
{ 37} CO    + OH            -->         HO2
{ 38} FORM  + OH            -->         HO2   +       CO
{ 39} FORM  + hv            -->   2.000*HO2   +       CO
{ 40} FORM  + hv            -->         CO
{ 41} FORM  + O             -->         OH    +       HO2   +       CO
{ 42} FORM  + NO3           -->         HNO3  +       HO2   +       CO
{ 43} ALD2  + O             -->         C2O3  +       OH
{ 44} ALD2  + OH            -->         C2O3
{ 45} ALD2  + NO3           -->         C2O3  +       HNO3
{ 46} ALD2  + hv            -->         XO2   + 2.000*HO2   +       CO
                              +         FORM
{ 47} C2O3  + NO            -->         NO2   +       XO2   +       FORM
                              +         HO2
{ 48} C2O3  + NO2           -->         PAN
{ 49} PAN                   -->         C2O3  +       NO2
{ 50} C2O3  + C2O3          -->   2.000*XO2   + 2.000*FORM  + 2.000*HO2
{ 51} C2O3  + HO2           -->   0.790*FORM  + 0.790*XO2   + 0.790*HO2
                              + 0.790*OH    + 0.210*PACD
{ 52} OH                    -->         XO2   +       FORM  +       HO2
{ 53} PAR   + OH            -->   0.870*XO2   + 0.130*XO2N  + 0.110*HO2
                              + 0.110*ALD2  + 0.760*ROR   - 0.110*PAR
{ 54} ROR                   -->   1.100*ALD2  + 0.960*XO2   + 0.940*HO2
                              - 2.100*PAR   + 0.040*XO2N  + 0.020*ROR
{ 55} ROR                   -->         HO2
{ 56} ROR   + NO2           -->         NTR
{ 57} OLE   + O             -->   0.630*ALD2  + 0.380*HO2   + 0.280*XO2
                              + 0.300*CO    + 0.200*FORM  + 0.020*XO2N
                              + 0.220*PAR   + 0.200*OH
{ 58} OLE   + OH            -->         FORM  +       ALD2  +       XO2
                              +         HO2   -       PAR
{ 59} OLE   + O3            -->   0.500*ALD2  + 0.740*FORM  + 0.330*CO
                              + 0.440*HO2   + 0.220*XO2   + 0.100*OH
                              + 0.200*FACD  + 0.200*AACD  -       PAR
{ 60} OLE   + NO3           -->   0.910*XO2   + 0.090*XO2N  +       FORM
                              +         ALD2  -       PAR   +       NO2
{ 61} ETH   + O             -->         FORM  + 0.700*XO2   +       CO
```

Table 8A-5. CB4_AQ Mechanism

```
                                  + 1.700*HO2   + 0.300*OH
{ 62} ETH   + OH            -->         XO2   + 1.560*FORM  +       HO2
                                  + 0.220*ALD2
{ 63} ETH   + O3            -->         FORM  + 0.420*CO    + 0.120*HO2
                                  + 0.400*FACD
{ 64} TOL   + OH            -->   0.080*XO2   + 0.360*CRES  + 0.440*HO2
                                  + 0.560*TO2
{ 65} TO2   + NO            -->   0.900*NO2   + 0.900*HO2   + 0.900*OPEN
                                  + 0.100*NTR
{ 66} TO2                   -->         CRES  +       HO2
{ 67} CRES  + OH            -->   0.400*CRO   + 0.600*XO2   + 0.600*HO2
                                  + 0.300*OPEN
{ 68} CRES  + NO3           -->         CRO   +       HNO3
{ 69} CRO   + NO2           -->         NTR
{ 70} XYL   + OH            -->   0.700*HO2   + 0.500*XO2   + 0.200*CRES
                                  + 0.800*MGLY  + 1.100*PAR   + 0.300*TO2
{ 71} OPEN  + OH            -->         XO2   + 2.000*CO    + 2.000*HO2
                                  +       C2O3  +       FORM
{ 72} OPEN  + hv            -->         C2O3  +       HO2   +       CO
{ 73} OPEN  + O3            -->   0.030*ALD2  + 0.620*C2O3  + 0.700*FORM
                                  + 0.030*XO2   + 0.690*CO    + 0.080*OH
                                  + 0.760*HO2   + 0.200*MGLY
{ 74} MGLY  + OH            -->         XO2   +       C2O3
{ 75} MGLY  + hv            -->         C2O3  +       HO2   +       CO
{ 76} ISOP  + O             -->   0.750*ISPD  + 0.500*FORM  + 0.250*XO2
                                  + 0.250*HO2   + 0.250*C2O3  + 0.250*PAR
{ 77} ISOP  + OH            -->   0.912*ISPD  + 0.629*FORM  + 0.991*XO2
                                  + 0.912*HO2   + 0.088*XO2N
{ 78} ISOP  + O3            -->   0.650*ISPD  + 0.600*FORM  + 0.200*XO2
                                  + 0.066*HO2   + 0.266*OH    + 0.200*C2O3
                                  + 0.150*ALD2  + 0.350*PAR   + 0.066*CO
{ 79} ISOP  + NO3           -->   0.200*ISPD  + 0.800*NTR   +       XO2
                                  + 0.800*HO2   + 0.200*NO2   + 0.800*ALD2
                                  + 2.400*PAR
{ 80} XO2   + NO            -->         NO2
{ 81} XO2   + XO2           -->
{ 82} XO2N  + NO            -->         NTR
{ 83} SO2   + OH            -->         SULF  +       HO2
{ 84} SO2                   -->         SULF
{ 85} XO2   + HO2           -->         UMHP
{ 86} XO2N  + HO2           -->
{ 87} XO2N  + XO2N          -->
{ 88} XO2N  + XO2           -->
{ 89} ISPD  + OH            -->   1.565*PAR   + 0.167*FORM  + 0.713*XO2
                                  + 0.503*HO2   + 0.334*CO    + 0.168*MGLY
                                  + 0.273*ALD2  + 0.498*C2O3
{ 90} ISPD  + O3            -->   0.114*C2O3  + 0.150*FORM  + 0.850*MGLY
                                  + 0.154*HO2   + 0.268*OH    + 0.064*XO2
                                  + 0.020*ALD2  + 0.360*PAR   + 0.225*CO
{ 91} ISPD  + NO3           -->   0.357*ALD2  + 0.282*FORM  + 1.282*PAR
                                  + 0.925*HO2   + 0.643*CO    + 0.850*NTR
                                  + 0.075*C2O3  + 0.075*XO2   + 0.075*HNO3
{ 92} ISPD  + hv            -->   0.333*CO    + 0.067*ALD2  + 0.900*FORM
                                  + 0.832*PAR   + 1.033*HO2   + 0.700*XO2
                                  + 0.967*C2O3
{ 93} ISOP  + NO2           -->   0.200*ISPD  + 0.800*NTR   +       XO2
                                  + 0.800*HO2   + 0.200*NO    + 0.800*ALD2
                                  + 2.400*PAR
>--------------------------------------------------------------------------<


Rate Expression                                                  Rate Constant
================================================================================
k(  1) uses photo table NO2_CBIV88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) is a falloff expression using:                             {1.37387E-14}
   k0   =  6.0000E-34 * (T/300)**(-2.30)
   kinf =  2.8000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  3) =  1.8000E-12 * exp( -1370.0/T)                            {1.81419E-14}
k(  4) =  9.3000E-12                                              {9.30000E-12}
k(  5) is a falloff expression using:                             {1.57527E-12}
   k0   =  9.0000E-32 * (T/300)**(-2.00)
   kinf =  2.2000E-11 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
```

Table 8A-5. CB4_AQ Mechanism

```
k(  6) is a falloff expression using:                                {1.66375E-12}
   k0   =  9.0000E-32 * (T/300)**(-1.50)
   kinf =  3.0000E-11 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  7) =  1.2000E-13 * exp( -2450.0/T)                               {3.22581E-17}
k(  8) uses photo table NO2_CBIV88      , scaled by 5.30000E-02      {0.00000E+00}
k(  9) uses photo table O3O1D_CBIV88    , scaled by 1.00000E+00      {0.00000E+00}
k( 10) =  1.8000E-11 * exp(   107.0/T)                               {2.57757E-11}
k( 11) =  3.2000E-11 * exp(    67.0/T)                               {4.00676E-11}
k( 12) =  2.2000E-10                                                 {2.20000E-10}
k( 13) =  1.6000E-12 * exp(  -940.0/T)                               {6.82650E-14}
k( 14) =  1.4000E-14 * exp(  -580.0/T)                               {1.99920E-15}
k( 15) uses photo table NO2_CBIV88      , scaled by 3.39000E+01      {0.00000E+00}
k( 16) =  1.3000E-11 * exp(   250.0/T)                               {3.00805E-11}
k( 17) =  2.5000E-14 * exp( -1230.0/T)                               {4.03072E-16}
k( 18) is a falloff expression using:                                {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 19) =  1.3000E-21                                                 {1.30000E-21}
k( 20) = k( 18) / Keq,  where Keq =  2.700E-27 * exp( 11000.0/T)     {4.36029E-02}
k( 21) =  3.3000E-39 * exp(   530.0/T)                               {1.95397E-38}
k( 22) =  4.4000E-40                                                 {4.39999E-40}
k( 23) is a falloff expression using:                                {6.69701E-12}
   k0   =  6.7000E-31 * (T/300)**(-3.30)
   kinf =  3.0000E-11 * (T/300)**(-1.00)
   F =  0.60,  n =  1.00
k( 24) uses photo table NO2_CBIV88      , scaled by 1.97500E-01      {0.00000E+00}
k( 25) =  6.6000E-12                                                 {6.60000E-12}
k( 26) =  1.0000E-20                                                 {1.00000E-20}
k( 27) is a falloff expression using:                                {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 28) is a special rate expression of the form:                     {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 29) =  3.7000E-12 * exp(   240.0/T)                               {8.27883E-12}
k( 30) is a falloff expression using:                                {1.48014E-12}
   k0   =  2.3000E-31 * (T/300)**(-4.60)
   kinf =  4.2000E-12 * (T/300)**( 0.20)
   F =  0.60,  n =  1.00
k( 31) = k( 30) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)     {9.17943E-02}
k( 32) =  1.3000E-12 * exp(   380.0/T)                               {4.65309E-12}
k( 33) =  5.9000E-14 * exp(  1150.0/T)                               {2.79783E-12}
k( 34) =  2.2000E-38 * exp(  5800.0/T)                               {6.23927E-30}
k( 35) uses photo table HCHOmol_CBIV88  , scaled by 2.55000E-01      {0.00000E+00}
k( 36) =  3.1000E-12 * exp(  -187.0/T)                               {1.65514E-12}
k( 37) =  1.5000E-13 * (1.0 + 0.6*Pressure)                          {2.40000E-13}
k( 38) =  1.0000E-11                                                 {1.00000E-11}
k( 39) uses photo table HCHOrad_CBIV88  , scaled by 1.00000E+00      {0.00000E+00}
k( 40) uses photo table HCHOmol_CBIV88  , scaled by 1.00000E+00      {0.00000E+00}
k( 41) =  3.0000E-11 * exp( -1550.0/T)                               {1.65275E-13}
k( 42) =  6.3000E-16                                                 {6.30000E-16}
k( 43) =  1.2000E-11 * exp(  -986.0/T)                               {4.38753E-13}
k( 44) =  7.0000E-12 * exp(   250.0/T)                               {1.61972E-11}
k( 45) =  2.5000E-15                                                 {2.50000E-15}
k( 46) uses photo table ALD_CBIV88      , scaled by 1.00000E+00      {0.00000E+00}
k( 47) =  3.4900E-11 * exp(  -180.0/T)                               {1.90766E-11}
k( 48) =  2.6300E-12 * exp(   380.0/T)                               {9.41356E-12}
k( 49) =  2.0000E+16 * exp(-13500.0/T)                               {4.23268E-04}
k( 50) =  2.5000E-12                                                 {2.50000E-12}
k( 51) =  6.5000E-12                                                 {6.50000E-12}
k( 52) =  1.1000E+02 * exp( -1710.0/T)                               {3.54242E-01}
k( 53) =  8.1000E-13                                                 {8.10000E-13}
k( 54) =  1.0000E+15 * exp( -8000.0/T)                               {2.19325E+03}
k( 55) =  1.6000E+03                                                 {1.60000E+03}
k( 56) =  1.5000E-11                                                 {1.50000E-11}
k( 57) =  1.2000E-11 * exp(  -324.0/T)                               {4.04572E-12}
k( 58) =  5.2000E-12 * exp(   504.0/T)                               {2.82173E-11}
k( 59) =  1.4000E-14 * exp( -2105.0/T)                               {1.19778E-17}
k( 60) =  7.7000E-15                                                 {7.70000E-15}
```

Table 8A-5. CB4_AQ Mechanism

```
k( 61) =  1.0000E-11 * exp(  -792.0/T)                          {7.01080E-13}
k( 62) =  2.0000E-12 * exp(   411.0/T)                          {7.94340E-12}
k( 63) =  1.3000E-14 * exp( -2633.0/T)                          {1.89105E-18}
k( 64) =  2.1000E-12 * exp(   322.0/T)                          {6.18715E-12}
k( 65) =  8.1000E-12                                            {8.10000E-12}
k( 66) =  4.2000E+00                                            {4.20000E+00}
k( 67) =  4.1000E-11                                            {4.10000E-11}
k( 68) =  2.2000E-11                                            {2.20000E-11}
k( 69) =  1.4000E-11                                            {1.40000E-11}
k( 70) =  1.7000E-11 * exp(   116.0/T)                          {2.50901E-11}
k( 71) =  3.0000E-11                                            {3.00000E-11}
k( 72) uses photo table HCHOrad_CBIV88  , scaled by 9.04000E+00   {0.00000E+00}
k( 73) =  5.4000E-17 * exp(  -500.0/T)                          {1.00858E-17}
k( 74) =  1.7000E-11                                            {1.70000E-11}
k( 75) uses photo table HCHOrad_CBIV88  , scaled by 9.64000E+00   {0.00000E+00}
k( 76) =  3.6000E-11                                            {3.60000E-11}
k( 77) =  2.5400E-11 * exp(   407.6/T)                          {9.97368E-11}
k( 78) =  7.8600E-15 * exp( -1912.0/T)                          {1.28512E-17}
k( 79) =  3.0300E-12 * exp(  -448.0/T)                          {6.73819E-13}
k( 80) =  8.1000E-12                                            {8.10000E-12}
k( 81) =  1.7000E-14 * exp(  1300.0/T)                          {1.33359E-12}
k( 82) =  8.1000E-12                                            {8.10000E-12}
k( 83) =  4.3900E-13 * exp(   160.0/T)                          {7.51005E-13}
k( 84) =  1.3600E-06                                            {1.36000E-06}
k( 85) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 86) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 87) =  1.7300E-14 * exp(  1300.0/T)                          {1.35712E-12}
k( 88) =  3.4500E-14 * exp(  1300.0/T)                          {2.70640E-12}
k( 89) =  3.3600E-11                                            {3.36000E-11}
k( 90) =  7.1100E-18                                            {7.11000E-18}
k( 91) =  1.0000E-15                                            {1.00000E-15}
k( 92) uses photo table ACROLEIN        , scaled by 3.60000E-03   {0.00000E+00}
k( 93) =  1.4900E-19                                            {1.49000E-19}
================================================================================
```

Table 8A-6. CB4_AE_AQ Mechanism

```
 Reaction List
>-------------------------------------------------------------------------------<
{  1} NO2     + hv                --> NO      +       O
{  2} O       + [O2]              --> O3
{  3} O3      + NO                --> NO2
{  4} O       + NO2               --> NO
{  5} O       + NO2               --> NO3
{  6} O       + NO                --> NO2
{  7} O3      + NO2               --> NO3
{  8} O3      + hv                --> O
{  9} O3      + hv                --> O1D
{ 10} O1D     + [N2]              --> O
{ 11} O1D     + [O2]              --> O
{ 12} O1D     + [H2O]             --> 2.000*OH
{ 13} O3      + OH                --> HO2
{ 14} O3      + HO2               --> OH
{ 15} NO3     + hv                --> 0.890*NO2     + 0.890*O       + 0.110*NO
{ 16} NO3     + NO                --> 2.000*NO2
{ 17} NO3     + NO2               --> NO      +       NO2
{ 18} NO3     + NO2               --> N2O5
{ 19} N2O5    + [H2O]             --> 2.000*HNO3
{ 20} N2O5                        --> NO3     +       NO2
{ 21} NO      + NO      + [O2]    --> 2.000*NO2
{ 22} NO      + NO2     + [H2O]   --> 2.000*HONO
{ 23} OH      + NO                --> HONO
{ 24} HONO    + hv                --> OH      +       NO
{ 25} HONO    + OH                --> NO2
{ 26} HONO    + HONO              --> NO      +       NO2
{ 27} OH      + NO2               --> HNO3
{ 28} OH      + HNO3              --> NO3
{ 29} HO2     + NO                --> OH      +       NO2
{ 30} HO2     + NO2               --> PNA
{ 31} PNA                         --> HO2     +       NO2
{ 32} PNA     + OH                --> NO2
{ 33} HO2     + HO2               --> H2O2
{ 34} HO2     + HO2     + [H2O]   --> H2O2
{ 35} H2O2    + hv                --> 2.000*OH
{ 36} H2O2    + OH                --> HO2
{ 37} CO      + OH                --> HO2
{ 38} FORM    + OH                --> HO2     +       CO
{ 39} FORM    + hv                --> 2.000*HO2     +       CO
{ 40} FORM    + hv                --> CO
{ 41} FORM    + O                 --> OH      +       HO2     +       CO
{ 42} FORM    + NO3               --> HNO3    +       HO2     +       CO
{ 43} ALD2    + O                 --> C2O3    +       OH
{ 44} ALD2    + OH                --> C2O3
{ 45} ALD2    + NO3               --> C2O3    +       HNO3
{ 46} ALD2    + hv                --> XO2     + 2.000*HO2     +       CO
                                    +       FORM
{ 47} C2O3    + NO                --> NO2     +       XO2     +       FORM
                                    +       HO2
{ 48} C2O3    + NO2               --> PAN
{ 49} PAN                         --> C2O3    +       NO2
{ 50} C2O3    + C2O3              --> 2.000*XO2     + 2.000*FORM    + 2.000*HO2
{ 51} C2O3    + HO2               --> 0.790*FORM    + 0.790*XO2     + 0.790*HO2
                                    + 0.790*OH      + 0.210*PACD
{ 52} OH                          --> XO2     +       FORM    +       HO2
{ 53} PAR     + OH                --> 0.870*XO2     + 0.130*XO2N    + 0.110*HO2
                                    + 0.110*ALD2    + 0.760*ROR     - 0.110*PAR
{ 54} ROR                         --> 1.100*ALD2    + 0.960*XO2     + 0.940*HO2
                                    - 2.100*PAR     + 0.040*XO2N    + 0.020*ROR
{ 55} ROR                         --> HO2
{ 56} ROR     + NO2               --> NTR
{ 57} OLE     + O                 --> 0.630*ALD2    + 0.380*HO2     + 0.280*XO2
                                    + 0.300*CO      + 0.200*FORM    + 0.020*XO2N
                                    + 0.220*PAR     + 0.200*OH
{ 58} OLE     + OH                --> FORM    +       ALD2    +       XO2
                                    +       HO2     -       PAR
{ 59} OLE     + O3                --> 0.500*ALD2    + 0.740*FORM    + 0.330*CO
                                    + 0.440*HO2     + 0.220*XO2     + 0.100*OH
                                    + 0.200*FACD    + 0.200*AACD    -       PAR
{ 60} OLE     + NO3               --> 0.910*XO2     + 0.090*XO2N    +       FORM
                                    +       ALD2    -       PAR     +       NO2
{ 61} ETH     + O                 --> FORM    + 0.700*XO2     +       CO
```

Table 8A-6. CB4_AE_AQ Mechanism

```
                                    + 1.700*HO2     + 0.300*OH
{ 62} ETH     + OH              -->         XO2     + 1.560*FORM    +       HO2
                                    + 0.220*ALD2
{ 63} ETH     + O3              -->         FORM    + 0.420*CO      + 0.120*HO2
                                    + 0.400*FACD
{ 64} TOL     + OH              -->   0.080*XO2     + 0.360*CRES    + 0.440*HO2
                                    + 0.560*TO2     +       TOLAER
{ 65} TO2     + NO              -->   0.900*NO2     + 0.900*HO2     + 0.900*OPEN
                                    + 0.100*NTR
{ 66} TO2                       -->         CRES    +       HO2
{ 67} CRES    + OH              -->   0.400*CRO     + 0.600*XO2     + 0.600*HO2
                                    + 0.300*OPEN    +       CSLAER
{ 68} CRES    + NO3             -->         CRO     +       HNO3    +       CSLAER
{ 69} CRO     + NO2             -->         NTR
{ 70} XYL     + OH              -->   0.700*HO2     + 0.500*XO2     + 0.200*CRES
                                    + 0.800*MGLY    + 1.100*PAR     + 0.300*TO2
                                    +       XYLAER
{ 71} OPEN    + OH              -->         XO2     + 2.000*CO      + 2.000*HO2
                                    +       C2O3    +       FORM
{ 72} OPEN    + hv              -->         C2O3    +       HO2     +       CO
{ 73} OPEN    + O3              -->   0.030*ALD2    + 0.620*C2O3    + 0.700*FORM
                                    + 0.030*XO2     + 0.690*CO      + 0.080*OH
                                    + 0.760*HO2     + 0.200*MGLY
{ 74} MGLY    + OH              -->         XO2     +       C2O3
{ 75} MGLY    + hv              -->         C2O3    +       HO2     +       CO
{ 76} ISOP    + O               -->   0.750*ISPD    + 0.500*FORM    + 0.250*XO2
                                    + 0.250*HO2     + 0.250*C2O3    + 0.250*PAR
{ 77} ISOP    + OH              -->   0.912*ISPD    + 0.629*FORM    + 0.991*XO2
                                    + 0.912*HO2     + 0.088*XO2N
{ 78} ISOP    + O3              -->   0.650*ISPD    + 0.600*FORM    + 0.200*XO2
                                    + 0.066*HO2     + 0.266*OH      + 0.200*C2O3
                                    + 0.150*ALD2    + 0.350*PAR     + 0.066*CO
{ 79} ISOP    + NO3             -->   0.200*ISPD    + 0.800*NTR     +       XO2
                                    + 0.800*HO2     + 0.200*NO2     + 0.800*ALD2
                                    + 2.400*PAR
{ 80} XO2     + NO              -->         NO2
{ 81} XO2     + XO2             -->
{ 82} XO2N    + NO              -->         NTR
{ 83} SO2     + OH              -->         SULF    +       HO2     +       SULAER
{ 84} SO2                       -->         SULF    +       SULAER
{ 85} XO2     + HO2             -->         UMHP
{ 86} XO2N    + HO2             -->
{ 87} XO2N    + XO2N            -->
{ 88} XO2N    + XO2             -->
{ 89} ISPD    + OH              -->   1.565*PAR     + 0.167*FORM    + 0.713*XO2
                                    + 0.503*HO2     + 0.334*CO      + 0.168*MGLY
                                    + 0.273*ALD2    + 0.498*C2O3
{ 90} ISPD    + O3              -->   0.114*C2O3    + 0.150*FORM    + 0.850*MGLY
                                    + 0.154*HO2     + 0.268*OH      + 0.064*XO2
                                    + 0.020*ALD2    + 0.360*PAR     + 0.225*CO
{ 91} ISPD    + NO3             -->   0.357*ALD2    + 0.282*FORM    + 1.282*PAR
                                    + 0.925*HO2     + 0.643*CO      + 0.850*NTR
                                    + 0.075*C2O3    + 0.075*XO2     + 0.075*HNO3
{ 92} ISPD    + hv              -->   0.333*CO      + 0.067*ALD2    + 0.900*FORM
                                    + 0.832*PAR     + 1.033*HO2     + 0.700*XO2
                                    + 0.967*C2O3
{ 93} ISOP    + NO2             -->   0.200*ISPD    + 0.800*NTR     +       XO2
                                    + 0.800*HO2     + 0.200*NO      + 0.800*ALD2
                                    + 2.400*PAR
{ 94} TERP    + OH              -->         TERPAER +       OH
{ 95} TERP    + NO3             -->         TERPAER +       NO3
{ 96} TERP    + O3              -->         TERPAER +       O3
>-------------------------------------------------------------------------------<

Rate Expression                                                  Rate Constant
 ================================================================================
 k(  1) uses photo table NO2_CBIV88      , scaled by 1.00000E+00   {0.00000E+00}
 k(  2) is a falloff expression using:                             {1.37387E-14}
    k0   =  6.0000E-34 * (T/300)**(-2.30)
    kinf =  2.8000E-12 * (T/300)**( 0.00)
    F =  0.60,  n =  1.00
 k(  3) =  1.8000E-12 * exp( -1370.0/T)                           {1.81419E-14}
 k(  4) =  9.3000E-12                                             {9.30000E-12}
```

Table 8A-6. CB4_AE_AQ Mechanism

```
k(  5) is a falloff expression using:                                {1.57527E-12}
   k0   =  9.0000E-32 * (T/300)**(-2.00)
   kinf =  2.2000E-11 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  6) is a falloff expression using:                                {1.66375E-12}
   k0   =  9.0000E-32 * (T/300)**(-1.50)
   kinf =  3.0000E-11 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k(  7) =  1.2000E-13 * exp( -2450.0/T)                               {3.22581E-17}
k(  8) uses photo table NO2_CBIV88      , scaled by 5.30000E-02      {0.00000E+00}
k(  9) uses photo table O3O1D_CBIV88    , scaled by 1.00000E+00      {0.00000E+00}
k( 10) =  1.8000E-11 * exp(   107.0/T)                               {2.57757E-11}
k( 11) =  3.2000E-11 * exp(    67.0/T)                               {4.00676E-11}
k( 12) =  2.2000E-10                                                 {2.20000E-10}
k( 13) =  1.6000E-12 * exp(  -940.0/T)                               {6.82650E-14}
k( 14) =  1.4000E-14 * exp(  -580.0/T)                               {1.99920E-15}
k( 15) uses photo table NO2_CBIV88      , scaled by 3.39000E+01      {0.00000E+00}
k( 16) =  1.3000E-11 * exp(   250.0/T)                               {3.00805E-11}
k( 17) =  2.5000E-14 * exp( -1230.0/T)                               {4.03072E-16}
k( 18) is a falloff expression using:                                {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 19) =  1.3000E-21                                                 {1.30000E-21}
k( 20) = k( 18) / Keq,  where Keq =  2.700E-27 * exp( 11000.0/T)     {4.36029E-02}
k( 21) =  3.3000E-39 * exp(   530.0/T)                               {1.95397E-38}
k( 22) =  4.4000E-40                                                 {4.39999E-40}
k( 23) is a falloff expression using:                                {6.69701E-12}
   k0   =  6.7000E-31 * (T/300)**(-3.30)
   kinf =  3.0000E-11 * (T/300)**(-1.00)
   F =  0.60,  n =  1.00
k( 24) uses photo table NO2_CBIV88      , scaled by 1.97500E-01      {0.00000E+00}
k( 25) =  6.6000E-12                                                 {6.60000E-12}
k( 26) =  1.0000E-20                                                 {1.00000E-20}
k( 27) is a falloff expression using:                                {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 28) is a special rate expression of the form:                     {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 29) =  3.7000E-12 * exp(   240.0/T)                               {8.27883E-12}
k( 30) is a falloff expression using:                                {1.48014E-12}
   k0   =  2.3000E-31 * (T/300)**(-4.60)
   kinf =  4.2000E-12 * (T/300)**( 0.20)
   F =  0.60,  n =  1.00
k( 31) = k( 30) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)     {9.17943E-02}
k( 32) =  1.3000E-12 * exp(   380.0/T)                               {4.65309E-12}
k( 33) =  5.9000E-14 * exp(  1150.0/T)                               {2.79783E-12}
k( 34) =  2.2000E-38 * exp(  5800.0/T)                               {6.23927E-30}
k( 35) uses photo table HCHOmol_CBIV88  , scaled by 2.55000E-01      {0.00000E+00}
k( 36) =  3.1000E-12 * exp(  -187.0/T)                               {1.65514E-12}
k( 37) =  1.5000E-13 * (1.0 + 0.6*Pressure)                          {2.40000E-13}
k( 38) =  1.0000E-11                                                 {1.00000E-11}
k( 39) uses photo table HCHOrad_CBIV88  , scaled by 1.00000E+00      {0.00000E+00}
k( 40) uses photo table HCHOmol_CBIV88  , scaled by 1.00000E+00      {0.00000E+00}
k( 41) =  3.0000E-11 * exp( -1550.0/T)                               {1.65275E-13}
k( 42) =  6.3000E-16                                                 {6.30000E-16}
k( 43) =  1.2000E-11 * exp(  -986.0/T)                               {4.38753E-13}
k( 44) =  7.0000E-12 * exp(   250.0/T)                               {1.61972E-11}
k( 45) =  2.5000E-15                                                 {2.50000E-15}
k( 46) uses photo table ALD_CBIV88      , scaled by 1.00000E+00      {0.00000E+00}
k( 47) =  3.4900E-11 * exp(  -180.0/T)                               {1.90766E-11}
k( 48) =  2.6300E-12 * exp(   380.0/T)                               {9.41356E-12}
k( 49) =  2.0000E+16 * exp(-13500.0/T)                               {4.23268E-04}
k( 50) =  2.5000E-12                                                 {2.50000E-12}
k( 51) =  6.5000E-12                                                 {6.50000E-12}
k( 52) =  1.1000E+02 * exp( -1710.0/T)                               {3.54242E-01}
k( 53) =  8.1000E-13                                                 {8.10000E-13}
k( 54) =  1.0000E+15 * exp( -8000.0/T)                               {2.19325E+03}
k( 55) =  1.6000E+03                                                 {1.60000E+03}
k( 56) =  1.5000E-11                                                 {1.50000E-11}
```

Table 8A-6. CB4_AE_AQ Mechanism

```
k( 57) =  1.2000E-11 * exp(  -324.0/T)                          {4.04572E-12}
k( 58) =  5.2000E-12 * exp(   504.0/T)                          {2.82173E-11}
k( 59) =  1.4000E-14 * exp( -2105.0/T)                          {1.19778E-17}
k( 60) =  7.7000E-15                                            {7.70000E-15}
k( 61) =  1.0000E-11 * exp(  -792.0/T)                          {7.01080E-13}
k( 62) =  2.0000E-12 * exp(   411.0/T)                          {7.94340E-12}
k( 63) =  1.3000E-14 * exp( -2633.0/T)                          {1.89105E-18}
k( 64) =  2.1000E-12 * exp(   322.0/T)                          {6.18715E-12}
k( 65) =  8.1000E-12                                            {8.10000E-12}
k( 66) =  4.2000E+00                                            {4.20000E+00}
k( 67) =  4.1000E-11                                            {4.10000E-11}
k( 68) =  2.2000E-11                                            {2.20000E-11}
k( 69) =  1.4000E-11                                            {1.40000E-11}
k( 70) =  1.7000E-11 * exp(   116.0/T)                          {2.50901E-11}
k( 71) =  3.0000E-11                                            {3.00000E-11}
k( 72) uses photo table HCHOrad_CBIV88  , scaled by 9.04000E+00 {0.00000E+00}
k( 73) =  5.4000E-17 * exp(  -500.0/T)                          {1.00858E-17}
k( 74) =  1.7000E-11                                            {1.70000E-11}
k( 75) uses photo table HCHOrad_CBIV88  , scaled by 9.64000E+00 {0.00000E+00}
k( 76) =  3.6000E-11                                            {3.60000E-11}
k( 77) =  2.5400E-11 * exp(   407.6/T)                          {9.97368E-11}
k( 78) =  7.8600E-15 * exp( -1912.0/T)                          {1.28512E-17}
k( 79) =  3.0300E-12 * exp(  -448.0/T)                          {6.73819E-13}
k( 80) =  8.1000E-12                                            {8.10000E-12}
k( 81) =  1.7000E-14 * exp(  1300.0/T)                          {1.33359E-12}
k( 82) =  8.1000E-12                                            {8.10000E-12}
k( 83) =  4.3900E-13 * exp(   160.0/T)                          {7.51005E-13}
k( 84) =  1.3600E-06                                            {1.36000E-06}
k( 85) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 86) =  7.6700E-14 * exp(  1300.0/T)                          {6.01684E-12}
k( 87) =  1.7300E-14 * exp(  1300.0/T)                          {1.35712E-12}
k( 88) =  3.4500E-14 * exp(  1300.0/T)                          {2.70640E-12}
k( 89) =  3.3600E-11                                            {3.36000E-11}
k( 90) =  7.1100E-18                                            {7.11000E-18}
k( 91) =  1.0000E-15                                            {1.00000E-15}
k( 92) uses photo table ACROLEIN        , scaled by 3.60000E-03 {0.00000E+00}
k( 93) =  1.4900E-19                                            {1.49000E-19}
k( 94) =  1.0700E-11 * exp(   549.0/T)                          {6.75269E-11}
k( 95) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k( 96) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
================================================================================
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
 Reaction List
>-----------------------------------------------------------------------------<
{  1} NO2   + hv            -->         O3P   +       NO
{  2} O3    + hv            -->         O1D
{  3} O3    + hv            -->         O3P
{  4} HONO  + hv            -->         HO    +       NO
{  5} HNO3  + hv            -->         HO    +       NO2
{  6} HNO4  + hv            -->         HO2   +       NO2
{  7} NO3   + hv            -->         NO
{  8} NO3   + hv            -->         NO2   +       O3P
{  9} H2O2  + hv            -->   2.000*HO
{ 10} HCHO  + hv            -->         CO
{ 11} HCHO  + hv            -->         HO2   +       HO2   +       CO
{ 12} ALD   + hv            -->         MO2   +       HO2   +       CO
{ 13} OP1   + hv            -->         HCHO  +       HO2   +       HO
{ 14} OP2   + hv            -->         ALD   +       HO2   +       HO
{ 15} PAA   + hv            -->         MO2   +       HO
{ 16} KET   + hv            -->         ACO3  +       ETHP
{ 17} GLY   + hv            -->   0.130*HCHO  + 1.870*CO
{ 18} GLY   + hv            -->   0.450*HCHO  + 1.550*CO    + 0.800*HO2
{ 19} MGLY  + hv            -->         ACO3  +       HO2   +       CO
{ 20} DCB   + hv            -->   0.980*HO2   + 0.020*ACO3  +       TCO3
{ 21} ONIT  + hv            -->   0.200*ALD   + 0.800*KET   +       HO2
                                +       NO2
{ 22} O3P   + [M]   + [O2]  -->         O3
{ 23} O3P   + NO2           -->         NO
{ 24} O1D   + [N2]          -->         O3P
{ 25} O1D   + [O2]          -->         O3P
{ 26} O1D   + [H2O]         -->   2.000*HO
{ 27} O3    + NO            -->         NO2
{ 28} O3    + HO            -->         HO2
{ 29} O3    + HO2           -->         HO
{ 30} HO2   + NO            -->         NO2   +       HO
{ 31} HO2   + NO2           -->         HNO4
{ 32} HNO4                  -->         HO2   +       NO2
{ 33} HO2   + HO2           -->         H2O2
{ 34} HO2   + HO2   + [H2O] -->         H2O2
{ 35} H2O2  + HO            -->         HO2
{ 36} NO    + HO            -->         HONO
{ 37} NO    + NO    + [O2]  -->   2.000*NO2
{ 38} O3    + NO2           -->         NO3
{ 39} NO3   + NO            -->   2.000*NO2
{ 40} NO3   + NO2           -->         NO    +       NO2
{ 41} NO3   + HO2           -->         HNO3
{ 42} NO3   + NO2           -->         N2O5
{ 43} N2O5                  -->         NO2   +       NO3
{ 44} N2O5  + [H2O]         -->   2.000*HNO3
{ 45} HO    + NO2           -->         HNO3
{ 46} HO    + HNO3          -->         NO3
{ 47} HO    + HNO4          -->         NO2
{ 48} HO    + HO2           -->
{ 49} HO    + SO2           -->         SULF  +       HO2
{ 50} CO    + HO            -->         HO2
{ 51} HO                    -->         MO2
{ 52} ETH   + HO            -->         ETHP
{ 53} HC3   + HO            -->   0.830*HC3P  + 0.170*HO2   + 0.009*HCHO
                                + 0.075*ALD   + 0.025*KET
{ 54} HC5   + HO            -->         HC5P  + 0.250*XO2
{ 55} HC8   + HO            -->         HC8P  + 0.750*XO2
{ 56} OL2   + HO            -->         OL2P
{ 57} OLT   + HO            -->         OLTP
{ 58} OLI   + HO            -->         OLIP
{ 59} TOL   + HO            -->   0.750*TOLP  + 0.250*CSL   + 0.250*HO2
{ 60} XYL   + HO            -->   0.830*XYLP  + 0.170*CSL   + 0.170*HO2
{ 61} CSL   + HO            -->   0.100*HO2   + 0.900*XO2   + 0.900*TCO3
{ 62} CSL   + HO            -->         CSL
{ 63} HCHO  + HO            -->         HO2   +       CO
{ 64} ALD   + HO            -->         ACO3
{ 65} KET   + HO            -->         KETP
{ 66} GLY   + HO            -->         HO2   + 2.000*CO
{ 67} MGLY  + HO            -->         ACO3  +       CO
{ 68} DCB   + HO            -->         TCO3
{ 69} OP1   + HO            -->   0.500*MO2   + 0.500*HCHO  + 0.500*HO
{ 70} OP2   + HO            -->   0.500*HC3P  + 0.500*ALD   + 0.500*HO
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
{ 71} PAA   + HO            -->         ACO3
{ 72} PAN   + HO            -->         HCHO  +       NO3   +       XO2
{ 73} ONIT  + HO            -->         HC3P  +       NO2
{ 74} ISO   + HO            -->         OLTP
{ 75} ACO3  + NO2           -->         PAN
{ 76} PAN                   -->         ACO3  +       NO2
{ 77} TCO3  + NO2           -->         TPAN
{ 78} TPAN                  -->         TCO3  +       NO2
{ 79} MO2   + NO            -->         HCHO  +       HO2   +       NO2
{ 80} HC3P  + NO            -->   0.750*ALD   + 0.250*KET   + 0.090*HCHO
                              + 0.036*ONIT  + 0.964*NO2   + 0.964*HO2
{ 81} HC5P  + NO            -->   0.380*ALD   + 0.690*KET   + 0.080*ONIT
                              + 0.920*NO2   + 0.920*HO2
{ 82} HC8P  + NO            -->   0.350*ALD   + 1.060*KET   + 0.040*HCHO
                              + 0.240*ONIT  + 0.760*NO2   + 0.760*HO2
{ 83} OL2P  + NO            -->   1.600*HCHO  +       HO2   +       NO2
                              + 0.200*ALD
{ 84} OLTP  + NO            -->         ALD   +       HCHO  +       HO2
                              +       NO2
{ 85} OLIP  + NO            -->         HO2   + 1.450*ALD   + 0.280*HCHO
                              + 0.100*KET   +       NO2
{ 86} ACO3  + NO            -->         MO2   +       NO2
{ 87} TCO3  + NO            -->         NO2   + 0.920*HO2   + 0.890*GLY
                              + 0.110*MGLY  + 0.050*ACO3  + 0.950*CO
                              + 2.000*XO2
{ 88} TOLP  + NO            -->         NO2   +       HO2   + 0.170*MGLY
                              + 0.160*GLY   + 0.700*DCB
{ 89} XYLP  + NO            -->         NO2   +       HO2   + 0.450*MGLY
                              + 0.806*DCB
{ 90} ETHP  + NO            -->         ALD   +       HO2   +       NO2
{ 91} KETP  + NO            -->         MGLY  +       NO2   +       HO2
{ 92} OLN   + NO            -->         HCHO  +       ALD   + 2.000*NO2
{ 93} HCHO  + NO3           -->         HO2   +       HNO3  +       CO
{ 94} ALD   + NO3           -->         ACO3  +       HNO3
{ 95} GLY   + NO3           -->         HNO3  +       HO2   + 2.000*CO
{ 96} MGLY  + NO3           -->         HNO3  +       ACO3  +       CO
{ 97} DCB   + NO3           -->         HNO3  +       TCO3
{ 98} CSL   + NO3           -->         HNO3  +       XNO2  + 0.500*CSL
{ 99} OL2   + NO3           -->         OLN
{100} OLT   + NO3           -->         OLN
{101} OLI   + NO3           -->         OLN
{102} ISO   + NO3           -->         OLN
{103} OL2   + O3            -->         HCHO  + 0.400*ORA1  + 0.420*CO
                              + 0.120*HO2
{104} OLT   + O3            -->   0.530*HCHO  + 0.500*ALD   + 0.330*CO
                              + 0.200*ORA1  + 0.200*ORA2  + 0.230*HO2
                              + 0.220*MO2   + 0.100*HO
{105} OLI   + O3            -->   0.180*HCHO  + 0.720*ALD   + 0.100*KET
                              + 0.230*CO    + 0.060*ORA1  + 0.290*ORA2
                              + 0.260*HO2   + 0.140*HO    + 0.310*MO2
{106} ISO   + O3            -->   0.530*HCHO  + 0.500*ALD   + 0.330*CO
                              + 0.200*ORA1  + 0.200*ORA2  + 0.230*HO2
                              + 0.220*MO2   + 0.100*HO
{107} HO2   + MO2           -->         OP1
{108} HO2   + ETHP          -->         OP2
{109} HO2   + HC3P          -->         OP2
{110} HO2   + HC5P          -->         OP2
{111} HO2   + HC8P          -->         OP2
{112} HO2   + OL2P          -->         OP2
{113} HO2   + OLTP          -->         OP2
{114} HO2   + OLIP          -->         OP2
{115} HO2   + KETP          -->         OP2
{116} HO2   + ACO3          -->         PAA
{117} HO2   + TOLP          -->         OP2
{118} HO2   + XYLP          -->         OP2
{119} HO2   + TCO3          -->         OP2
{120} HO2   + OLN           -->         ONIT
{121} MO2   + MO2           -->   1.500*HCHO  +       HO2
{122} MO2   + ETHP          -->   0.750*HCHO  +       HO2   + 0.750*ALD
{123} MO2   + HC3P          -->   0.840*HCHO  + 0.770*ALD   + 0.260*KET
                              +       HO2
{124} MO2   + HC5P          -->   0.770*HCHO  + 0.410*ALD   + 0.750*KET
                              +       HO2
{125} MO2   + HC8P          -->   0.800*HCHO  + 0.460*ALD   + 1.390*KET
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
                                  +       HO2
{126} MO2   + OL2P          -->   1.550*HCHO  + 0.350*ALD   +       HO2
{127} MO2   + OLTP          -->   1.250*HCHO  + 0.750*ALD   +       HO2
{128} MO2   + OLIP          -->   0.890*HCHO  + 0.725*ALD   +       HO2
                                  + 0.550*KET
{129} MO2   + KETP          -->   0.750*HCHO  + 0.750*MGLY  +       HO2
{130} MO2   + ACO3          -->         HCHO  + 0.500*HO2   + 0.500*MO2
                                  + 0.500*ORA2
{131} MO2   + TOLP          -->         HCHO  + 0.170*MGLY  + 0.160*GLY
                                  + 0.700*DCB   + 2.000*HO2
{132} MO2   + XYLP          -->         HCHO  + 0.450*MGLY  + 0.806*DCB
                                  + 2.000*HO2
{133} MO2   + TCO3          -->   0.500*HCHO  + 0.445*GLY   + 0.055*MGLY
                                  + 0.500*ORA2  + 0.025*ACO3  + 0.460*HO2
                                  + 0.475*CO    +       XO2
{134} MO2   + OLN           -->   1.750*HCHO  + 0.500*HO2   +       ALD
                                  +       NO2
{135} ETHP  + ACO3          -->         ALD   + 0.500*HO2   + 0.500*MO2
                                  + 0.500*ORA2
{136} HC3P  + ACO3          -->   0.770*ALD   + 0.260*KET   + 0.500*HO2
                                  + 0.500*MO2   + 0.500*ORA2
{137} HC5P  + ACO3          -->   0.410*ALD   + 0.750*KET   + 0.500*HO2
                                  + 0.500*MO2   + 0.500*ORA2
{138} HC8P  + ACO3          -->   0.460*ALD   + 1.390*KET   + 0.500*HO2
                                  + 0.500*MO2   + 0.500*ORA2
{139} OL2P  + ACO3          -->   0.800*HCHO  + 0.600*ALD   + 0.500*HO2
                                  + 0.500*MO2   + 0.500*ORA2
{140} OLTP  + ACO3          -->         ALD   + 0.500*HCHO  + 0.500*HO2
                                  + 0.500*MO2   + 0.500*ORA2
{141} OLIP  + ACO3          -->   0.725*ALD   + 0.550*KET   + 0.140*HCHO
                                  + 0.500*HO2   + 0.500*MO2   + 0.500*ORA2
{142} KETP  + ACO3          -->         MGLY  + 0.500*HO2   + 0.500*MO2
                                  + 0.500*ORA2
{143} ACO3  + ACO3          -->   2.000*MO2
{144} ACO3  + TOLP          -->         MO2   + 0.170*MGLY  + 0.160*GLY
                                  + 0.700*DCB   +       HO2
{145} ACO3  + XYLP          -->         MO2   + 0.450*MGLY  + 0.806*DCB
                                  +       HO2
{146} ACO3  + TCO3          -->         MO2   + 0.920*HO2   + 0.890*GLY
                                  + 0.110*MGLY  + 0.050*ACO3  + 0.950*CO
                                  + 2.000*XO2
{147} ACO3  + OLN           -->         HCHO  +       ALD   + 0.500*ORA2
                                  +       NO2   + 0.500*MO2
{148} OLN   + OLN           -->   2.000*HCHO  + 2.000*ALD   + 2.000*NO2
{149} XO2   + HO2           -->         OP2
{150} XO2   + MO2           -->         HCHO  +       HO2
{151} XO2   + ACO3          -->         MO2
{152} XO2   + XO2           -->
{153} XO2   + NO            -->         NO2
{154} XNO2  + NO2           -->         ONIT
{155} XNO2  + HO2           -->         OP2
{156} XNO2  + MO2           -->         HCHO  +       HO2
{157} XNO2  + ACO3          -->         MO2
{158} XNO2  + XNO2          -->
>---------------------------------------------------------------------<

Rate Expression                                                    Rate Constant
=====================================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                            {1.68671E-12}
k( 36) is a falloff expression using:                             {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                            {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                            {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                            {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                            {4.03072E-16}
k( 41) =  2.5000E-12                                              {2.50000E-12}
k( 42) is a falloff expression using:                             {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
k( 44) =  2.0000E-21                                              {2.00000E-21}
k( 45) is a falloff expression using:                             {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 46) is a special rate expression of the form:                  {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 47) =  1.3000E-12 * exp(   380.0/T)                            {4.65309E-12}
k( 48) =  4.6000E-11 * exp(   230.0/T)                            {9.95294E-11}
k( 49) is a falloff expression using:                             {8.88848E-13}
   k0   =  3.0000E-31 * (T/300)**(-3.30)
   kinf =  1.5000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                       {2.40000E-13}
k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)         {3.80672E-01}
k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)         {2.74210E-13}
k( 53) =  1.5900E-11 * exp(  -540.0/T)                            {2.59669E-12}
k( 54) =  1.7300E-11 * exp(  -380.0/T)                            {4.83334E-12}
k( 55) =  3.6400E-11 * exp(  -380.0/T)                            {1.01696E-11}
k( 56) =  2.1500E-12 * exp(   411.0/T)                            {8.53916E-12}
k( 57) =  5.3200E-12 * exp(   504.0/T)                            {2.88684E-11}
k( 58) =  1.0700E-11 * exp(   549.0/T)                            {6.75269E-11}
k( 59) =  2.1000E-12 * exp(   322.0/T)                            {6.18715E-12}
k( 60) =  1.8900E-11 * exp(   116.0/T)                            {2.78943E-11}
k( 61) =  4.0000E-11                                              {4.00000E-11}
k( 62) =  9.0000E-01 * k( 61)                                     {3.60000E-11}
k( 63) =  9.0000E-12                                              {9.00000E-12}
k( 64) =  6.8700E-12 * exp(   256.0/T)                            {1.62197E-11}
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
k( 65) =  1.2000E-11 * exp(  -745.0/T)                          {9.85020E-13}
k( 66) =  1.1500E-11                                            {1.15000E-11}
k( 67) =  1.7000E-11                                            {1.70000E-11}
k( 68) =  2.8000E-11                                            {2.80000E-11}
k( 69) =  1.0000E-11                                            {1.00000E-11}
k( 70) =  1.0000E-11                                            {1.00000E-11}
k( 71) =  1.0000E-11                                            {1.00000E-11}
k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)       {1.37105E-13}
k( 73) =  1.5500E-11 * exp(  -540.0/T)                          {2.53137E-12}
k( 74) =  2.5500E-11 * exp(   409.0/T)                          {1.00601E-10}
k( 75) =  2.8000E-12 * exp(   181.0/T)                          {5.13974E-12}
k( 76) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 77) =  4.7000E-12                                            {4.70000E-12}
k( 78) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 79) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 80) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 81) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 82) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 83) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 84) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 85) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 86) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 87) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 88) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 89) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 90) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 91) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 92) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 93) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 94) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 95) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 96) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 97) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 98) =  2.2000E-11                                            {2.20000E-11}
k( 99) =  2.0000E-12 * exp( -2923.0/T)                          {1.09940E-16}
k(100) =  1.0000E-11 * exp( -1895.0/T)                          {1.73099E-14}
k(101) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k(102) =  5.8100E-13                                            {5.81000E-13}
k(103) =  1.2000E-14 * exp( -2633.0/T)                          {1.74559E-18}
k(104) =  1.3200E-14 * exp( -2105.0/T)                          {1.12933E-17}
k(105) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
k(106) =  1.2300E-14 * exp( -2013.0/T)                          {1.43295E-17}
k(107) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(118) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(119) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(120) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(121) =  1.9000E-13 * exp(   220.0/T)                          {3.97533E-13}
k(122) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(123) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(124) =  3.4000E-14 * exp(   220.0/T)                          {7.11376E-14}
k(125) =  2.9000E-14 * exp(   220.0/T)                          {6.06762E-14}
k(126) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(127) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(128) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(131) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(132) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(133) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(134) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(135) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(136) =  1.0000E-13 * exp(   220.0/T)                          {2.09228E-13}
k(137) =  8.4000E-14 * exp(   220.0/T)                          {1.75752E-13}
k(138) =  7.2000E-14 * exp(   220.0/T)                          {1.50644E-13}
```

Table 8A-7. RADM2 and RADM2_AQ Mechanisms

```
k(139) =  3.4000E-13 * exp(   220.0/T)                              {7.11376E-13}
k(140) =  3.4000E-13 * exp(   220.0/T)                              {7.11376E-13}
k(141) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                              {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(145) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(146) =  1.1900E-12 * exp(   220.0/T)                              {2.48981E-12}
k(147) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(148) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
k(149) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(150) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(151) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(152) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
k(153) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k(154) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k(155) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(156) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(157) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(158) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
================================================================================
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
 Reaction List
>--------------------------------------------------------------------------------<
{  1} NO2     + hv                --> O3P     +  NO
{  2} O3      + hv                --> O1D
{  3} O3      + hv                --> O3P
{  4} HONO    + hv                --> HO      +  NO
{  5} HNO3    + hv                --> HO      +  NO2
{  6} HNO4    + hv                --> HO2     +  NO2
{  7} NO3     + hv                --> NO
{  8} NO3     + hv                --> NO2     +  O3P
{  9} H2O2    + hv                --> 2.000*HO
{ 10} HCHO    + hv                --> CO
{ 11} HCHO    + hv                --> HO2     +  HO2     +  CO
{ 12} ALD     + hv                --> MO2     +  HO2     +  CO
{ 13} OP1     + hv                --> HCHO    +  HO2     +  HO
{ 14} OP2     + hv                --> ALD     +  HO2     +  HO
{ 15} PAA     + hv                --> MO2     +  HO
{ 16} KET     + hv                --> ACO3    +  ETHP
{ 17} GLY     + hv                --> 0.130*HCHO  + 1.870*CO
{ 18} GLY     + hv                --> 0.450*HCHO  + 1.550*CO      + 0.800*HO2
{ 19} MGLY    + hv                --> ACO3    +  HO2     +  CO
{ 20} DCB     + hv                --> 0.980*HO2   + 0.020*ACO3    +  TCO3
{ 21} ONIT    + hv                --> 0.200*ALD   + 0.800*KET     +  HO2
                                    +  NO2
{ 22} O3P     + [M]     + [O2]    --> O3
{ 23} O3P     + NO2               --> NO
{ 24} O1D     + [N2]              --> O3P
{ 25} O1D     + [O2]              --> O3P
{ 26} O1D     + [H2O]             --> 2.000*HO
{ 27} O3      + NO                --> NO2
{ 28} O3      + HO                --> HO2
{ 29} O3      + HO2               --> HO
{ 30} HO2     + NO                --> NO2     +  HO
{ 31} HO2     + NO2               --> HNO4
{ 32} HNO4                        --> HO2     +  NO2
{ 33} HO2     + HO2               --> H2O2
{ 34} HO2     + HO2     + [H2O]   --> H2O2
{ 35} H2O2    + HO                --> HO2
{ 36} NO      + HO                --> HONO
{ 37} NO      + NO      + [O2]    --> 2.000*NO2
{ 38} O3      + NO2               --> NO3
{ 39} NO3     + NO                --> 2.000*NO2
{ 40} NO3     + NO2               --> NO      +  NO2
{ 41} NO3     + HO2               --> HNO3
{ 42} NO3     + NO2               --> N2O5
{ 43} N2O5                        --> NO2     +  NO3
{ 44} N2O5    + [H2O]             --> 2.000*HNO3
{ 45} HO      + NO2               --> HNO3
{ 46} HO      + HNO3              --> NO3
{ 47} HO      + HNO4              --> NO2
{ 48} HO      + HO2               -->
{ 49} HO      + SO2               --> SULF    +  HO2     +  SULAER
{ 50} CO      + HO                --> HO2
{ 51} HO                          --> MO2
{ 52} ETH     + HO                --> ETHP
{ 53} HC3     + HO                --> 0.830*HC3P  + 0.170*HO2     + 0.009*HCHO
                                    + 0.075*ALD   + 0.025*KET
{ 54} HC5     + HO                --> HC5P    + 0.250*XO2
{ 55} HC8     + HO                --> HC8P    + 0.750*XO2     +  HC8AER
{ 56} OL2     + HO                --> OL2P
{ 57} OLT     + HO                --> OLTP
{ 58} OLI     + HO                --> OLIP    +  OLIAER
{ 59} TOL     + HO                --> 0.750*TOLP  + 0.250*CSL     + 0.250*HO2
                                    +  TOLAER
{ 60} XYL     + HO                --> 0.830*XYLP  + 0.170*CSL     + 0.170*HO2
                                    +  XYLAER
{ 61} CSL     + HO                --> 0.100*HO2   + 0.900*XO2     + 0.900*TCO3
                                    +  CSLAER
{ 62} CSL     + HO                --> CSL
{ 63} HCHO    + HO                --> HO2     +  CO
{ 64} ALD     + HO                --> ACO3
{ 65} KET     + HO                --> KETP
{ 66} GLY     + HO                --> HO2     + 2.000*CO
{ 67} MGLY    + HO                --> ACO3    +  CO
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
{ 68} DCB     + HO              -->         TCO3
{ 69} OP1     + HO              -->   0.500*MO2     + 0.500*HCHO    + 0.500*HO
{ 70} OP2     + HO              -->   0.500*HC3P    + 0.500*ALD     + 0.500*HO
{ 71} PAA     + HO              -->         ACO3
{ 72} PAN     + HO              -->         HCHO    +       NO3     +       XO2
{ 73} ONIT    + HO              -->         HC3P    +       NO2
{ 74} ISO     + HO              -->         OLTP
{ 75} ACO3    + NO2             -->         PAN
{ 76} PAN                       -->         ACO3    +       NO2
{ 77} TCO3    + NO2             -->         TPAN
{ 78} TPAN                      -->         TCO3    +       NO2
{ 79} MO2     + NO              -->         HCHO    +       HO2     +       NO2
{ 80} HC3P    + NO              -->   0.750*ALD     + 0.250*KET     + 0.090*HCHO
                                    + 0.036*ONIT    + 0.964*NO2     + 0.964*HO2
{ 81} HC5P    + NO              -->   0.380*ALD     + 0.690*KET     + 0.080*ONIT
                                    + 0.920*NO2     + 0.920*HO2
{ 82} HC8P    + NO              -->   0.350*ALD     + 1.060*KET     + 0.040*HCHO
                                    + 0.240*ONIT    + 0.760*NO2     + 0.760*HO2
{ 83} OL2P    + NO              -->   1.600*HCHO    +       HO2     +       NO2
                                    + 0.200*ALD
{ 84} OLTP    + NO              -->         ALD     +       HCHO    +       HO2
                                    +       NO2
{ 85} OLIP    + NO              -->         HO2     + 1.450*ALD     + 0.280*HCHO
                                    + 0.100*KET     +       NO2
{ 86} ACO3    + NO              -->         MO2     +       NO2
{ 87} TCO3    + NO              -->         NO2     + 0.920*HO2     + 0.890*GLY
                                    + 0.110*MGLY    + 0.050*ACO3    + 0.950*CO
                                    + 2.000*XO2
{ 88} TOLP    + NO              -->         NO2     +       HO2     + 0.170*MGLY
                                    + 0.160*GLY     + 0.700*DCB
{ 89} XYLP    + NO              -->         NO2     +       HO2     + 0.450*MGLY
                                    + 0.806*DCB
{ 90} ETHP    + NO              -->         ALD     +       HO2     +       NO2
{ 91} KETP    + NO              -->         MGLY    +       NO2     +       HO2
{ 92} OLN     + NO              -->         HCHO    +       ALD     + 2.000*NO2
{ 93} HCHO    + NO3             -->         HO2     +       HNO3    +       CO
{ 94} ALD     + NO3             -->         ACO3    +       HNO3
{ 95} GLY     + NO3             -->         HNO3    +       HO2     + 2.000*CO
{ 96} MGLY    + NO3             -->         HNO3    +       ACO3    +       CO
{ 97} DCB     + NO3             -->         HNO3    +       TCO3
{ 98} CSL     + NO3             -->         HNO3    +       XNO2    + 0.500*CSL
                                    + 0.500*CSLAER
{ 99} OL2     + NO3             -->         OLN
{100} OLT     + NO3             -->         OLN
{101} OLI     + NO3             -->         OLN     +       OLIAER
{102} ISO     + NO3             -->         OLN
{103} OL2     + O3              -->         HCHO    + 0.400*ORA1    + 0.420*CO
                                    + 0.120*HO2
{104} OLT     + O3              -->   0.530*HCHO    + 0.500*ALD     + 0.330*CO
                                    + 0.200*ORA1    + 0.200*ORA2    + 0.230*HO2
                                    + 0.220*MO2     + 0.100*HO
{105} OLI     + O3              -->   0.180*HCHO    + 0.720*ALD     + 0.100*KET
                                    + 0.230*CO      + 0.060*ORA1    + 0.290*ORA2
                                    + 0.260*HO2     + 0.140*HO      + 0.310*MO2
                                    +       OLIAER
{106} ISO     + O3              -->   0.530*HCHO    + 0.500*ALD     + 0.330*CO
                                    + 0.200*ORA1    + 0.200*ORA2    + 0.230*HO2
                                    + 0.220*MO2     + 0.100*HO
{107} HO2     + MO2             -->         OP1
{108} HO2     + ETHP            -->         OP2
{109} HO2     + HC3P            -->         OP2
{110} HO2     + HC5P            -->         OP2
{111} HO2     + HC8P            -->         OP2
{112} HO2     + OL2P            -->         OP2
{113} HO2     + OLTP            -->         OP2
{114} HO2     + OLIP            -->         OP2
{115} HO2     + KETP            -->         OP2
{116} HO2     + ACO3            -->         PAA
{117} HO2     + TOLP            -->         OP2
{118} HO2     + XYLP            -->         OP2
{119} HO2     + TCO3            -->         OP2
{120} HO2     + OLN             -->         ONIT
{121} MO2     + MO2             -->   1.500*HCHO    +       HO2
{122} MO2     + ETHP            -->   0.750*HCHO    +       HO2     + 0.750*ALD
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
{123} MO2     + HC3P              -->   0.840*HCHO    + 0.770*ALD     + 0.260*KET
                                    +       HO2
{124} MO2     + HC5P              -->   0.770*HCHO    + 0.410*ALD     + 0.750*KET
                                    +       HO2
{125} MO2     + HC8P              -->   0.800*HCHO    + 0.460*ALD     + 1.390*KET
                                    +       HO2
{126} MO2     + OL2P              -->   1.550*HCHO    + 0.350*ALD     +       HO2
{127} MO2     + OLTP              -->   1.250*HCHO    + 0.750*ALD     +       HO2
{128} MO2     + OLIP              -->   0.890*HCHO    + 0.725*ALD     +       HO2
                                    + 0.550*KET
{129} MO2     + KETP              -->   0.750*HCHO    + 0.750*MGLY    +       HO2
{130} MO2     + ACO3              -->         HCHO    + 0.500*HO2     + 0.500*MO2
                                    + 0.500*ORA2
{131} MO2     + TOLP              -->         HCHO    + 0.170*MGLY    + 0.160*GLY
                                    + 0.700*DCB     + 2.000*HO2
{132} MO2     + XYLP              -->         HCHO    + 0.450*MGLY    + 0.806*DCB
                                    + 2.000*HO2
{133} MO2     + TCO3              -->   0.500*HCHO    + 0.445*GLY     + 0.055*MGLY
                                    + 0.500*ORA2    + 0.025*ACO3    + 0.460*HO2
                                    + 0.475*CO      +       XO2
{134} MO2     + OLN               -->   1.750*HCHO    + 0.500*HO2     +       ALD
                                    +       NO2
{135} ETHP    + ACO3              -->         ALD     + 0.500*HO2     + 0.500*MO2
                                    + 0.500*ORA2
{136} HC3P    + ACO3              -->   0.770*ALD     + 0.260*KET     + 0.500*HO2
                                    + 0.500*MO2     + 0.500*ORA2
{137} HC5P    + ACO3              -->   0.410*ALD     + 0.750*KET     + 0.500*HO2
                                    + 0.500*MO2     + 0.500*ORA2
{138} HC8P    + ACO3              -->   0.460*ALD     + 1.390*KET     + 0.500*HO2
                                    + 0.500*MO2     + 0.500*ORA2
{139} OL2P    + ACO3              -->   0.800*HCHO    + 0.600*ALD     + 0.500*HO2
                                    + 0.500*MO2     + 0.500*ORA2
{140} OLTP    + ACO3              -->         ALD     + 0.500*HCHO    + 0.500*HO2
                                    + 0.500*MO2     + 0.500*ORA2
{141} OLIP    + ACO3              -->   0.725*ALD     + 0.550*KET     + 0.140*HCHO
                                    + 0.500*HO2     + 0.500*MO2     + 0.500*ORA2
{142} KETP    + ACO3              -->         MGLY    + 0.500*HO2     + 0.500*MO2
                                    + 0.500*ORA2
{143} ACO3    + ACO3              -->   2.000*MO2
{144} ACO3    + TOLP              -->         MO2     + 0.170*MGLY    + 0.160*GLY
                                    + 0.700*DCB     +       HO2
{145} ACO3    + XYLP              -->         MO2     + 0.450*MGLY    + 0.806*DCB
                                    +       HO2
{146} ACO3    + TCO3              -->         MO2     + 0.920*HO2     + 0.890*GLY
                                    + 0.110*MGLY    + 0.050*ACO3    + 0.950*CO
                                    + 2.000*XO2
{147} ACO3    + OLN               -->         HCHO    +       ALD     + 0.500*ORA2
                                    +       NO2     + 0.500*MO2
{148} OLN     + OLN               -->   2.000*HCHO    + 2.000*ALD     + 2.000*NO2
{149} XO2     + HO2               -->         OP2
{150} XO2     + MO2               -->         HCHO    +       HO2
{151} XO2     + ACO3              -->         MO2
{152} XO2     + XO2               -->
{153} XO2     + NO                -->         NO2
{154} XNO2    + NO2               -->         ONIT
{155} XNO2    + HO2               -->         OP2
{156} XNO2    + MO2               -->         HCHO    +       HO2
{157} XNO2    + ACO3              -->         MO2
{158} XNO2    + XNO2              -->
{159} TERP    + HO                -->         TERPAER +       HO
{160} TERP    + NO3               -->         TERPAER +       NO3
{161} TERP    + O3                -->         TERPAER +       O3
>--------------------------------------------------------------------------------<

Rate Expression                                                  Rate Constant
================================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                            {1.68671E-12}
k( 36) is a falloff expression using:                             {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                            {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                            {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                            {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                            {4.03072E-16}
k( 41) =  2.5000E-12                                              {2.50000E-12}
k( 42) is a falloff expression using:                             {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
k( 44) =  2.0000E-21                                              {2.00000E-21}
k( 45) is a falloff expression using:                             {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 46) is a special rate expression of the form:                  {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 47) =  1.3000E-12 * exp(   380.0/T)                            {4.65309E-12}
k( 48) =  4.6000E-11 * exp(   230.0/T)                            {9.95294E-11}
k( 49) is a falloff expression using:                             {8.88848E-13}
   k0   =  3.0000E-31 * (T/300)**(-3.30)
   kinf =  1.5000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                       {2.40000E-13}
k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)         {3.80672E-01}
k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)         {2.74210E-13}
k( 53) =  1.5900E-11 * exp(  -540.0/T)                            {2.59669E-12}
k( 54) =  1.7300E-11 * exp(  -380.0/T)                            {4.83334E-12}
k( 55) =  3.6400E-11 * exp(  -380.0/T)                            {1.01696E-11}
k( 56) =  2.1500E-12 * exp(   411.0/T)                            {8.53916E-12}
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
k( 57) =  5.3200E-12 * exp(   504.0/T)                          {2.88684E-11}
k( 58) =  1.0700E-11 * exp(   549.0/T)                          {6.75269E-11}
k( 59) =  2.1000E-12 * exp(   322.0/T)                          {6.18715E-12}
k( 60) =  1.8900E-11 * exp(   116.0/T)                          {2.78943E-11}
k( 61) =  4.0000E-11                                            {4.00000E-11}
k( 62) =  9.0000E-01 * k( 61)                                   {3.60000E-11}
k( 63) =  9.0000E-12                                            {9.00000E-12}
k( 64) =  6.8700E-12 * exp(   256.0/T)                          {1.62197E-11}
k( 65) =  1.2000E-11 * exp(  -745.0/T)                          {9.85020E-13}
k( 66) =  1.1500E-11                                            {1.15000E-11}
k( 67) =  1.7000E-11                                            {1.70000E-11}
k( 68) =  2.8000E-11                                            {2.80000E-11}
k( 69) =  1.0000E-11                                            {1.00000E-11}
k( 70) =  1.0000E-11                                            {1.00000E-11}
k( 71) =  1.0000E-11                                            {1.00000E-11}
k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)       {1.37105E-13}
k( 73) =  1.5500E-11 * exp(  -540.0/T)                          {2.53137E-12}
k( 74) =  2.5500E-11 * exp(   409.0/T)                          {1.00601E-10}
k( 75) =  2.8000E-12 * exp(   181.0/T)                          {5.13974E-12}
k( 76) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 77) =  4.7000E-12                                            {4.70000E-12}
k( 78) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 79) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 80) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 81) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 82) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 83) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 84) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 85) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 86) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 87) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 88) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 89) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 90) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 91) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 92) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 93) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 94) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 95) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 96) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 97) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 98) =  2.2000E-11                                            {2.20000E-11}
k( 99) =  2.0000E-12 * exp( -2923.0/T)                          {1.09940E-16}
k(100) =  1.0000E-11 * exp( -1895.0/T)                          {1.73099E-14}
k(101) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k(102) =  5.8100E-13                                            {5.81000E-13}
k(103) =  1.2000E-14 * exp( -2633.0/T)                          {1.74559E-18}
k(104) =  1.3200E-14 * exp( -2105.0/T)                          {1.12933E-17}
k(105) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
k(106) =  1.2300E-14 * exp( -2013.0/T)                          {1.43295E-17}
k(107) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(118) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(119) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(120) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(121) =  1.9000E-13 * exp(   220.0/T)                          {3.97533E-13}
k(122) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(123) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(124) =  3.4000E-14 * exp(   220.0/T)                          {7.11376E-14}
k(125) =  2.9000E-14 * exp(   220.0/T)                          {6.06762E-14}
k(126) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(127) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(128) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
```

Table 8A-8. RADM2_AE and RADM2_AE_AQ Mechanisms

```
k(131) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(132) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(133) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(134) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(135) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(136) =  1.0000E-13 * exp(   220.0/T)                          {2.09228E-13}
k(137) =  8.4000E-14 * exp(   220.0/T)                          {1.75752E-13}
k(138) =  7.2000E-14 * exp(   220.0/T)                          {1.50644E-13}
k(139) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(140) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(141) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(145) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(146) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(147) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(148) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(149) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(150) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(151) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(152) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(153) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(154) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(155) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(156) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(157) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(158) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(159) =  1.0000E+00 * k( 58)                                   {6.75269E-11}
k(160) =  1.0000E+00 * k(101)                                   {1.22539E-12}
k(161) =  1.0000E+00 * k(105)                                   {1.61125E-16}
================================================================================
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Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
 Reaction List
>-----------------------------------------------------------------------------------------<
{  1} NO2      + hv                  -->         O3P      +       NO
{  2} O3       + hv                  -->         O1D
{  3} O3       + hv                  -->         O3P
{  4} HONO     + hv                  -->         HO       +       NO
{  5} HNO3     + hv                  -->         HO       +       NO2
{  6} HNO4     + hv                  -->         HO2      +       NO2
{  7} NO3      + hv                  -->         NO
{  8} NO3      + hv                  -->         NO2      +       O3P
{  9} H2O2     + hv                  -->   2.000*HO
{ 10} HCHO     + hv                  -->         CO
{ 11} HCHO     + hv                  -->         HO2      +       HO2      +       CO
{ 12} ALD      + hv                  -->         MO2      +       HO2      +       CO
{ 13} OP1      + hv                  -->         HCHO     +       HO2      +       HO
{ 14} OP2      + hv                  -->         ALD      +       HO2      +       HO
{ 15} PAA      + hv                  -->         MO2      +       HO
{ 16} KET      + hv                  -->         ACO3     +       ETHP
{ 17} GLY      + hv                  -->   0.130*HCHO     + 1.870*CO
{ 18} GLY      + hv                  -->   0.450*HCHO     + 1.550*CO       + 0.800*HO2
{ 19} MGLY     + hv                  -->         ACO3     +       HO2      +       CO
{ 20} DCB      + hv                  -->   0.980*HO2      + 0.020*ACO3     +       TCO3
{ 21} ONIT     + hv                  -->   0.200*ALD      + 0.800*KET      +       HO2
                                           +       NO2
{ 22} O3P      + [M]      + [O2]     -->         O3
{ 23} O3P      + NO2                 -->         NO
{ 24} O1D      + [N2]                -->         O3P
{ 25} O1D      + [O2]                -->         O3P
{ 26} O1D      + [H2O]               -->   2.000*HO
{ 27} O3       + NO                  -->         NO2
{ 28} O3       + HO                  -->         HO2
{ 29} O3       + HO2                 -->         HO
{ 30} HO2      + NO                  -->         NO2      +       HO
{ 31} HO2      + NO2                 -->         HNO4
{ 32} HNO4                           -->         HO2      +       NO2
{ 33} HO2      + HO2                 -->         H2O2
{ 34} HO2      + HO2      + [H2O]    -->         H2O2
{ 35} H2O2     + HO                  -->         HO2
{ 36} NO       + HO                  -->         HONO
{ 37} NO       + NO       + [O2]     -->   2.000*NO2
{ 38} O3       + NO2                 -->         NO3
{ 39} NO3      + NO                  -->   2.000*NO2
{ 40} NO3      + NO2                 -->         NO       +       NO2
{ 41} NO3      + HO2                 -->         HNO3
{ 42} NO3      + NO2                 -->         N2O5
{ 43} N2O5                           -->         NO2      +       NO3
{ 44} N2O5     + [H2O]               -->   2.000*HNO3
{ 45} HO       + NO2                 -->         HNO3
{ 46} HO       + HNO3                -->         NO3
{ 47} HO       + HNO4                -->         NO2
{ 48} HO       + HO2                 -->
{ 49} HO       + SO2                 -->         SULF     +       HO2
{ 50} CO       + HO                  -->         HO2
{ 51} HO                             -->         MO2
{ 52} ETH      + HO                  -->         ETHP
{ 53} HC3      + HO                  -->   0.830*HC3P     + 0.170*HO2      + 0.009*HCHO
                                         + 0.075*ALD      + 0.025*KET
{ 54} HC5      + HO                  -->         HC5P     + 0.250*XO2
{ 55} HC8      + HO                  -->         HC8P     + 0.750*XO2
{ 56} OL2      + HO                  -->         OL2P
{ 57} OLT      + HO                  -->         OLTP
{ 58} OLI      + HO                  -->         OLIP
{ 59} TOL      + HO                  -->   0.750*TOLP     + 0.250*CSL      + 0.250*HO2
{ 60} XYL      + HO                  -->   0.830*XYLP     + 0.170*CSL      + 0.170*HO2
{ 61} CSL      + HO                  -->   0.100*HO2      + 0.900*XO2      + 0.900*TCO3
{ 62} CSL      + HO                  -->         CSL
{ 63} HCHO     + HO                  -->         HO2      +       CO
{ 64} ALD      + HO                  -->         ACO3
{ 65} KET      + HO                  -->         KETP
{ 66} GLY      + HO                  -->         HO2      + 2.000*CO
{ 67} MGLY     + HO                  -->         ACO3     +       CO
{ 68} DCB      + HO                  -->         TCO3
{ 69} OP1      + HO                  -->   0.500*MO2      + 0.500*HCHO     + 0.500*HO
{ 70} OP2      + HO                  -->   0.500*HC3P     + 0.500*ALD      + 0.500*HO
```

Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
{ 71} PAA      + HO                --> 1.000*ACO3
{ 72} PAN      + HO                --> 1.000*HCHO     + 1.000*NO3      + 1.000*XO2
{ 73} ONIT     + HO                --> 1.000*HC3P     + 1.000*NO2
{ 74} ACO3     + NO2               --> 1.000*PAN
{ 75} PAN                          --> 1.000*ACO3     + 1.000*NO2
{ 76} TCO3     + NO2               --> 1.000*TPAN
{ 77} TPAN                         --> 1.000*TCO3     + 1.000*NO2
{ 78} MO2      + NO                --> 1.000*HCHO     + 1.000*HO2      + 1.000*NO2
{ 79} HC3P     + NO                --> 0.750*ALD      + 0.250*KET      + 0.090*HCHO
                                     + 0.036*ONIT     + 0.964*NO2      + 0.964*HO2
{ 80} HC5P     + NO                --> 0.380*ALD      + 0.690*KET      + 0.080*ONIT
                                     + 0.920*NO2      + 0.920*HO2
{ 81} HC8P     + NO                --> 0.350*ALD      + 1.060*KET      + 0.040*HCHO
                                     + 0.240*ONIT     + 0.760*NO2      + 0.760*HO2
{ 82} OL2P     + NO                --> 1.600*HCHO     + 1.000*HO2      + 1.000*NO2
                                     + 0.200*ALD
{ 83} OLTP     + NO                --> 1.000*ALD      + 1.000*HCHO     + 1.000*HO2
                                     + 1.000*NO2
{ 84} OLIP     + NO                --> 1.000*HO2      + 1.450*ALD      + 0.280*HCHO
                                     + 0.100*KET      + 1.000*NO2
{ 85} ACO3     + NO                --> 1.000*MO2      + 1.000*NO2
{ 86} TCO3     + NO                --> 1.000*NO2      + 0.920*HO2      + 0.890*GLY
                                     + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                     + 2.000*XO2
{ 87} TOLP     + NO                --> 1.000*NO2      + 1.000*HO2      + 0.170*MGLY
                                     + 0.160*GLY      + 0.700*DCB
{ 88} XYLP     + NO                --> 1.000*NO2      + 1.000*HO2      + 0.450*MGLY
                                     + 0.806*DCB
{ 89} ETHP     + NO                --> 1.000*ALD      + 1.000*HO2      + 1.000*NO2
{ 90} KETP     + NO                --> 1.000*MGLY     + 1.000*NO2      + 1.000*HO2
{ 91} OLN      + NO                --> 1.000*HCHO     + 1.000*ALD      + 2.000*NO2
{ 92} HCHO     + NO3               --> 1.000*HO2      + 1.000*HNO3     + 1.000*CO
{ 93} ALD      + NO3               --> 1.000*ACO3     + 1.000*HNO3
{ 94} GLY      + NO3               --> 1.000*HNO3     + 1.000*HO2      + 2.000*CO
{ 95} MGLY     + NO3               --> 1.000*HNO3     + 1.000*ACO3     + 1.000*CO
{ 96} DCB      + NO3               --> 1.000*HNO3     + 1.000*TCO3
{ 97} CSL      + NO3               --> 1.000*HNO3     + 1.000*XNO2     + 0.500*CSL
{ 98} OL2      + NO3               --> 1.000*OLN
{ 99} OLT      + NO3               --> 1.000*OLN
{100} OLI      + NO3               --> 1.000*OLN
{101} OL2      + O3                --> 1.000*HCHO     + 0.400*ORA1     + 0.420*CO
                                     + 0.120*HO2
{102} OLT      + O3                --> 0.530*HCHO     + 0.500*ALD      + 0.330*CO
                                     + 0.200*ORA1     + 0.200*ORA2     + 0.230*HO2
                                     + 0.220*MO2      + 0.100*HO
{103} OLI      + O3                --> 0.180*HCHO     + 0.720*ALD      + 0.100*KET
                                     + 0.230*CO       + 0.060*ORA1     + 0.290*ORA2
                                     + 0.260*HO2      + 0.140*HO       + 0.310*MO2
{104} HO2      + MO2               --> 1.000*OP1
{105} HO2      + ETHP              --> 1.000*OP2
{106} HO2      + HC3P              --> 1.000*OP2
{107} HO2      + HC5P              --> 1.000*OP2
{108} HO2      + HC8P              --> 1.000*OP2
{109} HO2      + OL2P              --> 1.000*OP2
{110} HO2      + OLTP              --> 1.000*OP2
{111} HO2      + OLIP              --> 1.000*OP2
{112} HO2      + KETP              --> 1.000*OP2
{113} HO2      + ACO3              --> 1.000*PAA
{114} HO2      + TOLP              --> 1.000*OP2
{115} HO2      + XYLP              --> 1.000*OP2
{116} HO2      + TCO3              --> 1.000*OP2
{117} HO2      + OLN               --> 1.000*ONIT
{118} MO2      + MO2               --> 1.500*HCHO     + 1.000*HO2
{119} MO2      + ETHP              --> 0.750*HCHO     + 1.000*HO2      + 0.750*ALD
{120} MO2      + HC3P              --> 0.840*HCHO     + 0.770*ALD      + 0.260*KET
                                     + 1.000*HO2
{121} MO2      + HC5P              --> 0.770*HCHO     + 0.410*ALD      + 0.750*KET
                                     + 1.000*HO2
{122} MO2      + HC8P              --> 0.800*HCHO     + 0.460*ALD      + 1.390*KET
                                     + 1.000*HO2
{123} MO2      + OL2P              --> 1.550*HCHO     + 0.350*ALD      + 1.000*HO2
{124} MO2      + OLTP              --> 1.250*HCHO     + 0.750*ALD      + 1.000*HO2
{125} MO2      + OLIP              --> 0.890*HCHO     + 0.725*ALD      + 1.000*HO2
                                     + 0.550*KET
```

Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
{126} MO2      + KETP               -->   0.750*HCHO     + 0.750*MGLY     +       HO2
{127} MO2      + ACO3               -->         HCHO     + 0.500*HO2      + 0.500*MO2
                                         + 0.500*ORA2
{128} MO2      + TOLP               -->         HCHO     + 0.170*MGLY     + 0.160*GLY
                                         + 0.700*DCB      + 2.000*HO2
{129} MO2      + XYLP               -->         HCHO     + 0.450*MGLY     + 0.806*DCB
                                         + 2.000*HO2
{130} MO2      + TCO3               -->   0.500*HCHO     + 0.445*GLY      + 0.055*MGLY
                                         + 0.500*ORA2     + 0.025*ACO3     + 0.460*HO2
                                         + 0.475*CO       +       XO2
{131} MO2      + OLN                -->   1.750*HCHO     + 0.500*HO2      +       ALD
                                         +       NO2
{132} ETHP     + ACO3               -->         ALD      + 0.500*HO2      + 0.500*MO2
                                         + 0.500*ORA2
{133} HC3P     + ACO3               -->   0.770*ALD      + 0.260*KET      + 0.500*HO2
                                         + 0.500*MO2      + 0.500*ORA2
{134} HC5P     + ACO3               -->   0.410*ALD      + 0.750*KET      + 0.500*HO2
                                         + 0.500*MO2      + 0.500*ORA2
{135} HC8P     + ACO3               -->   0.460*ALD      + 1.390*KET      + 0.500*HO2
                                         + 0.500*MO2      + 0.500*ORA2
{136} OL2P     + ACO3               -->   0.800*HCHO     + 0.600*ALD      + 0.500*HO2
                                         + 0.500*MO2      + 0.500*ORA2
{137} OLTP     + ACO3               -->         ALD      + 0.500*HCHO     + 0.500*HO2
                                         + 0.500*MO2      + 0.500*ORA2
{138} OLIP     + ACO3               -->   0.725*ALD      + 0.550*KET      + 0.140*HCHO
                                         + 0.500*HO2      + 0.500*MO2      + 0.500*ORA2
{139} KETP     + ACO3               -->         MGLY     + 0.500*HO2      + 0.500*MO2
                                         + 0.500*ORA2
{140} ACO3     + ACO3               -->   2.000*MO2
{141} ACO3     + TOLP               -->         MO2      + 0.170*MGLY     + 0.160*GLY
                                         + 0.700*DCB      +       HO2
{142} ACO3     + XYLP               -->         MO2      + 0.450*MGLY     + 0.806*DCB
                                         +       HO2
{143} ACO3     + TCO3               -->         MO2      + 0.920*HO2      + 0.890*GLY
                                         + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                         + 2.000*XO2
{144} ACO3     + OLN                -->         HCHO     +       ALD      + 0.500*ORA2
                                         +       NO2      + 0.500*MO2
{145} OLN      + OLN                -->   2.000*HCHO     + 2.000*ALD      + 2.000*NO2
{146} XO2      + HO2                -->         OP2
{147} XO2      + MO2                -->         HCHO     +       HO2
{148} XO2      + ACO3               -->         MO2
{149} XO2      + XO2                -->
{150} XO2      + NO                 -->         NO2
{151} XNO2     + NO2                -->         ONIT
{152} XNO2     + HO2                -->         OP2
{153} XNO2     + MO2                -->         HCHO     +       HO2
{154} XNO2     + ACO3               -->         MO2
{155} XNO2     + XNO2               -->
{156} ISO      + HO                 -->         ISO_RO2  + 0.079*XO2
{157} ISO_RO2  + NO                 -->   0.088*ONIT     + 0.912*NO2      + 0.912*HO2
                                         + 0.912*ISOPROD  + 0.629*HCHO
{158} ISO_RO2  + HO2                -->         OP2
{159} ISO_RO2  + ACO3               -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                         +       ISOPROD
{160} ISO_RO2  + MO2                -->   0.500*HCHO     + 0.500*HO2      +       ISOPROD
{161} ISO      + O3                 -->   0.600*HCHO     + 0.650*ISOPROD  + 0.390*ORA1
                                         + 0.270*HO       + 0.070*HO2      + 0.070*CO
                                         + 0.200*XO2      + 0.200*ACO3     + 0.150*ALD
{162} ISO      + O3P                -->   0.750*ISOPROD  + 0.250*ACO3     + 0.250*HCHO
                                         + 0.250*MO2
{163} ISO      + NO3                -->         ISON_RO2
{164} ISON_RO2 + NO                 -->         NO2      + 0.800*ALD      + 0.800*ONIT
                                         + 0.800*HO2      + 0.200*ISOPROD  + 0.200*NO2
{165} ISON_RO2 + HO2                -->         ONIT
{166} ISON_RO2 + ACO3               -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                         +       ALD      +       ONIT
{167} ISON_RO2 + MO2                -->   0.500*HCHO     + 0.500*HO2      +       ALD
                                         +       ONIT
{168} ISOPROD  + HO                 -->   0.500*ACO3     + 0.500*IP_RO2   + 0.200*XO2
{169} IP_RO2   + NO                 -->         NO2      +       HO2      + 0.590*CO
                                         + 0.550*ALD      + 0.250*HCHO     + 0.080*GLY
                                         + 0.340*MGLY     + 0.630*KET
{170} IP_RO2   + HO2                -->         OP2
```

Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
{171} IP_RO2   + ACO3               -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       + 0.500*ALD      + 0.500*KET
{172} IP_RO2   + MO2                -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                       + 0.500*KET
{173} ISOPROD  + O3                 -->   0.268*HO       + 0.100*HO2      + 0.114*ACO3
                                       + 0.054*MO2      + 0.070*XO2      + 0.155*CO
                                       + 0.146*HCHO     + 0.020*ALD      + 0.010*GLY
                                       + 0.850*MGLY     + 0.090*KET      + 0.462*ORA1
{174} ISOPROD  + hv                 -->   0.970*ACO3     + 0.333*HO2      + 0.700*MO2
                                       + 0.200*HCHO     + 0.333*CO       + 0.067*ALD
                                       + 0.033*KET
{175} ISOPROD  + NO3                -->   0.075*ACO3     + 0.075*HNO3     + 0.643*CO
                                       + 0.282*HCHO     + 0.925*ONIT     + 0.282*ALD
                                       + 0.925*HO2      + 0.925*XO2
>--------------------------------------------------------------------------------------<


Rate Expression                                                              Rate Constant
==============================================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                            {1.68671E-12}
k( 36) is a falloff expression using:                             {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                            {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                            {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                            {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                            {4.03072E-16}
k( 41) =  2.5000E-12                                              {2.50000E-12}
k( 42) is a falloff expression using:                             {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
```

Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
    kinf =  1.5000E-12 * (T/300)**(-0.50)
    F =  0.60,  n =  1.00
 k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
 k( 44) =  2.0000E-21                                             {2.00000E-21}
 k( 45) is a falloff expression using:                            {1.14885E-11}
    k0   =  2.6000E-30 * (T/300)**(-3.20)
    kinf =  2.4000E-11 * (T/300)**(-1.30)
    F =  0.60,  n =  1.00
 k( 46) is a special rate expression of the form:                 {1.47236E-13}
    k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
    k0 =  7.2000E-15 * exp(   785.0/T)
    k2 =  4.1000E-16 * exp(  1440.0/T)
    k3 =  1.9000E-33 * exp(   725.0/T)
 k( 47) =  1.3000E-12 * exp(   380.0/T)                           {4.65309E-12}
 k( 48) =  4.6000E-11 * exp(   230.0/T)                           {9.95294E-11}
 k( 49) is a falloff expression using:                            {8.88848E-13}
    k0   =  3.0000E-31 * (T/300)**(-3.30)
    kinf =  1.5000E-12 * (T/300)**( 0.00)
    F =  0.60,  n =  1.00
 k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                      {2.40000E-13}
 k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)        {3.80672E-01}
 k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)        {2.74210E-13}
 k( 53) =  1.5900E-11 * exp(  -540.0/T)                           {2.59669E-12}
 k( 54) =  1.7300E-11 * exp(  -380.0/T)                           {4.83334E-12}
 k( 55) =  3.6400E-11 * exp(  -380.0/T)                           {1.01696E-11}
 k( 56) =  2.1500E-12 * exp(   411.0/T)                           {8.53916E-12}
 k( 57) =  5.3200E-12 * exp(   504.0/T)                           {2.88684E-11}
 k( 58) =  1.0700E-11 * exp(   549.0/T)                           {6.75269E-11}
 k( 59) =  2.1000E-12 * exp(   322.0/T)                           {6.18715E-12}
 k( 60) =  1.8900E-11 * exp(   116.0/T)                           {2.78943E-11}
 k( 61) =  4.0000E-11                                             {4.00000E-11}
 k( 62) =  9.0000E-01 * k( 61)                                    {3.60000E-11}
 k( 63) =  9.0000E-12                                             {9.00000E-12}
 k( 64) =  6.8700E-12 * exp(   256.0/T)                           {1.62197E-11}
 k( 65) =  1.2000E-11 * exp(  -745.0/T)                           {9.85020E-13}
 k( 66) =  1.1500E-11                                             {1.15000E-11}
 k( 67) =  1.7000E-11                                             {1.70000E-11}
 k( 68) =  2.8000E-11                                             {2.80000E-11}
 k( 69) =  1.0000E-11                                             {1.00000E-11}
 k( 70) =  1.0000E-11                                             {1.00000E-11}
 k( 71) =  1.0000E-11                                             {1.00000E-11}
 k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)        {1.37105E-13}
 k( 73) =  1.5500E-11 * exp(  -540.0/T)                           {2.53137E-12}
 k( 74) =  2.8000E-12 * exp(   181.0/T)                           {5.13974E-12}
 k( 75) =  1.9500E+16 * exp(-13543.0/T)                           {3.57235E-04}
 k( 76) =  4.7000E-12                                             {4.70000E-12}
 k( 77) =  1.9500E+16 * exp(-13543.0/T)                           {3.57235E-04}
 k( 78) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 79) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 80) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 81) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 82) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 83) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 84) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 85) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 86) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 87) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 88) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 89) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 90) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 91) =  4.2000E-12 * exp(   180.0/T)                           {7.68378E-12}
 k( 92) =  6.0000E-13 * exp( -2058.0/T)                           {6.01030E-16}
 k( 93) =  1.4000E-12 * exp( -1900.0/T)                           {2.38307E-15}
 k( 94) =  6.0000E-13 * exp( -2058.0/T)                           {6.01030E-16}
 k( 95) =  1.4000E-12 * exp( -1900.0/T)                           {2.38307E-15}
 k( 96) =  1.4000E-12 * exp( -1900.0/T)                           {2.38307E-15}
 k( 97) =  2.2000E-11                                             {2.20000E-11}
 k( 98) =  2.0000E-12 * exp( -2923.0/T)                           {1.09940E-16}
 k( 99) =  1.0000E-11 * exp( -1895.0/T)                           {1.73099E-14}
 k(100) =  3.2300E-11 * exp(  -975.0/T)                           {1.22539E-12}
 k(101) =  1.2000E-14 * exp( -2633.0/T)                           {1.74559E-18}
 k(102) =  1.3200E-14 * exp( -2105.0/T)                           {1.12933E-17}
 k(103) =  7.2900E-15 * exp( -1136.0/T)                           {1.61125E-16}
 k(104) =  7.7000E-14 * exp(  1300.0/T)                           {6.04038E-12}
```

Table 8A-9. RADM2_CIS1 and RADM2_CIS1_AQ Mechanisms

```
k(105) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(106) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(107) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(118) =  1.9000E-13 * exp(   220.0/T)                          {3.97533E-13}
k(119) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(120) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(121) =  3.4000E-14 * exp(   220.0/T)                          {7.11376E-14}
k(122) =  2.9000E-14 * exp(   220.0/T)                          {6.06762E-14}
k(123) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(124) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(125) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(126) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(127) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(128) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(131) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(132) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(133) =  1.0000E-13 * exp(   220.0/T)                          {2.09228E-13}
k(134) =  8.4000E-14 * exp(   220.0/T)                          {1.75752E-13}
k(135) =  7.2000E-14 * exp(   220.0/T)                          {1.50644E-13}
k(136) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(137) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(138) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(139) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(140) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(141) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(145) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(146) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(147) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(148) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(149) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(150) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(151) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(152) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(153) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(154) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(155) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(156) =  2.5400E-11 * (T/300)**( 1.00) * exp(   407.6/T)       {9.90719E-11}
k(157) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(158) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(159) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(160) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(161) =  7.8600E-15 * (T/300)**( 1.00) * exp( -1912.2/T)       {1.27569E-17}
k(162) =  3.6000E-11                                            {3.60000E-11}
k(163) =  3.0300E-12 * (T/300)**( 1.00) * exp(  -447.9/T)       {6.69552E-13}
k(164) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(165) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(166) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(167) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(168) =  3.3600E-11                                            {3.36000E-11}
k(169) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(170) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(171) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(172) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(173) =  7.1100E-18                                            {7.11000E-18}
k(174) uses photo table ACROLEIN       , scaled by 3.60000E-03  {0.00000E+00}
k(175) =  1.0000E-15                                            {1.00000E-15}
================================================================================
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Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
 Reaction List
>-------------------------------------------------------------------------------------------<
{  1} NO2      + hv                  -->         O3P      +       NO
{  2} O3       + hv                  -->         O1D
{  3} O3       + hv                  -->         O3P
{  4} HONO     + hv                  -->         HO       +       NO
{  5} HNO3     + hv                  -->         HO       +       NO2
{  6} HNO4     + hv                  -->         HO2      +       NO2
{  7} NO3      + hv                  -->         NO
{  8} NO3      + hv                  -->         NO2      +       O3P
{  9} H2O2     + hv                  -->   2.000*HO
{ 10} HCHO     + hv                  -->         CO
{ 11} HCHO     + hv                  -->         HO2      +       HO2      +       CO
{ 12} ALD      + hv                  -->         MO2      +       HO2      +       CO
{ 13} OP1      + hv                  -->         HCHO     +       HO2      +       HO
{ 14} OP2      + hv                  -->         ALD      +       HO2      +       HO
{ 15} PAA      + hv                  -->         MO2      +       HO
{ 16} KET      + hv                  -->         ACO3     +       ETHP
{ 17} GLY      + hv                  -->   0.130*HCHO     + 1.870*CO
{ 18} GLY      + hv                  -->   0.450*HCHO     + 1.550*CO       + 0.800*HO2
{ 19} MGLY     + hv                  -->         ACO3     +       HO2      +       CO
{ 20} DCB      + hv                  -->   0.980*HO2      + 0.020*ACO3     +       TCO3
{ 21} ONIT     + hv                  -->   0.200*ALD      + 0.800*KET      +       HO2
                                           +       NO2
{ 22} O3P      + [M]      + [O2]     -->         O3
{ 23} O3P      + NO2                 -->         NO
{ 24} O1D      + [N2]                -->         O3P
{ 25} O1D      + [O2]                -->         O3P
{ 26} O1D      + [H2O]               -->   2.000*HO
{ 27} O3       + NO                  -->         NO2
{ 28} O3       + HO                  -->         HO2
{ 29} O3       + HO2                 -->         HO
{ 30} HO2      + NO                  -->         NO2      +       HO
{ 31} HO2      + NO2                 -->         HNO4
{ 32} HNO4                           -->         HO2      +       NO2
{ 33} HO2      + HO2                 -->         H2O2
{ 34} HO2      + HO2      + [H2O]    -->         H2O2
{ 35} H2O2     + HO                  -->         HO2
{ 36} NO       + HO                  -->         HONO
{ 37} NO       + NO       + [O2]     -->   2.000*NO2
{ 38} O3       + NO2                 -->         NO3
{ 39} NO3      + NO                  -->   2.000*NO2
{ 40} NO3      + NO2                 -->         NO       +       NO2
{ 41} NO3      + HO2                 -->         HNO3
{ 42} NO3      + NO2                 -->         N2O5
{ 43} N2O5                           -->         NO2      +       NO3
{ 44} N2O5     + [H2O]               -->   2.000*HNO3
{ 45} HO       + NO2                 -->         HNO3
{ 46} HO       + HNO3                -->         NO3
{ 47} HO       + HNO4                -->         NO2
{ 48} HO       + HO2                 -->
{ 49} HO       + SO2                 -->         SULF     +       HO2      +       SULAER
{ 50} CO       + HO                  -->         HO2
{ 51} HO                             -->         MO2
{ 52} ETH      + HO                  -->         ETHP
{ 53} HC3      + HO                  -->   0.830*HC3P     + 0.170*HO2      + 0.009*HCHO
                                         + 0.075*ALD      + 0.025*KET
{ 54} HC5      + HO                  -->         HC5P     + 0.250*XO2
{ 55} HC8      + HO                  -->         HC8P     + 0.750*XO2      +       HC8AER
{ 56} OL2      + HO                  -->         OL2P
{ 57} OLT      + HO                  -->         OLTP
{ 58} OLI      + HO                  -->         OLIP     +       OLIAER
{ 59} TOL      + HO                  -->   0.750*TOLP     + 0.250*CSL      + 0.250*HO2
                                           +       TOLAER
{ 60} XYL      + HO                  -->   0.830*XYLP     + 0.170*CSL      + 0.170*HO2
                                           +       XYLAER
{ 61} CSL      + HO                  -->   0.100*HO2      + 0.900*XO2      + 0.900*TCO3
                                           +       CSLAER
{ 62} CSL      + HO                  -->         CSL
{ 63} HCHO     + HO                  -->         HO2      +       CO
{ 64} ALD      + HO                  -->         ACO3
{ 65} KET      + HO                  -->         KETP
{ 66} GLY      + HO                  -->         HO2      + 2.000*CO
{ 67} MGLY     + HO                  -->         ACO3     +       CO
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
{ 68} DCB      + HO                --> 1.000*TCO3
{ 69} OP1      + HO                --> 0.500*MO2      + 0.500*HCHO     + 0.500*HO
{ 70} OP2      + HO                --> 0.500*HC3P     + 0.500*ALD      + 0.500*HO
{ 71} PAA      + HO                --> 1.000*ACO3
{ 72} PAN      + HO                --> 1.000*HCHO     + 1.000*NO3      + 1.000*XO2
{ 73} ONIT     + HO                --> 1.000*HC3P     + 1.000*NO2
{ 74} ACO3     + NO2               --> 1.000*PAN
{ 75} PAN                          --> 1.000*ACO3     + 1.000*NO2
{ 76} TCO3     + NO2               --> 1.000*TPAN
{ 77} TPAN                         --> 1.000*TCO3     + 1.000*NO2
{ 78} MO2      + NO                --> 1.000*HCHO     + 1.000*HO2      + 1.000*NO2
{ 79} HC3P     + NO                --> 0.750*ALD      + 0.250*KET      + 0.090*HCHO
                                     + 0.036*ONIT     + 0.964*NO2      + 0.964*HO2
{ 80} HC5P     + NO                --> 0.380*ALD      + 0.690*KET      + 0.080*ONIT
                                     + 0.920*NO2      + 0.920*HO2
{ 81} HC8P     + NO                --> 0.350*ALD      + 1.060*KET      + 0.040*HCHO
                                     + 0.240*ONIT     + 0.760*NO2      + 0.760*HO2
{ 82} OL2P     + NO                --> 1.600*HCHO     + 1.000*HO2      + 1.000*NO2
                                     + 0.200*ALD
{ 83} OLTP     + NO                --> 1.000*ALD      + 1.000*HCHO     + 1.000*HO2
                                     + 1.000*NO2
{ 84} OLIP     + NO                --> 1.000*HO2      + 1.450*ALD      + 0.280*HCHO
                                     + 0.100*KET      + 1.000*NO2
{ 85} ACO3     + NO                --> 1.000*MO2      + 1.000*NO2
{ 86} TCO3     + NO                --> 1.000*NO2      + 0.920*HO2      + 0.890*GLY
                                     + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                     + 2.000*XO2
{ 87} TOLP     + NO                --> 1.000*NO2      + 1.000*HO2      + 0.170*MGLY
                                     + 0.160*GLY      + 0.700*DCB
{ 88} XYLP     + NO                --> 1.000*NO2      + 1.000*HO2      + 0.450*MGLY
                                     + 0.806*DCB
{ 89} ETHP     + NO                --> 1.000*ALD      + 1.000*HO2      + 1.000*NO2
{ 90} KETP     + NO                --> 1.000*MGLY     + 1.000*NO2      + 1.000*HO2
{ 91} OLN      + NO                --> 1.000*HCHO     + 1.000*ALD      + 2.000*NO2
{ 92} HCHO     + NO3               --> 1.000*HO2      + 1.000*HNO3     + 1.000*CO
{ 93} ALD      + NO3               --> 1.000*ACO3     + 1.000*HNO3
{ 94} GLY      + NO3               --> 1.000*HNO3     + 1.000*HO2      + 2.000*CO
{ 95} MGLY     + NO3               --> 1.000*HNO3     + 1.000*ACO3     + 1.000*CO
{ 96} DCB      + NO3               --> 1.000*HNO3     + 1.000*TCO3
{ 97} CSL      + NO3               --> 1.000*HNO3     + 1.000*XNO2     + 0.500*CSL
                                     + 0.500*CSLAER
{ 98} OL2      + NO3               --> 1.000*OLN
{ 99} OLT      + NO3               --> 1.000*OLN
{100} OLI      + NO3               --> 1.000*OLN      + 1.000*OLIAER
{101} OL2      + O3                --> 1.000*HCHO     + 0.400*ORA1     + 0.420*CO
                                     + 0.120*HO2
{102} OLT      + O3                --> 0.530*HCHO     + 0.500*ALD      + 0.330*CO
                                     + 0.200*ORA1     + 0.200*ORA2     + 0.230*HO2
                                     + 0.220*MO2      + 0.100*HO
{103} OLI      + O3                --> 0.180*HCHO     + 0.720*ALD      + 0.100*KET
                                     + 0.230*CO       + 0.060*ORA1     + 0.290*ORA2
                                     + 0.260*HO2      + 0.140*HO       + 0.310*MO2
                                     + 1.000*OLIAER
{104} HO2      + MO2               --> 1.000*OP1
{105} HO2      + ETHP              --> 1.000*OP2
{106} HO2      + HC3P              --> 1.000*OP2
{107} HO2      + HC5P              --> 1.000*OP2
{108} HO2      + HC8P              --> 1.000*OP2
{109} HO2      + OL2P              --> 1.000*OP2
{110} HO2      + OLTP              --> 1.000*OP2
{111} HO2      + OLIP              --> 1.000*OP2
{112} HO2      + KETP              --> 1.000*OP2
{113} HO2      + ACO3              --> 1.000*PAA
{114} HO2      + TOLP              --> 1.000*OP2
{115} HO2      + XYLP              --> 1.000*OP2
{116} HO2      + TCO3              --> 1.000*OP2
{117} HO2      + OLN               --> 1.000*ONIT
{118} MO2      + MO2               --> 1.500*HCHO     + 1.000*HO2
{119} MO2      + ETHP              --> 0.750*HCHO     + 1.000*HO2      + 0.750*ALD
{120} MO2      + HC3P              --> 0.840*HCHO     + 0.770*ALD      + 0.260*KET
                                     + 1.000*HO2
{121} MO2      + HC5P              --> 0.770*HCHO     + 0.410*ALD      + 0.750*KET
                                     + 1.000*HO2
{122} MO2      + HC8P              --> 0.800*HCHO     + 0.460*ALD      + 1.390*KET
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
                                          +       HO2
{123} MO2      + OL2P             -->   1.550*HCHO     + 0.350*ALD      +       HO2
{124} MO2      + OLTP             -->   1.250*HCHO     + 0.750*ALD      +       HO2
{125} MO2      + OLIP             -->   0.890*HCHO     + 0.725*ALD      +       HO2
                                       + 0.550*KET
{126} MO2      + KETP             -->   0.750*HCHO     + 0.750*MGLY     +       HO2
{127} MO2      + ACO3             -->          HCHO     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{128} MO2      + TOLP             -->          HCHO     + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      + 2.000*HO2
{129} MO2      + XYLP             -->          HCHO     + 0.450*MGLY     + 0.806*DCB
                                       + 2.000*HO2
{130} MO2      + TCO3             -->   0.500*HCHO     + 0.445*GLY      + 0.055*MGLY
                                       + 0.500*ORA2     + 0.025*ACO3     + 0.460*HO2
                                       + 0.475*CO       +       XO2
{131} MO2      + OLN              -->   1.750*HCHO     + 0.500*HO2      +       ALD
                                       +       NO2
{132} ETHP     + ACO3             -->          ALD      + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{133} HC3P     + ACO3             -->   0.770*ALD      + 0.260*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{134} HC5P     + ACO3             -->   0.410*ALD      + 0.750*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{135} HC8P     + ACO3             -->   0.460*ALD      + 1.390*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{136} OL2P     + ACO3             -->   0.800*HCHO     + 0.600*ALD      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{137} OLTP     + ACO3             -->          ALD      + 0.500*HCHO     + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{138} OLIP     + ACO3             -->   0.725*ALD      + 0.550*KET      + 0.140*HCHO
                                       + 0.500*HO2      + 0.500*MO2      + 0.500*ORA2
{139} KETP     + ACO3             -->          MGLY     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{140} ACO3     + ACO3             -->   2.000*MO2
{141} ACO3     + TOLP             -->          MO2      + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      +       HO2
{142} ACO3     + XYLP             -->          MO2      + 0.450*MGLY     + 0.806*DCB
                                       +       HO2
{143} ACO3     + TCO3             -->          MO2      + 0.920*HO2      + 0.890*GLY
                                       + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                       + 2.000*XO2
{144} ACO3     + OLN              -->          HCHO     +       ALD      + 0.500*ORA2
                                       +       NO2      + 0.500*MO2
{145} OLN      + OLN              -->   2.000*HCHO     + 2.000*ALD      + 2.000*NO2
{146} XO2      + HO2              -->          OP2
{147} XO2      + MO2              -->          HCHO     +       HO2
{148} XO2      + ACO3             -->          MO2
{149} XO2      + XO2              -->
{150} XO2      + NO               -->          NO2
{151} XNO2     + NO2              -->          ONIT
{152} XNO2     + HO2              -->          OP2
{153} XNO2     + MO2              -->          HCHO     +       HO2
{154} XNO2     + ACO3             -->          MO2
{155} XNO2     + XNO2             -->
{156} TERP     + HO               -->          TERPAER  +       HO
{157} TERP     + NO3              -->          TERPAER  +       NO3
{158} TERP     + O3               -->          TERPAER  +       O3
{159} ISO      + HO               -->          ISO_RO2  + 0.079*XO2
{160} ISO_RO2  + NO               -->   0.088*ONIT     + 0.912*NO2      + 0.912*HO2
                                       + 0.912*ISOPROD  + 0.629*HCHO
{161} ISO_RO2  + HO2              -->          OP2
{162} ISO_RO2  + ACO3             -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       +       ISOPROD
{163} ISO_RO2  + MO2              -->   0.500*HCHO     + 0.500*HO2      +       ISOPROD
{164} ISO      + O3               -->   0.600*HCHO     + 0.650*ISOPROD  + 0.390*ORA1
                                       + 0.270*HO       + 0.070*HO2      + 0.070*CO
                                       + 0.200*XO2      + 0.200*ACO3     + 0.150*ALD
{165} ISO      + O3P              -->   0.750*ISOPROD  + 0.250*ACO3     + 0.250*HCHO
                                       + 0.250*MO2
{166} ISO      + NO3              -->          ISON_RO2
{167} ISON_RO2 + NO               -->          NO2      + 0.800*ALD      + 0.800*ONIT
                                       + 0.800*HO2      + 0.200*ISOPROD  + 0.200*NO2
{168} ISON_RO2 + HO2              -->          ONIT
{169} ISON_RO2 + ACO3             -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
                                        +       ALD      +       ONIT
{170} ISON_RO2 + MO2                -->   0.500*HCHO     + 0.500*HO2      +       ALD
                                        +       ONIT
{171} ISOPROD  + HO                 -->   0.500*ACO3     + 0.500*IP_RO2   + 0.200*XO2
{172} IP_RO2   + NO                 -->         NO2      +       HO2      + 0.590*CO
                                        + 0.550*ALD      + 0.250*HCHO     + 0.080*GLY
                                        + 0.340*MGLY     + 0.630*KET
{173} IP_RO2   + HO2                -->         OP2
{174} IP_RO2   + ACO3               -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                        + 0.500*ALD      + 0.500*KET
{175} IP_RO2   + MO2                -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                        + 0.500*KET
{176} ISOPROD  + O3                 -->   0.268*HO       + 0.100*HO2      + 0.114*ACO3
                                        + 0.054*MO2      + 0.070*XO2      + 0.155*CO
                                        + 0.146*HCHO     + 0.020*ALD      + 0.010*GLY
                                        + 0.850*MGLY     + 0.090*KET      + 0.462*ORA1
{177} ISOPROD  + hv                 -->   0.970*ACO3     + 0.333*HO2      + 0.700*MO2
                                        + 0.200*HCHO     + 0.333*CO       + 0.067*ALD
                                        + 0.033*KET
{178} ISOPROD  + NO3                -->   0.075*ACO3     + 0.075*HNO3     + 0.643*CO
                                        + 0.282*HCHO     + 0.925*ONIT     + 0.282*ALD
                                        + 0.925*HO2      + 0.925*XO2
>-------------------------------------------------------------------------------------------<

Rate Expression                                                              Rate Constant
================================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                           {1.68671E-12}
k( 36) is a falloff expression using:                            {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                              {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                              {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                              {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                              {4.03072E-16}
k( 41) =  2.5000E-12                                                {2.50000E-12}
k( 42) is a falloff expression using:                               {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
k( 44) =  2.0000E-21                                                {2.00000E-21}
k( 45) is a falloff expression using:                               {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 46) is a special rate expression of the form:                    {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 47) =  1.3000E-12 * exp(   380.0/T)                              {4.65309E-12}
k( 48) =  4.6000E-11 * exp(   230.0/T)                              {9.95294E-11}
k( 49) is a falloff expression using:                               {8.88848E-13}
   k0   =  3.0000E-31 * (T/300)**(-3.30)
   kinf =  1.5000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                         {2.40000E-13}
k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)           {3.80672E-01}
k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)           {2.74210E-13}
k( 53) =  1.5900E-11 * exp(  -540.0/T)                              {2.59669E-12}
k( 54) =  1.7300E-11 * exp(  -380.0/T)                              {4.83334E-12}
k( 55) =  3.6400E-11 * exp(  -380.0/T)                              {1.01696E-11}
k( 56) =  2.1500E-12 * exp(   411.0/T)                              {8.53916E-12}
k( 57) =  5.3200E-12 * exp(   504.0/T)                              {2.88684E-11}
k( 58) =  1.0700E-11 * exp(   549.0/T)                              {6.75269E-11}
k( 59) =  2.1000E-12 * exp(   322.0/T)                              {6.18715E-12}
k( 60) =  1.8900E-11 * exp(   116.0/T)                              {2.78943E-11}
k( 61) =  4.0000E-11                                                {4.00000E-11}
k( 62) =  9.0000E-01 * k( 61)                                       {3.60000E-11}
k( 63) =  9.0000E-12                                                {9.00000E-12}
k( 64) =  6.8700E-12 * exp(   256.0/T)                              {1.62197E-11}
k( 65) =  1.2000E-11 * exp(  -745.0/T)                              {9.85020E-13}
k( 66) =  1.1500E-11                                                {1.15000E-11}
k( 67) =  1.7000E-11                                                {1.70000E-11}
k( 68) =  2.8000E-11                                                {2.80000E-11}
k( 69) =  1.0000E-11                                                {1.00000E-11}
k( 70) =  1.0000E-11                                                {1.00000E-11}
k( 71) =  1.0000E-11                                                {1.00000E-11}
k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)           {1.37105E-13}
k( 73) =  1.5500E-11 * exp(  -540.0/T)                              {2.53137E-12}
k( 74) =  2.8000E-12 * exp(   181.0/T)                              {5.13974E-12}
k( 75) =  1.9500E+16 * exp(-13543.0/T)                              {3.57235E-04}
k( 76) =  4.7000E-12                                                {4.70000E-12}
k( 77) =  1.9500E+16 * exp(-13543.0/T)                              {3.57235E-04}
k( 78) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 79) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 80) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 81) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 82) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 83) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 84) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 85) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 86) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 87) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 88) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 89) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 90) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 91) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k( 92) =  6.0000E-13 * exp( -2058.0/T)                              {6.01030E-16}
k( 93) =  1.4000E-12 * exp( -1900.0/T)                              {2.38307E-15}
k( 94) =  6.0000E-13 * exp( -2058.0/T)                              {6.01030E-16}
k( 95) =  1.4000E-12 * exp( -1900.0/T)                              {2.38307E-15}
k( 96) =  1.4000E-12 * exp( -1900.0/T)                              {2.38307E-15}
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
k( 97) =  2.2000E-11                                                {2.20000E-11}
k( 98) =  2.0000E-12 * exp( -2923.0/T)                              {1.09940E-16}
k( 99) =  1.0000E-11 * exp( -1895.0/T)                              {1.73099E-14}
k(100) =  3.2300E-11 * exp(  -975.0/T)                              {1.22539E-12}
k(101) =  1.2000E-14 * exp( -2633.0/T)                              {1.74559E-18}
k(102) =  1.3200E-14 * exp( -2105.0/T)                              {1.12933E-17}
k(103) =  7.2900E-15 * exp( -1136.0/T)                              {1.61125E-16}
k(104) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(105) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(106) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(107) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(118) =  1.9000E-13 * exp(   220.0/T)                              {3.97533E-13}
k(119) =  1.4000E-13 * exp(   220.0/T)                              {2.92919E-13}
k(120) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(121) =  3.4000E-14 * exp(   220.0/T)                              {7.11376E-14}
k(122) =  2.9000E-14 * exp(   220.0/T)                              {6.06762E-14}
k(123) =  1.4000E-13 * exp(   220.0/T)                              {2.92919E-13}
k(124) =  1.4000E-13 * exp(   220.0/T)                              {2.92919E-13}
k(125) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(126) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(127) =  9.6000E-13 * exp(   220.0/T)                              {2.00859E-12}
k(128) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                              {2.00859E-12}
k(131) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(132) =  3.4000E-13 * exp(   220.0/T)                              {7.11376E-13}
k(133) =  1.0000E-13 * exp(   220.0/T)                              {2.09228E-13}
k(134) =  8.4000E-14 * exp(   220.0/T)                              {1.75752E-13}
k(135) =  7.2000E-14 * exp(   220.0/T)                              {1.50644E-13}
k(136) =  3.4000E-13 * exp(   220.0/T)                              {7.11376E-13}
k(137) =  3.4000E-13 * exp(   220.0/T)                              {7.11376E-13}
k(138) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(139) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(140) =  1.1900E-12 * exp(   220.0/T)                              {2.48981E-12}
k(141) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                              {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(145) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
k(146) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(147) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(148) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(149) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
k(150) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k(151) =  4.2000E-12 * exp(   180.0/T)                              {7.68378E-12}
k(152) =  7.7000E-14 * exp(  1300.0/T)                              {6.04038E-12}
k(153) =  1.7000E-14 * exp(   220.0/T)                              {3.55688E-14}
k(154) =  4.2000E-14 * exp(   220.0/T)                              {8.78758E-14}
k(155) =  3.6000E-16 * exp(   220.0/T)                              {7.53221E-16}
k(156) =  1.0000E+00 * k( 58)                                       {6.75269E-11}
k(157) =  1.0000E+00 * k(100)                                       {1.22539E-12}
k(158) =  1.0000E+00 * k(103)                                       {1.61125E-16}
k(159) =  2.5400E-11 * (T/300)**( 1.00) * exp(   407.6/T)           {9.90719E-11}
k(160) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)           {7.66335E-12}
k(161) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)           {5.96598E-12}
k(162) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)           {1.75402E-13}
k(163) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)           {7.09961E-14}
k(164) =  7.8600E-15 * (T/300)**( 1.00) * exp( -1912.2/T)           {1.27569E-17}
k(165) =  3.6000E-11                                                {3.60000E-11}
k(166) =  3.0300E-12 * (T/300)**( 1.00) * exp(  -447.9/T)           {6.69552E-13}
k(167) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)           {7.66335E-12}
k(168) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)           {5.96598E-12}
k(169) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)           {1.75402E-13}
k(170) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)           {7.09961E-14}
```

Table 8A-10. RADM2_CIS1_AE and RADM2_CIS1_AE_AQ Mechanisms

```
k(171) =  3.3600E-11                                                    {3.36000E-11}
k(172) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)               {7.66335E-12}
k(173) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)               {5.96598E-12}
k(174) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)               {1.75402E-13}
k(175) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)               {7.09961E-14}
k(176) =  7.1100E-18                                                    {7.11000E-18}
k(177) uses photo table ACROLEIN        , scaled by 3.60000E-03         {0.00000E+00}
k(178) =  1.0000E-15                                                    {1.00000E-15}
================================================================================
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
 Reaction List
>-------------------------------------------------------------------------------------------<
{  1} NO2      + hv                  -->         O3P      +       NO
{  2} O3       + hv                  -->         O1D
{  3} O3       + hv                  -->         O3P
{  4} HONO     + hv                  -->         HO       +       NO
{  5} HNO3     + hv                  -->         HO       +       NO2
{  6} HNO4     + hv                  -->         HO2      +       NO2
{  7} NO3      + hv                  -->         NO
{  8} NO3      + hv                  -->         NO2      +       O3P
{  9} H2O2     + hv                  -->   2.000*HO
{ 10} HCHO     + hv                  -->         CO
{ 11} HCHO     + hv                  -->         HO2      +       HO2      +       CO
{ 12} ALD      + hv                  -->         MO2      +       HO2      +       CO
{ 13} OP1      + hv                  -->         HCHO     +       HO2      +       HO
{ 14} OP2      + hv                  -->         ALD      +       HO2      +       HO
{ 15} PAA      + hv                  -->         MO2      +       HO
{ 16} KET      + hv                  -->         ACO3     +       ETHP
{ 17} GLY      + hv                  -->   0.130*HCHO     + 1.870*CO
{ 18} GLY      + hv                  -->   0.450*HCHO     + 1.550*CO       + 0.800*HO2
{ 19} MGLY     + hv                  -->         ACO3     +       HO2      +       CO
{ 20} DCB      + hv                  -->   0.980*HO2      + 0.020*ACO3     +       TCO3
{ 21} ONIT     + hv                  -->   0.200*ALD      + 0.800*KET      +       HO2
                                           +       NO2
{ 22} O3P      + [M]      + [O2]     -->         O3
{ 23} O3P      + NO2                 -->         NO
{ 24} O1D      + [N2]                -->         O3P
{ 25} O1D      + [O2]                -->         O3P
{ 26} O1D      + [H2O]               -->   2.000*HO
{ 27} O3       + NO                  -->         NO2
{ 28} O3       + HO                  -->         HO2
{ 29} O3       + HO2                 -->         HO
{ 30} HO2      + NO                  -->         NO2      +       HO
{ 31} HO2      + NO2                 -->         HNO4
{ 32} HNO4                           -->         HO2      +       NO2
{ 33} HO2      + HO2                 -->         H2O2
{ 34} HO2      + HO2      + [H2O]    -->         H2O2
{ 35} H2O2     + HO                  -->         HO2
{ 36} NO       + HO                  -->         HONO
{ 37} NO       + NO       + [O2]     -->   2.000*NO2
{ 38} O3       + NO2                 -->         NO3
{ 39} NO3      + NO                  -->   2.000*NO2
{ 40} NO3      + NO2                 -->         NO       +       NO2
{ 41} NO3      + HO2                 -->         HNO3
{ 42} NO3      + NO2                 -->         N2O5
{ 43} N2O5                           -->         NO2      +       NO3
{ 44} N2O5     + [H2O]               -->   2.000*HNO3
{ 45} HO       + NO2                 -->         HNO3
{ 46} HO       + HNO3                -->         NO3
{ 47} HO       + HNO4                -->         NO2
{ 48} HO       + HO2                 -->
{ 49} HO       + SO2                 -->         SULF     +       HO2
{ 50} CO       + HO                  -->         HO2
{ 51} HO                             -->         MO2
{ 52} ETH      + HO                  -->         ETHP
{ 53} HC3      + HO                  -->   0.830*HC3P     + 0.170*HO2      + 0.009*HCHO
                                         + 0.075*ALD      + 0.025*KET
{ 54} HC5      + HO                  -->         HC5P     + 0.250*XO2
{ 55} HC8      + HO                  -->         HC8P     + 0.750*XO2
{ 56} OL2      + HO                  -->         OL2P
{ 57} OLT      + HO                  -->         OLTP
{ 58} OLI      + HO                  -->         OLIP
{ 59} TOL      + HO                  -->   0.750*TOLP     + 0.250*CSL      + 0.250*HO2
{ 60} XYL      + HO                  -->   0.830*XYLP     + 0.170*CSL      + 0.170*HO2
{ 61} CSL      + HO                  -->   0.100*HO2      + 0.900*XO2      + 0.900*TCO3
{ 62} CSL      + HO                  -->         CSL
{ 63} HCHO     + HO                  -->         HO2      +       CO
{ 64} ALD      + HO                  -->         ACO3
{ 65} KET      + HO                  -->         KETP
{ 66} GLY      + HO                  -->         HO2      + 2.000*CO
{ 67} MGLY     + HO                  -->         ACO3     +       CO
{ 68} DCB      + HO                  -->         TCO3
{ 69} OP1      + HO                  -->   0.500*MO2      + 0.500*HCHO     + 0.500*HO
{ 70} OP2      + HO                  -->   0.500*HC3P     + 0.500*ALD      + 0.500*HO
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
{ 71} PAA      + HO                --> ACO3
{ 72} PAN      + HO                --> HCHO     +       NO3      +       XO2
{ 73} ONIT     + HO                --> HC3P     +       NO2
{ 74} ACO3     + NO2               --> PAN
{ 75} PAN                          --> ACO3     +       NO2
{ 76} TCO3     + NO2               --> TPAN
{ 77} TPAN                         --> TCO3     +       NO2
{ 78} MO2      + NO                --> HCHO     +       HO2      +       NO2
{ 79} HC3P     + NO                --> 0.750*ALD      + 0.250*KET      + 0.090*HCHO
                                     + 0.036*ONIT     + 0.964*NO2      + 0.964*HO2
{ 80} HC5P     + NO                --> 0.380*ALD      + 0.690*KET      + 0.080*ONIT
                                     + 0.920*NO2      + 0.920*HO2
{ 81} HC8P     + NO                --> 0.350*ALD      + 1.060*KET      + 0.040*HCHO
                                     + 0.240*ONIT     + 0.760*NO2      + 0.760*HO2
{ 82} OL2P     + NO                --> 1.600*HCHO     +       HO2      +       NO2
                                     + 0.200*ALD
{ 83} OLTP     + NO                --> ALD      +       HCHO     +       HO2
                                     +       NO2
{ 84} OLIP     + NO                --> HO2      + 1.450*ALD      + 0.280*HCHO
                                     + 0.100*KET      +       NO2
{ 85} ACO3     + NO                --> MO2      +       NO2
{ 86} TCO3     + NO                --> NO2      + 0.920*HO2      + 0.890*GLY
                                     + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                     + 2.000*XO2
{ 87} TOLP     + NO                --> NO2      +       HO2      + 0.170*MGLY
                                     + 0.160*GLY      + 0.700*DCB
{ 88} XYLP     + NO                --> NO2      +       HO2      + 0.450*MGLY
                                     + 0.806*DCB
{ 89} ETHP     + NO                --> ALD      +       HO2      +       NO2
{ 90} KETP     + NO                --> MGLY     +       NO2      +       HO2
{ 91} OLN      + NO                --> HCHO     +       ALD      + 2.000*NO2
{ 92} HCHO     + NO3               --> HO2      +       HNO3     +       CO
{ 93} ALD      + NO3               --> ACO3     +       HNO3
{ 94} GLY      + NO3               --> HNO3     +       HO2      + 2.000*CO
{ 95} MGLY     + NO3               --> HNO3     +       ACO3     +       CO
{ 96} DCB      + NO3               --> HNO3     +       TCO3
{ 97} CSL      + NO3               --> HNO3     +       XNO2     + 0.500*CSL
{ 98} OL2      + NO3               --> OLN
{ 99} OLT      + NO3               --> OLN
{100} OLI      + NO3               --> OLN
{101} OL2      + O3                --> HCHO     + 0.400*ORA1     + 0.420*CO
                                     + 0.120*HO2
{102} OLT      + O3                --> 0.530*HCHO     + 0.500*ALD      + 0.330*CO
                                     + 0.200*ORA1     + 0.200*ORA2     + 0.230*HO2
                                     + 0.220*MO2      + 0.100*HO
{103} OLI      + O3                --> 0.180*HCHO     + 0.720*ALD      + 0.100*KET
                                     + 0.230*CO       + 0.060*ORA1     + 0.290*ORA2
                                     + 0.260*HO2      + 0.140*HO       + 0.310*MO2
{104} HO2      + MO2               --> OP1
{105} HO2      + ETHP              --> OP2
{106} HO2      + HC3P              --> OP2
{107} HO2      + HC5P              --> OP2
{108} HO2      + HC8P              --> OP2
{109} HO2      + OL2P              --> OP2
{110} HO2      + OLTP              --> OP2
{111} HO2      + OLIP              --> OP2
{112} HO2      + KETP              --> OP2
{113} HO2      + ACO3              --> PAA
{114} HO2      + TOLP              --> OP2
{115} HO2      + XYLP              --> OP2
{116} HO2      + TCO3              --> OP2
{117} HO2      + OLN               --> ONIT
{118} MO2      + MO2               --> 1.500*HCHO     +       HO2
{119} MO2      + ETHP              --> 0.750*HCHO     +       HO2      + 0.750*ALD
{120} MO2      + HC3P              --> 0.840*HCHO     + 0.770*ALD      + 0.260*KET
                                     +       HO2
{121} MO2      + HC5P              --> 0.770*HCHO     + 0.410*ALD      + 0.750*KET
                                     +       HO2
{122} MO2      + HC8P              --> 0.800*HCHO     + 0.460*ALD      + 1.390*KET
                                     +       HO2
{123} MO2      + OL2P              --> 1.550*HCHO     + 0.350*ALD      +       HO2
{124} MO2      + OLTP              --> 1.250*HCHO     + 0.750*ALD      +       HO2
{125} MO2      + OLIP              --> 0.890*HCHO     + 0.725*ALD      +       HO2
                                     + 0.550*KET
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
{126} MO2      + KETP              -->   0.750*HCHO     + 0.750*MGLY     +       HO2
{127} MO2      + ACO3              -->         HCHO     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{128} MO2      + TOLP              -->         HCHO     + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      + 2.000*HO2
{129} MO2      + XYLP              -->         HCHO     + 0.450*MGLY     + 0.806*DCB
                                       + 2.000*HO2
{130} MO2      + TCO3              -->   0.500*HCHO     + 0.445*GLY      + 0.055*MGLY
                                       + 0.500*ORA2     + 0.025*ACO3     + 0.460*HO2
                                       + 0.475*CO       +       XO2
{131} MO2      + OLN               -->   1.750*HCHO     + 0.500*HO2      +       ALD
                                       +       NO2
{132} ETHP     + ACO3              -->         ALD      + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{133} HC3P     + ACO3              -->   0.770*ALD      + 0.260*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{134} HC5P     + ACO3              -->   0.410*ALD      + 0.750*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{135} HC8P     + ACO3              -->   0.460*ALD      + 1.390*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{136} OL2P     + ACO3              -->   0.800*HCHO     + 0.600*ALD      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{137} OLTP     + ACO3              -->         ALD      + 0.500*HCHO     + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{138} OLIP     + ACO3              -->   0.725*ALD      + 0.550*KET      + 0.140*HCHO
                                       + 0.500*HO2      + 0.500*MO2      + 0.500*ORA2
{139} KETP     + ACO3              -->         MGLY     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{140} ACO3     + ACO3              -->   2.000*MO2
{141} ACO3     + TOLP              -->         MO2      + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      +       HO2
{142} ACO3     + XYLP              -->         MO2      + 0.450*MGLY     + 0.806*DCB
                                       +       HO2
{143} ACO3     + TCO3              -->         MO2      + 0.920*HO2      + 0.890*GLY
                                       + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                       + 2.000*XO2
{144} ACO3     + OLN               -->         HCHO     +       ALD      + 0.500*ORA2
                                       +       NO2      + 0.500*MO2
{145} OLN      + OLN               -->   2.000*HCHO     + 2.000*ALD      + 2.000*NO2
{146} XO2      + HO2               -->         OP2
{147} XO2      + MO2               -->         HCHO     +       HO2
{148} XO2      + ACO3              -->         MO2
{149} XO2      + XO2               -->
{150} XO2      + NO                -->         NO2
{151} XNO2     + NO2               -->         ONIT
{152} XNO2     + HO2               -->         OP2
{153} XNO2     + MO2               -->         HCHO     +       HO2
{154} XNO2     + ACO3              -->         MO2
{155} XNO2     + XNO2              -->
{156} ISO      + HO                -->         ISO_RO2  + 0.079*XO2
{157} ISO_RO2  + NO                -->   0.088*ONIT     + 0.912*NO2      + 0.912*HO2
                                       + 0.362*ISOPROD  + 0.230*MACR     + 0.320*MVK
                                       + 0.629*HCHO     + 0.079*XO2
{158} ISO_RO2  + HO2               -->         OP2
{159} ISO_RO2  + ACO3              -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       + 0.362*ISOPROD  + 0.230*MACR     + 0.320*MVK
                                       + 0.629*HCHO
{160} ISO_RO2  + MO2               -->   0.500*HCHO     + 0.500*HO2      + 0.362*ISOPROD
                                       + 0.230*MACR     + 0.320*MVK      + 0.629*HCHO
{161} ISO      + O3                -->   0.600*HCHO     + 0.390*MACR     + 0.160*MVK
                                       + 0.390*ORA1     + 0.270*HO       + 0.070*HO2
                                       + 0.070*CO       + 0.200*XO2      + 0.200*MCO3
                                       + 0.150*ALD      + 0.100*ISOPROD
{162} ISO      + O3P               -->   0.750*ISOPROD  + 0.250*MCO3     + 0.250*HCHO
                                       + 0.250*MO2
{163} ISO      + NO3               -->         ISON_RO2
{164} ISON_RO2 + NO                -->         NO2      + 0.800*ALD      + 0.800*ONIT
                                       + 0.800*HO2      + 0.200*ISOPROD  + 0.200*NO2
{165} ISON_RO2 + HO2               -->         ONIT
{166} ISON_RO2 + ACO3              -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       +       ALD      +       ONIT
{167} ISON_RO2 + MO2               -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                       + 0.500*ONIT
{168} MACR     + HO                -->   0.500*MCO3     + 0.500*MACR_RO2
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
{169} MACR_RO2 + NO                  -->         NO2      +       HO2      + 0.840*KET
                                        + 0.840*CO       + 0.150*HCHO     + 0.150*MGLY
{170} MACR_RO2 + HO2                 -->         OP2
{171} MACR_RO2 + ACO3                -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                        + 0.840*KET      + 0.840*CO       + 0.150*HCHO
                                        + 0.150*MGLY
{172} MACR_RO2 + MO2                 -->   0.650*HCHO     + 0.500*HO2      + 0.840*KET
                                        + 0.840*CO       + 0.150*MGLY
{173} MACR     + O3                  -->   0.630*ORA1     + 0.210*HO       + 0.110*HO2
                                        + 0.110*CO       + 0.200*HCHO     + 0.100*XO2
                                        + 0.100*ACO3
{174} MACR     + hv                  -->   0.660*HO2      + 0.330*MCO3     + 0.670*CO
                                        + 0.670*HCHO     + 0.670*ACO3     + 0.340*HO
                                        + 0.340*XO2
{175} MACR     + NO3                 -->   0.500*MCO3     + 0.500*HNO3     + 0.500*CO
                                        + 0.500*HO2      + 0.500*ONIT     + 0.500*XO2
{176} MVK      + HO                  -->         MVK_RO2
{177} MVK_RO2  + NO                  -->         NO2      + 0.700*ALD      + 0.700*XO2
                                        + 0.700*ACO3     + 0.300*HCHO     + 0.300*MGLY
                                        + 0.300*HO2
{178} MVK_RO2  + HO2                 -->         OP2
{179} MVK_RO2  + ACO3                -->   0.500*HO2      + 1.200*MO2      + 0.500*ORA2
                                        + 0.700*ALD      + 0.300*HCHO     + 0.300*MGLY
{180} MVK_RO2  + MO2                 -->   0.800*HCHO     + 0.500*HO2      + 0.700*ALD
                                        + 0.700*MO2      + 0.300*MGLY
{181} MVK      + O3                  -->   0.670*ORA1     + 0.160*HO       + 0.110*HO2
                                        + 0.110*CO       + 0.950*MGLY     + 0.100*HCHO
                                        + 0.050*XO2      + 0.050*ACO3
{182} MVK      + hv                  -->   0.700*ISOPROD  + 0.700*CO       + 0.300*MO2
                                        + 0.300*MCO3
{183} MPAN                           -->         MCO3     +       NO2
{184} MCO3     + NO                  -->         NO2      +       HCHO     +       ACO3
{185} MCO3     + NO2                 -->         MPAN
{186} MCO3     + HO2                 -->         PAA
{187} MCO3     + MO2                 -->   2.250*HCHO     + 0.500*HO2      + 0.500*MO2
{188} MCO3     + ACO3                -->   2.000*MO2      +       HCHO
{189} MCO3     + MCO3                -->   2.000*MO2      + 2.000*HCHO
{190} ISOPROD  + HO                  -->   0.313*ACO3     + 0.687*IP_RO2
{191} IP_RO2   + NO                  -->         NO2      +       HO2      + 0.610*CO
                                        + 0.270*ALD      + 0.030*HCHO     + 0.180*GLY
                                        + 0.210*MGLY     + 0.700*KET
{192} IP_RO2   + HO2                 -->         OP2
{193} IP_RO2   + ACO3                -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                        + 0.500*ALD      + 0.500*KET
{194} IP_RO2   + MO2                 -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                        + 0.500*KET
{195} ISOPROD  + O3                  -->   0.476*HO       + 0.072*HO2      + 0.168*MO2
                                        + 0.237*ACO3     + 0.100*XO2      + 0.243*CO
                                        + 0.218*HCHO     + 0.062*ALD      + 0.278*KET
                                        + 0.031*GLY      + 0.653*MGLY     + 0.044*ORA1
{196} ISOPROD  + hv                  -->   1.216*CO       + 0.434*ALD      + 0.350*HCHO
                                        + 0.216*KET      + 1.216*HO2      + 0.784*ACO3
{197} ISOPROD  + NO3                 -->   0.668*CO       + 0.332*HCHO     + 0.332*ALD
                                        +       ONIT     +       HO2      +       XO2
>-------------------------------------------------------------------------------------<

Rate Expression                                                          Rate Constant
=========================================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                            {1.68671E-12}
k( 36) is a falloff expression using:                             {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                            {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                            {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                            {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                            {4.03072E-16}
k( 41) =  2.5000E-12                                              {2.50000E-12}
k( 42) is a falloff expression using:                             {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
k( 44) =  2.0000E-21                                              {2.00000E-21}
k( 45) is a falloff expression using:                             {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 46) is a special rate expression of the form:                  {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 47) =  1.3000E-12 * exp(   380.0/T)                            {4.65309E-12}
k( 48) =  4.6000E-11 * exp(   230.0/T)                            {9.95294E-11}
k( 49) is a falloff expression using:                             {8.88848E-13}
   k0   =  3.0000E-31 * (T/300)**(-3.30)
   kinf =  1.5000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                       {2.40000E-13}
k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)         {3.80672E-01}
k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)         {2.74210E-13}
k( 53) =  1.5900E-11 * exp(  -540.0/T)                            {2.59669E-12}
k( 54) =  1.7300E-11 * exp(  -380.0/T)                            {4.83334E-12}
k( 55) =  3.6400E-11 * exp(  -380.0/T)                            {1.01696E-11}
k( 56) =  2.1500E-12 * exp(   411.0/T)                            {8.53916E-12}
k( 57) =  5.3200E-12 * exp(   504.0/T)                            {2.88684E-11}
k( 58) =  1.0700E-11 * exp(   549.0/T)                            {6.75269E-11}
k( 59) =  2.1000E-12 * exp(   322.0/T)                            {6.18715E-12}
k( 60) =  1.8900E-11 * exp(   116.0/T)                            {2.78943E-11}
k( 61) =  4.0000E-11                                              {4.00000E-11}
k( 62) =  9.0000E-01 * k( 61)                                     {3.60000E-11}
k( 63) =  9.0000E-12                                              {9.00000E-12}
k( 64) =  6.8700E-12 * exp(   256.0/T)                            {1.62197E-11}
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
k( 65) =  1.2000E-11 * exp(  -745.0/T)                          {9.85020E-13}
k( 66) =  1.1500E-11                                            {1.15000E-11}
k( 67) =  1.7000E-11                                            {1.70000E-11}
k( 68) =  2.8000E-11                                            {2.80000E-11}
k( 69) =  1.0000E-11                                            {1.00000E-11}
k( 70) =  1.0000E-11                                            {1.00000E-11}
k( 71) =  1.0000E-11                                            {1.00000E-11}
k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)       {1.37105E-13}
k( 73) =  1.5500E-11 * exp(  -540.0/T)                          {2.53137E-12}
k( 74) =  2.8000E-12 * exp(   181.0/T)                          {5.13974E-12}
k( 75) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 76) =  4.7000E-12                                            {4.70000E-12}
k( 77) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 78) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 79) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 80) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 81) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 82) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 83) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 84) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 85) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 86) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 87) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 88) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 89) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 90) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 91) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 92) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 93) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 94) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 95) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 96) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 97) =  2.2000E-11                                            {2.20000E-11}
k( 98) =  2.0000E-12 * exp( -2923.0/T)                          {1.09940E-16}
k( 99) =  1.0000E-11 * exp( -1895.0/T)                          {1.73099E-14}
k(100) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k(101) =  1.2000E-14 * exp( -2633.0/T)                          {1.74559E-18}
k(102) =  1.3200E-14 * exp( -2105.0/T)                          {1.12933E-17}
k(103) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
k(104) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(105) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(106) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(107) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(118) =  1.9000E-13 * exp(   220.0/T)                          {3.97533E-13}
k(119) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(120) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(121) =  3.4000E-14 * exp(   220.0/T)                          {7.11376E-14}
k(122) =  2.9000E-14 * exp(   220.0/T)                          {6.06762E-14}
k(123) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(124) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(125) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(126) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(127) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(128) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(131) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(132) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(133) =  1.0000E-13 * exp(   220.0/T)                          {2.09228E-13}
k(134) =  8.4000E-14 * exp(   220.0/T)                          {1.75752E-13}
k(135) =  7.2000E-14 * exp(   220.0/T)                          {1.50644E-13}
k(136) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(137) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(138) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
```

Table 8A-11. RADM2_CIS4 and RADM2_CIS4_AQ Mechanisms

```
k(139) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(140) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(141) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(145) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(146) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(147) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(148) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(149) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(150) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(151) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(152) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(153) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(154) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(155) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(156) =  2.5400E-11 * (T/300)**( 1.00) * exp(   407.6/T)       {9.90719E-11}
k(157) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(158) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(159) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(160) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(161) =  7.8600E-15 * (T/300)**( 1.00) * exp( -1912.2/T)       {1.27569E-17}
k(162) =  3.6000E-11                                            {3.60000E-11}
k(163) =  3.0300E-12 * (T/300)**( 1.00) * exp(  -447.9/T)       {6.69552E-13}
k(164) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(165) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(166) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(167) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(168) =  1.8600E-11 * (T/300)**( 1.00) * exp(   176.1/T)       {3.33618E-11}
k(169) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(170) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(171) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(172) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(173) =  1.3600E-15 * (T/300)**( 1.00) * exp( -2113.5/T)       {1.12330E-18}
k(174) uses photo table ACROLEIN       , scaled by 3.60000E-03  {0.00000E+00}
k(175) =  1.5000E-12 * (T/300)**( 1.00) * exp( -1726.0/T)       {4.54753E-15}
k(176) =  4.1400E-12 * (T/300)**( 1.00) * exp(   452.9/T)       {1.87990E-11}
k(177) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(178) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(179) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(180) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(181) =  7.5100E-16 * (T/300)**( 1.00) * exp( -1519.7/T)       {4.54966E-18}
k(182) uses photo table ACROLEIN       , scaled by 1.11000E-02  {0.00000E+00}
k(183) =  1.6000E+16 * (T/300)**( 1.00) * exp(-13486.0/T)       {3.52536E-04}
k(184) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(185) =  2.8000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {5.10890E-12}
k(186) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(187) =  9.6000E-13 * (T/300)**( 1.00) * exp(   221.4/T)       {2.00460E-12}
k(188) =  1.1900E-12 * (T/300)**( 1.00) * exp(   221.4/T)       {2.48486E-12}
k(189) =  1.1900E-12 * (T/300)**( 1.00) * exp(   221.4/T)       {2.48486E-12}
k(190) =  3.3600E-11                                            {3.36000E-11}
k(191) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(192) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(193) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(194) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(195) =  7.1100E-18                                            {7.11000E-18}
k(196) uses photo table ACROLEIN       , scaled by 3.60000E-03  {0.00000E+00}
k(197) =  1.0000E-13                                            {1.00000E-13}
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Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
 Reaction List
>-------------------------------------------------------------------------------------------<
{  1} NO2      + hv                  -->         O3P      +       NO
{  2} O3       + hv                  -->         O1D
{  3} O3       + hv                  -->         O3P
{  4} HONO     + hv                  -->         HO       +       NO
{  5} HNO3     + hv                  -->         HO       +       NO2
{  6} HNO4     + hv                  -->         HO2      +       NO2
{  7} NO3      + hv                  -->         NO
{  8} NO3      + hv                  -->         NO2      +       O3P
{  9} H2O2     + hv                  -->   2.000*HO
{ 10} HCHO     + hv                  -->         CO
{ 11} HCHO     + hv                  -->         HO2      +       HO2      +       CO
{ 12} ALD      + hv                  -->         MO2      +       HO2      +       CO
{ 13} OP1      + hv                  -->         HCHO     +       HO2      +       HO
{ 14} OP2      + hv                  -->         ALD      +       HO2      +       HO
{ 15} PAA      + hv                  -->         MO2      +       HO
{ 16} KET      + hv                  -->         ACO3     +       ETHP
{ 17} GLY      + hv                  -->   0.130*HCHO     + 1.870*CO
{ 18} GLY      + hv                  -->   0.450*HCHO     + 1.550*CO       + 0.800*HO2
{ 19} MGLY     + hv                  -->         ACO3     +       HO2      +       CO
{ 20} DCB      + hv                  -->   0.980*HO2      + 0.020*ACO3     +       TCO3
{ 21} ONIT     + hv                  -->   0.200*ALD      + 0.800*KET      +       HO2
                                           +       NO2
{ 22} O3P      + [M]      + [O2]     -->         O3
{ 23} O3P      + NO2                 -->         NO
{ 24} O1D      + [N2]                -->         O3P
{ 25} O1D      + [O2]                -->         O3P
{ 26} O1D      + [H2O]               -->   2.000*HO
{ 27} O3       + NO                  -->         NO2
{ 28} O3       + HO                  -->         HO2
{ 29} O3       + HO2                 -->         HO
{ 30} HO2      + NO                  -->         NO2      +       HO
{ 31} HO2      + NO2                 -->         HNO4
{ 32} HNO4                           -->         HO2      +       NO2
{ 33} HO2      + HO2                 -->         H2O2
{ 34} HO2      + HO2      + [H2O]    -->         H2O2
{ 35} H2O2     + HO                  -->         HO2
{ 36} NO       + HO                  -->         HONO
{ 37} NO       + NO       + [O2]     -->   2.000*NO2
{ 38} O3       + NO2                 -->         NO3
{ 39} NO3      + NO                  -->   2.000*NO2
{ 40} NO3      + NO2                 -->         NO       +       NO2
{ 41} NO3      + HO2                 -->         HNO3
{ 42} NO3      + NO2                 -->         N2O5
{ 43} N2O5                           -->         NO2      +       NO3
{ 44} N2O5     + [H2O]               -->   2.000*HNO3
{ 45} HO       + NO2                 -->         HNO3
{ 46} HO       + HNO3                -->         NO3
{ 47} HO       + HNO4                -->         NO2
{ 48} HO       + HO2                 -->
{ 49} HO       + SO2                 -->         SULF     +       HO2      +       SULAER
{ 50} CO       + HO                  -->         HO2
{ 51} HO                             -->         MO2
{ 52} ETH      + HO                  -->         ETHP
{ 53} HC3      + HO                  -->   0.830*HC3P     + 0.170*HO2      + 0.009*HCHO
                                         + 0.075*ALD      + 0.025*KET
{ 54} HC5      + HO                  -->         HC5P     + 0.250*XO2
{ 55} HC8      + HO                  -->         HC8P     + 0.750*XO2      +       HC8AER
{ 56} OL2      + HO                  -->         OL2P
{ 57} OLT      + HO                  -->         OLTP
{ 58} OLI      + HO                  -->         OLIP     +       OLIAER
{ 59} TOL      + HO                  -->   0.750*TOLP     + 0.250*CSL      + 0.250*HO2
                                           +       TOLAER
{ 60} XYL      + HO                  -->   0.830*XYLP     + 0.170*CSL      + 0.170*HO2
                                           +       XYLAER
{ 61} CSL      + HO                  -->   0.100*HO2      + 0.900*XO2      + 0.900*TCO3
                                           +       CSLAER
{ 62} CSL      + HO                  -->         CSL
{ 63} HCHO     + HO                  -->         HO2      +       CO
{ 64} ALD      + HO                  -->         ACO3
{ 65} KET      + HO                  -->         KETP
{ 66} GLY      + HO                  -->         HO2      + 2.000*CO
{ 67} MGLY     + HO                  -->         ACO3     +       CO
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Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
{ 68} DCB      + HO                --->         TCO3
{ 69} OP1      + HO                --->   0.500*MO2      + 0.500*HCHO     + 0.500*HO
{ 70} OP2      + HO                --->   0.500*HC3P     + 0.500*ALD      + 0.500*HO
{ 71} PAA      + HO                --->         ACO3
{ 72} PAN      + HO                --->         HCHO     +       NO3      +       XO2
{ 73} ONIT     + HO                --->         HC3P     +       NO2
{ 74} ACO3     + NO2               --->         PAN
{ 75} PAN                          --->         ACO3     +       NO2
{ 76} TCO3     + NO2               --->         TPAN
{ 77} TPAN                         --->         TCO3     +       NO2
{ 78} MO2      + NO                --->         HCHO     +       HO2      +       NO2
{ 79} HC3P     + NO                --->   0.750*ALD      + 0.250*KET      + 0.090*HCHO
                                       + 0.036*ONIT     + 0.964*NO2      + 0.964*HO2
{ 80} HC5P     + NO                --->   0.380*ALD      + 0.690*KET      + 0.080*ONIT
                                       + 0.920*NO2      + 0.920*HO2
{ 81} HC8P     + NO                --->   0.350*ALD      + 1.060*KET      + 0.040*HCHO
                                       + 0.240*ONIT     + 0.760*NO2      + 0.760*HO2
{ 82} OL2P     + NO                --->   1.600*HCHO     +       HO2      +       NO2
                                       + 0.200*ALD
{ 83} OLTP     + NO                --->         ALD      +       HCHO     +       HO2
                                       +       NO2
{ 84} OLIP     + NO                --->         HO2      + 1.450*ALD      + 0.280*HCHO
                                       + 0.100*KET      +       NO2
{ 85} ACO3     + NO                --->         MO2      +       NO2
{ 86} TCO3     + NO                --->         NO2      + 0.920*HO2      + 0.890*GLY
                                       + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                       + 2.000*XO2
{ 87} TOLP     + NO                --->         NO2      +       HO2      + 0.170*MGLY
                                       + 0.160*GLY      + 0.700*DCB
{ 88} XYLP     + NO                --->         NO2      +       HO2      + 0.450*MGLY
                                       + 0.806*DCB
{ 89} ETHP     + NO                --->         ALD      +       HO2      +       NO2
{ 90} KETP     + NO                --->         MGLY     +       NO2      +       HO2
{ 91} OLN      + NO                --->         HCHO     +       ALD      + 2.000*NO2
{ 92} HCHO     + NO3               --->         HO2      +       HNO3     +       CO
{ 93} ALD      + NO3               --->         ACO3     +       HNO3
{ 94} GLY      + NO3               --->         HNO3     +       HO2      + 2.000*CO
{ 95} MGLY     + NO3               --->         HNO3     +       ACO3     +       CO
{ 96} DCB      + NO3               --->         HNO3     +       TCO3
{ 97} CSL      + NO3               --->         HNO3     +       XNO2     + 0.500*CSL
                                       + 0.500*CSLAER
{ 98} OL2      + NO3               --->         OLN
{ 99} OLT      + NO3               --->         OLN
{100} OLI      + NO3               --->         OLN      +       OLIAER
{101} OL2      + O3                --->         HCHO     + 0.400*ORA1     + 0.420*CO
                                       + 0.120*HO2
{102} OLT      + O3                --->   0.530*HCHO     + 0.500*ALD      + 0.330*CO
                                       + 0.200*ORA1     + 0.200*ORA2     + 0.230*HO2
                                       + 0.220*MO2      + 0.100*HO
{103} OLI      + O3                --->   0.180*HCHO     + 0.720*ALD      + 0.100*KET
                                       + 0.230*CO       + 0.060*ORA1     + 0.290*ORA2
                                       + 0.260*HO2      + 0.140*HO       + 0.310*MO2
                                       +       OLIAER
{104} HO2      + MO2               --->         OP1
{105} HO2      + ETHP              --->         OP2
{106} HO2      + HC3P              --->         OP2
{107} HO2      + HC5P              --->         OP2
{108} HO2      + HC8P              --->         OP2
{109} HO2      + OL2P              --->         OP2
{110} HO2      + OLTP              --->         OP2
{111} HO2      + OLIP              --->         OP2
{112} HO2      + KETP              --->         OP2
{113} HO2      + ACO3              --->         PAA
{114} HO2      + TOLP              --->         OP2
{115} HO2      + XYLP              --->         OP2
{116} HO2      + TCO3              --->         OP2
{117} HO2      + OLN               --->         ONIT
{118} MO2      + MO2               --->   1.500*HCHO     +       HO2
{119} MO2      + ETHP              --->   0.750*HCHO     +       HO2      + 0.750*ALD
{120} MO2      + HC3P              --->   0.840*HCHO     + 0.770*ALD      + 0.260*KET
                                       +       HO2
{121} MO2      + HC5P              --->   0.770*HCHO     + 0.410*ALD      + 0.750*KET
                                       +       HO2
{122} MO2      + HC8P              --->   0.800*HCHO     + 0.460*ALD      + 1.390*KET
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Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
                                          +       HO2
{123} MO2      + OL2P              -->   1.550*HCHO     + 0.350*ALD      +       HO2
{124} MO2      + OLTP              -->   1.250*HCHO     + 0.750*ALD      +       HO2
{125} MO2      + OLIP              -->   0.890*HCHO     + 0.725*ALD      +       HO2
                                       + 0.550*KET
{126} MO2      + KETP              -->   0.750*HCHO     + 0.750*MGLY     +       HO2
{127} MO2      + ACO3              -->         HCHO     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{128} MO2      + TOLP              -->         HCHO     + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      + 2.000*HO2
{129} MO2      + XYLP              -->         HCHO     + 0.450*MGLY     + 0.806*DCB
                                       + 2.000*HO2
{130} MO2      + TCO3              -->   0.500*HCHO     + 0.445*GLY      + 0.055*MGLY
                                       + 0.500*ORA2     + 0.025*ACO3     + 0.460*HO2
                                       + 0.475*CO       +       XO2
{131} MO2      + OLN               -->   1.750*HCHO     + 0.500*HO2      +       ALD
                                       +       NO2
{132} ETHP     + ACO3              -->         ALD      + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{133} HC3P     + ACO3              -->   0.770*ALD      + 0.260*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{134} HC5P     + ACO3              -->   0.410*ALD      + 0.750*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{135} HC8P     + ACO3              -->   0.460*ALD      + 1.390*KET      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{136} OL2P     + ACO3              -->   0.800*HCHO     + 0.600*ALD      + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{137} OLTP     + ACO3              -->         ALD      + 0.500*HCHO     + 0.500*HO2
                                       + 0.500*MO2      + 0.500*ORA2
{138} OLIP     + ACO3              -->   0.725*ALD      + 0.550*KET      + 0.140*HCHO
                                       + 0.500*HO2      + 0.500*MO2      + 0.500*ORA2
{139} KETP     + ACO3              -->         MGLY     + 0.500*HO2      + 0.500*MO2
                                       + 0.500*ORA2
{140} ACO3     + ACO3              -->   2.000*MO2
{141} ACO3     + TOLP              -->         MO2      + 0.170*MGLY     + 0.160*GLY
                                       + 0.700*DCB      +       HO2
{142} ACO3     + XYLP              -->         MO2      + 0.450*MGLY     + 0.806*DCB
                                       +       HO2
{143} ACO3     + TCO3              -->         MO2      + 0.920*HO2      + 0.890*GLY
                                       + 0.110*MGLY     + 0.050*ACO3     + 0.950*CO
                                       + 2.000*XO2
{144} ACO3     + OLN               -->         HCHO     +       ALD      + 0.500*ORA2
                                       +       NO2      + 0.500*MO2
{145} OLN      + OLN               -->   2.000*HCHO     + 2.000*ALD      + 2.000*NO2
{146} XO2      + HO2               -->         OP2
{147} XO2      + MO2               -->         HCHO     +       HO2
{148} XO2      + ACO3              -->         MO2
{149} XO2      + XO2               -->
{150} XO2      + NO                -->         NO2
{151} XNO2     + NO2               -->         ONIT
{152} XNO2     + HO2               -->         OP2
{153} XNO2     + MO2               -->         HCHO     +       HO2
{154} XNO2     + ACO3              -->         MO2
{155} XNO2     + XNO2              -->
{156} TERP     + HO                -->         TERPAER  +       HO
{157} TERP     + NO3               -->         TERPAER  +       NO3
{158} TERP     + O3                -->         TERPAER  +       O3
{159} ISO      + HO                -->         ISO_RO2  + 0.079*XO2
{160} ISO_RO2  + NO                -->   0.088*ONIT     + 0.912*NO2      + 0.912*HO2
                                       + 0.362*ISOPROD  + 0.230*MACR     + 0.320*MVK
                                       + 0.629*HCHO     + 0.079*XO2
{161} ISO_RO2  + HO2               -->         OP2
{162} ISO_RO2  + ACO3              -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       + 0.362*ISOPROD  + 0.230*MACR     + 0.320*MVK
                                       + 0.629*HCHO
{163} ISO_RO2  + MO2               -->   0.500*HCHO     + 0.500*HO2      + 0.362*ISOPROD
                                       + 0.230*MACR     + 0.320*MVK      + 0.629*HCHO
{164} ISO      + O3                -->   0.600*HCHO     + 0.390*MACR     + 0.160*MVK
                                       + 0.390*ORA1     + 0.270*HO       + 0.070*HO2
                                       + 0.070*CO       + 0.200*XO2      + 0.200*MCO3
                                       + 0.150*ALD      + 0.100*ISOPROD
{165} ISO      + O3P               -->   0.750*ISOPROD  + 0.250*MCO3     + 0.250*HCHO
                                       + 0.250*MO2
{166} ISO      + NO3               -->         ISON_RO2
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Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
{167} ISON_RO2 + NO                  -->         NO2      + 0.800*ALD      + 0.800*ONIT
                                       + 0.800*HO2      + 0.200*ISOPROD  + 0.200*NO2
{168} ISON_RO2 + HO2                 -->         ONIT
{169} ISON_RO2 + ACO3                -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       +       ALD      +       ONIT
{170} ISON_RO2 + MO2                 -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                       + 0.500*ONIT
{171} MACR     + HO                  -->   0.500*MCO3     + 0.500*MACR_RO2
{172} MACR_RO2 + NO                  -->         NO2      +       HO2      + 0.840*KET
                                       + 0.840*CO       + 0.150*HCHO     + 0.150*MGLY
{173} MACR_RO2 + HO2                 -->         OP2
{174} MACR_RO2 + ACO3                -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       + 0.840*KET      + 0.840*CO       + 0.150*HCHO
                                       + 0.150*MGLY
{175} MACR_RO2 + MO2                 -->   0.650*HCHO     + 0.500*HO2      + 0.840*KET
                                       + 0.840*CO       + 0.150*MGLY
{176} MACR     + O3                  -->   0.630*ORA1     + 0.210*HO       + 0.110*HO2
                                       + 0.110*CO       + 0.200*HCHO     + 0.100*XO2
                                       + 0.100*ACO3
{177} MACR     + hv                  -->   0.660*HO2      + 0.330*MCO3     + 0.670*CO
                                       + 0.670*HCHO     + 0.670*ACO3     + 0.340*HO
                                       + 0.340*XO2
{178} MACR     + NO3                 -->   0.500*MCO3     + 0.500*HNO3     + 0.500*CO
                                       + 0.500*HO2      + 0.500*ONIT     + 0.500*XO2
{179} MVK      + HO                  -->         MVK_RO2
{180} MVK_RO2  + NO                  -->         NO2      + 0.700*ALD      + 0.700*XO2
                                       + 0.700*ACO3     + 0.300*HCHO     + 0.300*MGLY
                                       + 0.300*HO2
{181} MVK_RO2  + HO2                 -->         OP2
{182} MVK_RO2  + ACO3                -->   0.500*HO2      + 1.200*MO2      + 0.500*ORA2
                                       + 0.700*ALD      + 0.300*HCHO     + 0.300*MGLY
{183} MVK_RO2  + MO2                 -->   0.800*HCHO     + 0.500*HO2      + 0.700*ALD
                                       + 0.700*MO2      + 0.300*MGLY
{184} MVK      + O3                  -->   0.670*ORA1     + 0.160*HO       + 0.110*HO2
                                       + 0.110*CO       + 0.950*MGLY     + 0.100*HCHO
                                       + 0.050*XO2      + 0.050*ACO3
{185} MVK      + hv                  -->   0.700*ISOPROD  + 0.700*CO       + 0.300*MO2
                                       + 0.300*MCO3
{186} MPAN                           -->         MCO3     +       NO2
{187} MCO3     + NO                  -->         NO2      +       HCHO     +       ACO3
{188} MCO3     + NO2                 -->         MPAN
{189} MCO3     + HO2                 -->         PAA
{190} MCO3     + MO2                 -->   2.250*HCHO     + 0.500*HO2      + 0.500*MO2
{191} MCO3     + ACO3                -->   2.000*MO2      +       HCHO
{192} MCO3     + MCO3                -->   2.000*MO2      + 2.000*HCHO
{193} ISOPROD  + HO                  -->   0.313*ACO3     + 0.687*IP_RO2
{194} IP_RO2   + NO                  -->         NO2      +       HO2      + 0.610*CO
                                       + 0.270*ALD      + 0.030*HCHO     + 0.180*GLY
                                       + 0.210*MGLY     + 0.700*KET
{195} IP_RO2   + HO2                 -->         OP2
{196} IP_RO2   + ACO3                -->   0.500*HO2      + 0.500*MO2      + 0.500*ORA2
                                       + 0.500*ALD      + 0.500*KET
{197} IP_RO2   + MO2                 -->   0.500*HCHO     + 0.500*HO2      + 0.500*ALD
                                       + 0.500*KET
{198} ISOPROD  + O3                  -->   0.476*HO       + 0.072*HO2      + 0.168*MO2
                                       + 0.237*ACO3     + 0.100*XO2      + 0.243*CO
                                       + 0.218*HCHO     + 0.062*ALD      + 0.278*KET
                                       + 0.031*GLY      + 0.653*MGLY     + 0.044*ORA1
{199} ISOPROD  + hv                  -->   1.216*CO       + 0.434*ALD      + 0.350*HCHO
                                       + 0.216*KET      + 1.216*HO2      + 0.784*ACO3
{200} ISOPROD  + NO3                 -->   0.668*CO       + 0.332*HCHO     + 0.332*ALD
                                       +       ONIT     +       HO2      +       XO2
>-------------------------------------------------------------------------------------<


Rate Expression                                                    Rate Constant
=============================================================================
k(  1) uses photo table NO2_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k(  2) uses photo table O3O1D_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  3) uses photo table O3O3P_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
k(  4) uses photo table HONO_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  5) uses photo table HNO3_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  6) uses photo table HNO4_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k(  7) uses photo table NO3NO_RADM88    , scaled by 1.00000E+00   {0.00000E+00}
```

Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
k(  8) uses photo table NO3NO2_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k(  9) uses photo table H2O2_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 10) uses photo table HCHOmol_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 11) uses photo table HCHOrad_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 12) uses photo table ALD_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 13) uses photo table MHP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 14) uses photo table HOP_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 15) uses photo table PAA_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 16) uses photo table KETONE_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 17) uses photo table GLYform_RADM88  , scaled by 1.00000E+00   {0.00000E+00}
k( 18) uses photo table GLYmol_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 19) uses photo table MGLY_RADM88     , scaled by 1.00000E+00   {0.00000E+00}
k( 20) uses photo table UDC_RADM88      , scaled by 1.00000E+00   {0.00000E+00}
k( 21) uses photo table ORGNIT_RADM88   , scaled by 1.00000E+00   {0.00000E+00}
k( 22) =  6.0000E-34 * (T/300)**(-2.30)                           {6.09302E-34}
k( 23) =  6.5000E-12 * exp(   120.0/T)                            {9.72293E-12}
k( 24) =  1.8000E-11 * exp(   110.0/T)                            {2.60365E-11}
k( 25) =  3.2000E-11 * exp(    70.0/T)                            {4.04730E-11}
k( 26) =  2.2000E-10                                              {2.20000E-10}
k( 27) =  2.0000E-12 * exp( -1400.0/T)                            {1.82272E-14}
k( 28) =  1.6000E-12 * exp(  -940.0/T)                            {6.82650E-14}
k( 29) =  1.1000E-14 * exp(  -500.0/T)                            {2.05452E-15}
k( 30) =  3.7000E-12 * exp(   240.0/T)                            {8.27883E-12}
k( 31) is a falloff expression using:                             {1.39058E-12}
   k0   =  1.8000E-31 * (T/300)**(-3.20)
   kinf =  4.7000E-12 * (T/300)**(-1.40)
   F =  0.60,  n =  1.00
k( 32) = k( 31) / Keq,  where Keq =  2.100E-27 * exp( 10900.0/T)  {8.62399E-02}
k( 33) is a special rate expression of the form:                  {3.01634E-12}
   k = k1 + k2[M], where
   k1 =  2.2000E-13 * exp(   620.0/T)
   k2 =  1.9000E-33 * exp(   980.0/T)
k( 34) is a special rate expression of the form:                  {6.78905E-30}
   k = k1 + k2[M], where
   k1 =  3.0800E-34 * exp(  2820.0/T)
   k2 =  2.6600E-54 * exp(  3180.0/T)
k( 35) =  3.3000E-12 * exp(  -200.0/T)                            {1.68671E-12}
k( 36) is a falloff expression using:                             {4.87144E-12}
   k0   =  7.0000E-31 * (T/300)**(-2.60)
   kinf =  1.5000E-11 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 37) =  3.3000E-39 * exp(   530.0/T)                            {1.95397E-38}
k( 38) =  1.4000E-13 * exp( -2500.0/T)                            {3.18213E-17}
k( 39) =  1.7000E-11 * exp(   150.0/T)                            {2.81225E-11}
k( 40) =  2.5000E-14 * exp( -1230.0/T)                            {4.03072E-16}
k( 41) =  2.5000E-12                                              {2.50000E-12}
k( 42) is a falloff expression using:                             {1.26440E-12}
   k0   =  2.2000E-30 * (T/300)**(-4.30)
   kinf =  1.5000E-12 * (T/300)**(-0.50)
   F =  0.60,  n =  1.00
k( 43) = k( 42) / Keq,  where Keq =  1.100E-27 * exp( 11200.0/T)  {5.47034E-02}
k( 44) =  2.0000E-21                                              {2.00000E-21}
k( 45) is a falloff expression using:                             {1.14885E-11}
   k0   =  2.6000E-30 * (T/300)**(-3.20)
   kinf =  2.4000E-11 * (T/300)**(-1.30)
   F =  0.60,  n =  1.00
k( 46) is a special rate expression of the form:                  {1.47236E-13}
   k = k0 + {k3[M] / (1 + k3[M]/k2)}, where
   k0 =  7.2000E-15 * exp(   785.0/T)
   k2 =  4.1000E-16 * exp(  1440.0/T)
   k3 =  1.9000E-33 * exp(   725.0/T)
k( 47) =  1.3000E-12 * exp(   380.0/T)                            {4.65309E-12}
k( 48) =  4.6000E-11 * exp(   230.0/T)                            {9.95294E-11}
k( 49) is a falloff expression using:                             {8.88848E-13}
   k0   =  3.0000E-31 * (T/300)**(-3.30)
   kinf =  1.5000E-12 * (T/300)**( 0.00)
   F =  0.60,  n =  1.00
k( 50) =  1.5000E-13 * (1.0 + 0.6*Pressure)                       {2.40000E-13}
k( 51) =  2.8300E+01 * (T/300)**( 2.00) * exp( -1280.0/T)         {3.80672E-01}
k( 52) =  1.2330E-12 * (T/300)**( 2.00) * exp(  -444.0/T)         {2.74210E-13}
k( 53) =  1.5900E-11 * exp(  -540.0/T)                            {2.59669E-12}
k( 54) =  1.7300E-11 * exp(  -380.0/T)                            {4.83334E-12}
k( 55) =  3.6400E-11 * exp(  -380.0/T)                            {1.01696E-11}
k( 56) =  2.1500E-12 * exp(   411.0/T)                            {8.53916E-12}
```

Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
k( 57) =  5.3200E-12 * exp(   504.0/T)                          {2.88684E-11}
k( 58) =  1.0700E-11 * exp(   549.0/T)                          {6.75269E-11}
k( 59) =  2.1000E-12 * exp(   322.0/T)                          {6.18715E-12}
k( 60) =  1.8900E-11 * exp(   116.0/T)                          {2.78943E-11}
k( 61) =  4.0000E-11                                            {4.00000E-11}
k( 62) =  9.0000E-01 * k( 61)                                   {3.60000E-11}
k( 63) =  9.0000E-12                                            {9.00000E-12}
k( 64) =  6.8700E-12 * exp(   256.0/T)                          {1.62197E-11}
k( 65) =  1.2000E-11 * exp(  -745.0/T)                          {9.85020E-13}
k( 66) =  1.1500E-11                                            {1.15000E-11}
k( 67) =  1.7000E-11                                            {1.70000E-11}
k( 68) =  2.8000E-11                                            {2.80000E-11}
k( 69) =  1.0000E-11                                            {1.00000E-11}
k( 70) =  1.0000E-11                                            {1.00000E-11}
k( 71) =  1.0000E-11                                            {1.00000E-11}
k( 72) =  6.1650E-13 * (T/300)**( 2.00) * exp(  -444.0/T)       {1.37105E-13}
k( 73) =  1.5500E-11 * exp(  -540.0/T)                          {2.53137E-12}
k( 74) =  2.8000E-12 * exp(   181.0/T)                          {5.13974E-12}
k( 75) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 76) =  4.7000E-12                                            {4.70000E-12}
k( 77) =  1.9500E+16 * exp(-13543.0/T)                          {3.57235E-04}
k( 78) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 79) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 80) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 81) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 82) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 83) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 84) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 85) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 86) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 87) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 88) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 89) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 90) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 91) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k( 92) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 93) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 94) =  6.0000E-13 * exp( -2058.0/T)                          {6.01030E-16}
k( 95) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 96) =  1.4000E-12 * exp( -1900.0/T)                          {2.38307E-15}
k( 97) =  2.2000E-11                                            {2.20000E-11}
k( 98) =  2.0000E-12 * exp( -2923.0/T)                          {1.09940E-16}
k( 99) =  1.0000E-11 * exp( -1895.0/T)                          {1.73099E-14}
k(100) =  3.2300E-11 * exp(  -975.0/T)                          {1.22539E-12}
k(101) =  1.2000E-14 * exp( -2633.0/T)                          {1.74559E-18}
k(102) =  1.3200E-14 * exp( -2105.0/T)                          {1.12933E-17}
k(103) =  7.2900E-15 * exp( -1136.0/T)                          {1.61125E-16}
k(104) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(105) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(106) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(107) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(108) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(109) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(110) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(111) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(112) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(113) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(114) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(115) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(116) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(117) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(118) =  1.9000E-13 * exp(   220.0/T)                          {3.97533E-13}
k(119) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(120) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(121) =  3.4000E-14 * exp(   220.0/T)                          {7.11376E-14}
k(122) =  2.9000E-14 * exp(   220.0/T)                          {6.06762E-14}
k(123) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(124) =  1.4000E-13 * exp(   220.0/T)                          {2.92919E-13}
k(125) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(126) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(127) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
k(128) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(129) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(130) =  9.6000E-13 * exp(   220.0/T)                          {2.00859E-12}
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Table 8A-12. RADM2_CIS4_AE and RADM2_CIS4_AE_AQ Mechanisms

```
k(131) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(132) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(133) =  1.0000E-13 * exp(   220.0/T)                          {2.09228E-13}
k(134) =  8.4000E-14 * exp(   220.0/T)                          {1.75752E-13}
k(135) =  7.2000E-14 * exp(   220.0/T)                          {1.50644E-13}
k(136) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(137) =  3.4000E-13 * exp(   220.0/T)                          {7.11376E-13}
k(138) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(139) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(140) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(141) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(142) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(143) =  1.1900E-12 * exp(   220.0/T)                          {2.48981E-12}
k(144) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(145) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(146) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(147) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(148) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(149) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(150) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(151) =  4.2000E-12 * exp(   180.0/T)                          {7.68378E-12}
k(152) =  7.7000E-14 * exp(  1300.0/T)                          {6.04038E-12}
k(153) =  1.7000E-14 * exp(   220.0/T)                          {3.55688E-14}
k(154) =  4.2000E-14 * exp(   220.0/T)                          {8.78758E-14}
k(155) =  3.6000E-16 * exp(   220.0/T)                          {7.53221E-16}
k(156) =  1.0000E+00 * k( 58)                                   {6.75269E-11}
k(157) =  1.0000E+00 * k(100)                                   {1.22539E-12}
k(158) =  1.0000E+00 * k(103)                                   {1.61125E-16}
k(159) =  2.5400E-11 * (T/300)**( 1.00) * exp(   407.6/T)       {9.90719E-11}
k(160) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(161) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(162) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(163) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(164) =  7.8600E-15 * (T/300)**( 1.00) * exp( -1912.2/T)       {1.27569E-17}
k(165) =  3.6000E-11                                            {3.60000E-11}
k(166) =  3.0300E-12 * (T/300)**( 1.00) * exp(  -447.9/T)       {6.69552E-13}
k(167) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(168) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(169) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(170) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(171) =  1.8600E-11 * (T/300)**( 1.00) * exp(   176.1/T)       {3.33618E-11}
k(172) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(173) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(174) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(175) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(176) =  1.3600E-15 * (T/300)**( 1.00) * exp( -2113.5/T)       {1.12330E-18}
k(177) uses photo table ACROLEIN       , scaled by 3.60000E-03  {0.00000E+00}
k(178) =  1.5000E-12 * (T/300)**( 1.00) * exp( -1726.0/T)       {4.54753E-15}
k(179) =  4.1400E-12 * (T/300)**( 1.00) * exp(   452.9/T)       {1.87990E-11}
k(180) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(181) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(182) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(183) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(184) =  7.5100E-16 * (T/300)**( 1.00) * exp( -1519.7/T)       {4.54966E-18}
k(185) uses photo table ACROLEIN       , scaled by 1.11000E-02  {0.00000E+00}
k(186) =  1.6000E+16 * (T/300)**( 1.00) * exp(-13486.0/T)       {3.52536E-04}
k(187) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(188) =  2.8000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {5.10890E-12}
k(189) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(190) =  9.6000E-13 * (T/300)**( 1.00) * exp(   221.4/T)       {2.00460E-12}
k(191) =  1.1900E-12 * (T/300)**( 1.00) * exp(   221.4/T)       {2.48486E-12}
k(192) =  1.1900E-12 * (T/300)**( 1.00) * exp(   221.4/T)       {2.48486E-12}
k(193) =  3.3600E-11                                            {3.36000E-11}
k(194) =  4.2000E-12 * (T/300)**( 1.00) * exp(   181.2/T)       {7.66335E-12}
k(195) =  7.7000E-14 * (T/300)**( 1.00) * exp(  1298.3/T)       {5.96598E-12}
k(196) =  8.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {1.75402E-13}
k(197) =  3.4000E-14 * (T/300)**( 1.00) * exp(   221.4/T)       {7.09961E-14}
k(198) =  7.1100E-18                                            {7.11000E-18}
k(199) uses photo table ACROLEIN       , scaled by 3.60000E-03  {0.00000E+00}
k(200) =  1.0000E-13                                            {1.00000E-13}
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