

Revisions to Photochemical Data for Use in Atmospheric Modeling

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Solar and stellar flux incident on an atmosphere can cause molecules to dissociate into highly reactive species and allows for photochemical processes to play a fundamental role in atmospheric chemistry. While models have tried to simulate such processes, they are extremely sensitive to photoabsorption cross-sections and quantum yields: two parameters that are important in determining the photodissociation rate, and hence the lifetime, of atmospheric compounds. Obtaining high-resolution and current data for these parameters is therefore highly desirable. Due to this, database and literature searches for high-quality cross-sections and quantum yields were performed and compiled for KINETICS, a Caltech/JPL Chemical Transport Model that can be used in modeling planetary atmospheres. Furthermore, photodissociation rates determined by running a Titan 1-D model were used to verify the completeness of these latest revisions.

Nomenclature

J	= photodissociation rate
z	= altitude
λ	= wavelength
q	= quantum yield (branching ratio)
σ	= photoabsorption cross-section
F	= incident UV solar or stellar flux
I_0	= incident light intensity
I	= transmitted light intensity
d	= absorption path length
n	= absorber concentration

I. Introduction

IN 1981, Allen, et al. developed the initial version of the Caltech/JPL KINETICS Chemical Transport Model (CTM) as a way to model the Earth's lower thermosphere and mesosphere.¹ The model was instrumental in producing the first photochemical model of Titan after the Voyager flybys² and has since been used to model the Martian atmosphere,³ Jupiter, Neptune, comets, exoplanets, molecular clouds, and protostellar disks.⁴

Written in FORTRAN 90, KINETICS can be run in several modes, the simplest being a 1-D mode where chemical abundances are calculated in a column extending vertically through an atmosphere. This method provides a global average of the atmosphere's chemical composition. More complex modes, such as 2-D and 3-D, consider air movement in a north-south direction and consider latitude-dependency by modeling the how the radiation field received by different latitudes in the atmosphere affect chemical composition. All modes account for the diurnal cycle between night and day.

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For inputs, the code requires a list of species and their abundances, a list of reactions, diffusion coefficients, boundary conditions, photoabsorption cross-sections, solar/stellar flux, and physical conditions such as density, temperature, and pressure. Chemical abundances are then output as a function of time and position.⁵

The following subsections provide motivation and theoretical background for the revisions made to the photochemical database that KINETICS uses for modeling.

A. Motivation

The unique chemical nature of Titan's atmosphere has intrigued researchers from across multiple scientific disciplines due to photochemical processes generating complex organic molecules throughout the atmosphere. Moreover, researchers are interested in the chemical evolution of Titan's atmosphere since it might provide insights into the atmosphere of early Earth.⁶

Titan is the only satellite in the solar system that has a dense atmosphere. In fact, the atmospheric pressure on Titan is greater than that on Earth with the pressure reaching 1.5 bars at the surface. Data from the Cassini Composite Infrared Spectrometer (CCIS) has shown that Titan's atmosphere is composed of 95-98% nitrogen, 1.8-5.0% methane, and 0.1-0.2% hydrogen along with trace amounts of CO, ⁴⁰Ar, and organics. Temperatures range from 70 to 180 K depending on the altitude as seen in Fig. 1.⁷

Hydrocarbon photochemistry on Titan is primarily driven by the photodissociation of methane at high altitudes for wavelengths less than 145 nm.⁸ Similarly, the formation of excited atomic nitrogen that forms from the dissociation of N₂ above 700 km can form nitriles when it reacts with hydrocarbons. Interestingly, long-wavelength UV radiation (>155 nm) can cause photolysis of light hydrocarbons, resulting in a mixture of more complex organic molecules known as the "photochemical haze" of Titan.⁷

As described by Vuitton and co-workers,⁹ Titan is of such great interest because it is one of the few places in the Solar System where such complex atmospheric organic chemistry is currently taking place. Also, the large amount of observational data obtained from the Cassini-Huygens mission in 2005 has sparked a renewed interest in Titan. Even with observational evidence, assessing the extent that organic chemistry plays in Titan's atmosphere still requires the development of a comprehensive model of the satellite's atmosphere.⁵

Interest in modeling Titan's atmosphere began in earnest after Voyagers 1 and 2 flew past the satellite in November 1981. In 1984, Yuk Yung and Mark Allen developed the first comprehensive photochemical model of Titan's atmosphere.² Their model showed that N₂ was readily dissociated by electrons and short-wavelength photons in the upper atmosphere and CH₄ dissociation occurring indirectly in the stratosphere. Later models were developed that improved upon the chemistry and physics but none of them have fully been able to reproduce the set of available observations.⁹ Part of this has been due to the experimental errors introduced in the model's parameters, which are covered in the next section.

Not to be mistaken, while Titan is one of the primary motivations for updating the photochemical database of KINETICS, these updates have wide applicability and could be used in modeling atmospheres such as those of Mars, Earth, and even exoplanets.

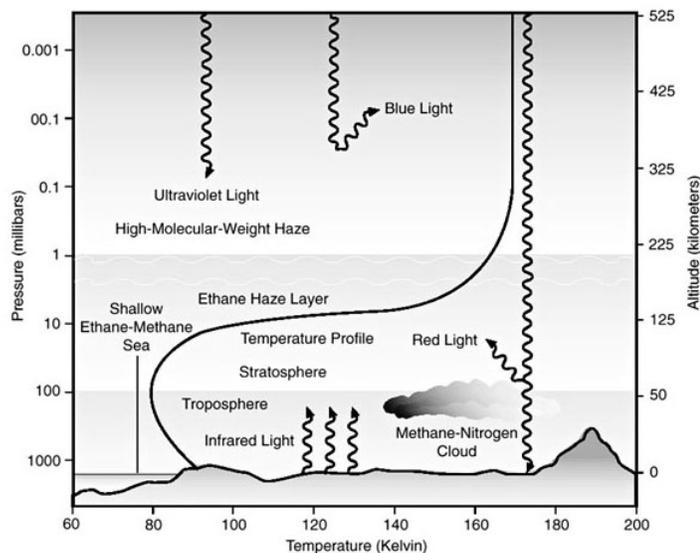


Figure 1. Schematic of Titan's atmosphere. This schematic of Titan's atmosphere shows how the temperature (in Kelvin) changes relative to altitude (in kilometers) as well as demonstrates that higher energy ultraviolet and blue light traverse less through the atmosphere than lower energy red light. Image credit: Penn State University.

B. Theoretical Background

Photodissociation rates for atmospheric molecules are necessary in order to determine the abundances, and hence evolution, of molecular species over time. For a particular photochemical pathway of a species, i , at altitude, z , the photodissociation rate is given by:

$$J_i(z) = \int_{\lambda_1}^{\lambda_2} q_i(\lambda, T) \sigma_i(\lambda, T) F(\lambda, z) d\lambda \quad (1)$$

where $q(\lambda, T)$ is the quantum yield, or branching ratio, for a particular photochemical pathway of a species, $\sigma(\lambda, T)$ is the photoabsorption cross-section of the species, and $F(\lambda, z)$ is the incident UV solar or stellar flux on the atmosphere.

The quantum yield is the probability that a particular pathway will proceed after a photon hits the parent species. As such, it is dimensionless, but it is also wavelength-dependent and can be temperature-dependent for some species.

Likewise, photoabsorption cross-sections represent the effective area that a photon must traverse in order to be absorbed by the molecule. It is defined by the Beer-Lambert law describing the attenuation of light by a homogeneous absorbing system:

$$I = I_0 e^{-\sigma dn} \quad (2)$$

Where I_0 and I are the incident and transmitted light intensities, respectively, d is the absorption path length (in cm), n is the concentration of the absorber (in molecules/cm³) and σ is the absorption cross-section.¹⁰ While the KINETICS model requires that cross-sections have units of cm²/molecule, cross-sections can also be measured in barns and other units.

Thus, the larger the cross-section, the easier it is to excite and/or dissociate the molecule. Like quantum yields, cross-sections are wavelength-dependent and can be temperature-dependent for some species as shown in Fig. 2.

At the present moment, a large amount of uncertainty is intrinsic in both cross-sections and quantum yields since photochemical reactions studied in the laboratory tend to be more representative of the conditions on Earth. As a result, there is a limited amount of low-temperature, low-pressure kinetic data available for modeling planetary atmospheres like that of Titan or Mars. As a result, modelers are often forced to extrapolate data for many species to low temperatures, which adds uncertainty into the data. Since photochemical systems are heavily coupled and strongly non-linear, even small errors can cause inaccurate results.⁸

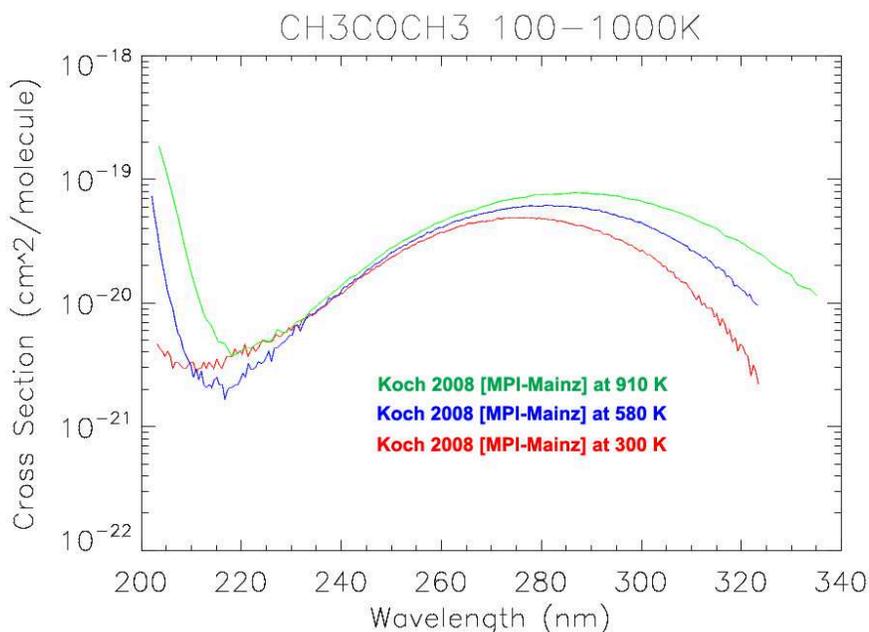
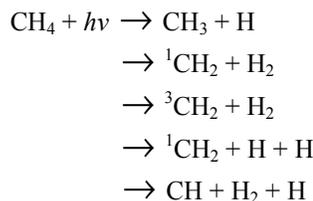


Figure 2. Temperature-Dependence of Acetone (CH₃COCH₃) Photoabsorption Cross-Section. This plot shows the temperature-dependence of the cross-section for acetone at three different temperatures ranging from 300 to 910 K.

To illustrate, consider the primary photodissociation channels of methane at Lyman- α :



The abundances of propylene (C_3H_6) and propyne ($\text{CH}_3\text{C}_2\text{H}$) have been shown to be quite sensitive to which photodissociation channels of methane are the most dominant. However, since there is already experimental error in the quantum yields for each channel at room temperature, extrapolating the data to lower temperatures introduces even larger amounts of uncertainty to the data, thus affecting the final abundances of species.⁸

Until experiments are done at lower temperatures and pressures to obtain kinetic data for a larger variety of atmospheric models, this issue will be present. Until then, the best alternative for atmospheric modelers is to incorporate the highest resolution and most current photoabsorption cross-sections and quantum yields in their models.

II. Methods

A. Data Collection

Database and literature searches have been completed to obtain high-quality photoabsorption cross-sections and quantum yields for use in KINETICS. While cross-sectional and quantum yield data exist for a multitude of molecules, the primary emphasis for this search has been focused on finding data for species that actually appear in KINDATA: the master list that contains all the species and reactions used by KINETICS. Cross-sectional data was still collected for molecules that are not yet in KINDATA, and their availability will be of use when reactions that refer to these species are added in the future. Furthermore, cross-sectional and quantum yield data was limited to the wavelength range between 20 and 800 nm, so most infrared data was excluded from the search.

This work continues and completes the work commenced by David Caratelli, an intern in the group in the summer of 2010. The current update necessitated the use of nine databases to find high-resolution cross-sections and quantum yields. Literature searches were also performed using Web of Science and SciFinder to find updates to species that the databases did not yet index. Furthermore, for the first time, the photochemical database now contains recommendations from both the IUPAC Subcommittee for Gas Kinetic Data Evaluation¹¹ as well as the NASA Panel for Data Evaluation,¹² which prepares and compiles kinetic and photochemical data. Observations and remarks on the nine databases used in the update follow. Moreover, Appendix A contains the website URLs for these databases as of August 2012.

MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules

Arguably the most comprehensive and complete of all the databases, MPI-Mainz contains photoabsorption cross-sections that are already in the format required by KINETICS with wavelength already in nanometers (or angstroms) and cross-sections in $\text{cm}^2/\text{molecule}$. Its database of over 900 species contains data for many families of molecules: from halogenated compounds to radicals to nitrogenous species to organics. However, it does not contain any cross-sections for ionized or atomic species at the present time. Furthermore, while it just started to catalog quantum yields in 2010, this part of the database is still being updated, so more quantum yields may appear in this database in the coming years.

science-softCon UV/Vis⁺ Spectra Database (UV/Vis⁺ Photochemistry Database)

Following MPI-Mainz in terms of comprehensiveness, science-softCon had updates to cross-sections that were just published in the past year, and it had the most accessible updates to quantum yield studies. Unfortunately, it commonly does not provide data files containing cross-sections or quantum yields for its references, even though a subscription to the database was recently purchased by JPL. Thus, a literature search is usually necessary to find the reference and extract the data from the article itself. Even with this downside, a dedicated science team

continually monitors the literature for updates to the database, and the database did provide useful data references that other databases did not index.

HITRAN on the Web

HITRAN is a compilation of useful spectroscopic parameters that can be used by atmospheric computer models and is currently being developed at the Harvard-Smithsonian Center for Astrophysics under the Atomic and Molecular Physics Division. The latest data set available at the time is HITRAN 2008 (Version 13). HITRAN on the Web allows users to access relevant parts of the HITRAN database online instead of via FTP. It also allows for easy visualization of data, but unfortunately mixes IR and UV-Vis spectra together, so it's important to be aware of the wavelength range. At the moment, it only contains the most commonly considered molecules in atmospheric models. Furthermore, all UV and visible data was extracted from this database.

Photo Ionization/Dissociation RATES (PHIDRATES) from the Southwest Research Institute:

Containing cross-sections for 38 atomic neutrals and 30 atomic ions, this database is useful for finding data for atomic neutrals and ions. Moreover, this database also lists high-resolution data for both total and partial cross-sections, which is of use when determining the quantum yield. Unfortunately, it contains only the most common polyatomic molecules, so it isn't as comprehensive as MPI-Mainz or science-softCon.

IUP-Bremen

IUP-Bremen contains high-resolution reference spectra available for download, and it also compiles a selection of cross-sections collected from around the web. However, the cross-sections under 'DLR-Database' are not the most recent and can usually be found on MPI-Mainz or science-softCon. All UV and visible data was extracted from this database.

Harvard-Smithsonian Center for Astrophysics (CFA)

Provided extremely high-resolution cross-sections for eight common atmospheric molecules, and data files were well organized. All UV and visible data was extracted from this database.

GEISA-2011

The 2011 edition contains extremely high-resolution cross-sections for some common atmospheric molecules. Moreover, it also easily displays what pressure a cross-section was measured at, which is something that many other databases do not track. All UV and visible data was extracted from this database.

Leiden Database

Excellent source for finding the cross-sections of small charged-species and unsaturated organic species. As stated in the database, no systematic updates have been made to the site since 1990, so more recent cross-sections are not indexed.

National Institute for Fusion Science (NIFS)

While a bit of time is needed to convert data into the necessary format for KINETICS, this database was useful in obtaining cross-sections for some atomic and polyatomic species. Moreover, the data was recently published in 2010. All UV and visible data was extracted from this database.

Steps have been taken to prevent cross-sectional data for isomers from accidentally being combined or merged. For instance, the previous naming system had no way of differentiating between benzene and dipropargyl (both have molecular formula of C_6H_6) or telling whether the double bond was located on the first or second carbon in pentene. When relevant, stereoisomerism was also mentioned. As such, molecular names have been added to files that have an ambiguous molecular formula.

Along with appending molecular names to some data files, a few other changes were added to the standard filename for both cross-sections and quantum yields. To start, the standard filename for cross-sections is:

MolecularFormula_Author(s)_Temperature(in Kelvin)_CROSS_hires.dat

Data sets that were updated or created this summer have *sum12* appended to the end of the file name. Furthermore, some sources provided cross-sections of molecules at the same temperature but were taken at different pressures. In these cases, the pressure that the cross-section was taken at is provided after the temperature. Considering quantum yields, the standard filename is:

PhotochemicalReaction_Author(s)_BR_hires.dat

Like the cross-sections, filenames ending in *sum12* means the file was created or updated during this summer. Moreover, temperature data was included, if available.

B. Analysis of Raw Data

Following the completion of collecting photoabsorption cross-sections and quantum yields from literature searches and across multiple databases, the resulting raw data files for each molecule were analyzed to determine whether they should be incorporated into KINETICS. A set of standards was developed that helped in guiding this analysis. The following standards were originally created to manage and account for the massive number of cross-sectional raw data, but the standards were also applied to quantum yields when applicable.

While cross-sectional data is temperature-dependent, data files that were in a similar temperature range were grouped together during analysis. All ranges are defined to begin when the last digit is a one and end when the last digit is a zero. Thus, any cross-sectional data that falls between 291 and 300 K, inclusively, are grouped together and analyzed. Moreover, all temperature ranges are labeled with the last digit as a five. Using the 291 to 300 K range as an example, that range would be labeled as 295 K.

The primary motive for grouping cross-sections together rather than analyzing each temperature separately was to avoid the scenario of having excellent, high-resolution data at one temperature and having less than prime data at a temperature only a few Kelvin away. Since both would have almost equal weighting, the poor quality data would have the same influence in KINETICS as the high quality data, which is unwanted. Thus, ranges were adopted to help prevent old and poor quality data from being incorporated into the final data set.

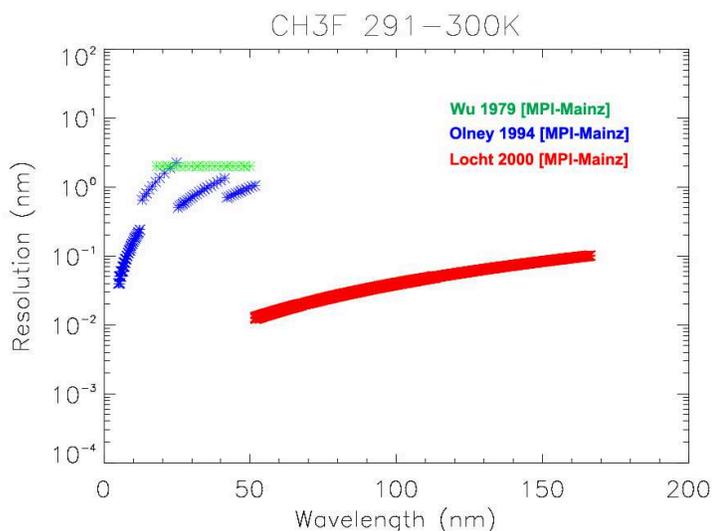


Figure 3. Wavelength coverage versus resolution for CH_3F . Since Locht 2000 has the largest wavelength coverage and, in this case, has the highest resolution data in this temperature region, it is listed first in the script file. Moreover, Olney 1994 would be listed second because it provides cross-sectional data in a wavelength region not covered by Locht. Wu 1979 would be excluded from the finalized data set because it is of lower resolution and provides no new information.

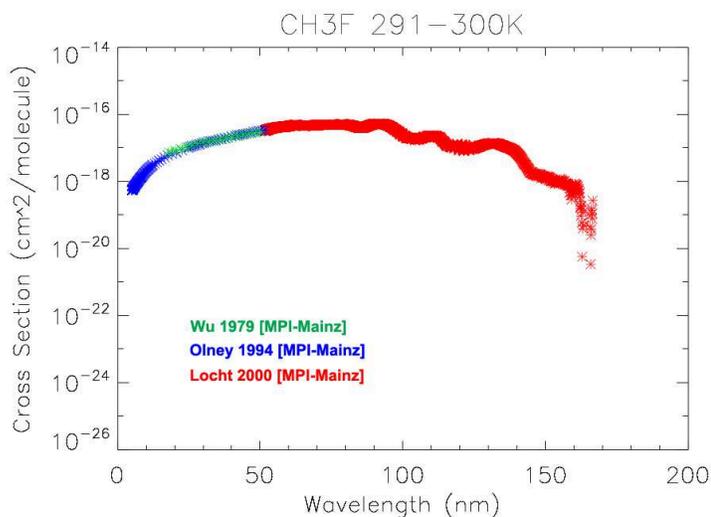


Figure 4. Wavelength coverage versus actual cross-section for CH_3F . This type of plot provides the opportunity to check for discontinuities or any poor-fitting data in one of the individual data sets. In the case for CH_3F , the data fit relatively well between Olney and Locht, so both were included in the finalized data set.

After grouping individual cross-sections into their respective temperature range, the resolution, wavelength coverage, and actual cross-section were considered for each individual data set in the group. Since it was uncommon for databases to readily list the resolution that a cross-section was taken at, the resolution was defined to be the wavelength interval between one data point and its immediate neighbor in the dataset.

Each group of cross-sections for a particular molecule and temperature range were first plotted according to wavelength coverage versus resolution, as in Fig. 3 depicting CH₃F. Data sets with the longest wavelength coverage were listed first in script files used by CROSSDISK¹ because CROSSDISK layers individual data sets on top of each other to create a single, merged file. Thus, the second file listed in the input script is layered on top of the first, the third on top of the second, and so on and so forth.

Listed below the file with the longest wavelength coverage were data sets that had higher resolution than the previously listed file but also shorter wavelength coverage. Sometimes data sets were added that may be of lower resolution, but provided data in a region where other data sets did not cover.

Data sets were not blindly included based solely on this type of plot. Along with plotting wavelength coverage versus resolution, graphs of the actual cross-sections were also plotted over the wavelength region to see whether proposed cross-sections to be included in the final, merged file fit relatively well with other studies. Figure 4 illustrates this by using CH₃F as an example. Thus, even if a cross-section covered a large wavelength range or had a high-resolution, it was not included if it contained poor quality data that didn't fit well with other studies and recommendations or was too old of a data set that its quality became questionable.

At times when two studies conflicted with each other, it was highly useful to check recommendations from both the IUPAC Subcommittee for Gas Kinetic Data Evaluation as well as the NASA Panel for Data Evaluation to resolve the discrepancy. If no recommendation was available, the cross-sections for that molecule at other temperature ranges were looked at to determine the general trend for the cross-section of that molecule.

If a single source for a molecule at the same temperature included cross-sections that were measured at different pressures, the data set that was created with the lowest pressure was analyzed. Also, when a database did not provide a temperature for a particular cross-section or quantum yield, it was assumed that the cross-section was taken at room temperature and is thus included in the 295 K temperature range. Files with an unknown temperature are labeled *boh* in the filename.

III. Preliminary Results

To determine how the updates affected the results generated by KINETICS, a simple 1-D model of the Titan atmosphere was run over a small time step of 10⁻¹⁵ seconds to see how the updates affected the photodissociation rates used in the model.

While a more comprehensive analysis of how the updates affected the model will be discussed in a future paper, a couple of preliminary photodissociation rates from a Titan 1-D model are presented to show the effect the update had on a few particular rates. For instance, the total photodissociation rate for N₂ and H₂ in altitudes greater than 837 kilometers in Titan's atmosphere changed by less than 20 percent of the old value; whereas, the change was greater than 20 percent in altitudes below 837 kilometers. Likewise, the change in the photodissociation rate of CH₄ was less than 20 percent in altitudes greater than 803 kilometers and more than 20 percent at lower altitudes.

As a result of this update, the total number of molecules having cross-sectional data in KINETICS has risen from 250 molecules to nearly 320 molecules. Moreover, 141 of the 250 molecules that already had cross-sectional data before this endeavor started had higher-resolution updates to their cross-sections. Multiple updates have also been made to quantum yields, especially those of some chlorine and nitrogen oxides. Furthermore, data for molecules not yet in KINDATA will be useful when new photodissociation reactions are added in the future. Moreover, it is evident that more experiments are needed to determine the photoabsorption cross-sections and quantum yields at lower temperatures as well as for more photodissociation channels and molecules, especially those of ionic species.

IV. Conclusion

High-resolution and current updates to photoabsorption cross-sections and quantum yields have been collected across multiple databases and literature sources as well as analyzed and compiled for use by KINETICS. As a result,

¹CROSSDISK was developed by Jason Weibel, a graduate student at the California Institute of Technology. The program compiles and merges individual cross-sectional data files for a particular molecule and temperature range together into a single high-resolution file, which is then converted to a low-resolution file that is used by KINETICS. Data is downsampled to average away minor differences that occur between data sets from different authors.

the current photochemical database represents the most comprehensive collection of data that KINETICS has ever used. Moreover, the update will allow for more complex models to be made of planetary atmospheres in the solar system and of molecular clouds and exoplanets.

Appendix A

The following list contains the URLs for the databases used in this update. Links are current as of August 2012.

- MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules: <http://www.atmosphere.mpg.de/enid/2295>
- science-softCon UV/Vis⁺ Spectra Database (UV/Vis⁺ Photochemistry Database): <http://www.science-softcon.de/spektrum> (spectra only available on JPL network)
- HITRAN on the Web: <http://hitran.iao.ru/en/en/xsect>
- Photo Ionization/Dissociation RATES (PHIDRATES) from the Southwest Research Institute: <http://phidrates.space.swri.edu>
- IUP-Bremen: <http://www.iup-physik.uni-bremen.de/gruppen/molspec/databases/referencespectra/index.html>
- Harvard-Smithsonian Center for Astrophysics (CFA): <http://www.cfa.harvard.edu/amp/ampdata/cfamols.html>
- GEISA-2011: <http://ether.ipsl.jussieu.fr/etherTypo/?id=1293&L=0>
- Leiden Database: <http://home.strw.leidenuniv.nl/~ewine/photo/index.php?file=pd.php>
- National Institute for Fusion Science (NIFS): http://dpc.nifs.ac.jp/photoab/d_list.html

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