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# The UMIST database for astrochemistry 1999*

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**Abstract.** We report a new version of the UMIST database for astrochemistry. The previous (1995) version has been updated and its format has been revised. The database contains the rate coefficients, temperature ranges and – where available – the temperature dependence of 4113 gas-phase reactions important in astrophysical environments. The data involve 396 species and 12 elements. We have also tabulated permanent electric dipole moments of the neutral species and heats of formation. A new table lists the photo process cross sections (ionisation, dissociation, fragmentation) for a few species for which these quantities have been measured. Data for Deuterium fractionation are given in a separate table. Finally, a new online Java applet for data extraction has been created and its use is explained in detail. The detailed new datafiles and associated software are available on the World Wide Web at http://www.rate99.co.uk.

**Key words:** molecular data — molecular processes — ISM: molecules — circumstellar matter

## 1. Introduction

The UMIST Database is widely used by the scientific community in modelling chemical kinetics in the interstellar medium. In this paper, we report on the latest release of the database and on electronic access to our full range of data and related codes. In recent years, some very large models, often containing up to 10 000 reactions, have been published. Our latest release takes a much more circumspect approach with the number of reactions extended by 249 compared to the previous release (Millar et al. 1997), to a total of 4113. Large systems often take a generic approach to the rate coefficients and chemical reactions included by extending particular reactions applicable to smaller species to much larger systems. While this is a useful approach in determining whether or not large molecules may form, it is not based generally on thermodynamics which can affect particular reactions.

In recent years, there has been an increasing need to model the chemical kinetics of hot circumstellar envelopes and interstellar shocks, with the result that we have reviewed the temperature dependence and temperature range validity of each reaction. Although not yet totally accurate, we believe this new piece of data should make models noticeably more reliable. In addition, we have included a number of three-body reactions which are of particular importance in high density environments, such as protoplanetary disks. In Sect. 2, the new conventions adopted to tabulate the species and their possible isomers are explained. Also, a few words of caution are given on the data, mainly concerning the lack of distinction between certain isomers. Section 3 describes the content of the database and the new format used. Section 4 gives details on the new data that have been included in our online database set. Finally, Sect. 5 reports on the use of the newly developed Java applet which has been designed to enable the user to select and save to a local disk particular data.

## 2. The species and related data

The whole set of reactions contains 396 species (excluding the electrons), made from the 12 following elements: H, He, C, N, O, Na, Mg, Si, P, S, Cl, Fe. The species are tabulated in Table 1 and their heats of formation, where available, are listed in Table 2, while the dipole moments of the neutral molecules are given in Table 3.

### *2.1. The nomenclature*

The functional site on the species has been highlighted whenever possible by writing it under a pseudo-developed

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* Table 8 is only available in electronic form at http://www.edpsciences.org and http://www.rate99.co.uk

form on the right of the species formula. Carboxylic acids end in "COOH", aldehydes in "CHO", alcohols in "COH", thiols in "SH", etc. For unsaturated or radical compounds the situation is more complex. For cyanopolyynes $HC_nN$, a condensed formula is sufficient to describe the molecule because its triple and single bonds are regularly alternated. For other species, the formula should appear obvious: the charge on C2H7O+ is not on the same atom as for C2H6OH+; HCN carries H on C, whereas HNC carries H on the N atom. All the $C_nH_m$ molecules are meant to be linear chains when written under their condensed form.

But there are difficult cases: for example, C3H3+ and H2C3H+ differ by their geometry: C3H3+ is a cycle, whereas H2C3H+ is linear with one triple bond ($H_2C$–C≡$CH^+$); Also, due to the lack of precision on the isomeric nature of $C_3H_n$, $n = 0..3$, used in experiments and mentioned in the literature, no distinction has been made between l-$C_3H_n$ and c-$C_3H_n$, as sometimes experiments cannot discriminate between the isomers (e.g., propyne HC≡C–$CH_3$ and allene $H_2C$=C=$CH_2$). Therefore for more detailed data, the user is encouraged to refer to the bibliographic references.

The other delicate isomer distinction is between H2CCC, which carries both H on the same carbon atom, and C3H2, where both H are on distinct C atoms.

### *2.2. The conventions*

Termolecular and collider reactions contain a catalyst species, the nature of which is not specified and is simply noted "M". Software – available on-line on http://www.rate99.co.uk – which turns kinetic reaction sets into differential equation subroutines, automatically replaces M by the medium number density. To increase data readability for the user, the names of the two-letter elements have been rewritten as a capital letter followed by a lower-case letter (e.g. HE → He; SI → Si) and the electrons have been changed from "ELECTR" to "e-".

## 3. The reaction set

Table 8 contains all the reactions and associated rate coefficients, and is available online at

http://www.rate99.co.uk
http://www.edpsciences.org

### *3.1. The new entry format*

The number of observed and predicted astrophysical species increases steadily with time, and with it, the size of their formula (e.g. ethyl methyl ether, $C_2H_5OCH_3$, has been discussed as a possible interstellar molecule). To account for this, we have altered the format for the names of the species by increasing by one letter, making them 8-character strings. Also, the smallest products in a four-product reaction are mostly H and/or He, therefore only 4 characters have been allocated for the last two products. The necessity to consider termolecular reactions for high density environments means that a third species must be included on the reactant side of these reactions. To account for that, each reaction now comprises *three* reactants and four products. Our new reaction format reads:

I, R1, R2, R3, P1, P2, P3, P4, $\alpha$, $\beta$, $\gamma$, *flags*

where I is the reaction number, R1 to R3 are the reactants, P1 to P4 are the products, and $\alpha$, $\beta$ and $\gamma$ are the constants used to determine the rate coefficients. The series of flags is a string of 16 characters and/or digits that store respectively:

- the kind of data: measured M, estimated E, calculated C or literature search L, with format A1. Here "literature search" means that the given datum is a compilation of several other data (measured and/or calculated). The sources of these data are mainly Baulch et al. (1992) and the NIST database (Mallard et al. 1998);
- the lowest and highest temperatures defining the temperature range, format 2(I5). Each temperature is given as an integer number of kelvins in the range $10 < T < 41\,000$ K;
- the error on the rate value, format A1. The following scheme has been used:
  - "A". Error < 25%
  - "B". Error < 50%
  - "C". Error within a factor of 2
  - "D". Error within an order of magnitude
  - "E". Highly uncertain;
- the reference code, format A4. The references are listed in Table 4.

The full entry format in Fortran is correspondingly written as:

```
I4, 5(1X, A8), 2(1X, A4), 1X, 1PE8.2, 3X,
0PF5.2, 2X, 0PF8.1, A1, 2(I5), A1, A4.
```

### *3.2. Calculation of the rates from $\alpha$, $\beta$ and $\gamma$*

For two- or three-body reactions, the rate coefficient is given by:

$$k = \alpha\,(T/300)^{\beta}\,\exp(-\gamma/T) \qquad \mathrm{cm^3\ s^{-1}} \tag{1}$$

where $T$ is the gas temperature.
For direct cosmic-ray ionisation (R2 = CRP):

$$k = \alpha \qquad \mathrm{s^{-1}} \tag{2}$$

whereas for cosmic-ray-induced photoreactions (R2 = CRPHOT):

$$k = \alpha\,(T/300)^{\beta}\,\gamma/(1-\omega) \qquad \mathrm{s^{-1}} \tag{3}$$

**Table 1.** List of the species found in the database. The 396 species are classified by their number of atoms and are vertically ordered by mass

| Number of atoms | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | $\geq 9$ |
| H− | H2+ | H3+ | CH3+ | CH4+ | CH5+ | C2H5+ | C2H6+ | C2H7+ |
| H+ | H2 | CH2+ | CH3 | CH4 | C2H4+ | C2H5 | C2H6 | CH3OCH3+ |
| H | HeH+ | CH2 | NH3+ | NH4+ | C2H4 | CH3OH2+ | C3H5+ | C2H5OH+ |
| He+ | CH+ | NH2+ | NH3 | C2H3+ | CH2NH2+ | C3H4+ | H5C2O+ | CH3OCH3 |
| He | CH | NH2 | H3O+ | C2H3 | CH4N+ | C3H4 | C4H4+ | C2H5OH |
| C− | NH+ | H2O+ | C2H2+ | CH2NH | CH3OH+ | H4C2N+ | H4C3N+ | C2H7O+ |
| C+ | NH | H2O | C2H2 | H3CO+ | CH3OH | CH3CHO+ | COOCH4+ | C2H6OH+ |
| C | OH+ | C2H+ | HCNH+ | SiH4+ | SiH5+ | CH3CHO | HCOOCH3 | C4H5+ |
| N+ | OH− | C2H | H2CN | SiH4 | C3H3+ | C4H3+ | C5H3+ | C2H6CO+ |
| N | OH | HCN+ | H2NC+ | C3H2+ | H2C3H+ | C4H3 | H3C4N+ | C2H6CO |
| O− | C2+ | HNC | H2CO+ | C3H2 | C3H3 | H3C3N | H3C4N | C3H6OH+ |
| O+ | C2 | HCN | H2CO | H2CCC | CH3CN | H3C3O+ | C6H2+ | H5C2O2+ |
| O | CN+ | HOC+ | HOCH | CH2CN+ | CH3CN+ | PC2H4+ | C6H2 | C5H4+ |
| Na+ | CN− | HCO+ | SiH3+ | CH2CN | CH3CO+ | C5H2+ | H2C5N+ | C5H4 |
| Na | CN | HCO | SiH3 | CH2CO+ | SiCH4+ | C5H2 | C7H+ | C5H5+ |
| Mg+ | CO+ | HN2+ | H2NO+ | CH2CO | PCH4+ | H2C4N+ | C7H | H4C4N+ |
| Mg | CO | SiH2+ | PH3+ | SiCH3+ | HCOOH2+ | C6H+ | C8+ | C6H3+ |
| Si+ | N2+ | SiH2 | H2O2 | SiCH3 | C4H2+ | C6H | C8 | C6H4+ |
| Si | N2 | HNO+ | H3S+ | CH2PH | C4H2 | HC5N+ | C7N+ | H3C5N+ |
| P+ | SiH+ | HNO | C3H+ | PCH3+ | H2C3N+ | HC5N | C7N | C6H5+ |
| P | SiH | PH2+ | C3H | HCOOH | C3H2O+ | C7+ | | C6H6 |
| S− | NO+ | PH2 | C2NH+ | H3CS+ | SiC2H3+ | C7 | | C6H7+ |
| S+ | NO | O2H+ | HC2O+ | H3SiO+ | PC2H3+ | | | C7H2+ |
| S | PH+ | O2H | SiCH2+ | PNH3+ | C5H+ | | | C7H2 |
| Cl+ | PH | H2S+ | SiCH2 | C4H+ | C5H | | | C7H3+ |
| Cl | O2+ | H2S | HNCO+ | C4H | HC4N+ | | | C7H4+ |
| Fe+ | O2 | C3+ | SiNH2+ | HC3N+ | SiC3H2+ | | | C7H4 |
| Fe | HS+ | C3 | PCH2+ | HC3N | C6+ | | | H3C6N |
| | HS | H2Cl+ | HCO2+ | HC3O+ | C6 | | | C7H5+ |
| | HCl | CNC+ | H2CS+ | SiC2H2+ | C5N+ | | | H4C6N+ |
| | HCl+ | C2N+ | H2CS | SiC2H2 | C5N | | | C8H+ |
| | SiC+ | C2N | H2SiO+ | PC2H2+ | SiC4H+ | | | C8H |
| | SiC | C2O+ | H2SiO | C5+ | PC4H+ | | | C8H2+ |
| | SiN+ | C2O | PNH2+ | C5 | HC4S+ | | | C8H2 |
| | SiN | HCSi+ | C4+ | C4N+ | | | | HC7N+ |
| | CP+ | HCSi | C4 | SiC3H+ | | | | HC7N |
| | CP | OCN+ | H2PO+ | SiC3H | | | | C8H3+ |
| | CS+ | OCN | H2CCl+ | H3S2+ | | | | H2C7N+ |
| | CS | HNSi+ | C3N+ | PC3H+ | | | | C8H4+ |
| | SiO+ | HNSi | C3N | HC3S+ | | | | H3C7N+ |
| | SiO | HCP+ | C3O+ | SiC4+ | | | | C8H5+ |
| | PN+ | HCP | C3O | SiC4 | | | | C9+ |
| | PN | CO2+ | C2N2+ | C4P+ | | | | C9 |
| | NS+ | CO2 | SiC2H+ | C4P | | | | C9H+ |
| | NS | N2O | SiC2H | C4S+ | | | | C9H |
| | PO+ | HCS+ | SiNCH+ | C4S | | | | C9H2+ |
| | PO | HCS | HC2P+ | | | | | C9H2 |
| | CCl+ | SiOH+ | HC2P | | | | | C9H3+ |
| | CCl | HPN+ | HC2S+ | | | | | C9H4+ |
| | SO+ | NO2+ | HOCS+ | | | | | H3C8N |
| | SO | NO2 | HSiO2+ | | | | | C9H5+ |
| | ClO+ | HNS+ | SiC3+ | | | | | H4C8N+ |
| | ClO | HPO+ | SiC3 | | | | | C10+ |
| | SiS | HPO | HSO2+ | | | | | C9N+ |
| | SiS+ | HSO+ | H2S2 | | | | | C9N |
| | S2+ | SiC2+ | H2S2+ | | | | | HC9N+ |
| | S2 | SiC2 | C3P | | | | | HC9N |
| | | SiNC+ | C3S+ | | | | | H2C9N+ |
| | | SiNC | C3S | | | | | H3C9N+ |
| | | CCP+ | | | | | | |
| | | CCP | | | | | | |
| | | C2S | | | | | | |
| | | C2S+ | | | | | | |
| | | OCS+ | | | | | | |
| | | OCS | | | | | | |
| | | SiO2 | | | | | | |
| | | HSiS+ | | | | | | |
| | | SO2+ | | | | | | |
| | | SO2 | | | | | | |
| | | HS2 | | | | | | |
| | | HS2+ | | | | | | |

**Table 2.** Species and heats of formation in kJ mol$^{-1}$ at 0 K

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| H | 216.0 | He | 0.0 | C | 711.2 | N | 470.8 | O | 246.8 |
| Na | 107.6 | Mg | 146.5 | Si | 446.0 | P | 315.6 | S | 274.7 |
| Cl | 119.6 | Fe | 414.0 | H2 | 0.0 | CH | 592.5 | NH | 376.5 |
| OH | 38.4 | SiH | 374.9 | PH | 237.0 | HS | 136.5 | HCl | −92.1 |
| C2 | 817.0 | CN | 436.8 | CO | −113.8 | SiC | 714.7 | CP | 447.6 |
| CS | 277.1 | CCl | 384.0 | N2 | 0.0 | NO | 89.8 | SiN | 371.2 |
| PN | 105.8 | NS | 263.0 | O2 | 0.0 | SiO | −101.6 | PO | −32.0 |
| SO | 5.0 | ClO | 101.8 | SiS | 104.6 | S2 | 128.3 | CH2 | 390.0 |
| NH2 | 191.6 | H2O | −238.9 | SiH2 | 289.0 | PH2 | 112.3 | H2S | −17.6 |
| C2H | 560.0 | HCN | 135.5 | HNC | 201.0 | HCO | 44.8 | HCSi | ..... |
| HCP | 167.0 | HCS | 310.0 | HNO | 100.0 | HNSi | 162.8 | O2H | 13.4 |
| HPO | ..... | HS2 | ..... | C3 | 831.0 | CCN | 556.0 | CCO | 282.6 |
| SiC2 | 610.0 | CCP | ..... | C2S | 586.0 | OCN | 154.0 | SiNC | ..... |
| CO2 | −393.1 | OCS | −142.0 | N2O | 85.5 | NO2 | 36.0 | SiO2 | −281.2 |
| SO2 | −294.3 | CH3 | 149.0 | NH3 | −38.9 | SiH3 | 202.9 | C2H2 | 228.6 |
| H2O2 | −130.0 | H2S2 | 16.0 | H2CN | 189.0 | H2CO | −104.7 | SiCH2 | ..... |
| H2CS | 105.0 | H2SiO | ..... | C3H | 602.5 | SiC2H | ..... | HCCP | ..... |
| C4 | 1052.0 | C3N | ..... | C3O | ..... | SiC3 | ..... | C3P | ..... |
| C3S | 567.0 | CH4 | −66.8 | SiH4 | 46.0 | C2H3 | 262.2 | CH2NH | 110.0 |
| SiCH3 | ..... | CH2PH | ..... | H2CCC | 512.0 | C3H2 | ..... | CH2CN | 245.0 |
| CH2CO | −44.6 | SiC2H2 | ..... | CHOOH | −378.8 | C4H | ..... | HC3N | 351.0 |
| SiC3H | ..... | C5 | 1081.0 | SiC4 | ..... | C4P | ..... | C4S | ..... |
| C2H4 | 60.7 | CH3OH | −190.7 | C3H3 | 343.0 | CH3CN | 81.0 | C4H2 | 440.0 |
| C5H | ..... | C6 | 1312.0 | C5N | ..... | C2H5 | 130.0 | C3H4 | 195.1 |
| CH3CHO | −155.0 | H3C3N | 184.0 | C5H2 | 723.0 | C6H | ..... | HC5N | ..... |
| C7 | 1325.0 | C2H6 | −69.1 | HCOOCH3 | −355.5 | H3C4N | 338.0 | C6H2 | 652.0 |
| C7H | ..... | C8 | 1487.0 | C7N | ..... | CH3OCH3 | −166.3 | C2H5OH | −217.1 |
| C5H4 | 425.0 | C7H2 | 933.0 | C8H | ..... | HC7N | ..... | C9 | 1554.0 |
| C2H6CO | −217.2 | H3C6N | ..... | C8H2 | 864.0 | C9H | ..... | C9N | ..... |
| C7H4 | ..... | C9H2 | 1142.0 | HC9N | ..... | H3C8N | ..... | H− | 143.2 |
| C− | 589.3 | O− | 105.4 | S− | 75.0 | OH− | −137.7 | CN− | 63.6 |
| H+ | 1528.0 | He+ | 2372.0 | C+ | 1797.6 | N+ | 1873.1 | O+ | 1560.7 |
| Na+ | 603.4 | Mg+ | 884.2 | Si+ | 1233.0 | P+ | 1328.0 | S+ | 1272.0 |
| Cl+ | 1371.0 | Fe+ | 1173.0 | H2+ | 1488.3 | HeH+ | 1352.0 | CH+ | 1619.1 |
| NH+ | 1678.1 | OH+ | 1292.7 | SiH+ | 1136.2 | PH+ | 1219.0 | HS+ | 1137.0 |
| HCl+ | 1137.7 | C2+ | 1992.0 | CN+ | 1796.3 | CO+ | 1238.3 | SiC+ | ..... |
| CP+ | 1529.0 | CS+ | 1356.0 | CCl+ | 1243.0 | N2+ | 1503.3 | NO+ | 984.0 |
| SiN+ | ..... | PN+ | 1249.0 | NS+ | 1119.0 | O2+ | 1164.7 | SiO+ | 1001.2 |
| PO+ | 778.0 | SO+ | 1000.7 | ClO+ | 1158.0 | SiS+ | ..... | S2+ | 1031.0 |
| H3+ | 1107.0 | CH2+ | 1386.0 | NH2+ | 1266.4 | H2O+ | 977.9 | SiH2+ | 1155.2 |
| PH2+ | 1090.0 | H2S+ | 991.0 | H2Cl+ | 867.0 | C2H+ | 1689.0 | HCN+ | 1448.0 |
| HCO+ | 825.6 | HOC+ | 963.0 | HCSi+ | ..... | HCP+ | 1208.0 | HCS+ | 1018.0 |
| N2H+ | 1035.5 | HNO+ | 1074.4 | HNSi+ | ..... | HPN+ | ..... | HNS+ | ..... |
| O2H+ | 1108.5 | SiOH+ | ..... | HPO+ | ..... | HSO+ | ..... | HSiS+ | ..... |
| S2H+ | ..... | C3+ | 2004.0 | CCN+ | 1715.0 | CNC+ | 1620.0 | C2O+ | ..... |
| SiC2+ | 1594.0 | CCP+ | ..... | C2S+ | ..... | NCO+ | 1289.0 | SiNC+ | ..... |
| CO2+ | 935.7 | OCS+ | 936.0 | NO2+ | 977.0 | SO2+ | 894.0 | CH3+ | 1098.0 |
| NH3+ | 941.0 | H3O+ | 597.0 | SiH3+ | 992.0 | PH3+ | 966.0 | H3S+ | 797.0 |
| C2H2+ | 1328.5 | HCNH+ | 947.0 | H2NC+ | 1109.0 | H2CO+ | 944.5 | SiCH2+ | ..... |
| PCH2+ | ..... | H2CS+ | 1006.0 | H2CCl+ | 962.1 | H2NO+ | 939.7 | SiNH2+ | 889.9 |
| PNH2+ | ..... | H2SiO+ | ..... | H2PO+ | ..... | H2S2+ | 913.0 | C3H+ | 1593.0 |
| CCNH+ | 1531.0 | HC2O+ | 1096.0 | C2HO+ | ..... | SiC2H+ | ..... | PC2H+ | ..... |
| HC2S+ | ..... | HNCO+ | 1015.0 | SiNCH+ | ..... | HCO2+ | 589.0 | HOCS+ | 757.0 |
| HSiO2+ | ..... | HSO2+ | 597.0 | C4+ | 2187.0 | C3N+ | ..... | C3O+ | ..... |
| SiC3+ | ..... | C3S+ | ..... | C2N2+ | 1594.8 | CH4+ | 1140.0 | NH4+ | 630.0 |
| SiH4+ | 1170.0 | C2H3+ | 1120.9 | H3CO+ | 703.0 | SiCH3+ | 977.0 | PCH3+ | ..... |
| H3CS+ | 901.0 | PNH3+ | ..... | H3SiO+ | ..... | H3S2+ | ..... | C3H2+ | 1381.0 |
| CH2CN+ | 1214.0 | CH2CO+ | 882.7 | SiC2H2+ | ..... | PC2H2+ | ..... | C4H+ | 1805.0 |

**Table 2.** continued

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| HC3N+ | 1474.0 | HC3O+ | 971.0 | SiC3H+ | ..... | PC3H+ | ..... | HC3S+ | ..... |
| C5+ | 2162.0 | C4N+ | ..... | SiC4+ | ..... | C4P+ | ..... | C4S+ | ..... |
| CH5+ | 905.0 | SiH5+ | 917.0 | C2H4+ | 1074.0 | CH4N+ | 745.0 | CH2NH2+ | ..... |
| CH3OH+ | 856.2 | SiCH4+ | 1015.0 | PCH4+ | ..... | C3H3+ | 1075.0 | H2C3H+ | ..... |
| CH3CN+ | 1258.0 | CH3CO+ | 653.0 | SiC2H3+ | ..... | PC2H3+ | ..... | CHOOH2+ | 403.0 |
| C4H2+ | 1422.0 | H2C3N+ | 1127.5 | C3H2O+ | 1157.0 | SiC3H2+ | ..... | C5H+ | ..... |
| HC4N+ | ..... | SiC4H+ | ..... | PC4H+ | ..... | HC4S+ | ..... | C6+ | ..... |
| C5N+ | ..... | C2H5+ | 914.0 | CH3OH2+ | 567.0 | C3H4+ | 1194.5 | H4C2N+ | 817.0 |
| CH3CHO+ | 831.9 | PC2H4+ | ..... | C4H3+ | 1217.0 | H3C3O+ | 751.0 | C5H2+ | ..... |
| H2C4N+ | ..... | PC4H2+ | ..... | C6H+ | ..... | HC5N+ | ..... | C7+ | 2299.0 |
| C2H6+ | 1043.0 | C3H5+ | 969.0 | C2H5O+ | 583.0 | H5C2O+ | ..... | H4C3N+ | 817.0 |
| COOCH4+ | 688.0 | C5H3+ | ..... | H3C4N+ | ..... | C6H2+ | 1569.0 | H2C5N+ | ..... |
| C7H+ | ..... | C8+ | ..... | C7N+ | ..... | C2H7+ | 856.4 | C2H5OH+ | 793.1 |
| C2H6O+ | 801.0 | C4H5+ | 1076.0 | H5C2O2+ | 386.0 | C5H4+ | 1332.0 | H4C4N+ | ..... |
| C6H3+ | ..... | H3C5N+ | ..... | C7H2+ | ..... | C8H+ | ..... | HC7N+ | ..... |
| C9+ | 2451.0 | C2H6OH+ | 542.0 | C2H7O+ | 507.0 | C2H6CO+ | 719.7 | C5H5+ | 1132.0 |
| C6H4+ | 1400.0 | C7H3+ | ..... | C8H2+ | 1741.0 | H2C7N+ | ..... | C9H+ | ..... |
| C10+ | ..... | C9N+ | ..... | C3H6OH+ | 490.0 | C6H5+ | 1141.3 | C7H4+ | ..... |
| H4C6N+ | ..... | C8H3+ | ..... | H3C7N+ | ..... | C9H2+ | ..... | HC9N+ | ..... |
| C7H5+ | ..... | C8H4+ | ..... | C9H3+ | ..... | H2C9N+ | ..... | C8H5+ | ..... |
| C9H4+ | ..... | H4C8N+ | ..... | H3C9N+ | ..... | C9H5+ | ..... | | |

Notes: These data were compiled from the NIST-JANAF tables, mostly by H.-H. Lee (Ohio State University), with the exception of the heats of formation for the carbon chains $C_n$, $n = 2 - 7$, which come from Gingerich et al. (1994), and for the carbenes, $H_2C_n$, which come from Bettens et al. (1995). The heat of formation for CH2NH is taken from the NIST Webbook (Afeefy et al. 2000), and for C2S and C3S from J.R. Flores (private communication). These three entries are values at 298 K not 0 K.

where $\alpha$ is the cosmic-ray ionisation rate, $\gamma$ is the probability per cosmic-ray ionisation that the appropriate photoreaction takes place, and $\omega$ is the dust grain albedo in the far ultraviolet (typically 0.6 at 150 nm). We note that because CO is destroyed by the line absorption, its rate of destruction is sensitive to its rotational level populations. To account for this we have included a temperature-dependence in the calculation of the rate coefficient.

For interstellar photoreactions (R2 = `PHOTON`), the rate is derived as:

$$k = \alpha \ \exp(-\gamma A_{\rm V}) \qquad {\rm s}^{-1} \tag{4}$$

where $\alpha$ represents the rate in the unshielded interstellar ultraviolet radiation field, $A_{\rm V}$ is the extinction at visible wavelengths caused by interstellar dust, and $\gamma$ is the parameter used to take into account the increased extinction of dust at ultraviolet wavelengths.

### *3.3. General form of the reaction set*

We have re-organised the order of reactions in this release. The reactions are divided into 14 categories or types, which are grouped together in the database. Table 5 summarizes these categories, along with their position in the database. Within each category, the reactions are listed by increasing total molar mass (total mass of the reactants).

- Photoprocesses: the temperature flags of the photoprocesses, which are just an artifact from the data revision software, are, of course, irrelevant. Also, the unshielded rates shown are valid only for the ISM UV field (from Draine 1978). These photorates can be rescaled to a stellar radiation field or calculated from cross sections when available (see Table 7 and Eq. (5));
- Neutral-neutral reactions: the reactions that were already present in the former UMIST Database have had their temperature dependence reviewed and temperature range defined when known. When not known, an arbitrary range of 10 to 300 K has been attributed, since these reactions were originally defined for these low temperatures;
- Cosmic-Ray reactions: reactions with `CRPHOT` (cosmic ray photons) and `CRP` (cosmic ray protons) have been left unchanged;
- Sundries: this section gathers all the reactions that cannot be classified by any of the other types because they are a combination of at least two different types.

### *3.4. Alterations present in this release*

- A major change brought to the database is the inclusion of the temperature dependence and temperature range for all the reactions. The maximum temperature range used in the database has been arbitrarily defined from 10 to 41 000 K. Where explicit information is not available, the rate coefficients have been attributed a

**Table 3.** Permanent electric dipole moments in Debye of the neutral molecules

| Species | $\mu_D$ | Species | $\mu_D$ | Species | $\mu_D$ |
|---|---|---|---|---|---|
| H2 | 0 | CH | 1.46 | NH | 1.3 |
| OH | 1.66 | SiH | 0.12 | PH | 0.64 |
| HS | 0.76 | HCl | 1.08 | C2 | 0 |
| CN | 1.45 | CO | 0.112 | SiC | 1.7 |
| CP | 0.86 | CS | 1.96 | CCl | $< 0.65$ |
| N2 | 0 | NO | 0.153 | SiN | $\sim 2.3$ |
| PN | 2.75 | NS | 1.81 | O2 | 0 |
| SiO | 3.1 | PO | 1.88 | SO | 1.55 |
| ClO | 1.24 | SiS | 1.73 | S2 | 0 |
| CH2 | 0.57 | NH2 | 1.83 | H2O | 1.85 |
| SiH2 | 0.18 | PH2 | .... | H2S | 0.97 |
| C2H | 0.8 | HCN | 2.98 | HNC | 2.7 |
| HCO | $\sim 1.0$ | HCSi | .... | HCP | 0.3 |
| HCS | .... | HNO | 1.67 | HNSi | 0.16 |
| O2H | 2.09 | HPO | 2.33 | HS2 | .... |
| C3 | 0 | CCN | 0.6 | CCO | 1.3 |
| SiC2 | 2.39 | CCP | .... | C2S | 2.8 |
| OCN | 0.64 | SiNC | 2.03 | CO2 | 0 |
| OCS | 0.71 | N2O | 0.16 | NO2 | 0.32 |
| SiO2 | $\sim 0.5$ | SO2 | 1.63 | CH3 | 0 |
| NH3 | 1.47 | SiH3 | 0 | C2H2 | 0 |
| H2O2 | 1.57 | H2S2 | 1.2 | H2CN | 2.54 |
| H2CO | 2.33 | SiCH2 | .... | H2CS | 1.65 |
| H2SiO | .... | l-C3H | 3.1 | SiC2H | 1.4 |
| HCCP | 0 | C4 | 0 | C3N | 2.2 |
| C3O | 2.39 | SiC3 | .... | C3P | .... |
| C3S | 3.7 | CH4 | 0 | SiH4 | 0 |
| C2H3 | $\sim 1.5$ | CH2NH | 2.02 | SiCH3 | .... |
| CH2PH | .... | c-C3H2 | 3.4 | CH2CN | 1.62 |
| CH2CO | 1.42 | SiC2H2 | 2.5 | CHOOH | 1.41 |
| C4H | 0.9 | HC3N | 3.6 | SiC3H | .... |
| C5 | 0 | SiC4 | 6.3 | C4P | .... |
| C4S | $\sim 3.0$ | C2H4 | 0 | CH3OH | 1.7 |
| C3H3 | 4.0 | CH3CN | 3.92 | H2CCCC | 4.5 |
| C5H | 4.3 | C6 | 0 | C5N | $\sim 2.7$ |
| C2H5 | .... | C3H4 [CH3CCH] | 0.78 | CH3CHO | 2.69 |
| H3C3N [CH2CHCN] | 3.89 | C5H2 | 2.5 | C6H | 5.0 |
| HC5N | 4.33 | C7 | 0 | C2H6 | 0 |
| HCOOCH3 | 1.77 | H3C4N [CH3C3N] | 4.91 | C6H2 | 0 |
| C7H | 4.5 | C8 | 0 | C7N | 3.0 |
| CH3OCH3 | 1.3 | C2H5OH | 1.44 | C5H4 [CH3C4H] | 1.21 |
| C7H2 | 2.5 | C8H | 5.0 | HC7N | 4.62 |
| C9 | 0 | C2H6CO | 2.8 | H3C6N [CH3C5N] | 5.75 |
| C8H2 | 0 | C9H | 4.7 | C9N | 3.3 |
| C7H4 [CH3C6H] | 1.5 | C9H2 | 2.5 | HC9N | 4.84 |
| H3C8N [CH3C7N] | 5.47 | | | | |

Notes: c-C3H = 2.4D; H2CCC = 4.1D; HCCCCH = 0D; H2C3H(propargyl) = 0.14D;
C3S from Suernam & Lovas (1994); CH3C3N and CH3C5N from Botschwina et al. (1994);
H2CCCC from Oswald & Botschwina (1995); C3N from Pauzat et al. (1991);
C5N from Botschwina (1996); HCN, HC3N, HC7N and HC9N from Botschwina & Horn (1997).

**Table 4.** List of the database reaction reference flags and their correspondance with the bibliographical references. Note: Any digit-only flag found in the database is the same flag as that used for referencing reactions in Anicich & Huntress (1986) and Anicich (1993)

| Flags | References | Flags | References |
|---|---|---|---|
| AA83 | Alge et al. 1983 | AM90 | Adams et al. 1990 |
| AS84 | Adams et al. 1984 | AS95 | Andreazza et al. 1995 |
| AS97 | Andreazza and Singh 1997 | BA84 | Barlow 1984 |
| BC92 | Baulch et al. 1992 | BH83 | Becker and Hong 1983 |
| BO90 | Bohme 1990 | BS97 | Brownsword and Sims 1997 |
| BW87 | Bohme et al. 1987 | CH82 | Copp et al. 1982 |
| CH94 | Clary et al. 1994 | DA97 | Decker and Adams 1997 |
| DD90 | Dalgarno et al. 1990 | DF86 | Dheandanoo et al. 1986 |
| DM77 | Mann 1977 | FA80 | Field et al. 1980 |
| DPFR | Donnelly and Pasternack 1979, Filseth et al. 1979, Reisler et al. 1980 | | |
| FO91 | Forst 1991 | FS91 | Frost et al. 1991 |
| FV86 | Federer et al. 1986 | GA89 | Giles et al. 1989 |
| GH92 | Gerlich and Horning 1992 | GI90 | Giles 1990 |
| GL87 | Gredel et al. 1987 | GL89 | Gredel et al. 1989 |
| HA89 | Herbst, Adams et al. 1989 | HA90 | Herd et al. 1990 |
| HA93 | Haider and Husain 1993a | HD89 | Herbst, DeFrees and Koch 1989 |
| HE85 | Herbst 1985 | HE87 | Herbst 1987 |
| HG90 | Herbst, Giles and Smith 1990 | HG93 | Harding et al. 1993 |
| HH93 | Haider and Husain 1993b | HL86 | Herbst and Leung 1986 |
| HL89 | Herbst and Leung 1989 | HL90 | Herbst and Leung 1990 |
| HL97 | Herbst and Lee 1997 | HM89 | Herbst, Millar et al. 1989 |
| HN79 | Husain and Norris 1979 | HT00 | Herbst et al. 2000 |
| IS89 | Smith I.W.M. 1989 | KD93 | Kimura and Dalgarno 1993 |
| KM89 | Karpas and Meot-ner 1989 | LG88 | Leen and Graff 1988 |
| LH84 | Leung et al. 1984 | LL98 | Larson et al. 1998 |
| MA85 | Millar et al. 1985 | MA86 | Millar, Adams et al. 1986 |
| MB73 | MacGregor & Berry 1973 | MB87 | Millar et al. 1987 |
| MD83 | Mitchell and Deveau 1983 | MH90 | Millar and Herbst 1990 |
| MH91 | Millar, Herbst and Charnley 1991 | MI84 | Mitchell 1984 |
| MI90 | Mitchell 1990 | MI91 | Millar 1991 |
| MM93 | Maluendes et al. 1993 | MN85 | Millar and Nejad 1985 |
| MN89 | Marston et al. 1989 | MS99 | McEwan et al. 1999 |
| NA99 | Nahar 1999 | NIST | Mallard et al. 1998 |
| NM90 | Nesbitt et al. 1990 | NP97 | Nahar and Pradhan 1997 |
| PD89 | Petuchowski et al. 1989 | PF92 | Petrie et al. 1992 |
| PH80 | Prasad and Huntress 1980 | PH82 | Prasad and Huntress 1982 |
| PR90 | Pineau des Forêts et al. 1990 | RA92 | Rawlings 1992 |
| RJ91 | Roberge et al. 1991 | RW80 | Raksit and Warneck 1980 |
| RW88 | Rawlings et al. 1988 | SA84 | Smith and Adams 1984 |
| SA88 | Smith, Adams et al. 1988 | SA92 | Sen et al. 1992 |
| SM88 | Stief et al. 1988 | SM89 | Smith et al. 1989 |
| SM93 | Smith M.A. 1993 | SQ93 | Sims et al. 1993 |
| SQ94 | Sims et al. 1994 | SS92 | Smith et al. 1992 |
| SS93 | Smith and Spanel 1993 | SS94 | Smith et al. 1994 |
| SS99 | Stancil et al. 1999 | SY92 | Suzuki et al. 1992 |
| TA84 | Thorne et al. 1984 | TE96 | Talbi et al. 1996 |
| TH86 | Tsang and Hampson 1986 | VD87 | van Dishoeck 1987 |
| VA99 | Vikor et al. 1999. The values of the total rates are from MI90 and AA83 (at 300 K). | | |
| VD88 | van Dishoeck 1988 | VP83 | Viggiano and Paulson 1983 |
| WB88 | Wlodek et al. 1988 | WM94 | Wilson et al. 1994 |
| ZD89 | Zygelman et al. 1989 | | |

range of 10−300 K. However, if their "$\gamma$" Arrhenius coefficient is too large, the lowest temperature has been defined as $T_{\rm l} = \gamma/30$ (in K), and the largest temperature $T_{\rm u}$ has been arbitrarily taken as 41 000 K (the value of such rates does not change significantly at higher temperatures), unless the rate's value becomes unphysical, in which case an appropriate upper temperature has been determined. Many Ion-Neutral and Ion-Ion reactions remain constant whatever the temperature, and where this is the case they have been arbitrarily defined from 10 to 41 000 K;

– Two new reaction types have been added, namely *Termolecular reactions* and *Collider reactions*, both of which become important at high density, typically above $10^{10}$ cm$^{-3}$. Termolecular reactions are catalysed bimolecular reactions and the catalyst is named "M". The nature of the third body is not important in general because it is only used as a de-excitation energy carrier:

  $$\mathrm{X + Y + M \rightarrow XY + M.}$$

  Collider reactions are collision-induced dissociations and the collider is also named "M" as its nature does not significantly alter the rate of the process:

  $$\mathrm{XY + M \rightarrow X + Y + M;}$$

– Because the reactions were chosen to be appropriate not only for the cold ISM, less discrimination has been operated so novel reactions have been added to all the types. The net result is a richer chemistry with multi-product reactions;
– Tables of cross section data appropriate for photo processes have been gathered and are included in the electronic tables to allow study of chemistry in a variety of radiation fields. Table 7 gives further information on these cross sections.

## 4. Other data

### *4.1. Deuterium chemistry*

A comprehensive description of deuterium chemistry requires that all D-bearing analogues of H-bearing species are included in a chemical model. This has the effect of approximately tripling the number of reactions in a model if it is to include deuterium. For our purposes, we have decided not to include a full deuterium chemistry in this release. Such a chemistry can be generated most efficiently using software but the detailed branching ratios adopted are a matter of individual choice at this time and we prefer to list only the most important reactions in Table 6. Rodgers & Millar (1996) have discussed many of the issues involved in generating a deuterium chemistry.

**Table 5.** List of the types of chemical reactions and their position in the database. The unclassifiable reactions are put in the category "Sundries". The first column XX is the abbreviation used for the types

| XX | Type of reaction | Position (index "I") |
|---|---|---|
| NN | Neutral - Neutral Reactions | 1 – 433 |
| IN | Ion - Neutral Reactions | 434 – 2606 |
| CE | Charge Exchange Reactions | 2607 – 3144 |
| II | Ion - Ion Neutralisations | 3145 – 3175 |
| DR | Dissociative Recombinations | 3176 – 3606 |
| RR | Radiative Recombinations | 3607 – 3631 |
| AD | Associative Detachments | 3632 – 3678 |
| RA | Radiative Associations | 3679 – 3760 |
| PH | Photoprocesses | 3761 – 3916 |
| CP | Cosmic-Ray Proton Reacs (CRP) | 3917 – 3927 |
| CR | Cosmic-Ray Photon Reacs (CRPHOT) | 3928 – 4059 |
| CL | Collider Reactions | 4060 – 4077 |
| TR | Termolecular Reactions | 4078 – 4107 |
| – | Sundries | 4108 – 4113 |

### *4.2. Cross sections for photoprocesses*

The necessity for having data on photo process cross sections arises from the fact that astrochemistry is not exclusive to the ISM but is now applied to circumstellar regions and comets as well. As a result, the rates of destruction of the species through exposure to the stellar radiation field can change by several orders of magnitude. For example, the photoionization rate of $He^0$ in interstellar clouds is negligible, whereas in the radiation field of a nearby Wolf-Rayet star it can be as large as $10^{-5}$ s$^{-1}$. Table 7 gives the list of the species and the data references compiled to date by us. The detailed cross-sections, which are available electronically, are given in megabarns (1 Mb = $10^{-18}$ cm$^2$). The photorate, $\beta(X,r)$ (s$^{-1}$), for species $X$ at a distance $r$ from a localised radiation source can be derived using Eq. (5):

$$\beta(X,r) = \frac{10^{-26}\, w(r)}{hc} \int_{\lambda<\lambda_0}^{\lambda_0} \lambda\, \mathcal{F}_\lambda\, \sigma_\lambda(X)\, \mathrm{d}\lambda \qquad (5)$$

where $w(r)$ is the dilution factor at the distance $r$ from the source, $\lambda_0$ (Å) is the photoprocess threshold wavelength, such that any photon with $\lambda < \lambda_0$ will take part to the process, $\mathcal{F}_\lambda$ is the source Spectral Energy Distribution in erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$, $\sigma_\lambda(X)$ is the cross section (Mb) for the species $X$ at the wavelength $\lambda$ (Å).

These data are not complete. Future work is aimed at updating these via the Opacity Project and other sources.

### *4.3. Dipole moments*

At low temperatures, the rates of ion-molecule reaction rate coefficients can increase dramatically through ion-dipole interactions, which are particularly important for

**Table 6.** Deuterium Reactions. NOTE: a*(b)* stands for $a\times10^b$. *(D-resc)* means that the equivalent H-only reaction rate has been rescaled by D reduced mass. * implies that the exponential term in the rate expression has the form $\exp(-T/\gamma)$. References: as: Adams & Smith 1985; cd: Crosswell & Dalgarno 1985; dl: Dalgarno & Lepp 1987; dmd: Dalgarno & McDowell 1956; fp: Frommhold & Pickett 1978; hasd: Herbst et al. 1987; kah: Karpas et al. 1979; lbh: Lee et al. 1996; ljb: Linder et al. 1995; lm: Larsson et al. 1996; pdf: Pineau des Forêts et al. 1986; rp: Ramaker & Peek 1976; s: Schilke et al. 1992; saa: Smith et al. 1982a,b; smt: Sidhu et al. 1992; str: Strömholm et al. 1995; w: Watson 1976; zm: Zhang & Miller 1989

| Reaction | | | | | | | $\alpha$ ($\mathrm{cm^3\ s^{-1}}$) | $\beta$ | $\gamma$ (K) | References |
|---|---|---|---|---|---|---|---|---|---|---|
| $H_3^+$ | + | HD | → | $H_2D^+$ | + | $H_2$ | 1.5(−09) | | | lbh |
| $H_2D^+$ | + | $H_2$ | → | $H_3^+$ | + | HD | 2.0(−09) | −0.8 | 230 | smt |
| $CH_2^+$ | + | HD | → | $CH_2D^+$ | + | $H_2$ | 1.3(−09) | – | – | saa |
| $CH_2D^+$ | + | $H_2$ | → | $CH_2^+$ | + | HD | 8.7(−10) | – | 370 | saa |
| $C_2H_2^+$ | + | HD | → | $C_2HD^+$ | + | $H_2$ | 1.0(−09) | – | – | hasd |
| $C_2HD^+$ | + | $H_2$ | → | $C_2H_2^+$ | + | HD | 2.5(−09) | – | 550 | hasd |
| $D^+$ | + | $H_2$ | → | $H^+$ | + | HD | 2.1(−09) | – | – | saa |
| $H^+$ | + | HD | → | $D^+$ | + | $H_2$ | 1.0(−09) | – | 464 | saa |
| $D^+$ | + | H | → | $H^+$ | + | D | 1.0(−09) | – | – | w |
| $H^+$ | + | D | → | $D^+$ | + | H | 1.0(−09) | – | 41 | w |
| $H_3^+$ | + | D | → | $H_2D^+$ | + | H | 1.0(−09) | – | – | as (estimate) |
| $H_2D^+$ | + | H | → | $H_3^+$ | + | D | 1.0(−09) | – | 632 | as (estimate) |
| $HCO^+$ | + | D | → | $DCO^+$ | + | H | 1.0(−09) | – | – | as |
| $DCO^+$ | + | H | → | $HCO^+$ | + | D | 2.2(−09) | – | 796 | as |
| $N_2H^+$ | + | D | → | $N_2D^+$ | + | H | 1.0(−09) | – | – | as |
| $N_2D^+$ | + | H | → | $N_2H^+$ | + | D | 2.2(−09) | – | 550 | as |
| OH | + | D | → | OD | + | H | 1.3(−10) | – | – | cd |
| OD | + | H | → | OH | + | D | 1.3(−10) | – | 810 | cd |
| $N^+$ | + | HD | → | $ND^+$ | + | H | 3.2(−10) | – | 16 | s |
| $N^+$ | + | HD | → | $NH^+$ | + | D | 3.2(−10) | – | 100 | s |
| $C_2H$ | + | D | → | $C_2D$ | + | H | 5.0(−11) | 0.5 | 250 | s |
| $C_2D$ | + | H | → | $C_2H$ | + | D | 5.0(−11) | 0.5 | 832 | s |
| HCN | + | D | → | DCN | + | H | 1.0(−10) | 0.5 | 500 | s (estimate) |
| DCN | + | H | → | HCN | + | D | 1.0(−10) | 0.5 | 500 | s (estimate) |
| $D^+$ | + | $D^-$ | → | D | + | D | 5.7(−08) | −0.5 | – | dl (D-resc) |
| $D^+$ | + | $H^-$ | → | D | + | H | 4.6(−08) | −0.5 | – | dl (D-resc) |
| $H^+$ | + | $D^-$ | → | D | + | H | 4.6(−08) | −0.5 | – | dl (D-resc) |
| D | + | $H^-$ | → | H | + | $D^-$ | 6.4(−09) | 0.41 | – | dmd (D-resc) |
| H | + | $D^-$ | → | D | + | $H^-$ | 6.4(−09) | 0.41 | – | dmd (D-resc) |
| $H_2^+$ | + | D | → | $HD^+$ | + | H | 1.07(−09) | 0.06 | 41400* | ljb |
| $H_2^+$ | + | D | → | $H_2$ | + | $D^+$ | 6.4(−10) | – | – | kah |
| $HD^+$ | + | H | → | $H_2^+$ | + | D | 1.0(−09) | – | 154 | dmd (D-resc) |
| $HD^+$ | + | $e^-$ | → | H | + | D | 3.4(−09) | −0.4 | – | str |
| $HD^+$ | + | H | → | HD | + | $H^+$ | 6.4(−10) | – | – | kah |
| $HD^+$ | + | $H_2$ | → | $H_3^+$ | + | D | 1.05(−09) | – | – | pdf |
| H | + | $D^+$ | → | $HD^+$ | + | h$\nu$ | 3.9(−19) | 1.8 | −20 | rp (D-resc) + fp |
| D | + | $H^+$ | → | $HD^+$ | + | h$\nu$ | 3.9(−19) | 1.8 | −20 | rp (D-resc) + fp |
| $H_2$ | + | D | → | HD | + | H | 7.5(−11) | – | 3820 | zm (fitted) |
| HD | + | H | → | $H_2$ | + | D | 7.5(−11) | – | 4240 | zm (fitted) |
| $H_2$ | + | $D^+$ | → | $H_2D^+$ | + | h$\nu$ | 1.0(−20) | – | – | dmd (D-resc) |
| HD | + | $H^+$ | → | $H_2D^+$ | + | h$\nu$ | 1.0(−20) | – | – | dmd (D-resc) |
| $H_2^+$ | + | D | → | $H_2D^+$ | + | h$\nu$ | 7.0(−18) | 1.8 | −20 | dmd (D-resc) |
| $HD^+$ | + | H | → | $H_2D^+$ | + | h$\nu$ | 1.2(−17) | 1.8 | −20 | dmd (D-resc) |
| $H_2D^+$ | + | $e^-$ | → | H | + H | + D | 4.38(−08) | −0.5 | – | lm |
| $H_2D^+$ | + | $e^-$ | → | $H_2$ | + | D | 4.2(−09) | −0.5 | – | lm |
| $H_2D^+$ | + | $e^-$ | → | H | + | HD | 1.2(−08) | −0.5 | – | lm |
| $HD^+$ | + | $H_2$ | → | $H_2D^+$ | + | H | 1.05(−09) | – | – | pdf |
| HD | + | $H_2^+$ | → | $H_2D^+$ | + | H | 1.05(−09) | – | – | dmd (D-resc) |
| HD | + | $H_2^+$ | → | $H_3^+$ | + | D | 1.05(−09) | – | – | dmd (D-resc) |

**Table 7.** List of the species for which photo processes can be derived using known cross sections. The photo processes are calculated only from the ground state

| Species | Processes | Products | References |
|---|---|---|---|
| He | ionisation | $He^+ + e^-$ | Band et al. 1990 |
| C | ionisation | $C^+ + e^-$ | Cantù et al. 1981, Hofmann et al. 1983 |
| $C^+$ | ionisation | $C^{++} + e^-$ | Henry 1970 |
| $C^{++}$ | ionisation | $C^{3+} + e^-$ | Osterbrock 1974 |
| N | ionisation | $N^+ + e^-$ | Henry 1970 |
| O | ionisation | $O^+ + e^-$ | Taylor & Burke 1976, Henry 1970 |
| Ne | ionisation | $Ne^+ + e^-$ | Henry 1970 |
| Si | ionisation | $Si^+ + e^-$ | Chapman & Henry 1972 |
| $C_2$ | ionisation | $C_2^+ + e^-$ | Padial et al. 1985 |
| | dissociation | C + C | Pouilly et al. 1983 |
| CO | ionisation | $CO^+ + e^-$ | Hudson 1971 |
| | dissociation | C + O | Letzelter et al. 1987 |
| $CO_2$ | ionisation | $CO_2^+ + e^-$ | Hudson 1971, Hitchcock et al. 1980 |
| | fragmentation | $CO + O^+ + e^-$ | Hitchcock et al. 1980 |
| | | $O + CO^+ + e^-$ | Hitchcock et al. 1980 |
| | | $O_2 + C^+ + e^-$ | Hitchcock et al. 1980 |
| $O_2$ | ionisation | $O_2^+ + e^-$ | Brion & Tan 1979, Ogawa & Ogawa 1975, Clarke & Wayne 1970 |
| | fragmentation | $O + O^+ + e^-$ | Brion & Tan 1979 |
| $N_2O$ | ionisation | $N_2O^+ + e^-$ | Hitchcock et al. 1980 |
| | fragmentation | $NO^+ + N + e^-$ | Hitchcock et al. 1980 |
| | fragmentation | $NO + N^+ + e^-$ | Hitchcock et al. 1980 |
| | fragmentation | $N_2^+ + O + e^-$ | Hitchcock et al. 1980 |
| | fragmentation | $N_2 + O^+ + e^-$ | Hitchcock et al. 1980 |

the interaction of light ions with neutrals possessing a permanent electric dipole moment in excess of about 1 Debye. Table 3 gives electric dipole moments for the neutral molecules contained in this database.

## 5. Database java applet

The database java applet can be found on the Rate99 web site at the following URL: http://www.rate99.co.uk. The user can perform searches for reactions which

- include a certain species, either as reactant, product or both;
- are valid at a certain temperature;
- were sourced from a particular reference;
- contain a certain element;

. . . and so on.

The searches can be made either on the whole database, or on the current results.

Information on an individual reaction can be displayed by selecting that reaction from the results list. The information displayed is an expansion of the *flag* field (see Sect. 3.1), and includes the formula for calculating the rate coefficient of the reaction, the reference from which the data are sourced and the temperature range over which the data are valid. At this point a graph can also be displayed showing the variation of the reaction rate with temperature, or in the case of interstellar photoreactions (`PHOTON`) or photoreactions induced by cosmic-rays (`CRPHOT`), the variation with visual extinction or grain albedo respectively.

A major function of the applet allows the user to build a ratefile interactively by choosing which elements and/or species it is to be composed from and optionally which temperature it is to be used for.

The current ratefile or selection of reactions can be saved at any time onto the user's local machine for use with an equation writer (the format of this file is described in Sect. 3.1). Normally, java applets are denied access to the local filesystem for security reasons. When the applet wants access to the filesystem, the user is alerted and can either grant or deny this permission. For this to work, the browser must support Java 1.1 or later. The implementations of security are (naturally) different between Netscape and Internet Explorer, so to begin with the applet only works with Netscape Navigator v4.5 or above. All this is explained in further detail on the web page itself.

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