

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 $\text{C}_2\text{H}_7\text{O}^+$ is not on the same atom as for $\text{C}_2\text{H}_6\text{OH}^+$; 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, C_3H_3^+ and $\text{H}_2\text{C}_3\text{H}^+$ differ by their geometry: C_3H_3^+ is a cycle, whereas $\text{H}_2\text{C}_3\text{H}^+$ is linear with one triple bond ($\text{H}_2\text{C}-\text{C}\equiv\text{CH}^+$); 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 $l\text{-C}_3\text{H}_n$ and $c\text{-C}_3\text{H}_n$, as sometimes experiments cannot discriminate between the isomers (e.g., propyne $\text{HC}\equiv\text{C}-\text{CH}_3$ and allene $\text{H}_2\text{C}=\text{C}=\text{CH}_2$). Therefore for more detailed data, the user is encouraged to refer to the bibliographic references.

The other delicate isomer distinction is between H_2CCC , which carries both H on the same carbon atom, and C_3H_2 , 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 \rightarrow He; SI \rightarrow 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, $\text{C}_2\text{H}_5\text{OCH}_3$, 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, α , β , γ , flags

where I is the reaction number, R1 to R3 are the reactants, P1 to P4 are the products, and α , β and γ 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,
 OPF5.2, 2X, OPF8.1, A1, 2(I5), A1, A4.

3.2. Calculation of the rates from α , β and γ

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

$$k = \alpha (T/300)^\beta \exp(-\gamma/T) \quad \text{cm}^3 \text{ s}^{-1} \quad (1)$$

where T is the gas temperature.

For direct cosmic-ray ionisation (R2 = CRP):

$$k = \alpha \quad \text{s}^{-1} \quad (2)$$

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

$$k = \alpha (T/300)^\beta \gamma / (1 - \omega) \quad \text{s}^{-1} \quad (3)$$

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	≥ 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	H ₂	0.0	CH	592.5	NH	376.5
OH	38.4	SiH	374.9	PH	237.0	HS	136.5	HCl	-92.1
C ₂	817.0	CN	436.8	CO	-113.8	SiC	714.7	CP	447.6
CS	277.1	CCl	384.0	N ₂	0.0	NO	89.8	SiN	371.2
PN	105.8	NS	263.0	O ₂	0.0	SiO	-101.6	PO	-32.0
SO	5.0	ClO	101.8	SiS	104.6	S ₂	128.3	CH ₂	390.0
NH ₂	191.6	H ₂ O	-238.9	SiH ₂	289.0	PH ₂	112.3	H ₂ S	-17.6
C ₂ H	560.0	HCN	135.5	HNC	201.0	HCO	44.8	HCSi
HCP	167.0	HCS	310.0	HNO	100.0	HNSi	162.8	O ₂ H	13.4
HPO	HS ₂	C ₃	831.0	CCN	556.0	CCO	282.6
SiC ₂	610.0	CCP	C ₂ S	586.0	OCN	154.0	SiNC
CO ₂	-393.1	OCS	-142.0	N ₂ O	85.5	NO ₂	36.0	SiO ₂	-281.2
SO ₂	-294.3	CH ₃	149.0	NH ₃	-38.9	SiH ₃	202.9	C ₂ H ₂	228.6
H ₂ O ₂	-130.0	H ₂ S ₂	16.0	H ₂ CN	189.0	H ₂ CO	-104.7	SiCH ₂
H ₂ CS	105.0	H ₂ SiO	C ₃ H	602.5	SiC ₂ H	HCCP
C ₄	1052.0	C ₃ N	C ₃ O	SiC ₃	C ₃ P
C ₃ S	567.0	CH ₄	-66.8	SiH ₄	46.0	C ₂ H ₃	262.2	CH ₂ NH	110.0
SiCH ₃	CH ₂ PH	H ₂ CCC	512.0	C ₃ H ₂	CH ₂ CN	245.0
CH ₂ CO	-44.6	SiC ₂ H ₂	CHOOH	-378.8	C ₄ H	HC ₃ N	351.0
SiC ₃ H	C ₅	1081.0	SiC ₄	C ₄ P	C ₄ S
C ₂ H ₄	60.7	CH ₃ OH	-190.7	C ₃ H ₃	343.0	CH ₃ CN	81.0	C ₄ H ₂	440.0
C ₅ H	C ₆	1312.0	C ₅ N	C ₂ H ₅	130.0	C ₃ H ₄	195.1
CH ₃ CHO	-155.0	H ₃ C ₃ N	184.0	C ₅ H ₂	723.0	C ₆ H	HC ₅ N
C ₇	1325.0	C ₂ H ₆	-69.1	HCOOCH ₃	-355.5	H ₃ C ₄ N	338.0	C ₆ H ₂	652.0
C ₇ H	C ₈	1487.0	C ₇ N	CH ₃ OCH ₃	-166.3	C ₂ H ₅ OH	-217.1
C ₅ H ₄	425.0	C ₇ H ₂	933.0	C ₈ H	HC ₇ N	C ₉	1554.0
C ₂ H ₆ CO	-217.2	H ₃ C ₆ N	C ₈ H ₂	864.0	C ₉ H	C ₉ N
C ₇ H ₄	C ₉ H ₂	1142.0	HC ₉ N	H ₃ C ₈ N	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	H ₂ +	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	C ₂ +	1992.0	CN+	1796.3	CO+	1238.3	SiC+
CP+	1529.0	CS+	1356.0	CCl+	1243.0	N ₂ +	1503.3	NO+	984.0
SiN+	PN+	1249.0	NS+	1119.0	O ₂ +	1164.7	SiO+	1001.2
PO+	778.0	SO+	1000.7	ClO+	1158.0	SiS+	S ₂ +	1031.0
H ₃ +	1107.0	CH ₂ +	1386.0	NH ₂ +	1266.4	H ₂ O+	977.9	SiH ₂ +	1155.2
PH ₂ +	1090.0	H ₂ S+	991.0	H ₂ Cl+	867.0	C ₂ H+	1689.0	HCN+	1448.0
HCO+	825.6	HOC+	963.0	HCSi+	HCP+	1208.0	HCS+	1018.0
N ₂ H+	1035.5	HNO+	1074.4	HNSi+	HPN+	HNS+
O ₂ H+	1108.5	SiOH+	HPO+	HSO+	HSiS+
S ₂ H+	C ₃ +	2004.0	CCN+	1715.0	CNC+	1620.0	C ₂ O+
SiC ₂ +	1594.0	CCP+	C ₂ S+	NCO+	1289.0	SiNC+
CO ₂ +	935.7	OCS+	936.0	NO ₂ +	977.0	SO ₂ +	894.0	CH ₃ +	1098.0
NH ₃ +	941.0	H ₃ O+	597.0	SiH ₃ +	992.0	PH ₃ +	966.0	H ₃ S+	797.0
C ₂ H ₂ +	1328.5	HCNH+	947.0	H ₂ NC+	1109.0	H ₂ CO+	944.5	SiCH ₂ +
PCH ₂ +	H ₂ CS+	1006.0	H ₂ CCl+	962.1	H ₂ NO+	939.7	SiNH ₂ +	889.9
PNH ₂ +	H ₂ SiO+	H ₂ PO+	H ₂ S ₂ +	913.0	C ₃ H+	1593.0
CCNH+	1531.0	HC ₂ O+	1096.0	C ₂ HO+	SiC ₂ H+	PC ₂ H+
HC ₂ S+	HNCO+	1015.0	SiNCH+	HCO ₂ +	589.0	HOCS+	757.0
HSiO ₂ +	HSO ₂ +	597.0	C ₄ +	2187.0	C ₃ N+	C ₃ O+
SiC ₃ +	C ₃ S+	C ₂ N ₂ +	1594.8	CH ₄ +	1140.0	NH ₄ +	630.0
SiH ₄ +	1170.0	C ₂ H ₃ +	1120.9	H ₃ CO+	703.0	SiCH ₃ +	977.0	PCH ₃ +
H ₃ CS+	901.0	PNH ₃ +	H ₃ SiO+	H ₃ S ₂ +	C ₃ H ₂ +	1381.0
CH ₂ CN+	1214.0	CH ₂ CO+	882.7	SiC ₂ H ₂ +	PC ₂ H ₂ +	C ₄ H+	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	C3OH2+	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 CH_2NH is taken from the NIST Webbook (Afeefy et al. 2000), and for C_2S and C_3S from J.R. Flores (private communication). These three entries are values at 298 K not 0 K.

where α is the cosmic-ray ionisation rate, γ is the probability per cosmic-ray ionisation that the appropriate photoreaction takes place, and ω 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 ($R_2 = \text{PHOTON}$), the rate is derived as:

$$k = \alpha \exp(-\gamma A_V) \quad \text{s}^{-1} \quad (4)$$

where α represents the rate in the unshielded interstellar ultraviolet radiation field, A_V is the extinction at visible wavelengths caused by interstellar dust, and γ 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	μ_D	Species	μ_D	Species	μ_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	~ 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	~ 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	~ 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	~ 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	~ 3.0	C2H4	0	CH3OH	1.7
C3H3	4.0	CH3CN	3.92	H2CCCC	4.5
C5H	4.3	C6	0	C5N	~ 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				

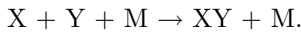
Notes: c-C3H = 2.4D; H2CCC = 4.1D; HCCCCH = 0D; H2C3H(propargyl) = 0.14D;
C3S from Suernam & Lovas (1994); CH3C3N and CH3C5N from Botschwina et al. (1994);
H2CCCC from Oswald & Botschwina (1995); C3N from Pauzat et al. (1991);
C5N from Botschwina (1996); HCN, HC3N, HC7N and HC9N from Botschwina & Horn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

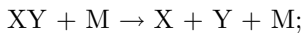
Flags	References	Flags	References
AA83	Alge et al. 1983	AM90	Adams et al. 1990
AS84	Adams et al. 1984	AS95	Andreazza et al. 1995
AS97	Andreazza and Singh 1997	BA84	Barlow 1984
BC92	Baulch et al. 1992	BH83	Becker and Hong 1983
BO90	Bohme 1990	BS97	Brownsword and Sims 1997
BW87	Bohme et al. 1987	CH82	Copp 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	FS91	Frost et al. 1991
FO91	Forst 1991	GA89	Giles et al. 1989
FV86	Federer et al. 1986	GI90	Giles 1990
GH92	Gerlich and Horning 1992	GL89	Gredel et al. 1989
GL87	Gredel et al. 1987	HA90	Herd et al. 1990
HA89	Herbst, Adams et al. 1989	HD89	Herbst, DeFrees and Koch 1989
HA93	Haider and Husain 1993a	HE87	Herbst 1987
HE85	Herbst 1985	HG93	Harding et al. 1993
HG90	Herbst, Giles and Smith 1990	HL86	Herbst and Leung 1986
HH93	Haider and Husain 1993b	HL90	Herbst and Leung 1990
HL89	Herbst and Leung 1989	HM89	Herbst, Millar et al. 1989
HL97	Herbst and Lee 1997	HT00	Herbst et al. 2000
HT79	Husain and Norris 1979	KD93	Kimura and Dalgarno 1993
IS89	Smith I.W.M. 1989	LG88	Leen and Graff 1988
KM89	Karpas and Meot-ner 1989	LL98	Larson et al. 1998
LH84	Leung et al. 1984	MA86	Millar, Adams et al. 1986
MA85	Millar et al. 1985	MB87	Millar et al. 1987
MB73	MacGregor & Berry 1973	MH90	Millar and Herbst 1990
MD83	Mitchell and Deveau 1983	MI84	Mitchell 1984
MH91	Millar, Herbst and Charnley 1991	MI91	Millar 1991
MI90	Mitchell 1990	MN85	Millar and Nejad 1985
MM93	Maluendes et al. 1993	MS99	McEwan et al. 1999
MN89	Marston et al. 1989	NIST	Mallard et al. 1998
NA99	Nahar 1999	NP97	Nahar and Pradhan 1997
NM90	Nesbitt et al. 1990	PF92	Petrie et al. 1992
PD89	Petuchowski et al. 1989	PH82	Prasad and Huntress 1982
PH80	Prasad and Huntress 1980	RA92	Rawlings 1992
PR90	Pineau des Forêts et al. 1990	RW80	Raksit and Warneck 1980
RJ91	Roberge et al. 1991	SA84	Smith and Adams 1984
RW88	Rawlings et al. 1988	SA92	Sen et al. 1992
SA88	Smith, Adams et al. 1988	SM89	Smith et al. 1989
SM88	Stief et al. 1988	SQ93	Sims et al. 1993
SM93	Smith M.A. 1993	SS92	Smith et al. 1992
SQ94	Sims et al. 1994	SS94	Smith et al. 1994
SS93	Smith and Spanel 1993	SY92	Suzuki et al. 1992
SS99	Stancil et al. 1999	TE96	Talbi et al. 1996
TA84	Thorne et al. 1984	VD87	van Dishoeck 1987
TH86	Tsang and Hampson 1986	VP83	Viggiano and Paulson 1983
VA99	Vikor et al. 1999. The values of the total rates are from MI90 and AA83 (at 300 K).	WM94	Wilson et al. 1994
VD88	van Dishoeck 1988		
WB88	Wlodek et al. 1988		
ZD89	Zygelman et al. 1989		

range of 10–300 K. However, if their “ γ ” Arrhenius coefficient is too large, the lowest temperature has been defined as $T_l = \gamma/30$ (in K), and the largest temperature T_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:



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:



- 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 ($1 \text{ Mb} = 10^{-18} \text{ cm}^2$). 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):

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

where $w(r)$ is the dilution factor at the distance r from the source, λ_0 (\AA) is the photoprocess threshold wavelength, such that any photon with $\lambda < \lambda_0$ will take part to the process, \mathcal{F}_λ is the source Spectral Energy Distribution in $\text{erg cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$, $\sigma_\lambda(X)$ is the cross section (Mb) for the species X at the wavelength λ (\AA).

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 $a \times 10^b$. (*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: Herbist 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	α ($\text{cm}^3 \text{s}^{-1}$)	β	γ (K)	References
$\text{H}_3^+ + \text{HD} \rightarrow \text{H}_2\text{D}^+ + \text{H}_2$	$1.5(-09)$			lbh
$\text{H}_2\text{D}^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{HD}$	$2.0(-09)$	-0.8	230	smt
$\text{CH}_2^+ + \text{HD} \rightarrow \text{CH}_2\text{D}^+ + \text{H}_2$	$1.3(-09)$	-	-	saa
$\text{CH}_2\text{D}^+ + \text{H}_2 \rightarrow \text{CH}_2^+ + \text{HD}$	$8.7(-10)$	-	370	saa
$\text{C}_2\text{H}_2^+ + \text{HD} \rightarrow \text{C}_2\text{HD}^+ + \text{H}_2$	$1.0(-09)$	-	-	hasd
$\text{C}_2\text{HD}^+ + \text{H}_2 \rightarrow \text{C}_2\text{H}_2^+ + \text{HD}$	$2.5(-09)$	-	550	hasd
$\text{D}^+ + \text{H}_2 \rightarrow \text{H}^+ + \text{HD}$	$2.1(-09)$	-	-	saa
$\text{H}^+ + \text{HD} \rightarrow \text{D}^+ + \text{H}_2$	$1.0(-09)$	-	464	saa
$\text{D}^+ + \text{H} \rightarrow \text{H}^+ + \text{D}$	$1.0(-09)$	-	-	w
$\text{H}^+ + \text{D} \rightarrow \text{D}^+ + \text{H}$	$1.0(-09)$	-	41	w
$\text{H}_3^+ + \text{D} \rightarrow \text{H}_2\text{D}^+ + \text{H}$	$1.0(-09)$	-	-	as (estimate)
$\text{H}_2\text{D}^+ + \text{H} \rightarrow \text{H}_3^+ + \text{D}$	$1.0(-09)$	-	632	as (estimate)
$\text{HCO}^+ + \text{D} \rightarrow \text{DCO}^+ + \text{H}$	$1.0(-09)$	-	-	as
$\text{DCO}^+ + \text{H} \rightarrow \text{HCO}^+ + \text{D}$	$2.2(-09)$	-	796	as
$\text{N}_2\text{H}^+ + \text{D} \rightarrow \text{N}_2\text{D}^+ + \text{H}$	$1.0(-09)$	-	-	as
$\text{N}_2\text{D}^+ + \text{H} \rightarrow \text{N}_2\text{H}^+ + \text{D}$	$2.2(-09)$	-	550	as
$\text{OH} + \text{D} \rightarrow \text{OD} + \text{H}$	$1.3(-10)$	-	-	cd
$\text{OD} + \text{H} \rightarrow \text{OH} + \text{D}$	$1.3(-10)$	-	810	cd
$\text{N}^+ + \text{HD} \rightarrow \text{ND}^+ + \text{H}$	$3.2(-10)$	-	16	s
$\text{N}^+ + \text{HD} \rightarrow \text{NH}^+ + \text{D}$	$3.2(-10)$	-	100	s
$\text{C}_2\text{H} + \text{D} \rightarrow \text{C}_2\text{D} + \text{H}$	$5.0(-11)$	0.5	250	s
$\text{C}_2\text{D} + \text{H} \rightarrow \text{C}_2\text{H} + \text{D}$	$5.0(-11)$	0.5	832	s
$\text{HCN} + \text{D} \rightarrow \text{DCN} + \text{H}$	$1.0(-10)$	0.5	500	s (estimate)
$\text{DCN} + \text{H} \rightarrow \text{HCN} + \text{D}$	$1.0(-10)$	0.5	500	s (estimate)
$\text{D}^+ + \text{D}^- \rightarrow \text{D} + \text{D}$	$5.7(-08)$	-0.5	-	dl (D-resc)
$\text{D}^+ + \text{H}^- \rightarrow \text{D} + \text{H}$	$4.6(-08)$	-0.5	-	dl (D-resc)
$\text{H}^+ + \text{D}^- \rightarrow \text{D} + \text{H}$	$4.6(-08)$	-0.5	-	dl (D-resc)
$\text{D} + \text{H}^- \rightarrow \text{H} + \text{D}^-$	$6.4(-09)$	0.41	-	dmd (D-resc)
$\text{H} + \text{D}^- \rightarrow \text{D} + \text{H}^-$	$6.4(-09)$	0.41	-	dmd (D-resc)
$\text{H}_2^+ + \text{D} \rightarrow \text{HD}^+ + \text{H}$	$1.07(-09)$	0.06	41400*	ljb
$\text{H}_2^+ + \text{D} \rightarrow \text{H}_2 + \text{D}^+$	$6.4(-10)$	-	-	kah
$\text{HD}^+ + \text{H} \rightarrow \text{H}_2^+ + \text{D}$	$1.0(-09)$	-	154	dmd (D-resc)
$\text{HD}^+ + \text{e}^- \rightarrow \text{H} + \text{D}$	$3.4(-09)$	-0.4	-	str
$\text{HD}^+ + \text{H} \rightarrow \text{HD} + \text{H}^+$	$6.4(-10)$	-	-	kah
$\text{HD}^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{D}$	$1.05(-09)$	-	-	pdf
$\text{H} + \text{D}^+ \rightarrow \text{HD}^+ + \text{h}\nu$	$3.9(-19)$	1.8	-20	rp (D-resc) + fp
$\text{D} + \text{H}^+ \rightarrow \text{HD}^+ + \text{h}\nu$	$3.9(-19)$	1.8	-20	rp (D-resc) + fp
$\text{H}_2 + \text{D} \rightarrow \text{HD} + \text{H}$	$7.5(-11)$	-	3820	zm (fitted)
$\text{HD} + \text{H} \rightarrow \text{H}_2 + \text{D}$	$7.5(-11)$	-	4240	zm (fitted)
$\text{H}_2 + \text{D}^+ \rightarrow \text{H}_2\text{D}^+ + \text{h}\nu$	$1.0(-20)$	-	-	dmd (D-resc)
$\text{HD} + \text{H}^+ \rightarrow \text{H}_2\text{D}^+ + \text{h}\nu$	$1.0(-20)$	-	-	dmd (D-resc)
$\text{H}_2^+ + \text{D} \rightarrow \text{H}_2\text{D}^+ + \text{h}\nu$	$7.0(-18)$	1.8	-20	dmd (D-resc)
$\text{HD}^+ + \text{H} \rightarrow \text{H}_2\text{D}^+ + \text{h}\nu$	$1.2(-17)$	1.8	-20	dmd (D-resc)
$\text{H}_2\text{D}^+ + \text{e}^- \rightarrow \text{H} + \text{H} + \text{D}$	$4.38(-08)$	-0.5	-	lm
$\text{H}_2\text{D}^+ + \text{e}^- \rightarrow \text{H}_2 + \text{D}$	$4.2(-09)$	-0.5	-	lm
$\text{H}_2\text{D}^+ + \text{e}^- \rightarrow \text{H} + \text{HD}$	$1.2(-08)$	-0.5	-	lm
$\text{HD}^+ + \text{H}_2 \rightarrow \text{H}_2\text{D}^+ + \text{H}$	$1.05(-09)$	-	-	pdf
$\text{HD} + \text{H}_2^+ \rightarrow \text{H}_2\text{D}^+ + \text{H}$	$1.05(-09)$	-	-	dmd (D-resc)
$\text{HD} + \text{H}_2^+ \rightarrow \text{H}_3^+ + \text{D}$	$1.05(-09)$	-	-	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	$\text{He}^+ + e^-$	Band et al. 1990
C	ionisation	$\text{C}^+ + e^-$	Cantù et al. 1981, Hofmann et al. 1983
C^+	ionisation	$\text{C}^{++} + e^-$	Henry 1970
C^{++}	ionisation	$\text{C}^{3+} + e^-$	Osterbrock 1974
N	ionisation	$\text{N}^+ + e^-$	Henry 1970
O	ionisation	$\text{O}^+ + e^-$	Taylor & Burke 1976, Henry 1970
Ne	ionisation	$\text{Ne}^+ + e^-$	Henry 1970
Si	ionisation	$\text{Si}^+ + e^-$	Chapman & Henry 1972
C_2	ionisation	$\text{C}_2^+ + e^-$	Padial et al. 1985
	dissociation	$\text{C} + \text{C}$	Pouilly et al. 1983
CO	ionisation	$\text{CO}^+ + e^-$	Hudson 1971
	dissociation	$\text{C} + \text{O}$	Letzelter et al. 1987
CO_2	ionisation	$\text{CO}_2^+ + e^-$	Hudson 1971, Hitchcock et al. 1980
	fragmentation	$\text{CO} + \text{O}^+ + e^-$	Hitchcock et al. 1980
		$\text{O} + \text{CO}^+ + e^-$	Hitchcock et al. 1980
		$\text{O}_2 + \text{C}^+ + e^-$	Hitchcock et al. 1980
O_2	ionisation	$\text{O}_2^+ + e^-$	Brion & Tan 1979, Ogawa & Ogawa 1975, Clarke & Wayne 1970
	fragmentation	$\text{O} + \text{O}^+ + e^-$	Brion & Tan 1979
N_2O	ionisation	$\text{N}_2\text{O}^+ + e^-$	Hitchcock et al. 1980
	fragmentation	$\text{NO}^+ + \text{N} + e^-$	Hitchcock et al. 1980
	fragmentation	$\text{NO} + \text{N}^+ + e^-$	Hitchcock et al. 1980
	fragmentation	$\text{N}_2^+ + \text{O} + e^-$	Hitchcock et al. 1980
	fragmentation	$\text{N}_2 + \text{O}^+ + e^-$	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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