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Thermodynamic Data

Dissociation Energy (1) = 672 kJ mol⁻¹ = 6.97 eV

Dissociation Energy (2) = 561 kJ mol⁻¹ = 5.81 eV

Dissociation Energy (3) = 1139 kJ mol⁻¹ = 11.80 eV

Ionisation Potential = 1061 kJ mol⁻¹ = 11.00 eV

Calculated DE from Diaz-Tendero et al (2006) (and good agreement with measurements of Gingerich et al (1994) within 0.3 eV estimated error bars); IP (vertical) estimated from Belau et al (2007) (estimated error barr 0.5 eV).

Rate Coefficient Data

$k / \text{molecule}^{-1} \text{ s}^{-1}$	T / K	Reference	Comments
<i>Rate Coefficient Measurement</i>			
<i>None</i>			
<i>Reviews and Evaluations</i>			
$1.0 \times 10^{-11} \times \exp(-1.7 \times A_V)$		OSU09 website	(a)
$1.0 \times 10^{-11} \times \exp(-1.7 \times A_V)$	10-41000	UMIST06 database	(a)
<i>Branching Fraction Measurement</i>			
(1)= 0.13 (±0.04)		Chabot 2006, 2010	(b)
(2)= 0.87 (±0.04)			
<i>Branching fraction Reviews and Evaluations</i>			
(1) = 1.0; (2) = 0.0		OSU09 website	(a)
(1) = 1.0; (2) = 0.0	10-41000	UMIST06 database	(a)

Comments

(a) Photodissociation rates are extrapolated from values recommended by van Dishoeck (1988) for large C_n (10 ≥ n ≥ 6). Lognormal factor 1.25 of accuracy is reported. According to van Hemert & van Dishoeck (2008), the photo-dissociation rates of carbon clusters may be larger than the one used up to now. In the absence of calculations for the specific species considered here, we prefer to use the

previous values but emphasize the need for future calculations or measurements.

Branching fractions reported in databases are those given in Bettens & Herbst (1995) although no details on how these were estimated for the photodissociation process were found anywhere in the literature. Channel (3) is assumed to be negligible because it requires photon energies close to the threshold of hydrogen H I emission (13.6 eV). For same reason photoionisation is neglected.

(b) Measurements have been performed with High Velocity Collision experiments on hot (3000°K) C₅ clusters produced by a sputtering source. Results have been interpreted satisfactorily within a statistical fragmentation behaviour (Martinet, 2004). Derivation of these experimental results in astrochemical context assumes that statistical fragmentation occurs under photodissociation process (Tuna 2007, Chabot 2010).

Preferred Values

Rate constant:

$$k = 1.0 \times 10^{-11} \times \exp(-1.7 \times A_V)$$

Reliability of rate constant:

$$F_0=2; g=0$$

Recommended Branching Fractions:

$$(1)=0.15$$

$$(2)=0.85$$

Reliability of Branching Fractions:

$$\pm 0.1(\text{uniform})$$

References

- S. Diàz-Tendero et al (2006), Int.J.Mass.Spectr. **252**, 126
- K.A.Gingerich et al (1994), JACS **116**, 3884
- L. Belau et al (2007) JACS **129**, 10229
- M. Chabot et al, (2006) J. Phys. B **39** 2593
- M. Chabot et al, (2010) A&A **524**, A39 (2010)
- E.F. van Dishoeck (1988) T.J.Millar and D.A. Williams(ed.), Kluwer Academic Publishers, 49.
- R. Bettens & E. Herbst(1995)IJMS/IP**149/150**,321
- G. Martinet et al, (2004) Phys.Rev.Lett. **93**, 063401
- T. Tuna et al, (2007) Mol. in Space& Lab. Conf., 303