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$$C_7 + h\nu \rightarrow C_6 + C \quad (1)$$
$$\rightarrow C_5 + C_2 \quad (2)$$
$$\rightarrow C_4 + C_3 \quad (3)$$
$$\rightarrow C_3 + C_3 + C \quad (4)$$
$$\rightarrow C_7 + e^- \quad (5)$$

Thermodynamic Data

Dissociation Energy (1) = 610 kJ mol^{-1} = 6.33 eV

Dissociation Energy (2) = 560 kJ mol^{-1}= 5.80 eV

Dissociation Energy (3) = 532 kJ mol^{-1} = 5.51 eV

Dissociation Energy (4) = 996 kJ mol^{-1} = 10.33 eV

Ionisation potential =973 kJ mol^{-1} = 10.10 eV

Calculated DE from Diaz-Tendero et al (2006) (and good agreement with measurements of Gingerich et al (1994) within 0.5 eV estimated error bars); IP (vertical) from Belau et al (2007) (estimated error bars 0.1).

Rate Coefficient Data

k / $molecule^{-1}$ s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurement			
None			
Reviews and Evaluations			
$2.0 \times 10^{-10} \times \exp(-2.5 \times A_V)$	10-41000	UMIST06 database	(a) photo ionisation
$1.0 \times 10^{-9} \times \exp(-1.7 \times A_V)$	10-41000	UMIST06 database	(a) photo dissociation
Branching Fraction Measurement			
(1) = 0.01 (±0.005)		Chabot 2006, 2010	(c)
(2) = 0.19 (±0.02)			
(3) = 0.80 (±0.04)			
Branching fraction Reviews and Evaluations			
(1) = 1.0	10-41000	UMIST06 database	(b) photo dissociation
(2) = (3) = (4) = 0.0	10-41000		

Comments

(a) Photoionisation and photodissociation rates are those recommended by van Dishoeck (1988) for large Cn (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.

(b) UMIST estimations for branching fractions 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 (4) is assumed to be negligible because it requires photon energies close to the threshold of hydrogen H I emission (13.6 eV).

(c) Measurements have been performed with High Velocity Collision experiments on hot (3000°K) C_7 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 constants:
Photo dissociation:
$k = 1.0 \times 10^{-9} \times \exp(-1.7 \times A_V)$
Photo ionisation:
$k = 2.0 \times 10^{-10} \times \exp(-2.5 \times A_V)$

Reliability of rate constants:
F0=2; g=0

Recommended Branching Fractions:
Photo dissociation:
(1) = 0.00
(2) = 0.20
(3) = 0.80
Photo ionisation:
(5) = 1.0

Reliability of Branching Fractions:
±0.1(uniform)

References

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