Authors: Marin Chabot & Karine Béroff (Orsay)

$$C_6 + CRPHOT \rightarrow C_5 + C \quad (1)$$
$$\rightarrow C_4 + C_2 \quad (2)$$
$$\rightarrow C_3 + C_3 \quad (3)$$
$$\rightarrow C_3 + C_2 + C \quad (4)$$

Thermodynamic Data

Dissociation Energy (1) = 527 kJ mol^{-1} = 5.46 eV

Dissociation Energy (2) = 621 kJ mol^{-1}= 6.44 eV

Dissociation Energy (3) = 386 kJ mol^{-1} = 4.00 eV

Dissociation Energy (4) = 1086 kJ mol^{-1} = 11.26 eV

Ionisation potential =936 kJ mol^{-1} = 9.70 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 (adiabatic) from Van Orden 1998 (estimated error bar: 0.2 eV).

Rate Coefficient Data

k / molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurement			
None			
Reviews and Evaluations			
$1.0 \times 10^3 \times \zeta$		OSU09 website	(a)
$0.5 \times 10^3 \times \zeta$	10-41000	UMIST06 database	(a)
Branching Fraction Measurement			
(1) = 0.09(±0.02)		Chabot 2006, 2010	(c)
(2) = 0.11(±0.02)			
(3) =0.80(±0.04)			
Branching fraction Reviews and Evaluations			
(1) = 1.0; (2) = (3) = 0.0		OSU09 website	(b)
(1) = 1.0; (2) = (3) = 0.0	10-41000	UMIST06 database	

Comments

(a) In OSU database the sum of CRPHOT and CRP is considered. The last one is expected to be negligible as compared to CRPHOT. Rate has been taken identical to the estimated rate of Gredel (1989) for the C_3.
Lognormal factor 1.25 of accuracy is reported.

(b) Branching fractions reported in OSU databases and UMIST are those given in Bettens & Herbst (1995) although no details on how these were estimated for the CRPHOT process were found anywhere in the literature.

(c) Measurements have been performed with high velocity collision experiments on hot (3000°K) C_6 clusters produced by a sputtering source. Results have been interpreted satisfactorily within statistical fragmentation behaviour (Martinet 2004). Derivation of these experimental results in astrochemical context assumes that statistical fragmentation occurs under CRPHOT process (Chabot 2010). Channel (4) is not relevant because it requires CRPHOT energies above or very close to the end of the emission spectrum of H_2 (Gredel 1989).

Preferred Values

Rate constant:
$k = 1.0 \times 10^3 \times \zeta$ molecule^{-1} s^{-1}

Reliability of rate constant:
Factor 2

Recommended Branching Fractions:
(1) = 0.10
(2) = 0.10
(3) = 0.80

Reliability of Branching Fractions:
±0.1 (uniform)

References

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