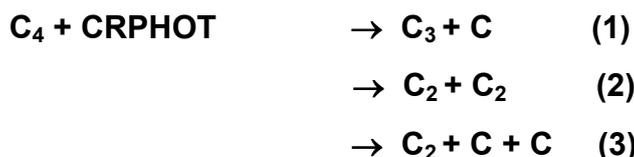


Authors: Marin Chabot & Karine Béroff (Orsay)



Thermodynamic Data

Dissociation Energy (1) = 465 kJ mol⁻¹ = 4.82 eV

Dissociation Energy (2) = 588 kJ mol⁻¹ = 6.09 eV

Dissociation Energy (3) = 1166 kJ mol⁻¹ = 12.08 eV

Ionisation Potential = 1206 kJ mol⁻¹ = 12.50 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: 0.3 eV).

Rate Coefficient Data

<i>k</i> / molecule ⁻¹ s ⁻¹	<i>T</i> / K	Reference	Comments
<i>Rate Coefficient Measurement</i>			
None			
<i>Reviews and Evaluations</i>			
1.0 × 10 ³ × ζ		OSU09 website	(a)
1.0 × 10 ³ × ζ	10-41000	UMIST06 database	(a)
<i>Branching Fraction Measurement</i>			
(1) = 0.77 (±0.04)		Chabot 2006, 2010	(c)
(2) = 0.23 (±0.02)			
<i>Branching fraction Reviews and Evaluations</i>			
(1) = 1.0; (2) = 0.0		OSU09 website	(b)
(1) = (2) = 0.5	10-41000	UMIST06 database	

Comments

(a) In OSU database the sum of CRPHOT and CR 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 C₃. Lognormal factor 1.25 of accuracy is reported.

(b) Branching fractions reported in OSU databases 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. UMIST estimations for branching fractions are identical to those used for Dissociative Recombination (Herbst 1989).

(c) Measurements have been performed with high velocity collision experiments on hot (3000°K) C₄ 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 (3) is not relevant because it requires CRPHOT energies above or very close to the end of the emission spectrum of H₂ (Gredel 1989).

Preferred Values

Rate constant:

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

Reliability of rate constant:

Factor 2

Recommended Branching Fractions:

(1)=0.75

(2)=0.25

Reliability of Branching Fractions:

±0.1 (uniform)

References

- S. Diàz-Tendero et al (2006), Int.J.Mass.Spectr. **252**, 126
- K.A.Gingerich et al (1994), JACS **116**, 3884
- A.Van Orden & R. Saykally 1998, Chem. Rev **98**, 2313
- M. Chabot et al, (2006) J. Phys. B **39** 2593
- M. Chabot et al, (2010) A&A in press
- R. Gredel, S. Lepp, A. Dalgarno, E. Herbst 1989, APJ**347**, 289.
- R. Bettens & E. Herbst(1995)IJMS/IP**149/150**,321
- E. Herbst & C.L. Leung, (1989) APJSS**69**, 271
- G. Martinet et al, (2004) Phys.Rev.Lett. **93**, 063401