Authors: Marin Chabot & Karine Béroff (Orsay)

$$C_4 + h\nu \rightarrow C_3 + C \quad (1)$$
$$\rightarrow C_2 + C_2 \quad (2)$$
$$\rightarrow C_2 + C + C \quad (3)$$

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 = 1109 kJ mol^{-1} = 11.5 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) : comment (a), (estimated error bar 1eV)

Rate Coefficient Data

k / molecule^{-1} s^{-1}	T / K	References	Comments
Rate Coefficient Calculation			
8.5×10^{-9}		van Hemert & van Dishoeck (2008)	(b)
Reviews and Evaluations			
$4.0 \times 10^{-10} \times \exp(-2.3\times A_V)$		OSU09 website	(c)
$4.0 \times 10^{-10} \times \exp(-2.3\times A_V)$	10-41000	UMIST06 database	(c)
Branching Fraction Measurement			
(1)= 0.89 (±0.06)		Choi et al, (2000)	(d)
(2)= 0.11 (±0.06)		Choi et al, (2000)	
Branching fraction Reviews and Evaluations			
(1) = (2) = 0.5		OSU09 website	(c)
(1) = (2) = 0.5	10-41000	UMIST06 database	

Comments

(a) The experimental measurements of IP are well above all calculations for C4. Lot of activities are currently undergoing (Belau 2008). We propose 11.5 eV with an error bar of 1 eV, this value covering both calculations and experiments.

(b) Quantum chemistry calculation with MRDCI package programs has been performed for small carbon and hydrocarbon molecules. Calculated rates in standard Draine field are, according to the authors, expected to be upper limits. They are higher by more than one order of magnitude than the currently used estimated rates in data bases for other Cn.

(c) Photodissociation rates are extrapolated from values recommended by van Dishoeck (1988) for large Cn ($10 \geq n \geq 6$). Lognormal factor 1.25 of accuracy is reported. In regard of recent calculation of van Hemert & van

Dishoeck (2008), accuracy could be underestimated. 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.

(d) Photodissociation measurements have been performed with photon energy between 2 and 5.2 eV on cold C_4 molecules produced by discharge in an expanding supersonic jet. Multiphoton absorption is also contributing. Error bars may be underestimated. Results have been interpreted as statistical fragmentation behaviour.

Preferred Values

Rate constant:
$k = 8.5\times 10^{-9}\times \exp(-2.3\times A_V)$

Reliability of rate constant:
F0=5 ; g=0

Recommended Branching Fractions:
(1)=0.85
(2)=0.15

Reliability of Branching Fractions:
±0.1(uniform)

References

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