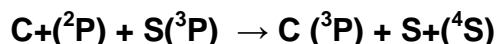


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Thermodynamic Data

$$\Delta H (1) = - 88.68 \text{ kJ mol}^{-1}$$

$$\Delta H (2) = \text{kJ mol}^{-1}$$

$$\Delta S (1) =$$

$$\Delta S (2) =$$

$$Kc(2) =$$

$$Kc(2) =$$

Thermochemical data are taken from ref. 1

Rate Coefficient Data *k*

<i>k</i> / cm ³ s ⁻¹	T / K	Reference	Comments
<i>Rate Coefficient calculations</i>			
Kooij formulae	500-5000	1	(a)
Alpha = 5.54 x 10 ⁻¹²			
Beta = 0.857847			
Gamma = 680.70			
<i>k</i> (500 K) = 2.2 10 ⁻¹²			
<i>k</i> (1000 K) = 7.8 10 ⁻¹²			
<i>Reviews and Evaluations</i>			
Alpha = 1.5 x 10 ⁻⁹			
Beta = 0.0			
Gamma = 0.0	10-41000	UMIST database	(*)

Comments

(a) We have performed rate constant calculations for this charge transfer reaction using accurate ab initio methods and semi-classical dynamics that gives reasonably accurate value for the 500-50000 K temperature range. These calculations have been completed by quantum wave packet dynamics in the 0.01-10 eV range. From these

values we have deduced the alpha, beta and gamma coefficients of the Kooij expression. Quantum dynamics have to be performed for the low 10-100 K temperature range. Our calculated values for this process are much smaller than the proposed UMIST value for the high temperatures. (*) The UMIST looks for us overestimated for such a process even at low temperature. The origin of the proposed value

has not been identified

Preferred Values

Until quantum dynamic calculations are performed we suggest a rate constant for the 10 -100 K temperature range of 10^{-10} - 5×10^{-11} cm^3s^{-1}

References

- 1-MC. Bacchus-Montabonel and D. Talbi, 2008, Chemical Phycis Letters, 467, 28-3
- 2-A. Chenel, E. Mangaud, Y. Justum. D. Talbi, M.C. Bacchus-Montabonel, M. Desouter-Lecomte, 2010, Journal of Physics B, 43, 245701 (11)

