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$C+(^2P) + S(^3P) \rightarrow C(^3P) + S+(^4S)$

Thermodynamic Data

ΔH *(1)* = − 88.68 kJ mol^{-1}

ΔS *(1)* =

Kc(2) =

ΔH (2) = kJ mol^{-1}

ΔS (2) =

Kc(2) =

Thermochemical data are taken from ref. 1

Rate Coefficient Data *k*

k / cm^3 s^{-1}	*T* / K	Reference	Comments
Rate Coefficient calculations			
Kooij formulae	500-5000	1	(a)
Alpha = 5.54 x 10^{-12} Beta = 0.857847 Gamma = 680.70			
k (500 k) = 2.2 10 $^{-12}$ *k (1000 k) = 7.8 10 $^{-12}$*			
Reviews and Evaluations			
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 x10^{-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)