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$H(^2S) + CH_2(^3B_1) \rightarrow CH(^2\Pi) + H_2(^1\Sigma_g^+)$ (1)

Thermodynamic Data

$\Delta H^o_{298}(1) = -\ 11.96$ kJ mol^{-1}

Thermochemical data are taken from ref. (*)

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	*T* / K	Reference	Comments
Rate Coefficient Measurements			
2.7×10^{-10}	298	Bohland & Temps., 1984	(a)
1.8×10^{-10}	298	Bohland *et al*., 1987	(b)
2.7×10^{-10}	298	Boullart & Peeters, 1992	©
Reviews and Evaluations			
2×10^{-10}	298 – 3000	Baulch *et al*., 2005 (p. 953)	(*)
6.64×10^{-11}	300-2500	UMIST database	
2.7×10^{-10}	all temperatures	OSU website	

Comments

The reactants correlate with doublet and quartet states, the products with only doublet states Therefore, there is an electronic degeneracy factor of *ca*. 1/3. The reaction probably proceeds via an energised CH_3 intermediate. Measurements on the reaction between CH and H_2 confirm that there is no barrier in the PES leading from CH_3 to CH + H_2. In assessing the high value of the recommended rate coefficient, the light mass of H (and therefore the small reduced mass of the reactants) should be kept in mind.

The three measurements, (a), (b), (c), of the rate coefficient at 298 K agree well. Other experimental results (and theoretical estimates) are summarised and discussed in ref. (d). At room temperature, they agree quite well with values in (a) to (c). Fulle and Hippler (d) infer a very mild positive *T*-dependence. I prefer to assume no *T*-dependence below room temperature.

Preferred Values

$k(298\ K) = 2.2 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}
$k(10\ K) = 2.2 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}
$k(T) = 2.2 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}

Reliability

$\Delta \log k_1$ (298 K) $= \pm 0.3$
$\Delta \log k_1$ (10 K) $= \pm 0.6$
$F_0 = 2$; $g = 7$

Comments on Preferred Values

I accept the recommendation of Baulch *et al.* for *k*(298 K) – essentially an average of the room temperature measurements and assume no *T*-dependence.

References

(*) D. L. Baulch *et al*., J. Phys. Chem. Ref. Data **34**, 575 (2005).
(a) T. Bohland and F. Temps, Ber. Bunsenges. Phys. Chem. **88**, 459 (1984).

(b) T. Bohland, H. Gg. Wagner and F. Temps, J. Phys. Chem. **91**, 1205 (1987).
(c) W. Boullart and J. Peeters, J. Phys. Chem. **96**, 9810 (19892).
(d) D. Fulle and H. Hippler, J. Chem. Phys., **106**, 8691 (1997).