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## $CH(^2\prod) + CH_4 \rightarrow C_2H_4 + H(^2S)$ (1)

*Thermodynamic Data*

$\Delta H^o_{298}(1) = -251.1$ kJ mol$^{-1}$

Thermochemical data are taken from Baulch *et al*. (a)

### Rate Coefficient Data

| $k$ / cm$^3$ molecule$^{-1}$ s$^{-1}$ | $T$ / K | Reference | Comments |
|---|---|---|---|
| *Rate Coefficient Measurements* | | | |
| Several experimental studies at room temperature and above are reported in the review by Baulch *et al* (a). These show good agreement in the overlapping range of temperature. | | | |
| $3.96 \times 10^{-8}\ T^{-1.04} \exp(-36.1/T)$ | 23 – 295 | Canosa et al., 1997 | (b) |
| *Reviews and Evaluations* | | | |
| $2.2 \times 10^{-8}\ T^{-0.94} \exp(-29/T)$ | 160 – 750 | Baulch et al., 2005 | (a) |
| $k(298\ K) = 9.4 \times 10^{-11}$ | | | |
| $3.96 \times 10^{-8}\ T^{-1.04} \exp(-36.1/T)$ | | Hébrard et al., 2009 | (c) |
| $1.05 \times 10^{-10}\ (T/300)^{-1.04} \exp(-36/T)$ | 23 – 300 | UMIST database | |
| $2.23 \times 10^{-12}$ | all temperatures | OSU website | |

## Comments

The experiments reviewed by Baulch *et al*.(a) agree well in respect of $k$(298 K). Moreover, these results agree well with the rate coefficient of Canosa *et al* (b) at room temperature. In their review of rate coefficients for reactions that may be important in the chemistry of Titan's atmosphere, Hébrard *et al*. (c) adopt the expression of Canosa et al. (b) and carefully evaluate the errors associated with this and similar measurements.

## Preferred Values

$k(298\ K) = 9.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$
$k(10\ K) = 9.8 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$

$k(T) = 1.06 \times 10^{-10}\ (T/300)^{-1.04} \exp(-36.1/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$

*Reliability*

$\Delta \log k\ (298\ K) = \pm 0.12$
$\Delta \log k(10\ K) = \pm 0.3$

$F_0 = 1.3$ ; $g = 4.45$

*Comments on Preferred Values*

The dependence of the rate coefficient for this reaction is well-established over a wide range of temperature (see ref. (c)). The uncertainty in $k$(298) is small. However, in view of the fact that the CRESU measurements of Canosa et al. (b) only go down to 23 K, there is some uncertainty in the extrapolation to 10 K.

The anomalously low value of $k$ given in the OSU data base disagrees with the available

measurements and is unexplained. The expression in the UMIST database is essentially that given by Canosa *et al*. (b).

## References


(a) D. L. Baulch *et al*., J. Phys. Chem. Ref. Data **34**, 575 (2005).

(b) A. Canosa, I. R. Sims, D. Travers, I. W. M. Smith and B. R. Rowe, Astron. Astrophys., **323**, 644 (1997).

(c) E. Hébrard *et al*., J. Phys. Chem. *A*, **113**, 11227 (2009).