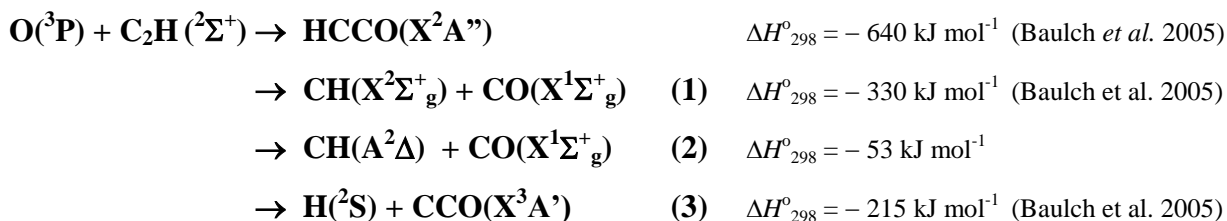


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Rate Coefficient Data k

$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T / K	Reference
<i>Rate Coefficient Measurements</i>		
$9.0 \pm 4 \times 10^{-11}$	600	(Boullart <i>et al.</i> 1996)
$k_2 = 1.8 \pm 0.7 \times 10^{-11}$	295	(Devriendt <i>et al.</i> 1996)
$k_2 = 2.4 \times 10^{-11} \times \exp(-230/T)$	290-925	(Devriendt & Peeters 1997)
$k_2 = 4.5 \pm 1.8 \times 10^{-12}$	295	(Devriendt <i>et al.</i> 1996, Carl <i>et al.</i> 2003)
<i>Reviews and Evaluations</i>		
3.0×10^{-11}	300–2500	(Tsang & Hampson 1986) (p 1219)
<i>Theoretical calculations</i>		
$2\text{-}3 \times 10^{-10}$	5-500	(Georgievskii & Klippenstein 2011)
Preferred value		
$k_1 = 1.8 \times 10^{-10}$	10-300	$F_0 = 2, g = 3$
$k_2 = 1.0 \times 10^{-11}$	10-300	$F_0 = 3, g = 3$
$k_3 = 1.0 \times 10^{-11}$	10-300	$F_0 = 3, g = 3$

k comprised between $k(T)/F$ and $k(T) \times F$, g defined by $F(T) = F_0 \times \exp(g \times |1/T - 1/300|)$

Comments

There is only one measurement of the global rate constant at 600 K (Boullart *et al.* 1996) relative to the known kinetic coefficients of $\text{C}_2\text{H} + \text{C}_2\text{H}_2$ and $\text{C}_2\text{H} + \text{O}_2$ using complex kinetic simulation. The estimation of (Tsang & Hampson 1986) is based only by analogy with similar reactions. Peeters's team determined the rate constant for the $\text{O} + \text{C}_2\text{H} \rightarrow \text{CH}(\text{A}^2\Delta) + \text{CO}(\text{X}^1\Sigma_g^+)$ reaction in the 290-925 K range leading to the excited state of CH responsible for the blue color in flame (Devriendt *et al.* 1996) (Devriendt & Peeters

1997). This partial rate constant was determined using absolute $\text{CH}(\text{A}^2\Delta)$ concentration through calibration via the known spectral photon yield of the $\text{NO} + \text{O} + \text{M} \rightarrow \text{NO}_2 + \text{M}$ reaction. Recently this partial rate constant has been re-evaluated to a lower value (Carl *et al.* 2003). Chickan *et al.* (2004) have studied the nascent vibrational distribution of the CO products from $\text{C}_2\text{H} + \text{O}$, suggesting the participation of both $\text{CH}(\text{A}^2\Delta)$ and $\text{CH}(\text{X}^2\Sigma_g^+)$ products, in the ratio of 3/2 and then a $\text{CH}(\text{A}^2\Delta)/\text{CH}(\text{X}^2\Sigma_g^+)$ branching fraction larger than previously

reported but with potential secondary sources of CO in their system ($O + CH$, $O + CCO$). There are obviously large uncertainties for the $O + C_2H \rightarrow CH(A^2\Delta) + CO(X^1\Sigma_g^+)$ branching ratio despite the fact that this channel is very likely to be far from negligible.

Zhao et al. (2007) performed theoretical calculations (at the DFT level) showing no barrier in the entrance valley leading to HCCO.

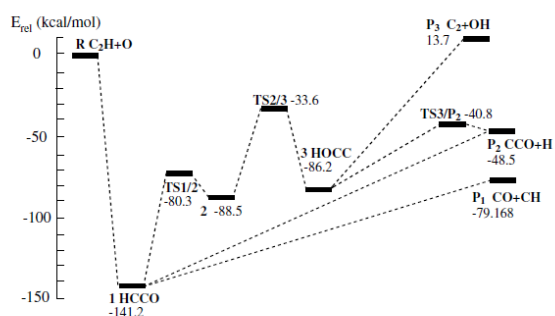
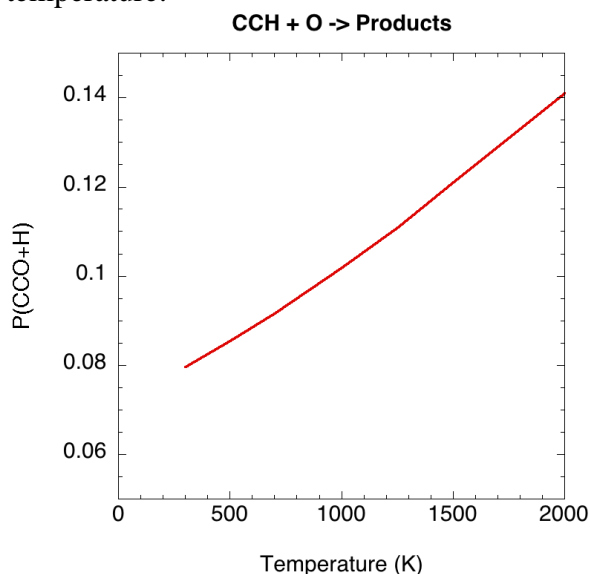


Fig. 2. Schematic singlet potential energy surface of the reaction channels for the $C_2H + O$ reaction at the CCSD(T)//B3LYP/6-311G(d,p) + ZPE level. E_{rel} represents the relative energies (kcal/mol).

Further evolution of HCCO leads to $CO + CH$, CH in its ground state, and $CCO + H$. Recent high level calculations of this rate constant by Georgievskii and Klippenstein (2011) leads to a value between 2 and $3 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ in the $5\text{-}500 \text{ K}$ range. S. Klippenstein performed, for this datasheet, a semiquantitative exploration of the CCO branching ratio using PST calculations leading to a branching ratio around 7% at low temperature:



We consider than the most accurate determination is the theoretical one from (Georgievskii & Klippenstein 2011) and that

the primary product is $CH(X^2\Sigma_g^+) + CO(X^1\Sigma_g^+)$. We consider a branching ratio equal to 5% for the $O + C_2H \rightarrow CH(A^2\Delta) + CO(X^1\Sigma_g^+)$ and 5% for the $H(^2S) + CCO(X^3A')$ channels.

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