

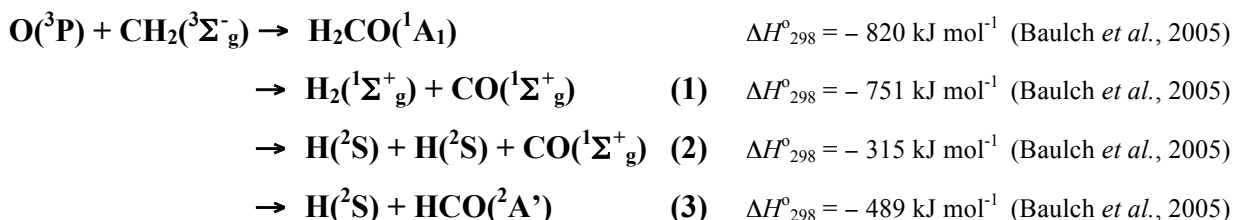
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### Rate Coefficient Data $k$

$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$T / \text{K}$	Reference	Comments
<i>Rate Coefficient Measurements</i>			
$1.3 \times 10^{-10}$	390-600	(Vinckier & Debruyne 1979)	
$8.4 \times 10^{-11}$	298	(Homann & Schweinfurth 1981)	
$1.4 \times 10^{-10}$	296	(Bohland <i>et al.</i> 1984)	
$k_1 = 1.0 \times 10^{-10}$	1500-2500	(Frank <i>et al.</i> 1987)	
$k_2 = 2.0 \times 10^{-10}$	1500-2500	(Frank <i>et al.</i> 1987)	
<i>Reviews and Evaluations</i>			
$3.4 \times 10^{-10} \times \exp(-270/T)$	300 – 3000	(Baulch <i>et al.</i> 2005) (p. 839)	
<b>Preferred value</b>			
$k_1 = 4.0 \times 10^{-11}$	10-300	$F_0 = 1.6, g = 3$	
$k_2 = 1.0 \times 10^{-10}$	10-300	$F_0 = 1.4, g = 3$	
$k_3 = 2.0 \times 10^{-12}$	10-300	$F_0 = 3.0, g = 3$	

$k$  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

The reactants correlate with singlet, triplet and quintet states. S. Klippenstein performed preliminary CASPT2 scans of the interaction between rigid fragments and found no barrier on both the singlet and triplet electronic surfaces in agreement with expectations for such radical-radical reactions as well as with the high experimental rate constant at room temperature. The rate constant from (Bohland *et al.* 1984) is a direct kinetic study and is likely reliable. The weak temperature

dependency adopted by (Baulch *et al.* 2005) was designed to fit the (Bohland *et al.* 1984) room temperature value and the high temperature values from (Frank *et al.* 1987). This expression may give realistic values above 300 K, but certainly does not at low temperature. Considering the absence of barrier found by S. Klippenstein, we recommend the use of a constant value between 10 and 300 K close to the (Bohland *et al.* 1984) value. The first step of the reaction is the formation of singlet and triplet  $\text{H}_2\text{CO}$ . Dissociation of the singlet  $\text{H}_2\text{CO}$

produced can be roughly deduced from H<sub>2</sub>CO photodissociation (Zhang *et al.* 2004, Lee & Lewis 1980), which is supposed to arise from the ground electronic state after internal conversion (so involving only singlet surfaces). The primary competition is between formation of HCO + H and CO + H<sub>2</sub>, the HCO + H formation being favored at high energy. For the O + CH<sub>2</sub> reaction there is so much energy in the HCO product that most of it will dissociate (Song *et al.* 2013, Neyer *et al.* 1992, Peters *et al.* 2013, Wang *et al.* 1973). It is difficult to estimate the amount of HCO produced with less than 70 kJ/mol (barrier for HCO dissociation). Moreover the dissociation of energized HCO has been found to be non-statistical (Neyer *et al.* 1992). The amount of non dissociating HCO is likely quite low but even if only 5% of HCO is stabilized  $k_3$  is as high as  $5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . For the H<sub>2</sub> + CO channel, there is also so much energy that some of the H<sub>2</sub> can also dissociate. Then H + H + CO will be the prominent product. As in interstellar chemistry the branching ratio between H + H and H<sub>2</sub> of the O + CH<sub>2</sub> reaction is not important (H/H<sub>2</sub> ratio is fully driven by H<sub>2</sub> formation on grain) we use the high temperature  $k_1/k_2$  ratio deduced from (Frank *et al.* 1987) even at low temperature. One critical point is the rate constant for the H + HCO channel which should only account for few percent of the total rate. This reaction could therefore be a minor source of HCO radical under interstellar conditions.

## References

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