Author: Ian Smith (Cambridge University, UK)

$$C(^3P) + C_3O() \rightarrow C_3(^1\Sigma_g^+) + CO(^1\Sigma^+) \qquad (1)$$

Thermodynamic Data

$\Delta H^o_{298}(1) \approx -360$ kJ mol^{-1}

Thermochemical data are quite hard to establish for C_3O. I combine data hidden away in (a) with data on C_n species given in (b).

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
Reviews and Evaluations			
1.0×10^{-10}	10 – 300	UMIST database	
1.0×10^{-10}	T-independent	OSU website	

Comments

C_3O is isoelectronic with NCCN and I assume that it has a singlet ground state. If so, the reactants correlate with triplet states, the products in their ground states with only singlet states. Consequently, as written, the reaction is spin-forbidden. However, C_3 has a relatively low-lying triplet state (energy 202.5 kJ mol^{-1} above the ground state (a)) which should be accessible to this reaction.

There are apparently no rate measurements on this reaction. It seems reasonable to suppose that it occurs rapidly via an adduct like those of radicals + alkenes (see (c) for discussion) but uncertainty is high.

Preferred Values

There seem no reason to change the estimates in the UMIST and OSU databases.

k(298 K) = 1×10^{-10} cm^3 molecule^{-1} s^{-1}
k(10 K) = 1×10^{-10} cm^3 molecule^{-1} s^{-1}
k(T) = 1×10^{-10} cm^3 molecule^{-1} s^{-1}

Reliability
$\Delta \log k_1$ (298 K) = ± 0.6
$\Delta \log k_1$ (10 K) = ± 0.6
$F_0 = 4$; $g = 0$
Comments on Preferred Values

References

(a) S. Eckern and M. Vala, J. Phys. Chem. A **101**, 3601 (1997)
(b) A. van Orden and R. J. Saykally, Chem. Rev. **98**, 2313 (1998).
(c) I. W. M. Smith *et al.*, Faraday Discuss. **133**, 137 (2006).