Supporting Information for

Catalytic Effect of Carbon Dioxide on Reaction OH+CO→H+CO_2 in Supercritical Environment: Master Equation Study

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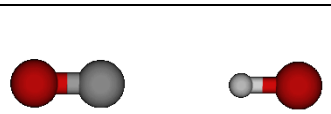
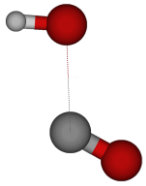
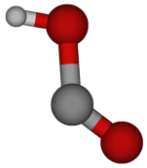
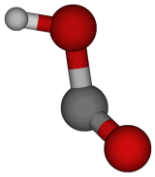
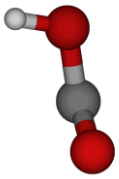
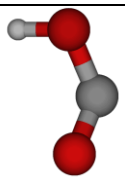
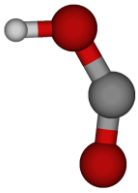
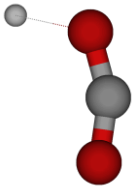
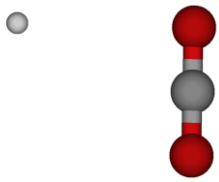
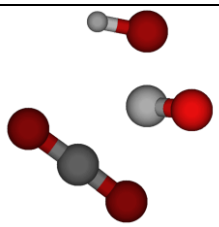
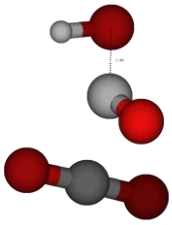
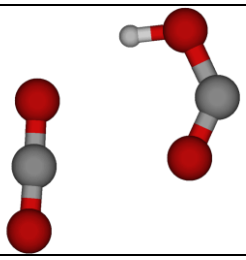
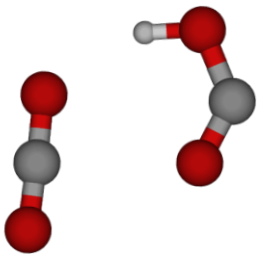
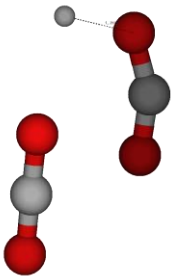
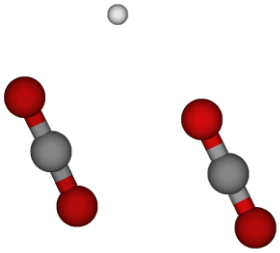
Table S1: Intrinsic Reaction Coordinate (IRC) analyses for R1 and R2. Geometries predicted at M11D3 theory level and energies predicted at CBS-QM11 theory level.[1]

Reverse	**Transition State**	**Forward**
OH..CO	TS1	trans-HOCO
		
-1.65 kcal/mol	1.01 kcal/mol	-25.71 kcal/mol
trans-HOCO	TS4	cis-HOCO
		
-25.71 kcal/mol	-17.9 kcal/mol	-23.71 kcal/mol
cis-HOCO	TS2	$H..CO_2$
		
PRC121	TS122	IN123
		
-1.33 kcal/mol	-1.27 kcal/mol	-26.78 kcal/mol
IN123	TS124	PC125
		
-26.78 kcal/mol	0.15 kcal/mol	-25.30 kcal/mol

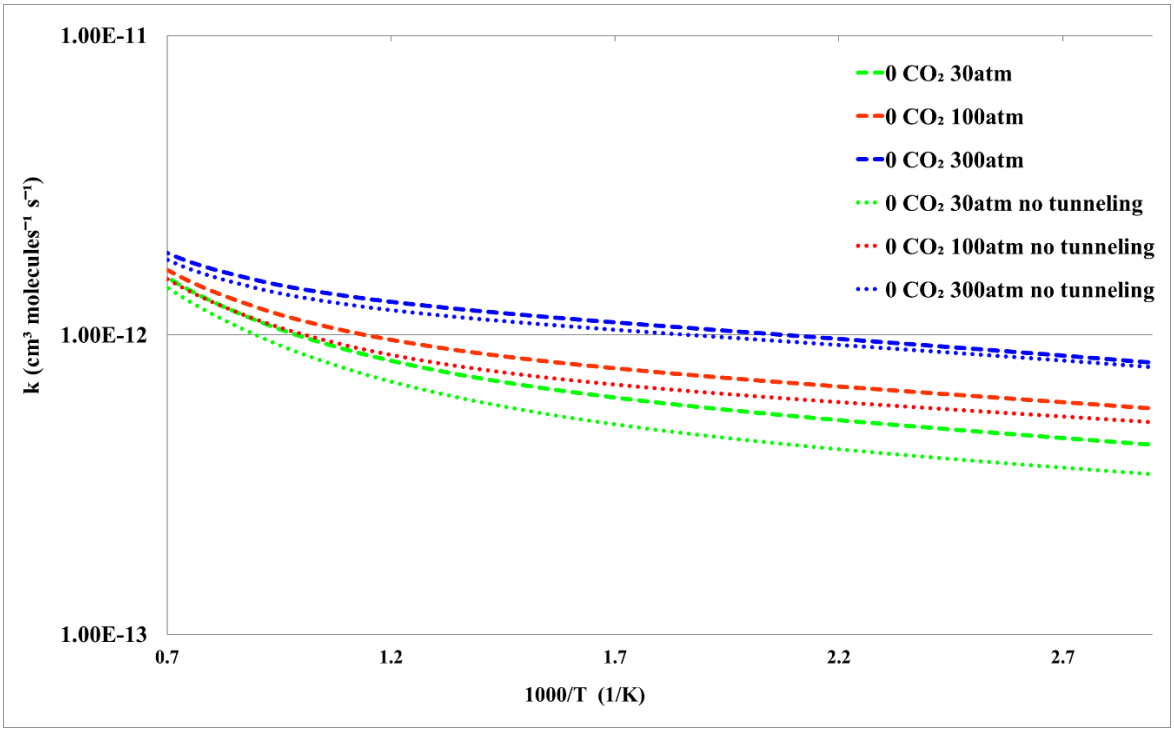


Figure S1. Bimolecular rate constants, calculated at 30 atm, 100 atm, and 300 atm for reaction R1 with (dashed) and without (dotted) Eckart tunneling correction. Turning Eckart tunneling correction off for the exit channel slows the rate of the reaction by 22% at room temperature, and 30 atm. This effect decreases as temperature and pressure increase. This is consistent with calculation by Nguyen et al.[2]

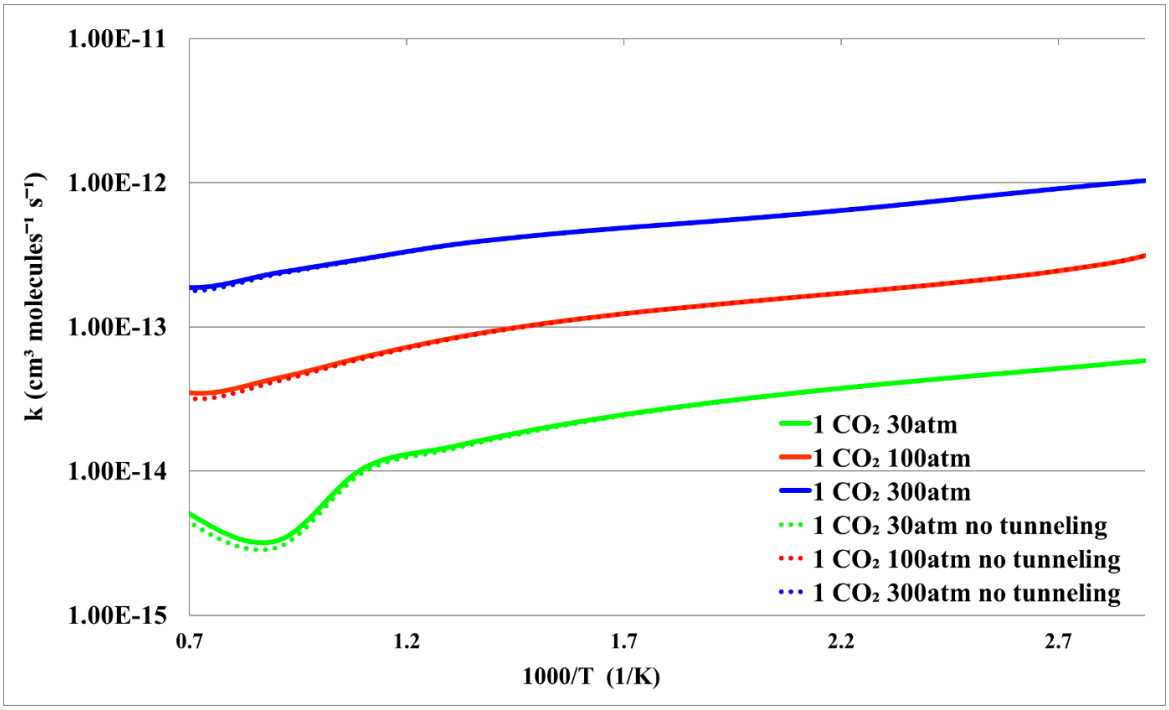


Figure S2. Bimolecular rate constants, calculated at 30 atm, 100 atm, and 300 atm for reaction R2 with (solid) and without (dotted) Eckart tunneling correction.

References

1. Masunov, A. E.; Wait, E.; Vasu, S. S., Chemical Reaction CO+OH → CO_2+H Autocatalyzed by Carbon Dioxide: Quantum Chemical Study of the Potential Energy Surfaces. *J. Phys. Chem. A* **2016**, *120*, 6023-6028.
2. Nguyen, T. L.; Xue, B. C.; Weston, R. E. J.; Barker, J. R.; Stanton, J. F., Reaction of HO with CO: Tunneling Is Indeed Important. *J. Phys. Chem. Lett.* **2012**, *3*, 1549-1553.