

Probing the Potential Energy Profile of the $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ Forward and Reverse Reactions: High Level CCSD(T) Studies with Spin-Orbit Coupling Included

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Figure S1. Three pathways of the water trimer reaction $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ with the MPW1K/cc-pVTZ(-PP) method.

Table S1. Harmonic vibrational frequencies and zero-point energies for the stationary points of the $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ reaction obtained at the CCSD(T)/cc-pVTZ(-PP) level of theory.

Table S2. Relative Gibbs free energies for all stationary points of the $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ reaction at various conditions.

Complete Gaussian 16 reference.

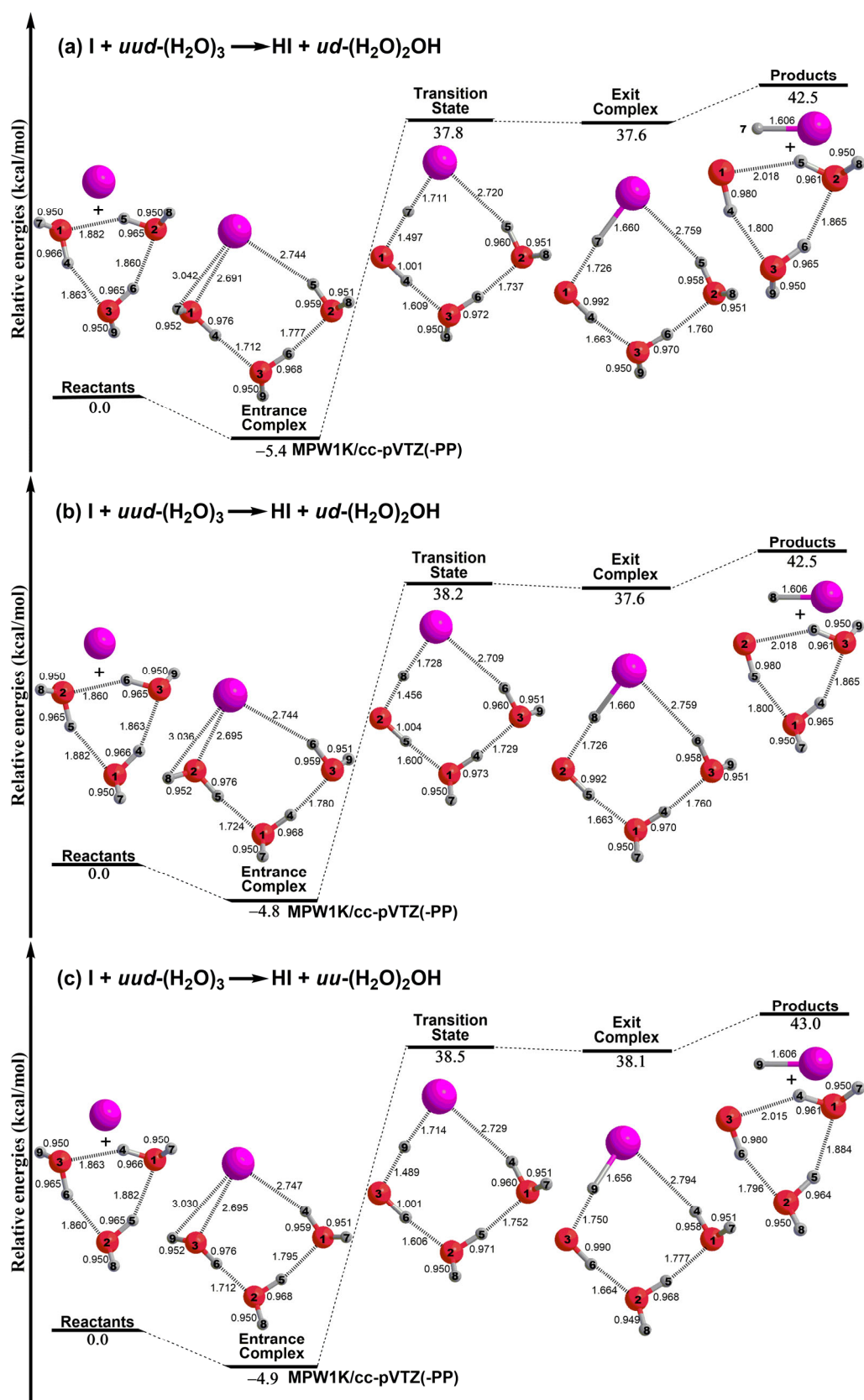


Figure S1 Three pathways of the water trimer reaction $I + (H_2O)_3 \rightarrow HI + (H_2O)_2OH$ with the MPW1K/cc-pVTZ(-PP) method. All bond distances were given in angstroms.

Table S1. Harmonic vibrational frequencies (in cm^{-1}) and zero-point energies (ZPE, in kcal/mol) for the stationary points of the $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ reaction obtained at the CCSD(T)/cc-pVTZ(-PP) level of theory. Experimental results are also shown for comparison.

	ZPE	ΔZPE	Vibrational Frequencies
$(\text{H}_2\text{O})_3$	46.46	0.00	188, 194, 202, 209, 228, 253, 360, 372, 471, 614, 689, 926, 1685, 1690, 1707, 3613, 3683, 3689, 3903, 3907, 3909
Entrance Complex	46.43	-0.03	30, 53, 100, 151, 180, 220, 237, 250, 261, 343, 390, 445, 491, 755, 903, 1670, 1689, 1706, 3521, 3635, 3769, 3876, 3900, 3901
Transition State	41.66	-4.80	307i, 30, 63, 101, 186, 214, 252, 277, 286, 406, 481, 493, 577, 689, 814, 1016, 1451, 1669, 1700, 3271, 3598, 3766, 3900, 3902
Exit Complex	42.05	-4.41	28, 46, 95, 115, 167, 215, 240, 267, 270, 331, 366, 446, 480, 597, 758, 903, 1670, 1698, 2093, 3410, 3626, 3780, 3901, 3907
$(\text{H}_2\text{O})_2\text{OH}$	37.85	-5.30	163, 196, 211, 230, 252, 291, 375, 534, 557, 668, 916, 1667, 1687, 3498, 3675, 3736, 3908, 3911
HI	3.31		2314
Experiment			
Bonded OH in $(\text{H}_2\text{O})_3$			3533, ^a 3544/3529, ^b 3528, ^c 3531.8 \pm 1.2, ^d 3516.7 \pm 2.3 ^d
Free OH in $(\text{H}_2\text{O})_3$			3726, ^a 3717 ^b
OH radical in $(\text{H}_2\text{O})_2\text{OH}$			3365.2 ^c
HI			2309 ^e

^a In gas phase from Ref. 26. ^b In liquid He from Ref. 26. ^c In solid Ne from Ref. 27.

^d From Ref. 28. ^e From Ref. 29, which is a harmonic vibrational frequency.

Table S2. Relative Gibbs free energies (ΔG , in kcal/mol) for all stationary points of the $\text{I} + (\text{H}_2\text{O})_3 \rightarrow \text{HI} + (\text{H}_2\text{O})_2\text{OH}$ reaction, as shown in Figure 1, at various conditions.^a

	T = 600 K p = 160 atm	T = 298.15 K p = 1.0 atm	T = 200 K p = 0.2 atm
I + (H₂O)₃	0.0	0.0	0.0
Entrance Complex	1.6	2.1	0.8
Transtion State	46.1	45.3	43.7
Exit Complex	42.1	43.4	42.3
HI + (H₂O)₂OH	37.1	39.3	40.0

^a Total energies (E) were obtained at the CCSD(T)/cc-pVTZ(-PP) level of theory.

Complete Gaussian 16 reference

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT, **2016**.