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***Supporting Information***

# Potential Energy Profile for the Cl + $(H_2O)_3$ → HCl + $(H_2O)_2OH$ Reaction. A CCSD(T) Study

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**Figure S1.** Four pathways of the water *trimer* reaction Cl + $(H_2O)_3$ → HCl + $(H_2O)_2OH$ with the MPW1K/cc-pVTZ method.

Complete Gaussian 16 reference.

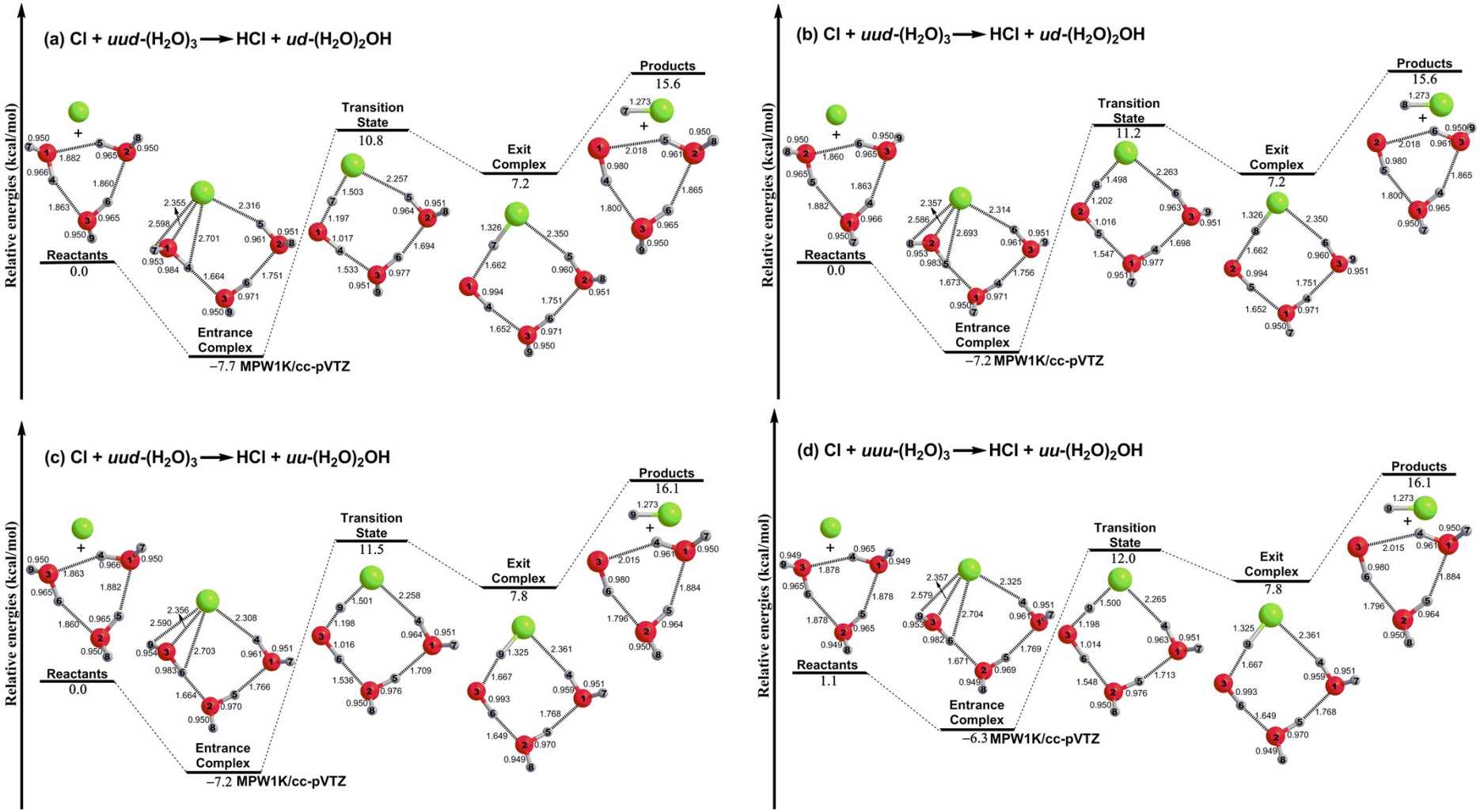


**Figure S1** Four pathways of the water *trimer* reaction Cl + $(H_2O)_3$ → HCl + $(H_2O)_2OH$ with the MPW1K/cc-pVTZ method. All bond distances were given in angstroms and all energies, relative to separated Cl + *uud*-$(H_2O)_3$, were given in kcal/mol.

**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**.