Supporting Information

Theoretical Study on the Water-Assisted Reaction of NCO with HCHO

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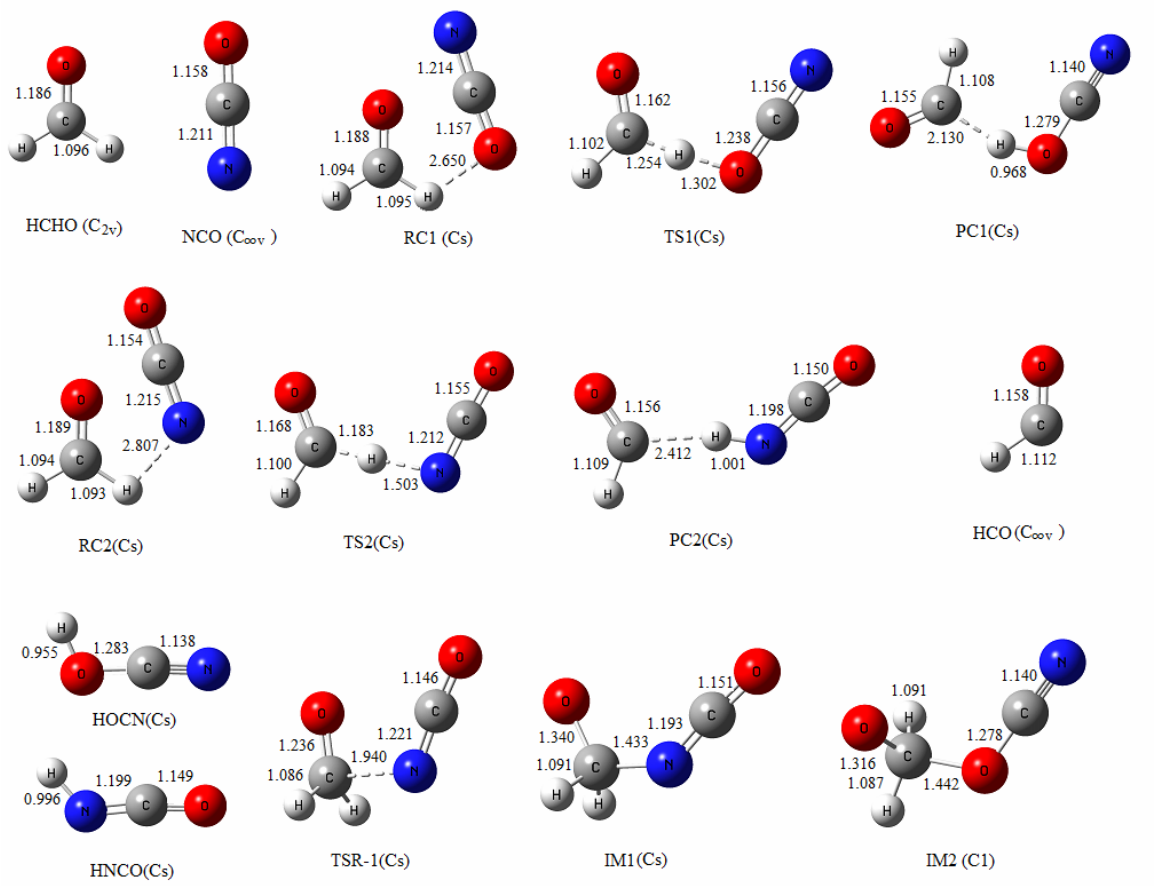

Figure. S1 Optimized geometries for reactants, reactant complexes, intermediates, transition states, product complexes and products involved in the H abstraction and addition reactions of NCO+HCHO without water at the BH&HLYP/6-311++G(3df,3pd) level. Bond lengths are given in angstrom.

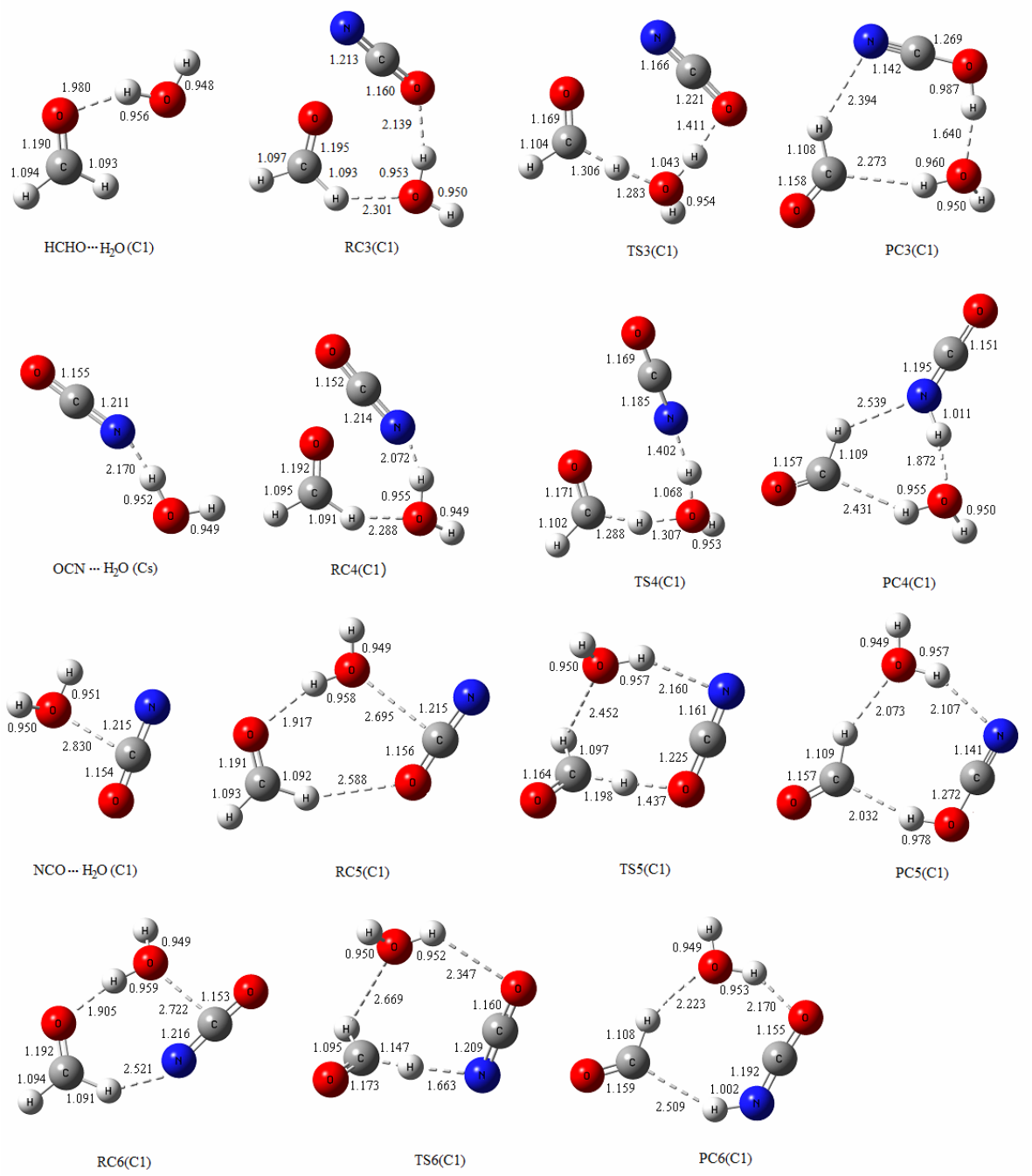

Figure. S2 Optimized geometries for reactant complexes, transition states, product complexes and products involved in the H abstraction reactions of NCO+HCHO with water at the BH&HLYP/6-311++G(3df,3pd) level. Bond lengths are given in angstrom.

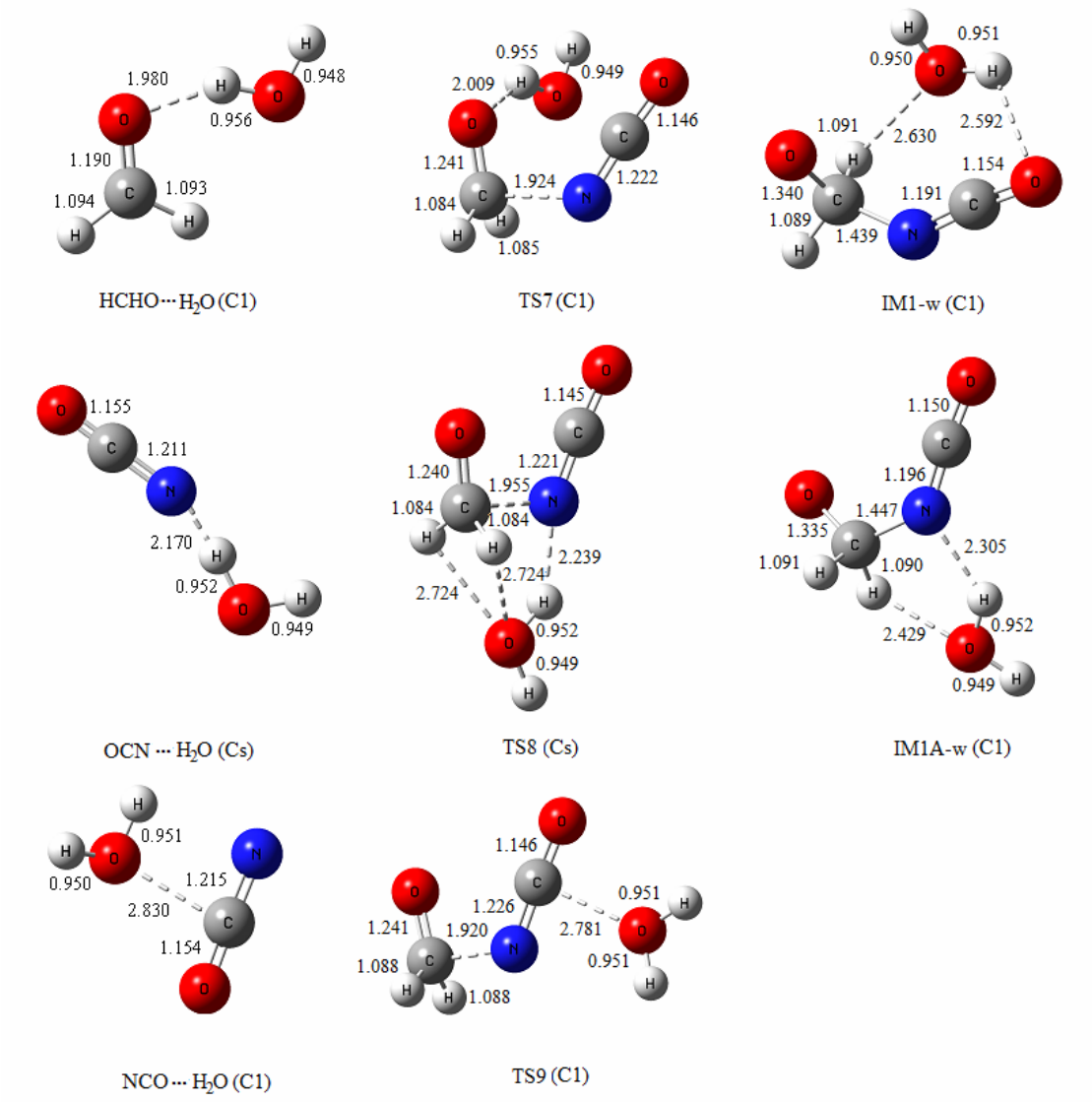

Figure. S3 Optimized geometries for intermediates and transition states involved in the addition reactions of NCO+HCHO with water at the BH&HLYP/6-311++G(3df,3pd) level. Bond lengths are given in angstrom.

Complete Reference of 37

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Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O¨ .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision C.01; Gaussian Inc, Wallingford, CT, 2010.