

Supporting Information for:

Mechanism of fixation of CO<sub>2</sub> into epoxide catalyzed by ZnBr<sub>2</sub> and

Choline Chloride co-catalyst: A DFT study

Tengfei Huang<sup>a</sup>, Lei Fang<sup>a</sup>, Ya Li<sup>a</sup>, Hongqing He<sup>b</sup>, Li Wang<sup>a\*</sup>, Jinglai Zhang<sup>a\*</sup>

*<sup>a</sup>Institute of Environmental and Analytical Sciences, College of Chemistry and Chemical*

*Engineering, Henan University, Kaifeng, Henan 475004, P.R. China*

*<sup>b</sup>Wuhan Center for Magnetic Resonance, State Key Laboratory of Magnetic Resonance and  
Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of*

*Sciences, Wuhan 430071, P. R. China*

---

\*Corresponding author. E-mail: [zhangjinglai@henu.edu.cn](mailto:zhangjinglai@henu.edu.cn), [chemwangl@henu.edu.cn](mailto:chemwangl@henu.edu.cn)

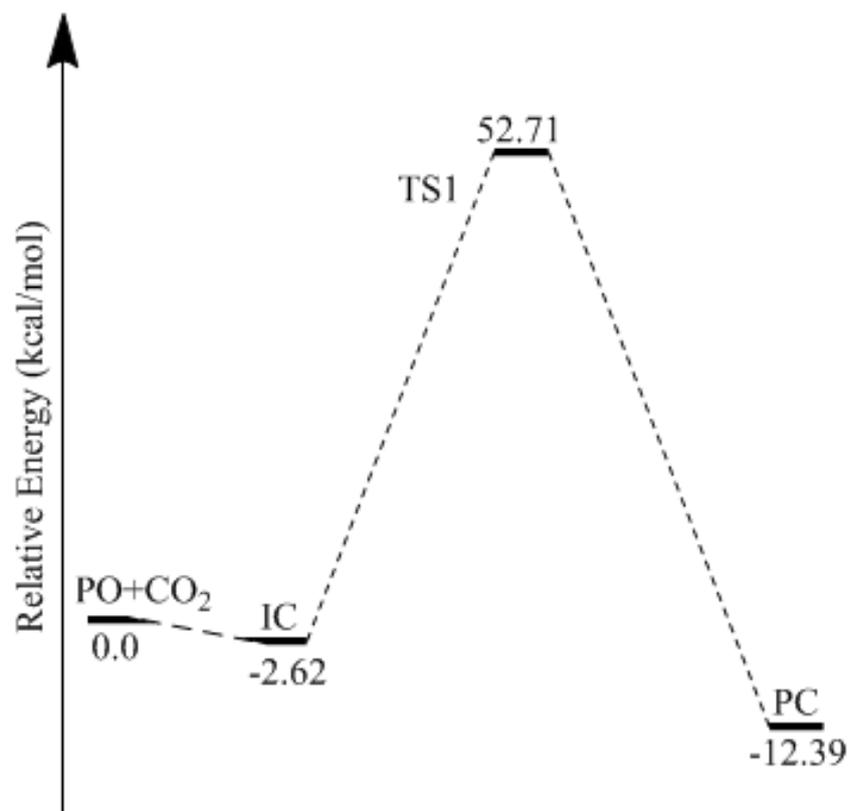


Figure S1 Potential energy surface profile for the preferential route of the uncatalyzed cycloaddition reaction calculated at the M06/6-31+G(d,p) level.

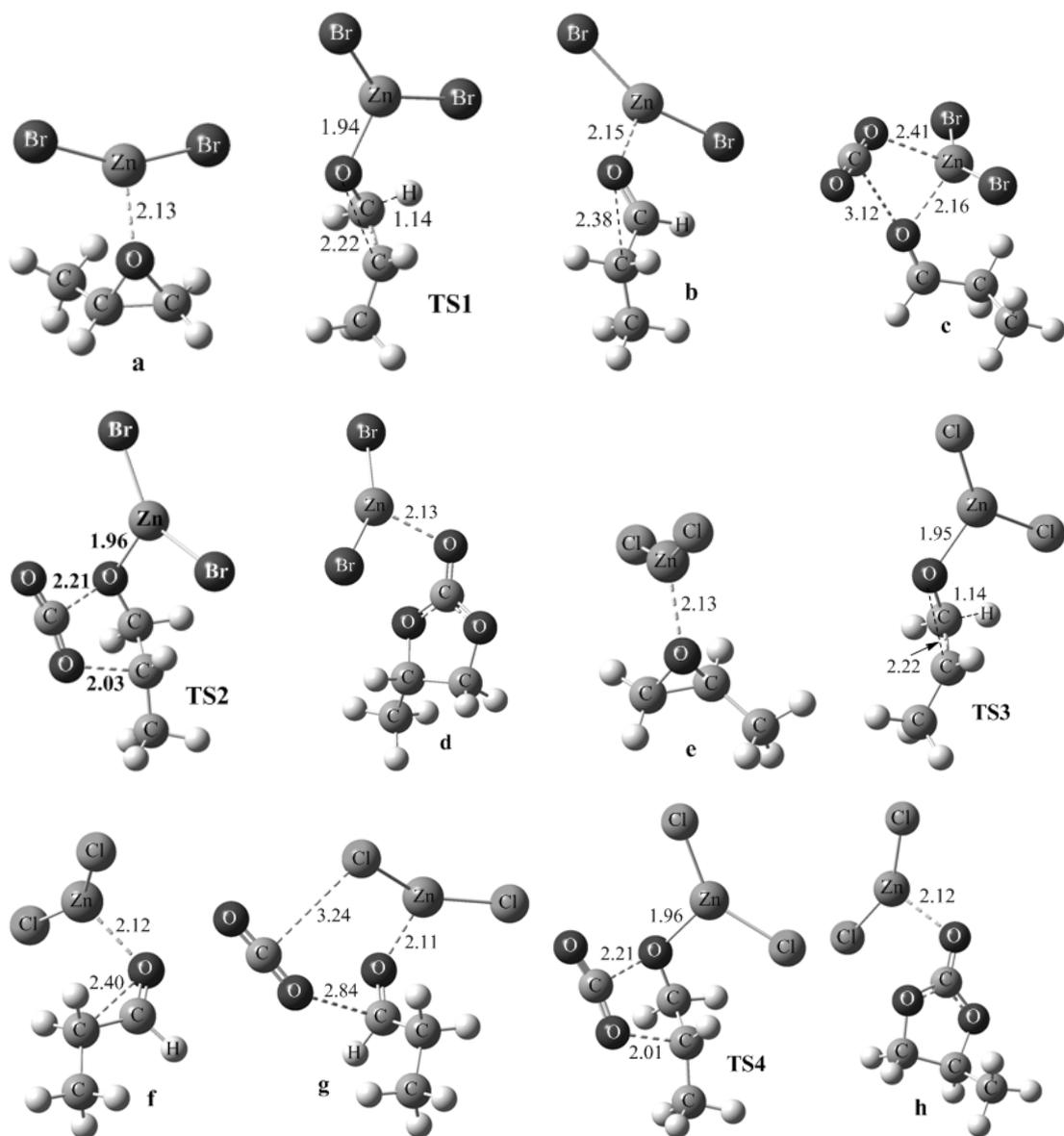


Figure S2 Optimized geometries for the intermediates and transition states involved in the routes of the cycloaddition reaction catalyzed by ZnBr<sub>2</sub> or ZnCl<sub>2</sub>.

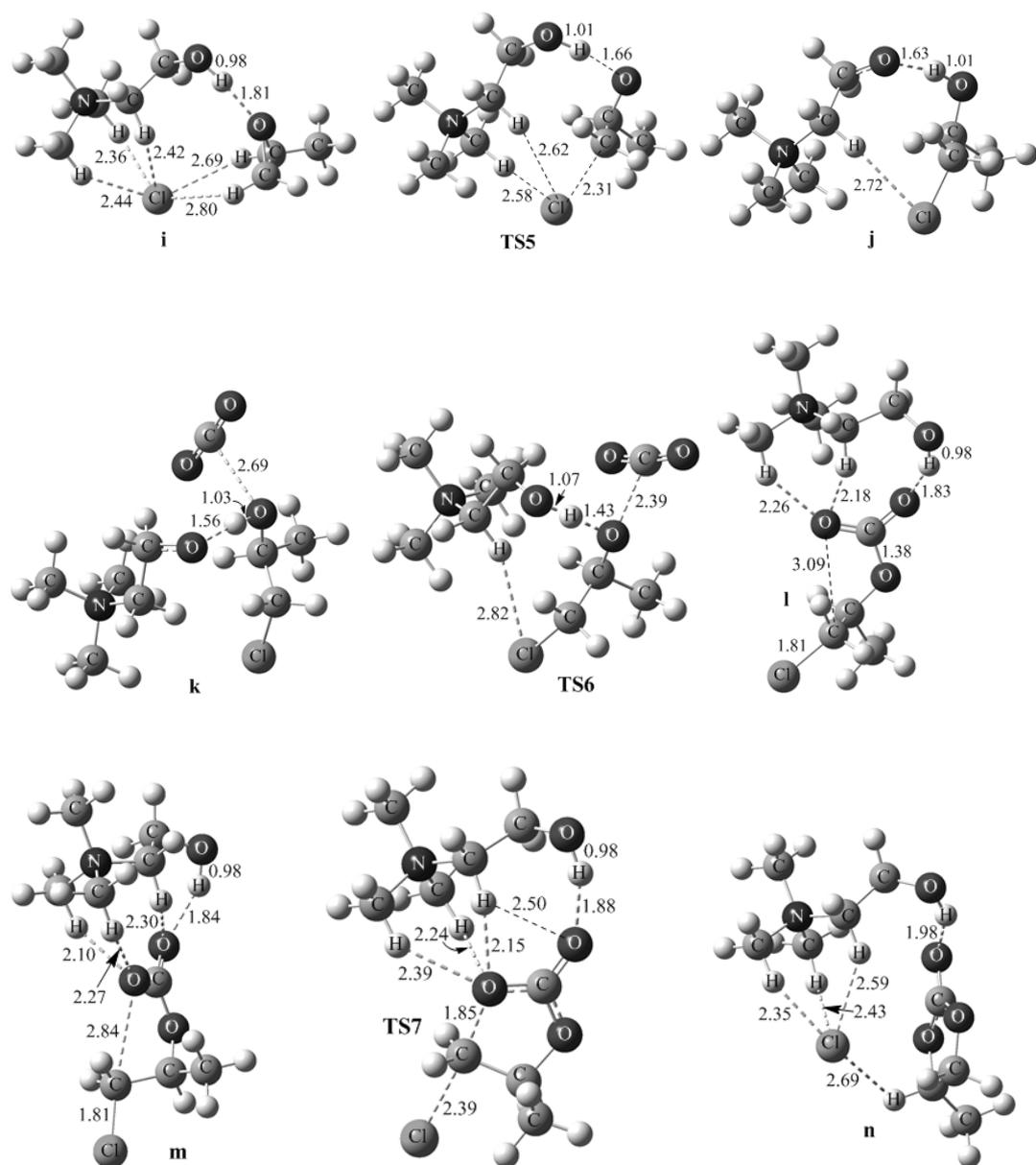
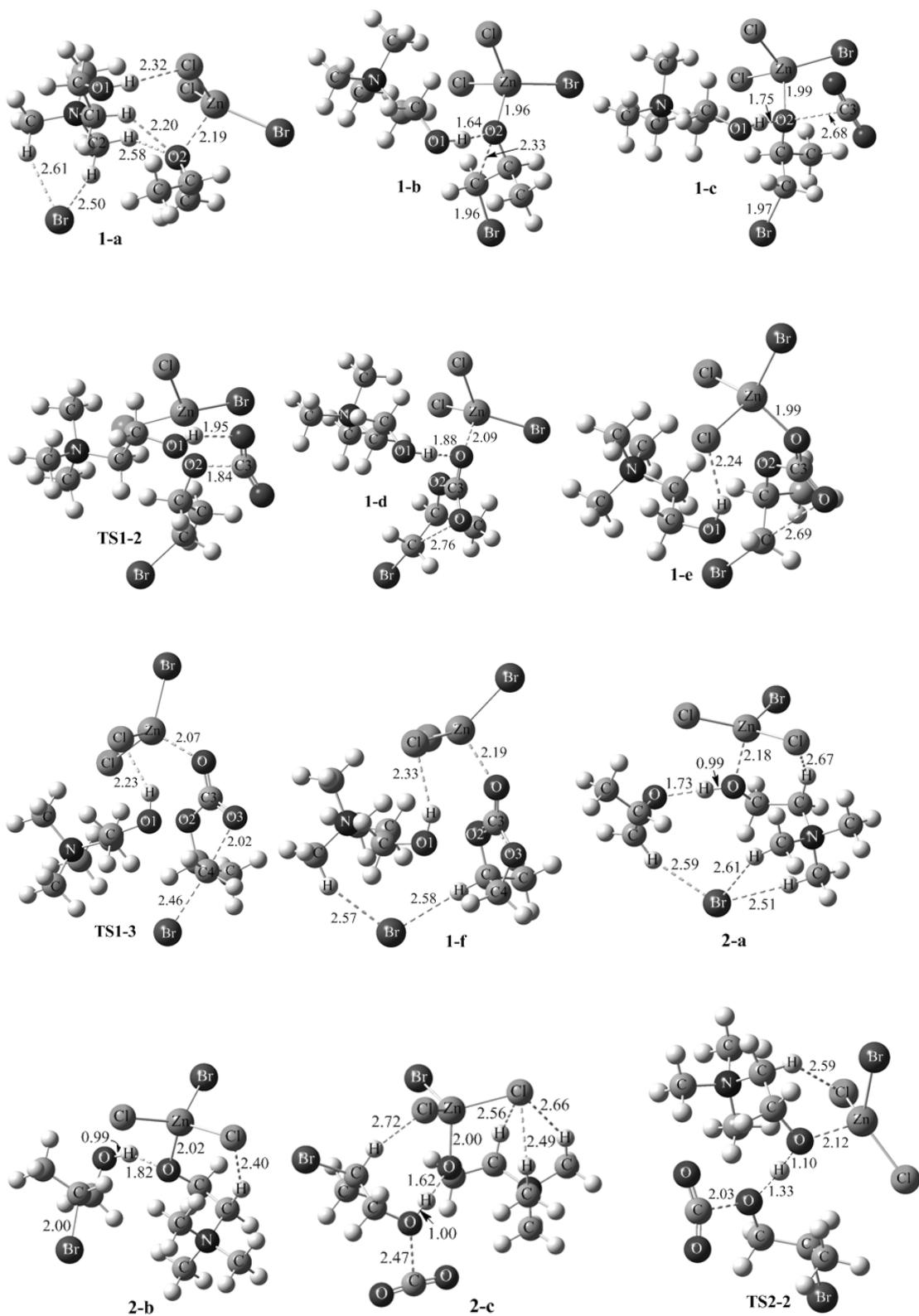
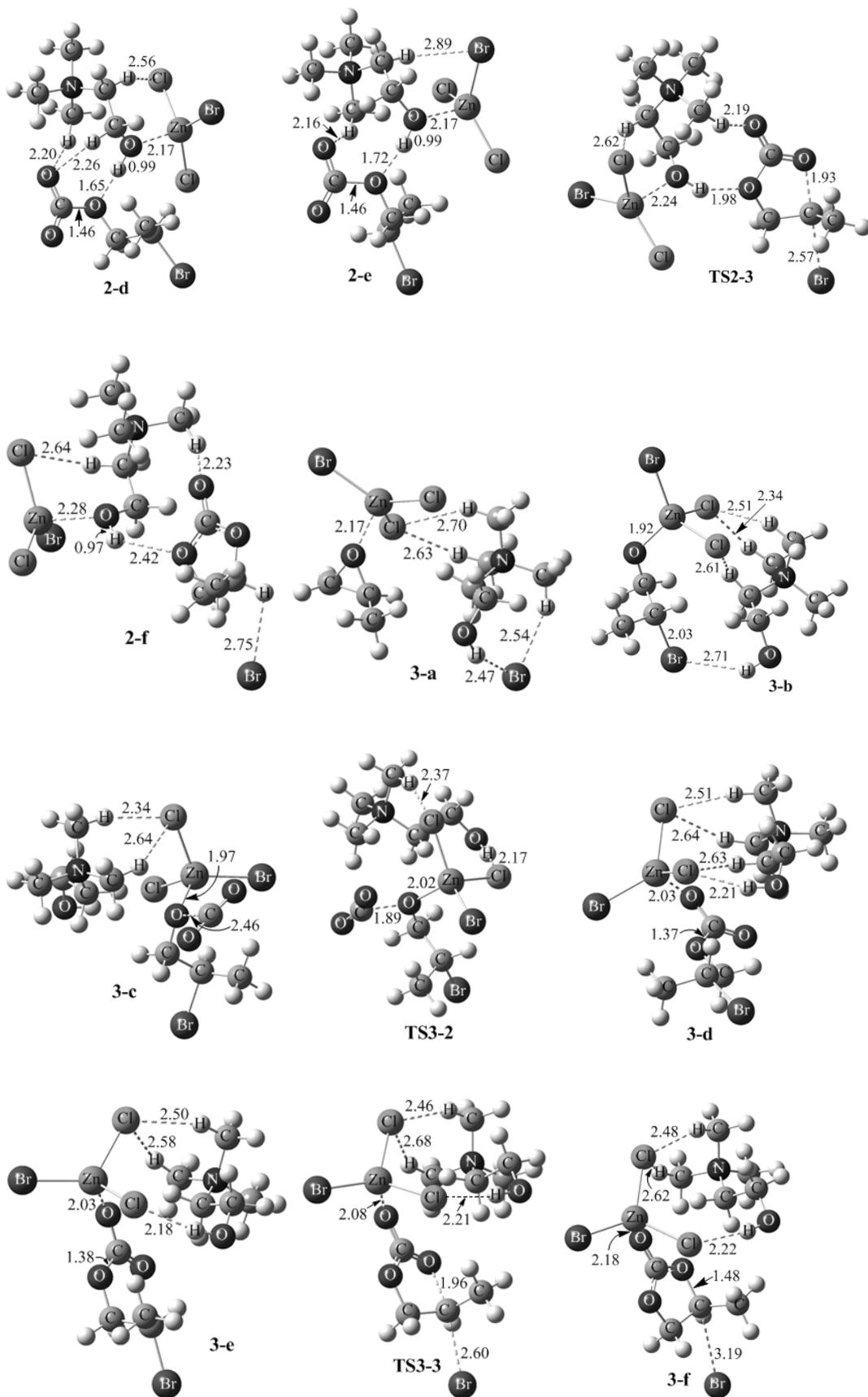


Figure S3 Optimized geometries for the intermediates and transition states involved in the optimal route of the cycloaddition reaction catalyzed by CH (choline chloride).





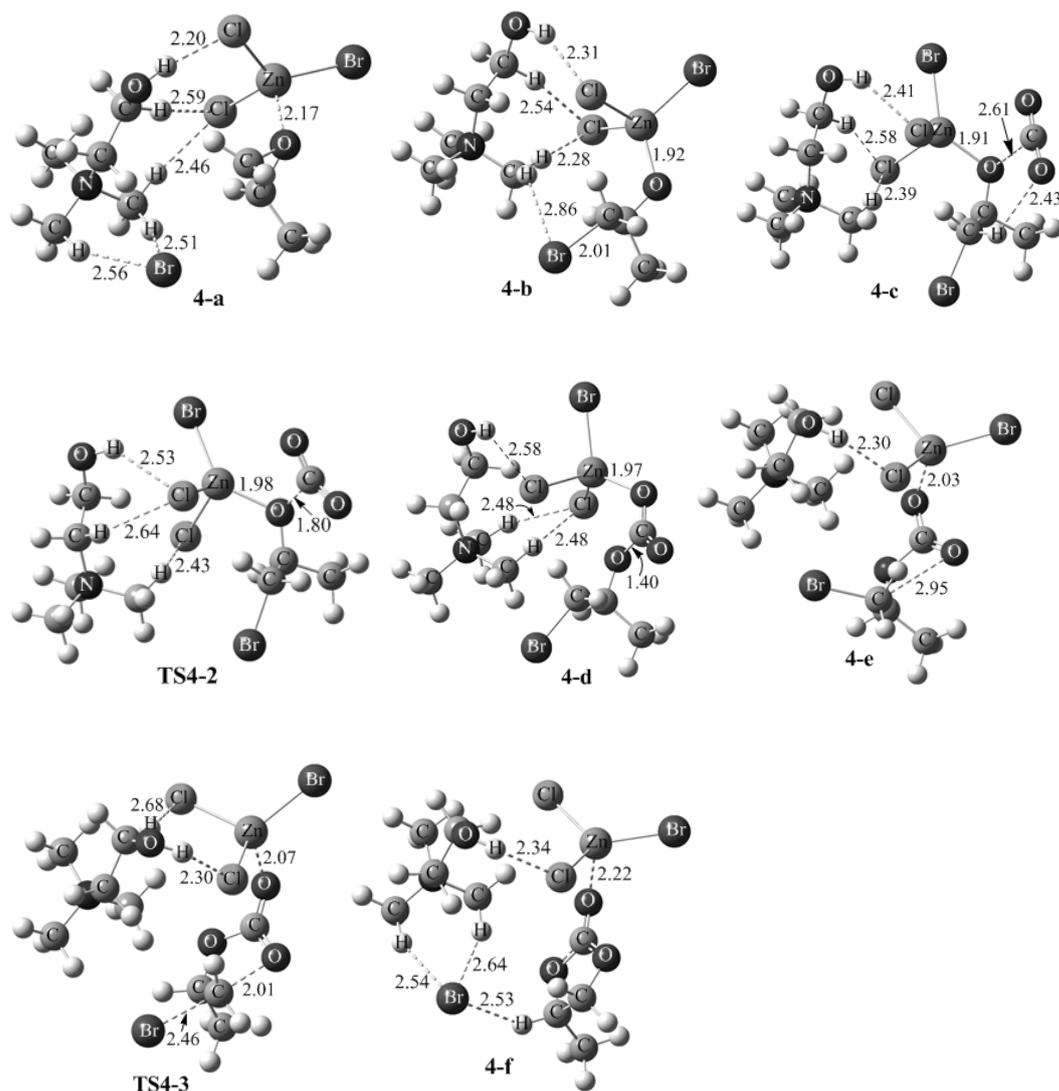


Figure S4 Optimized geometries for the intermediates and other transition states included in routes 1-4 of the cycloaddition reaction catalyzed by  $\text{Ch}^+$ ,  $\text{Br}^-$ , and  $\text{ZnBrCl}_2^-$ . TSm-n ( $n=2$  or  $3$ ) denotes the second or third transition state involved in route m, and m-n ( $n=a, b,$  or  $c$ ) denotes the intermediate in route m.



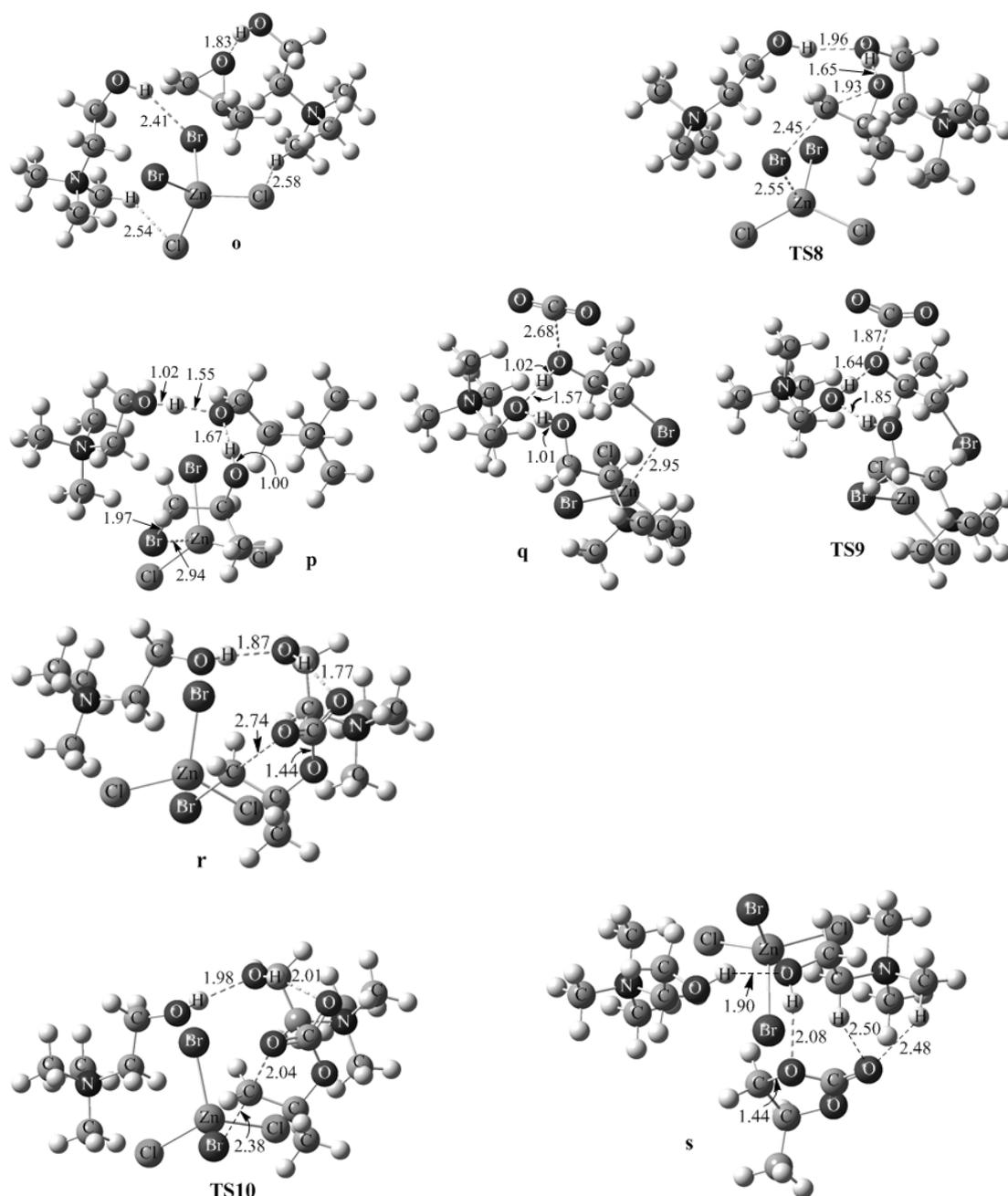


Figure S6 Optimized geometries for the intermediates and transition states included in route 5 of the cycloaddition reaction catalyzed by  $[\text{Ch}]_2[\text{ZnBr}_2\text{Cl}_2]$ .