

ADDITIONS AND CORRECTIONS

2009, Volume 113A

Solvejg Jørgensen* and Allan Gross: Theoretical Investigation of the Reaction between Carbonyl Oxides and Ammonia

Page 10284. Figures 2–5 should be the following figures.

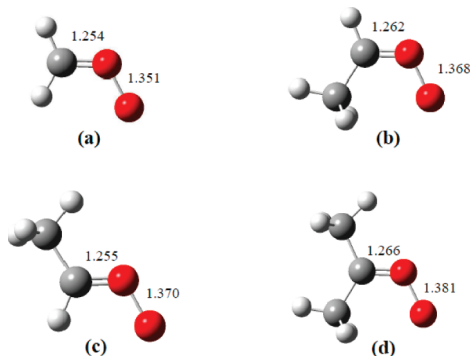


Figure 2. Structures of the carbonyl oxides studied in this work optimized at B3LYP/6-311++G(2d,2p) (white = hydrogen, gray = carbon, and red = oxygen atoms): (a) H_2COO , (b) *syn*-(CH_3) HCOO , (c) *anti*-(CH_3) HCOO , and (d) $(\text{CH}_3)_2\text{COO}$.

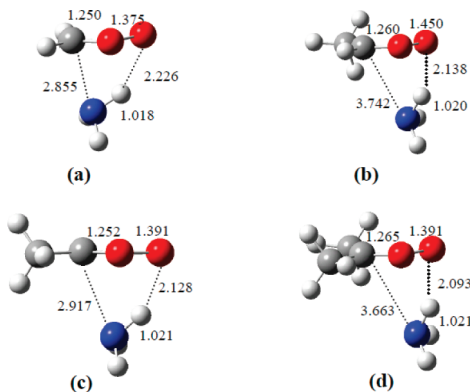


Figure 3. Structures of the prereactive complex studied in this work optimized at B3LYP/6-311++G(2d,2p) (blue = nitrogen atoms): (a) $\text{H}_2\text{COO}\cdots\text{H}-\text{NH}_2$, (b) *syn*-(CH_3) $\text{HCOO}\cdots\text{H}-\text{NH}_2$, (c) *anti*-(CH_3) $_2\text{COO}\cdots\text{H}-\text{NH}_2$, and (d) $(\text{CH}_3)_2\text{COO}\cdots\text{H}-\text{NH}_2$. Distances are given in angstroms.

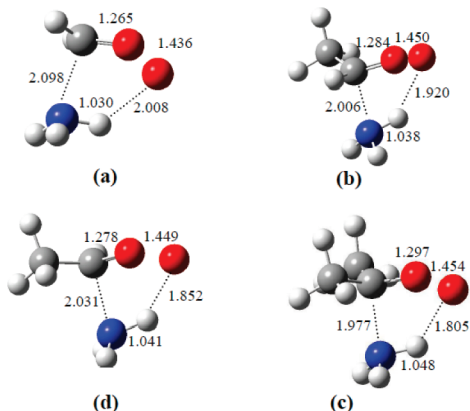


Figure 4. Structures of the transition-state complex studied in this work optimized at B3LYP/6-311++G(2d,2p): (a) $[\text{H}_2\text{COO}\cdots\text{H}\cdots\text{NH}_2]^\ddagger$, (b) $[\text{syn}-(\text{CH}_3)\text{HCOO}\cdots\text{H}\cdots\text{NH}_2]^\ddagger$, (c) $[\text{anti}-(\text{CH}_3)\text{HCOO}\cdots\text{H}\cdots\text{NH}_2]^\ddagger$, and (d) $[(\text{CH}_3)_2\text{COO}\cdots\text{H}\cdots\text{NH}_2]^\ddagger$. Distances are given in angstroms.

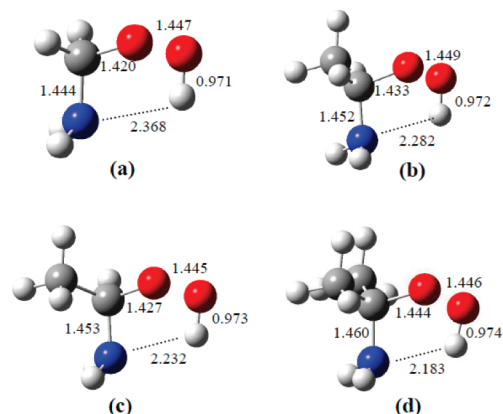


Figure 5. Structures of the products studied in this work optimized at B3LYP/6-311++G(2d,2p): (a) $\text{H}_2\text{C}(\text{OOH})(\text{NH}_2)$, (b) *syn*-(CH_3) $\text{HC}(\text{OOH})(\text{NH}_2)$, (c) *anti*-(CH_3) $\text{HC}(\text{OOH})(\text{NH}_2)$, and (d) $(\text{CH}_3)_2\text{C}(\text{OOH})(\text{NH}_2)$. Distances are given in angstroms.

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