Supplementary Material

A Theoretical Study of 1,3-Dipolar Cycloadditions of Nitrone and Fulminic Acid with Substituted Ethylenes
Eric C. Magnuson and Julianto Pranata *
Figure 3. Nitrone/Vinylamine Transition State Geometries

\[ \text{E(RHF)} = 100.35 \text{ kJ/mol} \]
\[ \text{E(B3LYP)} = 51.17 \text{ kJ/mol} \]

\[ \text{E(RHF)} = 113.13 \text{ kJ/mol} \]
\[ \text{E(B3LYP)} = 40.54 \text{ kJ/mol} \]

\[ \text{E(RHF)} = 149.46 \text{ kJ/mol} \]
\[ \text{E(B3LYP)} = 81.42 \text{ kJ/mol} \]

\[ \text{E(RHF)} = 156.11 \text{ kJ/mol} \]
\[ \text{E(B3LYP)} = 79.35 \text{ kJ/mol} \]
Figure 4. Nitrone/Acrylonitrile Transition State Geometries

\begin{align*}
\text{E(RHF)} &= 113.13 \text{ kJ/mol} \\
\text{E(B3LYP)} &= 35.23 \text{ kJ/mol} \\
\text{E(RHF)} &= 117.57 \text{ kJ/mol} \\
\text{E(B3LYP)} &= 38.96 \text{ kJ/mol} \\
\text{E(RHF)} &= 92.29 \text{ kJ/mol} \\
\text{E(B3LYP)} &= 38.89 \text{ kJ/mol} \\
\text{E(RHF)} &= 89.03 \text{ kJ/mol} \\
\text{E(B3LYP)} &= 35.18 \text{ kJ/mol}
\end{align*}
Figure 5. Nitrone/Acrolein (s-cis) Transition State Geometries

\[ \begin{align*}
E(\text{RHF}) &= 87.62 \text{ kJ/mol} \\
E(\text{B3LYP}) &= 5.03 \text{ kJ/mol}
\end{align*} \]

\[ \begin{align*}
E(\text{RHF}) &= 103.88 \text{ kJ/mol} \\
E(\text{B3LYP}) &= 24.45 \text{ kJ/mol}
\end{align*} \]
Figure 6. Nitrone/Acrolein (s-trans) Transition State Geometries

E(RHF) = 115.42 kJ/mol  
E(B3LYP) = 36.94 kJ/mol

E(RHF) = 117.41 kJ/mol  
E(B3LYP) = 41.10 kJ/mol

E(RHF) = 96.71 kJ/mol  
E(B3LYP) = 38.43 kJ/mol

E(RHF) = 96.46 kJ/mol  
E(B3LYP) = 36.42 kJ/mol
Figure 7. Fulminic Acid/Propene Transition State Geometries

\[ E(RHF) = 135.64 \text{ kJ/mol} \]
\[ E(B3LYP) = 50.41 \text{ kJ/mol} \]

\[ E(RHF) = 150.76 \text{ kJ/mol} \]
\[ E(B3LYP) = 60.46 \text{ kJ/mol} \]
Figure 8. Fulminic Acid/Vinylamine Transition State Geometries

E(RHF)=110.38 kJ/mol
E(B3LYP)=36.87 kJ/mol

E(RHF)=165.99 kJ/mol
E(B3LYP)=77.48 kJ/mol
Figure 9. Fulminic Acid/Acrylonitrile Transition State Geometries

$E_{\text{RHF}} = 146.34\text{ kJ/mol}$
$E_{\text{B3LYP}} = 46.59\text{ kJ/mol}$

$E_{\text{RHF}} = 135.83\text{ kJ/mol}$
$E_{\text{B3LYP}} = 54.85\text{ kJ/mol}$
Figure 10. Fulminic Acid/Acrolein ($s$-cis) Transition State Geometries

E(RHF)=130.48 kJ/mol
E(B3LYP)=35.46 kJ/mol

E(RHF)=132.94 kJ/mol
E(B3LYP)=49.18 kJ/mol
Figure 11. Fulminic Acid/Acrolein \( (s\text{-}trans) \) Transition State Geometries

\[
\begin{align*}
E(RHF) &= -209.54 \text{ kJ/mol} \\
E(B3LYP) &= -169.19 \text{ kJ/mol}
\end{align*}
\]

\[
\begin{align*}
E(RHF) &= -194.55 \text{ kJ/mol} \\
E(B3LYP) &= -159.73 \text{ kJ/mol}
\end{align*}
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