

Characterisation of the reaction mechanism between ammonia and formaldehyde from the topological analysis of ELF and catastrophe theory perspective.

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A prototypical reaction between ammonia and formaldehyde has been investigated at the DFT(M06)/6-311++G(d,p) computational level using the Bonding Evolution Theory (BET). BET is a very useful tool for studying reaction mechanisms as it combines topological analysis of electron localisation function with the catastrophe theory. Each of two studied reactions: $\text{H}_2\text{C}=\text{O} + \text{NH}_3 \leftrightarrow \text{HO}-\text{C}(\text{H}_2)-\text{NH}_2$ (hemiaminal) and $\text{HO}-\text{C}(\text{H}_2)-\text{NH}_2 \leftrightarrow \text{HN}=\text{CH}_2$ (Schiff base) + H_2O consists of six steps. Formation of hemiaminal starts from a nucleophilic attack of nitrogen lone pair in NH_3 on the carbon atom in $\text{H}_2\text{C}=\text{O}$ and is subsequently followed by hydrogen transfer within the $\text{N}-\text{H}\cdots\text{O}$ bridge. A Schiff base is formed via the dehydration reaction of the hemiaminal, where the $\text{C}-\text{O}$ bond is broken first, followed by hydrogen transfer towards the $[\text{HO}]\delta^-$ moiety, resulting in water and methanimine. The present paper focuses on differences in reaction mechanisms for the processes described above. The results have been compared to the reaction mechanism for stable hemiaminal synthesis from benzaldehyde and 4-amine-4H-1,2,4-triazole studied previously using the BET theory.

Słowa kluczowe

Hemiaminal, Schiff, Electron localization function (ELF), reaction mechanisms, chemical bond, topology, catastrophe, Methanimine, attractor

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