

Computational Studies on Molecular Structures and Carbonyl and Ketene Groups' Effects of Singlet and Triplet Energies of Azidoketene $O=C=CH-N=NN$ and Isocyanatoketene $O=C=CH-N=C=O$

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Editorial

Highly reactive intermediates, Azidoketene $O=C=CH-N=NN$ and Isocyanatoketene $O=C=CH-N=C=O$ have attracted much attention in computational chemistry [1–25]. Full geometry optimizations are carried out on singlet and triplet states of ketene substituted Azidoketene $O=C=CH-N=NN$ and Isocyanatoketene $O=C=CH-N=C=O$ by HF, HF+ MP2, LDA, BLYP, B3LYP, MP2, MP3 and MP4 methods using 6–311++G (d, p) basis set of the Gaussian 09. For Azidoketene $O=C=CH-N=NN$, the triplet state is ground state while other large substituted ketenes, the singlet state is ground state. By comparing Natural Bond Orbital (NBO) charges on Azidoketene $O=C=CH-N=NN$ and other large substituted ketenes, the role of carbonyl group is electron withdrawing more than Oxygen atom. Higher electronegativity of carbonyl group leads to stabilize the singlet respect to triplet state as well as decreasing the singlet–triplet splitting energies. In contrast to Azidoketene $O=C=CH-N=NN$, the singlet state of Isocyanatoketene $O=C=CH-N=C=O$ is ground state. Similar to Azidoketene $O=C=CH-N=NN$, stability of singlet state is increased with substituting of ketene groups on Isocyanatoketene $O=C=CH-N=C=O$ center. Furthermore, by comparing Natural Bond Orbital (NBO) charges on Isocyanatoketene $O=C=CH-N=C=O$ center and other large substituted ketenes, the role of carbonyl group is electron withdrawing respect to Oxygen atom. Here is also similar to Azidoketene $O=C=CH-N=NN$, higher electronegativity of carbonyl group leads to stabilize the singlet respect to triplet state as well as decreasing the singlet–triplet splitting energies.

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