

A Class of Non-Kekulé Molecules with Low Excitation Energies

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A class of non-Kekulé molecular systems with a new structural principle and low excitation energies or with a triplet ground state was investigated theoretically. The systems consist of a non-Kekulé monoradical, possessing a non-bonding molecular orbital linked in a specific way to another monoradical.

Key words: Non-Kekulé Molecules, Triplet Diradicals, Molecular Systems with Low Excitation Energies