

A New Type of Non-Kekulé Diradicals with Triplet Ground States.

I. Polymethine Systems

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It is shown theoretically that the ground state of a new class of non-Kekulé polymethine molecules can be a triplet state with non-degenerate singly occupied MOs. The investigated polymethine cyanine cations, polymethine oxonol anions, and neutral polymethine merocyanines are derivatives of the stable 2-azaphenalenyl radical whose pentamethine fragment is part of the polymethine chain.

Key words: Non-Kekulé Polymethines, Triplet Diradicals, Polymethines with Low Excitation Energies