Decomposition Mechanisms and Dynamics of N₆: Bond Orders and Partial Charges along Classical Trajectories

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Abstract:

Ab initio molecular dynamics simulations using B3LYP combined with Natural Bond Orbitals analysis of partial charges and bond orders along trajectories are used to study the decomposition dynamics of three theoretically known isomers of N₆. The results show that significant changes in bonding and in charge distribution occur in intervals of about 10 fs during the process. The decomposition of one isomer proceeds in two steps through a retro Diels Alder mechanism while the other isomers decompose to 3N₂ directly. It is suggested that this approach may provide useful insights into reactions in general.