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B_2P_2 Rings: Through-space π Bond or Stable Diradical? A Theoretical Study

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Abstract

Theoretical study of a series of B_2P_2 ring molecules shows that bulky substituent groups facilitate the existence of bond-stretch isomers. With the largest substituent group, the long bond (LB) isomer is more stable and adopts a mainly through-space B-B bond. Among these LB isomers we observed extraordinarily large singlet-triplet energy separation, a small number of effectively unpaired electrons, and the convergence of spin symmetry-broken (UDFT) computations to RDFT. The T_1 diagnostic for the LB isomer of prototype compound obtained at the CCSD/6-311G** level of theory is smaller than 0.02. We thus conclude that these B_2P_2 ring molecules do not characterize as diradicals.