

Aromatic B3 Ring Stabilized Group 2 Dimer, B3-Y-Y-B3 (Y = Be, Mg, Ca)

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December 15, 2021

Abstract

Quantum chemical calculations have been performed on B3 ring stabilized Y-Y interaction (Y = Be, Mg, Ca) to understand the possibility of binuclear sandwich type complex formation. Calculations indicate single reference character of the studied systems. The complexes have been found to be stable towards dissociation into different fragments. Thermodynamic consideration also indicates the favourability of their formation. Increase in aromaticity of the parent B3 ring upon complexation is observed which is expected to provide extra stability to the complexes.

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