Exploring the Potential Energy Surface of E_2P_4 clusters (E = Group 13 Element): The quest of inverse carbon-free sandwiches

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ABSTRACT

Inverse carbon-free sandwich structures with formula E_2P_4 (E = Al, Ga, In, Tl) have been proposed as a promising new target in main group chemistry. Our computational exploration of their corresponding potential energy surfaces at the S12h/TZ2P level shows that indeed stable carbon inverse-sandwiches can be obtained if one chooses an appropriate Group 13 element for E. The boron analogue B_2P_4 does not form the D_{4h}-symmetric inverse-sandwich structure, but instead prefers a D_{2d} structure of two perpendicular BP_2 units with the formation of a double B-B bond. For the other elements of Group 13, Al-Tl, the most favorable isomer is indeed the D_{4h} inverse-sandwich structure. The preference for the D_{2d} isomer for B_2P_4 and D_{4h} for the other clusters has been rationalized in terms of an isomerization energy decomposition analysis, and further corroborated by determination of the aromaticity of these species.