

Endohedral cluster of Li₁₀O with T_d symmetry

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A detailed numerical study of several isomers of the Li₁₀ cluster has been done. The analysis of the electronic localization function and the analysis of energy diagrams revealed the existence of one cluster with an inner space capable to suit a heteroatom. The perfect candidate is the Li₁₀O cluster due to the experimental evidence of the [Li₆O]⁴⁺ core, the same core present in Li₁₀O. In order to check the thermodynamic stability of this cluster, an analysis of its dissociation channels has been done. The IR and UV-vis spectra have been calculated to help in the further identification of this new cluster. © 2009 American Chemical Society.