

$[\text{Bi}_6\text{Mo}_3(\text{CO})_9]^{4-}$: a multiple local σ -aromatic cluster containing a distorted Bi_6 triangular prism

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Abstract

The first Zintl cluster containing a distorted Bi_6 triangular prism, $[\text{Bi}_6\text{Mo}_3(\text{CO})_9]^{4-}$, has been synthesized and structurally characterized. Quantum chemical calculations indicated that the distorted cage cluster features multiple local σ -aromaticity.

Indexed keywords

Engineering controlled terms:

Quantum chemistry