

# Viability of half-sandwich complex of heavier group-14 elements (Si-Pb) with neutral Be<sub>3</sub> ring and its potential application as H<sub>2</sub> storage material

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## Abstract

Quantum chemical calculations were carried out to establish the half-sandwich structural behaviour between heavier group-14 elements (Si-Pb) and neutral Be<sub>3</sub> ring. The proposed complexes are found to be global minima on the potential energy surface. Quantum chemical investigation revealed that the complexes found possess high bond dissociation energy and also favorable thermodynamics of their formation. The complexes were also found to possess significant aromatic behaviour. In addition, the half-sandwich complexes were found to possess promising chemical properties to be useful for potential H<sub>2</sub> storage material under reversible conditions.

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