He Incorporation into a Cage Compound $C_{14}H_{16}$: A Computational Study

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Since it was first reported in 1961, a symmetric cage compound built from 14 sp^3 carbon atoms (the summary formula $C_{14}H_{16}$, eight five-membered rings, a D_{2d} symmetry) and its derivatives have been studied in organic chemistry. Recently, Cross, Saunders and Prinzbach reported incorporation of He inside dodecahedrane, $He@C_{20}H_{20}$ (Org. Lett. 1 (1999) 1479). This first He containing endohedral species with its cage exclusively built only from sp^3 carbon atoms, was prepared by shooting a beam of helium ions at a continuously deposited surface of dodecahedrane.

In this report, computations are carried out on a hypothetical endohedral system $He@C_{14}H_{16}$, still smaller than $He@C_{20}H_{20}$. The full geometry optimizations have been carried out at several *ab initio* levels, followed by vibrational analysis in order to confirm that a local energy minimum has been localized. Then, the GIAO NMR computations have been carried out for several selected vawefunctions.