

Non-Central Location of Li in Li@C₆₀

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There has been a renewed interest in alkali metal containing endo-fullerenes, in particular Li@C₆₀ and Li@C₇₀. The species can be now produced by the low-energy bombardment method in bulk amounts. This experimental progress makes computations of the species at higher levels of theory interesting, too. In the report, the computations are carried out on Li@C₆₀ with the *ab initio* unrestricted Hartree-Fock (UHF) SCF method in the standard 3-21G basis set (UHF/3-21G) and the restricted open-shell Hartree-Fock (ROHF) treatment in the 4-31G basis set (ROHF/4-31G). At both levels of theory, the Li atom exhibits a non-central location relatively close to the cage.