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The photoabsorption spectra of a Xe atom encapsulated inside C_{54}, C_{56}, and C_{58} fullerenes[1] ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — The photoabsorption spectra of a Xe atom encapsulated inside C_{54}, C_{56}, and C_{58} have been investigated using the time-dependent-density-functional-theory (TDDFT). The most stable isomers for these fullerenes are respectively, C_{54} C_{2v}:540, C_{56} C_s:864, and C_{58} C_{3v}:1205. The stuctures of these fullerenes have been created using the Fullerene4.4 [1] package. The structures are then optimized using $DMol_3$ software. The absolute photoabsorption cross sections of C_{54}, C_{56}, C_{58} and Xe@C_{54}, Xe@C_{56}, Xe@C_{58} are evaluated using TDDFT. The results demonstrate that, except for the Xe atom inside C_{58}, which has similar confinement resonances as those of Xe@C_{60}, the Xe atoms inside C_{54} and C_{56} have totally different spectra. Because of this the measured spectra, with the loss of one or more pairs of C atoms, may be affected by the spectra of the Xe inside C_{54} (or C_{56}, C_{58}). More discussions about the spectra of fullerenes and endohedral fullerenes will be presented at the conference.

[1] P. Schwerdtfeger et al J. Comput. Chem. 35 1508 (2013).

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