DFT study on hydrogenated and deuterated derivatives of interstellar fullerenes

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The credible detection of C_{60}, C_{70} and C_{60}^{+} in astronomical environments enables the search for other fullerene molecules and their derivatives (Zhang et al. 2017). The high reaction rates of fullerenes with atomic H, the most abundant element in the universe, suggest the dominance of their hydrogeneted forms (García-Hernández et al. 2010), which can go through deuterium enrichment as well (Cataldo et al. 2009c).

Here, we present theoretical infrared (IR) spectra and standard enthalpy of formation for neutral and singly ionized $C_{60}H_m$, $C_{60}D_m$, $C_{70}H_n$ and $C_{70}D_n$ using Density Functional Theory (DFT). The calculated IR spectra is then compared with observations.

References

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