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Energy and rovibrational spectroscopic constants for fullerenes dimers $(C_{20})_2$, $(C_{24})_2$, $(C_{36})_2$, $(C_{60})_2$, $(C_{70})_2$ and $(C_{84})_2$

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Abstract: Fullerenes have been studied both experimentally and theoretically for the last years. Several applications have been done, such as: in material science area [1], in the production or transportation of drugs [2], and to build up solar cells [3]. Nevertheless, there are only some small works reporting spectroscopic data of fullerenes dimers. The main goal of this work is to calculate the rovibrational energies and spectroscopic constants of fullerenes dimers $(C_{20})_2$, $(C_{24})_2$, $(C_{36})_2$, $(C_{60})_2$, $(C_{70})_2$ and $(C_{84})_2$. To achieve this goal, we built up potential energies curves for the related systems and employed the Rydberg analytic function [4]. The spectroscopic constants were obtained employing the Dunham's [5] and the Discrete Variable Representation (DVR) methods [6]. The results found to the dissociation energy values D_e indicate that, in overall, these values increase as the carbon atoms number increase. Analysis by employing the Quantum Theory of Atoms in Molecules (QTAIM) [7] allowed us to verify that the fullerenes studied here, were stabilized by a non-covalent interaction.

Key-words: Fullerene dimers, Spectroscopic properties, QTAIM
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