Energy and rovibrational spectroscopic constants for fullerenes dimers \((\text{C}_{20})_2, (\text{C}_{24})_2, (\text{C}_{36})_2, (\text{C}_{60})_2, (\text{C}_{70})_2\) and \((\text{C}_{84})_2\)

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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 \((\text{C}_{20})_2, (\text{C}_{24})_2, (\text{C}_{36})_2, (\text{C}_{60})_2, (\text{C}_{70})_2\) and \((\text{C}_{84})_2\). 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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References: