

Spectroscopic Analysis of the(C₇₀)₂ Dimer on Different Relative Configurations

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Abstract: The present work is dedicated to study the spectroscopic property of the $(C_{70})_2$ dimers [1–3]. Based on this study, we built up the potential energy curves for the dimer formation. The spectroscopic constants were obtained by means of the Dunham's and Discrete Variable Representation methods [4,5]. For the full intermolecular potential representation, we employed the Rydberg analytical function [6]. As it is possible to modify the intermolecular interaction potential could be modified, as a result of the different faces that constitute the fullerenes, the spectroscopic properties of the $(C_{70})_2$ were examined for different intermolecular configurations. After running all calculations, it is possible to observe that the system's symmetry is reflected in both the potential energy curves and spectroscopic properties of the different. The small variations observed in the spectroscopic constants and in the dissociation energy values for the different configurations of the dimers can be attributed to the fact that the interaction between the monomer is most influenced by the hexagonal faces that make up the fullerene interacting units.

Key-words: $(C_{70})_2$ dimers, Spectroscopic properties, Dunham, DVR **Support**: This work was financially supported by CAPES, PrP-UEG and FAPEG-GO. **References**:

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