

B-01-S**INSIGHTS FROM NUMERICALLY EXACT APPROACHES FOR THE CALCULATION OF THE ROVIBRATIONAL ENERGY STRUCTURE OF TRI- AND TETRATOMIC MOLECULES**

M. Mladenović

*MSME, Univ Gustave Eiffel, CNRS UMR 8208, Univ Paris Est Créteil,
F-77454 Marne-la-Vallée, France (mirjana.mladenovic@univ-eiffel.fr)*

Numerically exact rotation-vibration solutions to the molecular Schrödinger equation for tri- and tetratomic molecules are applied. As a first example, the torsional structure of HOCO is analyzed using several adiabatic projection techniques. The torsional structure is found to exhibit two limiting cases associated with oscillator and rotor spectral patterns. Combining full-dimensional rovibrational calculations for N_2H^+ with the available experimental values for B_0 , the r_0 and r_e structures of the ion are additionally determined and analyzed.

B-02-S**STUDY OF NONCOVALENT INTERACTIONS USING CRYSTAL STRUCTURE DATA AND QUANTUM CHEMICAL CALCULATIONS**

M. R. Milovanović¹, J. M. Živković¹, D. B. Ninković¹, J. P. Blagojević Filipović¹, D. Z. Vojislavljević–Vasilev¹, I. S. Veljković², I. M. Stanković², D. P. Malenov³, V. B. Medaković³, D. Ž. Veljković³, S. D. Zarić³

¹*Innovation center of the Faculty of Chemistry, Studentski trg 12-16, Belgrade, 11000, Serbia,*

²*Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia,*

³*Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, 11000, Serbia (szaric@chem.bg.ac.rs)*

The analysis of the crystal structures in the CSD was used to recognize and characterize new types of noncovalent interactions. It was also used to study already known noncovalent interactions. Based on the data from the CSD we can determine existence of the interactions, frequency of the interactions, and preferred geometries of the interactions in the crystal structures [1,2].

The quantum chemical calculations were performed to evaluate the energies of the interactions. For the preferred geometries in the crystal structures we can calculate the interaction energies. By calculating potential energy surfaces for the interactions, we can determine the most stable geometries, as well as stability of various geometries [1,2].

Using this methodology our group recognized stacking interactions of planar metal-chelate rings; stacking interactions with organic aromatic rings, and stacking interactions between two chelate rings. The calculated energies showed that the stacking of metal-chelate rings is stronger than stacking between two benzene molecules. Studies of interactions of coordinated ligands indicate stronger noncovalent interactions than interactions of noncoordinated molecules [2].

REFERENCES

- [1] Ninković, D. B., Blagojević Filipović, J. P., Hall, M. B., Brothers, E. N., Zarić, S. D. (2020) *ACS Central Science*, **6**, 420.
[2] Malenov, D. P., Zarić, S. D. (2020) *Cood. Chem. Rev.* **419**, 213338.

B-03-O**FORMATION OF THE METHANE HALIDES FLUID-LIKE LAYERS AT AMBIENT CONDITIONS**

I.I. Grinvald, R.V. Kapustin

*Nizhny Novgorod State Technical University n.a. R.E. Alekseev
Minin str. 24, 603950 Nizhniy Novgorod, Russia
(grinwald@mts-nn.ru)*

The work presents the IR-study of fluid-like methane halides (methyl iodide, carbon tetrachloride, chloroform, and methane dichloride) layers formation in the near-surface area at ambient conditions. It was shown that at vapors compression-expansion procedure in variable-thickness spectral cell, the phase state of matter, exhibiting both gas and liquid spectral properties appears. The reversible and continuous transition of gas-like and liquid-like shapes, not depending on thermodynamic characteristics of studied substances, was revealed.

B-04-O**STRUCTURAL TRANSFORMATIONS OF DICHLORO-ALKANES AT THE LIQUID-TO-GAS TRANSITION**

I.I. Grinvald, R.V. Kapustin

*Nizhny Novgorod State Technical University n.a. R.E. Alekseev
Minin str. 24, 603950 Nizhniy Novgorod, Russia
(grinwald@mts-nn.ru)*

The work discusses the data obtained by IR study referring to the dual gas-liquid properties of thin layers forming in the cell near-surface (optical windows) area for dichloromethane, 1,2-dichloroethane and 1,2-dichloropropane. These layers represent the combination of gas-like and liquid-like states, which can be considered as the intermediate stage of the phase transition from gas to liquid. It was shown that the molecular interactions in dual gas-liquid systems of chloroalkanes are changing due to the restructuring of Cl...H hydrogen bonding.