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

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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 $r_{\square}$ and r_e structures of the ion are additionally determined and analyzed.

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

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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 that interactions of noncoordinated molecules [2].