BOOK OF ABSTRACTS

25th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV)

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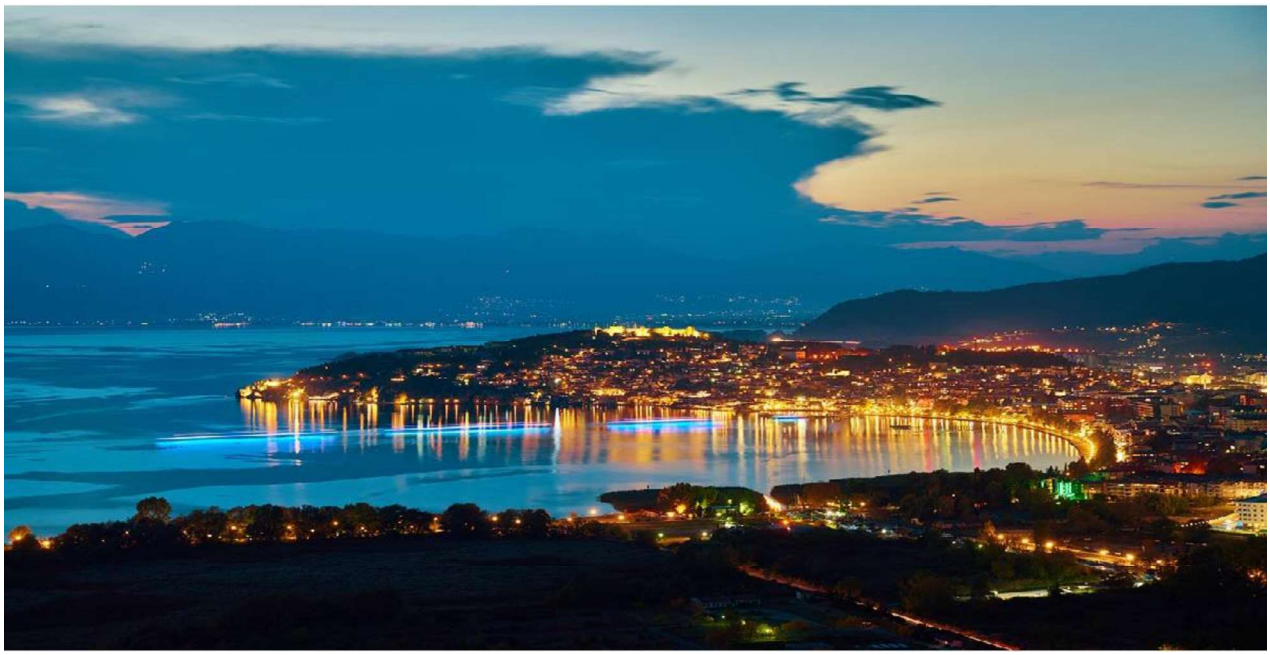

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P-36 Joint Crystal Structure and Computational Study of Hydrogen Bonds of Ethylenediamine

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The hydrogen bonds of coordinated ethylenediamine (en) play important roles in catalytic activity [1], the aim of this work was to study geometrical parameters and strength of these interactions. The search of crystal structures archived in Cambridge Structural Database (CSD) was performed in order to find crystal structures containing at least one coordinated en to a transition metal, and at least one free water molecule interacting with en via NH···O hydrogen bond. All calculations were performed at M06L-GD3/def2-TZVPP/BSSE level of theory since it was confirmed that this level gives a good agreement with the CCSD(T)/CBS level. The distribution of d_{OH} (Fig. 1) showed the maximum is at 2.0 Å - 2.1 Å, with a relatively large number of structures with distances shorter than 2.0 Å. The distribution of α (Fig 1.) revealed the maximum at 150º - 160. The d_{OH} and α are correlated, i.e. shorter distances correspond to larger angles. Most of en complexes contain cobalt, followed with palladium, nickel, and copper and most of them are in octahedral geometry. The coordination of en to the metal ions strengthens its hydrogen bonds with a water molecule. Namely, the energy of hydrogen bond of noncoordianted ethylenediamine is -2.3 kcal/mol, while the interaction energies for neutral metal complexes are in the range of -4.0 kcal/mol to -6.7 kcal/mol. Increasing of charge of complexes increases the energy of hydrogen bond. For singly charged complexes energy spans from -8.5 to -11.8 kcal/mol; for doubly charged complexes it spans from -15.6 kcal/mol to -19.9 kcal/mol; while triply charged complex has the strongest interaction of -28.0 kcal/mol [2]. In addition, the energies of hydrogen bond have a good correlation with the electrostatic potential on interacting hydrogen atom.

[1] Ghosh, S. K.; Ehnbom, A.; Lewis, K. G.; Gladysz, J. A. Coord. Chem. Rev. 2017, 350, 30–48.
[2] Živković, J. M; Milovanović, M. R.; Zarić, S. D., submitted to Cryst. Growth Des. 2022.