MS32-03 | CAN MEP VALUES BE USED TO PREDICT THE SUPRAMOLECULAR CONNECTIVITY IN THE CRYSTAL STRUCTURE?

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Research based on Margaret Etter's Rules [1] has shown that hydrogen and halogen bond donor-acceptor pairings follow a hierarchy based on their strengths which can be correlated with calculated molecular electrostatic potential (MEP) values. Studies conducted on organic systems have shown that it is possible to predict the donor-acceptor pairing if the difference in MEP values is significant. It still remains to be determined if insights obtained for organic systems can be used in a tandem with metal centers.

We have shown in our previous work that MEP values can be used to rationalize the supramolecular connectivity in the metal-organic setting for both hydrogen [2] and halogen [3] bonds. We have also shown that it is possible to use MEP values to predict the supramolecular connectivity in 2,4-pentanedionate (acac)-based complexes (Ni^{II}, Co^{II}, Cu^{II}), equipped with the lactam moiety [4]. The goal of our current research is to determine if it is possible to use MEP values to predict the supramolecular connectivity in systems displaying more conformational freedom. To assess this hypothesis, we used acac-based complexes of Co(II) and Ni(II) with small heterocyclic ligands equipped with the amide functionality, and here we are reporting on the results.

[1] M. C. Etter, *Acc. Chem. Res.* **23** (1990) 120–126.
[2] M. Đaković et al.; *IUCrJ* **5** (2018) 13–21.
[3] M. Borovina, I. Kodrin, M. Đaković, *CrystEngComm*, **20** (2018) 539–549.
[4] M. Borovina, I. Kodrin, M. Đaković, *Cryst. Growth Des.*, **19** (2019) 1985–1995.