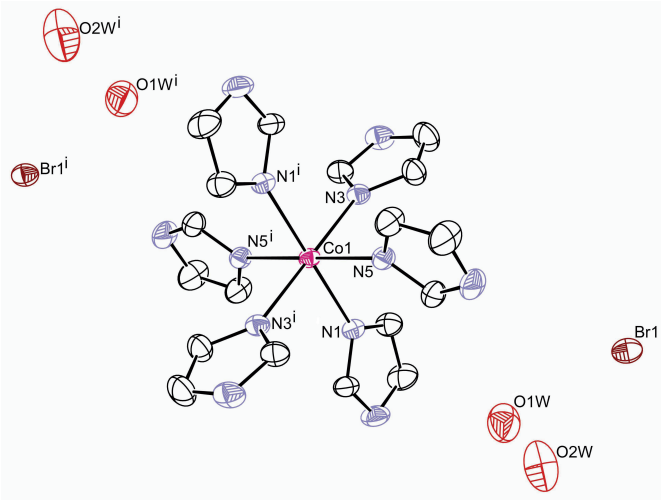

Keywords: X-ray_diffraction, cobalt, Ýmidazole

MS17.P19

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Structural Analysis of Hexa-4-methylimidazole nickel II 5-aminoisopthalate tetrahydrate.

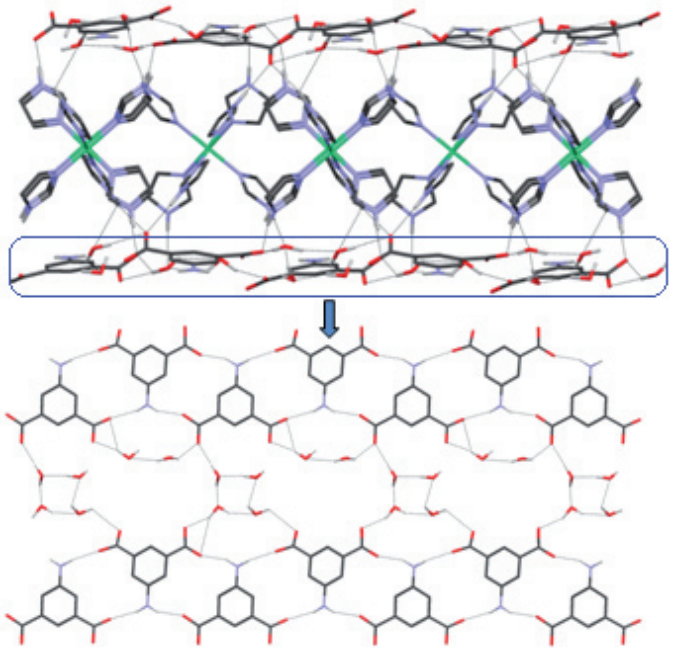
Ersin Temel,[a] Alper Tolga Çolak,[b] Okan Zafer Yeşilel,[c] Handan Günay,[c] Orhan Büyükgüngör,[a] [a]*Departament of Physics, Faculty of Arts and Sciences, Ondokuz Mayýs University, 55139, Kurupelit/ Samsun, (Turkey).* [b]*Department of Chemistry, Faculty of Arts and Sciences, Dumlupýnar University, Kütahya, (Turkey).* [c]*Department of Chemistry, Faculty of Arts and Sciences, Eskişehir Osmangazi University, Eskişehir, (Turkey).* E-mail: etemel@omu.edu.tr

The title compound is composed of $[Ni(4\text{-methyl imidazole})]^{+2}$ complex cations, 5-amino isopthalato anions and water molecules. Two nickel atoms are located at special positions. Each Ni atom has a slightly distorted octahedral coordination geometry defined by 4-methyl imidazole rings coordinated through N atoms. In the 5-amino isopthalato anions, while aniline parts are planar, carboxylate groups deviates from planarity.

The crystal packing is achieved by strong and moderate hydrogen bonds which play an important role in the formation of the 3D network. These interactions are drawn in Figure.

The packing is formed by periodic repeatation of 2D A- and B-layers which are paralel to *ab*-plane. While layer A is composed of only nickel complexes, layer B is composed of the combination of 5-amino pthalato and water molecules. In the layer A, nickel complexes with each other linked by C-H…π interaction. On the other hand, B-layers act as a bridge between nickel complexes along c-axis. Layers A and B are linked by N-H…O type hydrogen bonds.

It can be seen from figure that N-H…O and O-H…O hydrogen bonds construct 2D network in layer B. 5-amino isopthalato anions linked to each other by N-H…O type hydrogen bonds, generating adjacent $R_2^2(14)$ ring motifs along a-axis [1]. Tetrameric water clusters connect 5-amino isopthalato anions along b-axis. While the cyclic water tetramer is formed by O2W, O3W, O5W and O8W atoms, the dimeric clusters are formed by O1W, O4W and O6W, O7W atoms. Oxygen atoms of carboxylate groups are hydrogen bonded to dimeric and tetrameric clusters.



[1] J. Bernstein, R.E. Davis, L. Shimoni, N.L. Chang, *Angew. Chem. Int. Ed. Engl.* **1995,** *34,* 1555-1573.

Keywords: X-ray_diffraction, nickel, cluster

MS17.P20

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When organic and metal-organic molecules cease to crystallize?

Jan Fábry,[a] Radmila Krupková,[a] Miloš Kopecký[a.] [a]*Inst. Of Physcics of the Academy of Sciences of the Czech Republic. Na Slovance 2, 182 21 Praha 8, Czech Republic.* . E-mail: fabry@fzu.cz

The dependences of occurrences of the most frequent space-group types $P\bar{1}$, $P2_1$, $P2_1/c$, $C2/c$, $P2_12_12_1$ and $Pbca$ on reduced unit-cell volumes up to 8000 Å^3 were investigated for organic and metal-organic compounds with different number of residues, *i.e.* with different number of molecular constituents (1-3)**.** The dependences for these space-group types are similar, single-peaked; their maxima are proportional to the number of asymmetric units, affected by Z' (number of formula units *per* asymmetric unit) in the pertinent space-group types. The dependences of Z'<1, Z'=1, Z'>1 within each space group type on reduced unit-cell volumes are also similar in shape. From these dependences it can be inferred that ability for crystallization of organic and metal-organic molecules ceases for the structures with the reduced unit-cell volumes above 8000 Å^3. This volume corresponds roughly to 450 non-hydrogen atoms in a unit cell, i.e. to non-hydrogen 56 atoms *per* molecule [1].

The loosing ability for crystallization for large molecules is also manifested by the deviation from linearity of the Kempster-Lipson [2] rule for the structures composed from C, H, N, O at most. The present analysis has the following implications:

While a broadly shared view that the more symmetric is a molecule the more symmetric is a crystal arrangement seems to be correct [3,4] the opposite conclusion has been shown not to be quite true because the larger organic or metal-organic molecules tend to crystallize in a more symmetric space-group type such as *Pbca*. The present analysis shows influence of the molecular size on the symmetry of the crystalline state. It is known that biological macromolecules often contain huge dummy parts the function of which is unclear while active centres are surprisingly small. Can be the size of the biological