

MS10-P7 Pressure induced C-H agostic interactions in a Uranium complexAlessandro Prescimone^{1,2}, Simon Parsons², Polly L. Arnold²1. University of Basel
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The diuranium(III) compound [UN²]2(μ-η(6)-η(6)-C₆H₆) (N²=N(SiMe₃)₂) has been studied using variable, high-pressure single-crystal X-ray crystallography, and density functional theory. In this compound, the low-coordinate metal cations are coupled through π- and δ-symmetric arene overlap and show close metal-CH contacts with the flexible methyl CH groups of the sterically encumbered amido ligands. The metal-metal separation decreases with increasing pressure, but the most significant structural changes are to the close contacts between ligand CH bonds and the U centers. Although the interatomic distances are suggestive of agostic-type interactions between the U and ligand peripheral CH groups, QTAIM (quantum theory of atoms-in-molecules) computational analysis suggests that there is no such interaction at ambient pressure. However, QTAIM and NBO analyses indicate that the interaction becomes agostic at 3.2 GPa.

Keywords: extreme conditions, agostic interactions, high pressure, Uranium

MS10-P8 Syntheses, Molecular Structures and Supramolecular Assembly in Three Mixed-Ligands Cobalt(II) Complexes

trans-[Co(HOOC-(C₆H₄)-COO)₂(H₂O)₂(C₃N₂H₄)₂],
cis-mer-[Co(C₈H₄O₄)(H₂O)₂(C₃H₄N₂)₃], H₂O
and
trans-[Co(H₂O)₂(C₃N₂H₄)₄][OOC-C₄H₂S-COO]

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Carboxylate ligands, alone or combined with nitrogen ligands such as imidazole, have proven to be excellent candidates for the coordination polymers construction and multidimensional supramolecular structures [1-2]. Continuing our work on mixed ligand carboxylate complexes [3], three compounds from reactions between of cobalt salts, aromatic dicarboxylic acids and imidazole were synthesized, characterized by IR and TGA and their structures determined by single crystal XRD. Our syntheses have not achieved to expected mixed coordination polymers but led to 0D complexes. All the three crystallize in centrosymmetric spaces groups P2₁/n, P-1 and P2₁/c. The asymmetric unit consists of one Co(II) ion, one terephthalato dianion, three imidazole molecules, two coordination water molecules, one lattice water for complex 1, one Co(II) ion located on a center of inversion, one hydrogenisophthalato ligand, one imidazole molecule and one coordination water molecule for the second complex. In the salt complex, the structure consists unit of [Co(H₂O)₂(C₃N₂H₄)₂]²⁺ cation and a thiophenato ligand [OOC-C₄H₂S-COO]²⁻. All Co²⁺ cations have a slightly distorted octahedral environment with all ligands adopting monocoordination mode except the dianion [OOC-C₄H₂S-COO]²⁻ which remains uncoordinated. In the complex [Co(C₈H₄O₄)(H₂O)₂(C₃H₄N₂)₃], the backbone of the architecture is an helical hydrogen-bonded ladder composed of alternating R₂⁴(10), R₃³(8) and R₂²(6) heterosynthons running along [010]. In [Co(HOOC-(C₆H₄)-COO)₂(H₂O)₂(C₃N₂H₄)₂], the hydrogen bond network is not as dense as the previous complex but there are files of R₂²(8) synthons parallel to the [100] direction and connected by R₂²(16) synthons. In the complex salt, water molecules and cationic molecules are linked by hydrogen bonds forming R₄⁴(8) synthons, running in parallel lines at the b axis. This interconnected by thiophen dianion, engaged itself in a dense network of hydrogen bonds, in the three directions to form a three-dimensional supramolecular architecture. [1] Chen, P. K., Che, Y-X & Zheng, J-M. (2007). *Inorg. Chem. Comm.*, 10, 187-190. [2] Fu, X-C., Wang, X-Y., Li, M-T., Wang, C-G. & Deng, X-T. (2006). *Acta Cryst.*, C62, m343-345. [4] Benkanoun, A., Balegroune, F., Guehria-Laidoudi, A., Dahaoui, S. & Lecomte, C. (2012). *Acta Cryst.*, E68, m480-m481.

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