DSCM 30P STRUCTURE – MECHANICAL PROPERTIES CORRELATION FOR THE LAMINAR SOLID $\{[Co(OAc)_2(bpe)(H_2O)]\cdot 0.5(dmf)\}_n$

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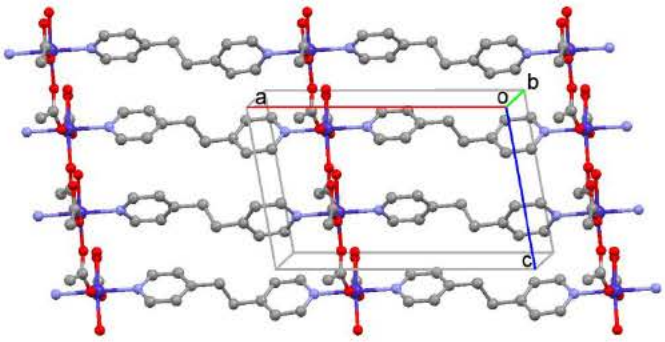
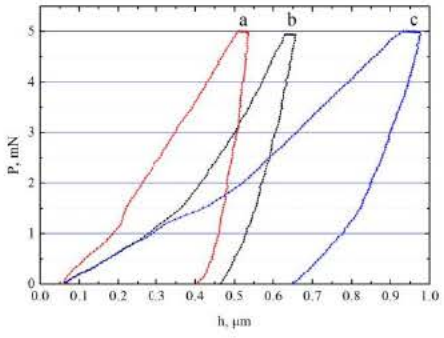
Mechanical properties of metal-organic materials (MOMs) deserve growing attention since they are essential variables for a majority of possible applications. The nanoindentation allows estimating the stability limits of MOMs, anisotropy of hardness on different planes, and contribution of different types of interatomic and intermolecular interactions to the overall crystal stability. Laminar title compound **1** crystallizes in the monoclinic space group $P2_1/c$ [1]. The Co(II) cation coordinates three AcO^- anions, one water and two bpe molecules. The N_2O_4-coordination surrounding of Co(II) atom represents the distorted octahedron that comprises four oxygen atoms in the equatorial plane [Co(1)-O: 2.071(2)–2.107(2) Å], and two nitrogen atoms in axial positions [Co(1)-N: 2.163(3) and 2.175(3) Å]. The extension of structural motif occurs *via* bridging AcO^- anions and bpe ligands and affords the 2D (4,4) coordination network. The Co···Co separation across AcO^- is 5.145 Å, and across bpe is 13.617 Å. The layer is running parallel to the (010) plane (Figure, left). The disordered dmf solvent molecules accumulated in the interlayered space are held there by the π-π interactions with the bpe aromatic systems.

To estimate the mechanical anisotropy of the layered material **1,** the three planes (001), (100) and (010) were indented for which the indexing of the planes was performed by X-ray method. Representative *P-h* curves obtained on three planes are shown in Figure, right.





An essential anisotropy is observed if the mechanical parameter values are compared for all investigated planes. The (001) plane is the hardest one, with the maximal values of E and H: 13.07 GPa and 0.73 GPa, respectively. The (010) plane is the least hard one: E = 4.92 GPa, H = 0.24 GPa. Thereby, the maximal anisotropy coefficient for Young modulus amounts to $k_E = E_{(001)}/E_{(010)}$ = 2.66, and for hardness: $k_H = H_{(001)}/H_{(010)}$ = 3.04. The mechanical parameters for the (100) plane is closed to the same for the (001): E = 12.54 GPa, H =0.61 GPa, i.e. $k_E = E_{(001)}/E_{(100)}$ =1.04, and $k_H = H_{(001)}/H_{(100)}$=1.2. Our results present convincing evidence that the crystal orientation dominated by the metal-organic layers with the van der Waals and π-π stacking interactions between the layers is the least robust from the mechanical properties standpoint.

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[1] Croitor et al., *Cryst. Growth Des.* 2014, **14**, 3015–3025.