

In Fc@MIL-53(Al) crystal structure, there are no strong guest-guest and guest-host interactions. The existing short contact of 3.12 Å between the Cp-ring and the benzene-ring of the linker has to be noted. Fc molecules are oriented around perpendicularly to the channel's direction. In all Fc-derivation's structures, strong guest-host interactions between substitute groups and μ -OH-groups of the host framework are present. The guest molecules are oriented in the channel's direction. As the fact, the packing of the guest molecules depends on guest-host but not on guest-guest interactions. MIL-47(V) framework does not give a strong breathing effect like MIL-53(Al). Therefore, Fc@MIL-47(V) absorbate structure is similar to Fcaa@MIL-53(Al) and both guest molecules are oriented in the channel's direction.

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Keywords: X-ray powder diffraction; structure determination; framework structures; guest-host structures

FA4-MS08-O4

Alkali Metal Complexes with Diphenylacetic Acid. Manuela Ramos Silva^a, Sérgio R. Domingos^b, Ana Matos Beja^a, José A. Paixão^a, Jesús Martín-Gil^c. ^aDepartment of Physics, University of Coimbra, Coimbra, Portugal. ^bMolecular Photonics Group, Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Netherlands. ^cETSIA, Universidad de Valladolid, Avda Madrid 57, Palencia, Spain.

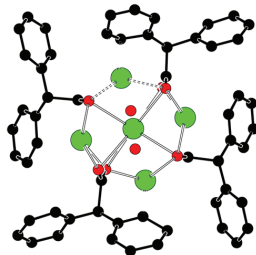
E-mail: manuela@pollux.fis.uc.pt

Diphenylacetic acid (DPA) does not contain a chiral center but can induce chiral assemblings by assuming a propeller-like conformation [1].

In the Na-DPA crystal structure the carboxylate oxygen atoms and the Na⁺ ions alternate at the vertices of a distorted cube centered at the origin of the -4 axis, forming an infinite columnar structure [2].

In the Rb-DPA crystal structure, the rotoinversion axis is lost and there is the formation of a ladder climbing along an -1 axis [3].

In the K-DPA crystal structure, there is the formation of a columnar structure although some of its constituting atoms are disordered, the following figure shows the columns as viewed from the top (H atoms were omitted for clarity).



This new compound crystallizes in the centrosymmetric

space group *Cc* with cell parameters: $a = 29.0438(10)$ Å, $b = 5.959(3)$ Å, $c = 29.9002(19)$ Å, $\beta = 106.902(2)^\circ$, $V = 4951(3)$ Å³. Structural features will be presented and discussed.

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FA4-MS08-O5

Powder Diffraction Structural Studies at Ambient and Non-Ambient Conditions on Porous Coordination Polymers. Simona Galli. Dipartimento di Scienze Chimiche e Ambientali, Università dell'Insubria, Como, Italy.

E-mail: simona.galli@uninsubria.it

The increasing industrial and environmental importance of applications such as gas storage, gas or liquid selective separation, heterogeneous catalysis, and drug delivery promoted the investigation of porous coordination polymers (PCPs) as promising materials [1-3] to overcome some of the limits of 'classical' porous species (e.g. activated carbons, metal hydrides, inorganic zeolites).

With the aim of engineering novel PCPs featuring (hydrogen, carbon dioxide, methane) gas storage or separation, our research group explored the coordination capabilities of polyazaaromatic ligands toward transition metal ions. Pioneering, remarkable results were obtained with the $M(5-X-2-pymo)_2$ materials ($M = Co, Zn, Cu, Pd$; 5-X-2-Hpymo = 5-X-pyrimidin-2-ole) [4-6]. Tuning either the coordination possibilities or the length of the organic spacer, led to the isolation and characterization of the $M(\text{Hoxonic})(4,4'\text{-bipy})_{0.5}$ ($M = Cu, Zn$; H₂oxonic = oxonic acid; 4,4'-bipy = 4,4'-bipyridine) and $M(\text{bpb})$ ($M = Ni, Zn$; H₂bpb = 1,4-(4-pyrazolyl)benzene) species, respectively.

Selected examples from the three families will be presented to highlight the effectiveness of powder diffraction structure solution methods *applied to laboratory data*, juxtaposed to thermogravimetric studies even in conditioned atmosphere, in providing a structural frame to the investigated functional properties.

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