

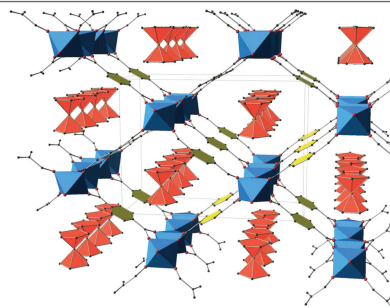
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**The adsorbate structure of ferrocene inside [Al(OH)(bdc)]<sub>x</sub> (MIL-53): a powder X-ray diffraction study**

Mikhail Meilikhov, Kirill Yusenko and Roland A. Fischer\*

Q1

The ferrocene molecules are arranged in a 1D chain-like fashion and their cyclopentadienyl rings are oriented almost parallel to the O<sub>3</sub>Al faces of the {AlO<sub>6</sub>} octahedra without  $\pi$ -stacking to the bdc.



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# The adsorbate structure of ferrocene inside [Al(OH)(bdc)]<sub>x</sub> a powder X-ray diffraction study†

Mikhail Meilikhov, Kirill Yusenko and Roland A. Fischer\*

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5 Ferrocene is strongly adsorbed by the highly porous metal-organic framework compound [Al(OH)(bdc)]<sub>x</sub> (MIL-53; bdc = 1,4-benzenedicarboxylate). The structure of the crystalline phase  $\{[\text{Fe}(\eta^5\text{-C}_5\text{H}_5)_2][\text{Al}(\text{OH})(\text{bdc})]_2\}_x$  was determined by X-ray powder diffraction and Rietveld methods. The ferrocene molecules are arranged in a 1D chain-like fashion and their cyclopentadienyl rings are oriented almost parallel to the O<sub>3</sub>Al faces of the {AlO<sub>6</sub>} octahedra without  $\pi$ -stacking to the bdc.

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