



	<b>Experiment title:</b> High resolution powder X-ray diffraction study of UiO12	<b>Experiment number:</b> 1-01-156
<b>Beamline:</b> BM01	<b>Date of experiment:</b> from: 10/11-98 to: 11/11-98	<b>Date of report:</b> 04/02-00
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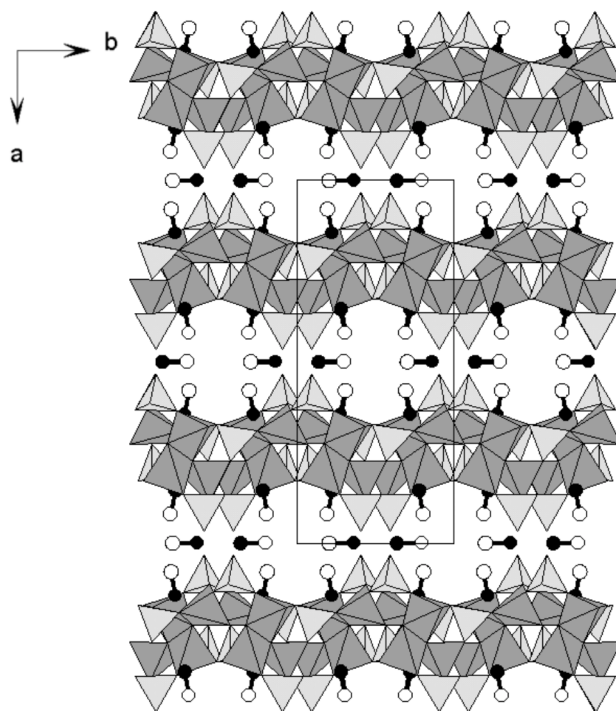
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**Report:** High-resolution powder patterns were collected on two layered aluminophosphates UiO-25 and UiO-30.

**UiO-25:** The crystal structure could be solved from direct methods using the program EXTRA. A monoclinic unit cell:  $a = 21.7487(6)\text{\AA}$ ,  $b = 9.3649(2)$ ,  $c = 9.7738(2)$  and  $\beta = 93.260(2)^\circ$  in space group  $C2/c$ . UiO-25,  $0.5[\text{NH}_2\text{CH}_3][\text{NH}_3\text{CH}_3]^+[\text{HAl}_2\text{P}_2\text{O}_9]^-$ , is a hybrid organic-inorganic structure with inorganic, anionic layers of aluminophosphates stacked in a ABAB sequence along [100] separated by partly protonated methylamine molecules (Fig. 1). The atomic arrangement in the inorganic layers are identical to that in UiO-13 and UiO-14 [1]. UiO-25 and the two structurally related compounds have been further characterized by high-field (14.1 T) solid-state 1-D  $^{27}\text{Al}$  MAS NMR and 2D 3QMAS NMR spectroscopy. A publication focusing both on the synchrotron powder diffraction data and the NMR data is in preparation.

[1] K.O. Kongshaug, H. Fjellvåg, K.P. Lillerud, *Microporous Mesoporous Mater.* 32 (1999) 17.

**UiO-30:** No structure for this aluminophosphate compound has been found.  $^{27}\text{Al}$  MAS NMR spectroscopy indicates one octahedral Al site. Further work will be done to solve the structure for this compound.



**Figure 1.** Polyhedral representation of UiO-25 seen along [001]. AlO<sub>5</sub> trigonal bipyramids with darker shading, PO<sub>4</sub> tetrahedra with lighter shading, C atoms with open circles and N atoms with solid circles.