Supplementary Information for

Influence of secondary ligand on structures and topologies of lanthanide coordination polymers with 1,3,5-triazine-2,4,6-triamine hexaacetic acid

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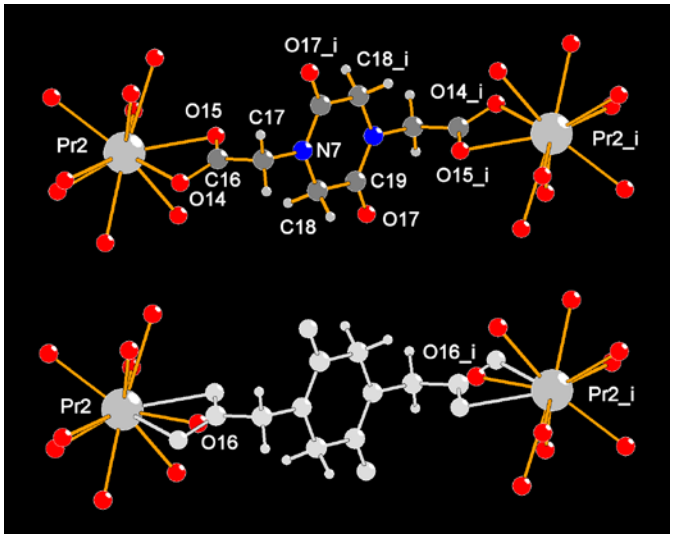
Supplementary Information 1 Disorder of the pzac^{2-} anion in **Ia**. Symmetry equivalent atoms are generated by the symmetry operator (*i*) = -*x*, 2-*y*, 2-*z*.

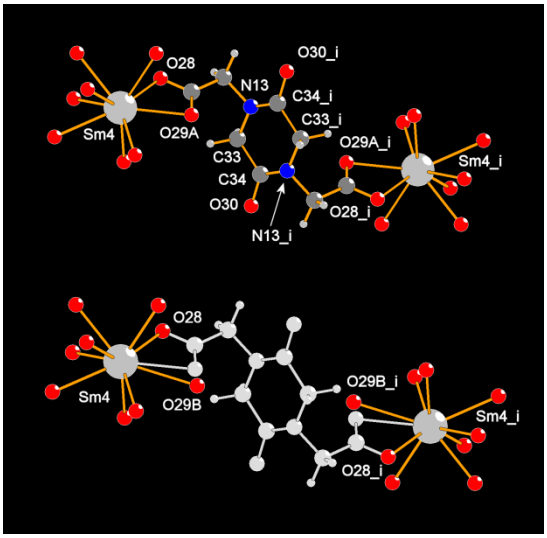


The anion is present at 50 % of the Pr2 sites. It is generated by inversion symmetry. The upper diagram shows the ligand linking two symmetry-related Pr2 ions.

In the lower diagram, the pzac ligand has been coloured grey to indicate that it is not present when O16 is present. The coordination about the Pr2 is completed by the water centred on O16.

Each of the two orientations is 50 % occupied in a random arrangement throughout the crystal.

Supplementary Information 2 Disorder of the pzac^{2-} anion in **II**. Symmetry equivalent atoms are generated by the symmetry operator (*i*) = 1-*x*, -*y*, 1-*z*.

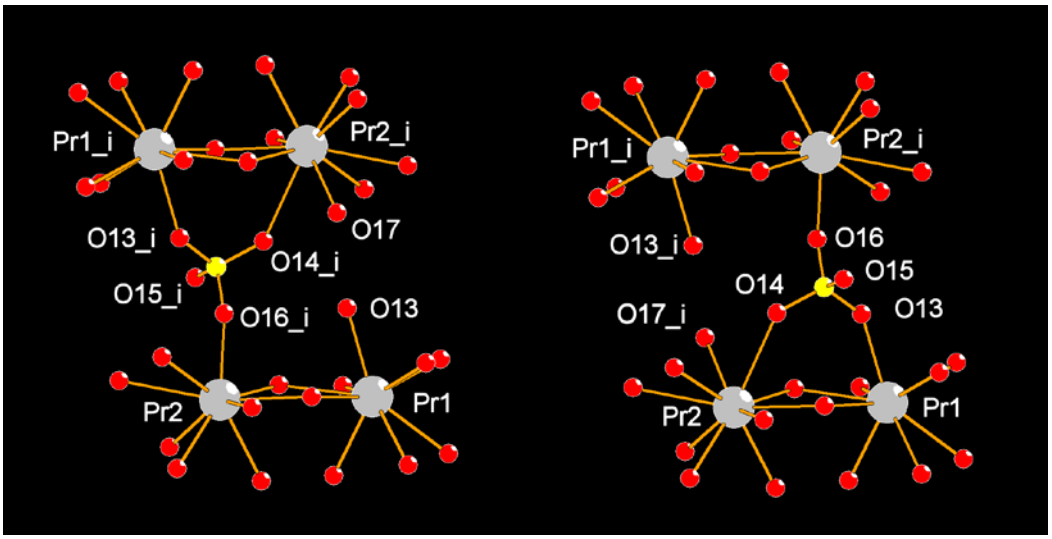


The anion is present at 50 % of the Sm4 sites. It is generated by inversion symmetry. The upper diagram shows the ligand linking two symmetry-related Sm4 ions.

In the lower diagram, the pzac ligand has been coloured grey to indicate that it is not present when water molecules centred on O28 and O29B are present.

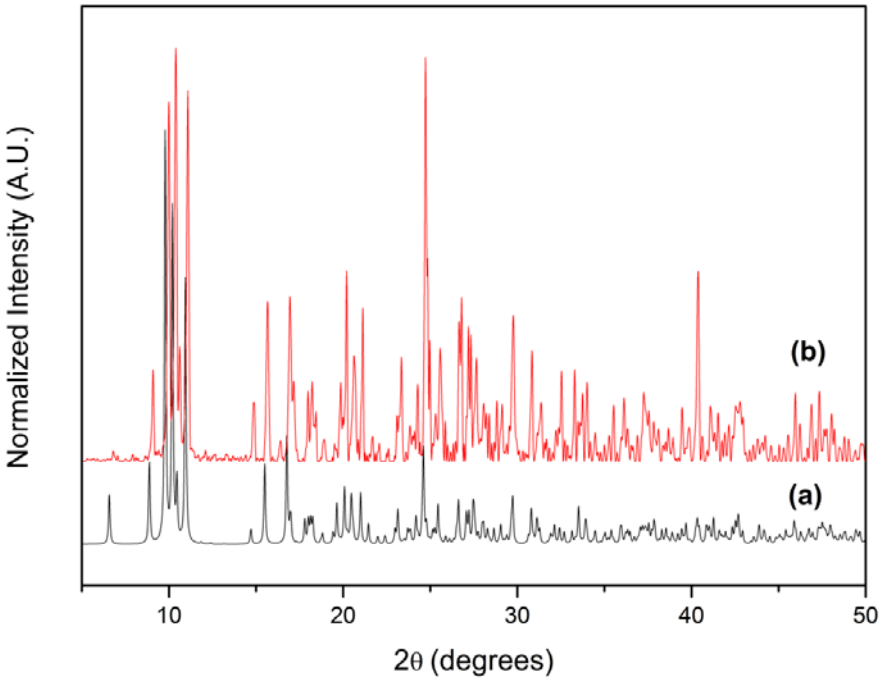
Each of the two orientations is 50 % occupied in a random arrangement throughout the crystal.

Supplementary Information 3 Disorder of the sulphate group in **IIIa**. Symmetry equivalent atoms are generated by the symmetry operator (*i*) = -*x*, -*y*, 1-*z*.

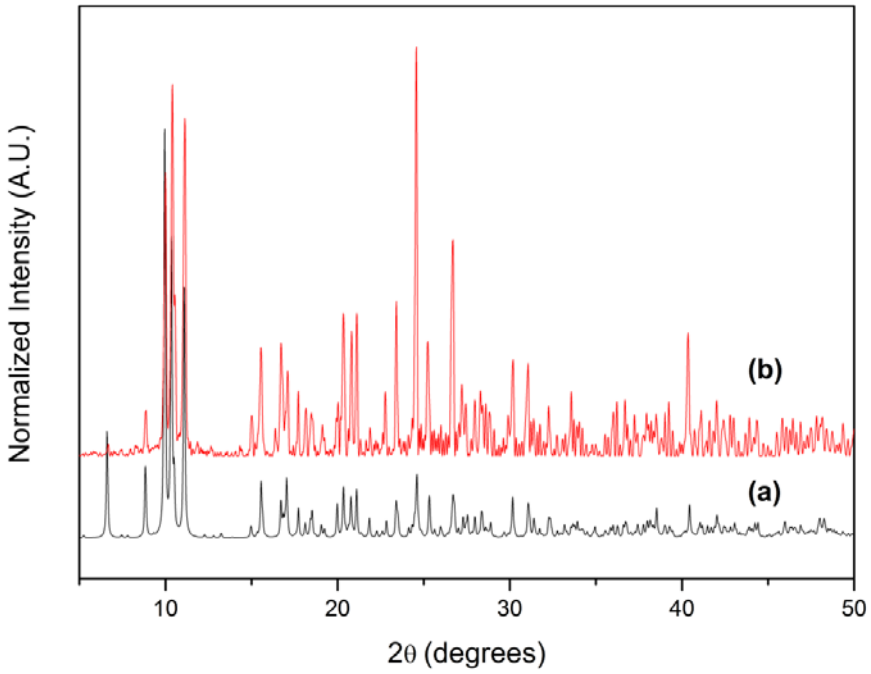


The sulphate adopts two different orientations that are related by inversion symmetry. In the first orientation (left) O13 and O17 are water molecules. In the second orientation O13_i and O17_i are the water molecules. Each of the two orientations is 50 % occupied in a random arrangement throughout the crystal.

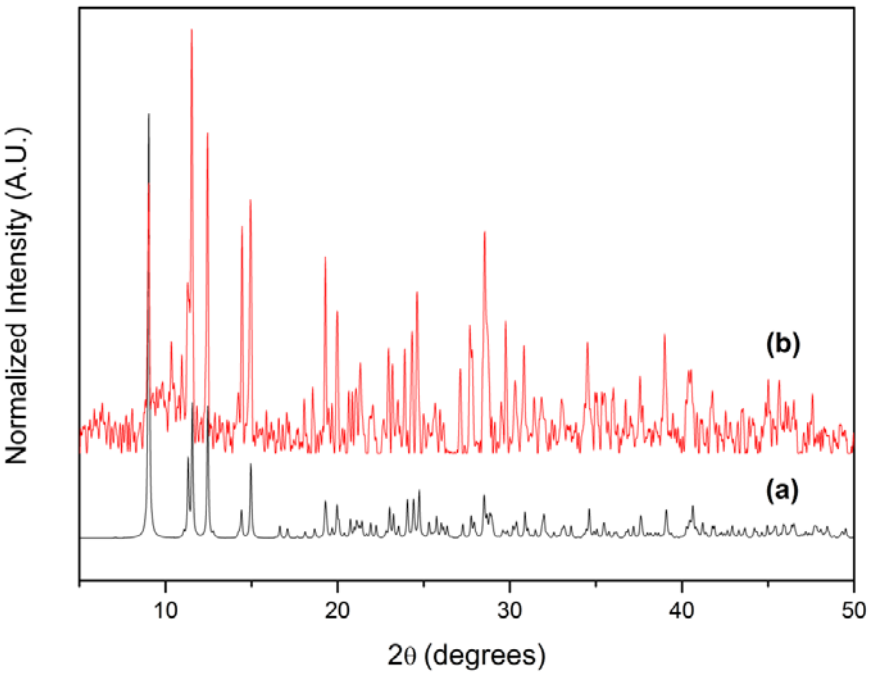
Supplementary Information 4 Powder X-ray diffraction patterns of **Ia**: (a) simulated (b) experimental



Supplementary Information 5 Powder X-ray diffraction patterns of **II**: (a) simulated (b) experimental



Supplementary Information 6 Powder X-ray diffraction patterns of **IIIa**: (a) simulated (b) experimental



Supplementary Information 7 List of band assignments for the IR spectra of **Ia**, **II** and **IIIa**.

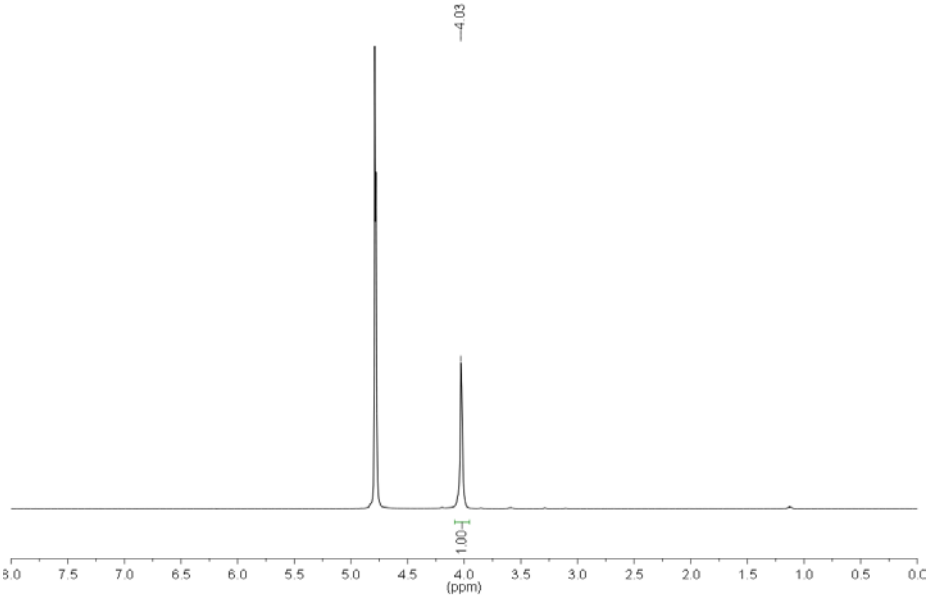
Band assignments[†]	**Ia**	**II**	**III**a
ν(O-H)	3472s,br	3472s,br	3456s,br
$\nu_s(CH_2)$	2935w	2935w	2935w
$\nu(H_3O^+)$	1882w	1851w	1843w
$\nu_{as}(COO)$	1627m	1635m	1621m
Quadrant ring stretching	1553vs	1553vs	1550vs
Semi-circle ring stretching	1487s	1487s	1487s
$\delta_{as}(CH_2)$	1432s	1435s	1439s
ν_s(C-C)	1400s	1401s	1385s
ν(C-N), aromatic	1300vs	1299vs	1300vs
ν(C-N), aliphatic	1197m	1198m	1192m
$\nu_4(SO_4^{2-})$	-	-	1097s
N-radial in phase stretching	991m	991m	991m
Triazine ring breathing	902w	902w	886w
Ring sextant out-of-plane bending	821m	821m	821m
Ring sextant out-of-plane bending	748m	748m	723m
Quadrant in-plane bending	613s	614s	609s
δ(C-N), side chain	539w	538w	540w

[†]w=weak, m=medium, s=strong, vs=very strong, br=broad

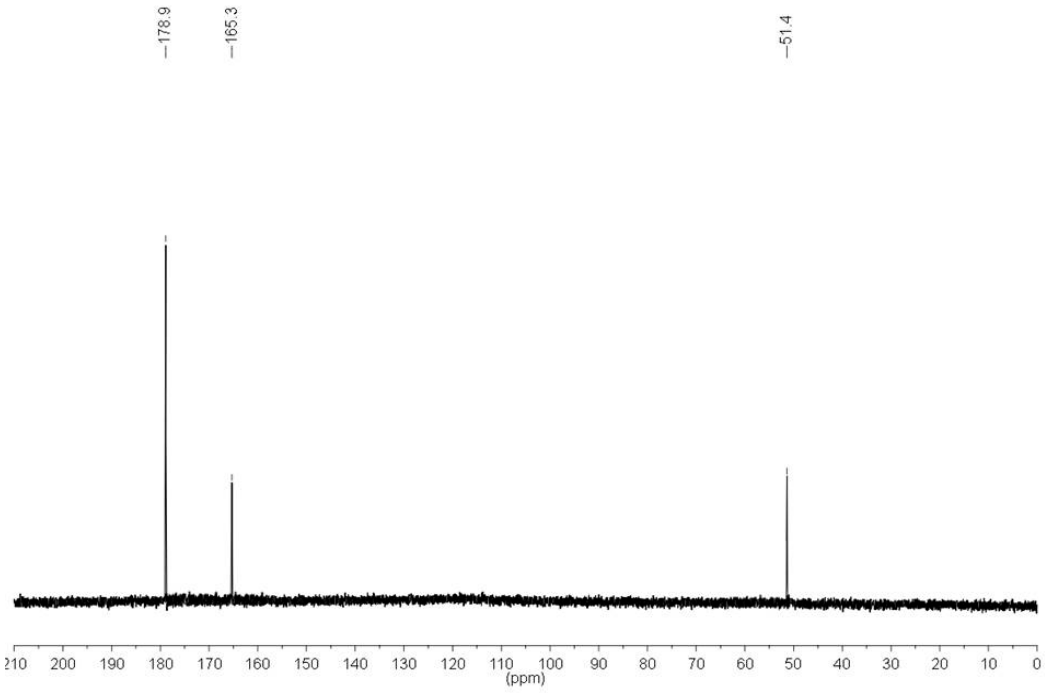
Supplementary Information 8

***N,N′,N″*-1,3,5-triazine-2,4,6-triyltrishexaacetic acid (TTHA)[1]** White powder (0.228 g, 89% yield); R_f 0.08 (60%MeOH/EtOAc); m.p. (dec.) ≥ 270 °C; FTIR (KBr): υmax 1720, 1558, 1497, 1397, 1231 cm^{-1}; ^{1}H NMR (2% NaOH in D_2O, 400 MHz) δ 4.03 (s, 12H)); ^{13}C NMR (2% NaOH in D_2O, 100 MHz) δ 51.4, 165.3, 178.9.

^{1}H NMR (400 MHz, 2% NaOH in D_2O)



^{13}C NMR (100 MHz, 2% NaOH in D_2O)



Reference: Zhu, Q.; Sheng, T.; Fu, R.; Hu, S.; Chen, J.; Xiang, S.; Shen, C.; Wu, X. *Cryst. Growth Des.* **2009,** *9*, 5128-5134.