Electronic Supplementary Material for CrystEngComm
This journal is © The Royal Society of Chemistry 2008

Supplementary information

A new class of 3-D porous framework: $[Ln(H_2O)_n]^{3+}$ ions act as pillars between π-stacked and H-bonded sheets of (*m*-BDTH)$^-$ organic anions in $[Ln(H_2O)_n](m\text{–}BDTH)_3 \cdot 9(H_2O)$ (Ln = Pr, n = 9; Ln = Gd, n = 8).

George E. Kostakis,[a] Ghulam Abbas,[a] Christopher E. Anson[a] and Annie K. Powell*[a]

Electronic Supplementary Material for CrystEngComm
This journal is © The Royal Society of Chemistry 2008

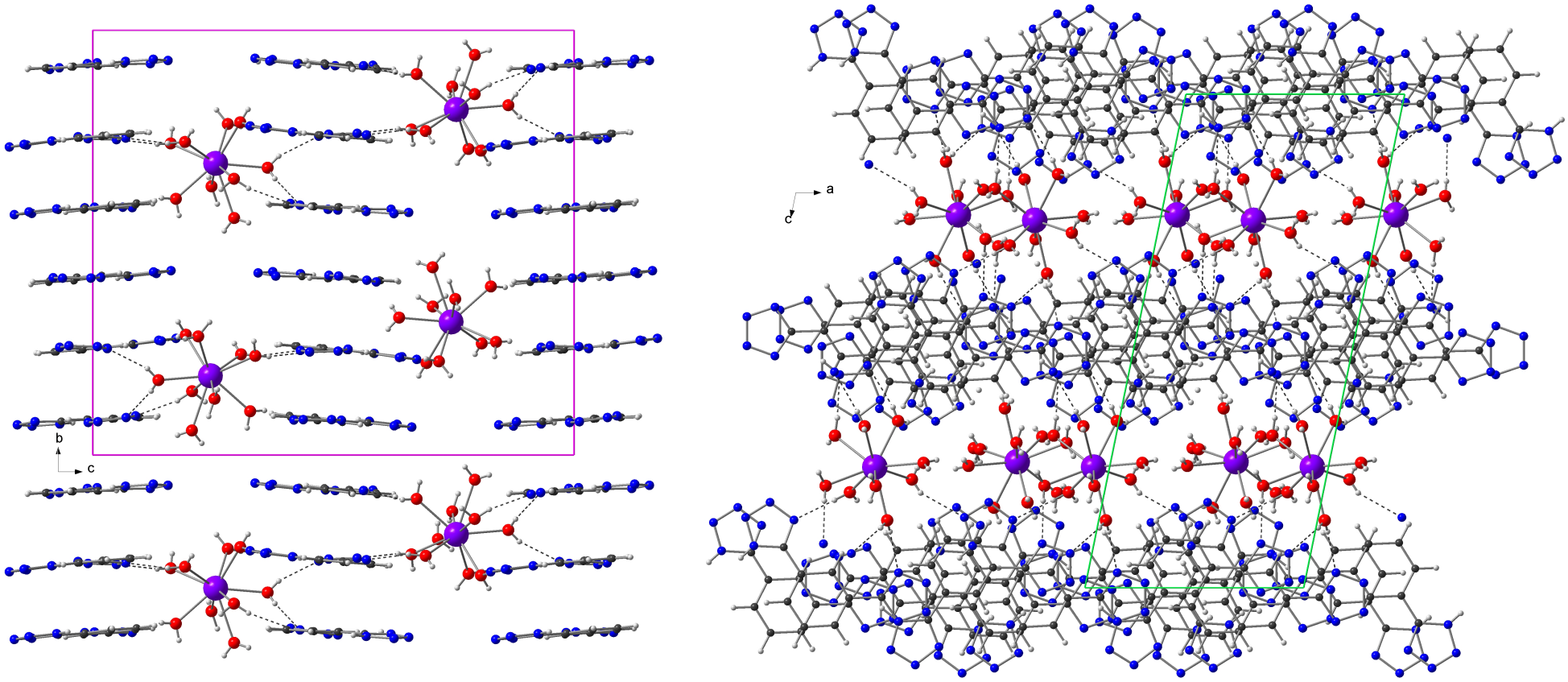

Fig. S1 The three dimensional framework of compound **1**, viewed down the *a*-axis (left) and down the *b*-axis (right), showing the H-bonding between the coordinated waters and the organic anions. Pr purlpe, O red, N blue, C grey. The lattice water molecules are omitted for clarity.

This journal is © The Royal Society of Chemistry 2008

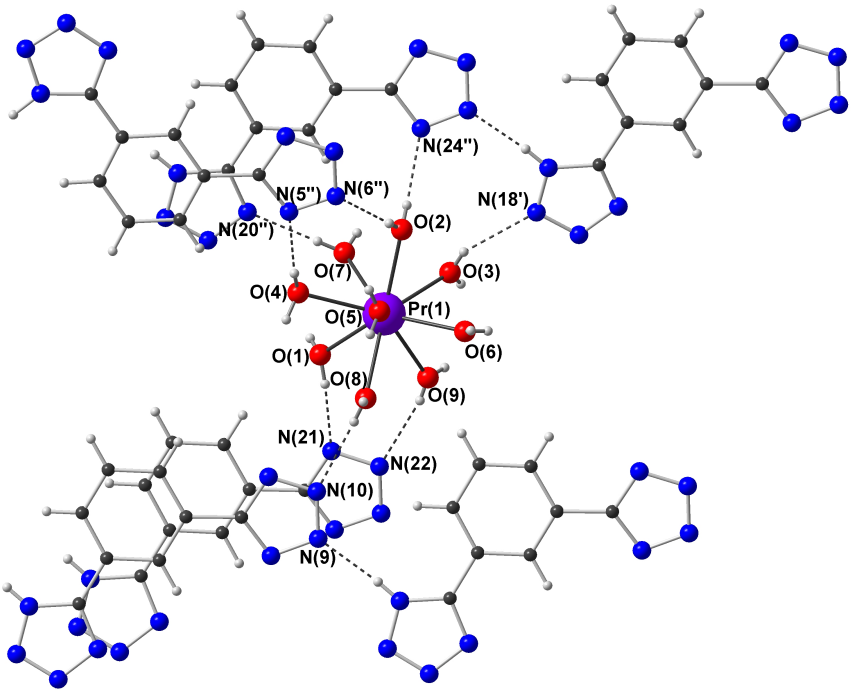

Fig.S2 Hydrogen-bonding between a $[Pr(OH_2)_9]^{3+}$ pillar and (*m*–BDTH)$^-$ anions from the two adjacent organic layers in **1**.

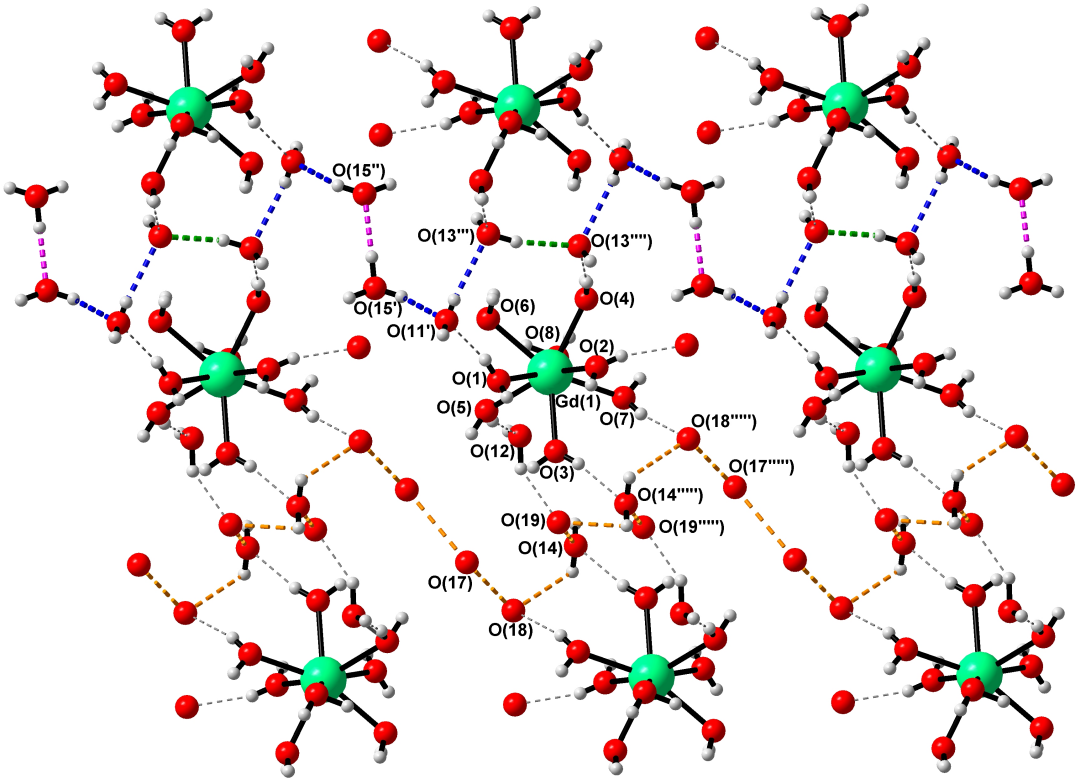

Fig. S3 A hydrogen-bonded layer in the structure of **2** showing the lattice waters between the $[Gd(OH_2)_9]^{3+}$ cationic pillars. Gd green, O red, H pale grey. In the structure of **2**, crystal waters also associate to form two independent helical chains. One of these can best be described as $\cdot\cdot(H_2O)\cdot\cdot(H_5O_2)^+\cdot\cdot(H_2O)\cdot\cdot(H_3O_2)^-\cdot\cdot(H_2O)\cdot\cdot$ in which hydrogen bonds highlighted in blue and pink, while the second water infinite tape is highlighted in orange

Electronic Supplementary Material for CrystEngComm
This journal is © The Royal Society of Chemistry 2008

This journal is © The Royal Society of Chemistry 2008

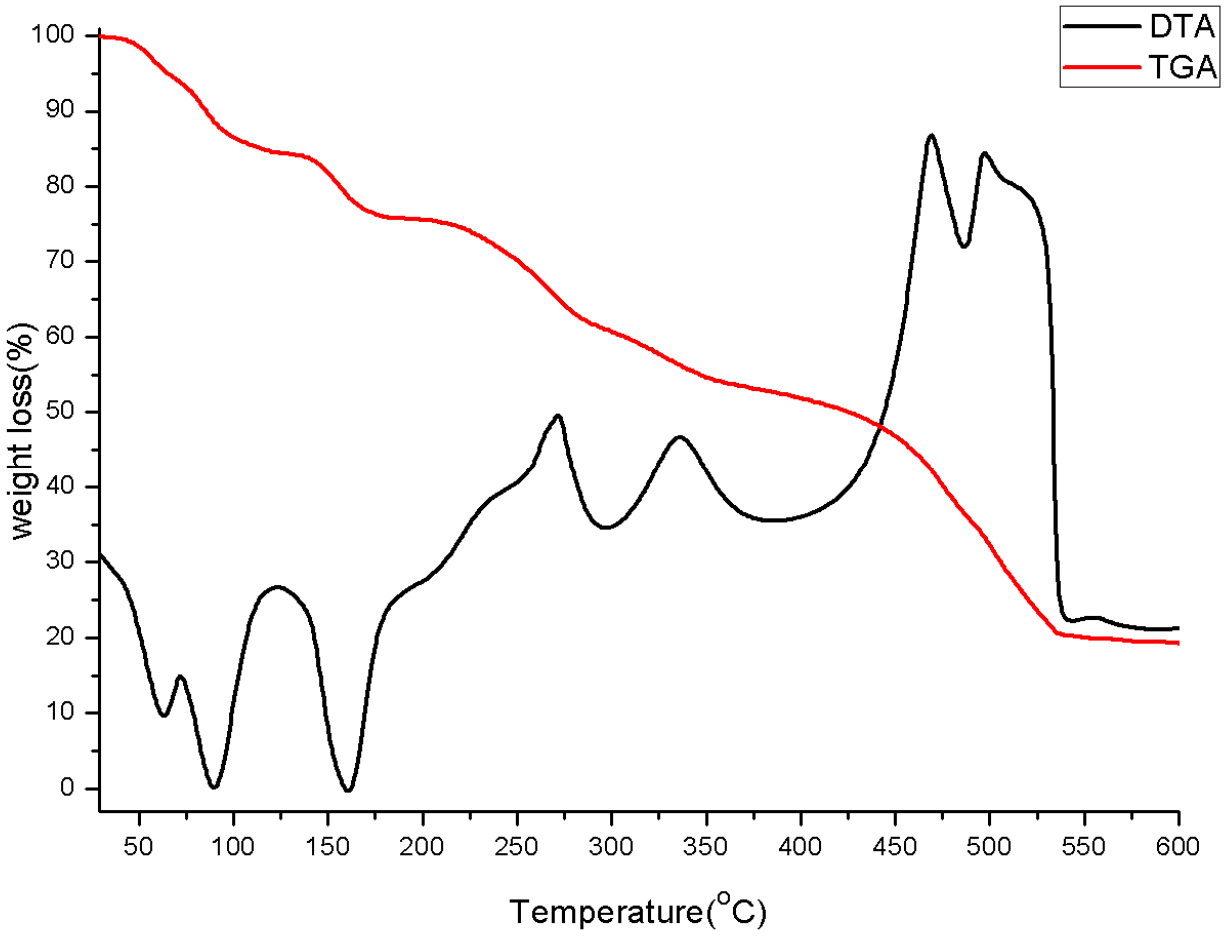

Fig. S4 Thermogravimetric data for compound **2**

This journal is © The Royal Society of Chemistry 2008

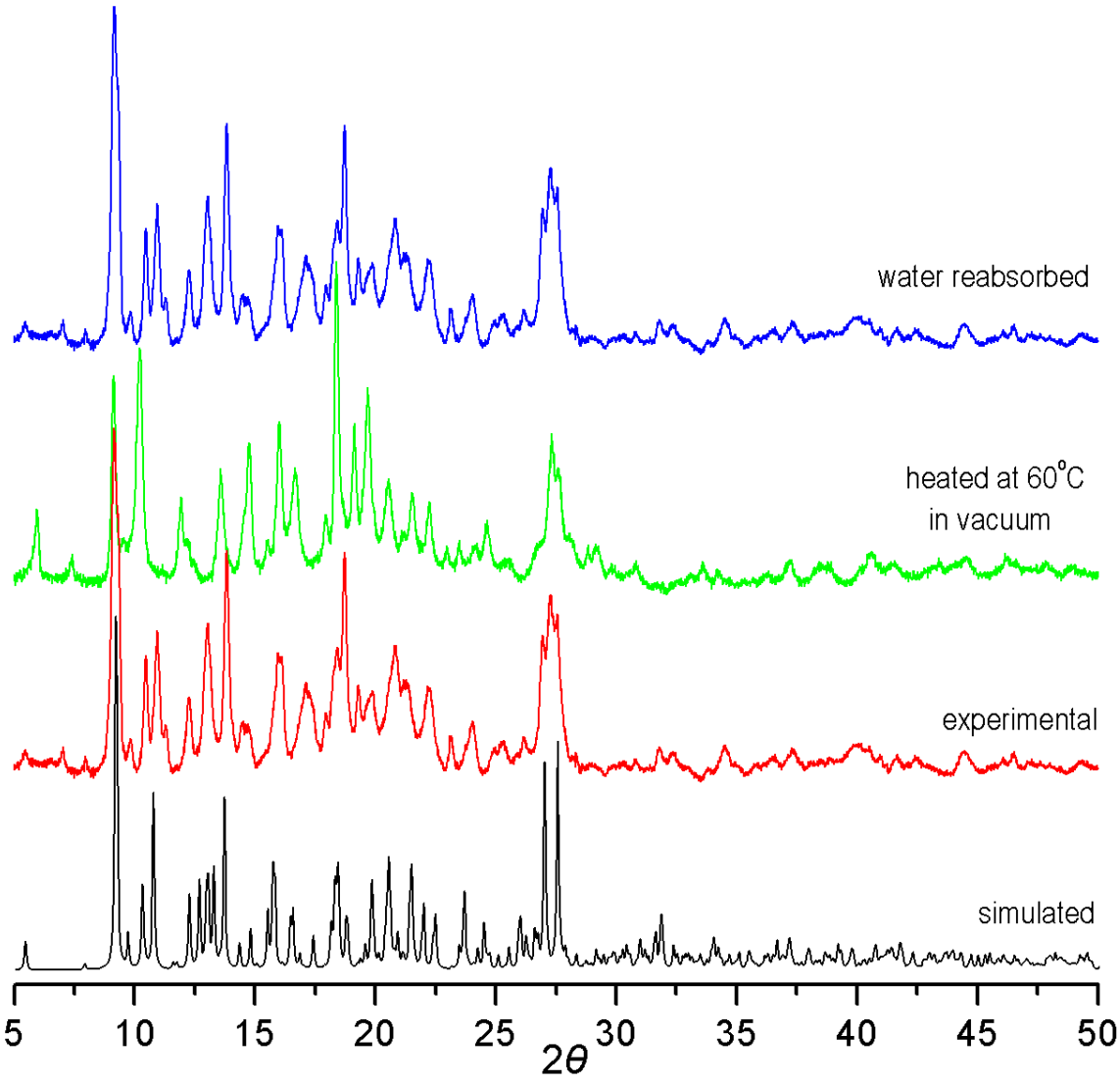

Fig. S5 X-ray powder patterns for compound **2**