A Neutron Diffraction Study of Hydrogen Bonding in Isostructural Potassium and Ammonium Lanthanoidates

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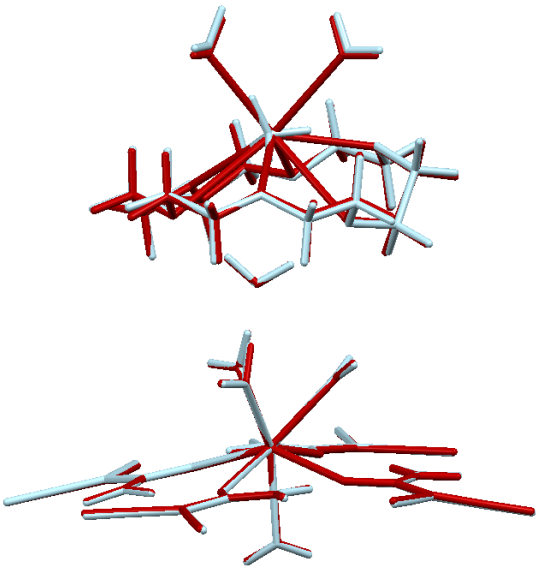
Supporting Information

Overlay Plot of 1Dy and 2Dy (from neutron data)

The diagram below show the overlay of the asymmetric units from the neutron structures of **1Dy** (blue) and **2Dy** (red). The overlay was calculated using Mercury with the fit being calculated on the overlay of the Dy atoms and the oxygen atoms of the four coordinated water molecules.



Geometries of Dy Aqua Ligands (from neutron data)

Angles were calculated using the distance of the Dy atom from the mean H-O-H plane of the aqua ligands (x) and the O-Dy bond length (y). This equals the angle subtended between the mean-plane of the aqua ligand and the Dy-O bond.

	1Dy			2Dy		
Water	**x**	**y**	**θ**	**x**	**y**	**θ**
O5	1.56	2.45	39.6	1.59	2.45	40.4
O6	0.62	2.43	14.9	0.55	2.43	13.1
O7	0.56	2.42	13.4	0.65	2.42	15.5
O8	0.12	2.36	2.8	0.01	2.36	0.2

Nitrile Interactions

The tables below list all of the hydrogen-bonding parameters for the interactions involving nitrile groups in the structures of **1Dy** and **2Dy**, as determined from neutron diffraction data, including the angle subtended at the nitrile nitrogen atom.

	D-H / Å	H···A / Å	D···A / Å	D-H···A / °	C≡N···H / °
O5···N2	0.966(10)	1.926(8)	2.892(5)	178.1(7)	159.6
O5···N5	0.965(7)	1.897(6)	2.852(4)	169.7(6)	146.4
O6···N12	0.958(7)	1.916(6)	2.854(4)	165.5(6)	163.0
O7···N3	0.958(9)	1.978(8)	2.918(5)	166.4(6)	166.7
O8···N8	0.972(6)	1.797(5)	2.768(3)	176.0(6)	155.2
O8···N11	0.974(6)	1.789(6)	2.759(4)	173.7(6)	150.8
O16···N6	0.914(11)	2.019(9)	2.909(7)	164.1(10)	169.0
O17···N9	0.968(9)	1.911(7)	2.819(4)	155.2(6)	157.7

Table SXX: Hydrogen-bond parameters involving nitrile groups in **1Dy** from neutron diffraction data.

	D-H / Å	H···A / Å	D···A / Å	D-H···A / °	C≡N···H / °
O5···N2	0.953(9)	1.933(8)	2.886(4)	177.5(8)	159.4
O5···N5	0.964(9)	1.896(8)	2.849(5)	169.6(8)	146.3
O6···N12	0.965(9)	1.906(8)	2.848(5)	164.8(8)	162.1
O7···N3	0.981(8)	1.958(7)	2.915(4)	164.4(8)	165.9
O8···N8	0.977(9)	1.800(8)	2.776(5)	176.6(8)	155.9
O8···N11	0.963(8)	1.795(7)	2.754(5)	173.3(8)	148.7
O16···N6	0.926(14)	2.022(10)	2.932(7)	167.2(11)	170.1
O17···N9	0.965(10)	1.922(8)	2.828(6)	155.4(8)	159.2

Table SXX: Hydrogen-bond parameters involving nitrile groups in **2Dy** from neutron diffraction data.

Crystal Packing Diagrams

Packing diagrams of **1Dy** and **2Dy** (from neutron data) show the extent of hydrogen bonding in the extended structure.

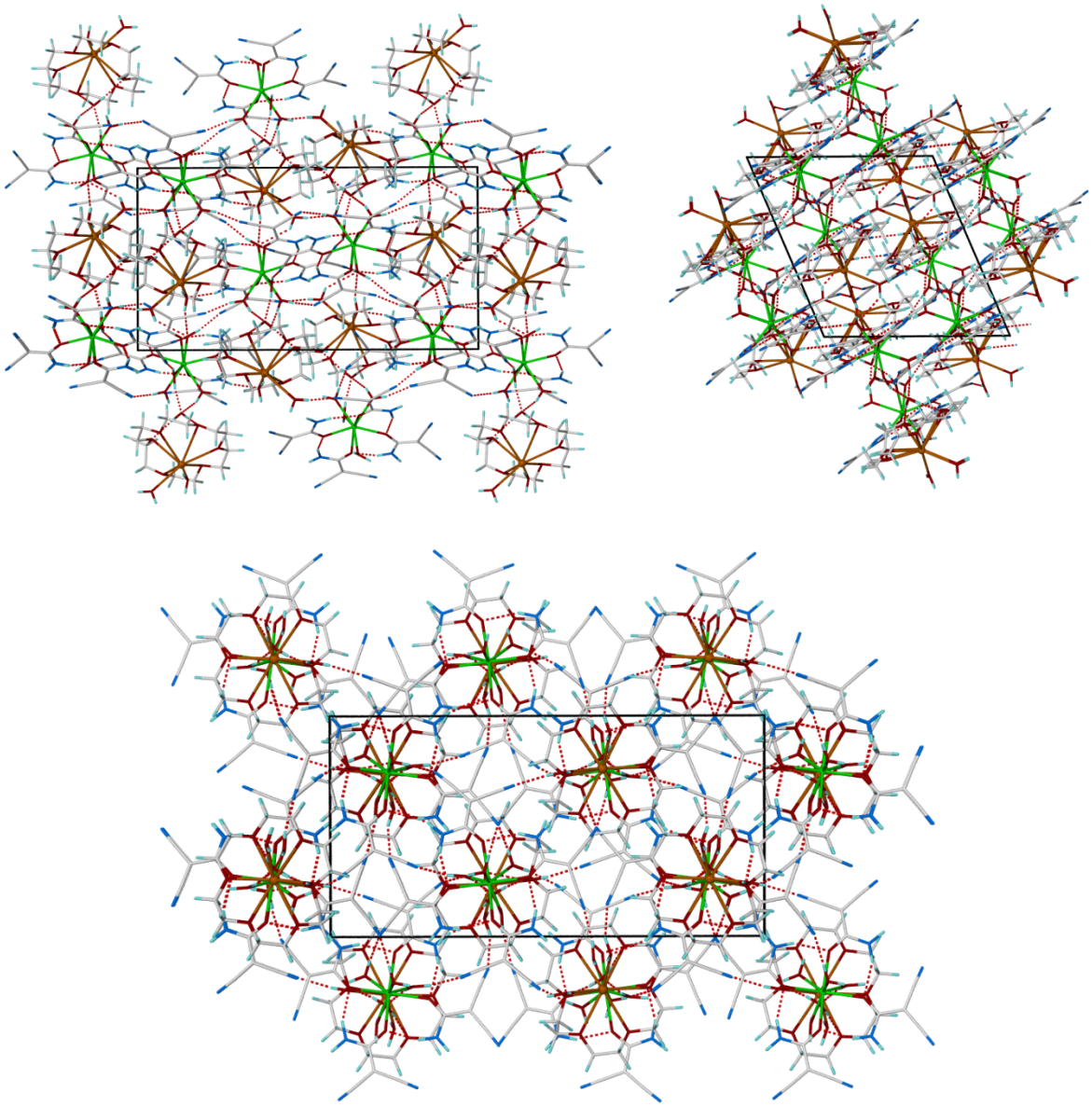


Figure SXX: Packing of **2Dy** viewed along the *a*-, *b*- and *c*-axes (clockwise from top left).

Thermogravimetric Analysis (TGA)

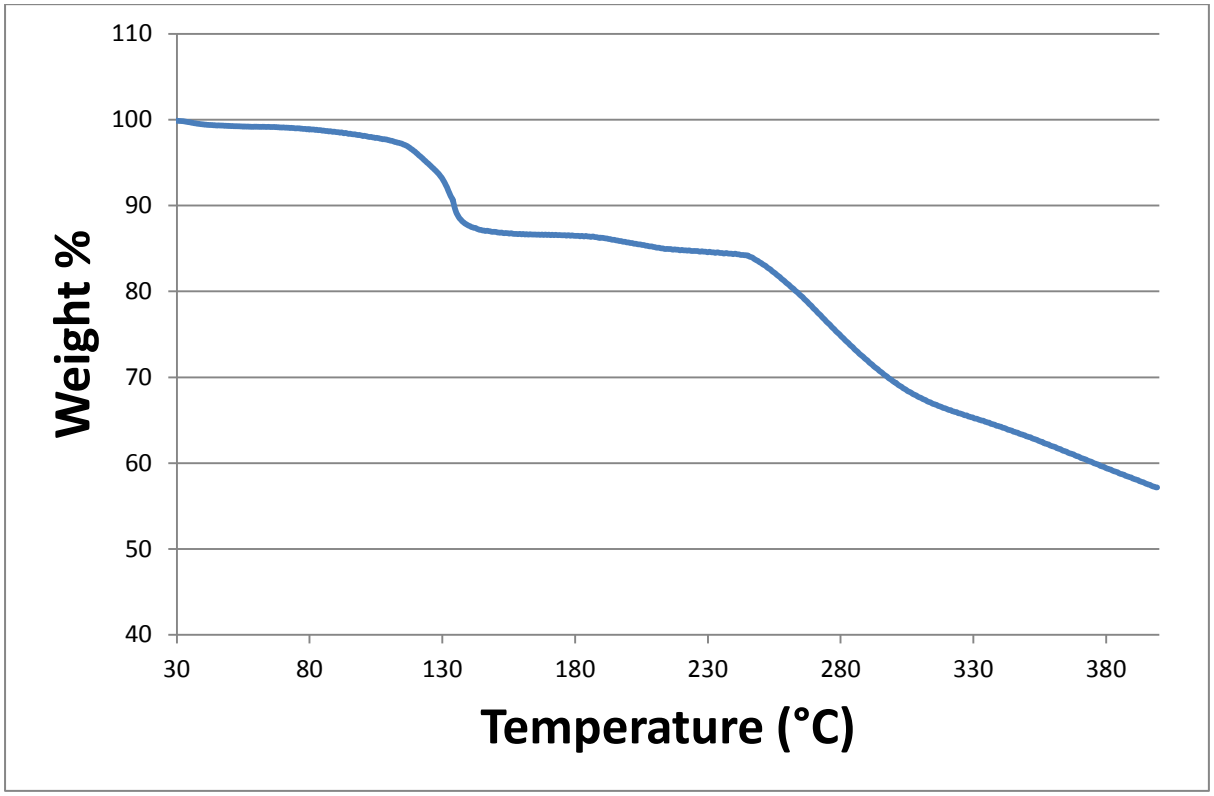


Figure SXX: Thermogravimetric trace for **1Dy**.

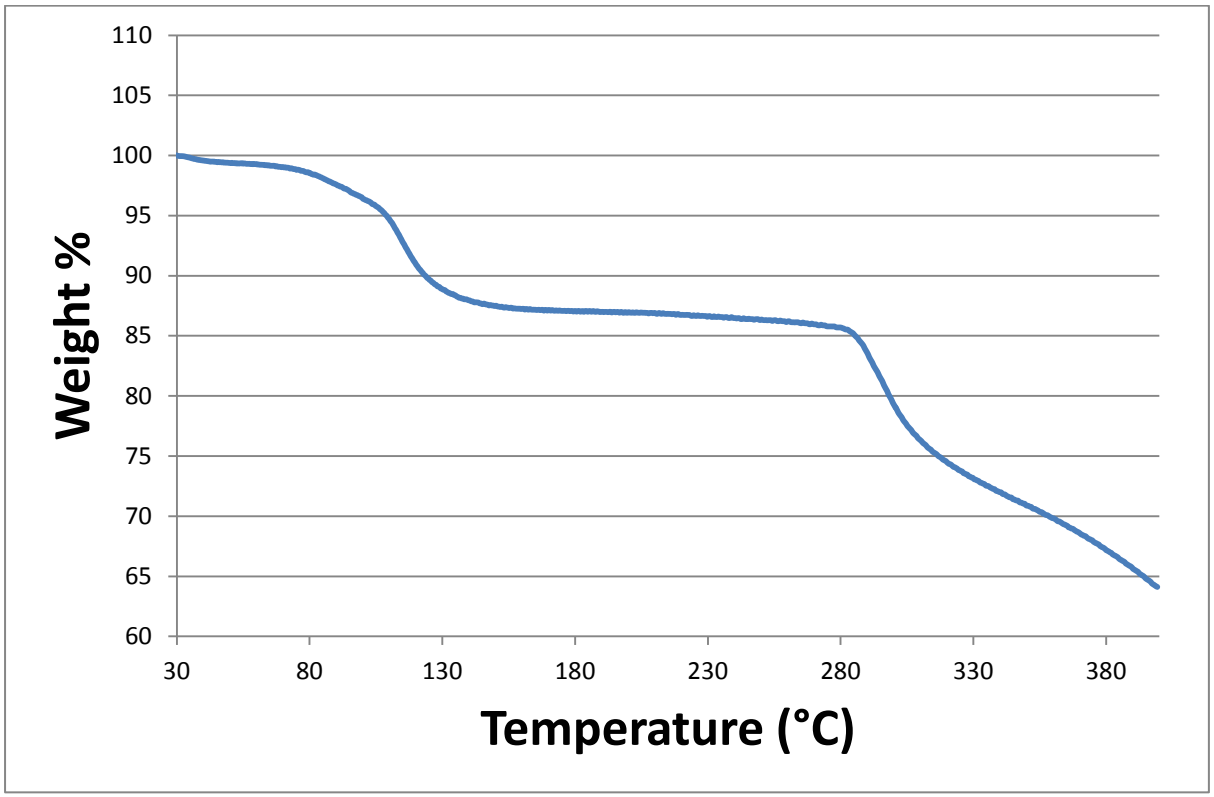


Figure SXX: Thermogravimetric trace for **2Dy**.