Electronic Supplementary Material (ESI) for Dalton Transactions.

Strong spin frustration and negative magnetization in $LnCu_3(OH)_6Cl_3$ (Ln = Nd and Sm) with triangular lattices: The effects of lanthanides

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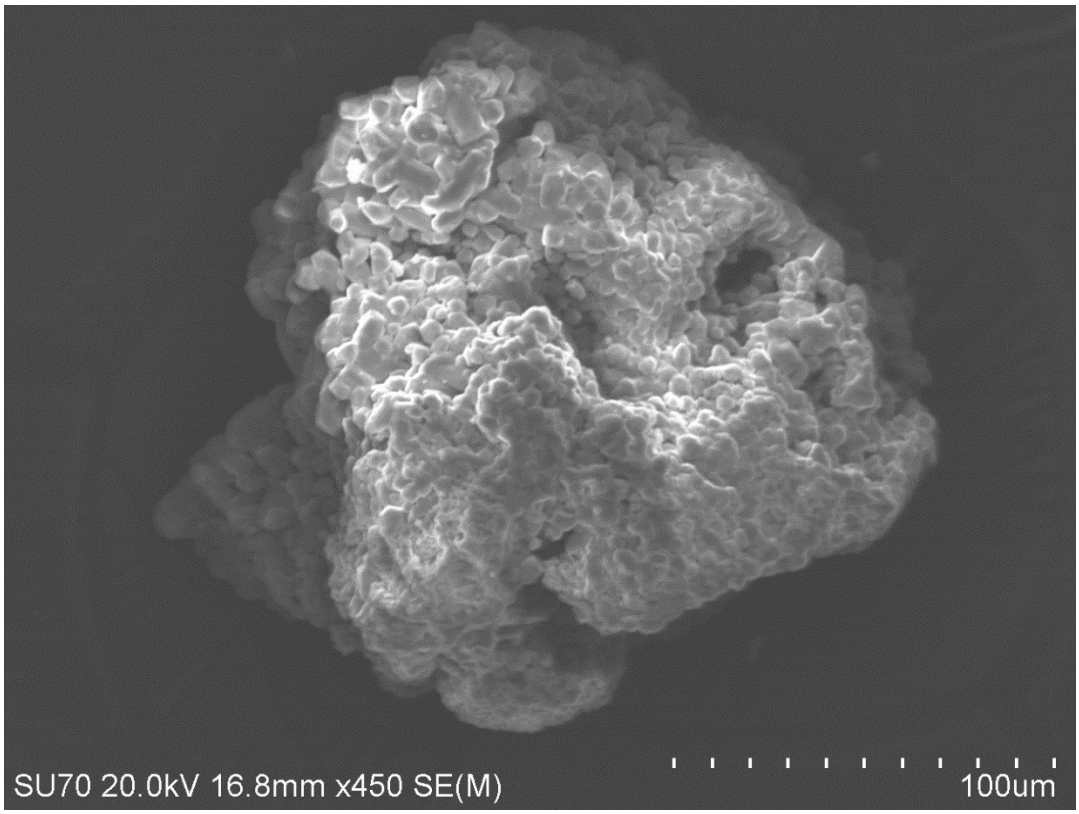

Figure S1. SEM image of $SmCu_3(OH)_6Cl_3$.

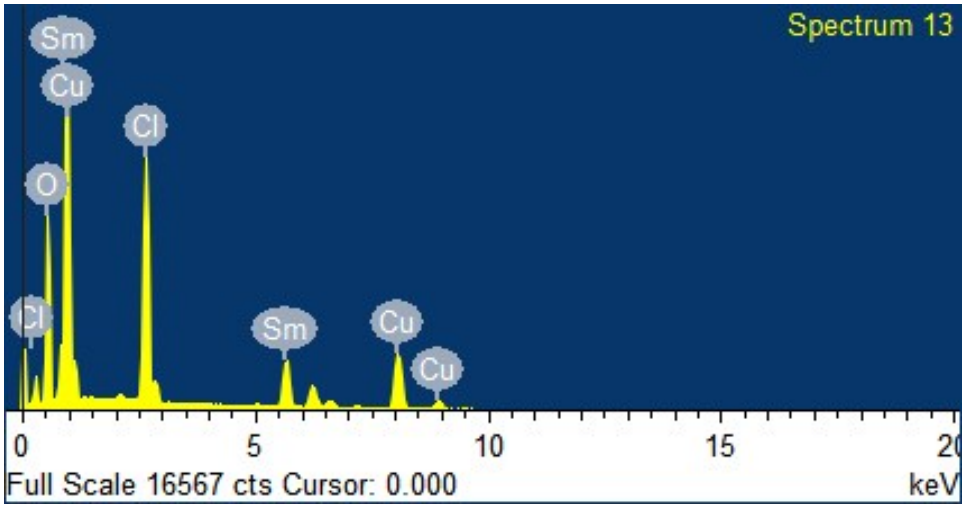

Figure S2. EDX of $SmCu_3(OH)_6Cl_3$.

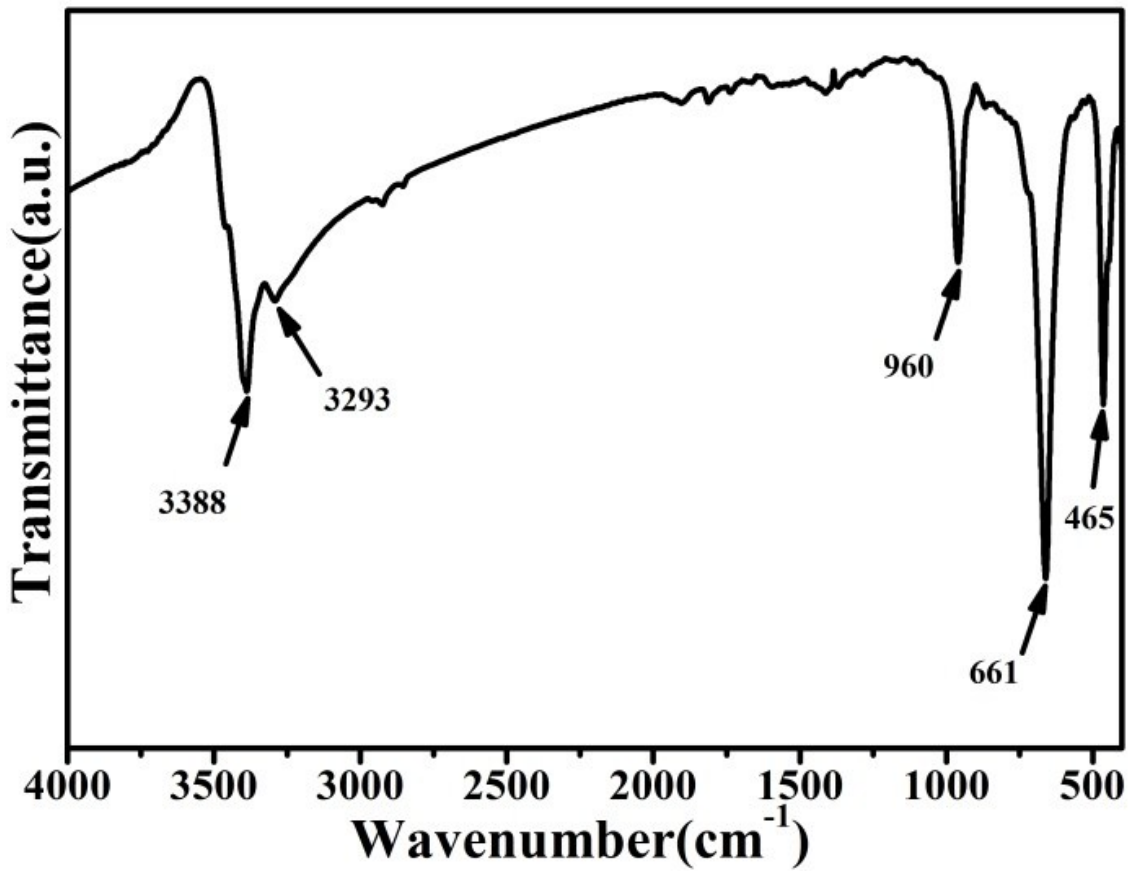

Figure S3. FTIR spectrum of $SmCu_3(OH)_6Cl_3$.

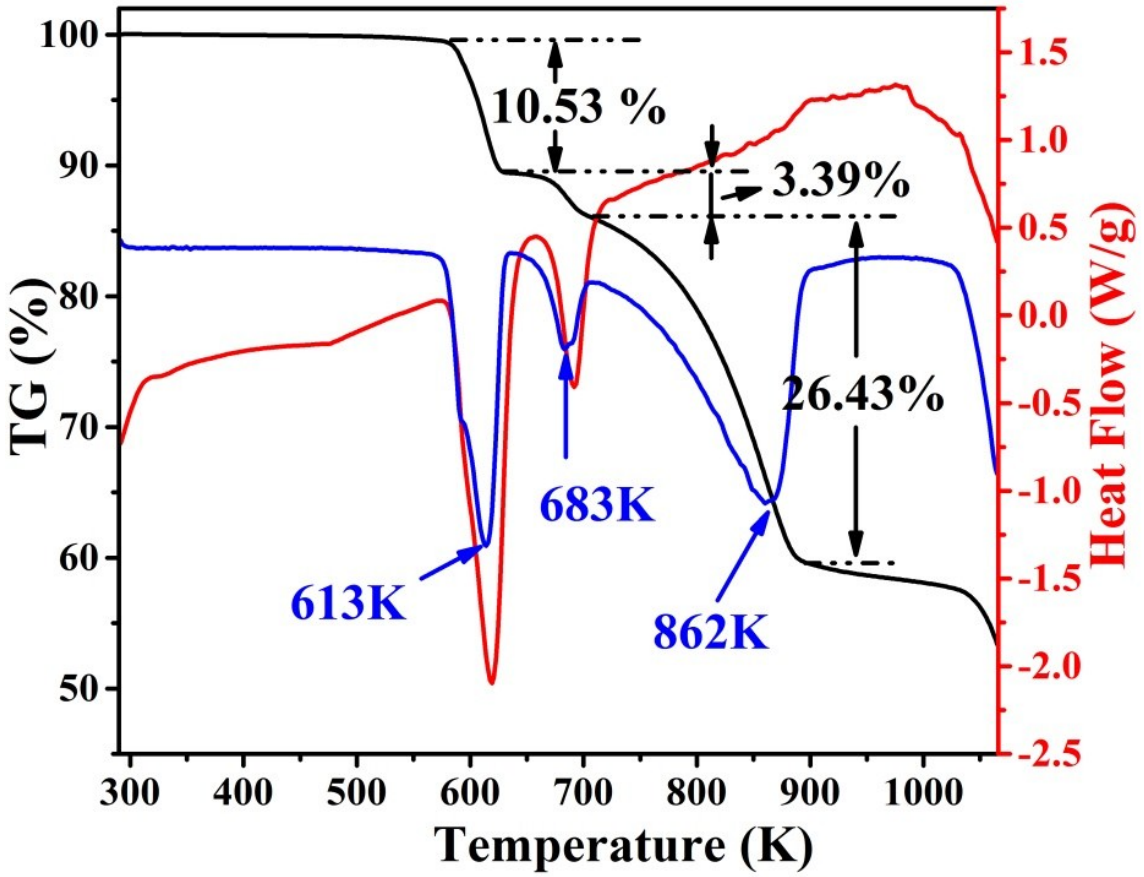

Figure S4. TG (black), DTG (blue) and DSC (red) curves of $SmCu_3(OH)_6Cl_3$.

Table S1 Atomic displacement parameters (Å^2) of $LnCu_3(OH)_6Cl_3$ (*Ln* = Nd, Sm and Gd)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00306 (16)	0.00306 (16)	0.0067 (2)	0.00153 (8)	0.000	0.000
Cu1	0.0029 (2)	0.0029 (2)	0.0067 (3)	0.00059 (15)	−0.00100 (6)	0.00100 (6)
Cl1	0.0161 (3)	0.0161 (3)	0.0049 (4)	0.00803 (17)	0.000	0.000
Cl2	0.0131 (4)	0.0131 (4)	0.0037 (5)	0.0065 (2)	0.000	0.000
O1	0.0051 (6)	0.0046 (7)	0.0035 (7)	0.0023 (4)	0.0002 (3)	0.0004 (7)
Sm1	0.00369 (17)	0.00369 (17)	0.0093 (2)	0.00185 (8)	0.000	0.000
Cu1	0.0029 (2)	0.0029 (2)	0.0071 (3)	0.00069 (18)	−0.00101 (8)	0.00101 (8)
Cl1	0.0151 (4)	0.0151 (4)	0.0052 (5)	0.0075 (2)	0.000	0.000
Cl2	0.0123 (5)	0.0123 (5)	0.0049 (7)	0.0061 (3)	0.000	0.000
O1	0.0049 (7)	0.0053 (9)	0.0042 (9)	0.0027 (5)	0.0000 (4)	0.0000 (8)
Gd1	0.00290 (12)	0.00290 (12)	0.00982 (16)	0.00145 (6)	0.000	0.000
Cu1	0.00271 (15)	0.00271 (15)	0.0081 (2)	0.00043 (13)	−0.00097 (6)	0.00097 (6)
Cl1	0.0142 (3)	0.0142 (3)	0.0064 (4)	0.00711 (15)	0.000	0.000
Cl2	0.0116 (4)	0.0116 (4)	0.0056 (5)	0.00581 (19)	0.000	0.000
O1	0.0049 (5)	0.0058 (7)	0.0049 (7)	0.0029 (4)	0.0002 (3)	0.0003 (6)

Table S2 Hydrogen-bond geometry (Å, °) of $LnCu_3(OH)_6Cl_3$ (*Ln* = Nd, Sm and Gd)

compounds	*D*—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
Nd	O1—H1···Cl1^{xi}	0.78 (2)	2.59 (3)	3.2814 (19)	148 (4)
	O1—H1···Cl2	0.78 (2)	2.73 (4)	3.1136 (18)	113 (4)
Sm	O1—H1···Cl1^{xi}	0.81 (2)	2.51 (3)	3.280 (2)	159 (6)
Gd	O1—H1···Cl1^{xi}	0.80 (2)	2.57 (3)	3.2712 (18)	147 (4)
	O1—H1···Cl2	0.80 (2)	2.66 (4)	3.0635 (16)	113 (3)

Symmetry code: (xi) *x*, *y*, *z*−1.