Supporting Information for

Sodalite-like Rare-Earth Carbonate: A Study of Structural Transformation and Diluted Magnetism

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Table of Contents

Table S1. Crystal data and structure refinement for 1a.

Compound	**1**
Empirical formula	$CH_6ClDy_3O_9$
Formula weight	685.01
Temperature	296(2) K
Wavelength (Å)	0.71073
Crystal system, space group	Cubic, *Im*-3
Unit cell dimensions	
a (Å)	12.4754(6)
b (Å)	12.4754(6)
c (Å)	12.4754(6)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å^3)	1941.62(16)
Z, calculated density (mg m^{-3})	8, 4.687
Absorption coefficient (mm^{-1})	23.150
F(000)	2392
Crystal size (mm^3)	0.32 × 0.21 × 0.15
θ range (°) for data collection	2.31 − 27.46
Limiting indices	$-13 \le h \le 16$, $-16 \le k \le 15$, $-16 \le l \le 12$
Reflections collected/unique	8032/426, [R_{int} = 0.0272]
Completeness to *θ* (%)	27.46, 100.0
Absorption correction	Semi-empirical from equivalents
Max and min transmission	0.1288 and 0.0505
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	426/7/32
Goodness-of-fit on F^2	0.989
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0395, wR_2 = 0.1005
R indices (all data)	R_1 = 0.0401, wR_2 = 0.1010
Largest diff. peak and hole (e Å^{-3})	3.028 and −2.256

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

Table S2. Crystal data and structure refinement for **2**[a].

Compound	**2**
Empirical formula	$CH_6ClEr_3O_9$
Formula weight	699.29
Temperature	296(2) K
Wavelength (Å)	0.71073
Crystal system, space group	Cubic, *Im*-3*m*
Unit cell dimensions	
a (Å)	12.4127(4)
b (Å)	12.4127(4)
c (Å)	12.4127(4)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å^3)	1912.49(11)
Z, calculated density (mg m^{-3})	8, 4.857
Absorption coefficient (mm^{-1})	26.389
F(000)	2440
Crystal size (mm^3)	0.07 × 0.07 × 0.05
θ range (°) for data collection	2.32 − 27.49
Limiting indices	$-10 \le h \le 9$, $-4 \le k \le 16$, $-12 \le l \le 16$
Reflections collected/unique	1614/252, [R_{int} = 0.0199]
Completeness to *θ* (%)	27.49, 100.0
Absorption correction	Semi-empirical from equivalents
Max and min transmission	0.3521 and 0.2595
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	252/7/21
Goodness-of-fit on F^2	1.115
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0490, wR_2 = 0.1261
R indices (all data)	R_1 = 0.0553, wR_2 = 0.1313
Largest diff. peak and hole (e Å^{-3})	3.584 and −3.019

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

Table S3. Crystal data and structure refinement for **3**[a].

Compound	**3**
Empirical formula	$CH_6ClY_3O_9$
Formula weight	464.24
Temperature	296(2) K
Wavelength (Å)	0.71073
Crystal system, space group	Cubic, *Im*-3*m*
Unit cell dimensions	
a (Å)	12.665(9)
b (Å)	12.665(9)
c (Å)	12.665(9)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å^3)	2032(2)
Z, calculated density (mg m^{-3})	8, 3.035
Absorption coefficient (mm^{-1})	17.281
F(000)	1744
Crystal size (mm^3)	0.05 × 0.05 × 0.05
θ range (°) for data collection	2.27 – 26.90
Limiting indices	$-16 \le h \le 5$, $-14 \le k \le 15$, $-11 \le l \le 7$
Reflections collected/unique	2253/251, [R_{int} = 0.0526]
Completeness to *θ* (%)	26.90, 99.6
Absorption correction	Semi-empirical from equivalents
Max and min transmission	0.4787 and 0.4787
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	251/7/21
Goodness-of-fit on F^2	1.117
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0701, wR_2 = 0.1868
R indices (all data)	R_1 = 0.0884, wR_2 = 0.2061
Largest diff. peak and hole (e Å^{-3})	2.923 and −1.350

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

Table S4. Selected bond lengths [Å] for **1**, **2**, **3** and **1-c**.

1		**2**		**3**		**1-c**	
Dy(1)-O(2)	2.304(11)	Er(1)-O(2)	2.290(13)	Y(1)-O(2)	2.333(10)	Dy(1)-O(1)	2.34(5)
Dy(1)-O(2)#5	2.347(7)	Er(1)-O(2)#7	2.290(13)	Y(1)-O(2)#7	2.333(10)	Dy(1)-O(2)	2.31(2)
Dy(1)-O(2)#6	2.347(7)	Er(1)-O(2)#8	2.328(8)	Y(1)-O(2)#8	2.379(6)	Dy(1)-O(3)	2.36(6)
Dy(1)-O(3)	2.302(11)	Er(1)-O(2)#2	2.328(8)	Y(1)-O(2)#1	2.379(6)	Dy(1)-O(4)	2.13(4)
Dy(1)-O(3)#1	2.347(7)	Er(1)-O(2)#9	2.328(8)	Y(1)-O(2)#9	2.379(6)	Dy(1)-O(2)#4	2.16(5)
Dy(1)-O(3)#7	2.347(7)	Er(1)-O(2)#10	2.328(8)	Y(1)-O(2)#10	2.379(6)	Dy(1)-O(4)#4	2.33(4)
Dy(1)-O(1)	2.536(13)	Er(1)-O(1)	2.522(16)	Y(1)-O(1)	2.565(12)	Dy(2)-O(1)	2.206(19)
Dy(1)-O(1)#1	2.539(14)	Er(1)-O(1)#11	2.522(16)	Y(1)-O(1)#11	2.565(12)	Dy(2)-O(2)	2.41(6)
Dy(1)-O(1)#7	2.539(14)	Er(1)-O(1)#12	2.522(16)	Y(1)-O(1)#12	2.565(12)	Dy(2)-O(1)#5	2.31(4)
Dy(1)-O(1)#8	2.536(14)	Er(1)-O(1)#2	2.522(16)	Y(1)-O(1)#1	2.565(12)	Dy(2)-O(3) #2	2.27(6)
C(1)-O(1)#1	1.274(13)	C(1)-O(1)#1	1.28(2)	C(1)-O(1)#1	1.311(18)	Dy(2)-O(3) #3	2.25(5)
C(1)-O(1)#2	1.274(13)	C(1)-O(1)#2	1.28(2)	C(1)-O(1)#3	1.311(18)	Dy(2)-O(4)#5	2.40(5)
C(1)-O(1)#3	1.274(13)	C(1)-O(1)#3	1.28(2)	C(1)-O(1)#4	1.311(18)	Dy(3)-O(1)	2.215(19)
C(1)-O(1)#4	1.274(13)	C(1)-O(1)#4	1.28(2)	C(1)-O(1)#5	1.311(18)	Dy(3)-O(3)#3	2.21(5)
C(1)-O(1)	1.274(13)	C(1)-O(1)#5	1.28(2)	C(1)-O(1)#2	1.311(18)	Dy(3)-O(4)#4	2.27(5)
C(1)-O(1)#5	1.274(13)	C(1)-O(1)	1.28(2)	C(1)-O(1)	1.311(18)	Dy(3)-O(2)#3	2.24(5)

Symmetry transformations used to generate equivalent atoms:

For **1**:

#1 -z+3/2,-x+3/2,-y+3/2 #2 y,z,x #3 -x+3/2,-y+3/2,-z+3/2 #4 z,x,y #5 -y+3/2,-z+3/2,-x+3/2 #6 y-1/2,-z+3/2,x+1/2 #7 z-1/2,-x+3/2,-y+3/2 #8 -x+1,y,z

For **2**:

#1 -y+1/2,-z+1/2,-x+1/2 #2 -z+1/2,-x+1/2,-y+1/2 #3 z,x,y #4 y,z,x #5 -x+1/2,-y+1/2,-z+1/2 #6 -y+1/2,z+1/2,-x+1/2 #7 z,-y+1,x #8 -y+1/2,-x+1/2,-z+1/2 #9 y-1/2,x+1/2,-z+1/2 #10 -z+1/2,x+1/2,y-1/2 #11 x,-y+1,z #12 -z+1/2,x+1/2,-y+1/2

For **3**:

#1 -z+1/2,-x+1/2,-y+1/2 #2 -y+1/2,-z+1/2,-x+1/2 #3 y,z,x #4 -x+1/2,-y+1/2,-z+1/2 #5 z,x,y #6 -y+1/2,z+1/2,-x+1/2 #7 z,-y+1,x #8 -y+1/2,-x+1/2,-z+1/2 #9 -z+1/2,x+1/2,y-1/2 #10 y-1/2,x+1/2,-z+1/2 #11 x,-y+1,z #12 -z+1/2,x+1/2,-y+1/2

For **1-c**:

#1 x-y,x-1,-z+1 #2 -x+y+4/3,-x+2/3,z-1/3 #3 -x+5/3,-y+1/3,-z+4/3 #4 -y+2/3,x-y-2/3,z+1/3 #5 y+1,-x+y+1,-z+1

Table S5. Crystal data and structure refinement for **1-c**[a].

Compound	**1-c**
Empirical formula	$ClDy_3O_5$
Formula weight	586.95
Temperature	296(2) K
Wavelength (Å)	0.71073
Crystal system, space group	Trigonal, *R*-3
Unit cell dimensions	
a (Å)	16.64(3)
b (Å)	16.64(3)
c (Å)	10.217(19)
α (°)	90
β (°)	90
γ (°)	120
Volume (Å^3)	2451(8)
Z, calculated density (mg m^{-3})	18, 7.158
Absorption coefficient (mm^{-1})	41.134
F(000)	4446
Crystal size (mm^3)	0.06 × 0.06 × 0.03
θ range (°) for data collection	2.45 – 24.83
Limiting indices	$-18 \le h \le 19$, $-19 \le k \le 19$, $-12 \le l \le 9$
Reflections collected/unique	3945/894, [R_{int} = 0.1268]
Completeness to *θ* (%)	24.83, 96.6
Absorption correction	Semi-empirical from equivalents
Max and min transmission	0.3717 and 0.1916
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	894/27/81
Goodness-of-fit on F^2	0.950
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0927, wR_2 = 0.2245
R indices (all data)	R_1 = 0. 2356, wR_2 = 0.3476
Largest diff. peak and hole (e Å^{-3})	4.214 and −2.427

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

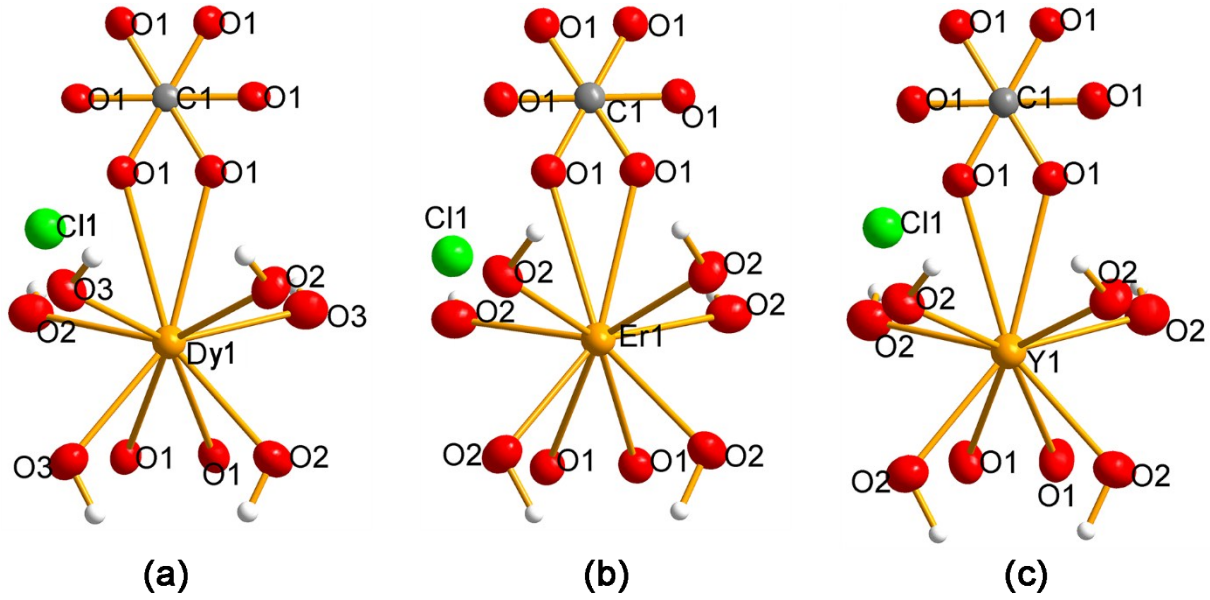


Fig. S1 Thermal ellipsoids given at 50% probability, showing the atomic labeling scheme of **1**, **2** and **3**, with white H atoms signed as white balls.

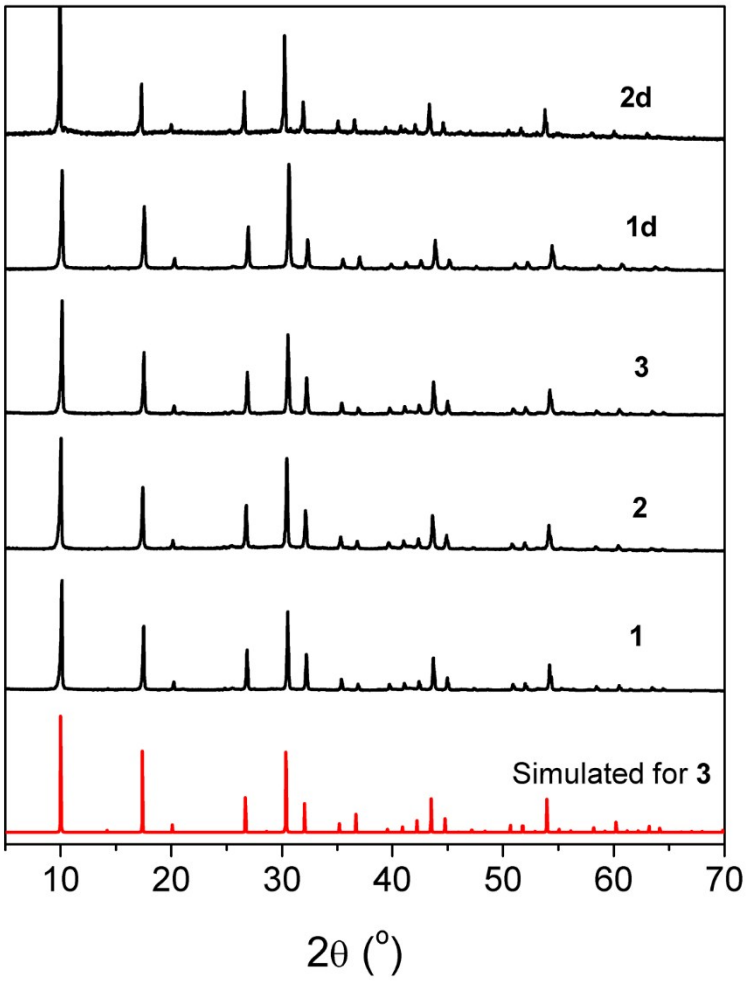


Fig. S2 Experimental PXRD patterns of **1**, **2**, **3**, **1d** and **2d**, comparing with the simulated one for **3**.

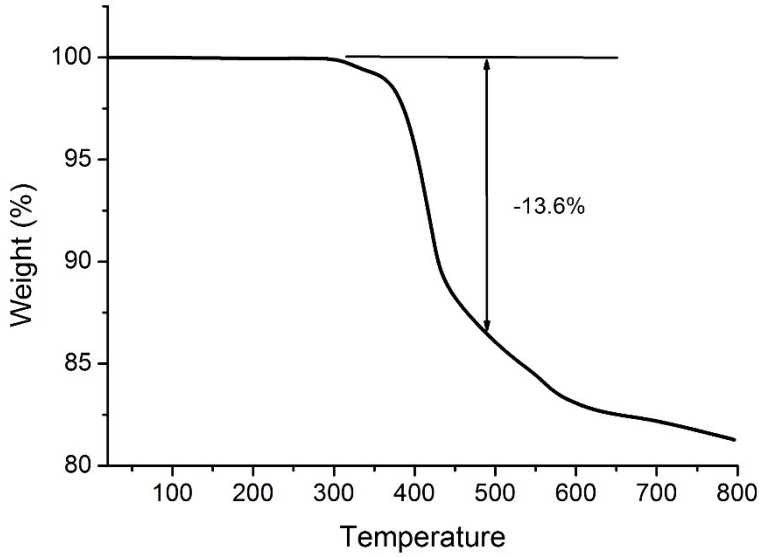


Fig. S3 TGA curves of as-synthesized **1**.

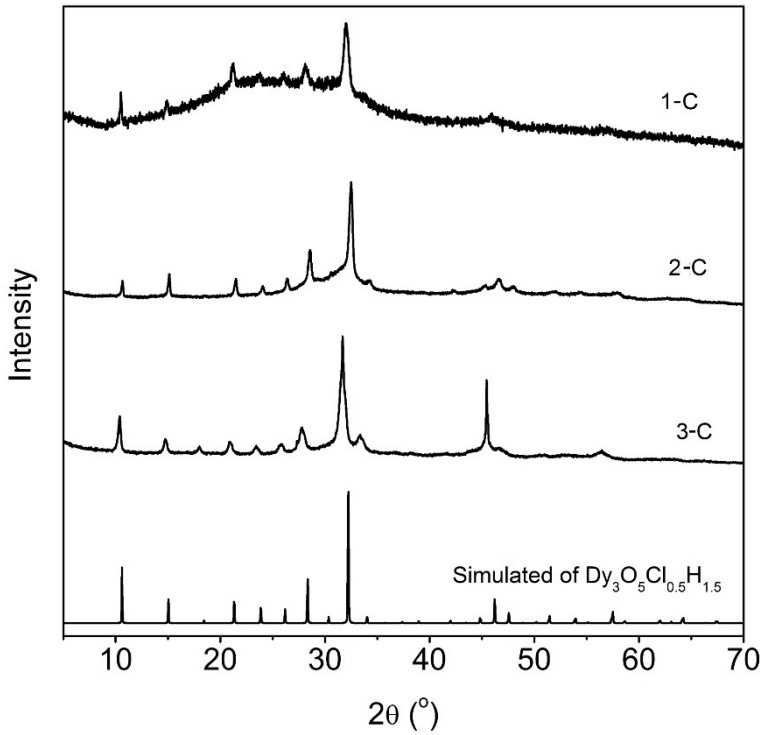
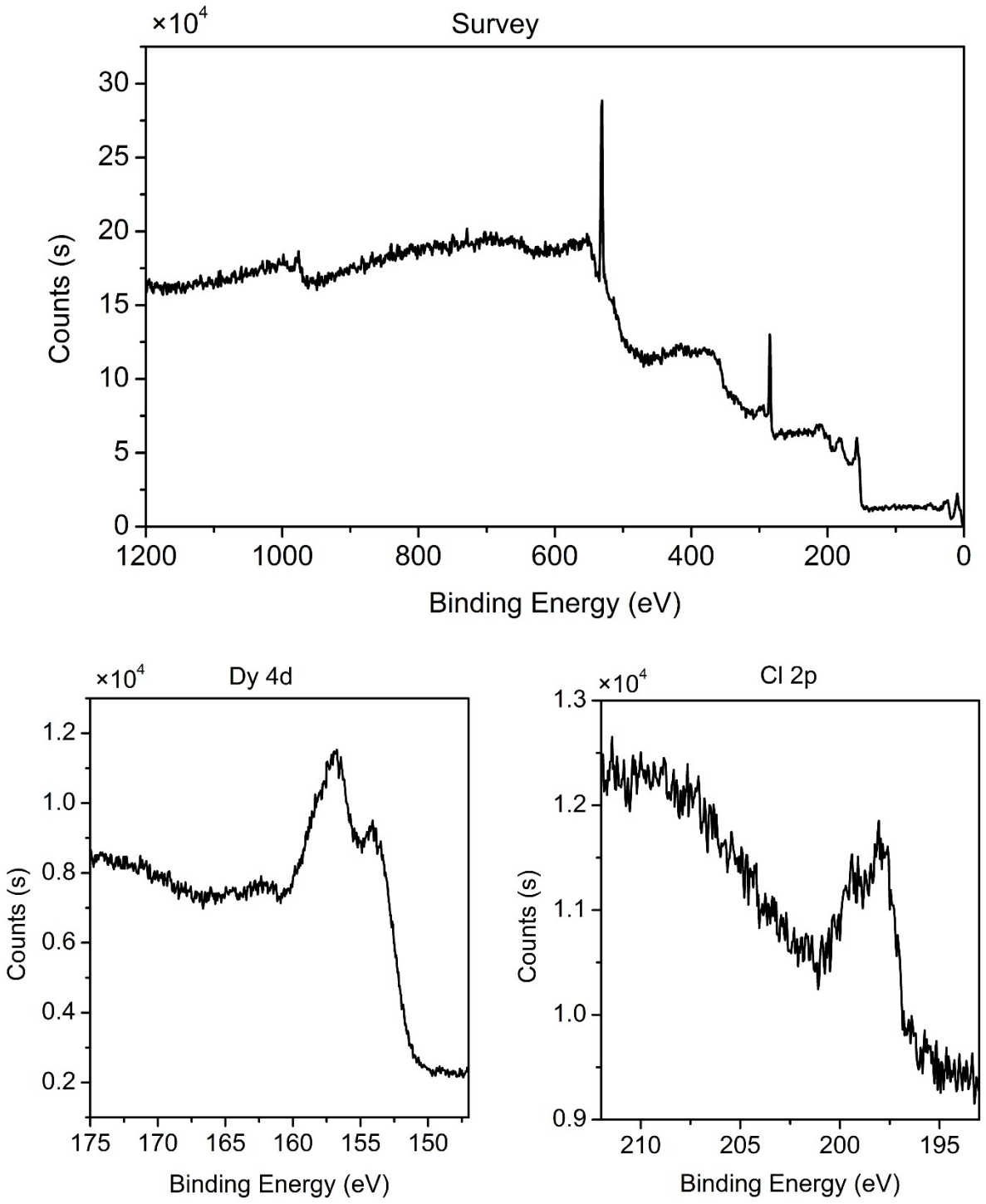
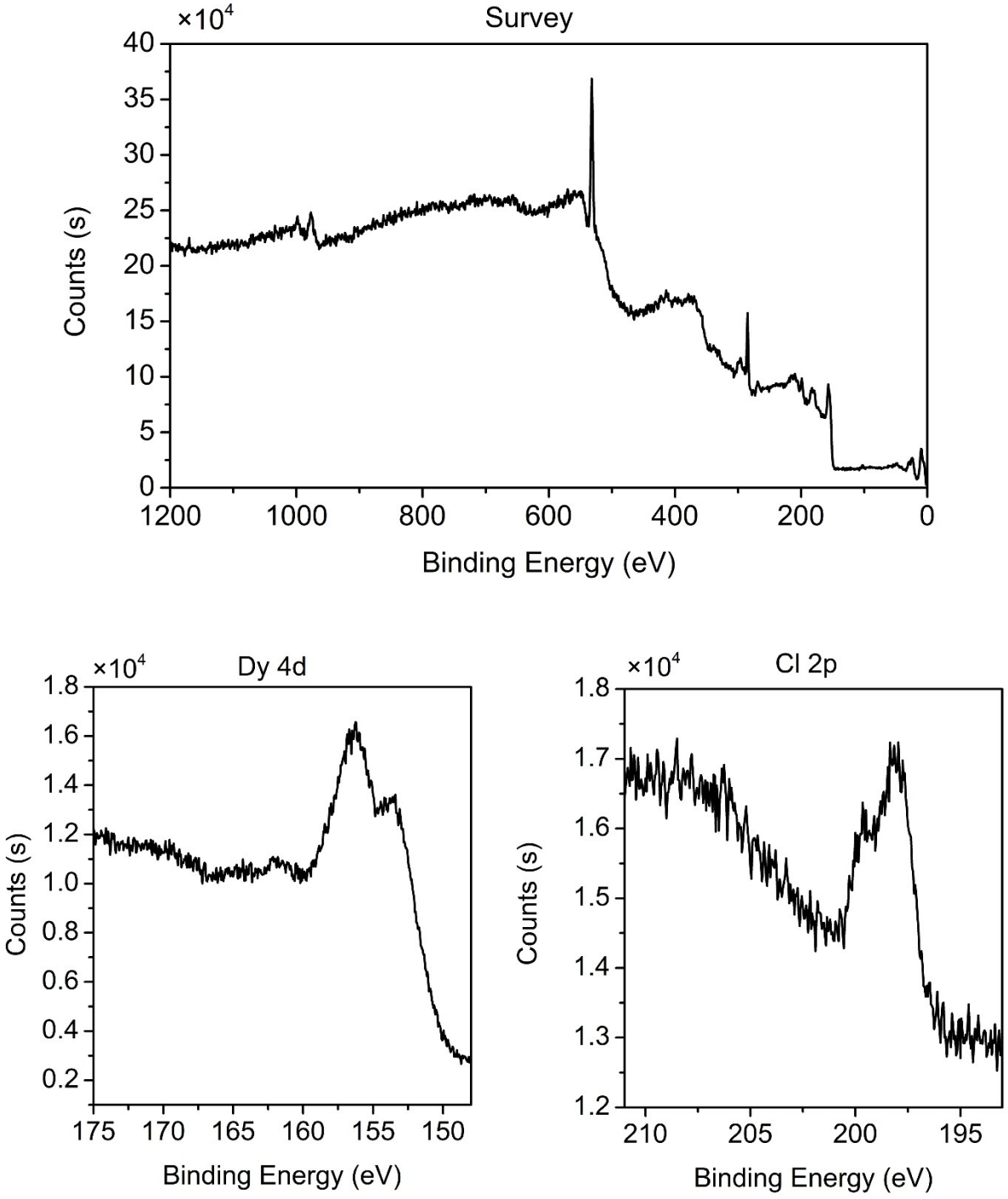


Fig. S4 Experimental PXRD for **1-c**, **2-c** and **3-c** and simulated PXRD pattern of **1-c**.



(a)



(b)

Fig. S5 X-ray photoelectron spectra of (a) **1** and (b) **1-c**, the signal around 198 eV, which corresponding to Cl 2p, indicating the existence of Cl for the crystals.

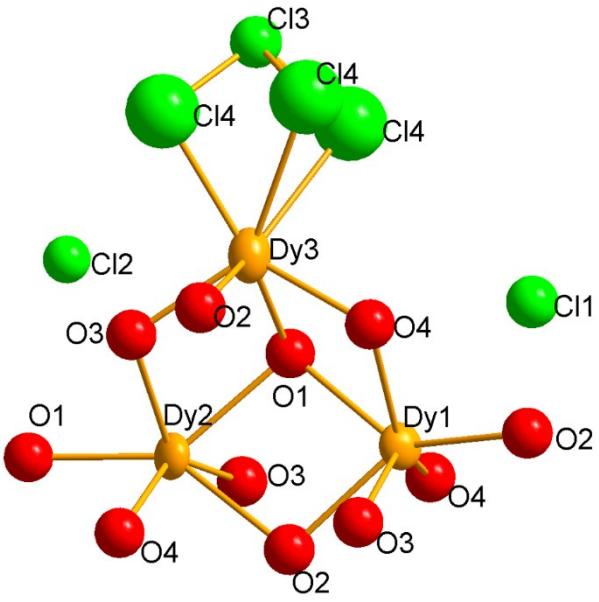


Fig. S6 Asymmetric unit of **1-c**, shows three crystallographically distinct of Dy atoms.

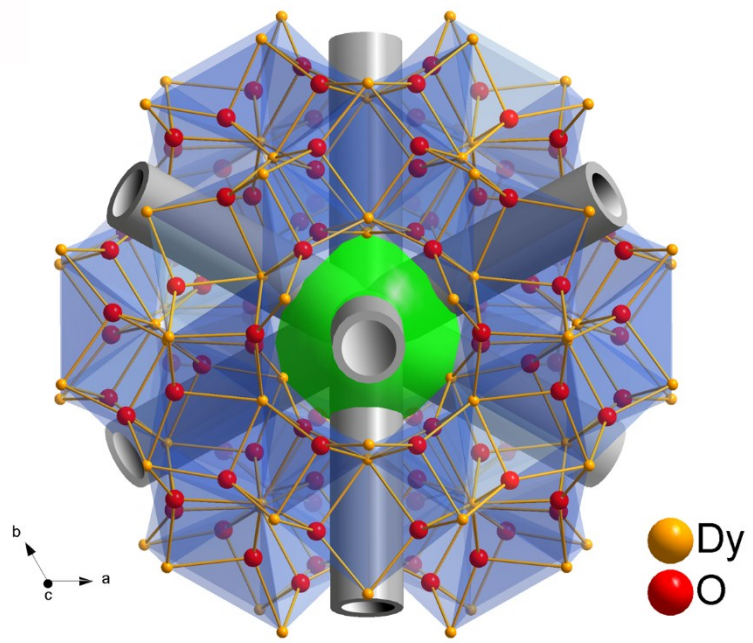


Fig. S7 Structure of **1-c** along [001] direction, with 3-D intersection 6-ring channels along [001], [11], [211] and [12].

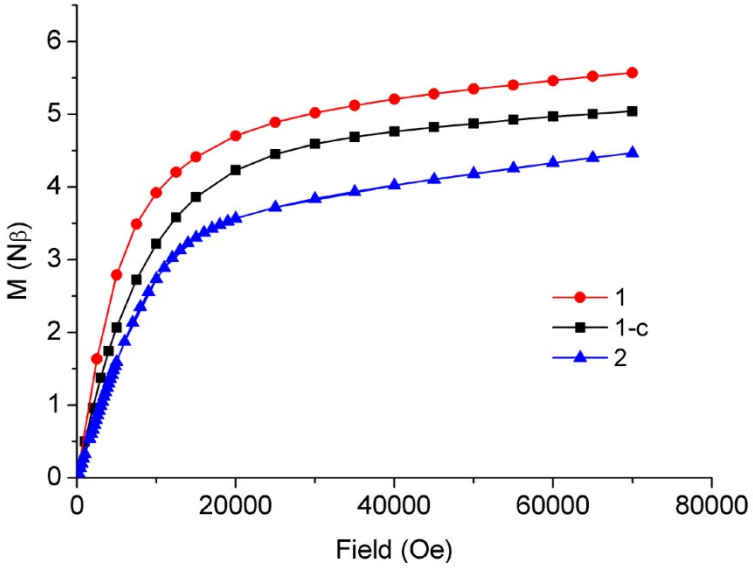


Fig. S8 M-H curve for (a) **1**; (b) **1-c** and (c) **2** at 2.00 K.

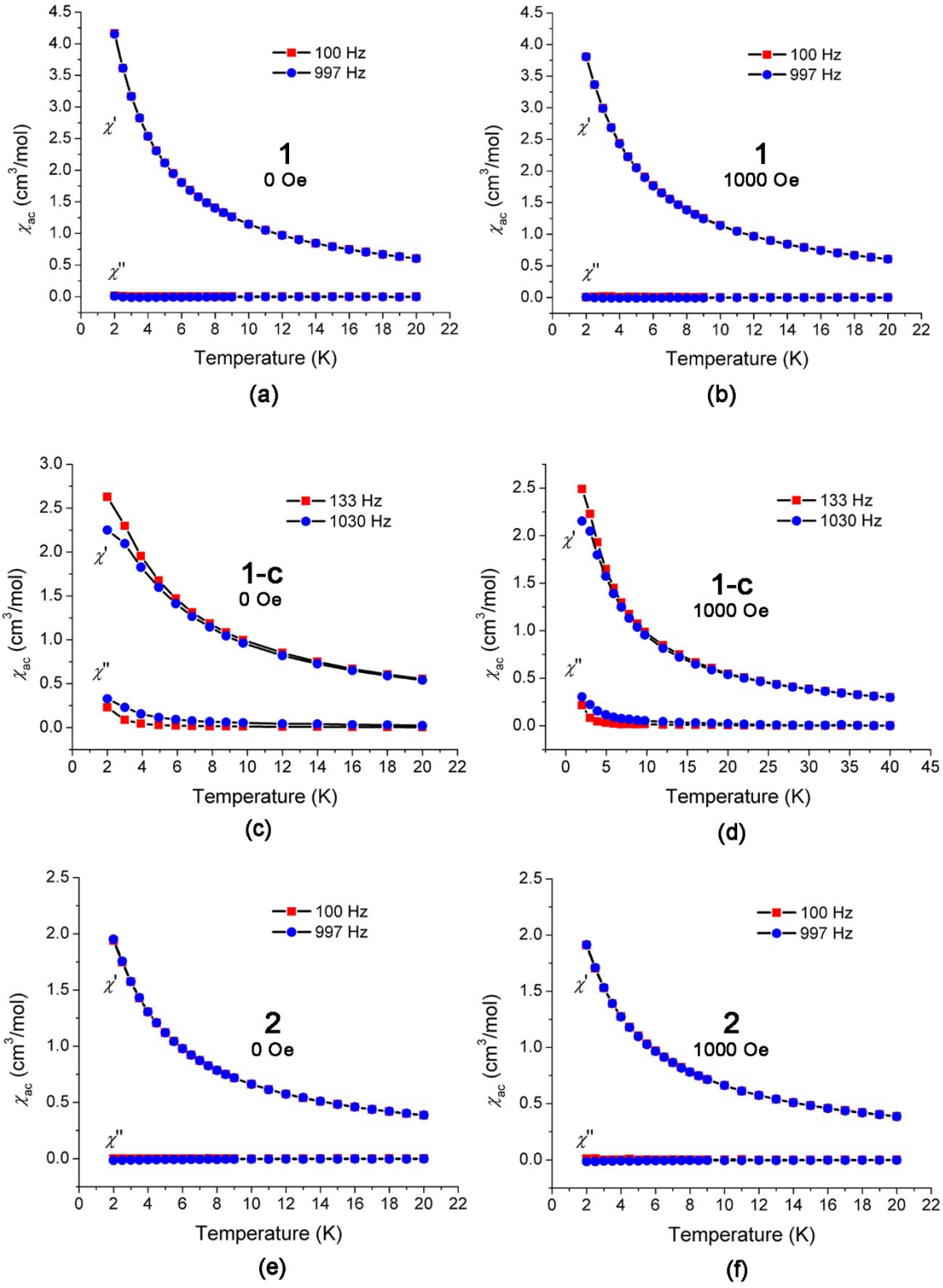


Fig. S9 Temperature-dependent in-phase (χ'_M) (up) and out-of-phase (χ''_M) (down) ac susceptibility components at different frequencies for complex **1** ((a) and (b)), **1-c** ((c) and (d)) and **2** ((e) and (f)) with applied dc field of 0 Oe (left) and 1000 Oe (right). The solid lines join the data points.

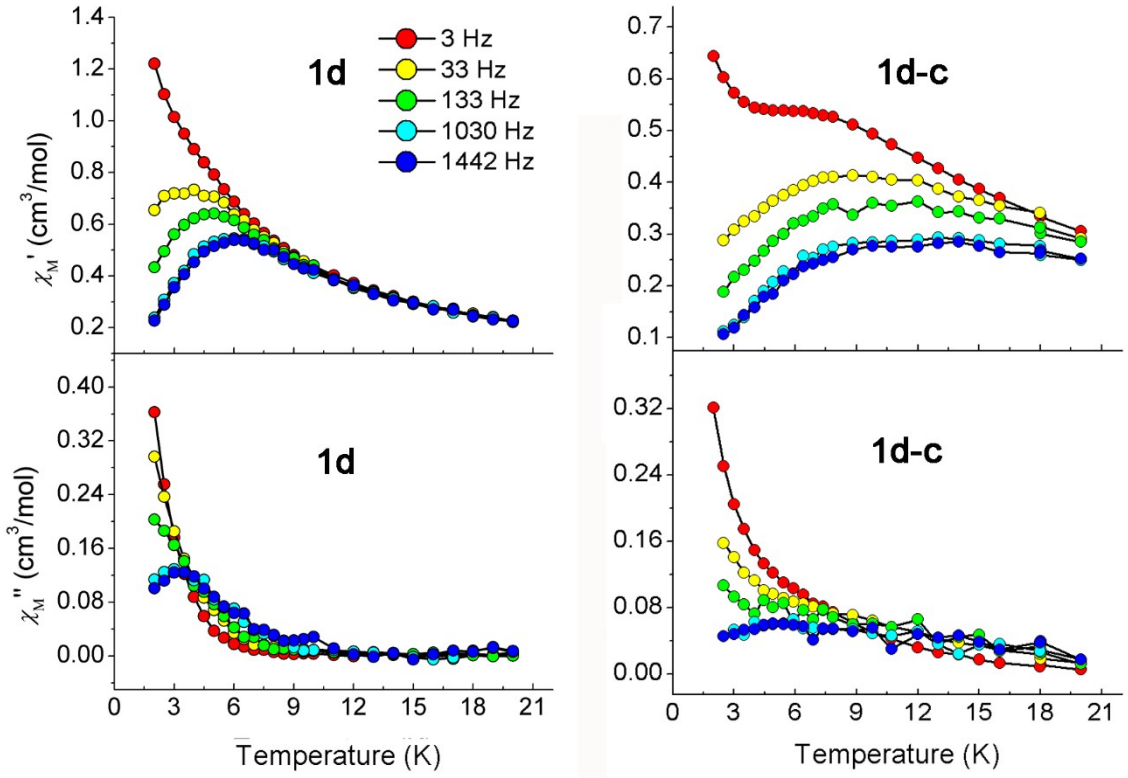


Fig. S10 Temperature dependent in-phase (χ'_M) (up) and out-of-phase (χ''_M) (down) ac susceptibility components at different frequencies for the diluted sample **1d** (with Dy/Y = 1/440) and the corresponding calcined sample **1d-c** with 500 Oe applied dc field. The solid lines join the data points.

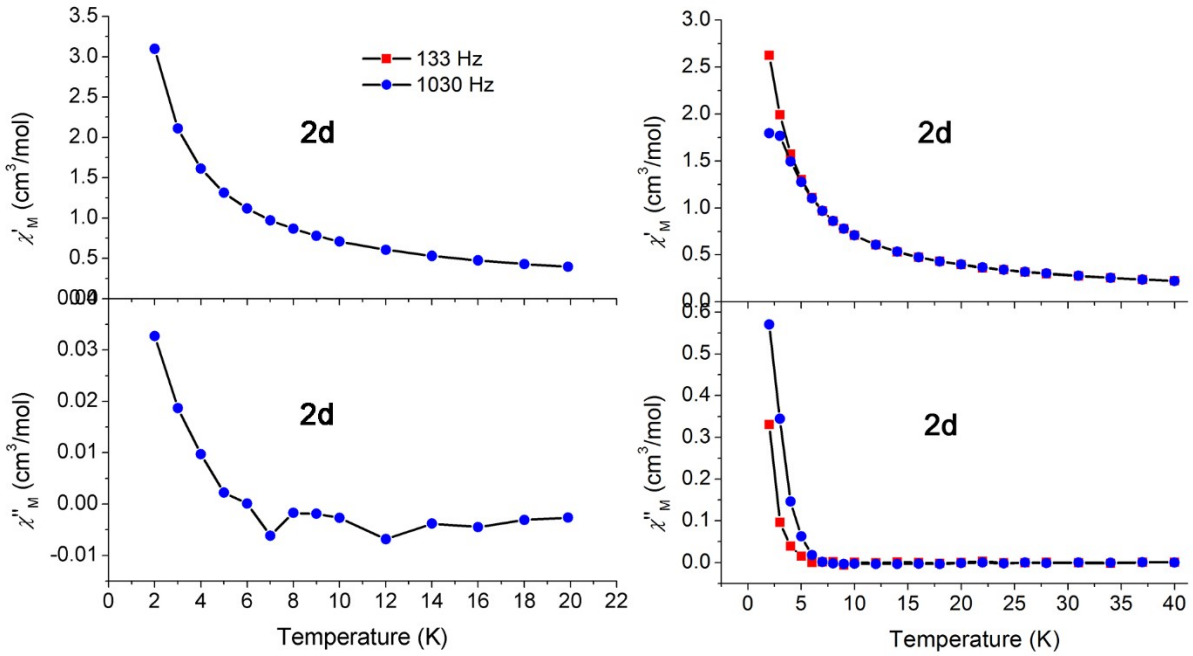


Fig. S11 Temperature dependent in-phase (χ'_M) (up) and out-of-phase (χ''_M) (down) AC susceptibility components at different frequencies for the diluted sample **2d** (with Er/Y = 1/15) with applied DC field of 0 Oe (left) and 1000 Oe (right). The solid lines join the data points. Ac in the presence of a small external dc field of 1000 Oe show the presence of an out-of-phase signal, χ'', for **2d** in contrast with **2**.