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Article

Cyano-bridged Dy(III) and Ho(III) complexes with square-wave structure of the chains

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Table S1. *SHAPE*[*] analysis.

Complex	Polyhedra [ML9]						
	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	
DyCr (**1**)	31.792	23.894	17.057	14.958	7.933	6.846	
DyFe (**2**)	31.867	23.816	17.270	14.612	8.077	7.029	
HoCr (**3**)	31.927	23.935	17.080	14.956	7.994	6.899	
HoFe (**4**)	31.877	23.752	17.382	14.747	8.292	7.227	
Dy [ref. 19]	32.388	23.609	16.548	15.736	7.880	6.716	
Ho [ref. 19]	32.527	23.615	16.593	15.750	7.913	6.751	
	JCSAPR-9	**CSAPR-9**	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
DyCr (**1**)	2.771	**1.986**	2.473	2.040	12.687	7.861	2.152
DyFe (**2**)	2.655	**1.861**	2.377	1.933	12.915	8.222	2.118
HoCr (**3**)	2.717	**1.937**	2.435	1.974	12.764	7.942	2.119
HoFe (**4**)	2.607	**1.808**	2.366	1.919	12.839	8.261	2.068
Dy [ref. 19]	2.342	1.470	3.009	2.475	11.924	8.343	***1.417***
Ho [ref. 19]	2.290	1.419	2.997	2.439	11.931	8.423	***1.370***

EP-9 – Enneagon (D_{9h}); OPY-9 - Octagonal pyramid (C_{8v}); HBPY-9 - Heptagonal bipyramid (D_{7h}); JTC-9 - Johnson triangular cupola (C_{3v}); JCCU-9 - Capped cube (C_{4v}); CCU-9 - Spherical-relaxed capped cube (C_{4v}); JCSAPR-9 - Capped square antiprism (C_{4v}); **CSAPR-9 - Spherical capped square antiprism (C_{4v})**; JTCTPR-9 - Tricapped trigonal prism (D_{3h}); TCTPR-9 - Spherical tricapped trigonal prism (D_{3h}); JTDIC-9 - Tridiminished icosahedron (C_{3v}); HH-9 - Hula-hoop (C_{2v}); ***MFF-9 - Muffin (C_s)***

[*] [M. Llunell, D. Casanova, J. Cirera, P. Alemany, S. Alvarez, 'SHAPE: Program for the Stereochemical Analysis of Molecular Fragments by Means of Continuous Shape Measures and Associated Tools', Version 2.1, 2013, Barcelona]

Capped square antiprism (C_{4v})

Muffin (C_s)

Tricapped trigonal prism (D_{3h})

Table S2. Hydrogen bond geometry in DyCr complex **1**.

D	H	A	Symmetry code for A	D-H, Å	H…A, Å	D…A, Å	D-H…A, º
O3	H3wa	N14	x, y+1, z	0.76(2)	1.97(2)	2.722(2)	170(2)
O3	H3wb	N15	2-x, y+1/2, 1/2-z	0.76(2)	2.09(2)	2.843(2)	170(2)
O4	H4wa	O5	x, y, z	0.77(1)	1.98(1)	2.754 (2)	175(2)
O4	H4wb	O5	-x+1, -y+1, -z	0.80(1)	2.07(1)	2.859(2)	171(2)
N1	H1a	O6	-x+2, -y+1, -z	0.86(2)	2.12(2)	2.944(2)	161(2)
N1	H1b	O6	x, y, z	0.83(2)	2.15(2)	2.954(2)	162(2)
N2	H2a	N16	-x+1, -y+1, -z	0.85(2)	2.17(2)	3.007(2)	167(2)
N3	H3	N14	2-x, y+1/2, 1/2-z	0.80(2)	2.64(2)	3.380(2)	154(2)
O5	H5wa	N16	-x+1, -y+1, -z	0.79(1)	2.24(1)	3.037(2)	178(2)
O5	H5wb	N17	1-x, y+1/2, 1/2-z	0.78(1)	2.36(2)	3.098(2)	158(2)
O6	H6wa	O7	x, -y+1/2, z-1/2	0.80(1)	1.99(2)	2.767(2)	164(3)
O6	H6wb	N14	2-x, y+1/2, 1/2-z	0.78(1)	2.32(2)	3.061(2)	158(3)
O7	H7wa	N17	x, y, z	0.79(1)	2.13(2)	2.914(2)	170(3)
O7	H7wb	N15	x, -y+1/2, z-1/2	0.77(1)	2.15(2)	2.915(2)	171(3)
C3	H3b	O7	x, y, z	0.98	2.61	3.462(2)	145.4
C6	H6	O7	x, y, z	0.95	2.63	3.584(2)	177.7
C8	H8	O2	x, -y+3/2, z+1/2	0.95	2.61	3.5339(18)	163.6

Table S3. Hydrogen bond geometry in DyFe complex **2**.

D	H	A	Symmetry code for A	D-H, Å	H…A, Å	D…A, Å	D-H…A, º
O3	H3wa	N14	x, y+1, z	0.77(3)	2.03(6)	2.743(9)	153(11)
O3	H3wb	N15	2-x, y+1/2, 1/2-z	0.78(3)	2.09(4)	2.864(9)	176(10)
O4	H4wa	O5	x, y, z	0.78(3)	1.97(4)	2.728(8)	164(10)
O4	H4wb	O5	-x+1, -y+1, -z	0.78(3)	2.10(4)	2.866(10)	166(10)
N1	H1a	O6	-x+2, -y+1, -z	0.79(4)	2.22(6)	2.928(11)	149(10)
N1	H1b	O6	x, y, z	0.79(4)	2.22(6)	2.923(10)	148(10)
N2	H2a	N16	-x+1, -y+1, -z	0.79(4)	2.28(4)	3.060(12)	177(10)
N3	H3	N14	2-x, y+1/2, 1/2-z	0.78(4)	2.64(5)	3.365(10)	155(9)
N4	H4	N12	1-x, y+1/2, 1/2-z	0.78(4)	2.63(7)	3.230(9)	134(8)
N4	H4	N13	1-x, y+1/2, 1/2-z	0.78(4)	2.60(6)	3.311(10)	151(8)
O5	H5wa	N16	-x+1, -y+1, -z	0.78(3)	2.21(4)	2.988(10)	175(10)
O5	H5wb	N17	1-x, y+1/2, 1/2-z	0.78(3)	2.42(8)	3.058(11)	140(11)
O6	H6wa	O7	x, -y+1/2, z-1/2	0.78(3)	2.00(5)	2.756(11)	163(12)
O6	H6wb	N14	2-x, y+1/2, 1/2-z	0.78(3)	2.32(6)	3.044(12)	154(12)
O7	H7wa	N17	x, y, z	0.78(4)	2.21(6)	2.938(11)	157(12)
O7	H7wb	N15	x, -y+1/2, z-1/2	0.78(4)	2.14(4)	2.911(12)	172(12)
C3	H3b	O7	x, y, z	0.98	2.57	3.440(12)	147.3
C6	H6	O7	x, y, z	0.95	2.55	3.500(12)	178.0
C8	H8	O2	x, -y+3/2, z+1/2	0.95	2.54	3.464(11)	163.7

Table S4. Hydrogen bond geometry in HoCr complex **3**.

D	H	A	Symmetry code for A	D-H, Å	H…A, Å	D…A, Å	D-H…A, º
O3	H3wa	N14	x, y+1, z	0.80(2)	1.932(15)	2.729(2)	173(3)
O3	H3wb	N15	2-x, y+1/2, 1/2-z	0.79(2)	2.069(16)	2.846(2)	167(3
O4	H4wa	O5	x, y, z	0.78(2)	1.978(15)	2.760(2)	176(3)
O4	H4wb	O5	-x+1, -y+1, -z	0.79(2)	2.084(15)	2.875(2)	174(3)
N1	H1a	O6	-x+2, -y+1, -z	0.83(3)	2.13(3)	2.941(3)	165(3)
N1	H1b	O6	x, y, z	0.85(3)	2.15(3)	2.963(3)	160(3)
N2	H2a	N16	-x+1, -y+1, -z	0.80(3)	2.21(3)	3.002(3)	169(3)
N3	H3	N14	2-x, y+1/2, 1/2-z	0.84(2)	2.64(3)	3.389(3)	149(2)
N4	H4	N12	1-x, y+1/2, 1/2-z	0.86(3)	2.66(3)	3.332(2)	137(2)
O5	H5wa	N16	-x+1, -y+1, -z	0.80(2)	2.249(16)	3.045(3)	176(3)
O5	H5wb	N17	1-x, y+1/2, 1/2-z	0.79(2)	2.351(18)	3.105(3)	160(3)
O6	H6wa	O7	x, -y+1/2, z-1/2	0.80(2)	2.010(19)	2.772(3)	158(3)
O6	H6wb	N14	2-x, y+1/2, 1/2-z	0.80(2)	2.294(19)	3.063(3)	163(4
O7	H7wa	N17	x, y, z	0.81(2)	2.109(17)	2.910(3)	170(3)
O7	H7wb	N15	x, -y+1/2, z-1/2	0.80(2)	2.124(17)	2.921(3)	171(3)
C3	H3b	O7	x, y, z	0.98	2.61	3.465(3)	145.2
C6	H6	O7	x, y, z	0.95	2.63	3.583(3)	177.2
C8	H8	O2	x, -y+3/2, z+1/2	0.95	2.62	3.538(2)	163.9

Table S5. Hydrogen bond geometry in HoFe complex **4**.

D	H	A	Symmetry code for A	D-H, Å	H…A, Å	D…A, Å	D-H…A, º
O3	H3wa	N14	x, y+1, z	0.83(2)	1.93(3)	2.742(6)	166(6)
O3	H3wb	N15	2-x, y+1/2, 1/2-z	0.82(2)	2.12(3)	2.904(7)	159(6)
O4	H4wa	O5	x, y, z	0.80	1.99	2.784(6)	170.6
O4	H4wb	O5	-x+1, -y+1, -z	0.82(2)	2.06(2)	2.868(5)	169(6)
N1	H1a	O6	-x+2, -y+1, -z	0.87(3)	2.19(5)	2.977(9)	151(8)
N1	H1b	O6	x, y, z	0.87(3)	2.15(4)	2.966(10)	155(7)
N2	H2a	N16	-x+1, -y+1, -z	0.86(3)	2.30(4)	3.110(8)	157(6)
N3	H3	N14	2-x, y+1/2, 1/2-z	0.88(4)	2.62(5)	3.373(8)	144(5)
N4	H4	N12	1-x, y+1/2, 1/2-z	0.85(4)	2.46(4)	3.252(6)	154(5)
O5	H5wa	N16	-x+1, -y+1, -z	0.82(2)	2.24(3)	3.038(7)	163(8)
O5	H5wb	N17	1-x, y+1/2, 1/2-z	0.82(2)	2.30(4)	3.040(7)	150(5)
O6	H6wa	O7	x, -y+1/2, z-1/2	0.82(2)	1.99(4)	2.785(10)	165(10)
O6	H6wb	N14	2-x, y+1/2, 1/2-z	0.82(2)	2.30(3)	3.102(9)	167(11)
O7	H7wa	N17	x, y, z	0.82(2)	2.16(3)	2.973(9)	171(8)
O7	H7wb	N15	x, -y+1/2, z-1/2	0.83(2)	2.12(3)	2.911(8)	160(9)
C6	H6	O7	x, y, z	0.93	2.64	3.565(9)	179.0
C8	H8	O2	x, -y+3/2, z+1/2	0.93	2.62	3.506(7)	160.5

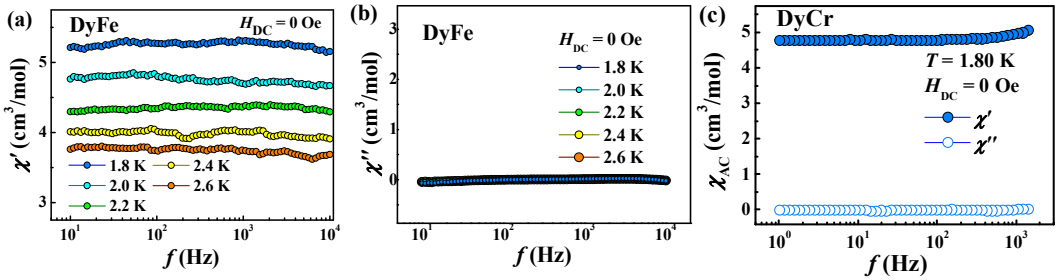

Figure S1. Real and imaginary parts of ac magnetic susceptibility for the **1** (DyCr) and **2** (DyFe) complexes, measured without an externally applied magnetic field.

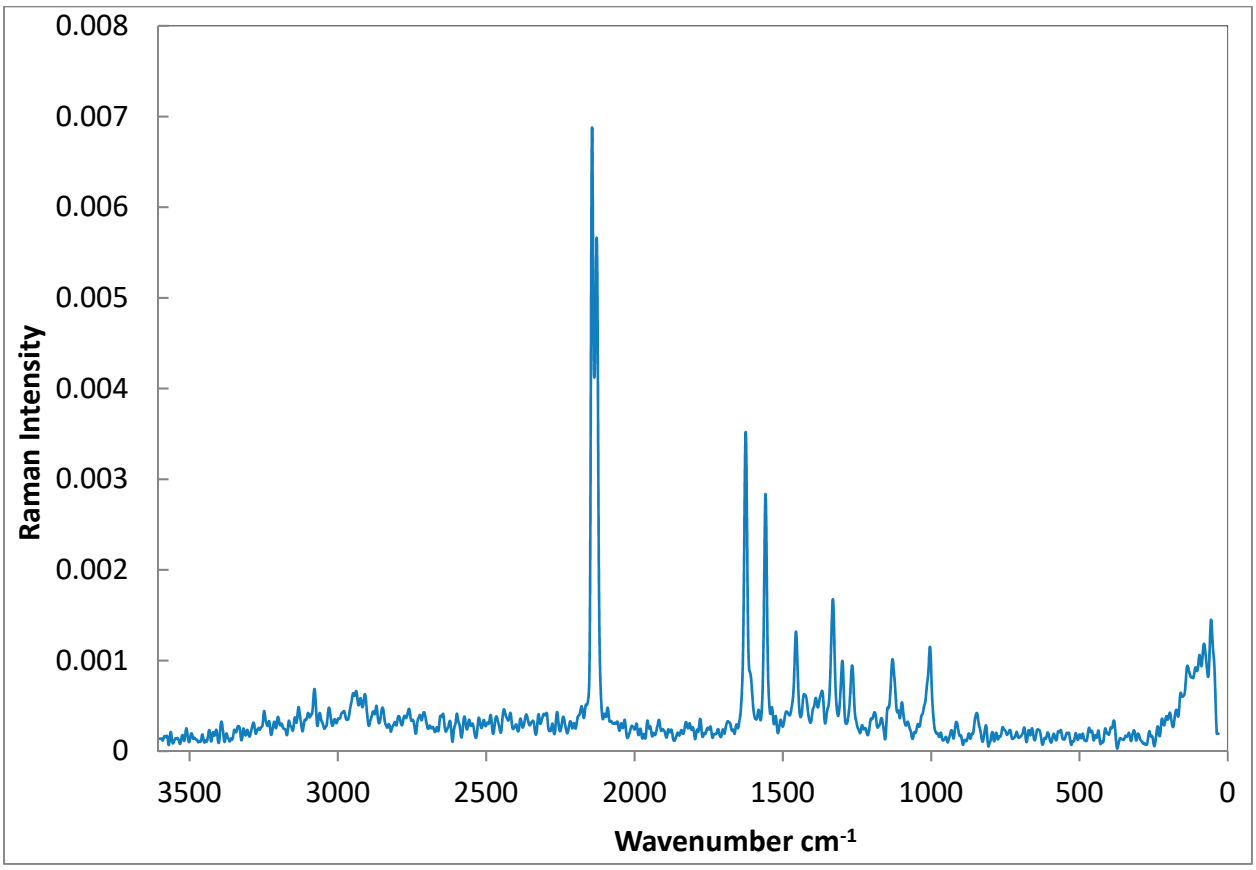

Figure S2. Raman spectrum of the complex **2** (DyFe).

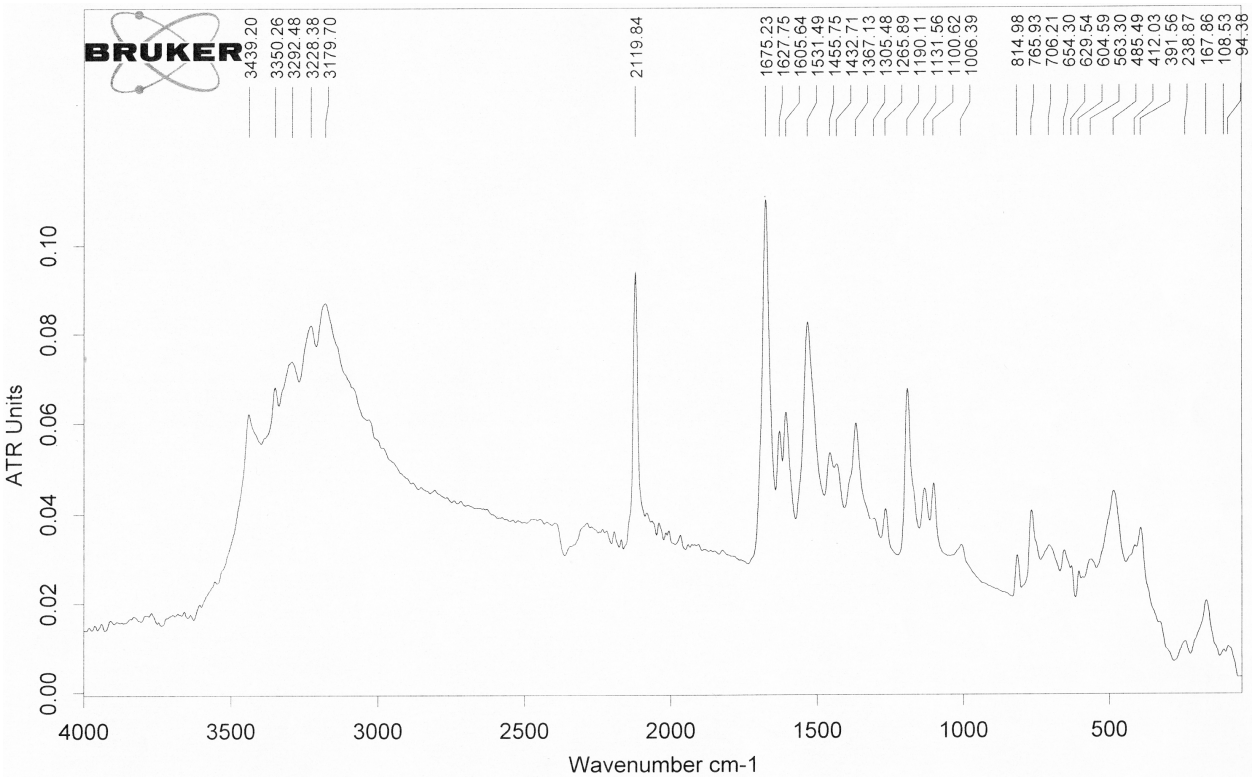

Figure S3. IR spectrum of the complex **2** (DyFe).

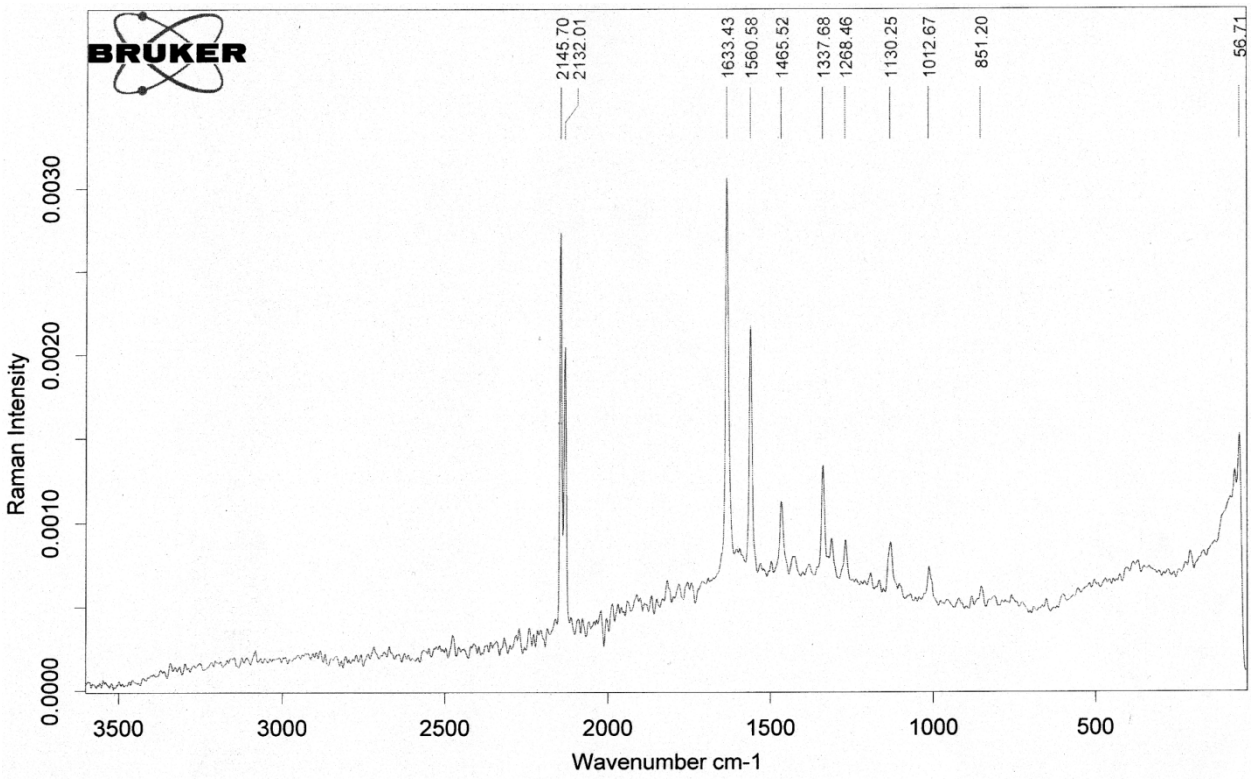

Figure S4. Raman spectrum of the complex **3** (HoCr).

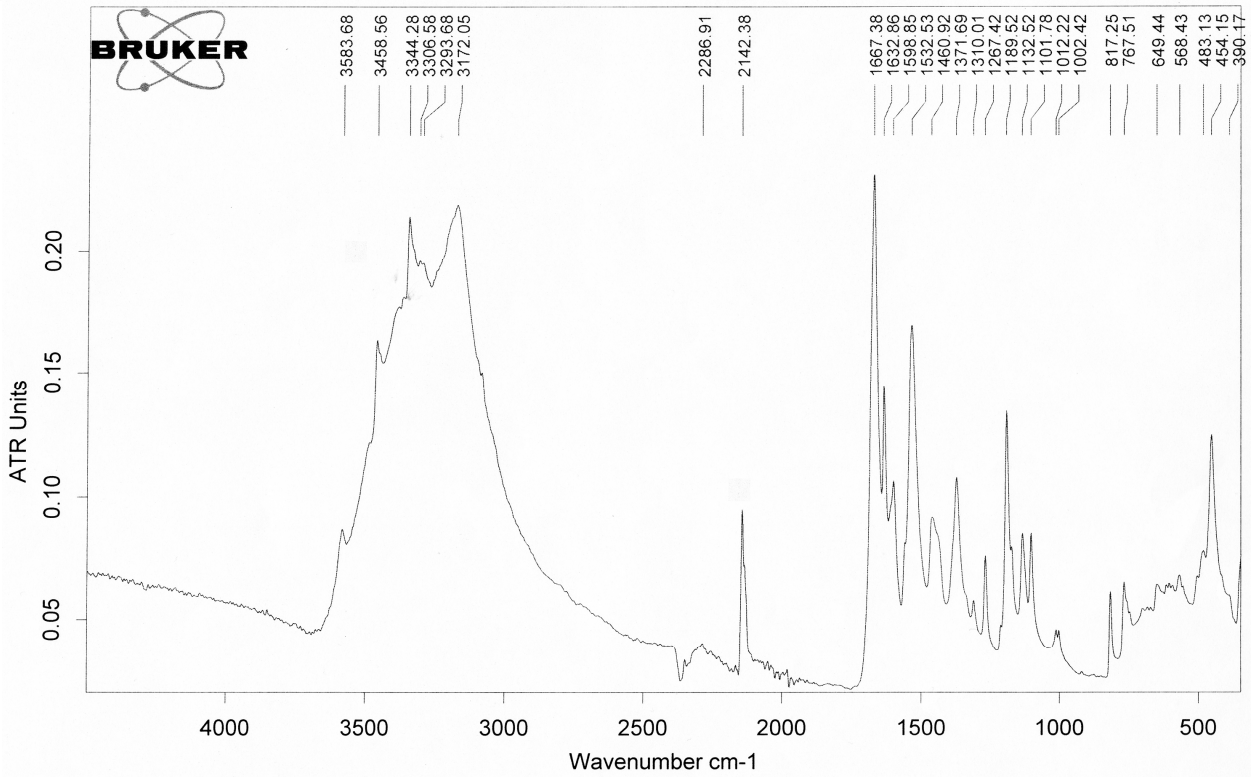

Figure S5. IR spectrum of the complex **3** (HoCr).

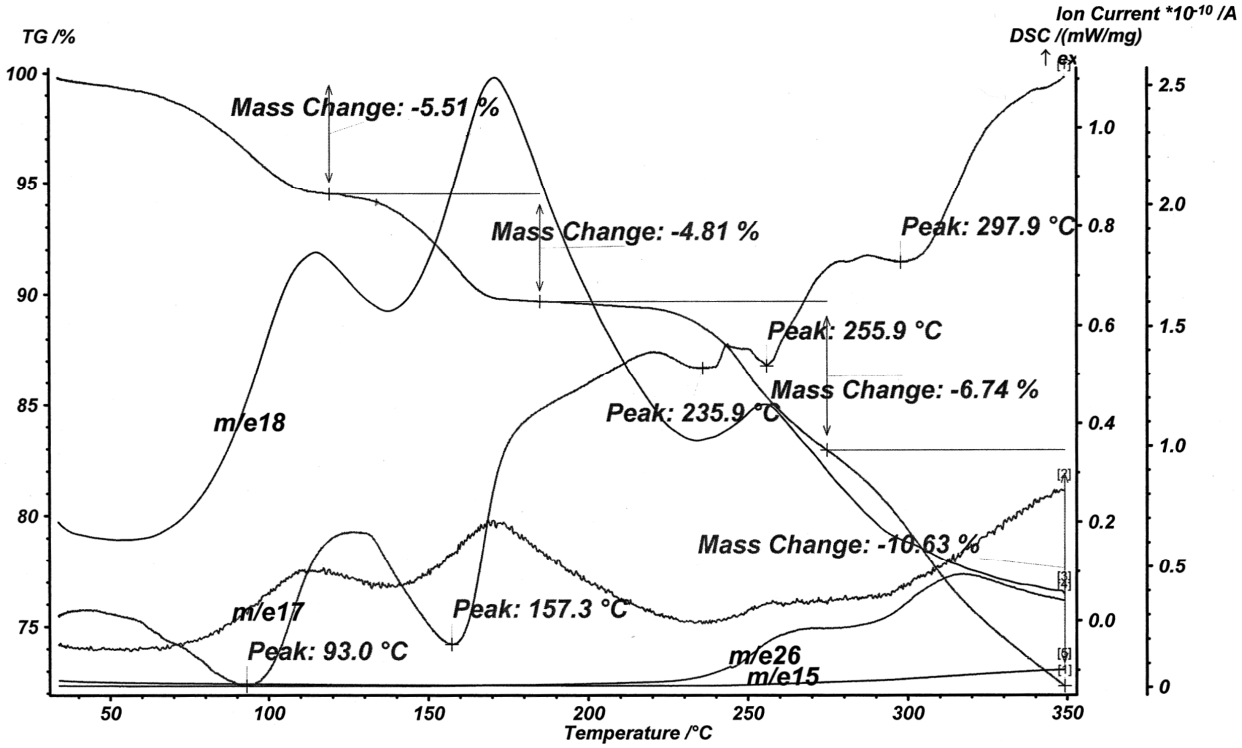

Figure S6. TG-DSC curves and mass spectra for complex **3** (HoCr) after drying in vacuum.

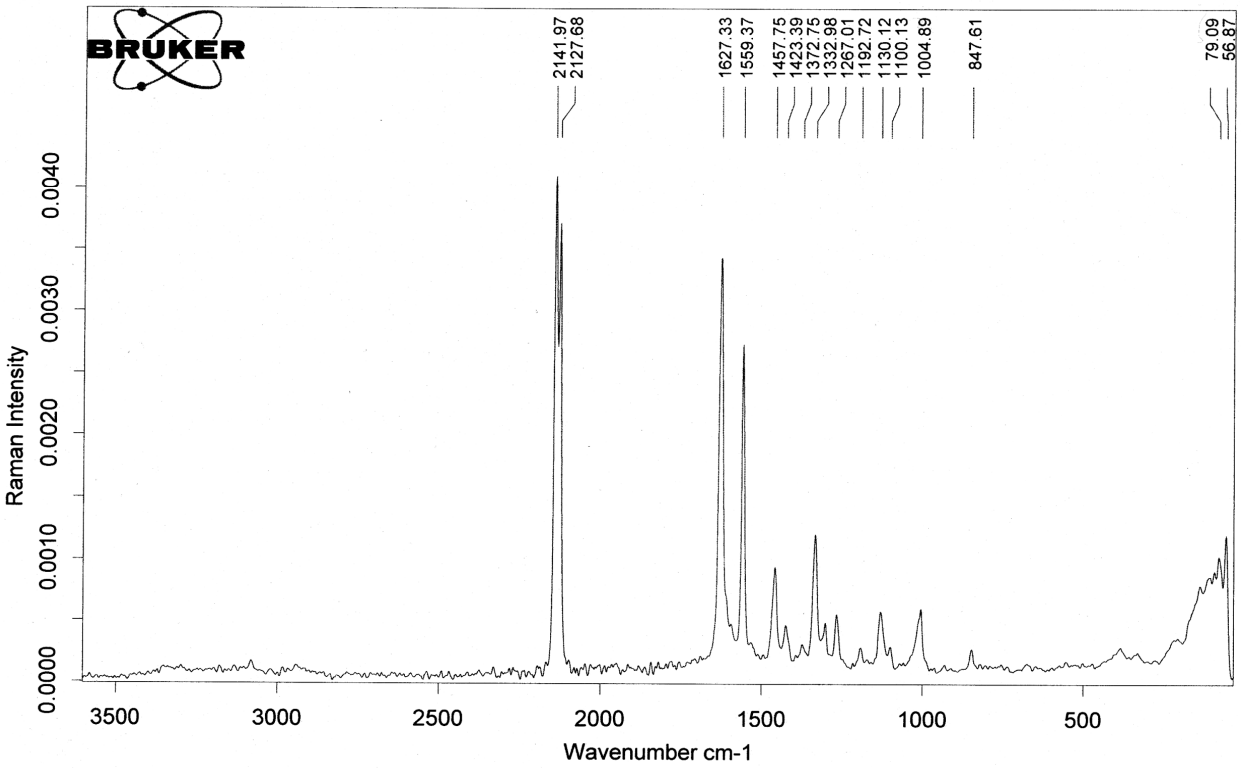

Figure S7. Raman spectrum of the complex **4** (HoFe).

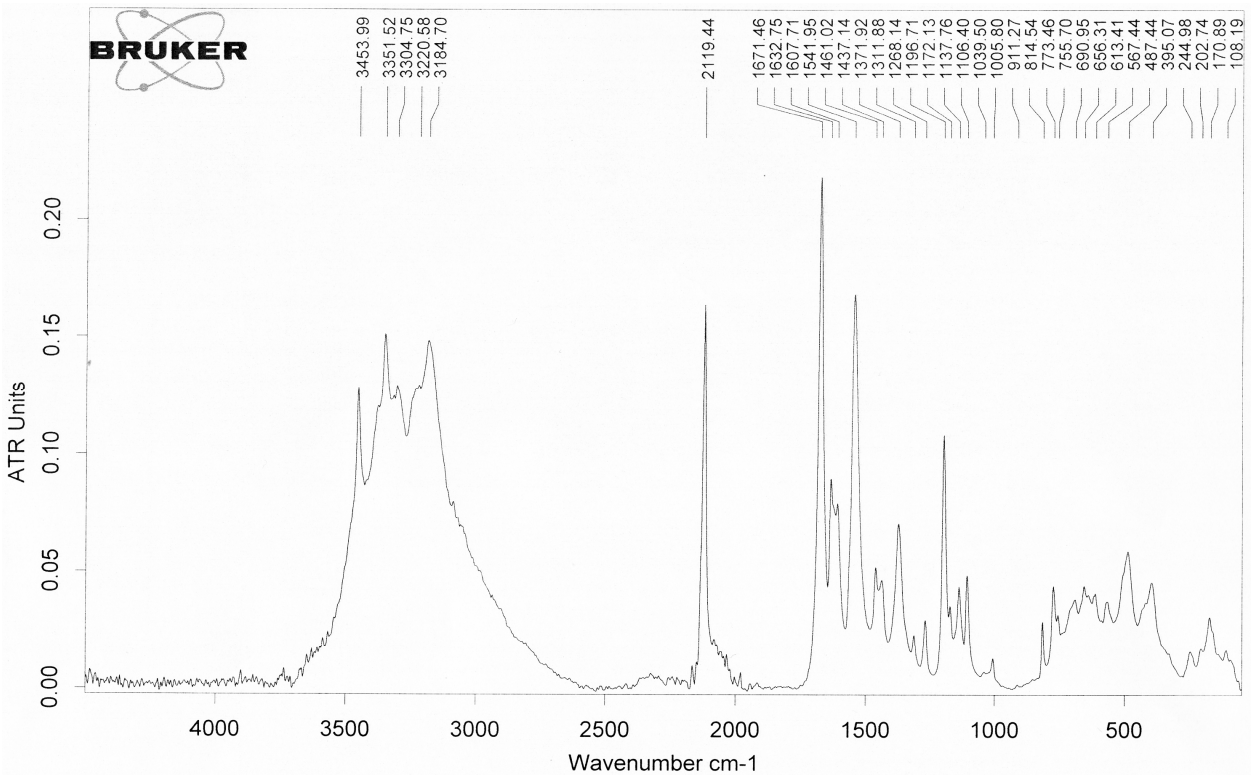

Figure S8. IR spectrum of the complex **4** (HoFe).

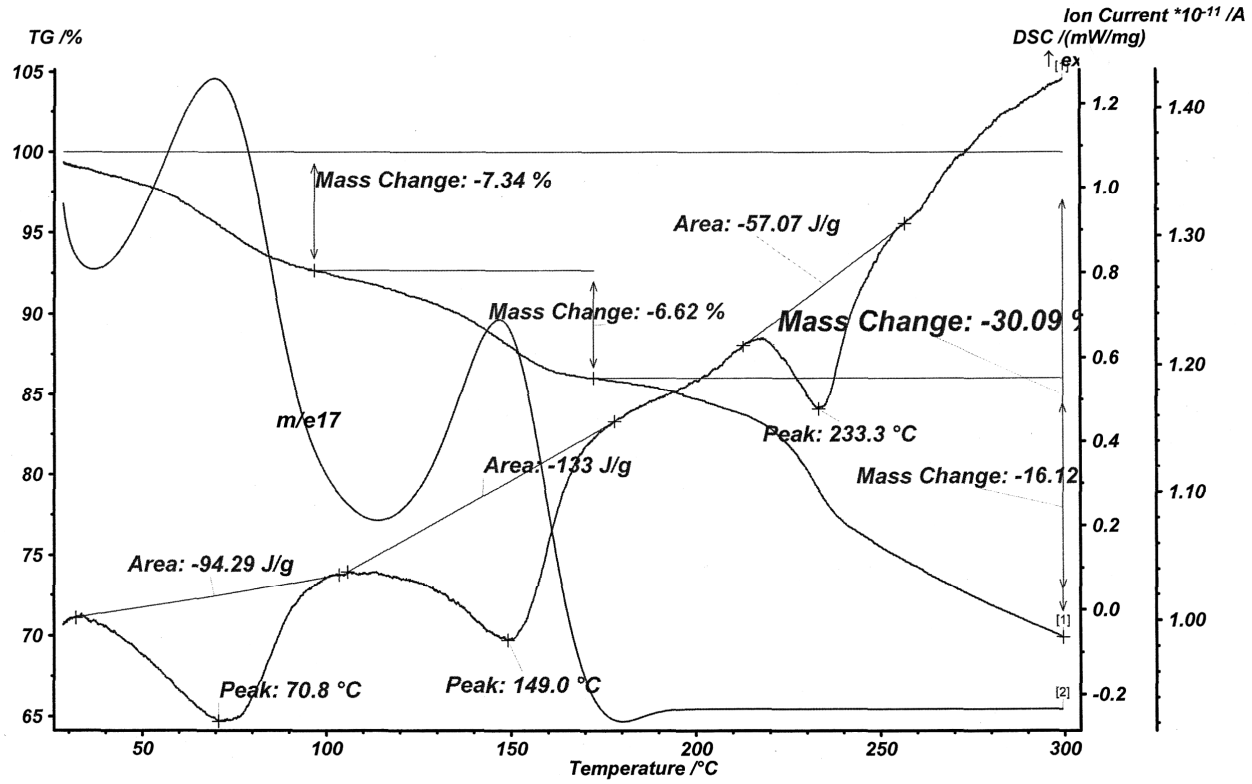

Figure S9. TG-DSC curves and mass spectra for complex **4** (HoFe) after drying in vacuum.