Synthesis and Magnetochemistry of Heterometallic Triangular $Fe^{III}_2Ln^{III}$ (Ln = La, Gd, Tb, Dy, and Ho) and $Fe^{III}_2Y^{III}$ Complexes

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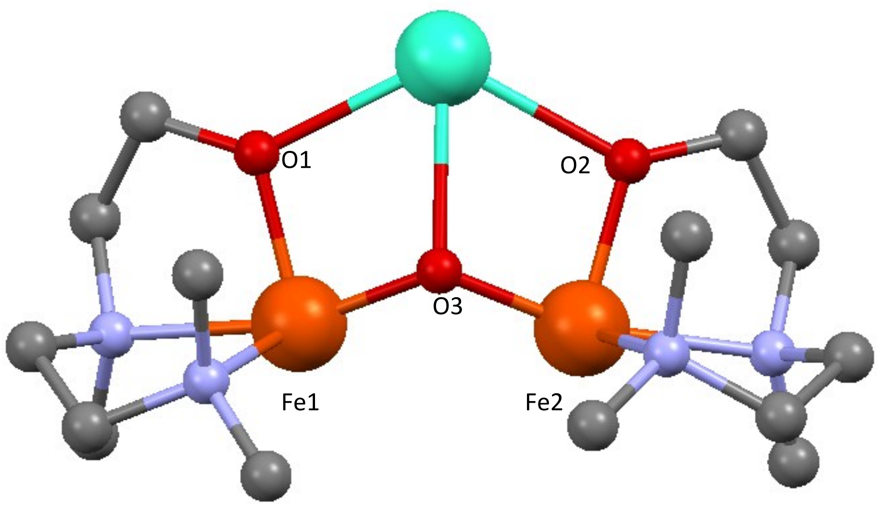

Figure S1. Structure of Fe_2LnO core. Ln^{III} green, Fe^{III} orange, N blue, O, red and C grey.

Table S1. Some important bond distances in Angstroms (Å)

Ln	Ln-O1/O2	Ln-O3	Ln-Fe1/Fe2	Fe1-O1	Fe2-O2	Fe1/Fe2-O3	Fe1-Fe2
La	2.499/2.475	2.534	3.483/3.471	1.950	1.965	1.837/1.836	3.191
Gd	2.408/2.377	2.446	3.412/3.401	1.956	1.964	1.834/1.838	3.188
Tb	2.348/2.385	2.432	3.381/3.398	1.965	1.949	1.828/1.832	3.174
Dy	2.376/2.338	2.416	3.389/3.376	1.941	1.965	1.836/1.832	3.177
Ho	2.376/2.340	2.412	3.390/3.374	1.949	1.967	1.836/1.830	3.177
Y	2.334/2.364	2.402	3.366/3.377	1.966	1.947	1.825/1.830	3.168

Table S2. Some important bond angles in degrees (º)

Ln	Ln-Fe1-Ln	Ln-Fe2-Ln	Ln-O3-Fe1	Ln-O3-Fe2
La	62.50	62.87	104.52	104.02
Gd	61.92	62.29	104.81	104.19
Tb	62.35	61.81	104.13	104.78
Dy	61.77	62.20	104.89	104.40
Ho	61.73	62.24	1045.06	104.52
Y	62.14	61.81	104.74	105.07

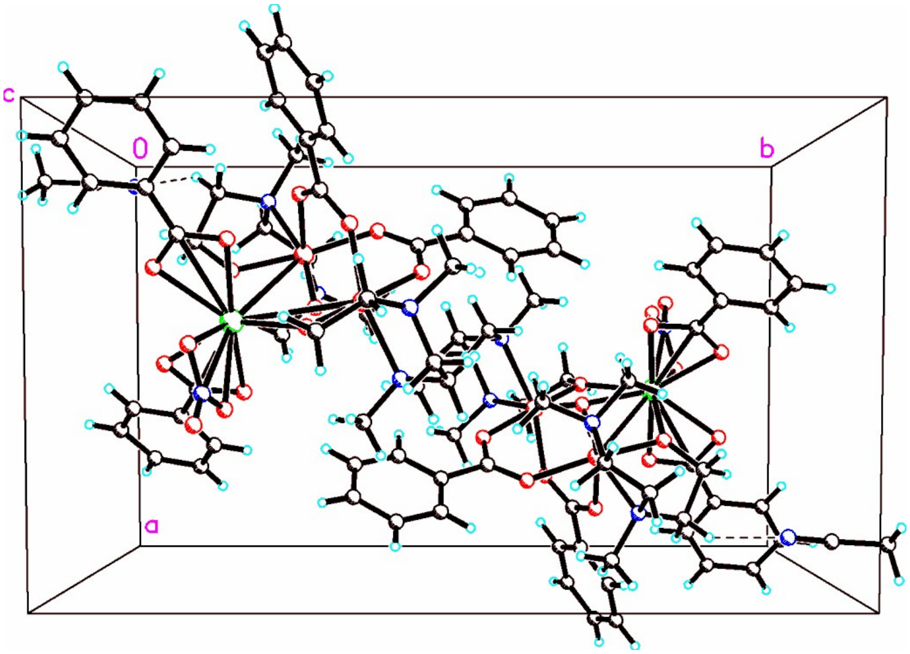

Figure S2. Molecular packing in unit cell.

Table S3. N---H bond distance in Angstroms (Å). (Hydrogen bond between acetonitrile 'N' and dmem CH_2)

Ln	**N---H bond distance**
La	3.816
Gd	3.788
Tb	3.807
Dy	3.833
Ho	3.842
Y	3.841

Table S4. Coupling constant (J) values for Fe cluster with structural parameters.

S. No.	Molecular Formula	Fe-μ-O (Å)	Fe-μ-O-Fe (°)	J (cm^{-1})	Ref .
1	$[Fe_3O(O_2CBu^t)_2(N_3)_3(dmem)_2]$	1.8716(19)/1.8647(19)	162.82(11)	-45.9	1
2	$[Fe_2CaO(O_2CCl_3)_6(THF)_4]$.THF	1.827(1)	124.09	-58.9	2
3	$[Fe_2SrO(O_2CCl_3)_6(THF)_6]$.0.5THF	--	--	-75.4	2
4	$[Fe_2BaO(O_2CCl_3)_6(THF)_6]$.0.5THF0.5$H_2O$	1.816(3)	123.55	-60.40	2
5	$[Fe_3O(TIEO)_2(O_2CPh)_2Cl_3]$ (Isosceles)	1.862(7)/1.867(7)	159.1(3)	-55.0(6)	3
6	$[Fe_2Gd_2(O)(OH)(TBC[4])_2(dmf)_4(MeOH)_2(H_2O)_2]Cl$	1.87	144.7	-85.0	4
7	$[Fe_2MgO(O_2CCH_3)_6(Py)_3]$	1.890(3)	120	-62(3)	5
8	$[Fe_2MnO(O_2CCH_3)_6(Py)_3]$	1.867(2)/1.862(2)	122.85	-64(3)	5
9	$[Fe_2NiO(O_2CCH_3)_6(Py)_3]$	--	--	-73(3)	5
10	$[Fe_2NiO(O_2CCH_3)_6(H_2O)_3]$	1.875/1.891	119.8	-71(3)	5
11	$[Fe_3Gd(\mu_3\text{-}O)_2(CCl_3CO_2)_8(H_2O)(THF)_3]$	~1.8	~125	-35	6
12	$[Fe_3Y(\mu_3\text{-}O)_2(CCl_3CO_2)_8(H_2O)(THF)_3]$	~1.8	~125	-35	6
13	$[Fe_3Lu(\mu_3\text{-}O)_2(CCl_3CO_2)_8(H_2O)(THF)_3]$	~1.8	~125	-35	6
14	$[Fe_3O(Etsao)(benz)_5(MeOH)_2$	1.887	120.65	-38	7
15	$[Fe_3O(Etsao)(benz)_5(MeOH)_2$	1.905	122.65	-29.3	7

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