Supporting Information

## Synthesis, Structures, and Magnetic Properties of Three 3d-4f [Na<sub>2</sub>Fe<sup>III</sup><sub>6</sub>Dy<sup>III</sup><sub>2</sub>] Complexes: Effect of Organic Ligands on the Connection of Inorganic Subunits

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Dy(1)-O(8)	2.312(5)	Fe(4)-O(11)	1.943(6)
Dy(1)-O(3)	2.320(5)	Fe(4)-O(36)	1.972(6)
Dy(1)-O(29)	2.329(6)	Fe(4)-N(11)	1.987(7)
Dy(1)-O(27)	2.333(5)	Fe(4)-O(12)	2.025(6)
Dy(1)-O(25)	2.355(5)	Fe(4)-N(3)	2.097(8)
Dy(1)-O(22)	2.366(6)	Fe(4)-O(34)	2.113(5)
Dy(1)-O(23)	2.414(5)	Fe(5)-O(16)	1.927(7)
Dy(1)-O(24)	2.580(6)	Fe(5)-N(14)	1.979(15)
Dy(2)-O(30)	2.277(6)	Fe(5)-O(36)	2.002(6)
Dy(2)-O(18)	2.285(6)	Fe(5)-N(14')	2.00(3)
Dy(2)-O(26)	2.298(7)	Fe(5)-O(17)	2.017(7)
Dy(2)-O(28)	2.309(6)	Fe(5)-N(4)	2.121(8)
Dy(2)-O(13)	2.316(5)	Fe(5)-O(34)	2.141(5)
Dy(2)-O(24)	2.352(6)	Fe(6)-O(18)	1.941(5)
Dy(2)-O(31)	2.370(7)	Fe(6)-O(13)	1.950(6)
Fe(1)-O(1)	1.932(6)	Fe(6)-O(17)	1.972(7)
Fe(1)-N(5)	1.978(8)	Fe(6)-O(32)	2.001(6)
Fe(1)-O(35)	1.997(6)	Fe(6)-O(12)	2.009(5)
Fe(1)-O(2)	2.013(6)	Fe(6)-O(34)	2.102(5)
Fe(1)-O(33)	2.121(5)	Na(1)-O(37)	2.277(8)
Fe(1)-N(1)	2.136(7)	Na(1)-O(6)	2.372(7)
Fe(2)-O(6)	1.926(6)	Na(1)-O(1)	2.378(6)
Fe(2)-N(8)	1.993(9)	Na(1)-O(10)	2.379(8)
Fe(2)-O(35)	1.998(6)	Na(1)-O(5)	2.399(8)
Fe(2)-O(7)	1.999(6)	Na(1)-O(35)	2.870(7)
Fe(2)-O(33)	2.130(5)	Na(2)-O(38')	2.231(19)
Fe(2)-N(2)	2.142(7)	Na(2)-O(16)	2.338(6)
Fe(3)-O(8)	1.939(5)	Na(2)-O(11)	2.349 (7)
Fe(3)-O(3)	1.947(5)	Na(2)-O(38)	2.35(2)
Fe(3)-O(2)	1.989(5)	Na(2)-O(20)	2.411(7)
Fe(3)-O(21)	2.000(6)	Na(2)-O(15)	2.475(7)
Fe(3)-O(7)	2.007(5)	Na(2)-O(36)	2.809(7)
Fe(3)-O(33)	2.098(6)		

Table S1. Selected bond lengths (Å) for complex 1

Dy(1)-O(12)	2.284(6)	Fe(2)-O(11)	2.022(8)	
Dy(1)-O(15)#1	2.305(6)	Fe(2)-N(7)	2.130(9)	
Dy(1)-O(6)	2.331(5)	Fe(2)-O(10)	2.142(6)	
Dy(1)-O(3)	2.334(6)	Fe(3)-O(5)	1.942(8)	
Dy(1)-O(13)#1	2.337(6)	Fe(3)-N(6)	1.988(11)	
Dy(1)-O(14)	2.345(6)	Fe(3)-O(7)	2.019(6)	
Dy(1)-O(17)	2.380(6)	Fe(3)-O(11)	2.021(8)	
Fe(1)-O(3)	1.954(6)	Fe(3)-N(8)	2.124(9)	
Fe(1)-O(6)	1.977(6)	Fe(3)-O(10)	2.126(6)	
Fe(1)-O(7)	2.001(6)	Na(1)-O(9)	2.29(4)	
Fe(1)-O(2)	2.008(6)	Na(1)-O(5)	2.370(12)	
Fe(1)-O(16)	2.011(6)	Na(1)-O(1)	2.409(13)	
Fe(1)-O(10)	2.104(6)	Na(1)-O(4)	2.442(16)	
Fe(2)-O(1)	1.936(8)	Na(1)-O(8)	2.461(16)	
Fe(2)-O(2)	2.009(6)	Na(1)-O(11)	2.732(9)	
Fe(2)-N(1)	2.017(12)			

Table S2. Selected bond lengths (Å) for complex  $\mathbf{2}$ 

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+1

Dy(1)-O(15)	2.167(5)	Fe(2)-O(6)	2.071(5)	
Dy(1)-O(16)#1	2.236(5)	Fe(2)-O(9)	2.143(5)	
Dy(1)-O(7)	2.314(5)	Fe(2)-N(2)	2.152(7)	
Dy(1)-O(3)	2.335(4)	Fe(3)-O(3)	1.909(5)	
Dy(1)-O(12)	2.352(5)	Fe(3)-O(6)	1.990(5)	
Dy(1)-O(14)#1	2.418(7)	Fe(3)-O(11)	1.992(5)	
Dy(1)-O(13)	2.460(6)	Fe(3)-O(7)	2.007(5)	
Fe(1)-O(1)	1.861(6)	Fe(3)-O(2)	2.056(5)	
Fe(1)-O(2)	2.001(5)	Fe(3)-O(9)	2.130(5)	
Fe(1)-O(10)	2.046(7)	Na(1)-O(4)	2.261(9)	
Fe(1)-N(3)	2.063(8)	Na(1)-N(5)#2	2.349(11)	
Fe(1)-N(1)	2.153(7)	Na(1)-O(5)	2.370(8)	
Fe(1)-O(9)	2.184(5)	Na(1)-O(1)	2.561(9)	
Fe(2)-N(6)	1.927(11)	Na(1)-O(8)	2.617(10)	
Fe(2)-O(5)	1.948(6)	Na(1)-O(10)	2.691(7)	
Fe(2)-O(10)	2.043(6)			

Table S3. Selected bond lengths (Å) for complex 3

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+1 #2 x,-y+3/2,z+1/2

Y(1)-O(12)	2.271(5)	Fe(2)-O(11)	2.016(5)	
Y(1)-O(15)	2.283(4)	Fe(2)-N(7)	2.124(5)	
Y(1)-O(13)	2.308(4)	Fe(2)-O(10)	2.151(4)	
Y(1)-O(6)	2.313(4)	Fe(3)-N(6)	1.986(6)	
Y(1)-O(3)	2.326(4)	Fe(3)-O(5)	1.938(5)	
Y(1)-O(14)	2.331(4)	Fe(3)-O(7)	2.013(4)	
Y(1)-O(17)	2.356(4)	Fe(3)-O(11)	2.014(5)	
Fe(1)-O(3)	1.948(4)	Fe(3)-N(8)	2.119(6)	
Fe(1)-O(6)	1.976(4)	Fe(3)-O(10)	2.121(4)	
Fe(1)-O(2)	2.003(4)	Na(1)-O(9)	2.45(3)	
Fe(1)-O(7)	2.001(4)	Na(1)-O(1)	2.418(7)	
Fe(1)-O(10)	2.094(4)	Na(1)-O(5)	2.380(7)	
Fe(1)-O(16)	2.016(4)	Na(1)-O(4)	2.452(8)	
Fe(2)-O(1)	1.926(5)	Na(1)-O(8)	2.457(9)	
Fe(2)-N(1)	2.006(8)	Na(1)-O(11)	2.696(6)	
Fe(2)-O(2)	2.006(4)			

Table S4. Selected bond lengths (Å) for complex 4

**Table S5.** Selected bond lengths (Å) for complex 5

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Gd(1)-O(15)	2.316(4)	Fe(2)-O(9)	2.016(6)	
Gd(1)-O(7)	2.347(4)	Fe(2)-O(10)	2.119(5)	
Gd(1)-O(16)	2.347(5)	Fe(2)-N(2)	2.119(6)	
Gd(1)-O(3)	2.370(5)	Fe(3)-O(1)	1.933(7)	
Gd(1)-O(17)	2.370(5)	Fe(3)-O(9)	2.007(7)	
Gd(1)-O(14)	2.375(4)	Fe(3)-N(3)	2.010(9)	
Gd(1)-O(13)	2.409(4)	Fe(3)-O(2)	2.007(6)	
Fe(1)-O(3)	1.932(5)	Fe(3)-O(10)	2.129(5)	
Fe(1)-O(7)	1.965(4)	Fe(3)-N(1)	2.137(9)	
Fe(1)-O(6)	1.989(5)	Na(1)-O(11)	2.339(14)	
Fe(1)-O(12)	1.998(5)	Na(1)-O(5)	2.352(8)	
Fe(1)-O(2)	2.017(5)	Na(1)-O(1)	2.414(12)	
Fe(1)-O(10)	2.105(5)	Na(1)-O(8)	2.436(12)	
Fe(2)-O(5)	1.945(6)	Na(1)-O(4)	2.442(15)	
Fe(2)-N(6)	1.951(9)	Na(1)-O(9)	2.705(7)	
Fe(2)-O(6)	2.020(5)			



Scheme S1. Schiff base ligand  $H_3L$ <sup>"</sup>.



**Fig.S1.** Plots of the temperature dependence of  $\mathbf{x}_{M}^{-1}$  for **1** at 1000 Oe. The red line is a simulation of the experimental data.



**Fig.S2.** Plots of the temperature dependence of  $\mathbf{x}_{M}^{-1}$  for **2** at 1000 Oe. The red line is a simulation of the experimental data.



**Fig.S3.** Plots of the temperature dependence of  $\chi_{M}^{-1}$  for **3** at 1000 Oe. The red line is a simulation of the experimental data.



**Fig.S4.** Plots of the temperature dependence of  $\chi_{M}^{-1}$  for **4** at 1000 Oe. The red line is a simulation of the experimental data.



**Fig.S5.** Plots of the temperature dependence of  $\chi_{M}^{-1}$  for **5** at 1000 Oe. The red line is a simulation of the experimental data.



Fig.S6. Field dependence of the magnetization for compounds 1-5 at 2K.



Figure S7. XRPD pattern for compound 1.



Figure S8. XRPD pattern for compound 2.



Figure S9. XRPD pattern for compound 3.



Figure S10. XRPD pattern for compound 4.



Figure S11. XRPD pattern for compound 5.