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Supporting Information

Observation of Current Rectification by the Bimetallic Iron(III) Hydrophobe $[Fe^{III}_2(L^{N4O6})]$ on Au|LB-Molecule|Au Devices

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Figure S1. Mass spectrum for $[Fe^{III}_2(L^{N4O6})]$ (**1**). Left: in bulk mass spectrum with experimental (bars) and simulated (line) isotopic distribution. Right: Mass spectrum from $[Fe^{III}_2(L^{N4O6})]$ **(1)** recovered (scraped) from LB films. Both spectra show the same distinctive envelope, confirming that the deposited species has retained its molecular identity.

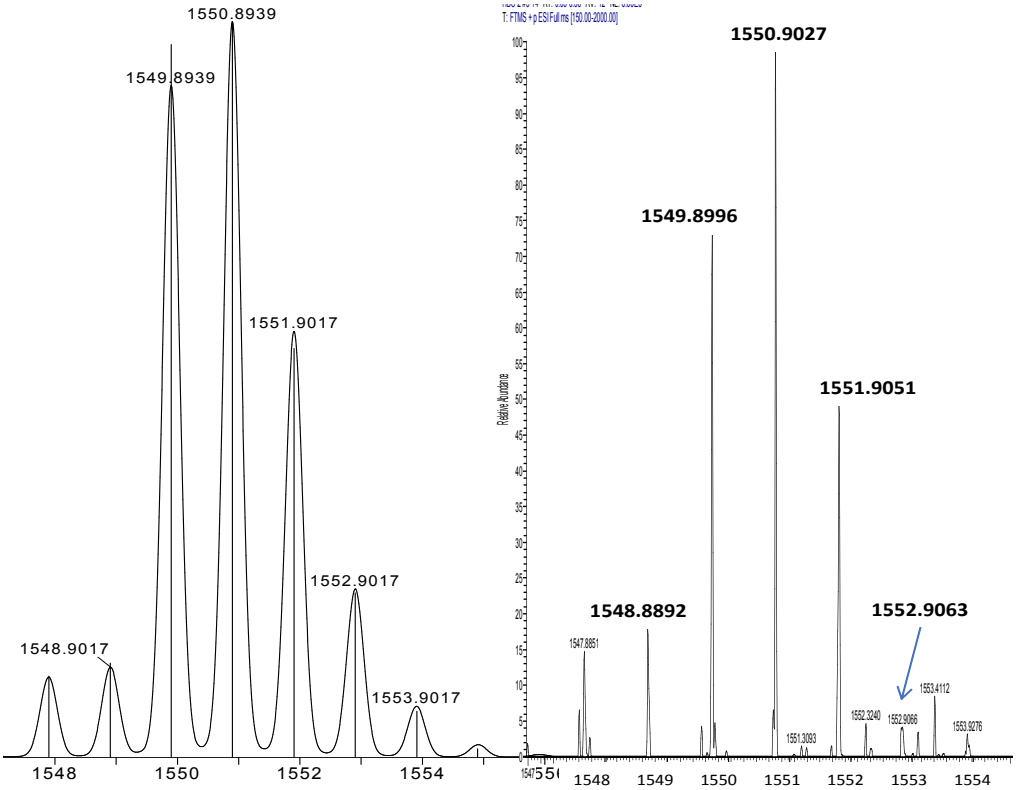


Figure S2. Formula and mass spectrum for $[Ga^{III}_2(L^{N4O6})]$ (**2**).

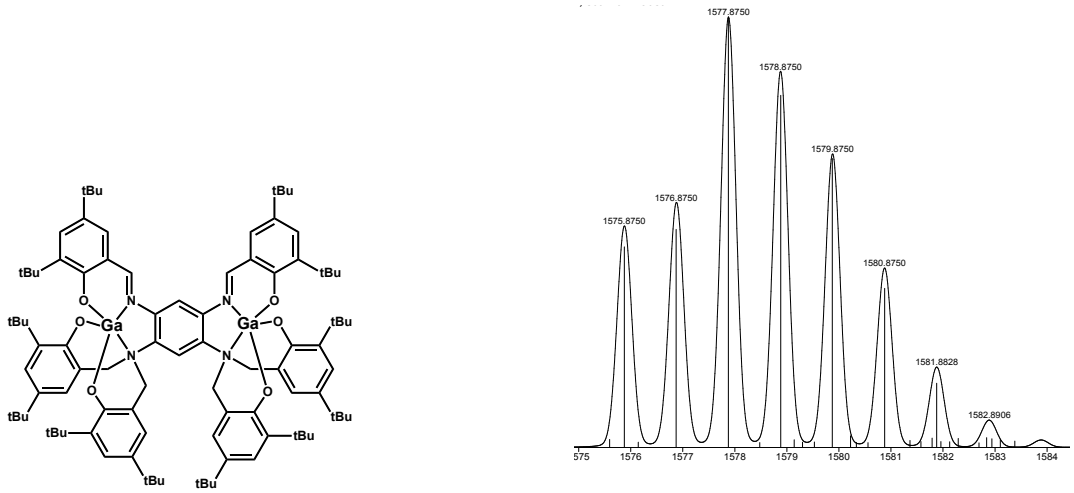
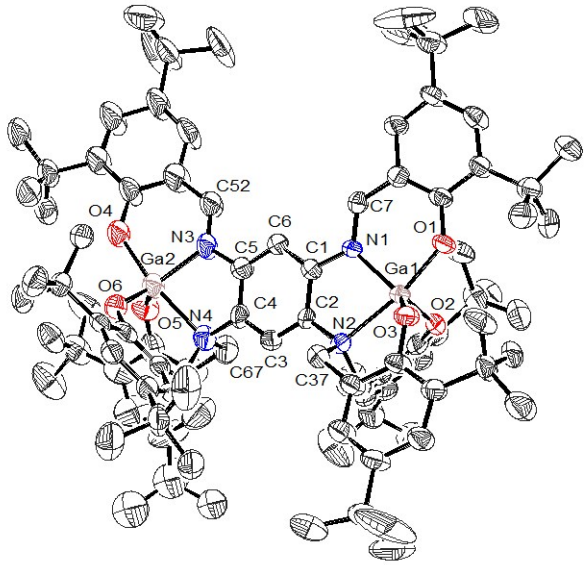


Figure S3. Crystal structure and selected bond lengths (Å) and angles (°) for [$Ga^{III}_2(L^{N4O6})$] (**2**).



Selected bond lengths (Å) and angles (°)	
O(6)-C(88)	1.367(6)
O(4)-C(58)	1.327(7)
O(2)-C(28)	1.367(6)
O(1)-C(13)	1.303(6)
Ga(1)-O(3)	1.867(4)
Ga(1)-N(1)	1.968(4)
Ga(2)-O(5)	1.825(4)
Ga(2)-N(4)	2.182(5)
N(1)-C(7)	1.314(6)
N(2)-C(22)	1.518(6)
O(2)-Ga(1)-O(3)	117.51(16)
N(1)-Ga(1)-N(2)	81.42(15)
τ_{Ga1}	0.73
τ_{Ga2}	0.81

Figure S4. Comparative electrochemistry for [$Fe^{III}_2(L^{N4O6})$] (**1**) and [$Ga^{III}_2(L^{N4O6})$] (**2**). Conditions: Dichloromethane, glassy carbon; Ag/AgCl; Pt wire; $TBAPF_6$; Scan rate: 100 mV/s, Ferrocene as internal standard.

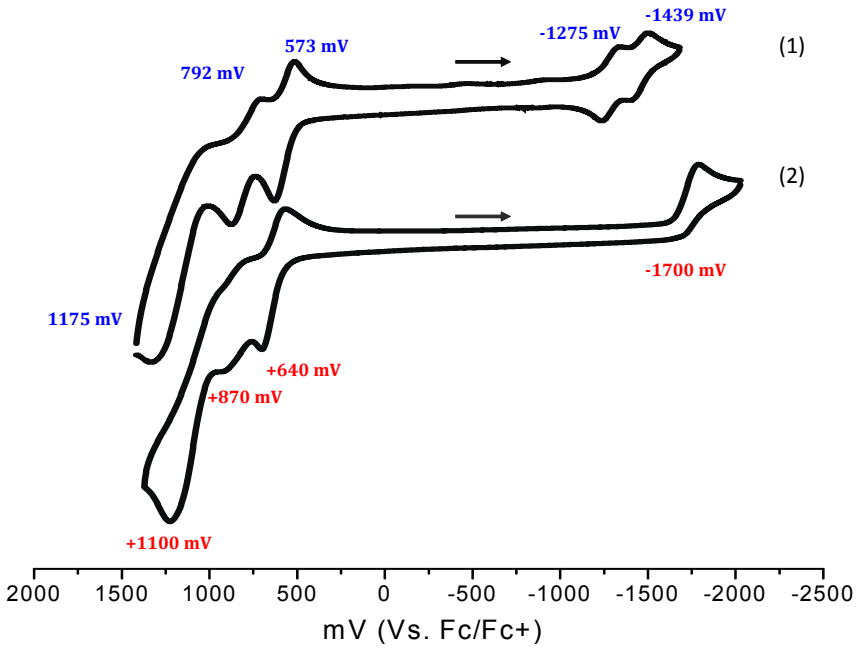


Figure S5. Measurement of $\Delta E_{1/2}$ for calculation of the comproportionation constant.

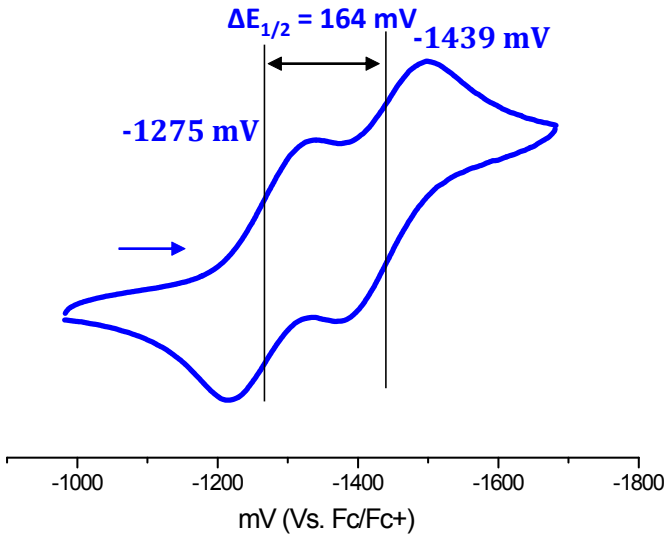


Figure S6. UV-visible spectrum of the $[Fe^{III}_2(L^{N4O6})]$ in dichloromethane.

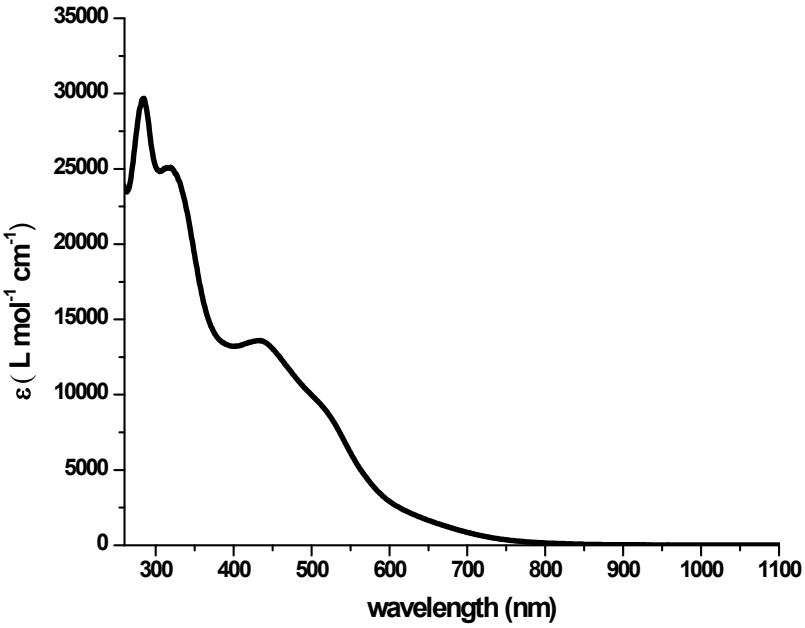


Figure S7. AFM height images of the 9-layer deposited film on quartz substrate for [$Fe^{III}_2(L^{N4O6})$] : (a) 2D view, (b) 3D view, (c) sectional analysis, (d) plot between the thickness (nm) vs. number of layers from monolayer to 9 layers.

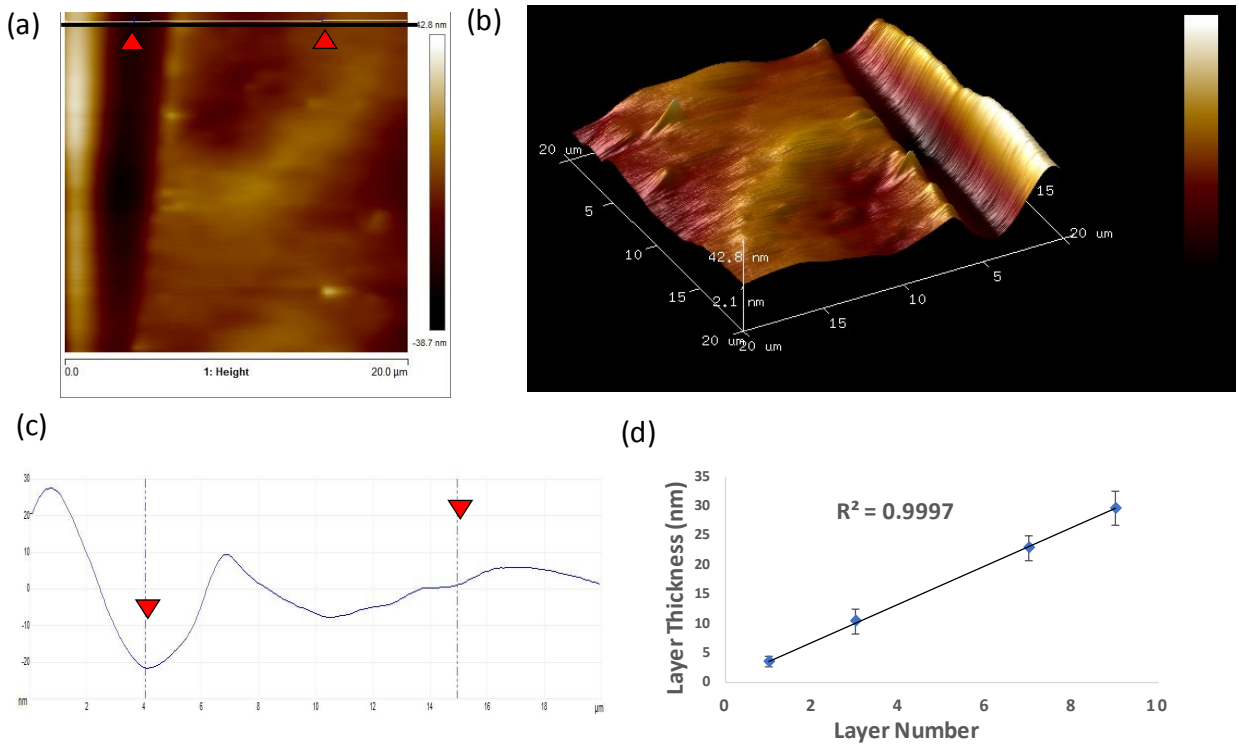


Figure S8. Approximate model for calculation of molecular area. The molecule is considered as roughly cylindrical with a radius $r \approx 8$ Å and height $h \approx 17$ Å, thus yielding a sectional area $2r * h \approx 272$ Å^2.

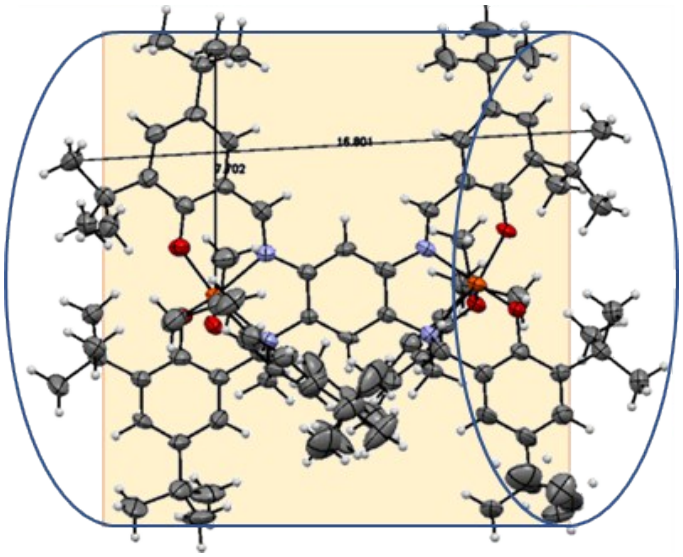


Figure S9. I-V characteristics of [$Fe^{III}_2(L^{N4O6})$] (**1**). (a) from 3.0 to -3.0V; (b) response observed after multiple scans between 4.0 to -4.0V (c) response observed for reversed applied potentials (d) Symmetric response observed after multiple scans.

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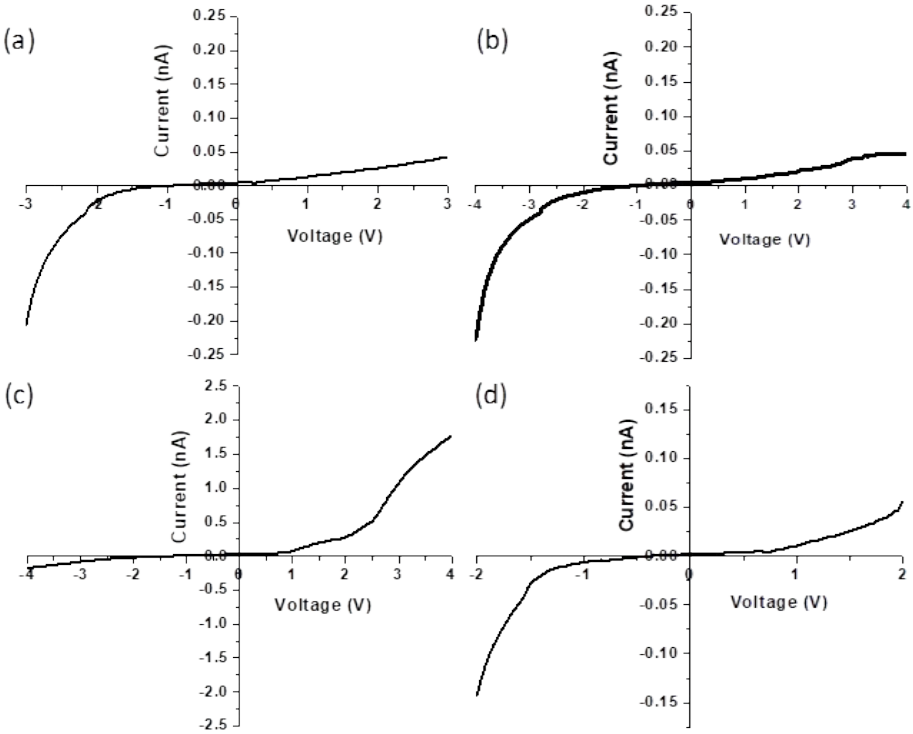


Figure S10. I-V measurements for [Fe^{III}_2(L^{N4O6})] (**1**) in five independent devices.

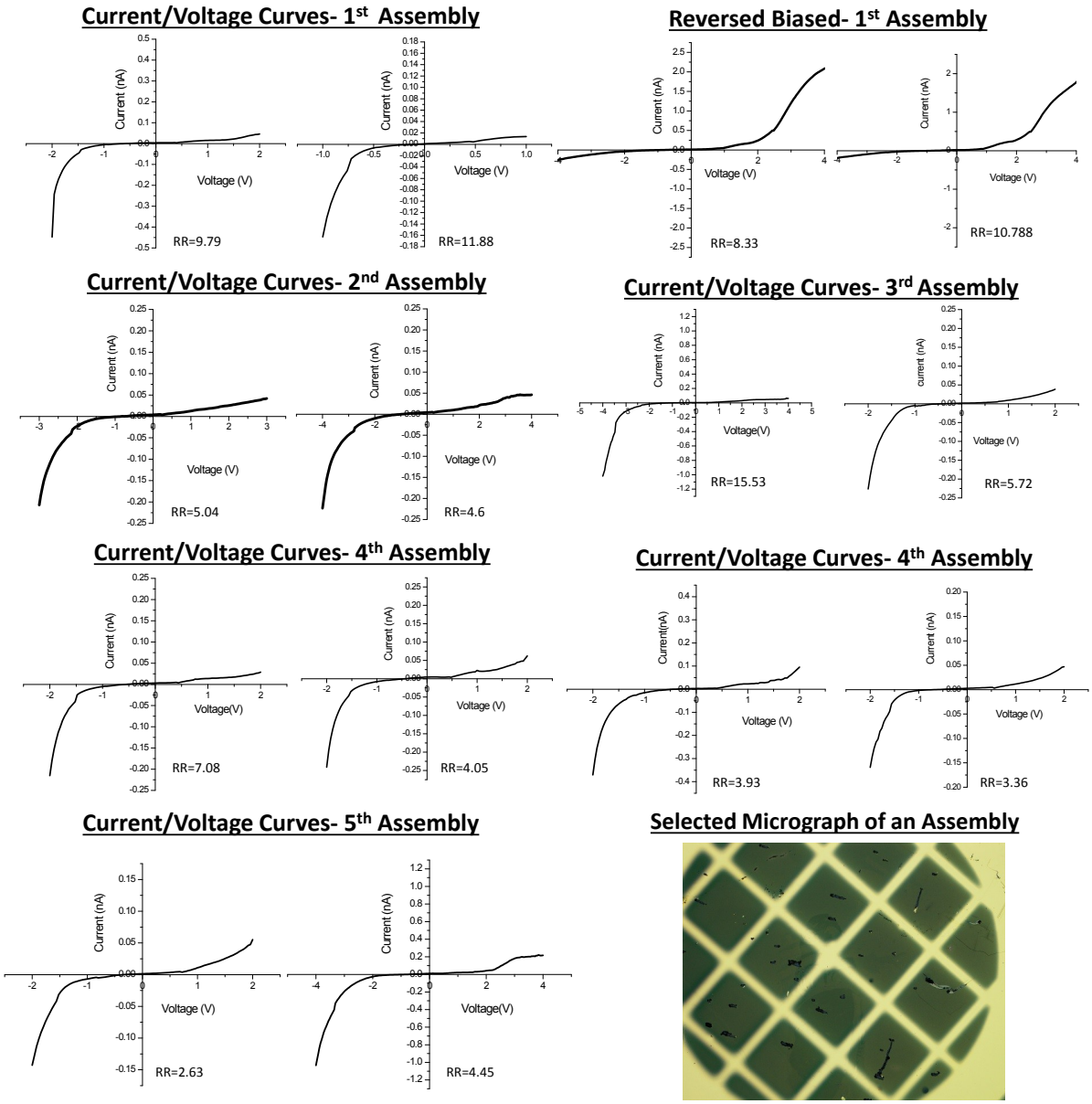
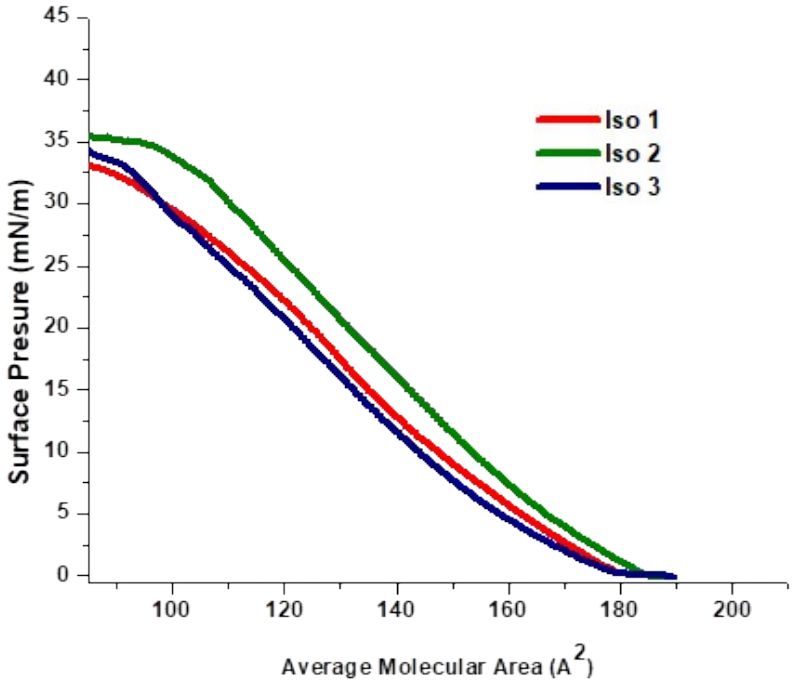


Figure S11. Triplicate measurement of isothermal compressions for [$Fe^{III}_2(L^{N4O6})$] (1), along with transfer ratiosin five independent devices.



Experiment	Transfer ratio
Monolayer 1	1.262
Monolayer 2	1.161
Monolayer 3	1.109
Monolayer 4	1.072
Monolayer 5	1.133

Table T1. Crystal data and structure refinement for $[Fe^{III}_2(L^{N4O6})]$ **(1)**

Identification code	frag
Empirical formula	$C_{96}H_{132}N_4O_6Fe_2$
Formula weight	1549.75
Temperature/K	100.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	19.1511(14)
b/Å	24.2553(16)
c/Å	23.9442(15)
α/°	90.00
β/°	108.925(4)
γ/°	90.00
Volume/Å^3	10521.2(12)
Z	4
ρ_{calc}mg/mm^3	0.978
m/mm^{-1}	0.321
F(000)	3344.0
Crystal size/mm^3	0.46 × 0.32 × 0.23
2Θ range for data collection	2.8 to 56.6°
Index ranges	-25 ≤ h ≤ 24, 0 ≤ k ≤ 32, 0 ≤ l ≤ 31
Reflections collected	25481
Independent reflections	25442[R(int) = 0.0000]
Data/restraints/parameters	25481/0/999
Goodness-of-fit on F^2	0.766
Final R indexes [I>=2σ (I)]	R_1 = 0.0955, wR_2 = 0.2211
Final R indexes [all data]	R_1 = 0.2600, wR_2 = 0.2742
Largest diff. peak/hole / e Å^{-3}	1.33/-0.41
CCDC number	1842912

Table T2. Bond lengths for $[Fe^{III}_2(L^{N4O6})]$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe01	O003	1.831(4)	C00W	C011	1.499(7)
Fe01	O005	1.850(3)	C00W	C023	1.372(7)
Fe01	O006	1.895(3)	C00X	C010	1.418(7)
Fe01	N009	2.224(4)	C00X	C01U	1.376(7)
Fe01	N00C	2.067(4)	C00Y	C01K	1.565(7)
Fe02	O004	1.843(4)	C00Y	C01P	1.509(7)
Fe02	O007	1.879(3)	C00Y	C020	1.531(7)
Fe02	O008	1.890(4)	C012	C01L	1.386(7)
Fe02	N00A	2.237(4)	C012	C01O	1.499(7)
Fe02	N00B	2.054(4)	C013	C01I	1.546(7)
O003	C00D	1.352(6)	C013	C01Z	1.521(7)
O004	C00O	1.387(6)	C013	C02I	1.542(7)
O005	C010	1.340(6)	C014	C015	1.506(7)
O006	C00Q	1.319(6)	C014	C01W	1.406(7)
O007	C00P	1.370(6)	C015	C025	1.547(7)
O008	C00U	1.309(6)	C015	C02E	1.521(7)
N009	C00G	1.454(6)	C015	C02F	1.543(7)
N009	C00Z	1.501(6)	C018	C01R	1.375(7)
N009	C011	1.502(6)	C019	C01Q	1.402(8)
N00A	C00F	1.456(6)	C01A	C01L	1.417(8)
N00A	C016	1.495(6)	C01A	C01M	1.366(7)
N00A	C017	1.499(6)	C01A	C01N	1.529(7)
N00B	C00I	1.415(6)	C01B	C01O	1.535(7)
N00B	C01E	1.308(6)	C01C	C01J	1.372(7)
N00C	C00N	1.414(6)	C01D	C01Q	1.369(7)
N00C	C01V	1.312(6)	C01F	C01H	1.512(8)
C00D	C00J	1.395(7)	C01F	C01X	1.397(8)
C00D	C00V	1.404(7)	C01H	C028	1.537(8)
C00E	C00F	1.381(7)	C01H	C02D	1.539(8)
C00E	C00G	1.379(6)	C01H	C02G	1.513(8)
C00F	C00I	1.386(6)	C01J	C022	1.546(8)
C00G	C00N	1.397(7)	C01J	C029	1.392(7)
C00H	C00P	1.380(7)	C01N	C024	1.531(7)
C00H	C016	1.503(7)	C01N	C02C	1.534(8)
C00H	C029	1.392(7)	C01N	C02M	1.511(8)
C00I	C00R	1.393(7)	C01O	C027	1.545(7)
C00J	C00Z	1.478(7)	C01O	C02A	1.534(7)
C00J	C01D	1.373(7)	C01Q	C026	1.531(8)
C00K	C00O	1.375(7)	C01R	C01X	1.387(8)
C00K	C017	1.486(7)	C01R	C02H	1.549(8)
C00K	C018	1.394(7)	C01U	C021	1.416(8)
C00L	C00P	1.404(7)	C01W	C01Y	1.399(8)
C00L	C013	1.553(7)	C01Y	C02B	1.363(7)
C00L	C01C	1.382(7)	C01Y	C02J	1.561(8)
C00M	C00Q	1.394(7)	C021	C023	1.395(8)
C00M	C01V	1.433(7)	C021	C1	1.491(8)
C00M	C02B	1.422(7)	C022	C02K	1.498(9)
C00N	C00R	1.370(7)	C022	C02L	1.524(9)
C00O	C01F	1.386(7)	C022	C02T	1.561(8)
C00Q	C014	1.455(7)	C026	C02P	1.511(9)
C00S	C00X	1.530(7)	C026	C02S	1.559(9)
C00S	C01G	1.537(7)	C026	C02W	1.528(9)
C00S	C01S	1.515(7)	C02H	C02R	1.527(9)
C00S	C01T	1.547(7)	C02H	C02X	1.606(10)
C00T	C00U	1.411(7)	C02H	C02Y	1.466(10)
C00T	C01E	1.405(7)	C02J	C02Q	1.512(8)
C00T	C01M	1.413(7)	C02J	C02U	1.549(11)
C00U	C012	1.449(7)	C02J	C02V	1.559(10)
C00V	C00Y	1.523(7)	C02O	C1	1.444(8)
C00V	C019	1.400(7)	C02Z	C1	1.360(13)
C00W	C010	1.411(7)	C1	C3	1.688(14)

Table T3. Bond angles for $[Fe^{III}_2(L^{N4O6})]$

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O003	Fe01	O005	116.56(15)	C01P	C00Y	C020	107.6(4)
O003	Fe01	O006	100.49(15)	C020	C00Y	C01K	110.1(4)
O003	Fe01	N009	89.77(15)	C00J	C00Z	N009	114.0(4)
O003	Fe01	N00C	120.53(16)	O005	C010	C00W	119.3(5)
O005	Fe01	O006	97.35(14)	O005	C010	C00X	121.3(5)
O005	Fe01	N009	89.12(15)	C00W	C010	C00X	119.4(5)
O005	Fe01	N00C	120.66(16)	C00W	C011	N009	112.9(4)
O006	Fe01	N009	163.75(16)	C00U	C012	C01O	122.2(5)
O006	Fe01	N00C	87.40(16)	C01L	C012	C00U	115.7(5)
N00C	Fe01	N009	76.50(16)	C01L	C012	C01O	122.1(5)
O004	Fe02	O007	119.34(15)	C01I	C013	C00L	110.0(4)
O004	Fe02	O008	101.82(15)	C01Z	C013	C00L	110.6(4)
O004	Fe02	N00A	89.43(15)	C01Z	C013	C01I	109.9(5)
O004	Fe02	N00B	116.59(15)	C01Z	C013	C02I	108.9(5)
O007	Fe02	O008	94.53(15)	C02I	C013	C00L	111.6(5)
O007	Fe02	N00A	88.30(15)	C02I	C013	C01I	105.7(5)
O007	Fe02	N00B	122.14(16)	C00Q	C014	C015	120.5(5)
O008	Fe02	N00A	165.08(15)	C01W	C014	C00Q	114.4(6)
O008	Fe02	N00B	87.65(16)	C01W	C014	C015	125.1(5)
N00B	Fe02	N00A	78.49(16)	C014	C015	C025	109.8(5)
C00D	O003	Fe01	132.8(3)	C014	C015	C02E	111.5(5)
C00O	O004	Fe02	128.3(3)	C014	C015	C02F	111.4(4)
C010	O005	Fe01	129.3(3)	C02E	C015	C025	110.6(5)
C00Q	O006	Fe01	132.4(4)	C02E	C015	C02F	106.8(5)
C00P	O007	Fe02	127.3(3)	C02F	C015	C025	106.7(4)
C00U	O008	Fe02	136.2(4)	N00A	C016	C00H	111.4(4)
C00G	N009	Fe01	108.3(3)	C00K	C017	N00A	112.7(4)
C00G	N009	C00Z	113.0(4)	C01R	C018	C00K	120.2(6)
C00G	N009	C011	108.7(4)	C00V	C019	C01Q	123.5(5)
C00Z	N009	Fe01	108.1(3)	C01L	C01A	C01N	121.8(5)
C00Z	N009	C011	111.2(4)	C01M	C01A	C01L	117.1(5)
C011	N009	Fe01	107.4(3)	C01M	C01A	C01N	121.1(5)
C00F	N00A	Fe02	107.7(3)	C01J	C01C	C00L	123.5(5)
C00F	N00A	C016	109.2(4)	C01Q	C01D	C00J	123.4(5)
C00F	N00A	C017	112.5(4)	N00B	C01E	C00T	127.9(5)
C016	N00A	Fe02	109.7(3)	C00O	C01F	C01H	123.1(5)
C016	N00A	C017	109.7(4)	C00O	C01F	C01X	113.4(6)
C017	N00A	Fe02	108.0(3)	C01X	C01F	C01H	123.3(5)
C00I	N00B	Fe02	115.6(3)	C01F	C01H	C028	110.4(5)
C01E	N00B	Fe02	124.5(4)	C01F	C01H	C02D	109.2(5)
C01E	N00B	C00I	119.9(4)	C01F	C01H	C02G	111.9(5)
C00N	N00C	Fe01	116.8(3)	C028	C01H	C02D	110.8(5)
C01V	N00C	Fe01	124.6(4)	C02G	C01H	C028	107.7(5)
C01V	N00C	C00N	118.5(5)	C02G	C01H	C02D	106.8(5)
O003	C00D	C00J	119.3(5)	C01C	C01J	C022	122.6(5)
O003	C00D	C00V	119.7(5)	C01C	C01J	C029	117.7(5)
C00J	C00D	C00V	121.0(5)	C029	C01J	C022	119.6(5)
C00G	C00E	C00F	120.5(4)	C012	C01L	C01A	125.3(5)
C00E	C00F	N00A	121.5(4)	C01A	C01M	C00T	121.9(5)
C00E	C00F	C00I	120.4(4)	C01A	C01N	C024	109.4(4)
C00I	C00F	N00A	118.1(4)	C01A	C01N	C02C	110.0(5)
C00E	C00G	N009	123.6(4)	C024	C01N	C02C	108.1(5)
C00E	C00G	C00N	119.4(5)	C02M	C01N	C01A	113.1(5)
C00N	C00G	N009	117.1(4)	C02M	C01N	C024	108.5(5)
C00P	C00H	C016	119.8(5)	C02M	C01N	C02C	107.7(5)
C00P	C00H	C029	119.4(5)	C012	C01O	C01B	110.3(4)
C029	C00H	C016	120.9(5)	C012	C01O	C027	109.9(5)
C00F	C00I	N00B	117.2(4)	C012	C01O	C02A	111.9(5)
C00F	C00I	C00R	118.8(5)	C01B	C01O	C027	108.8(4)
C00R	C00I	N00B	124.0(4)	C02A	C01O	C01B	107.8(5)
C00D	C00J	C00Z	119.4(5)	C02A	C01O	C027	108.1(5)
C01D	C00J	C00D	119.0(5)	C019	C01Q	C026	119.5(5)
C01D	C00J	C00Z	120.9(5)	C01D	C01Q	C019	116.4(5)
C00O	C00K	C017	121.4(5)	C01D	C01Q	C026	124.1(5)
C00O	C00K	C018	119.0(5)	C018	C01R	C01X	117.6(5)
C018	C00K	C017	119.6(5)	C018	C01R	C02H	122.9(6)

C00P	C00L	C013	121.2(5)	C01X	C01R	C02H	119.4(6)	C00P	C00L	C013	121.2(5)
C01C	C00L	C00P	117.4(5)	C00X	C01U	C021	123.3(6)	C01C	C00L	C00P	117.4(5)
C01C	C00L	C013	121.4(5)	N00C	C01V	C00M	124.7(6)	C00Q	C00M	C01V	123.5(5)
C01Y	C01W	C014	126.1(5)	C00Q	C00M	C02B	121.0(5)	C01R	C01X	C01F	125.3(6)
C02B	C00M	C01V	115.2(5)	C01W	C01Y	C02J	121.2(5)	C00G	C00N	N00C	115.0(5)
C02B	C01Y	C01W	117.4(5)	C00R	C00N	N00C	124.9(5)	C02B	C01Y	C02J	121.4(6)
C00R	C00N	C00G	119.9(5)	C01U	C021	C1	122.4(6)	C00K	C00O	O004	116.4(5)
C023	C021	C01U	116.7(5)	C00K	C00O	C01F	124.3(5)	C023	C021	C1	120.9(5)
C01F	C00O	O004	119.2(5)	C01J	C022	C02T	110.5(5)	O007	C00P	C00H	118.3(5)
C02K	C022	C01J	110.2(6)	O007	C00P	C00L	120.7(5)	C02K	C022	C02L	110.9(6)
C00H	C00P	C00L	120.9(5)	C02K	C022	C02T	111.6(6)	O006	C00Q	C00M	122.5(5)
C02L	C022	C01J	108.1(5)	O006	C00Q	C014	117.3(5)	C02L	C022	C02T	105.5(6)
C00M	C00Q	C014	120.1(5)	C00W	C023	C021	122.0(5)	C00N	C00R	C00I	121.0(5)
C01Q	C026	C02S	109.5(5)	C00X	C00S	C01G	109.8(4)	C02P	C026	C01Q	109.9(5)
C00X	C00S	C01T	109.2(5)	C02P	C026	C02S	109.3(6)	C01G	C00S	C01T	109.8(4)
C02P	C026	C02W	108.8(6)	C01S	C00S	C00X	111.8(4)	C02W	C026	C01Q	111.1(5)
C01S	C00S	C01G	107.4(5)	C02W	C026	C02S	108.1(6)	C01S	C00S	C01T	108.8(4)
C00H	C029	C01J	121.1(5)	C00U	C00T	C01M	119.7(5)	C01Y	C02B	C00M	120.8(6)
C01E	C00T	C00U	123.0(5)	C01R	C02H	C02X	106.5(6)	C01E	C00T	C01M	117.1(5)
C02R	C02H	C01R	111.2(6)	O008	C00U	C00T	120.4(5)	C02R	C02H	C02X	107.9(6)
O008	C00U	C012	119.4(5)	C02Y	C02H	C01R	111.9(6)	C00T	C00U	C012	120.2(5)
C02Y	C02H	C02R	110.1(7)	C00D	C00V	C00Y	122.0(5)	C02Y	C02H	C02X	109.1(7)
C019	C00V	C00D	116.7(5)	C02Q	C02J	C01Y	111.5(5)	C019	C00V	C00Y	121.3(5)
C02Q	C02J	C02U	110.9(6)	C010	C00W	C011	118.1(5)	C02Q	C02J	C02V	109.9(6)
C023	C00W	C010	120.2(5)	C02U	C02J	C01Y	107.4(6)	C023	C00W	C011	121.6(5)
C02U	C02J	C02V	109.9(6)	C010	C00X	C00S	120.8(5)	C02V	C02J	C01Y	107.2(6)
C01U	C00X	C00S	121.1(5)	C021	C1	C3	105.0(8)	C01U	C00X	C010	118.2(5)
C02O	C1	C021	116.1(5)	C00V	C00Y	C01K	108.2(4)	C02O	C1	C3	98.6(8)
C02Z	C1	C021	116.9(8)	C00V	C00Y	C02O	110.9(4)	C02Z	C1	C02O	120.2(9)
C01P	C00Y	C00V	113.0(5)	C02Z	C1	C3	92.8(8)	C01P	C00Y	C01K	107.1(4)

Table T4. Geometry optimized structures of the simplified models of **1** and [$Cu^{II}Fe^{III}$].

[$Cu^{II}Fe^{III}$] complex						
	Broken Symmetry, S = 2			Ferromagnetic, S = 3		
	x	*y*	*z*	*x*	*y*	*z*
Fe	0.05185640	0.05727785	-0.11703562	0.05216548	0.05740268	-0.11701062
O	1.82727068	-0.19654089	0.30560266	1.82749680	-0.19680309	0.30560661
C	2.58127959	-0.95174531	1.14543640	2.58144735	-0.95212592	1.14539289
C	3.89450235	-0.56319743	1.45083921	3.89471608	-0.56371754	1.45076797
C	4.66452295	-1.32973893	2.32305126	4.66470030	-1.33038131	2.32290554
H	5.67652089	-1.02358557	2.55283047	5.67673613	-1.02433673	2.55266182
C	4.13713055	-2.49087572	2.89980002	4.13721881	-2.49149995	2.89960593
C	2.83137790	-2.87868073	2.59264971	2.83141425	-2.87915790	2.59248792
H	2.42517224	-3.78303472	3.02943614	2.42513888	-3.78349792	3.02923887
C	2.03853302	-2.12438831	1.71908201	2.03860281	-2.12474184	1.71899671
C	0.66604558	-2.58453744	1.30243164	0.66604156	-2.58473667	1.30239945
H	0.64274109	-2.76303418	0.22711111	0.64267442	-2.76317718	0.22706830
H	0.43336468	-3.54124771	1.77200247	0.43332074	-3.54146723	1.77192216
N	-0.43845135	-1.56897861	1.55051957	-0.43833839	-1.56910875	1.55059572
C	-0.40594822	-0.85055047	2.81932594	-0.40569218	-0.85062294	2.81938526
C	-0.32122735	-1.50751842	4.10434957	-0.32087407	-1.50751517	4.10443563
C	-0.38558329	-2.91055656	4.31435004	-0.38531142	-2.91055086	4.31444449
H	-0.48921381	-3.58345930	3.48123391	-0.48889257	-3.58344161	3.48131424
C	-0.33710834	-3.42468817	5.59492846	-0.33699235	-3.42468104	5.59502011
H	-0.39372505	-4.48978495	5.76232832	-0.39366642	-4.48977452	5.76242224
C	-0.21874160	-2.56199790	6.69853890	-0.21853024	-2.56198273	6.69862852
H	-0.16967801	-2.91234021	7.71819119	-0.16929036	-2.91234544	7.71826723
N	-0.17405258	-1.23687375	6.53382671	-0.17383713	-1.23687699	6.53392902
C	-0.23400783	-0.71129537	5.27309777	-0.23377050	-0.71129468	5.27318306
C	-0.21008202	0.71472294	5.17995686	-0.20996726	0.71472610	5.18003498
N	-0.02798681	1.40475723	6.34732123	-0.02793809	1.40481400	6.34738723
C	0.06061049	2.73908906	6.31693253	0.06040704	2.73916456	6.31696051
H	0.18387395	3.22113432	7.27518391	0.18370338	3.22125809	7.27518220
C	0.00496599	3.44446914	5.10209642	0.00455401	3.44451316	5.10212007
H	0.13034949	4.51660121	5.10775413	0.12973015	4.51666976	5.10775654
C	-0.19824237	2.76426074	3.91622072	-0.19845868	2.76423208	3.91624673
H	-0.20848885	3.30681580	2.98385388	-0.20877732	3.30676154	2.98386447
C	-0.35115720	1.35446381	3.92881939	-0.35106950	1.35440879	3.92886657
C	-0.54121067	0.52685503	2.75047873	-0.54104435	0.52677489	2.75052010
N	-0.79376911	1.09576438	1.48037711	-0.79366606	1.09568247	1.48043953
C	-1.63818958	2.10385883	1.32346457	-1.63824232	2.10361269	1.32346678
H	-2.24071963	2.40315826	2.18012174	-2.24096339	2.40275946	2.18005116

C	-1.83787818	2.85525161	0.13392471	-1.83787502	2.85501739	0.13390657
C	-2.82363090	3.88517068	0.13347124	-2.82388349	3.88468261	0.13329462
H	-3.43248141	4.02177679	1.01950019	-3.43293160	4.02111437	1.01921454
C	-3.00465771	4.69907646	-0.96248210	-3.00492653	4.69856476	-0.96267989
C	-2.18825094	4.51371442	-2.10483942	-2.18827797	4.51342954	-2.10489254
H	-2.32583561	5.15639907	-2.96448564	-2.32587183	5.15609175	-2.96455399
C	-1.22091449	3.52810171	-2.14265660	-1.22067916	3.52806138	-2.14254971
C	-1.02999703	2.65955352	-1.03990129	-1.02972023	2.65956419	-1.03977097
O	-0.10842796	1.71253064	-1.09360712	-0.10781425	1.71282770	-1.09330131
C	-1.83195014	-2.10098697	1.24181015	-1.83187572	-2.10094321	1.24190366
H	-2.47917732	-1.22121269	1.21478705	-2.47905350	-1.22112756	1.21506623
H	-2.17079149	-2.73159472	2.06887501	-2.17072488	-2.73168283	2.06887001
C	-1.94063935	-2.86895578	-0.04879203	-1.94070887	-2.86867946	-0.04883306
C	-2.50738166	-4.14885840	-0.08731250	-2.50750911	-4.14855104	-0.08752223
H	-2.82213571	-4.61695879	0.83840405	-2.82220697	-4.61678743	0.83814412
C	-2.68305946	-4.82167401	-1.29831510	-2.68330905	-4.82116814	-1.29861826
C	-2.28509002	-4.20571423	-2.49074617	-2.28540690	-4.20503862	-2.49098195
H	-2.41820186	-4.71871717	-3.43413289	-2.41861233	-4.71788436	-3.43444071
C	-1.71265145	-2.93505188	-2.47406178	-1.71291358	-2.93440232	-2.47413492
C	-1.53511308	-2.25883068	-1.25681414	-1.53525167	-2.25838690	-1.25679311
O	-0.96871521	-1.02693307	-1.22940318	-0.96880462	-1.02650670	-1.22924435
Cu	0.11589327	0.18591237	7.98957217	0.11592530	0.18599366	7.98969204
Cl	0.02911376	-1.45195062	9.70720794	0.02947078	-1.45187956	9.70735225
Cl	0.12513252	2.02052423	9.43928901	0.12455942	2.02056728	9.43939662
O	2.37874447	-0.22085759	8.09101706	2.37882839	-0.22034847	8.09117205
H	2.35887061	-0.81527317	8.86511440	2.35908541	-0.81488500	8.86517944
C	3.41362054	0.79992002	8.23599949	3.41349688	0.80061897	8.23630070
H	3.20355889	1.44853313	9.08626276	3.20330338	1.44906970	9.08665571
H	4.39735547	0.33896539	8.34140249	4.39732466	0.33984904	8.34164247
H	3.39565886	1.38598377	7.32163679	3.39541993	1.38680895	7.32202168
H	-3.12464360	-5.80837104	-1.31266908	-3.12493513	-5.80784473	-1.31309273
H	-1.39531853	-2.44447008	-3.38285722	-1.39563018	-2.44368796	-3.38287622
H	-0.59615043	3.37649242	-3.01006222	-0.59571566	3.37663313	-3.00984340
H	-3.75651470	5.47471838	-0.95348882	-3.75698488	5.47401300	-0.95380342
H	4.73474604	-3.08561121	3.57637009	4.73480365	-3.08633411	3.57611655
H	4.28203414	0.33440742	0.99114662	4.28231421	0.33387662	0.99111059

[Fe^{III}_2], complex **1**

	Broken Symmetry			Ferromagnetic		
	x	*y*	*z*	*x*	*y*	*z*
Fe	-0.202236088	0.007872840	-0.013792024	-0.202114918	0.007639855	-0.014065599
Fe	0.353408927	-0.257511207	8.164470075	0.353088902	-0.257477240	8.164805656
O	-1.470114955	1.323572763	0.271721876	-1.470681891	1.322660704	0.271363740

O	2.178571631	-0.349549757	7.877554087	2.178214994	-0.350535903	7.878095906
O	1.287265072	0.211763903	-1.115716540	1.287488647	0.212296525	-1.115677200
O	-1.080147816	-1.413778641	-0.972774509	-1.079057209	-1.414533982	-0.973080225
O	-0.478506107	0.992380584	9.269059286	-0.478432085	0.993042269	9.268960011
O	-0.132702298	-1.858078600	9.119300311	-0.134104394	-1.857592657	9.119750277
N	1.045476425	1.096351162	1.602111694	1.045101831	1.096949821	1.601971583
N	0.356493275	1.404607869	6.553635968	0.357218428	1.404711535	6.553770967
N	-0.689128049	-1.103832168	6.542153898	-0.689159066	-1.103635449	6.542154657
N	-0.154910214	-1.337908953	1.606538198	-0.154640486	-1.337849814	1.606557211
C	-1.647622019	2.440058799	1.020926198	-1.648945730	2.438941639	1.020701328
C	0.704399718	1.268945668	4.077501097	0.704510453	1.269106080	4.077502711
H	1.149280393	2.250715613	4.078617671	1.149365211	2.250898534	4.078609223
C	0.274543753	0.708108845	5.278572648	0.274908950	0.708200153	5.278631620
C	0.566903170	0.578555481	2.874994008	0.566821416	0.578849147	2.874943088
C	-0.923256795	3.012911957	8.061865098	-0.921652784	3.013895485	8.061700290
C	-0.315047675	-0.570915475	5.280053374	-0.314818264	-0.570739610	5.280104027
C	-0.546352546	3.075176844	1.641333837	-0.548109914	3.074677738	1.641239660
C	2.894391103	1.490970770	6.502257916	2.895190006	1.489276036	6.502463368
C	-0.846203227	3.016592037	10.497643918	-0.845055375	3.017471372	10.497490835
C	-0.562032525	-3.380770144	0.318379189	-0.560949873	-3.381096610	0.318745707
C	-0.008254561	-0.706924351	2.870243568	-0.008139442	-0.706695839	2.870212975
C	3.136249081	0.242695822	7.122042175	3.136262756	0.240947627	7.122444923
C	-0.747046172	2.320963921	9.281947300	-0.746113309	2.321806290	9.281798256
C	-1.015553409	-2.731590656	-0.880470970	-1.014297754	-2.732315551	-0.880382438
C	-0.448763835	-1.268614161	4.073929586	-0.448567009	-1.268395953	4.073940688
H	-0.894074653	-2.251805462	4.072373668	-0.893865417	-2.251586351	4.072381771
C	-1.941396218	-2.776950157	7.820249549	-1.942264868	-2.776403205	7.819905469
C	-1.154341945	-2.691835227	9.019199635	-1.155753896	-2.691290478	9.019207959
C	-2.940149129	2.964225570	1.190677459	-2.941815495	2.962263194	1.190436264
C	3.109181590	1.175128303	0.104856481	3.108783363	1.176954482	0.104849463
C	3.073418194	1.248266088	-2.330775517	3.073046959	1.249729374	-2.330791908
C	0.856308021	2.579475198	1.396505431	0.854887429	2.579936593	1.396382977
H	1.151702155	2.764297828	0.363265007	1.150129166	2.765002492	0.363140134
H	1.562438208	3.134537981	2.024296566	1.560621688	3.135503873	2.024183531
C	2.473414395	0.867418665	-1.119676722	2.473236681	0.868689335	-1.119658599
C	2.503712885	0.689592329	1.394371356	2.503588150	0.691236628	1.394438597
H	2.511279563	-0.401492156	1.433712406	2.511962569	-0.399842128	1.433959901
H	3.087906423	1.056733782	2.243969856	3.087509060	1.058923630	2.244000032
C	-1.477214349	-3.548908272	10.100295510	-1.479211732	-3.548244000	10.100218881
C	-1.427512484	-3.538730741	-1.969662524	-1.425869909	-3.539809864	-1.969453376
C	-0.901732412	2.244329184	6.768255156	-0.900379570	2.245340256	6.768056170

H	-1.005384671	2.930853687	5.922205406	-1.003374637	2.931972705	5.922002759
H	-1.734736585	1.539808399	6.727632175	-1.733914595	1.541450593	6.727229519
C	1.605101153	2.228196490	6.758845900	1.606408593	2.227398570	6.759030027
H	1.558307958	2.564627653	7.795085423	1.559850365	2.563847825	7.795275925
H	1.562084446	3.130550267	6.138602490	1.564072941	3.129799171	6.138799962
C	3.903975441	2.064424822	5.718717550	3.905119836	2.061923892	5.718777199
H	3.725604530	3.027275862	5.252858510	3.727374890	3.024814840	5.252765337
C	-3.142499716	4.104687558	1.964018392	-3.144933941	4.102503735	1.963904013
H	-4.142953846	4.499633939	2.083289800	-4.145644875	4.496801863	2.083167842
C	-3.335056775	-4.501966407	8.844296397	-3.336607604	-4.501163429	8.843461063
C	-1.114544437	4.384226589	10.501524716	-1.112513659	4.385281395	10.501359266
H	-1.189382763	4.910713641	11.444155343	-1.187182660	4.911792492	11.443990459
C	-0.774643368	4.219152807	2.417025660	-0.777176225	4.218412347	2.417062952
H	0.069154472	4.715826590	2.883114357	0.066280166	4.715569710	2.883253246
C	-1.629103983	-2.023823269	6.653162576	-1.629398852	-2.023375607	6.652899001
H	-2.226984247	-2.254375708	5.771237598	-2.227089828	-2.253773537	5.770798132
C	4.376072000	-0.394057699	6.944914450	4.375653853	-0.396656875	6.945383943
C	-1.283179970	5.079017864	9.297805621	-1.280480324	5.080206016	9.297628258
C	-2.543887021	-4.423504882	10.014832814	-2.545954527	-4.422718349	10.014342886
H	-2.778415367	-5.060242227	10.858015904	-2.780938396	-5.059364686	10.857468350
C	-3.029329891	-3.693879144	7.770302287	-3.030300589	-3.693184435	7.769547462
H	-3.619142671	-3.749713915	6.862730533	-3.619716772	-3.749007773	6.861717657
C	-2.059694597	4.740670530	2.582717455	-2.062567565	4.739092275	2.582743844
C	5.136937169	1.431431843	5.545129951	5.137657456	1.428087956	5.545253604
C	4.290766772	1.926926703	-2.325810660	4.289986610	1.929126561	-2.325896300
H	4.745008640	2.215136084	-3.264918498	4.744074030	2.217479969	-3.265035201
C	-0.217979466	-2.651138710	1.491487684	-0.217272409	-2.651112459	1.491754067
H	0.000527309	-3.254029798	2.373110214	0.001349684	-3.253757861	2.373522666
C	-1.363016066	-4.917103762	-1.892251203	-1.361136686	-4.918153456	-1.891673269
H	-1.671497279	-5.512400185	-2.741887961	-1.669311668	-5.513724721	-2.741229287
C	5.366594287	0.196956895	6.164220533	5.366532297	0.193570832	6.164544854
H	6.318448753	-0.302611365	6.039491800	6.318053548	-0.306643617	6.039860906
C	-0.901286211	-5.564565778	-0.721853477	-0.899544985	-5.565224652	-0.721009817
C	4.924732140	2.240633904	-1.117606781	4.923729413	2.243381470	-1.117722572
C	4.328202281	1.863680308	0.087700674	4.327393955	1.866225331	0.087620246
H	4.815408475	2.097976537	1.027091742	4.814440111	2.100942753	1.026989888
C	-1.185176828	4.388113287	8.087906513	-1.182707106	4.389259340	8.087732477
H	-1.320776092	4.917441461	7.151876795	-1.317797716	4.918695393	7.151689868
C	-0.515236145	-4.802940579	0.360251708	-0.513882262	-4.803244594	0.360986716
H	-0.168978648	-5.283798440	1.267748909	-0.167738387	-5.283802739	1.268685837
H	-3.760527081	2.458193101	0.702474712	-3.761843204	2.455768865	0.702124050

H	-2.213357247	5.630361942	3.177957568	-2.216831400	5.628603471	3.178097365
H	-1.489289898	6.140467028	9.302502109	-1.485899794	6.141789279	9.302307503
H	-0.709065705	2.463106653	11.415423287	-0.708450358	2.463875453	11.415283066
H	-0.867523033	-3.479768972	10.988844821	-0.869916620	-3.479108235	10.989040077
H	-4.165491361	-5.191490472	8.795244497	-4.167108728	-5.190584195	8.794084496
H	5.867970474	2.769299114	-1.115273843	5.866645626	2.772621460	-1.115433501
H	2.566471367	1.000014625	-3.252100772	2.566277782	1.001037304	-3.252096192
H	-0.857298340	-6.643323099	-0.679307256	-0.855359834	-6.643962449	-0.678174746
H	-1.777235903	-3.034378313	-2.858108001	-1.775475849	-3.035751985	-2.858112113
H	5.907009099	1.895201257	4.943984384	5.908005597	1.891240175	4.943986626
H	4.532410628	-1.344986184	7.433498915	4.531385713	-1.347601208	7.434131047

Table T5. Coupling results: X-ray and simplified models of **1** and [$Cu^{II}Fe^{III}$].

Model	**State**	**SCF Energies** [a.u.]	**Rel. Energ.** [cm^{-1}]	**J** [cm^{-1}]	$\langle S_t^2 \rangle$	**Mulliken Charges**		**Mulliken Spin**	
[$Cu^{II}Fe^{III}$]						Fe	Cu	Fe	Cu
simplified	BS	-5656.56139567	0.00	2.01	7.015	1.734	1.173	4.135	-0.632
	F	-5656.56137273	5.03		12.015	1.734	1.173	4.135	0.632
X-ray	BS	-6599.00133064	0.00	1.79	7.015	1.741	1.144	4.118	-0.614
	F	-6599.00131021	4.48		12.015	1.741	1.144	4.118	0.614
[Fe^{III}_2], complex **1**						Fe	Fe	Fe	Fe
simplified	BS	-5048.70848817	0.00	0.83	5.022	1.75	1.75	4.15	-4.15
	F	-5048.70844074	10.41		30.022	1.75	1.75	4.15	4.15
X-ray	BS	-6934.24898507	0.00	0.65	5.021	1.74	1.74	4.14	-4.14
	F	-6934.24894780	8.18		30.022	1.74	1.74	4.14	4.14