Supporting Information for
A comparative study of NHC-functionalized ternary Se/Te−Fe−Cu compounds: synthesis, catalysis, and the effect of chalcogens

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Contents

Explanations for the checkCIF Alerts for 5:

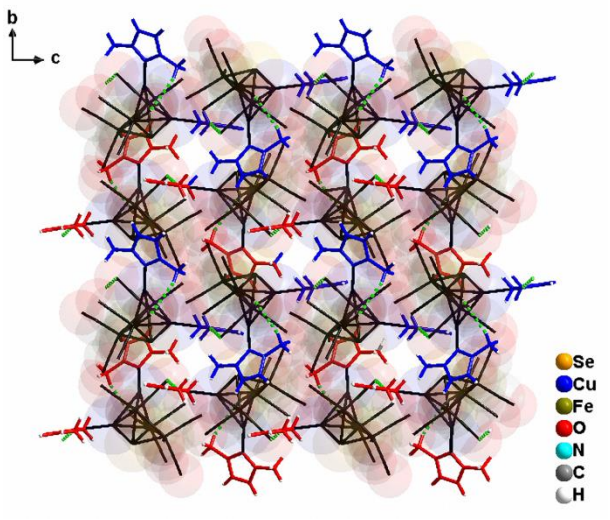
Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density			5.14 eA-3
PLAT430_ALERT_2_B Short Inter D...A Contact	O3···O3		2.82 Ang.
	1-x,1-y,1-z	=	3_666 Check

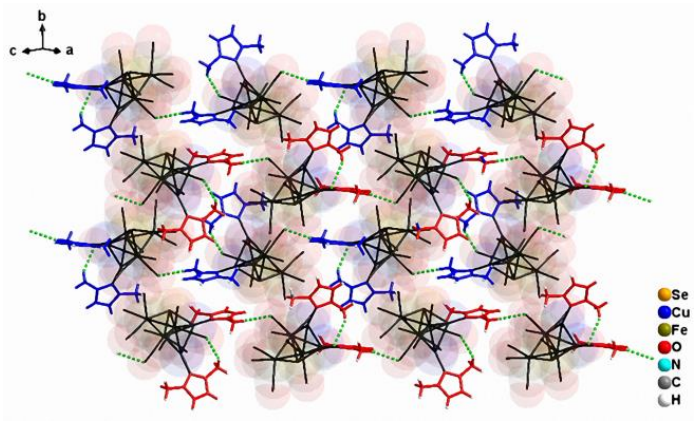
Explanation: There was no serious problem with the refinement. The largest residual electron density was near to the Fe_3 ring, which was likely due to the inefficient absorption correction for the heavier iron atoms. In addition, the O3 atom in the carbonyl group of **5** was close to the other O3 atom of the neighboring CO. Although recrystallization and data collection for different crystals were attempted repeatedly, this structure represented the best of the all.

Fig. S1 Two views of portions of the 1D supramolecular structures for **2** (a, b) and **3** (c, d). Green dashed lines represent nonclassical C−H···O(carbonyl) interactions and the $SeFe_3(CO)_9Cu_2$-based clusters are represented by space-filling spheres.

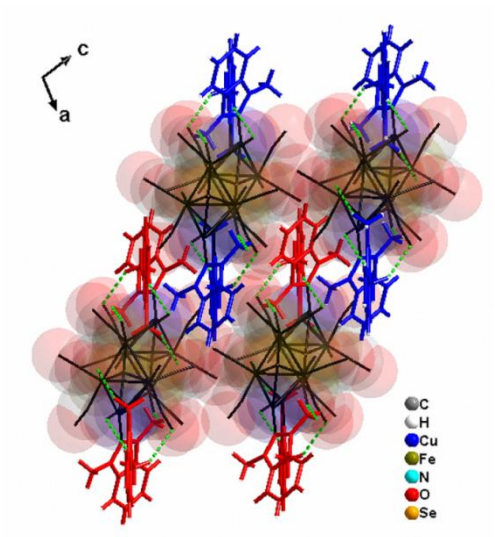
(a)



(b)



(c)



(d)

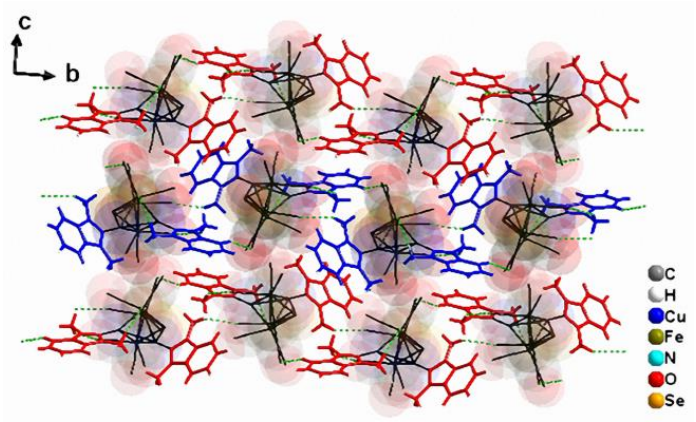
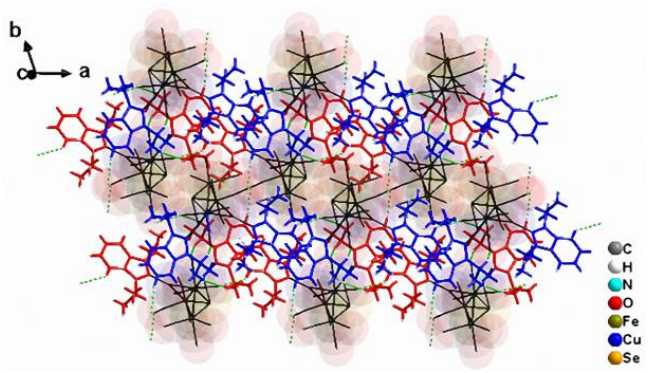
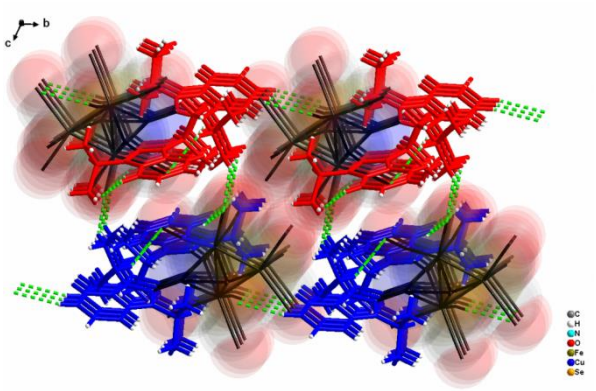


Fig. S2 Two views of portions of the 2D supramolecular structures for **4** (a, b) and **5** (c, d). Green and pink dashed lines represent nonclassical C−H···O(carbonyl) and the Cl···H interactions, respectively, and the $SeFe_3(CO)_9Cu_2$-based clusters are represented by space-filling spheres.

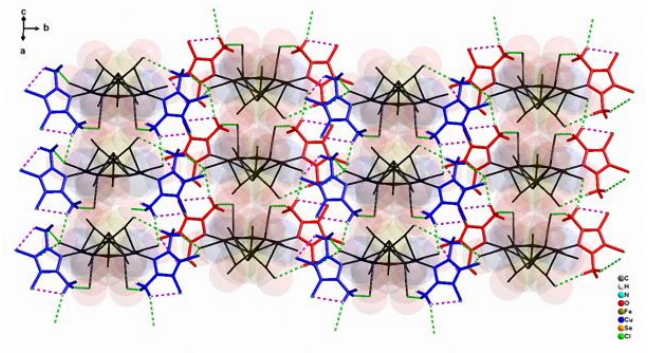
(a)



(b)



(c)



(d)

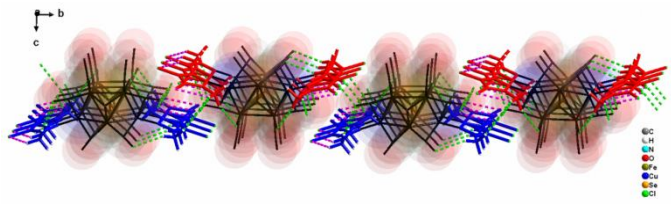


Fig. S3 Powder X-ray diffraction (PXRD) patterns for (a) crystals of **2** exposed to water for 5 days. (b) crystals of **2** exposed to air for 5 days. (c) simulated pattern for **2**.

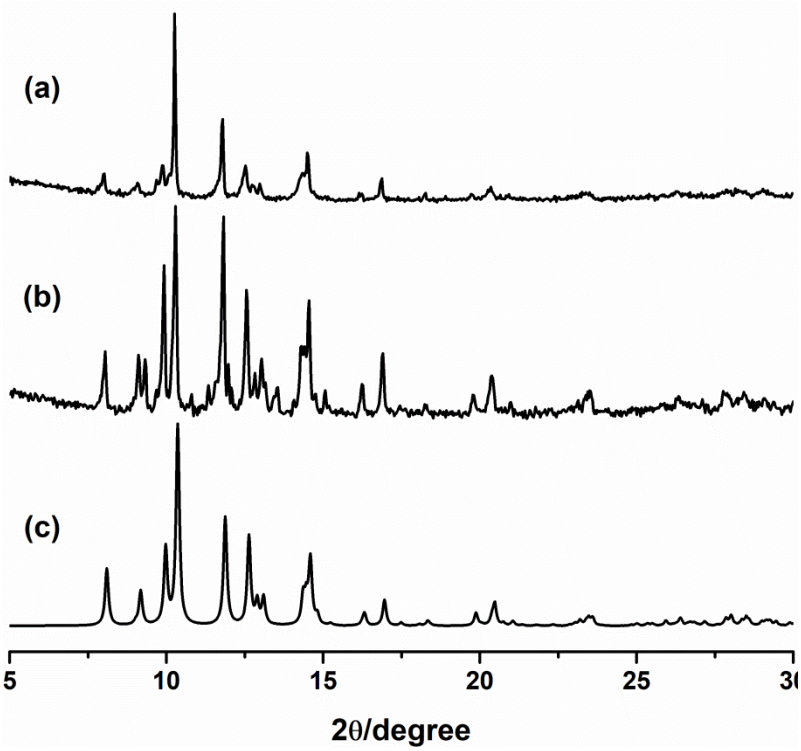


Fig. S4 DPV in MeCN of **2** (black line), **3** (red line), **4** (blue line), and **5** (green line). Conditions: electrolyte, 0.1 M Bu_4NClO_4; working electrode, glassy carbon; scan rate, 100 mV/s. Potentials are vs. SCE.

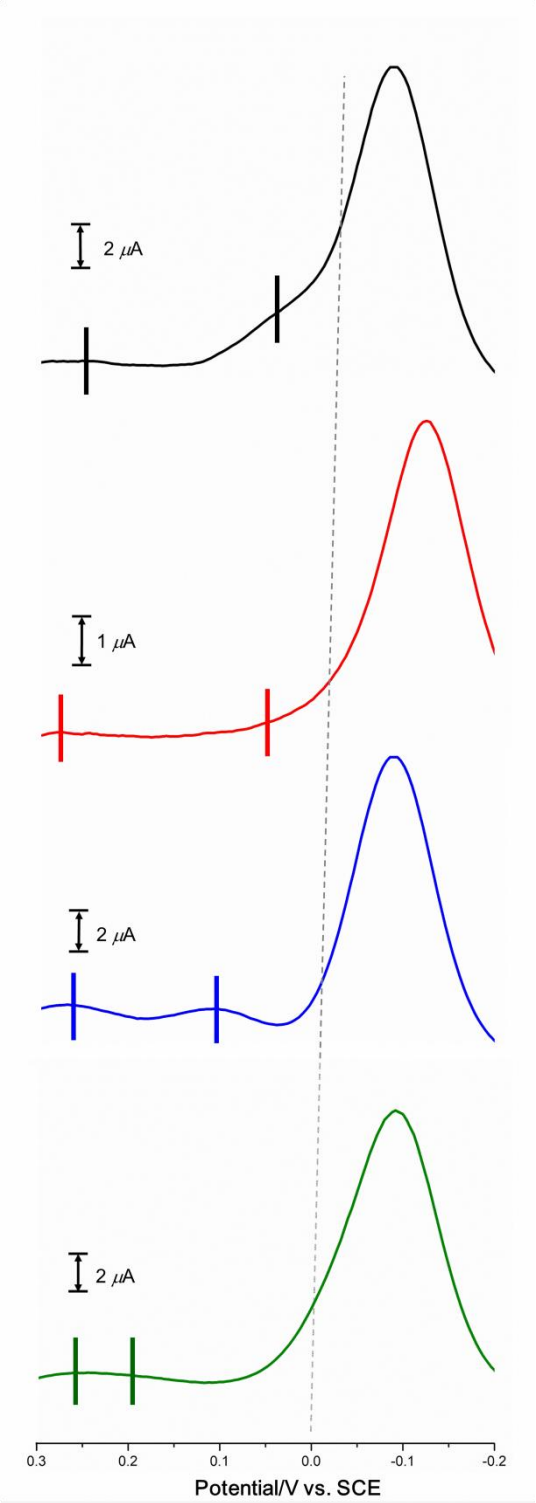


Table S1 Important C−H···O(carbonyl) contacts (Å) for **2**, **3**, **4**, and **5**

complex	C−H···O	H···O (Å)	C···O (Å)	C−H···O (deg)	C−O···H (deg)	symmetry operation
2	C(16)−H(16A)···O(2)	2.617(6)	3.47(1)	148.8(6)	101.3(5)	−0.5+x, 1.5−y, 0.5+z
3	C(13)−H(13)···O(7)	2.544(5)	3.441(9)	157.7(4)	97.7(4)	1.5−x, −0.5+y, 0.5−z
	C(27)−H(27A)···O(9)	2.600(6)	3.307(8)	129.2(4)	168.9(5)	1.5−x, 0.5+y, 0.5−z
4	C(17)−H(17)···O(3)	2.451(4)	3.376(8)	164.8(5)	120.4(4)	1+x, 1+y, z
	C(22)−H(22A)···O(6)	2.634(5)	3.455(9)	141.5(4)	100.6(4)	−x, −y, −z
	C(31)−H(31)···O(6)	2.535(5)	3.283(9)	135.7(5)	113.3(5)	−1+x, y, z
5	C(11)−H(11C)···O(5)	2.577(7)	3.49(1)	155.0(7)	119.8(7)	1−x, −0.5+y, 0.5−z
	C(16)−H(16A)···O(5)	2.543(9)	3.49(2)	162.7(7)	96.4(7)	−1+x, y, z
	C(14)−H(14A)···O(8)	2.494(9)	3.42(1)	156.7(6)	97.6(7)	−1+x, y, z

[a] Only the close contacts with H···O distances < 2.65 Å are listed. [b] Intramolecular C−H···O contacts are not listed.

Table S2 Differential pulse voltammetry of **2**, **3**, **4**, and **5**

Complex	Oxidation processes	Reduction processes
	E_p^{red}/V[a] ($W_{1/2}$/mV[b])	E_p^{red}/V[a] ($W_{1/2}$/mV[b])
2	0.042(70)	−0.090(102)
	0.252(107)	
3	0.074(74)	−0.126(106)
	0.270(74)	
4	0.104(81)	−0.090(98)
	0.266(150)	
5	0.192(145)	−0.092(118)
	0.265(147)	

[a] Ep^{red} = reductive peak potential. [b] $W_{1/2}$ = width at half-height.

Table S3 Selected bond distances (Å) and bond angles (deg) for **1**, **2**, **3**, **4**, and **5**

1			
Fe(1)−Fe(2)	2.7456(5)	Fe(1)−Cu(2)	2.4819(6)
Fe(1)−Fe(3)	2.6366(6)	Fe(2)−Cu(1)	2.5139(5)
Fe(2)−Fe(3)	2.7141(6)	Fe(2)−Cu(2)	2.4934(5)
Fe(1)−Se(1)	2.3276(4)	Fe(3)−Cu(1)	2.4894(5)
Fe(2)−Se(1)	2.3041(5)	Cu(1)−Cu(2)	2.6682(5)
Fe(3)−Se(1)	2.2992(5)	N(1)−Cu(1)	1.926(2)
Fe(1)−Cu(1)	2.5842(5)	N(2)−Cu(2)	1.891(2)
Se(1)−Fe(1)−Cu(2)	103.72(2)	Se(1)−Fe(3)−Fe(1)	55.77(1)
Se(1)−Fe(1)−Cu(1)	97.46(2)	Cu(1)−Fe(3)−Fe(1)	60.47(2)
Cu(2)−Fe(1)−Cu(1)	63.53(2)	Se(1)−Fe(3)−Fe(2)	53.96(1)
Se(1)−Fe(1)−Fe(3)	54.75(2)	Cu(1)−Fe(3)−Fe(2)	57.58(2)
Cu(2)−Fe(1)−Fe(3)	109.59(2)	Fe(1)−Fe(3)−Fe(2)	61.73(1)
Cu(1)−Fe(1)−Fe(3)	56.95(1)	Fe(3)−Cu(1)−Fe(2)	65.70(2)
Se(1)−Fe(1)−Fe(2)	53.25(1)	N(1)−Cu(1)−Fe(1)	139.76(7)
Cu(2)−Fe(1)−Fe(2)	56.71(2)	Fe(3)−Cu(1)−Fe(1)	62.59(2)
Cu(1)−Fe(1)−Fe(2)	56.19(1)	Fe(2)−Cu(1)−Fe(1)	65.15(2)
Fe(3)−Fe(1)−Fe(2)	60.53(2)	N(1)−Cu(1)−Cu(2)	106.94(8)
Se(1)−Fe(2)−Cu(2)	104.07(2)	Fe(2)−Cu(1)−Cu(2)	57.43(1)
Se(1)−Fe(2)−Cu(1)	100.09(2)	Fe(1)−Cu(1)−Cu(2)	56.37(2)
Cu(2)−Fe(2)−Cu(1)	64.40(2)	N(2)−Cu(2)−Fe(1)	146.97(8)
Se(1)−Fe(2)−Fe(3)	53.79(2)	N(2)−Cu(2)−Fe(2)	146.04(8)
Cu(2)−Fe(2)−Fe(3)	106.82(2)	Fe(1)−Cu(2)−Fe(3)	66.99(1)
Cu(1)−Fe(2)−Fe(3)	56.72(1)	N(2)−Cu(2)−Cu(1)	128.32(8)
Se(1)−Fe(2)−Fe(1)	54.04(1)	Fe(1)−Cu(2)−Cu(1)	60.10(1)
Cu(2)−Fe(2)−Fe(1)	56.31(1)	Fe(2)−Cu(2)−Cu(1)	58.17(1)
Cu(1)−Fe(2)−Fe(1)	58.66(1)	Fe(3)−Se(1)−Fe(2)	72.26(2)
Fe(3)−Fe(2)−Fe(1)	57.75(1)	Fe(3)−Se(1)−Fe(1)	69.48(2)
Se(1)−Fe(3)−Cu(1)	100.95(2)	Fe(2)−Se(1)−Fe(1)	72.71(2)

2			
Se(1)−Fe(1)	2.342(1)	Cu(2)−Fe(2)	2.516(1)
Se(1)−Fe(2)	2.359(1)	Fe(1)−Fe(2)	2.685(1)
Se(1)−Fe(3)	2.306(1)	Fe(1)−Fe(3)	2.628(1)
Se(1)−Cu(2)	2.429(1)	Fe(2)−Fe(3)	2.623(1)
Cu(1)−Fe(1)	2.507(1)	Cu(1)−Cu(2)	2.869(1)

Cu(1)−Fe(2)	2.532(1)	Cu(1)−C(10)	1.928(6)
Cu(2)−Fe(1)	2.780(1)	Cu(2)−C(15)	1.926(7)
Fe(3)−Se(1)−Fe(1)	68.86(3)	Se(1)−Fe(1)−Fe(3)	54.93(3)
Fe(3)−Se(1)−Fe(2)	68.41(3)	Cu(1)−Fe(1)−Fe(3)	108.42(4)
Fe(1)−Se(1)−Fe(2)	69.66(3)	Se(1)−Fe(1)−Fe(2)	55.48(3)
Fe(3)−Se(1)−Cu(2)	125.22(4)	Cu(1)−Fe(1)−Fe(2)	58.26(3)
Fe(1)−Se(1)−Cu(2)	71.27(3)	Fe(3)−Fe(1)−Fe(2)	59.16(3)
Fe(2)−Se(1)−Cu(2)	63.38(3)	Se(1)−Fe(1)−Cu(2)	55.82(3)
C(10)−Cu(1)−Fe(1)	150.6(2)	Cu(1)−Fe(1)−Cu(2)	65.50(3)
C(10)−Cu(1)−Fe(2)	144.7(2)	Fe(3)−Fe(1)−Cu(2)	102.01(4)
Fe(1)−Cu(1)−Fe(2)	64.39(3)	Fe(2)−Fe(1)−Cu(2)	54.79(3)
C(10)−Cu(1)−Cu(2)	131.2(2)	Se(1)−Fe(2)−Cu(2)	59.65(3)
Fe(1)−Cu(1)−Cu(2)	61.84(3)	Se(1)−Fe(2)−Cu(1)	106.73(4)
Fe(2)−Cu(1)−Cu(2)	55.09(3)	Cu(2)−Fe(2)−Cu(1)	69.28(4)
C(15)−Cu(2)−Se(1)	125.2(2)	Se(1)−Fe(2)−Fe(3)	54.84(3)
C(15)−Cu(2)−Fe(2)	163.0(2)	Cu(2)−Fe(2)−Fe(3)	109.78(4)
Se(1)−Cu(2)−Fe(2)	56.97(3)	Cu(1)−Fe(2)−Fe(3)	107.81(4)
C(15)−Cu(2)−Fe(1)	135.6(2)	Se(1)−Fe(2)−Fe(1)	54.86(3)
Se(1)−Cu(2)−Fe(1)	52.91(3)	Cu(2)−Fe(2)−Fe(1)	64.53(3)
Fe(2)−Cu(2)−Fe(1)	60.68(3)	Cu(1)−Fe(2)−Fe(1)	57.35(3)
C(15)−Cu(2)−Cu(1)	134.4(2)	Fe(3)−Fe(2)−Fe(1)	59.35(3)
Se(1)−Cu(2)−Cu(1)	95.30(3)	Se(1)−Fe(3)−Fe(2)	56.75(3)
Fe(2)−Cu(2)−Cu(1)	55.63(3)	Se(1)−Fe(3)−Fe(1)	56.21(3)
Fe(1)−Cu(2)−Cu(1)	52.66(3)	Fe(2)−Fe(3)−Fe(1)	61.50(3)
Se(1)−Fe(1)−Cu(1)	108.10(4)		

3			
Fe(1)−Fe(2)	2.696(1)	Cu(1)−Fe(2)	2.495(1)
Fe(1)−Fe(3)	2.615(1)	Cu(2)−Fe(1)	2.531(1)
Fe(2)−Fe(3)	2.620(1)	Cu(2)−Fe(2)	2.780(1)
Fe(1)−Se(1)	2.358(1)	Cu(2)−Se(1)	2.469(1)
Fe(2)−Se(1)	2.341(1)	Cu(1)−Cu(2)	2.832(1)
Fe(3)−Se(1)	2.315(1)	C(10)−Cu(1)	1.929(6)
Cu(1)−Fe(1)	2.560(1)	C(19)−Cu(2)	1.946(6)
C(10)−Cu(1)−Fe(2)	149.8(2)	Cu(2)−Fe(1)−Fe(2)	64.16(3)
C(10)−Cu(1)−Fe(1)	145.7(2)	Cu(1)−Fe(1)−Fe(2)	56.59(3)

Fe(2)−Cu(1)−Fe(1)	64.45(3)	Fe(3)−Fe(1)−Fe(2)	59.09(3)
C(10)−Cu(1)−Cu(2)	126.4(2)	Se(1)−Fe(2)−Cu(1)	108.47(4)
Fe(2)−Cu(1)−Cu(2)	62.53(3)	Se(1)−Fe(2)−Fe(3)	55.28(3)
Fe(1)−Cu(1)−Cu(2)	55.71(3)	Cu(1)−Fe(2)−Fe(3)	108.60(4)
C(19)−Cu(2)−Se(1)	125.2(2)	Se(1)−Fe(2)−Fe(1)	55.28(3)
C(19)−Cu(2)−Fe(1)	162.1(2)	Cu(1)−Fe(2)−Fe(1)	58.95(3)
Se(1)−Cu(2)−Fe(1)	56.26(3)	Fe(3)−Fe(2)−Fe(1)	58.91(3)
Se(1)−Cu(2)−Fe(2)	52.56(3)	Se(1)−Fe(2)−Cu(2)	56.89(3)
Fe(1)−Cu(2)−Fe(2)	60.81(3)	Cu(1)−Fe(2)−Cu(2)	64.69(3)
C(19)−Cu(2)−Cu(1)	134.6(2)	Fe(3)−Feu(2)−Cu(2)	102.99(4)
Se(1)−Cu(2)−Cu(1)	95.27(3)	Fe(1)−Fe(2)−Cu(2)	55.03(3)
Fe(1)−Cu(2)−Cu(1)	56.70(3)	Se(1)−Fe(3)−Fe(1)	56.76(3)
Fe(2)−Cu(2)−Cu(1)	52.78(3)	Se(1)−Fe(3)−Fe(2)	56.22(3)
Se(1)−Fe(1)−Cu(2)	60.55(3)	Fe(1)−Fe(3)−Fe(2)	62.00(3)
Se(1)−Fe(1)−Cu(1)	105.80(4)	Fe(3)−Se(1)−Fe(2)	68.50(4)
Cu(2)−Fe(1)−Cu(1)	67.59(4)	Fe(3)−Se(1)−Fe(1)	68.06(3)
Se(1)−Fe(1)−Fe(3)	55.18(3)	Fe(2)−Se(1)−Fe(1)	70.04(4)
Cu(2)−Fe(1)−Fe(3)	110.43(4)	Fe(3)−Se(1)−Cu(2)	124.12(4)
Cu(1)−Fe(1)−Fe(3)	106.78(4)	Fe(2)−Se(1)−Cu(2)	70.55(3)
Se(1)−Fe(1)−Fe(2)	54.68(3)	Fe(1)−Se(1)−Cu(2)	63.20(3)

4			
Fe(1)−Fe(2)	2.716(1)	Fe(1)−Se(1)	2.334(1)
Fe(1)−Fe(3)	2.615(1)	Fe(2)−Se(1)	2.331(1)
Fe(2)−Fe(3)	2.616(2)	Fe(3)−Se(1)	2.314(1)
Fe(1)−Cu(1)	2.596(1)	Cu(1)−Se(1)	2.501(1)
Fe(1)−Cu(2)	2.504(1)	C(10)−Cu(1)	1.919(6)
Fe(2)−Cu(1)	2.568(1)	C(23)−Cu(2)	1.917(6)
Fe(2)−Cu(2)	2.489(1)		
Se(1)−Fe(1)−Cu(2)	111.12(4)	Fe(3)−Fe(2)−Fe(1)	58.72(3)
Se(1)−Fe(1)−Cu(1)	60.68(4)	Se(1)−Fe(3)−Fe(1)	56.13(3)
Cu(2)−Fe(1)−Cu(1)	83.14(4)	Se(1)−Fe(3)−Fe(2)	56.04(3)
Se(1)−Fe(1)−Fe(3)	55.39(3)	Fe(1)−Fe(3)−Fe(2)	62.55(4)
Cu(2)−Fe(1)−Fe(3)	89.98(5)	C(10)−Cu(1)−Se(1)	128.3(2)
Cu(1)−Fe(1)−Fe(3)	107.24(4)	C(10)−Cu(1)−Fe(2)	150.5(2)
Se(1)−Fe(1)−Fe(2)	54.34(3)	Se(1)−Cu(1)−Fe(2)	54.74(3)
Cu(2)−Fe(1)−Fe(2)	56.79(4)	C(10)−Cu(1)−Fe(1)	145.5(2)

Cu(1)−Fe(1)−Fe(2)	57.76(3)	Se(1)−Cu(1)−Fe(1)	54.46(3)
Fe(3)−Fe(1)−Fe(2)	58.73(4)	Fe(2)−Cu(1)−Fe(1)	63.45(3)
Se(1)−Fe(2)−Cu(2)	111.78(4)	C(23)−Cu(2)−Fe(2)	147.3(2)
Se(1)−Fe(2)−Cu(1)	61.17(4)	C(23)−Cu(2)−Fe(1)	146.6(2)
Cu(2)−Fe(2)−Cu(1)	84.03(4)	Fe(2)−Cu(2)−Fe(1)	65.88(4)
Se(1)−Fe(2)−Fe(3)	55.42(3)	Fe(3)−Se(1)−Fe(2)	68.55(4)
Cu(2)−Fe(2)−Fe(3)	90.31(4)	Fe(3)−Se(1)−Fe(1)	68.48(4)
Cu(1)−Fe(2)−Fe(3)	108.09(4)	Fe(2)−Se(1)−Fe(1)	71.20(4)
Se(1)−Fe(2)−Fe(1)	54.45(4)	Fe(3)−Se(1)−Cu(1)	121.21(4)
Cu(2)−Fe(2)−Fe(1)	57.33(3)	Fe(2)−Se(1)−Cu(1)	64.09(4)
Cu(1)−Fe(2)−Fe(1)	58.79(4)	Fe(1)−Se(1)−Cu(1)	64.85(3)

5			
Fe(1)−Se(1)	2.322(2)	Fe(2)−Cu(2)	2.556(2)
Fe(2)−Se(1)	2.304(2)	Fe(3)−Cu(1)	2.567(2)
Fe(3)−Se(1)	2.313(2)	C(10)−Cu(1)	1.94(1)
Fe(1)−Fe(2)	2.660(2)	C(15)−Cu(2)	1.97(1)
Fe(1)−Fe(3)	2.678(2)	C(12)−Cl(1)	1.703(9)
Fe(2)−Fe(3)	2.617(2)	C(13)−Cl(2)	1.69(1)
Fe(1)−Cu(1)	2.470(2)	C(17)−Cl(3)	1.699(9)
Fe(1)−Cu(2)	2.531(2)	C(18)−Cl(4)	1.71(1)
Se(1)−Fe(1)−Cu(1)	106.46(6)	Se(1)−Fe(3)−Cu(1)	103.67(6)
Se(1)−Fe(1)−Cu(2)	104.11(6)	Se(1)−Fe(3)−Fe(2)	55.31(5)
Cu(1)−Fe(1)−Cu(2)	129.03(7)	Cu(1)−Fe(3)−Fe(2)	109.79(6)
Se(1)−Fe(1)−Fe(2)	54.59(5)	Se(1)−Fe(3)−Fe(1)	54.85(5)
Cu(1)−Fe(1)−Fe(2)	111.47(6)	Cu(1)−Fe(3)−Fe(1)	56.15(5)
Cu(2)−Fe(1)−Fe(2)	58.93(5)	Fe(2)−Fe(3)−Fe(1)	60.29(5)
Se(1)−Fe(1)−Fe(3)	54.54(4)	C(10)−Cu(1)−Fe(1)	157.2(3)
Cu(1)−Fe(1)−Fe(3)	59.65(5)	C(10)−Cu(1)−Fe(3)	138.6(3)
Cu(2)−Fe(1)−Fe(3)	112.45(6)	Fe(1)−Cu(1)−Fe(3)	64.21(5)
Fe(2)−Fe(1)−Fe(3)	58.71(5)	C(15)−Cu(2)−Fe(1)	157.2(3)
Se(1)−Fe(2)−Cu(2)	103.85(6)	C(15)−Cu(2)−Fe(2)	139.7(3)
Se(1)−Fe(2)−Fe(3)	55.63(4)	Fe(1)−Cu(2)−Fe(2)	63.06(5)
Cu(2)−Fe(2)−Fe(3)	113.69(6)	Fe(2)−Se(1)−Fe(3)	69.05(5)
Se(1)−Fe(2)−Fe(1)	55.22(5)	Fe(2)−Se(1)−Fe(1)	70.19(5)
Cu(2)−Fe(2)−Fe(1)	58.01(5)	Fe(3)−Se(1)−Fe(1)	70.60(5)
Fe(3)−Fe(2)−Fe(1)	61.00(5)		

Table S4 Cartesian coordinates of all calculated geometries
$[SeFe_3(CO)_9\{Cu(MeCN)\}_2]$ (**1**)
E = −10759.5767999 a.u.

	x	y	z
C	3.13594	8.33645	2.36137
O	2.00203	8.42725	2.28705
Fe	4.90907	8.20342	2.40925
C	5.32386	9.49254	1.2531
O	5.51881	10.37709	0.54444
C	4.86296	6.75942	1.37398
O	4.67403	5.92281	0.59615
Cu	6.08266	6.0995	3.34422
C	8.21861	6.90925	3.89573
O	9.08069	6.14763	3.85863
Fe	7.08005	8.2838	4.08806
C	8.01266	9.58667	3.2997
O	8.56586	10.48976	2.87123
C	7.65853	8.60119	5.74246
O	8.04967	8.82214	6.7891
C	5.19142	7.17581	6.58624
O	5.47394	7.02458	7.68434
Fe	4.64772	7.40144	4.9073
C	2.98425	7.84703	5.36306
O	1.9375	8.14836	5.69219
C	4.22737	5.70055	4.59588
O	3.77566	4.64801	4.50253
C	6.94801	3.3021	2.47148
N	6.58385	4.32622	2.78625
C	7.41473	1.98838	2.05857
H	6.64516	1.4142	1.86349
H	7.94582	1.59003	2.77907
H	7.96937	2.07738	1.25549
C	9.10076	7.12821	-0.61638
N	8.38494	7.41533	0.19389
C	10.03834	6.75309	-1.67319
H	10.66657	6.08361	-1.33089
H	10.53504	7.54636	-1.96642
H	9.54378	6.37882	-2.43079
Cu	7.23672	7.80376	1.64626

Se	5.16784	9.55356	4.28758

$[SeFe_3(CO)_9\{Cu(Me_2\text{-imy})\}_2]$ (**2**)
E = −11103.5294624 a.u.

	x	y	z
Se	11.20403	8.01196	2.87327
Fe	10.56645	8.50931	5.03306
Fe	10.72185	10.29157	3.10778
Fe	12.93022	9.09758	4.05984
Cu	12.79657	9.28575	1.55445
Cu	12.89084	11.52622	3.34454
C	13.90672	13.16372	3.27814
C	14.38688	9.6132	3.20669
C	11.07695	11.27102	1.66288
C	13.1167	9.05143	-0.33062
C	9.00497	10.21205	2.75279
C	10.54693	11.51413	4.39326
C	13.78464	7.67655	4.72248
C	13.0242	10.11315	5.528
C	8.83388	8.23694	4.94102
C	11.0062	6.92661	5.73113
C	10.46051	9.44838	6.56608
O	7.85947	10.1832	2.53285
O	10.33972	12.29429	5.20719
O	11.14574	11.96739	0.73828
O	13.18939	10.7642	6.4428
O	15.48639	9.89477	2.87327
O	14.3627	6.80025	5.13434
O	7.69708	8.06525	4.89759
O	11.29326	5.90609	6.1416
O	10.32363	9.97855	7.55232
N	13.92665	14.1705	4.1481
C	14.74391	15.18553	3.72503
C	13.15234	14.21995	5.38371
N	14.73919	13.56753	2.28629
C	15.25078	14.81056	2.57348
C	15.0842	12.786	1.11653
N	14.27749	8.95254	-1.01706
C	14.01099	8.74651	-2.35914
C	15.58825	9.00885	-0.43148

N	12.18563	8.90721	-1.27343
C	12.68767	8.70943	-2.50763
C	10.73702	8.90721	-1.02687
H	13.33281	15.04405	5.8418
H	12.21543	14.16776	5.17637
H	13.39676	13.481	5.94547
H	14.90689	15.98628	4.16771
H	15.84643	15.29541	2.04813
H	15.68845	13.28734	0.56317
H	15.50622	11.96877	1.38971
H	14.28791	12.58547	0.6192
H	16.25125	8.91545	-1.12073
H	15.70538	9.85081	0.01261
H	15.68631	8.296	0.20313
H	14.64236	8.65174	-3.03578
H	12.21176	8.57345	-3.29635
H	10.27127	8.78772	-1.85761
H	10.51549	8.19024	-0.42868
H	10.48059	9.74368	-0.63181

$[SeFe_3(CO)_9\{Cu(Me_2\text{-bimy})\}_2]$ (**3**)
E = −114 10.821075 a.u.

	x	y	z
C	5.15852	3.9896	0.8956
O	4.27074	3.70897	0.21455
Fe	6.52368	4.46498	1.91457
C	6.15675	6.17592	1.96024
O	5.84668	7.30985	1.91798
Cu	8.51312	5.85622	2.72809
C	7.69434	4.50158	0.53964
O	8.24863	4.67413	-0.46324
Cu	8.65097	3.10351	2.07711
C	7.15783	5.86305	4.92824
O	6.90334	6.92303	5.33947
Fe	7.58602	4.23478	4.38194
C	9.36965	4.25887	4.3496
O	10.52498	4.25128	4.53814
C	7.62805	3.42454	5.95225
O	7.70336	2.93152	6.98276
C	4.71966	3.59899	5.69219
O	4.49837	3.3449	6.79909
Fe	5.00237	4.03341	3.99721
C	3.55507	3.22733	3.34022
O	2.63227	2.67743	2.955
C	4.32942	5.67722	4.10741
O	3.81189	6.70496	4.20006
C	9.80772	7.20935	2.2642
N	11.05563	6.98181	1.81233
N	9.67414	8.56324	2.25607
C	8.48171	9.28948	2.72906
H	8.62192	10.25275	2.62341
H	7.70131	9.01264	2.20406
H	8.32794	9.08469	3.67505
C	10.83311	9.16623	1.76357
C	11.71638	8.16314	1.49863
C	11.14263	10.52391	1.53926
C	12.38583	10.76093	1.03376
H	10.52884	11.22361	1.72619

C	13.30594	9.73319	0.78345
H	12.63859	11.65594	0.84521
C	12.98435	8.42292	0.99963
H	14.17038	9.95315	0.45674
H	13.60031	7.72322	0.81596
C	11.67486	5.65257	1.74732
H	12.58234	5.73221	1.38647
H	11.71327	5.26575	2.64779
H	11.14081	5.07234	1.16542
C	10.09678	1.86965	1.65954
N	10.94281	1.7976	0.62416
N	10.38333	0.8002	2.45925
C	11.01183	2.71725	-0.486
H	11.71901	2.43093	-1.10365
H	10.15242	2.72674	-0.95737
H	11.21208	3.61605	-0.15441
C	11.82513	0.71676	0.76557
C	11.47071	0.07395	1.92611
C	12.88296	0.27116	-0.0065
C	13.57623	-0.83622	0.45999
H	13.12334	0.70349	-0.81758
C	13.17759	-1.47904	1.62541
H	14.32977	-1.15668	-0.02113
C	12.11932	-1.0486	2.39911
H	13.65437	-2.25269	1.90173
H	11.85652	-1.49041	3.19881
C	9.74937	0.49112	3.72707
H	10.13851	-0.32804	4.09603
H	9.89463	1.23253	4.35285
H	8.78753	0.36407	3.58891
Se	6.5438	2.49616	3.21165

$[SeFe_3(CO)_9\{Cu(^iPr_2\text{-bimy})\}_2]$ (**4**)
E = −11725.2010467 a.u.

	x	y	z
C	0.87071	3.66831	6.42685
O	0.67225	4.14356	7.45374
Fe	1.21178	2.98567	4.8417
C	1.55763	1.3525	5.4716
O	1.93329	0.38863	5.98153
Cu	-0.2991	1.02158	4.06683
C	2.85024	3.63818	4.77624
O	3.90363	4.11091	4.93076
Cu	2.72256	2.14225	3.03108
C	0.63912	0.98319	1.86554
O	0.82786	-0.06816	1.40478
Fe	0.42181	2.69685	2.25972
C	1.65605	3.41791	1.24042
O	2.38797	3.84215	0.43969
C	-0.88419	2.94227	1.07887
O	-1.71427	3.09923	0.3245
C	2.18021	5.70605	2.87136
O	3.18494	6.1819	2.54967
Fe	0.60426	5.05871	3.36809
C	-0.38218	5.86766	2.13385
O	-1.02711	6.38506	1.34999
C	0.34089	6.16697	4.7074
O	0.14469	6.88101	5.59382
C	-1.36743	-0.46902	4.63014
N	-2.50895	-0.36686	5.33815
N	-1.24025	-1.79646	4.36604
C	-3.00973	0.91445	5.89303
C	-4.28384	1.32932	5.21874
C	-3.10299	0.84216	7.40598
H	-2.32635	1.61035	5.6781
H	-4.59512	2.17634	5.60225
H	-4.12232	1.44445	4.25928
H	-4.96625	0.63928	5.355
H	-3.43513	1.6956	7.75436
H	-3.71852	0.12296	7.66305

H	-2.21523	0.66033	7.77965
C	-3.15432	-1.60889	5.4997
C	-4.33243	-1.97948	6.09251
C	-2.31913	-2.51694	4.86474
C	-4.64535	-3.33438	6.06301
H	-4.90627	-1.34441	6.50411
C	-3.8129	-4.23196	5.44772
H	-5.44558	-3.64084	6.47321
C	-2.65289	-3.87768	4.84929
H	-4.06303	-5.14785	5.4407
H	-2.09045	-4.52206	4.43769
C	-0.07341	-2.36152	3.64258
C	-0.47915	-2.98804	2.34317
C	0.69119	-3.30753	4.5894
H	0.53777	-1.60099	3.42625
H	1.46286	-3.68579	4.12021
H	0.99816	-2.80713	5.37327
H	0.0965	-4.03257	4.87738
H	0.31313	-3.34826	1.89223
H	-1.11674	-3.71245	2.51455
H	-0.89906	-2.31061	1.77142
C	4.43941	1.41025	2.59041
N	5.52444	2.0399	2.07766
N	4.79917	0.10767	2.73791
C	3.90654	-0.90047	3.28156
C	3.63195	-2.01389	2.27995
C	4.41113	-1.42335	4.6175
H	3.03208	-0.44871	3.45856
H	3.02872	-2.6726	2.68031
H	3.21585	-1.63506	1.47642
H	4.47552	-2.44815	2.03552
H	3.79002	-2.10067	4.95886
H	5.2976	-1.82331	4.49809
H	4.4704	-0.68241	5.25667
C	6.1048	-0.08719	2.2954
C	6.57161	1.14331	1.87538
C	6.93449	-1.20686	2.26028
C	8.18867	-1.04303	1.77283

H	6.63216	-2.05303	2.56793
C	8.67254	0.19097	1.34156
H	8.76101	-1.79937	1.72085
C	7.8636	1.30074	1.37528
H	9.56424	0.26448	1.02408
H	8.17333	2.14516	1.06903
C	5.56082	3.50264	1.85852
C	5.7791	3.86778	0.39474
C	6.57101	4.1561	2.80393
H	4.65967	3.85363	2.11278
H	6.58503	5.12331	2.648
H	6.31366	3.9781	3.73249
H	7.46248	3.78586	2.63536
H	5.79544	4.84311	0.30062
H	6.63196	3.49527	0.0885
H	5.04942	3.49945	-0.1461
Se	-0.9213	3.44294	4.01218

$[SeFe_3(CO)_9\{Cu(Me_2\text{-}Cl_2\text{-}imy)\}_2]$ (**5**)
E = −12941.925486 a.u.

	x	y	z
C	3.35334	15.80195	6.36432
O	2.81717	16.54812	7.10295
Fe	4.00258	14.51185	5.33626
Cu	4.98193	16.7536	4.99211
C	5.78444	14.56532	5.40258
O	6.9557	14.55369	5.48549
Cu	5.09652	12.24198	5.102
C	3.65699	13.28684	6.54671
O	3.38122	12.59879	7.44664
C	5.57614	13.04974	2.61989
O	6.71183	12.98466	2.28223
Fe	3.86355	13.14993	3.05599
C	3.48029	11.47606	3.52283
O	3.14047	10.36959	3.70222
C	3.28975	12.91027	1.40341
O	2.90407	12.70339	0.3452
C	3.0066	15.86704	1.35517
O	2.54134	15.98326	0.32711
Fe	3.72768	15.7622	2.98378
C	3.29136	17.44072	3.34797
O	2.96958	18.56113	3.46555
C	5.42175	15.94142	2.48875
O	6.51172	16.09716	2.10888
C	5.95464	18.36355	5.4463
N	7.23688	18.65179	5.14331
N	5.44605	19.53742	5.92566
C	4.04767	19.70014	6.3809
H	3.57399	18.84705	6.29045
H	4.04092	19.97908	7.31851
H	3.60399	20.37889	5.8322
C	6.39261	20.51371	5.91058
C	7.5137	19.9814	5.386
Cl	6.09391	22.11436	6.40682
Cl	9.00101	20.69805	5.01171
C	8.20692	17.70107	4.65189

H	9.06366	18.15435	4.50718
H	8.32385	16.9828	5.30762
H	7.89253	17.32217	3.80472
C	6.08964	10.63691	5.6694
N	5.60075	9.49791	6.17438
N	7.37274	10.37424	5.3453
C	8.2914	11.34821	4.78303
H	9.16288	10.92515	4.63229
H	7.93683	11.67596	3.92984
H	8.39458	12.0967	5.4056
C	7.65491	9.0423	5.58649
C	6.55852	8.52162	6.13669
Cl	9.15475	8.33473	5.21551
Cl	6.287	6.9126	6.6551
C	4.24901	9.32357	6.69595
H	4.13599	8.40074	7.00647
H	4.10389	9.93956	7.44212
H	3.59902	9.50953	5.98595
Se	2.14065	14.38796	3.95471