Versatile N2S2 nickel-dithiolates as mono-and bridging bidentate, S-donor ligands to gold(I)

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Supporting Information

Versatile N_2S_2 Nickel-dithiolates as Mono- and Bridging Bidentate, S-donor Ligands to Gold(I)

Tiffany A. Pinder, Steven K. Montalvo, Allen M. Lunsford, Chung-Hung Hsieh, Joseph H. Reibenspies, and Marcetta Y. Darensbourg*

Department of Chemistry, Texas A&M University, College Station, Texas 77843
Email: marcetta@chem.tamu.edu

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Table S1. Crystal data and structure refinement for [{Ni(bme-daco)}$AuPPh_3$]$^+$ Cl^- (**1**).

Identification code	datax	
Empirical formula	C28 H37 Au Cl N2 Ni O P S2	
Formula weight	803.81	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 16.697(3) Å	α = 90°.
	b = 11.0833(19) Å	β = 102.978(2)°.
	c = 16.059(3) Å	γ = 90°.
Volume	2896.1(8) $Å^3$	
Z	4	
Density (calculated)	1.844 Mg/m^3	
Absorption coefficient	6.027 mm^{-1}	
F(000)	1592	
Crystal size	0.11 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.22 to 28.33°.	
Index ranges	-22<=h<=22, -14<=k<=14, -21<=l<=21	
Reflections collected	33863	
Independent reflections	7153 [R(int) = 0.0370]	
Completeness to theta = 28.33°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6442 and 0.5569	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7153 / 0 / 342	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0214, wR2 = 0.0508	
R indices (all data)	R1 = 0.0244, wR2 = 0.0517	
Largest diff. peak and hole	0.813 and -1.292 e.$Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for [{Ni(bme-daco)}$AuPPh_3$]$^+$ Cl^- (**1**).

Au(1)-P(1)	2.2542(7)	C(6)-H(6B)	0.9900
Au(1)-S(1)	2.3329(7)	C(7)-H(7A)	0.9900
Au(1)-Ni(1)	2.9533(6)	C(7)-H(7B)	0.9900
Ni(1)-N(2)	1.974(2)	C(8)-C(9)	1.524(4)
Ni(1)-N(1)	1.980(2)	C(8)-H(8A)	0.9900
Ni(1)-S(2)	2.1706(8)	C(8)-H(8B)	0.9900
Ni(1)-S(1)	2.1854(7)	C(9)-C(10)	1.523(4)
S(1)-C(1)	1.829(3)	C(9)-H(9A)	0.9900
S(2)-C(3)	1.820(3)	C(9)-H(9B)	0.9900
N(1)-C(5)	1.502(3)	C(10)-H(10A)	0.9900
N(1)-C(8)	1.503(3)	C(10)-H(10B)	0.9900
N(1)-C(2)	1.506(3)	C(11)-C(16)	1.394(3)
N(2)-C(4)	1.506(3)	C(11)-C(12)	1.399(3)
N(2)-C(7)	1.508(3)	C(12)-C(13)	1.389(4)
N(2)-C(10)	1.509(3)	C(12)-H(12)	0.9500
P(1)-C(11)	1.807(2)	C(13)-C(14)	1.383(4)
P(1)-C(23)	1.811(2)	C(13)-H(13)	0.9500
P(1)-C(17)	1.815(2)	C(14)-C(15)	1.389(4)
C(1)-C(2)	1.501(4)	C(14)-H(14)	0.9500
C(1)-H(1A)	0.9900	C(15)-C(16)	1.389(4)
C(1)-H(1B)	0.9900	C(15)-H(15)	0.9500
C(2)-H(2A)	0.9900	C(16)-H(16)	0.9500
C(2)-H(2B)	0.9900	C(17)-C(22)	1.393(3)
C(3)-C(4)	1.504(4)	C(17)-C(18)	1.397(3)
C(3)-H(3A)	0.9900	C(18)-C(19)	1.390(4)
C(3)-H(3B)	0.9900	C(18)-H(18)	0.9500
C(4)-H(4A)	0.9900	C(19)-C(20)	1.385(4)
C(4)-H(4B)	0.9900	C(19)-H(19)	0.9500
C(5)-C(6)	1.513(3)	C(20)-C(21)	1.387(4)
C(5)-H(5A)	0.9900	C(20)-H(20)	0.9500
C(5)-H(5B)	0.9900	C(21)-C(22)	1.383(4)
C(6)-C(7)	1.508(4)	C(21)-H(21)	0.9500
C(6)-H(6A)	0.9900	C(22)-H(22)	0.9500

C(23)-C(28)	1.392(3)	C(2)-N(1)-Ni(1)	112.15(15)
C(23)-C(24)	1.397(3)	C(4)-N(2)-C(7)	109.2(2)
C(24)-C(25)	1.380(3)	C(4)-N(2)-C(10)	107.7(2)
C(24)-H(24)	0.9500	C(7)-N(2)-C(10)	109.6(2)
C(25)-C(26)	1.393(4)	C(4)-N(2)-Ni(1)	110.35(16)
C(25)-H(25)	0.9500	C(7)-N(2)-Ni(1)	108.47(15)
C(26)-C(27)	1.390(4)	C(10)-N(2)-Ni(1)	111.47(16)
C(26)-H(26)	0.9500	C(11)-P(1)-C(23)	105.64(11)
C(27)-C(28)	1.386(3)	C(11)-P(1)-C(17)	105.11(11)
C(27)-H(27)	0.9500	C(23)-P(1)-C(17)	105.00(11)
C(28)-H(28)	0.9500	C(11)-P(1)-Au(1)	114.19(8)
O(1)-H(1)	0.79(5)	C(23)-P(1)-Au(1)	110.46(8)
O(1)-H(2)	0.81(5)	C(17)-P(1)-Au(1)	115.56(8)
		C(2)-C(1)-S(1)	108.65(17)
P(1)-Au(1)-S(1)	176.16(2)	C(2)-C(1)-H(1A)	110.0
P(1)-Au(1)-Ni(1)	129.446(17)	S(1)-C(1)-H(1A)	110.0
S(1)-Au(1)-Ni(1)	47.052(17)	C(2)-C(1)-H(1B)	110.0
N(2)-Ni(1)-N(1)	90.69(9)	S(1)-C(1)-H(1B)	110.0
N(2)-Ni(1)-S(2)	91.18(7)	H(1A)-C(1)-H(1B)	108.3
N(1)-Ni(1)-S(2)	170.72(6)	C(1)-C(2)-N(1)	111.2(2)
N(2)-Ni(1)-S(1)	171.05(6)	C(1)-C(2)-H(2A)	109.4
N(1)-Ni(1)-S(1)	90.52(6)	N(1)-C(2)-H(2A)	109.4
S(2)-Ni(1)-S(1)	89.05(3)	C(1)-C(2)-H(2B)	109.4
N(2)-Ni(1)-Au(1)	137.36(6)	N(1)-C(2)-H(2B)	109.4
N(1)-Ni(1)-Au(1)	93.21(6)	H(2A)-C(2)-H(2B)	108.0
S(2)-Ni(1)-Au(1)	79.30(2)	C(4)-C(3)-S(2)	106.78(19)
S(1)-Ni(1)-Au(1)	51.385(18)	C(4)-C(3)-H(3A)	110.4
C(1)-S(1)-Ni(1)	97.53(9)	S(2)-C(3)-H(3A)	110.4
C(1)-S(1)-Au(1)	106.57(9)	C(4)-C(3)-H(3B)	110.4
Ni(1)-S(1)-Au(1)	81.56(2)	S(2)-C(3)-H(3B)	110.4
C(3)-S(2)-Ni(1)	96.92(9)	H(3A)-C(3)-H(3B)	108.6
C(5)-N(1)-C(8)	111.53(19)	C(3)-C(4)-N(2)	111.2(2)
C(5)-N(1)-C(2)	105.16(18)	C(3)-C(4)-H(4A)	109.4
C(8)-N(1)-C(2)	109.14(19)	N(2)-C(4)-H(4A)	109.4
C(5)-N(1)-Ni(1)	108.02(15)	C(3)-C(4)-H(4B)	109.4
C(8)-N(1)-Ni(1)	110.74(15)	N(2)-C(4)-H(4B)	109.4

H(4A)-C(4)-H(4B)	108.0	H(10A)-C(10)-H(10B)	107.8
N(1)-C(5)-C(6)	115.0(2)	C(16)-C(11)-C(12)	119.7(2)
N(1)-C(5)-H(5A)	108.5	C(16)-C(11)-P(1)	121.29(18)
C(6)-C(5)-H(5A)	108.5	C(12)-C(11)-P(1)	118.96(18)
N(1)-C(5)-H(5B)	108.5	C(13)-C(12)-C(11)	119.7(2)
C(6)-C(5)-H(5B)	108.5	C(13)-C(12)-H(12)	120.1
H(5A)-C(5)-H(5B)	107.5	C(11)-C(12)-H(12)	120.1
C(7)-C(6)-C(5)	114.2(2)	C(14)-C(13)-C(12)	120.2(2)
C(7)-C(6)-H(6A)	108.7	C(14)-C(13)-H(13)	119.9
C(5)-C(6)-H(6A)	108.7	C(12)-C(13)-H(13)	119.9
C(7)-C(6)-H(6B)	108.7	C(13)-C(14)-C(15)	120.4(2)
C(5)-C(6)-H(6B)	108.7	C(13)-C(14)-H(14)	119.8
H(6A)-C(6)-H(6B)	107.6	C(15)-C(14)-H(14)	119.8
C(6)-C(7)-N(2)	113.3(2)	C(16)-C(15)-C(14)	119.8(2)
C(6)-C(7)-H(7A)	108.9	C(16)-C(15)-H(15)	120.1
N(2)-C(7)-H(7A)	108.9	C(14)-C(15)-H(15)	120.1
C(6)-C(7)-H(7B)	108.9	C(15)-C(16)-C(11)	120.2(2)
N(2)-C(7)-H(7B)	108.9	C(15)-C(16)-H(16)	119.9
H(7A)-C(7)-H(7B)	107.7	C(11)-C(16)-H(16)	119.9
N(1)-C(8)-C(9)	113.3(2)	C(22)-C(17)-C(18)	119.8(2)
N(1)-C(8)-H(8A)	108.9	C(22)-C(17)-P(1)	118.28(19)
C(9)-C(8)-H(8A)	108.9	C(18)-C(17)-P(1)	121.80(18)
N(1)-C(8)-H(8B)	108.9	C(19)-C(18)-C(17)	119.8(2)
C(9)-C(8)-H(8B)	108.9	C(19)-C(18)-H(18)	120.1
H(8A)-C(8)-H(8B)	107.7	C(17)-C(18)-H(18)	120.1
C(10)-C(9)-C(8)	116.3(2)	C(20)-C(19)-C(18)	120.0(3)
C(10)-C(9)-H(9A)	108.2	C(20)-C(19)-H(19)	120.0
C(8)-C(9)-H(9A)	108.2	C(18)-C(19)-H(19)	120.0
C(10)-C(9)-H(9B)	108.2	C(19)-C(20)-C(21)	120.3(2)
C(8)-C(9)-H(9B)	108.2	C(19)-C(20)-H(20)	119.8
H(9A)-C(9)-H(9B)	107.4	C(21)-C(20)-H(20)	119.8
N(2)-C(10)-C(9)	113.0(2)	C(22)-C(21)-C(20)	120.1(3)
N(2)-C(10)-H(10A)	109.0	C(22)-C(21)-H(21)	119.9
C(9)-C(10)-H(10A)	109.0	C(20)-C(21)-H(21)	119.9
N(2)-C(10)-H(10B)	109.0	C(21)-C(22)-C(17)	120.0(2)
C(9)-C(10)-H(10B)	109.0	C(21)-C(22)-H(22)	120.0

C(17)-C(22)-H(22)	120.0	C(27)-C(26)-C(25)	120.1(2)
C(28)-C(23)-C(24)	119.8(2)	C(27)-C(26)-H(26)	119.9
C(28)-C(23)-P(1)	122.66(18)	C(25)-C(26)-H(26)	119.9
C(24)-C(23)-P(1)	117.49(18)	C(28)-C(27)-C(26)	120.1(3)
C(25)-C(24)-C(23)	120.2(2)	C(28)-C(27)-H(27)	119.9
C(25)-C(24)-H(24)	119.9	C(26)-C(27)-H(27)	119.9
C(23)-C(24)-H(24)	119.9	C(27)-C(28)-C(23)	119.8(2)
C(24)-C(25)-C(26)	119.8(2)	C(27)-C(28)-H(28)	120.1
C(24)-C(25)-H(25)	120.1	C(23)-C(28)-H(28)	120.1
C(26)-C(25)-H(25)	120.1	H(1)-O(1)-H(2)	109(4)

Symmetry transformations used to generate equivalent atoms:

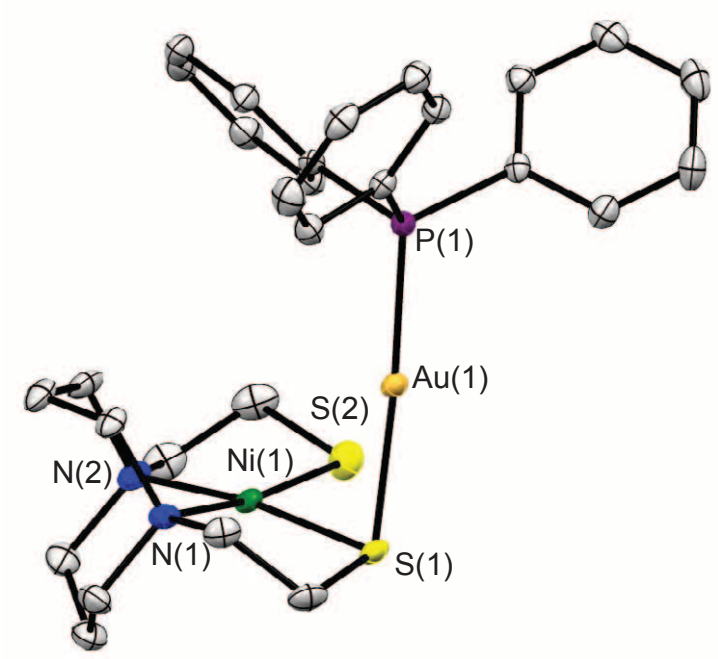

Figure S1. TEP of complex **1** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, the Cl^- counterion, and the H_2O of crystallization are not shown.

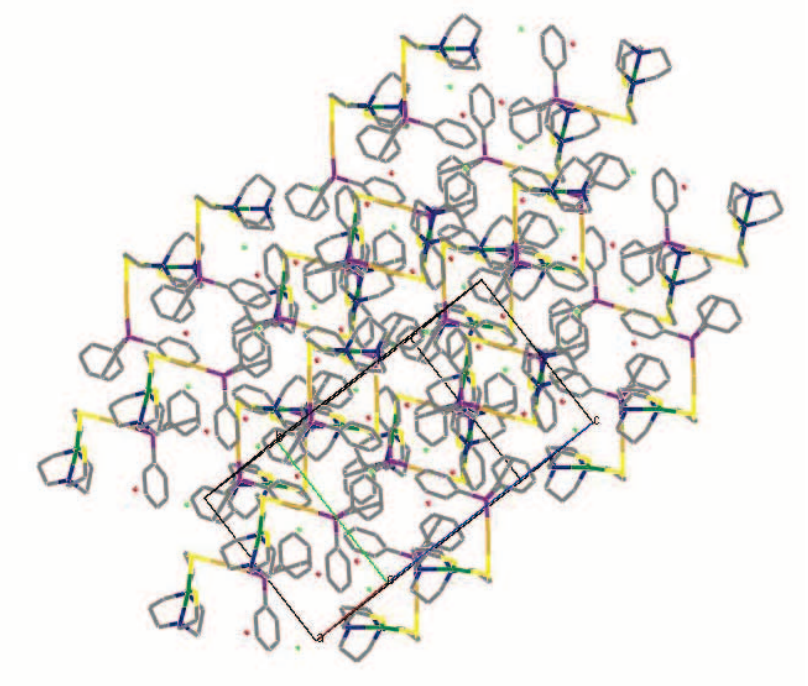

Figure S2. The packing diagram of complex **1** in capped stick drawing.

Table S3. Crystal data and structure refinement for $[Au_2\{Ni(bme\text{-}daco)\}_2]^{2+}(Cl^-)_2$ (**2**).

Identification code	041213nibmedacoapph3inmeoh_0m-sr	
Empirical formula	C22 H48 Au2 Cl2 N4 Ni2 O2 S4	
Formula weight	1111.14	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 8.661(2) Å	α = 90°.
	b = 15.988(4) Å	β = 100.346(3)°.
	c = 13.637(3) Å	γ = 90°.
Volume	1857.5(8) $Å^3$	
Z	2	
Density (calculated)	1.987 Mg/m^3	
Absorption coefficient	9.265 mm^{-1}	
F(000)	1072	
Crystal size	0.30 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.98 to 28.28°.	
Index ranges	-11<=h<=11, 0<=k<=21, 0<=l<=18	
Reflections collected	4584	
Independent reflections	4584 [R(int) = 0.0000]	
Completeness to theta = 28.28°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4576 and 0.1676	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4584 / 0 / 174	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0198, wR2 = 0.0474	
R indices (all data)	R1 = 0.0234, wR2 = 0.0483	
Largest diff. peak and hole	1.041 and -1.301 $e.Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for $[Au_2\{Ni(bme\text{-}daco)\}_2]^{2+}(Cl^-)_2$ (**2**).

Au(1)-S(2)#1	2.3000(8)	C(7)-H(7B)	0.9700
Au(1)-S(1)	2.3040(8)	C(8)-C(9)	1.507(4)
Au(1)-Au(1)#1	3.1273(5)	C(8)-H(8A)	0.9700
Au(1)-Ni(1)	3.1782(6)	C(8)-H(8B)	0.9700
Ni(1)-N(2)	1.968(2)	C(9)-C(10)	1.510(4)
Ni(1)-N(1)	1.985(2)	C(9)-H(9A)	0.9700
Ni(1)-S(1)	2.1800(8)	C(9)-H(9B)	0.9700
Ni(1)-S(2)	2.1921(9)	C(10)-H(10A)	0.9700
N(1)-C(8)	1.500(3)	C(10)-H(10B)	0.9700
N(1)-C(2)	1.504(3)	C(11)-O(1)	1.413(3)
N(1)-C(7)	1.509(3)	C(11)-H(11A)	0.9600
N(2)-C(4)	1.498(3)	C(11)-H(11B)	0.9600
N(2)-C(10)	1.504(3)	C(11)-H(11C)	0.9600
N(2)-C(5)	1.511(3)	O(1)-H(1)	0.8200
S(1)-C(1)	1.829(3)		
S(2)-C(3)	1.827(3)	S(2)#1-Au(1)-S(1)	177.98(2)
S(2)-Au(1)#1	2.3000(8)	S(2)#1-Au(1)-Au(1)#1	87.601(19)
C(1)-C(2)	1.505(4)	S(1)-Au(1)-Au(1)#1	90.47(2)
C(1)-H(1A)	0.9700	S(2)#1-Au(1)-Ni(1)	134.891(19)
C(1)-H(1B)	0.9700	S(1)-Au(1)-Ni(1)	43.308(18)
C(2)-H(2A)	0.9700	Au(1)#1-Au(1)-Ni(1)	61.631(14)
C(2)-H(2B)	0.9700	N(2)-Ni(1)-N(1)	90.47(8)
C(3)-C(4)	1.501(4)	N(2)-Ni(1)-S(1)	174.46(6)
C(3)-H(3A)	0.9700	N(1)-Ni(1)-S(1)	90.44(6)
C(3)-H(3B)	0.9700	N(2)-Ni(1)-S(2)	90.17(6)
C(4)-H(4A)	0.9700	N(1)-Ni(1)-S(2)	175.23(7)
C(4)-H(4B)	0.9700	S(1)-Ni(1)-S(2)	88.47(3)
C(5)-C(6)	1.523(3)	N(2)-Ni(1)-Au(1)	138.87(6)
C(5)-H(5A)	0.9700	N(1)-Ni(1)-Au(1)	94.42(6)
C(5)-H(5B)	0.9700	S(1)-Ni(1)-Au(1)	46.46(2)
C(6)-C(7)	1.530(3)	S(2)-Ni(1)-Au(1)	88.20(2)
C(6)-H(6A)	0.9700	C(8)-N(1)-C(2)	104.81(19)
C(6)-H(6B)	0.9700	C(8)-N(1)-C(7)	109.89(19)
C(7)-H(7A)	0.9700	C(2)-N(1)-C(7)	110.0(2)

C(8)-N(1)-Ni(1)	113.50(16)	N(2)-C(4)-H(4B)	109.2
C(2)-N(1)-Ni(1)	111.96(15)	C(3)-C(4)-H(4B)	109.2
C(7)-N(1)-Ni(1)	106.71(15)	H(4A)-C(4)-H(4B)	107.9
C(4)-N(2)-C(10)	104.50(19)	N(2)-C(5)-C(6)	113.8(2)
C(4)-N(2)-C(5)	109.87(18)	N(2)-C(5)-H(5A)	108.8
C(10)-N(2)-C(5)	110.40(19)	C(6)-C(5)-H(5A)	108.8
C(4)-N(2)-Ni(1)	112.47(15)	N(2)-C(5)-H(5B)	108.8
C(10)-N(2)-Ni(1)	113.53(15)	C(6)-C(5)-H(5B)	108.8
C(5)-N(2)-Ni(1)	106.12(15)	H(5A)-C(5)-H(5B)	107.7
C(1)-S(1)-Ni(1)	98.35(8)	C(5)-C(6)-C(7)	118.6(2)
C(1)-S(1)-Au(1)	106.11(10)	C(5)-C(6)-H(6A)	107.7
Ni(1)-S(1)-Au(1)	90.23(3)	C(7)-C(6)-H(6A)	107.7
C(3)-S(2)-Ni(1)	97.82(9)	C(5)-C(6)-H(6B)	107.7
C(3)-S(2)-Au(1)#1	105.62(9)	C(7)-C(6)-H(6B)	107.7
Ni(1)-S(2)-Au(1)#1	91.93(3)	H(6A)-C(6)-H(6B)	107.1
C(2)-C(1)-S(1)	108.48(18)	N(1)-C(7)-C(6)	112.8(2)
C(2)-C(1)-H(1A)	110.0	N(1)-C(7)-H(7A)	109.0
S(1)-C(1)-H(1A)	110.0	C(6)-C(7)-H(7A)	109.0
C(2)-C(1)-H(1B)	110.0	N(1)-C(7)-H(7B)	109.0
S(1)-C(1)-H(1B)	110.0	C(6)-C(7)-H(7B)	109.0
H(1A)-C(1)-H(1B)	108.4	H(7A)-C(7)-H(7B)	107.8
N(1)-C(2)-C(1)	111.8(2)	N(1)-C(8)-C(9)	114.7(2)
N(1)-C(2)-H(2A)	109.2	N(1)-C(8)-H(8A)	108.6
C(1)-C(2)-H(2A)	109.2	C(9)-C(8)-H(8A)	108.6
N(1)-C(2)-H(2B)	109.2	N(1)-C(8)-H(8B)	108.6
C(1)-C(2)-H(2B)	109.2	C(9)-C(8)-H(8B)	108.6
H(2A)-C(2)-H(2B)	107.9	H(8A)-C(8)-H(8B)	107.6
C(4)-C(3)-S(2)	107.84(17)	C(8)-C(9)-C(10)	113.1(2)
C(4)-C(3)-H(3A)	110.1	C(8)-C(9)-H(9A)	109.0
S(2)-C(3)-H(3A)	110.1	C(10)-C(9)-H(9A)	109.0
C(4)-C(3)-H(3B)	110.1	C(8)-C(9)-H(9B)	109.0
S(2)-C(3)-H(3B)	110.1	C(10)-C(9)-H(9B)	109.0
H(3A)-C(3)-H(3B)	108.5	H(9A)-C(9)-H(9B)	107.8
N(2)-C(4)-C(3)	111.8(2)	N(2)-C(10)-C(9)	114.3(2)
N(2)-C(4)-H(4A)	109.2	N(2)-C(10)-H(10A)	108.7
C(3)-C(4)-H(4A)	109.2	C(9)-C(10)-H(10A)	108.7

N(2)-C(10)-H(10B)	108.7	H(11A)-C(11)-H(11B)	109.5
C(9)-C(10)-H(10B)	108.7	O(1)-C(11)-H(11C)	109.5
H(10A)-C(10)-H(10B)	107.6	H(11A)-C(11)-H(11C)	109.5
O(1)-C(11)-H(11A)	109.5	H(11B)-C(11)-H(11C)	109.5
O(1)-C(11)-H(11B)	109.5	C(11)-O(1)-H(1)	109.5

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

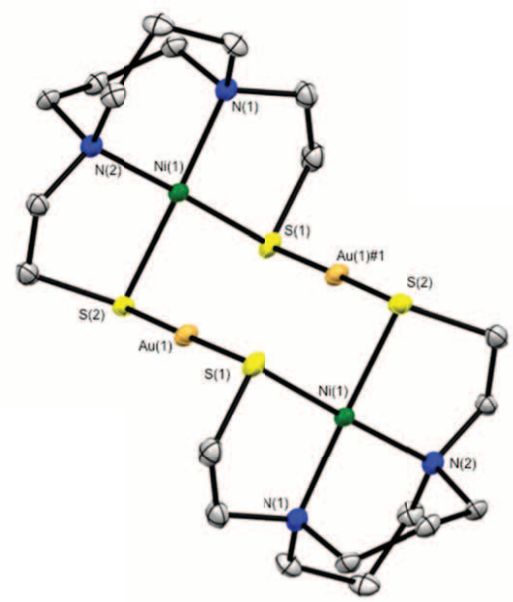

Figure S3. TEP of complex **2** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, the Cl^- counterion, and the MeOH of crystallization are not shown.

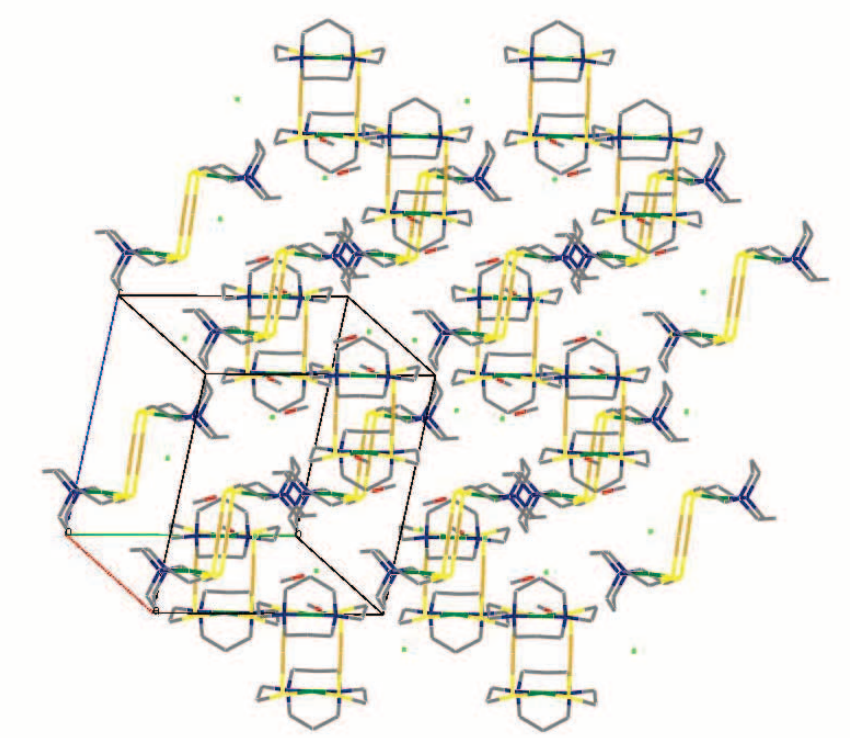

Figure S4. The packing diagram of complex **2** in capped stick drawing.

Table S5. Crystal data and structure refinement for $[Au_2\{Ni(bme\text{-}dach)\}_2]^{2+}(Cl^-)_2$ (**3**).

Identification code	mdau	
Empirical formula	C10 H22 Au Cl N2 Ni O S2	
Formula weight	541.54	
Temperature	110(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 8.3017(7) Å	α = 90°.
	b = 8.6040(8) Å	β = 95.316(5)°.
	c = 21.8658(17) Å	γ = 90°.
Volume	1555.1(2) $Å^3$	
Z	4	
Density (calculated)	2.313 Mg/m^3	
Absorption coefficient	22.996 mm^{-1}	
F(000)	1040	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	5.53 to 64.01°.	
Index ranges	-9<=h<=9, -9<=k<=9, -24<=l<=25	
Reflections collected	25177	
Independent reflections	2554 [R(int) = 0.0626]	
Completeness to theta = 64.01°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2331 and 0.0259	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2554 / 0 / 164	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0607	
R indices (all data)	R1 = 0.0292, wR2 = 0.0617	
Largest diff. peak and hole	0.797 and -1.532 $e.Å^{-3}$	

Table S6. Bond lengths [Å] and angles [°] for $[Au_2\{Ni(bme\text{-}dach)\}_2]^{2+}(Cl^-)_2$ (**3**).

Au(1)-S(2)#1	2.2946(13)	C(7)-H(7A)	0.9900
Au(1)-S(1)	2.2995(12)	C(7)-H(7B)	0.9900
Au(1)-Au(1)#1	3.1103(5)	C(8)-C(9)	1.534(7)
Ni(1)-N(2)	1.922(4)	C(8)-H(8A)	0.9900
Ni(1)-N(1)	1.926(4)	C(8)-H(8B)	0.9900
Ni(1)-S(2)	2.1802(14)	C(9)-H(9A)	0.9900
Ni(1)-S(1)	2.1845(15)	C(9)-H(9B)	0.9900
S(1)-C(1)	1.848(5)	C(1ME)-H(1MA)	0.9800
S(2)-C(5)	1.829(5)	C(1ME)-H(1MB)	0.9800
S(2)-Au(1)#1	2.2946(13)	C(1ME)-H(1MC)	0.9800
O(1ME)-C(1ME)	1.418(7)		
O(1ME)-H(1ME)	0.8653	S(2)#1-Au(1)-S(1)	177.35(4)
N(1)-C(7)	1.498(6)	S(2)#1-Au(1)-Au(1)#1	90.33(3)
N(1)-C(6)	1.498(6)	S(1)-Au(1)-Au(1)#1	92.28(3)
N(1)-C(4)	1.503(6)	N(2)-Ni(1)-N(1)	82.57(17)
N(2)-C(3)	1.494(6)	N(2)-Ni(1)-S(2)	173.42(13)
N(2)-C(9)	1.495(7)	N(1)-Ni(1)-S(2)	91.03(13)
N(2)-C(2)	1.515(6)	N(2)-Ni(1)-S(1)	91.34(13)
C(1)-C(2)	1.489(7)	N(1)-Ni(1)-S(1)	172.17(13)
C(1)-H(1A)	0.9900	S(2)-Ni(1)-S(1)	94.90(6)
C(1)-H(1B)	0.9900	C(1)-S(1)-Ni(1)	96.90(17)
C(2)-H(2A)	0.9900	C(1)-S(1)-Au(1)	103.18(18)
C(2)-H(2B)	0.9900	Ni(1)-S(1)-Au(1)	93.13(5)
C(3)-C(4)	1.544(7)	C(5)-S(2)-Ni(1)	97.57(17)
C(3)-H(3A)	0.9900	C(5)-S(2)-Au(1)#1	105.16(17)
C(3)-H(3B)	0.9900	Ni(1)-S(2)-Au(1)#1	94.40(5)
C(4)-H(4A)	0.9900	C(1ME)-O(1ME)-H(1ME)	133.1
C(4)-H(4B)	0.9900	C(7)-N(1)-C(6)	110.8(4)
C(5)-C(6)	1.512(7)	C(7)-N(1)-C(4)	110.1(4)
C(5)-H(5A)	0.9900	C(6)-N(1)-C(4)	110.2(4)
C(5)-H(5B)	0.9900	C(7)-N(1)-Ni(1)	104.0(3)
C(6)-H(6A)	0.9900	C(6)-N(1)-Ni(1)	112.8(3)
C(6)-H(6B)	0.9900	C(4)-N(1)-Ni(1)	108.7(3)
C(7)-C(8)	1.531(7)	C(3)-N(2)-C(9)	111.1(4)

C(3)-N(2)-C(2)	110.6(4)	S(2)-C(5)-H(5B)	109.8
C(9)-N(2)-C(2)	109.6(4)	H(5A)-C(5)-H(5B)	108.3
C(3)-N(2)-Ni(1)	107.6(3)	N(1)-C(6)-C(5)	110.0(4)
C(9)-N(2)-Ni(1)	106.4(3)	N(1)-C(6)-H(6A)	109.7
C(2)-N(2)-Ni(1)	111.6(3)	C(5)-C(6)-H(6A)	109.7
C(2)-C(1)-S(1)	108.9(3)	N(1)-C(6)-H(6B)	109.7
C(2)-C(1)-H(1A)	109.9	C(5)-C(6)-H(6B)	109.7
S(1)-C(1)-H(1A)	109.9	H(6A)-C(6)-H(6B)	108.2
C(2)-C(1)-H(1B)	109.9	N(1)-C(7)-C(8)	112.2(4)
S(1)-C(1)-H(1B)	109.9	N(1)-C(7)-H(7A)	109.2
H(1A)-C(1)-H(1B)	108.3	C(8)-C(7)-H(7A)	109.2
C(1)-C(2)-N(2)	109.8(4)	N(1)-C(7)-H(7B)	109.2
C(1)-C(2)-H(2A)	109.7	C(8)-C(7)-H(7B)	109.2
N(2)-C(2)-H(2A)	109.7	H(7A)-C(7)-H(7B)	107.9
C(1)-C(2)-H(2B)	109.7	C(7)-C(8)-C(9)	114.5(4)
N(2)-C(2)-H(2B)	109.7	C(7)-C(8)-H(8A)	108.6
H(2A)-C(2)-H(2B)	108.2	C(9)-C(8)-H(8A)	108.6
N(2)-C(3)-C(4)	109.4(4)	C(7)-C(8)-H(8B)	108.6
N(2)-C(3)-H(3A)	109.8	C(9)-C(8)-H(8B)	108.6
C(4)-C(3)-H(3A)	109.8	H(8A)-C(8)-H(8B)	107.6
N(2)-C(3)-H(3B)	109.8	N(2)-C(9)-C(8)	112.5(4)
C(4)-C(3)-H(3B)	109.8	N(2)-C(9)-H(9A)	109.1
H(3A)-C(3)-H(3B)	108.3	C(8)-C(9)-H(9A)	109.1
N(1)-C(4)-C(3)	109.3(4)	N(2)-C(9)-H(9B)	109.1
N(1)-C(4)-H(4A)	109.8	C(8)-C(9)-H(9B)	109.1
C(3)-C(4)-H(4A)	109.8	H(9A)-C(9)-H(9B)	107.8
N(1)-C(4)-H(4B)	109.8	O(1ME)-C(1ME)-H(1MA)	109.5
C(3)-C(4)-H(4B)	109.8	O(1ME)-C(1ME)-H(1MB)	109.5
H(4A)-C(4)-H(4B)	108.3	H(1MA)-C(1ME)-H(1MB)	109.5
C(6)-C(5)-S(2)	109.4(4)	O(1ME)-C(1ME)-H(1MC)	109.5
C(6)-C(5)-H(5A)	109.8	H(1MA)-C(1ME)-H(1MC)	109.5
S(2)-C(5)-H(5A)	109.8	H(1MB)-C(1ME)-H(1MC)	109.5
C(6)-C(5)-H(5B)	109.8		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

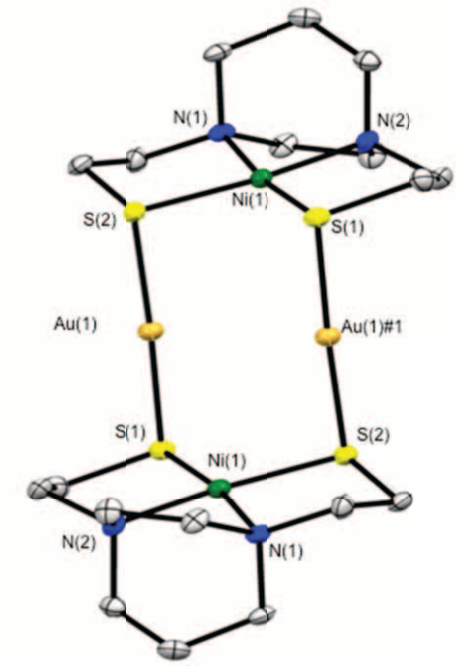

Figure S5. TEP of complex **3** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, the Cl^- counterion, and the MeOH of crystallization are not shown.

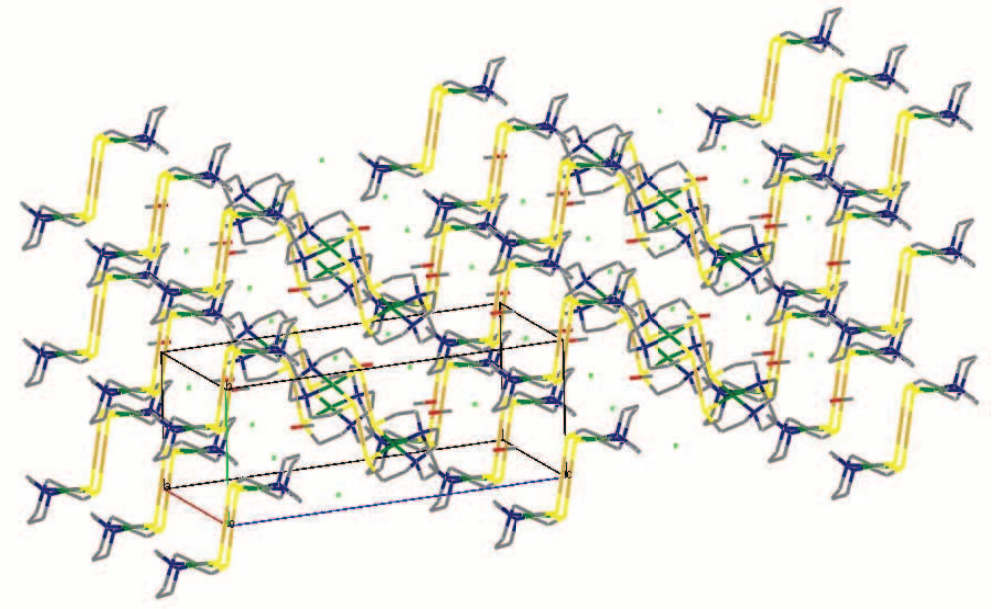

Figure S6. The packing diagram of complex **3** in capped stick drawing.

Table S7. Crystal data and structure refinement for $(Et_4N^+)_2[Au_2\{Ni(ema)\}_2]$ (**4**).

Identification code	data_0m	
Empirical formula	C28 H56 Au2 N6 Ni2 O4 S4	
Formula weight	1180.38	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 8.308(2) Å	α = 90°.
	b = 24.096(6) Å	β = 110.431(3)°.
	c = 10.191(3) Å	γ = 90°.
Volume	1911.6(9) $Å^3$	
Z	2	
Density (calculated)	2.051 Mg/m^3	
Absorption coefficient	8.880 mm^{-1}	
F(000)	1152	
Crystal size	0.30 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.29 to 28.64°.	
Index ranges	-11<=h<=11, -32<=k<=31, -13<=l<=13	
Reflections collected	22917	
Independent reflections	4844 [R(int) = 0.0487]	
Completeness to theta = 28.64°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5369 and 0.1759	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4844 / 0 / 212	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0269, wR2 = 0.0501	
R indices (all data)	R1 = 0.0418, wR2 = 0.0545	
Largest diff. peak and hole	0.814 and -0.970 $e.Å^{-3}$	

Table S8. Bond lengths [Å] and angles [°] for $(Et_4N^+)_2[Au_2\{Ni(ema)\}_2]$ (**4**).

Au(1)-S(2)#1	2.2914(11)	C(8)-H(8A)	0.9600
Au(1)-S(1)	2.2952(11)	C(8)-H(8B)	0.9600
Au(1)-Au(1)#1	3.1169(7)	C(8)-H(8C)	0.9600
Ni(1)-N(1)	1.849(3)	C(9)-C(10)	1.511(5)
Ni(1)-N(2)	1.854(3)	C(9)-H(9A)	0.9700
Ni(1)-S(1)	2.1854(11)	C(9)-H(9B)	0.9700
Ni(1)-S(2)	2.1991(11)	C(10)-H(10A)	0.9600
S(1)-C(1)	1.831(4)	C(10)-H(10B)	0.9600
S(2)-C(3)	1.830(4)	C(10)-H(10C)	0.9600
S(2)-Au(1)#1	2.2914(11)	C(11)-C(12)	1.514(5)
N(1)-C(2)	1.327(5)	C(11)-H(11A)	0.9700
N(1)-C(6)	1.461(5)	C(11)-H(11B)	0.9700
N(2)-C(4)	1.330(5)	C(12)-H(12A)	0.9600
N(2)-C(5)	1.460(5)	C(12)-H(12B)	0.9600
N(3)-C(7)	1.510(5)	C(12)-H(12C)	0.9600
N(3)-C(9)	1.514(5)	C(13)-C(14)	1.512(6)
N(3)-C(13)	1.515(5)	C(13)-H(13A)	0.9700
N(3)-C(11)	1.517(4)	C(13)-H(13B)	0.9700
O(1)-C(2)	1.245(4)	C(14)-H(14A)	0.9600
O(2)-C(4)	1.239(5)	C(14)-H(14B)	0.9600
C(1)-C(2)	1.510(5)	C(14)-H(14C)	0.9600
C(1)-H(1A)	0.9700		
C(1)-H(1B)	0.9700	S(2)#1-Au(1)-S(1)	175.35(3)
C(3)-C(4)	1.518(6)	S(2)#1-Au(1)-Au(1)#1	90.72(3)
C(3)-H(3A)	0.9700	S(1)-Au(1)-Au(1)#1	93.90(3)
C(3)-H(3B)	0.9700	N(1)-Ni(1)-N(2)	85.61(14)
C(5)-C(6)	1.521(6)	N(1)-Ni(1)-S(1)	88.29(10)
C(5)-H(5A)	0.9700	N(2)-Ni(1)-S(1)	173.59(11)
C(5)-H(5B)	0.9700	N(1)-Ni(1)-S(2)	173.52(11)
C(6)-H(6A)	0.9700	N(2)-Ni(1)-S(2)	88.48(11)
C(6)-H(6B)	0.9700	S(1)-Ni(1)-S(2)	97.70(4)
C(7)-C(8)	1.513(6)	C(1)-S(1)-Ni(1)	98.15(13)
C(7)-H(7A)	0.9700	C(1)-S(1)-Au(1)	104.13(14)
C(7)-H(7B)	0.9700	Ni(1)-S(1)-Au(1)	92.44(4)

C(3)-S(2)-Ni(1)	96.61(14)	N(2)-C(5)-H(5B)	110.3
C(3)-S(2)-Au(1)#1	103.27(13)	C(6)-C(5)-H(5B)	110.3
Ni(1)-S(2)-Au(1)#1	95.12(4)	H(5A)-C(5)-H(5B)	108.6
C(2)-N(1)-C(6)	118.2(3)	N(1)-C(6)-C(5)	107.6(3)
C(2)-N(1)-Ni(1)	125.4(3)	N(1)-C(6)-H(6A)	110.2
C(6)-N(1)-Ni(1)	115.3(2)	C(5)-C(6)-H(6A)	110.2
C(4)-N(2)-C(5)	119.0(3)	N(1)-C(6)-H(6B)	110.2
C(4)-N(2)-Ni(1)	124.4(3)	C(5)-C(6)-H(6B)	110.2
C(5)-N(2)-Ni(1)	114.7(3)	H(6A)-C(6)-H(6B)	108.5
C(7)-N(3)-C(9)	111.4(3)	N(3)-C(7)-C(8)	115.0(3)
C(7)-N(3)-C(13)	106.1(3)	N(3)-C(7)-H(7A)	108.5
C(9)-N(3)-C(13)	110.9(3)	C(8)-C(7)-H(7A)	108.5
C(7)-N(3)-C(11)	110.9(3)	N(3)-C(7)-H(7B)	108.5
C(9)-N(3)-C(11)	106.6(3)	C(8)-C(7)-H(7B)	108.5
C(13)-N(3)-C(11)	111.1(3)	H(7A)-C(7)-H(7B)	107.5
C(2)-C(1)-S(1)	112.8(3)	C(7)-C(8)-H(8A)	109.5
C(2)-C(1)-H(1A)	109.0	C(7)-C(8)-H(8B)	109.5
S(1)-C(1)-H(1A)	109.0	H(8A)-C(8)-H(8B)	109.5
C(2)-C(1)-H(1B)	109.0	C(7)-C(8)-H(8C)	109.5
S(1)-C(1)-H(1B)	109.0	H(8A)-C(8)-H(8C)	109.5
H(1A)-C(1)-H(1B)	107.8	H(8B)-C(8)-H(8C)	109.5
O(1)-C(2)-N(1)	126.0(4)	C(10)-C(9)-N(3)	116.0(3)
O(1)-C(2)-C(1)	119.1(3)	C(10)-C(9)-H(9A)	108.3
N(1)-C(2)-C(1)	114.9(3)	N(3)-C(9)-H(9A)	108.3
C(4)-C(3)-S(2)	111.9(3)	C(10)-C(9)-H(9B)	108.3
C(4)-C(3)-H(3A)	109.2	N(3)-C(9)-H(9B)	108.3
S(2)-C(3)-H(3A)	109.2	H(9A)-C(9)-H(9B)	107.4
C(4)-C(3)-H(3B)	109.2	C(9)-C(10)-H(10A)	109.5
S(2)-C(3)-H(3B)	109.2	C(9)-C(10)-H(10B)	109.5
H(3A)-C(3)-H(3B)	107.9	H(10A)-C(10)-H(10B)	109.5
O(2)-C(4)-N(2)	126.5(4)	C(9)-C(10)-H(10C)	109.5
O(2)-C(4)-C(3)	120.4(4)	H(10A)-C(10)-H(10C)	109.5
N(2)-C(4)-C(3)	113.0(3)	H(10B)-C(10)-H(10C)	109.5
N(2)-C(5)-C(6)	107.1(3)	C(12)-C(11)-N(3)	114.5(3)
N(2)-C(5)-H(5A)	110.3	C(12)-C(11)-H(11A)	108.6
C(6)-C(5)-H(5A)	110.3	N(3)-C(11)-H(11A)	108.6

C(12)-C(11)-H(11B)	108.6	N(3)-C(13)-H(13A)	108.4
N(3)-C(11)-H(11B)	108.6	C(14)-C(13)-H(13B)	108.4
H(11A)-C(11)-H(11B)	107.6	N(3)-C(13)-H(13B)	108.4
C(11)-C(12)-H(12A)	109.5	H(13A)-C(13)-H(13B)	107.5
C(11)-C(12)-H(12B)	109.5	C(13)-C(14)-H(14A)	109.5
H(12A)-C(12)-H(12B)	109.5	C(13)-C(14)-H(14B)	109.5
C(11)-C(12)-H(12C)	109.5	H(14A)-C(14)-H(14B)	109.5
H(12A)-C(12)-H(12C)	109.5	C(13)-C(14)-H(14C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(14A)-C(14)-H(14C)	109.5
C(14)-C(13)-N(3)	115.3(3)	H(14B)-C(14)-H(14C)	109.5
C(14)-C(13)-H(13A)	108.4		

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

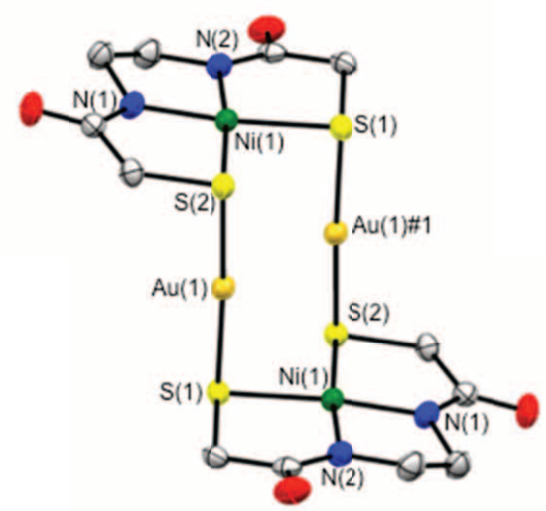

Figure S7. TEP of complex **4** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms and the Et_4N^+ counterion are not shown.

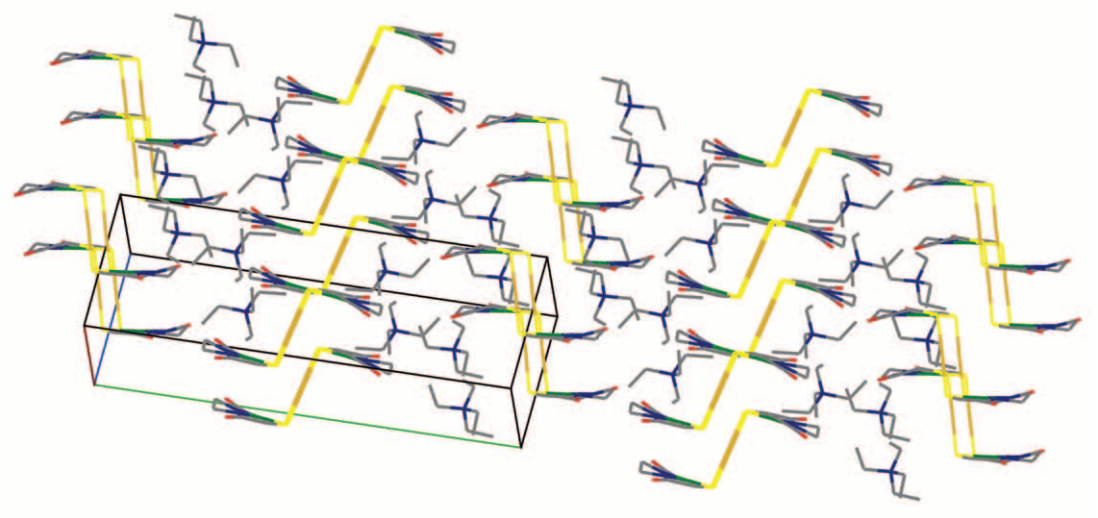

Figure S8. The packing diagram of complex **4** in capped stick drawing.

Table S9. Crystal data and structure refinement for [{Ni(ema)}$_2$Au$_4$(PPh$_3$)$_4$] (**5**).

Identification code	niau	
Empirical formula	C96 H100 Au4 N10 Ni2 O7 P4 S4	
Formula weight	2663.26	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.465(2) Å	α = 75.987(2)°.
	b = 16.178(2) Å	β = 78.277(2)°.
	c = 25.137(4) Å	γ = 71.395(2)°.
Volume	4987.9(13) Å^3	
Z	2	
Density (calculated)	1.773 Mg/m^3	
Absorption coefficient	6.436 mm^{-1}	
F(000)	2596	
Crystal size	0.100 x 0.100 x 0.050 mm^3	
Theta range for data collection	2.101 to 28.382°.	
Index ranges	-17<=h<=18, -21<=k<=21, -33<=l<=33	
Reflections collected	59144	
Independent reflections	24138 [R(int) = 0.0455]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.3136	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	24138 / 171 / 1159	
Goodness-of-fit on F^2	1.125	
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.0993	
R indices (all data)	R1 = 0.0567, wR2 = 0.1039	
Extinction coefficient	0	
Largest diff. peak and hole	3.615 and -1.925 e.Å^{-3}	

Table S10. Bond lengths [Å] and angles [°] for [{Ni(ema)}$_2$Au$_4$(PPh$_3$)$_4$] (**5**).

Au(1)-Au(3)	3.0544(6)	C(27)-C(28)	1.38(1)
Au(2)-Au(4)	3.1268(5)	C(28)-C(29)	1.38(1)
C(9)-C(10)	1.52(1)	C(1A)-C(2A)	1.22(2)
S(4)-C(10)	1.835(8)	C(1B)-C(2B)	1.34(2)
N(4)-C(11)	1.458(9)	C(1C)-C(2C)	1.35(2)
C(11)-C(12)	1.527(9)	C(1D)-C(2D)	1.20(1)
N(3)-C(12)	1.45(1)	C(1E)-C(2E)	1.34(1)
P(1)-C(13)	1.812(7)	C(1F)-C(2F)	1.24(2)
C(13)-C(14)	1.385(9)	N(2)-C(3)	1.469(8)
C(14)-C(15)	1.38(1)	C(25)-C(30)	1.41(1)
C(15)-C(16)	1.36(1)	C(29)-C(30)	1.38(1)
C(16)-C(17)	1.39(1)	P(2)-C(31)	1.807(7)
C(17)-C(18)	1.38(1)	C(31)-C(32)	1.40(1)
C(13)-C(18)	1.38(1)	C(32)-C(33)	1.38(1)
N(1A)-C(1A)	1.34(2)	C(33)-C(34)	1.39(1)
N(1B)-C(1B)	1.20(2)	C(34)-C(35)	1.38(2)
N(1C)-C(1C)	1.21(2)	C(31)-C(36)	1.384(9)
N(1D)-C(1D)	1.35(2)	C(35)-C(36)	1.40(1)
N(1E)-C(1E)	1.23(1)	P(2)-C(37)	1.826(7)
N(1F)-C(1F)	1.34(2)	C(37)-C(38)	1.39(1)
S(2)-C(1I)	1.828(8)	C(38)-C(39)	1.38(1)
N(2)-C(1J)	1.313(8)	N(9)-C(4)	1.46(1)
C(1I)-C(1J)	1.510(9)	C(3)-C(4)	1.506(9)
O(2)-C(1J)	1.270(9)	C(39)-C(40)	1.38(1)
C(19)-C(20)	1.37(1)	C(40)-C(41)	1.37(2)
C(20)-C(21)	1.37(1)	C(41)-C(42)	1.39(1)
C(21)-C(22)	1.37(1)	C(37)-C(42)	1.394(9)
C(22)-C(23)	1.40(1)	P(2)-C(43)	1.815(7)
C(19)-C(24)	1.41(1)	C(43)-C(44)	1.39(1)
C(23)-C(24)	1.38(1)	C(44)-C(45)	1.38(1)
P(1)-C(24)	1.807(7)	C(45)-C(46)	1.39(1)
P(1)-C(25)	1.808(7)	C(46)-C(47)	1.37(1)
C(25)-C(26)	1.39(1)	C(47)-C(48)	1.40(1)
C(26)-C(27)	1.40(1)	C(43)-C(48)	1.40(1)

P(3)-C(49)	1.808(6)	C(75)-C(76)	1.39(2)
N(9)-C(5)	1.306(8)	C(76)-C(77)	1.38(1)
O(1)-C(5)	1.259(8)	C(73)-C(78)	1.39(1)
C(49)-C(50)	1.399(8)	C(77)-C(78)	1.39(1)
C(50)-C(51)	1.382(9)	P(4)-C(79)	1.808(8)
C(51)-C(52)	1.38(1)	C(7)-C(8)	1.52(1)
C(52)-C(53)	1.39(1)	O(3)-C(8)	1.235(8)
C(49)-C(54)	1.38(1)	N(3)-C(8)	1.311(8)
C(53)-C(54)	1.37(1)	C(79)-C(80)	1.39(1)
P(3)-C(55)	1.797(7)	C(80)-C(81)	1.40(1)
C(55)-C(56)	1.41(1)	C(81)-C(82)	1.37(1)
C(56)-C(57)	1.38(1)	C(82)-C(83)	1.37(1)
C(57)-C(58)	1.39(1)	C(83)-C(84)	1.39(1)
C(58)-C(59)	1.38(1)	C(79)-C(84)	1.40(1)
C(5)-C(6)	1.51(1)	N(4)-C(9)	1.316(7)
S(1)-C(6)	1.817(7)	O(4)-C(9)	1.24(1)
C(55)-C(60)	1.393(8)	C(10)-H(10A)	0.990(7)
C(59)-C(60)	1.39(1)	C(10)-H(10B)	0.989(5)
P(3)-C(61)	1.830(8)	C(11)-H(11A)	0.990(6)
C(61)-C(62)	1.388(9)	C(11)-H(11B)	0.989(8)
C(62)-C(63)	1.39(1)	C(12)-H(12A)	0.991(6)
C(63)-C(64)	1.38(1)	C(12)-H(12B)	0.989(7)
C(64)-C(65)	1.37(1)	C(14)-H(14)	0.949(6)
C(65)-C(66)	1.39(1)	C(15)-H(15)	0.950(7)
C(61)-C(66)	1.39(1)	C(16)-H(16)	0.951(8)
P(4)-C(67)	1.808(6)	C(17)-H(17)	0.950(7)
C(67)-C(68)	1.40(1)	C(18)-H(18)	0.950(7)
C(68)-C(69)	1.37(1)	C(19)-H(19)	0.950(7)
S(3)-C(7)	1.836(6)	C(1I)-H(1IA)	0.990(7)
C(69)-C(70)	1.37(1)	C(1I)-H(1IB)	0.990(6)
C(70)-C(71)	1.38(1)	O(1W)-H(1WA)	0.870(6)
C(67)-C(72)	1.386(9)	O(1W)-H(1WB)	0.871(8)
C(71)-C(72)	1.41(1)	C(20)-H(20)	0.95(1)
P(4)-C(73)	1.813(7)	C(21)-H(21)	0.949(8)
C(73)-C(74)	1.38(1)	C(22)-H(22)	0.948(9)
C(74)-C(75)	1.40(1)	C(23)-H(23)	0.950(8)

C(26)-H(26)	0.949(8)	C(40)-H(40)	0.950(9)
C(27)-H(27)	0.95(1)	C(41)-H(41)	0.951(8)
C(28)-H(28)	0.949(8)	C(42)-H(42)	0.949(9)
C(29)-H(29))	0.950(8)	C(44)-H(44)	0.950(7)
C(2A)-H(2AA)	0.98(1)	C(45)-H(45)	0.949(9)
C(2A)-H(2AB)	0.98(1)	C(46)-H(46)	0.949(9)
C(2A)-H(2AC)	0.98(1)	C(47)-H(47)	0.950(7)
C(2B)-H(2BA)	0.98(1)	C(48)-H(48)	0.951(8)
C(2B)-H(2BB)	0.98(1)	C(4)-H(4A)	0.988(7)
C(2B)-H(2BC)	0.98(1)	C(4)-H(4B)	0.991(6)
C(2C)-H(2CA)	0.98(1)	C(50)-H(50)	0.950(6)
C(2C)-H(2CB)	0.98(1)	C(51)-H(51)	0.951(7)
C(2C)-H(2CC)	0.98(1)	C(52)-H(52)	0.951(7)
C(2D)-H(2DA)	0.98(1)	C(53)-H(53)	0.950(8)
C(2D)-H(2DB)	0.98(1)	C(54)-H(54)	0.950(7)
C(2D)-H(2DC)	0.98(1)	C(56)-H(56)	0.950(6)
C(2E)-H(2EA)	0.98(1)	C(57)-H(57)	0.95(1)
C(2E)-H(2EB)	0.98(1)	C(58)-H(58)	0.949(8)
C(2E)-H(2EC)	0.98(1)	C(59)-H(59)	0.950(7)
C(2F)-H(2FA)	0.98(1)	C(60)-H(60)	0.949(8)
C(2F)-H(2FB)	0.98(1)	C(62)-H(62)	0.950(7)
C(2F)-H(2FC)	0.98(2)	C(63)-H(63)	0.951(8)
O(2W)-H(2WA)	0.870(8)	C(64)-H(64)	0.950(9)
O(2W)-H(2WB)	0.870(5)	C(65)-H(65)	0.951(8)
C(30)-H(30)	0.95(1)	C(66)-H(66)	0.950(8)
C(32)-H(32)	0.950(6)	C(68)-H(68)	0.950(7)
C(33)-H(33)	0.95(1)	C(69)-H(69)	0.950(9)
C(34)-H(34)	0.95(1)	C(6)-H(6A)	0.990(8)
C(35)-H(35)	0.950(7)	C(6)-H(6B)	0.990(6)
C(36)-H(36)	0.950(8)	C(70)-H(70)	0.950(7)
C(38)-H(38)	0.949(6)	C(71)-H(71)	0.949(8)
C(39)-H(39)	0.95(1)	C(72)-H(72)	0.949(8)
C(3)-H(3A)	0.991(7)	C(74)-H(74)	0.950(9)
C(3)-H(3B)	0.990(9)	C(75)-H(75)	0.950(9)
O(3W)-H(3WA)	0.870(7)	C(76)-H(76)	0.950(8)
O(3W)-H(3WB)	0.870(6)	C(77)-H(77)	0.95(1)

C(78)-H(78)	0.948(8)	N(1B)-C(1B)-C(2B)	177(1)
C(7)-H(7A)	0.989(7)	C(1B)-C(2B)-H(2BA)	110(1)
C(7)-H(7B)	0.990(6)	C(1B)-C(2B)-H(2BB)	109(1)
C(80)-H(80)	0.949(7)	C(1B)-C(2B)-H(2BC)	110(1)
C(81)-H(81)	0.95(1)	H(2BA)-C(2B)-H(2BB)	110(1)
C(82)-H(82)	0.95(1)	H(2BA)-C(2B)-H(2BC)	109(1)
C(83)-H(83)	0.950(8)	H(2BB)-C(2B)-H(2BC)	109(1)
C(84)-H(84)	0.95(1)	N(1C)-C(1C)-C(2C)	174(1)
Ni(1)-N(2)	1.848(5)	C(1C)-C(2C)-H(2CA)	109(1)
Ni(2)-N(3)	1.861(5)	C(1C)-C(2C)-H(2CB)	109(1)
Ni(2)-N(4)	1.852(6)	C(1C)-C(2C)-H(2CC)	109(1)
Ni(1)-N(9)	1.861(5)	H(2CA)-C(2C)-H(2CB)	110(1)
Au(2)-Ni(1)	2.9227(9)	H(2CA)-C(2C)-H(2CC)	110(1)
Au(1)-Ni(1)	3.1411(8)	H(2CB)-C(2C)-H(2CC)	109(1)
Au(4)-Ni(2)	3.3127(9)	N(1D)-C(1D)-C(2D)	173(1)
Au(3)-Ni(2)	2.9040(9)	C(1D)-C(2D)-H(2DA)	109(1)
Au(1)-P(1)	2.269(2)	C(1D)-C(2D)-H(2DB)	110(1)
Au(2)-P(2)	2.266(2)	C(1D)-C(2D)-H(2DC)	109(1)
Au(3)-P(3)	2.259(2)	H(2DA)-C(2D)-H(2DB)	110(1)
Au(4)-P(4)	2.268(2)	H(2DA)-C(2D)-H(2DC)	109(1)
Au(1)-S(1)	2.330(2)	H(2DB)-C(2D)-H(2DC)	110(1)
Ni(1)-S(1)	2.186(2)	N(1E)-C(1E)-C(2E)	176(1)
Ni(1)-S(2)	2.207(2)	C(1E)-C(2E)-H(2EA)	109(1)
Au(2)-S(2)	2.350(2)	C(1E)-C(2E)-H(2EB)	110(1)
Ni(2)-S(3)	2.204(2)	C(1E)-C(2E)-H(2EC)	109(1)
Au(3)-S(3)	2.352(2)	H(2EA)-C(2E)-H(2EB)	109(1)
Au(4)-S(4)	2.324(2)	H(2EA)-C(2E)-H(2EC)	109(1)
Ni(2)-S(4)	2.198(2)	H(2EB)-C(2E)-H(2EC)	110(1)
		N(1F)-C(1F)-C(2F)	172(2)
N(1A)-C(1A)-C(2A)	178(1)	C(1F)-C(2F)-H(2FA)	109(1)
C(1A)-C(2A)-H(2AA)	110(1)	C(1F)-C(2F)-H(2FB)	109(1)
C(1A)-C(2A)- H(2AB)	109(1)	C(1F)-C(2F)-H(2FC)	110(1)
C(1A)-C(2A)-H(2AC)	109(1)	H(2FA)-C(2F)-H(2FB)	109(1)
H(2AA)-C(2A)-H(2AB)	109(1)	H(2FA)-C(2F)-H(2FC)	110(1)
H(2AA)-C(2A)-H(2AC)	109(1)	H(2FB)-C(2F)-H(2FC)	110(1)
H(2AB)-C(2A)-H(2AC)	109(1)	H(1WA)-O(1W)-H(1WB)	109.4(7)

H(2WA)-O(2W)-H(2WB)	109.5(7)	S(1)-Ni(1)-N(9)	87.9(2)
H(3WA)-O(3W)-H(3WB)	109.5(8)	S(1)-Ni(1)-N(2)	173.5(2)
Au(3)-Au(1)-Ni(1)	116.09(2)	S(2)-Ni(1)-N(9)	173.4(2)
Au(3)-Au(1)-S(1)	80.67(4)	S(2)-Ni(1)-N(2)	87.9(2)
Au(3)-Au(1)-P(1)	101.95(5)	N(9)-Ni(1)-N(2)	85.6(2)
Ni(1)-Au(1)-S(1)	44.07(4)	Au(3)-Ni(2)-Au(4)	117.61(3)
Ni(1)-Au(1)-P(1)	131.23(5)	Au(3)-Ni(2)-S(3)	52.68(5)
S(1)-Au(1)-P(1)	174.95(6)	Au(3)-Ni(2)-S(4)	92.92(5)
Au(4)-Au(2)-Ni(1)	116.32(2)	Au(3)-Ni(2)-N(3)	90.3(2)
Au(4)-Au(2)-S(2)	78.18(4)	Au(3)-Ni(2)-N(4)	127.6(2)
Au(4)-Au(2)-P(2)	114.40(4)	Au(4)-Ni(2)-S(3)	85.95(5)
Ni(1)-Au(2)-S(2)	47.99(4)	Au(4)-Ni(2)-S(4)	44.40(5)
Ni(1)-Au(2)-P(2)	120.19(5)	Au(4)-Ni(2)-N(3)	137.9(2)
S(2)-Au(2)-P(2)	167.14(6)	Au(4)-Ni(2)-N(4)	98.6(2)
Au(1)-Au(3)-Ni(2)	116.66(2)	S(3)-Ni(2)-S(4)	98.72(7)
Au(1)-Au(3)-S(3)	84.17(4)	S(3)-Ni(2)-N(3)	87.9(2)
Au(1)-Au(3)-P(3)	103.57(4)	S(3)-Ni(2)-N(4)	173.6(2)
Ni(2)-Au(3)-S(3)	48.19(4)	S(4)-Ni(2)-N(3)	173.4(2)
Ni(2)-Au(3)-P(3)	125.69(5)	S(4)-Ni(2)-N(4)	87.7(2)
S(3)-Au(3)-P(3)	172.22(6)	N(3)-Ni(2)-N(4)	85.7(2)
Au(2)-Au(4)-Ni(2)	112.77(2)	Au(1)-S(1)-Ni(1)	88.07(6)
Au(2)-Au(4)-S(4)	76.45(4)	Au(1)-S(1)-C(6)	106.5(2)
Au(2)-Au(4)-P(4)	106.91(5)	Ni(1)-S(1)-C(6)	98.3(2)
Ni(2)-Au(4)-S(4)	41.43(4)	Au(2)-S(2)-Ni(1)	79.71(6)
Ni(2)-Au(4)-P(4)	133.64(5)	Au(2)-S(2)-C(1I)	102.5(2)
S(4)-Au(4)-P(4)	174.76(6)	Ni(1)-S(2)-C(1I)	96.1(2)
Au(1)-Ni(1)-Au(2)	118.52(3)	Au(3)-S(3)-Ni(2)	79.13(6)
Au(1)-Ni(1)-S(1)	47.86(5)	Au(3)-S(3)-C(7)	100.9(2)
Au(1)-Ni(1)-S(2)	80.89(5)	Ni(2)-S(3)-C(7)	97.6(2)
Au(1)-Ni(1)-N(9)	104.5(2)	Au(4)-S(4)-Ni(2)	94.17(7)
Au(1)-Ni(1)-N(2)	134.1(2)	Au(4)-S(4)-C(10)	104.8(2)
Au(2)-Ni(1)-S(1)	97.37(5)	Ni(2)-S(4)-C(10)	98.3(2)
Au(2)-Ni(1)-S(2)	52.29(5)	Au(1)-P(1)-C(13)	114.5(2)
Au(2)-Ni(1)-N(9)	126.0(2)	Au(1)-P(1)-C(24)	114.9(2)
Au(2)-Ni(1)-N(2)	86.6(2)	Au(1)-P(1)-C(25)	109.0(2)
S(1)-Ni(1)-S(2)	98.61(7)	C(13)-P(1)-C(24)	104.0(3)

C(13)-P(1)-C(25)	106.9(3)	H(1IA)-C(1I)-C(1J)	109.2(6)
C(24)-P(1)-C(25)	106.9(3)	H(1IB)-C(1I)-C(1J)	109.2(6)
Au(2)-P(2)-C(31)	119.6(2)	O(2)-C(1J)-N(2)	125.8(6)
Au(2)-P(2)-C(37)	109.2(2)	O(2)-C(1J)-C(1I)	119.4(6)
Au(2)-P(2)-C(43)	111.3(2)	N(2)-C(1J)-C(1I)	114.8(6)
C(31)-P(2)-C(37)	107.3(3)	N(2)-C(3)-H(3A)	110.3(6)
C(31)-P(2)-C(43)	104.3(3)	N(2)-C(3)-H(3B)	110.3(6)
C(37)-P(2)-C(43)	104.1(3)	N(2)-C(3)-C(4)	107.0(6)
Au(3)-P(3)-C(49)	112.4(2)	H(3A)-C(3)-H(3B)	108.5(7)
Au(3)-P(3)-C(55)	115.6(2)	H(3A)-C(3)-C(4)	110.4(6)
Au(3)-P(3)-C(61)	112.3(2)	H(3B)-C(3)-C(4)	110.3(6)
C(49)-P(3)-C(55)	105.2(3)	N(9)-C(4)-C(3)	108.8(6)
C(49)-P(3)-C(61)	104.9(3)	N(9)-C(4)-H(4A)	110.0(6)
C(55)-P(3)-C(61)	105.6(3)	N(9)-C(4)-H(4B)	109.7(6)
Au(4)-P(4)-C(67)	108.8(2)	C(3)-C(4)-H(4A)	110.0(6)
Au(4)-P(4)-C(73)	115.7(2)	C(3)-C(4)-H(4B)	109.9(6)
Au(4)-P(4)-C(79)	113.8(2)	H(4A)-C(4)-H(4B)	108.3(6)
C(67)-P(4)-C(73)	105.4(3)	O(1)-C(5)-N(9)	125.0(6)
C(67)-P(4)-C(79)	106.7(3)	O(1)-C(5)-C(6)	119.3(6)
C(73)-P(4)-C(79)	105.8(3)	N(9)-C(5)-C(6)	115.7(6)
Ni(1)-N(9)-C(4)	114.8(4)	S(1)-C(6)-C(5)	112.4(5)
Ni(1)-N(9)-C(5)	124.4(5)	S(1)-C(6)-H(6A)	109.1(5)
C(4)-N(9)-C(5)	118.7(5)	S(1)-C(6)-H(6B)	109.1(5)
Ni(1)-N(2)-C(1J)	125.0(5)	C(5)-C(6)-H(6A)	109.2(6)
Ni(1)-N(2)-C(3)	114.8(4)	C(5)-C(6)-H(6B)	109.1(6)
C(1J)-N(2)-C(3)	119.8(6)	H(6A)-C(6)-H(6B)	107.9(6)
Ni(2)-N(3)-C(8)	125.8(5)	S(3)-C(7)-H(7A)	109.3(5)
Ni(2)-N(3)-C(12)	114.7(4)	S(3)-C(7)-H(7B)	109.2(5)
C(8)-N(3)-C(12)	118.7(5)	S(3)-C(7)-C(8)	111.9(5)
Ni(2)-N(4)-C(9)	125.6(5)	H(7A)-C(7)-H(7B)	107.9(6)
Ni(2)-N(4)-C(11)	115.1(4)	H(7A)-C(7)-C(8)	109.2(6)
C(9)-N(4)-C(11)	117.2(5)	H(7B)-C(7)-C(8)	109.2(6)
S(2)-C(1I)-H(1IA)	109.3(5)	O(3)-C(8)-N(3)	125.5(6)
S(2)-C(1I)-H(1IB)	109.2(5)	O(3)-C(8)-C(7)	119.6(6)
S(2)-C(1I)-C(1J)	111.9(5)	N(3)-C(8)-C(7)	114.9(6)
H(1IA)-C(1I)-H(1IB)	108.0(6)	O(4)-C(9)-N(4)	126.1(6)

O(4)-C(9)-C(10)	119.4(6)	C(13)-C(18)-H(18)	119.9(8)
N(4)-C(9)-C(10)	114.5(6)	C(17)-C(18)-H(18)	119.8(8)
S(4)-C(10)-C(9)	111.6(5)	H(19)-C(19)-C(20)	120.4(7)
S(4)-C(10)-H(10A)	109.3(5)	H(19)-C(19)-C(24)	120.5(7)
S(4)-C(10)-H(10B)	109.3(5)	C(20)-C(19)-C(24)	119.1(7)
C(9)-C(10)-H(10A)	109.3(6)	C(19)-C(20)-H(20)	119.2(9)
C(9)-C(10)-H(10B)	109.3(6)	C(19)-C(20)-C(21)	121.6(8)
H(10A)-C(10)-H(10B)	108.0(6)	H(20)-C(20)-C(21)	119.2(9)
N(4)-C(11)-H(11A)	110.2(6)	C(20)-C(21)-H(21)	120.1(9)
N(4)-C(11)-H(11B)	110.2(6)	C(20)-C(21)-C(22)	120.0(9)
N(4)-C(11)-C(12)	107.7(5)	H(21)-C(21)-C(22)	119.9(9)
H(11A)-C(11)-H(11B)	108.5(6)	C(21)-C(22)-H(22)	120.2(9)
H(11A)-C(11)-C(12)	110.1(6)	C(21)-C(22)-C(23)	119.7(9)
H(11B)-C(11)-C(12)	110.2(6)	H(22)-C(22)-C(23)	120.2(9)
N(3)-C(12)-C(11)	107.4(5)	C(22)-C(23)-H(23)	119.9(8)
N(3)-C(12)-H(12A)	110.3(6)	C(22)-C(23)-C(24)	120.2(7)
N(3)-C(12)-H(12B)	110.2(6)	H(23)-C(23)-C(24)	119.9(8)
C(11)-C(12)-H(12A)	110.1(6)	P(1)-C(24)-C(19)	117.1(5)
C(11)-C(12)-H(12B)	110.2(6)	P(1)-C(24)-C(23)	123.7(6)
H(12A)-C(12)-H(12B)	108.5(6)	C(19)-C(24)-C(23)	119.3(7)
P(1)-C(13)-C(14)	120.1(5)	P(1)-C(25)-C(26)	122.6(6)
P(1)-C(13)-C(18)	120.5(6)	P(1)-C(25)-C(30)	118.5(5)
C(14)-C(13)-C(18)	119.3(7)	C(26)-C(25)-C(30)	118.7(7)
C(13)-C(14)-H(14)	119.9(7)	C(25)-C(26)-H(26)	119.8(8)
C(13)-C(14)-C(15)	120.3(7)	C(25)-C(26)-C(27)	120.0(7)
H(14)-C(14)-C(15)	119.8(7)	H(26)-C(26)-C(27)	120.2(8)
C(14)-C(15)-H(15)	120.1(8)	C(26)-C(27)-H(27)	119.8(8)
C(14)-C(15)-C(16)	119.9(7)	C(26)-C(27)-C(28)	120.3(8)
H(15)-C(15)-C(16)	120.0(8)	H(27)-C(27)-C(28)	119.9(9)
C(15)-C(16)-H(16)	119.4(8)	C(27)-C(28)-H(28)	120.2(8)
C(15)-C(16)-C(17)	121.1(8)	C(27)-C(28)-C(29)	119.7(8)
H(16)-C(16)-C(17)	119.5(8)	H(28)-C(28)-C(29)	120.0(8)
C(16)-C(17)-H(17)	120.5(8)	C(28)-C(29)-H(29)	119.7(8)
C(16)-C(17)-C(18)	119.0(7)	C(28)-C(29)-C(30)	120.6(7)
H(17)-C(17)-C(18)	120.5(8)	H(29)-C(29)-C(30)	119.7(8)
C(13)-C(18)-C(17)	120.3(7)	C(25)-C(30)-C(29)	120.6(7)

C(25)-C(30)-H(30)	119.7(8)	C(37)-C(42)-H(42)	120.0(8)
C(29)-C(30)-H(30)	119.7(8)	C(41)-C(42)-H(42)	120.1(8)
P(2)-C(31)-C(32)	117.7(5)	P(2)-C(43)-C(44)	123.0(6)
P(2)-C(31)-C(36)	122.0(5)	P(2)-C(43)-C(48)	117.6(5)
C(32)-C(31)-C(36)	119.8(7)	C(44)-C(43)-C(48)	119.3(7)
C(31)-C(32)-H(32)	119.8(7)	C(43)-C(44)-H(44)	119.6(8)
C(31)-C(32)-C(33)	120.5(7)	C(43)-C(44)-C(45)	120.8(7)
H(32)-C(32)-C(33)	119.8(8)	H(44)-C(44)-C(45)	119.6(8)
C(32)-C(33)-H(33)	120.5(9)	C(44)-C(45)-H(45)	119.9(9)
C(32)-C(33)-C(34)	119.2(8)	C(44)-C(45)-C(46)	120.3(8)
H(33)-C(33)-C(34)	120.3(9)	H(45)-C(45)-C(46)	119.8(9)
C(33)-C(34)-H(34)	119.6(9)	C(45)-C(46)-H(46)	120.3(9)
C(33)-C(34)-C(35)	121.1(9)	C(45)-C(46)-C(47)	119.3(8)
H(34)-C(34)-C(35)	119.4(9)	H(46)-C(46)-C(47)	120.4(9)
C(34)-C(35)-H(35)	120.3(9)	C(46)-C(47)-H(47)	119.2(8)
C(34)-C(35)-C(36)	119.4(8)	C(46)-C(47)-C(48)	121.7(8)
H(35)-C(35)-C(36)	120.3(8)	H(47)-C(47)-C(48)	119.1(8)
C(31)-C(36)-C(35)	119.9(7)	C(43)-C(48)-C(47)	118.6(7)
C(31)-C(36)-H(36)	120.1(7)	C(43)-C(48)-H(48)	120.6(8)
C(35)-C(36)-H(36)	120.0(7)	C(47)-C(48)-H(48)	120.7(8)
P(2)-C(37)-C(38)	118.8(5)	P(3)-C(49)-C(50)	118.6(5)
P(2)-C(37)-C(42)	121.3(5)	P(3)-C(49)-C(54)	122.6(6)
C(38)-C(37)-C(42)	119.9(7)	C(50)-C(49)-C(54)	118.8(7)
C(37)-C(38)-H(38)	120.4(7)	C(49)-C(50)-H(50)	120.0(7)
C(37)-C(38)-C(39)	118.9(7)	C(49)-C(50)-C(51)	120.1(7)
H(38)-C(38)-C(39)	120.7(7)	H(50)-C(50)-C(51)	120.0(7)
C(38)-C(39)-H(39)	119.2(8)	C(50)-C(51)-H(51)	119.8(8)
C(38)-C(39)-C(40)	121.4(8)	C(50)-C(51)-C(52)	120.6(7)
H(39)-C(39)-C(40)	119.4(9)	H(51)-C(51)-C(52)	119.6(8)
C(39)-C(40)-H(40)	120.2(9)	C(51)-C(52)-H(52)	120.4(8)
C(39)-C(40)-C(41)	119.7(8)	C(51)-C(52)-C(53)	119.3(8)
H(40)-C(40)-C(41)	120.1(9)	H(52)-C(52)-C(53)	120.3(8)
C(40)-C(41)-H(41)	120.1(9)	C(52)-C(53)-H(53)	119.9(9)
C(40)-C(41)-C(42)	120.2(8)	C(52)-C(53)-C(54)	120.2(8)
H(41)-C(41)-C(42)	119.8(8)	H(53)-C(53)-C(54)	119.9(9)
C(37)-C(42)-C(41)	119.9(7)	C(49)-C(54)-C(53)	121.0(7)

C(49)-C(54)-H(54)	119.5(8)	C(61)-C(66)-H(66)	120.1(8)
C(53)-C(54)-H(54)	119.5(8)	C(65)-C(66)-H(66)	119.9(8)
P(3)-C(55)-C(56)	118.1(5)	P(4)-C(67)-C(68)	121.6(5)
P(3)-C(55)-C(60)	123.4(5)	P(4)-C(67)-C(72)	118.9(5)
C(56)-C(55)-C(60)	118.5(6)	C(68)-C(67)-C(72)	119.5(7)
C(55)-C(56)-H(56)	119.6(7)	C(67)-C(68)-H(68)	120.0(8)
C(55)-C(56)-C(57)	120.8(7)	C(67)-C(68)-C(69)	119.9(7)
H(56)-C(56)-C(57)	119.6(7)	H(68)-C(68)-C(69)	120.1(8)
C(56)-C(57)-H(57)	120.1(8)	C(68)-C(69)-H(69)	119.1(8)
C(56)-C(57)-C(58)	119.8(8)	C(68)-C(69)-C(70)	121.5(8)
H(57)-C(57)-C(58)	120.1(9)	H(69)-C(69)-C(70)	119.4(8)
C(57)-C(58)-H(58)	120.1(9)	C(69)-C(70)-H(70)	120.2(9)
C(57)-C(58)-C(59)	120.0(8)	C(69)-C(70)-C(71)	119.5(8)
H(58)-C(58)-C(59)	119.9(9)	H(70)-C(70)-C(71)	120.3(9)
C(58)-C(59)-H(59)	119.7(9)	C(70)-C(71)-H(71)	119.8(8)
C(58)-C(59)-C(60)	120.6(8)	C(70)-C(71)-C(72)	120.5(8)
H(59)-C(59)-C(60)	119.7(8)	H(71)-C(71)-C(72)	119.7(8)
C(55)-C(60)-C(59)	120.4(7)	C(67)-C(72)-C(71)	119.1(7)
C(55)-C(60)-H(60)	119.8(7)	C(67)-C(72)-H(72)	120.5(8)
C(59)-C(60)-H(60)	119.8(7)	C(71)-C(72)-H(72)	120.4(8)
P(3)-C(61)-C(62)	119.3(5)	P(4)-C(73)-C(74)	120.8(6)
P(3)-C(61)-C(66)	120.6(5)	P(4)-C(73)-C(78)	118.6(6)
C(62)-C(61)-C(66)	120.1(7)	C(74)-C(73)-C(78)	119.6(7)
C(61)-C(62)-H(62)	120.4(7)	C(73)-C(74)-H(74)	119.4(8)
C(61)-C(62)-C(63)	119.2(7)	C(73)-C(74)-C(75)	121.4(7)
H(62)-C(62)-C(63)	120.5(7)	H(74)-C(74)-C(75)	119.2(8)
C(62)-C(63)-H(63)	119.9(8)	C(74)-C(75)-H(75)	121.2(9)
C(62)-C(63)-C(64)	120.3(7)	C(74)-C(75)-C(76)	117.6(8)
H(63)-C(63)-C(64)	119.8(8)	H(75)-C(75)-C(76)	121.2(9)
C(63)-C(64)-H(64)	119.6(8)	C(75)-C(76)-H(76)	119.1(9)
C(63)-C(64)-C(65)	120.9(7)	C(75)-C(76)-C(77)	121.8(9)
H(64)-C(64)-C(65)	119.5(8)	H(76)-C(76)-C(77)	119.1(9)
C(64)-C(65)-H(65)	120.3(8)	C(76)-C(77)-H(77)	120.2(9)
C(64)-C(65)-C(66)	119.5(7)	C(76)-C(77)-C(78)	119.5(8)
H(65)-C(65)-C(66)	120.2(8)	H(77)-C(77)-C(78)	120.2(9)
C(61)-C(66)-C(65)	120.0(7)	C(73)-C(78)-C(77)	120.0(8)

C(73)-C(78)-H(78)	119.9(8)	H(82)-C(82)-C(83)	119.5(9)
C(77)-C(78)-H(78)	120.1(9)	C(82)-C(83)-H(83)	120.0(9)
P(4)-C(79)-C(80)	123.1(6)	C(82)-C(83)-C(84)	119.8(8)
P(4)-C(79)-C(84)	119.4(6)	H(83)-C(83)-C(84)	120.2(8)
C(80)-C(79)-C(84)	117.5(7)	C(79)-C(84)-C(83)	121.2(8)
C(79)-C(80)-H(80)	119.5(8)	C(79)-C(84)-H(84)	119.4(8)
C(79)-C(80)-C(81)	121.1(7)	C(83)-C(84)-H(84)	119.4(8)
H(80)-C(80)-C(81)	119.5(8)		
C(80)-C(81)-H(81)	120.2(9)		
C(80)-C(81)-C(82)	119.7(8)		
H(81)-C(81)-C(82)	120.1(9)		
C(81)-C(82)-H(82)	119.7(9)		
C(81)-C(82)-C(83)	120.7(9)		

Symmetry transformations used to generate equivalent atoms:

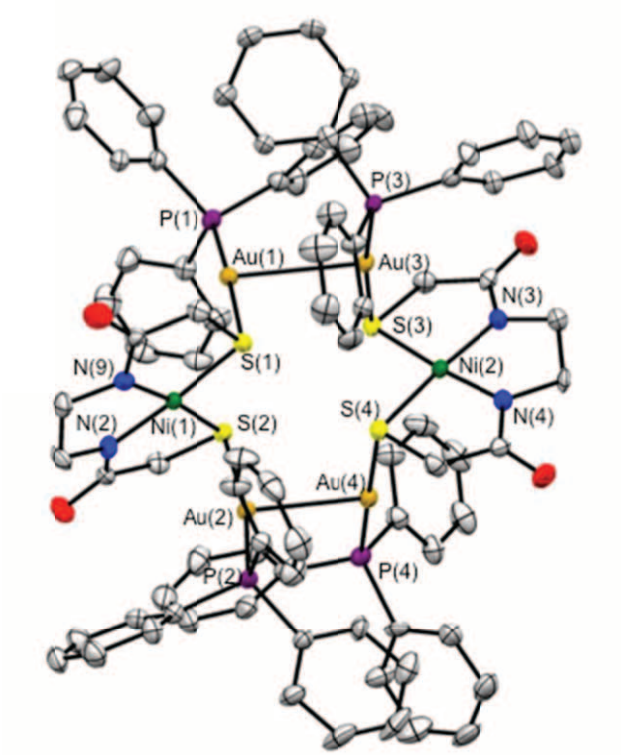

Figure S9. TEP of complex **5** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, H_2O and MeCN of crystallization are not shown.

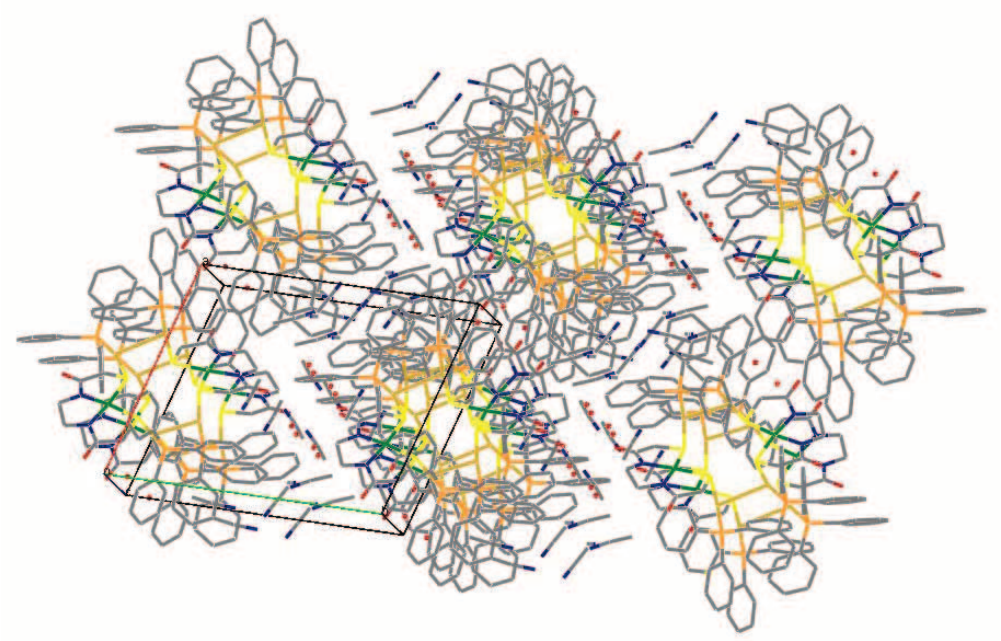

Figure S10. The packing diagram of complex **5** in capped stick drawing.

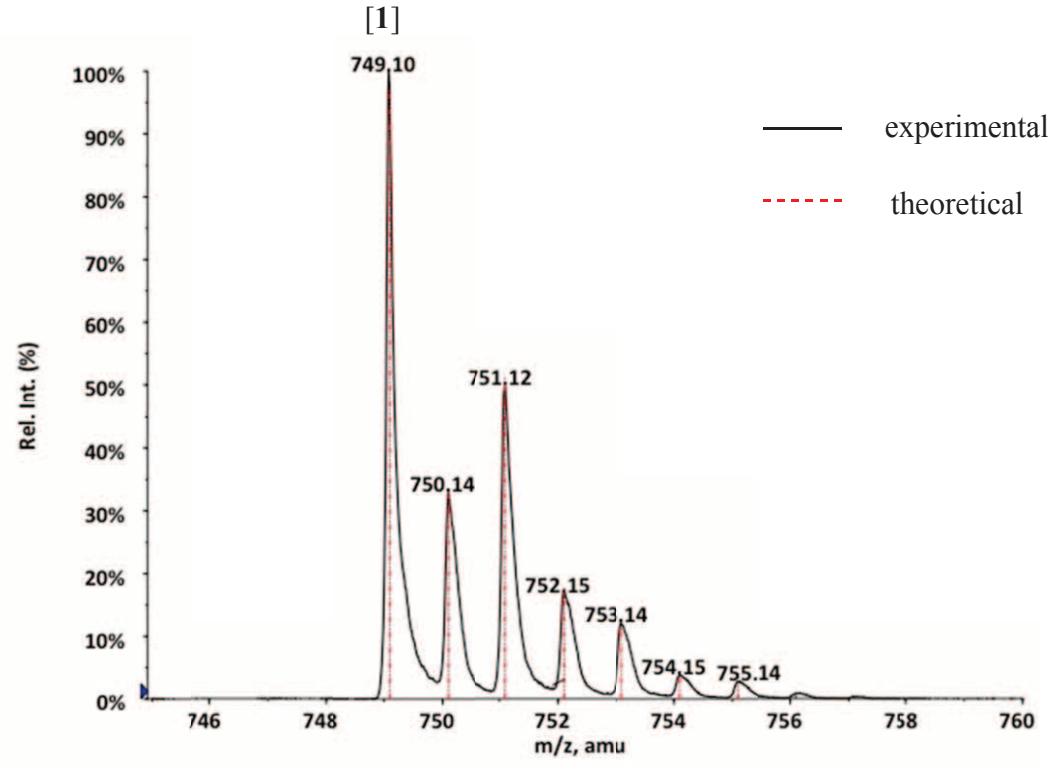

Figure S11. $^{+}$ESI-MS of complex **1,** $[Au\{Ni(bme\text{-}daco)PPh_3\}]^{+}$, m/z $[M\text{-}Cl^{-}]^{+}$ = 749, in MeCN.

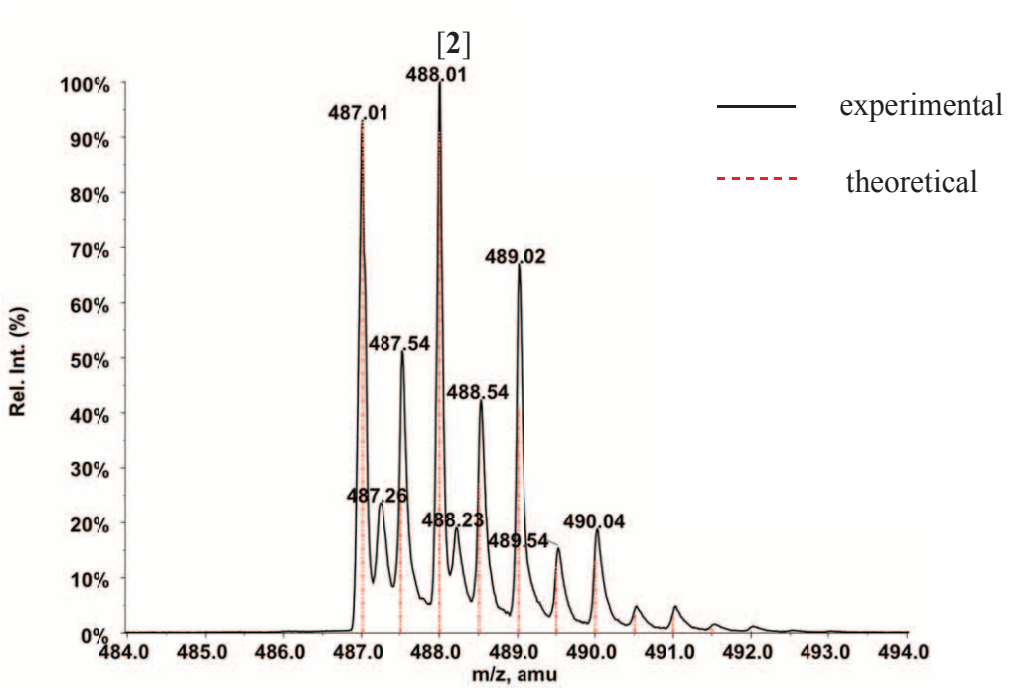

Figure S12. $^{+}$ESI-MS of complex **2,** $[Au_2\{Ni(bme\text{-}daco)\}_2]^{2+}$, m/z $[M\text{-}2Cl^{-}]^{2+}$ = 488 ,in MeOH.

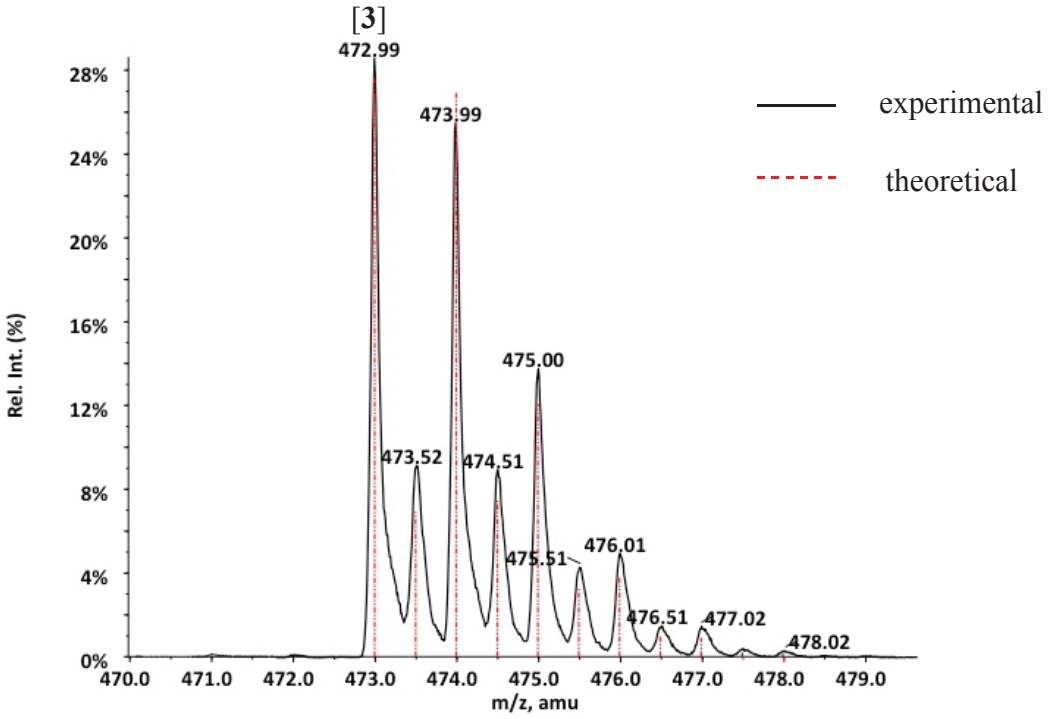

Figure S13. $^{+}$ESI-MS of complex **3,** $[Au_2\{Ni(bme\text{-}dach)\}_2]^2$, m/z $[M\text{-}2Cl^-]^{2+}$ = 473, in MeOH.

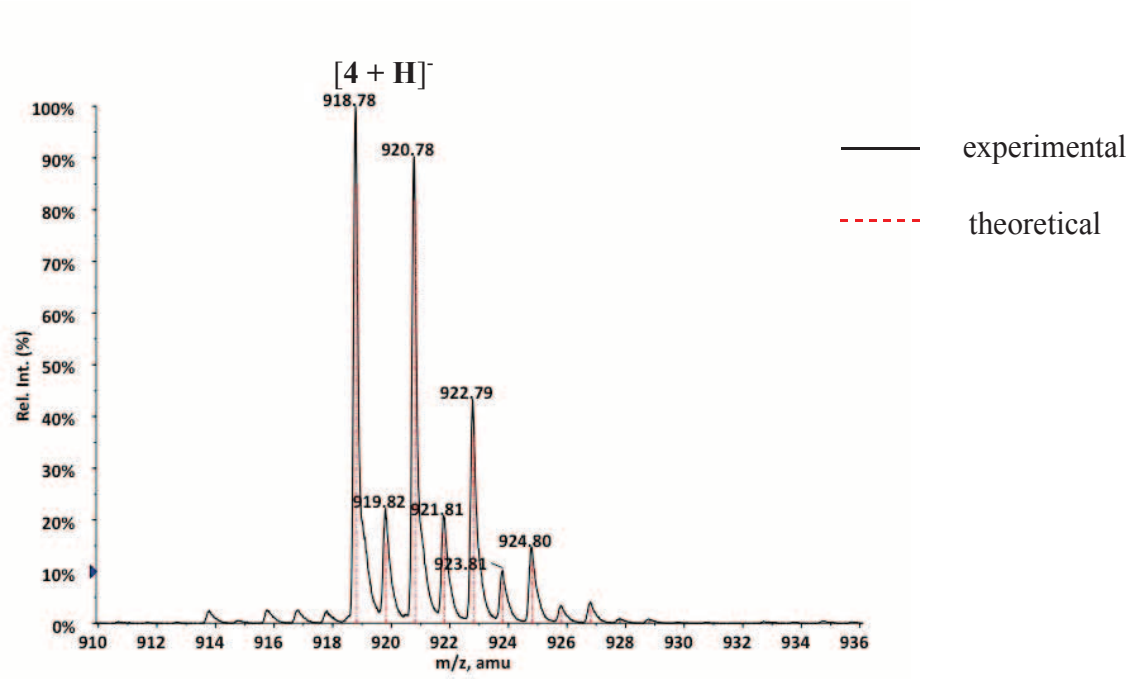

Figure S14. $^{-}$ESI-MS of complex **4,** $[Au_2\{Ni(ema)\}_2]^{2-}$, m/z $[M+H]^-$ = 919, in MeCN.

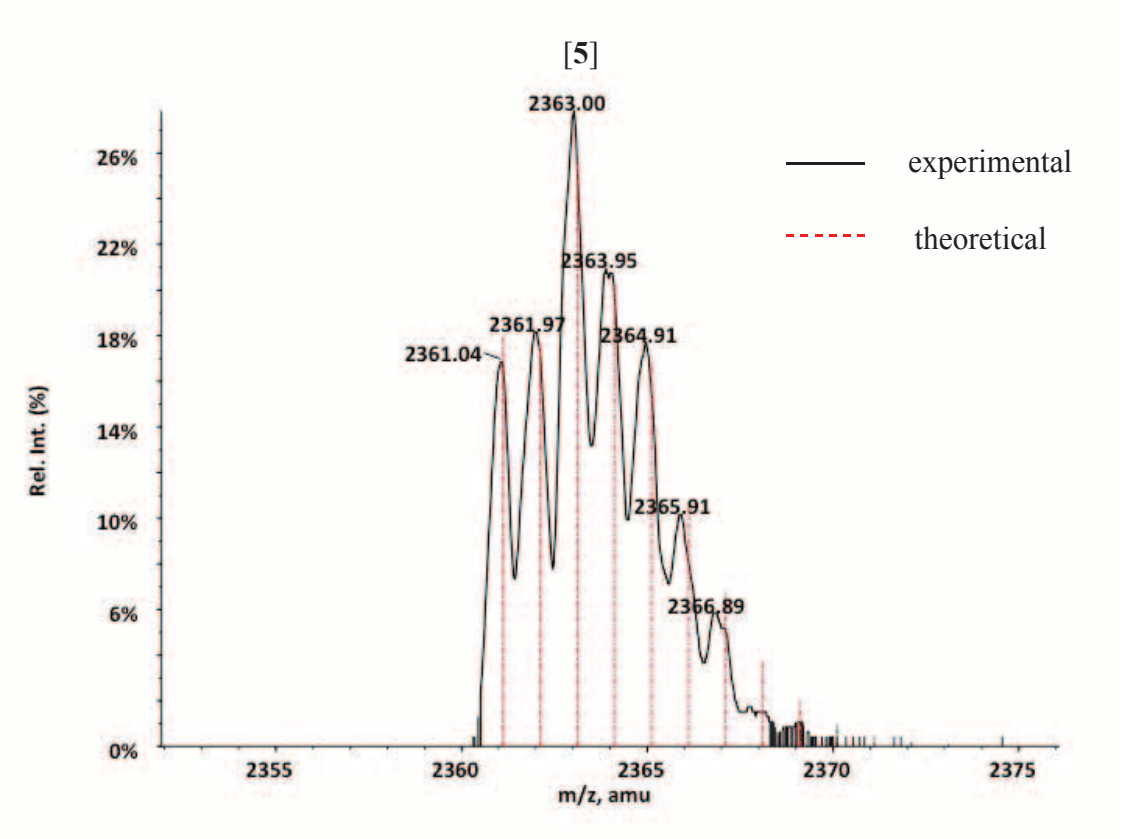

Figure S15. $^{+}$ESI-MS of complex **5,** [{Ni(ema)}$_2$Au$_4$(PPh$_3$)$_4$], m/z [M] = 2363, in CD_2Cl_2.

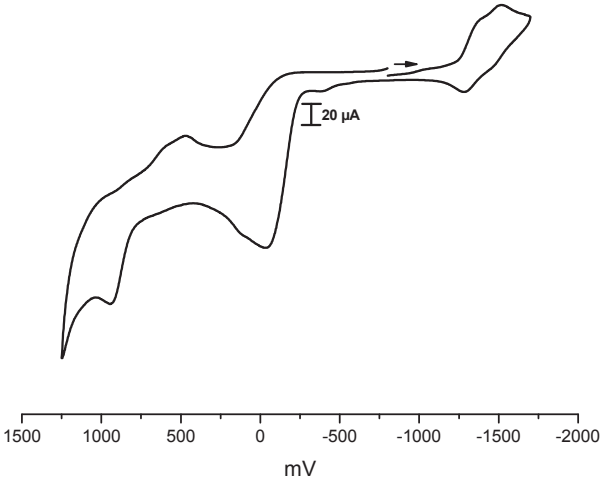

Figure S16. Full cyclic voltammogram measured on a solution of complex **1** (2mM) at a scan rate of 150 mV/s in MeCN.

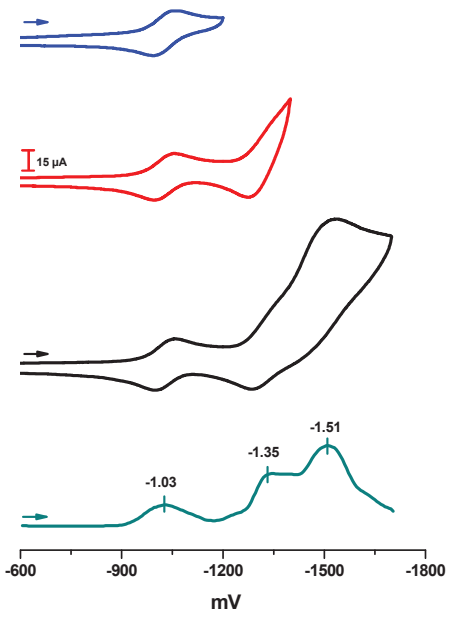

Figure S17. Cyclic voltammograms initiated in the oxidation region (with scan reversals to isolate successive waves) of 2 mM solutions of **1** in 0.1 mM TBAHFP/CH_3CN with a glassy carbon working electrode at 150 mV/s scan rate. Scans of the squarewave voltammograms are initiated in the negative direction; square-wave voltammogram amplitude = 25 mV; frequency = 15 Hz; *E*step = 4 mV.

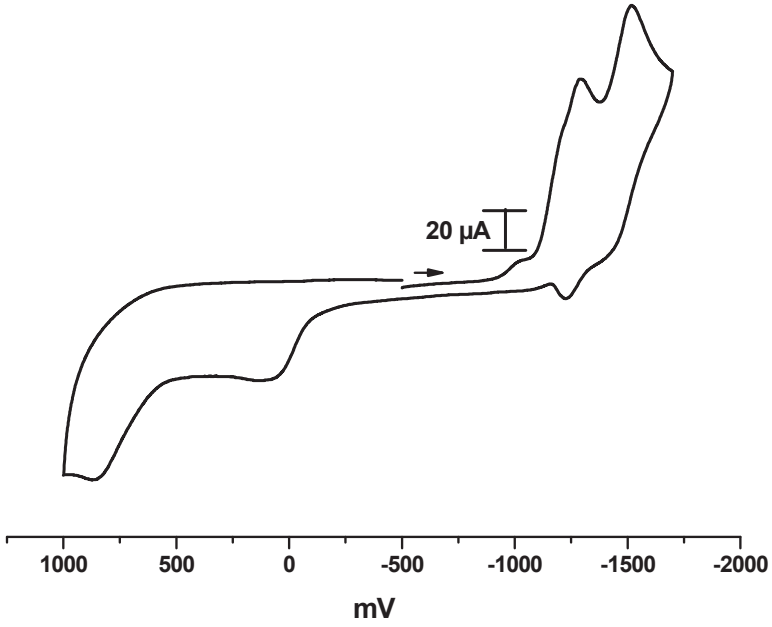

Figure S18. Full cyclic voltammogram measured on a solution of complex **2** (2mM) at a scan rate of 150 mV/s in MeCN.

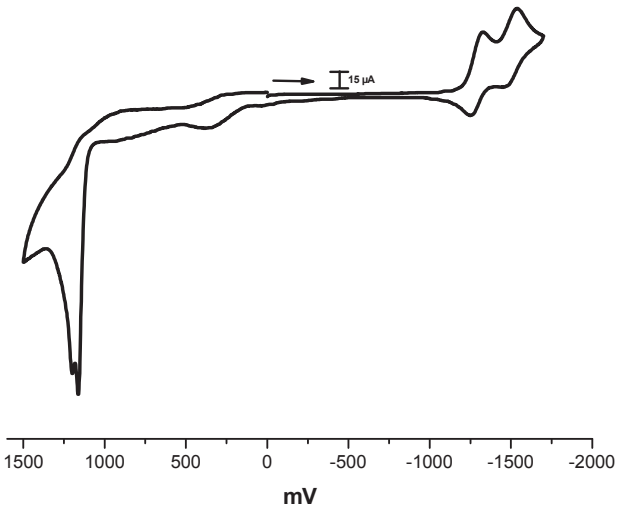

Figure S19. Full cyclic voltammogram measured on a solution of complex **3** (2mM) at a scan rate of 150 mV/s in MeCN.

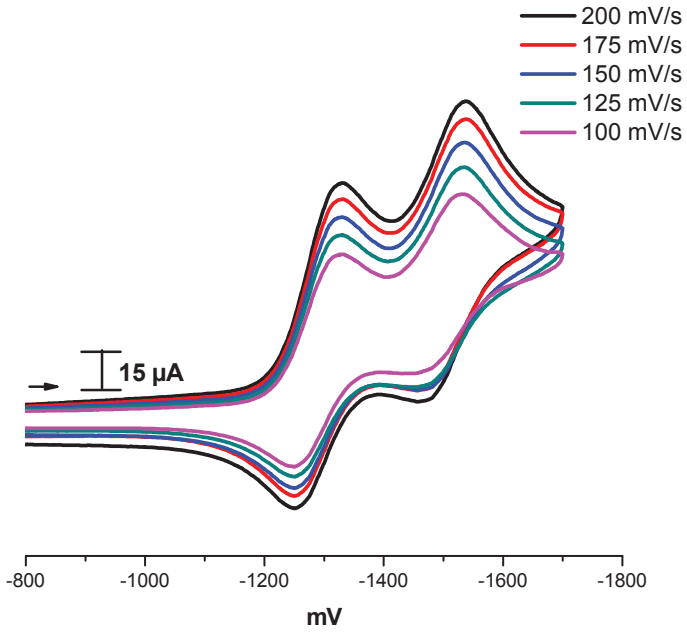

Figure S20. Cyclic voltammogram of complex **3** (2mM) at varied scan rates in MeCN.

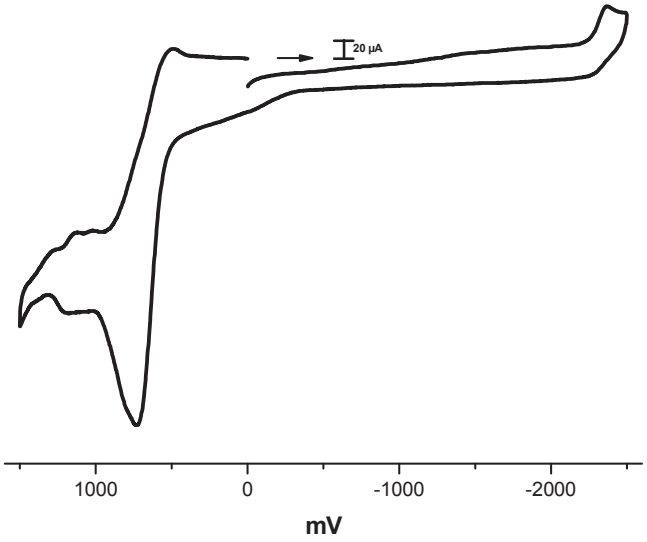

Figure S21. Full cyclic voltammogram measured on a solution of complex **4** (2mM) at a scan rate of 150 mV/s in MeCN.

Table S11. Solubility properties of complexes **1 – 4**

	H_2O	MeCN	MeOH	DCM
1	✓	✓	✓	✓
2	✓	✓	✓	✓
3	✓	✓	✓	✗
4	✓	✗ [a]	✓	✗ [a]

[a]Slightly soluble in solvent. Cyclic voltammetry measurements for complex **4** (2mM) was conducted in both MeCN and MeOH giving identical results.

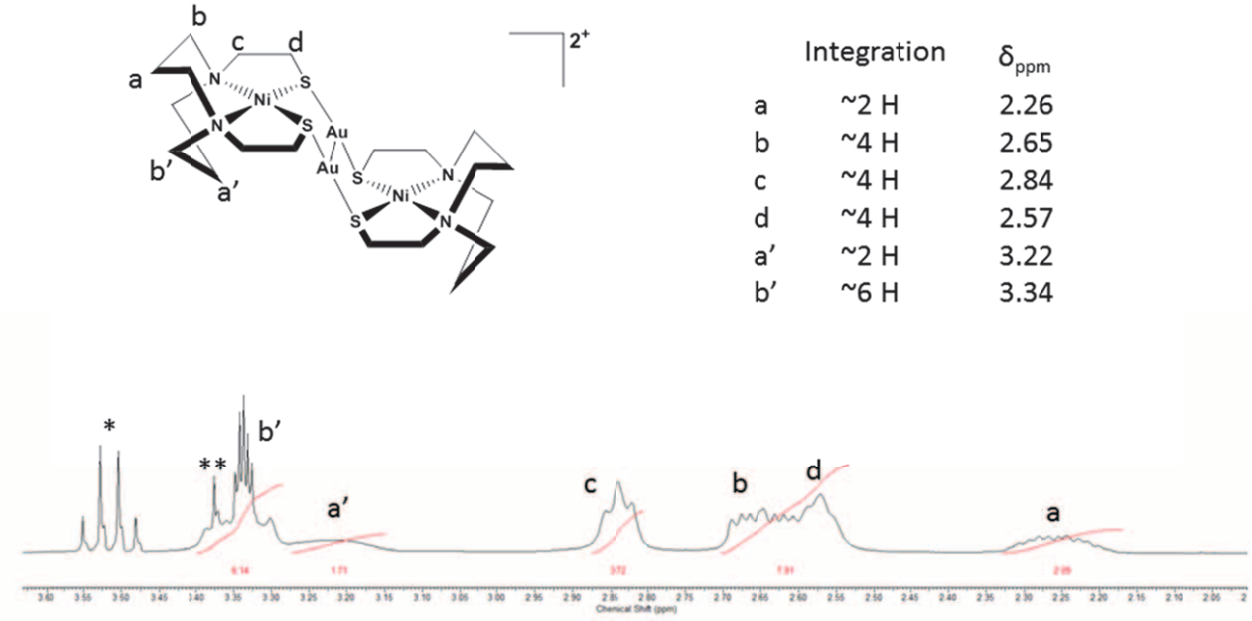

Figure S22. ^{1}H NMR of complex **2** taken at rt (22°C) in CD_3OD. * Quartet centered at 3.52 ppm is assigned to diethyl ether impurity. ** Sharp singlet at 3.38 ppm is an unknown impurity.

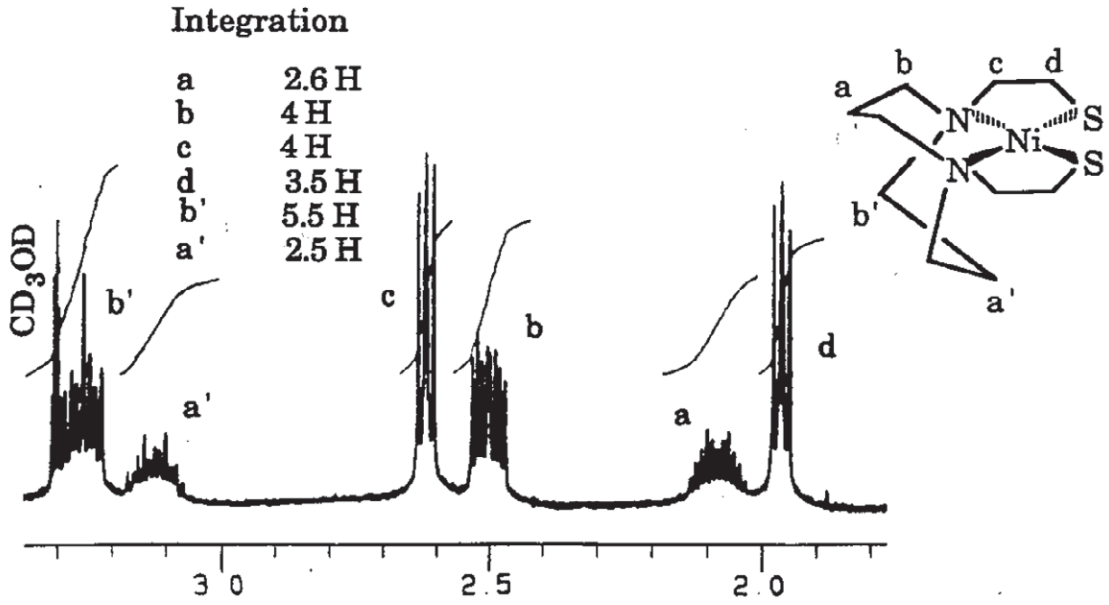

Figure S23. The graphic was taken from the dissertation of Daniel Mills at Texas A&M University. The spectrum was recorded on an Inova 300 mHz spectrometer in CD_3OD.