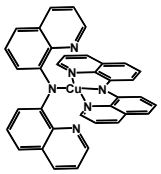
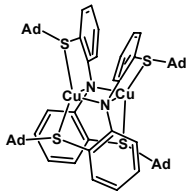
Appendix B

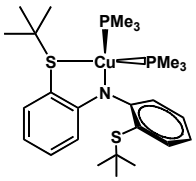
Undiscussed solid-state molecular structures



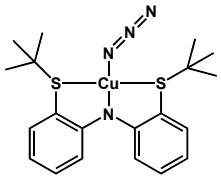
$(BQA)_2Cu$ B-4



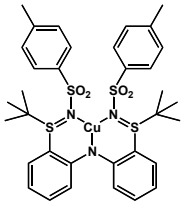
$\{(^{Ad}SNS)Cu\}_2$ B-5



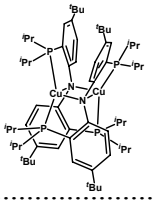
$(PMe_3)_2Cu(SNS)$ B-6



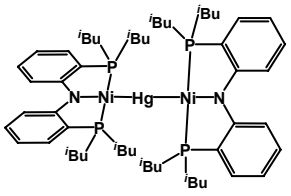
$(SNS)CuN_3$ B-7



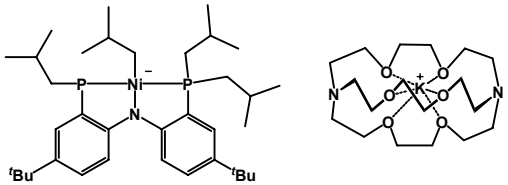
$((TosN)_2\text{-}SNS)Cu$ B-8



$\{(^tBu_2\text{-}^{iPr}PNP)Cu\}_2$ B-9



$\{(PNP)Ni\}_2Hg$ B-10



$[(PNP')Ni\text{-}CH_2CH(CH_3)_2][(crypt)K]$..... B-11

Table B.1: X-ray parameters for assorted copper and nickel amide complexes.[a]

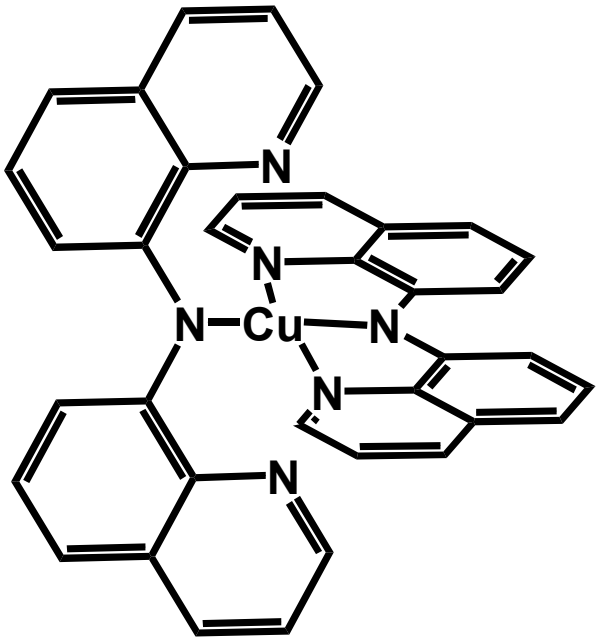
	Page B-4	Page B-5	Page B-6	Page B-7	Page B-8	Page B-9	Page B-10	Page B-11
Chemical Formula	$C_{36}H_{24}CuN_6$	$C_{64}H_{76}Cu_2N_2S_4$	$C_{26}H_{44}CuNP_2S_2$	$C_{20}H_{26}CuN_4S_2$	$C_{34}H_{40}CuN_3O_4S_4$	$C_{64}H_{104}Cu_2N_2P_4$	$C_{56}H_{88}HgN_2Ni_2P_4$	$[C_{36}H_{60}NP_2Ni][C_{18}H_{36}KN_2O_6]$
Formula Weight	604.15	1128.65	560.22	499.09	746.47	1152.45	1231.17	1043.09
T (K)	100(2)	98(2)	98(2)	98(2)	100(2)	100(2)	100(2)	100(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
a (Å)	14.0498(9)	23.875(6)	9.7826(8)	8.9030(6)	10.979(3)	22.778(2)	20.2832(5)	13.297(5)
b (Å)	29.936(2)	21.522(5)	9.8845(8)	25.869(2)	20.300(4)	14.334(1)	16.7095(4)	21.98(1)
c (Å)	13.4935(8)	25.877(7)	16.210(1)	9.0191(6)	16.544(3)	38.483(3)	16.7667(5)	20.600(9)
α (°)	90	90	82.890(1)	90	90	90	90	90
β (°)	104.211(1)	90	79.295(1)	91.2610(10)	109.19(2)	94.282(1)	93.390(1)	102.17(3)
γ (°)	90	90	73.818(1)	90	90	90	90	90
V ($Å^3$)	5501.5(6)	13297(6)	1474.8(2)	2076.7(2)	3482.4(13)	12529(2)	5672.7(3)	5886(5)
Crystal System	Monoclinic	Orthorhombic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	Cc (#9)	Pbca (#61)	P-1 (#2)	P2(1)/n (#14)	P2(1)/c (#14)	P 2(1)/c (#14)	C 2/c (#15)	P 2(1)/c (#14)
Z	8	8	2	2	4	8	4	4
D_{calcd} (g/cm^3)	1.459	1.350	1.262	1.440	1.424	1.222	1.442	1.177
μ (mm^{-1})	0.833	1.017	1.005	1.265	0.909	0.820	3.506	0.501
R1	0.0473	0.0842	0.0254	0.0320	0.0513	0.0514	0.0335	0.0470
wR2 (I>2σ(I))	0.0707	0.1836	0.0667	0.0656	0.0765	0.0888	0.0665	0.0796

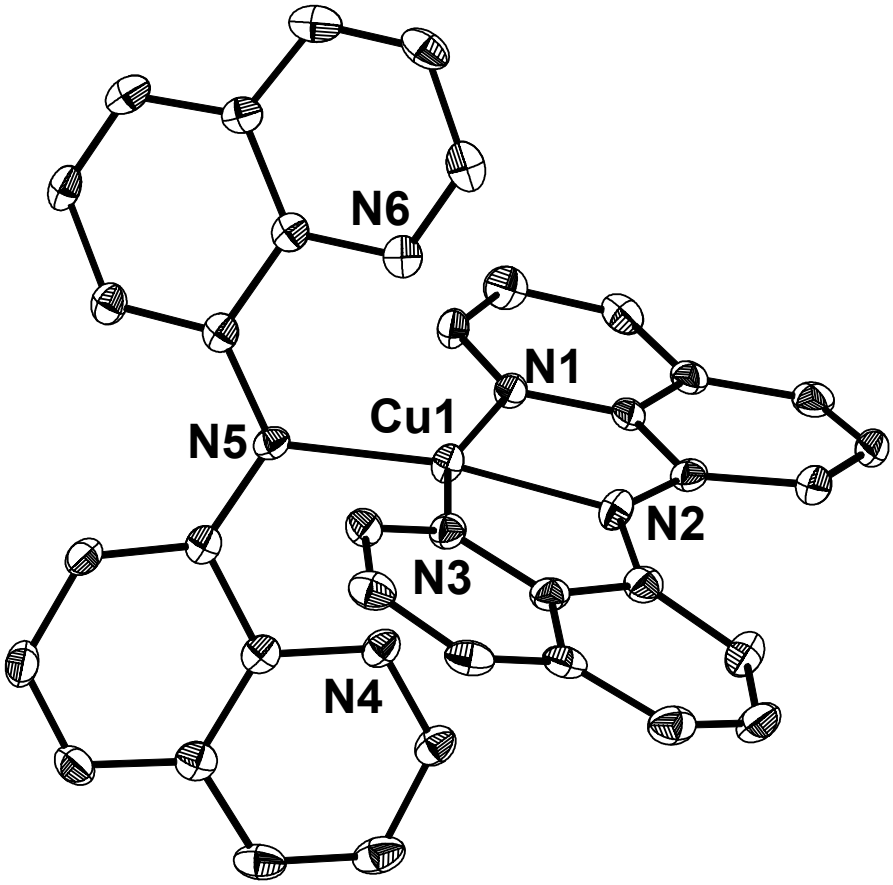
[a] $R1 = \Sigma ||F_o|-|F_c|| / \Sigma |F_o|$, $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

$(BQA)_2Cu$

Bond Lengths and Angles

Cu1−N1	2.070(2) Å
Cu1−N3	2.053(2) Å
Cu1−N2	1.969(2) Å
Cu1−N5	2.002(2) Å
Cu1−N6	2.482(2) Å
Cu1−N4	2.359(2) Å
N1−Cu1−N3	159.76(8)°
N2−Cu1−N5	171.12(9)°
N1−Cu1−N2	80.50(9)°
N3−Cu1−N2	80.60(8)°
N3−Cu1−N5	96.58(8)°
N1−Cu1−N5	103.17(8)°

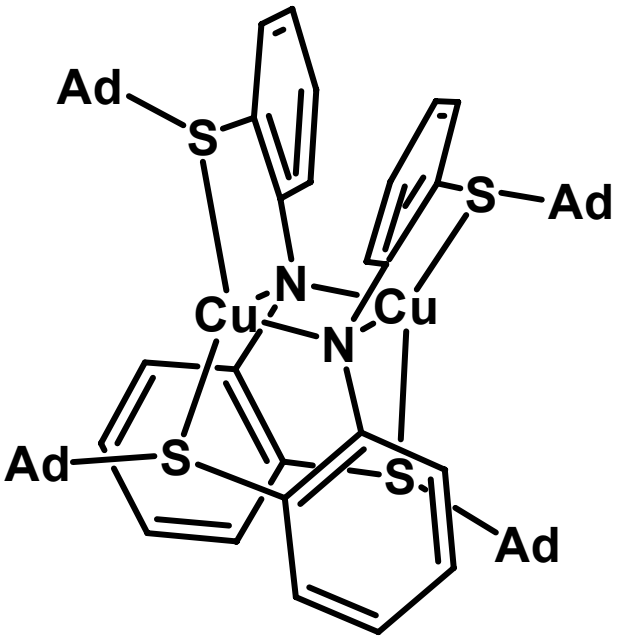


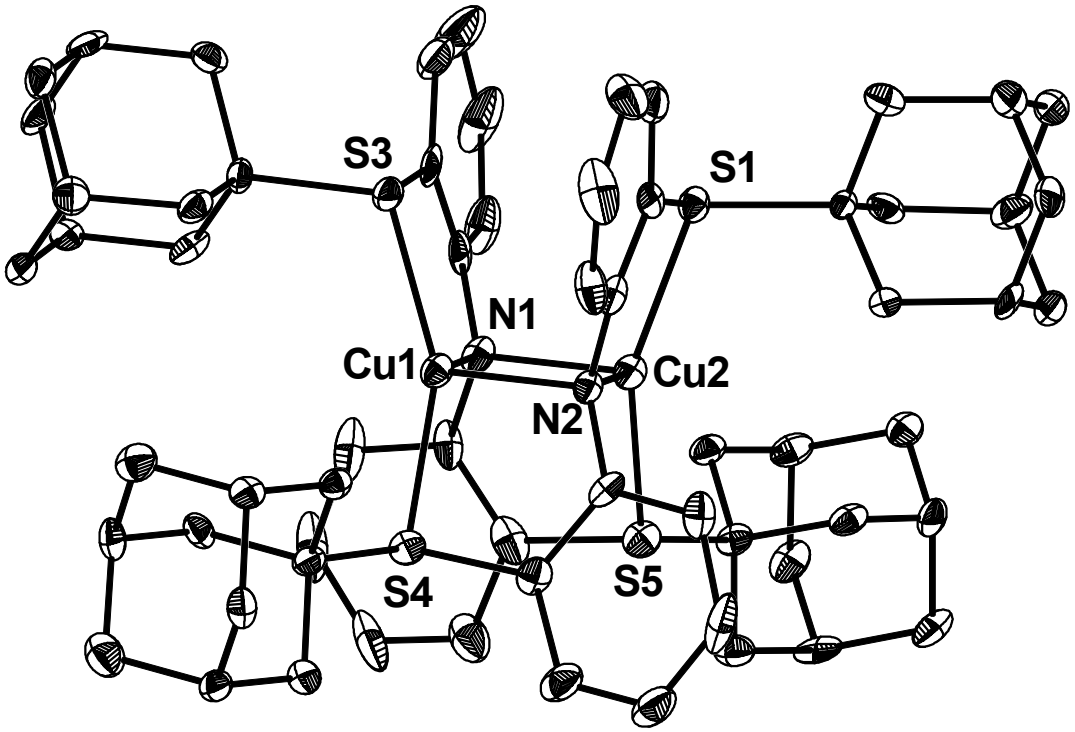


$\{(^{Ad}SNS)Cu\}_2$

Bond Lengths and Angles

Cu1−Cu2	2.6184(12) Å
N1−Cu1	2.119(5) Å
N1−Cu2	2.137(4) Å
N2−Cu1	2.132(4) Å
N2−Cu2	2.128(5) Å
Cu1−S4	2.263(2) Å
Cu1−S3	2.267(2) Å
Cu2−S1	2.267(2) Å
Cu2−S5	2.265(2) Å
N1−Cu1−N2	104.35(18)°
N1−Cu2−N2	103.87(18)°
Cu1−N1−Cu2	75.92(16)°
Cu1−N2−Cu2	75.85(16)°
S3−Cu1−S4	152.95(7)°
S1−Cu2−S5	153.54(8)°

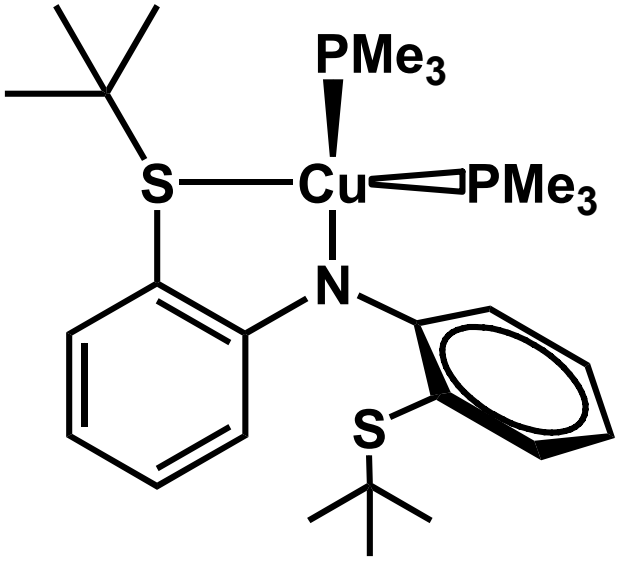


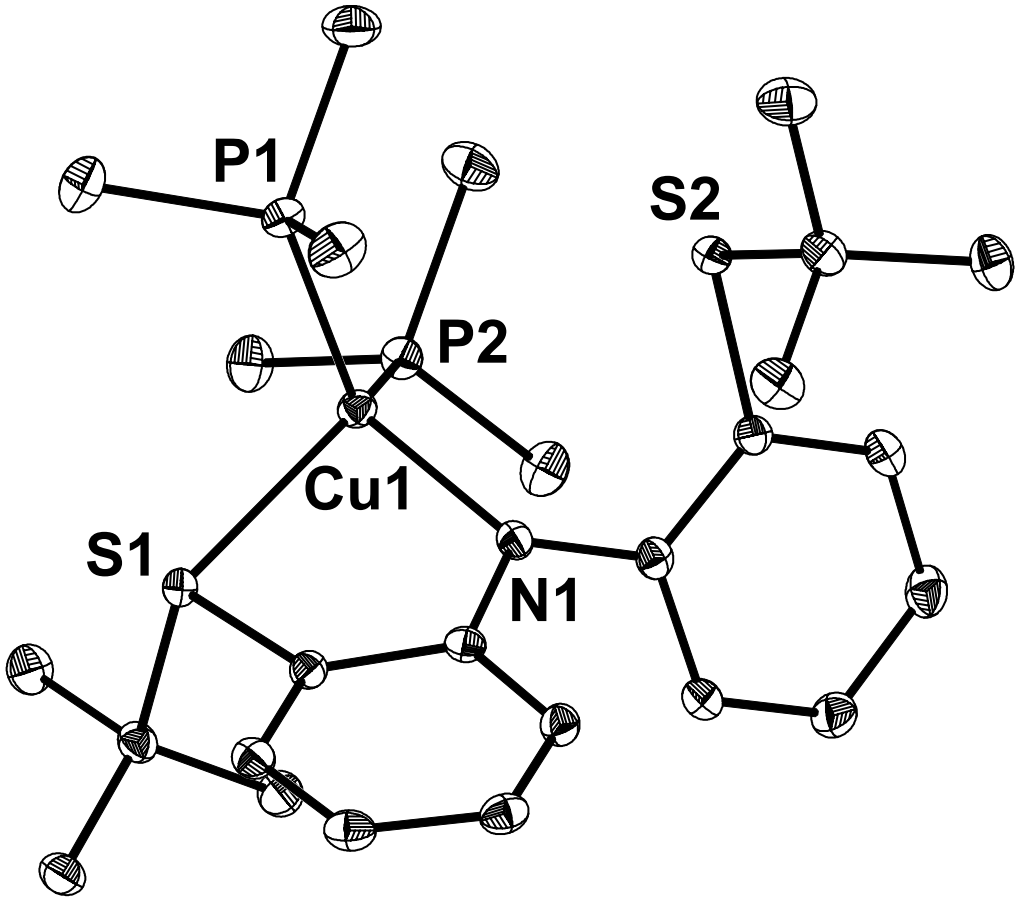


$(PMe_3)_2Cu(SNS)$

Bond Lengths and Angles

Cu1−N1	2.043(1) Å
Cu1−S1	2.393(1) Å
Cu1−P1	2.275(2) Å
Cu1−P2	2.229(1) Å
Cu1−S2	3.536(1) Å
N1−Cu1−S1	85.28(3)°
N1−Cu1−P1	111.26(3)°
N1−Cu1−P2	114.85(4)°
P2−Cu1−P1	118.39(2)°
P1−Cu1−S1	95.58(1)°
S1−Cu1−P2	126.15(1)°

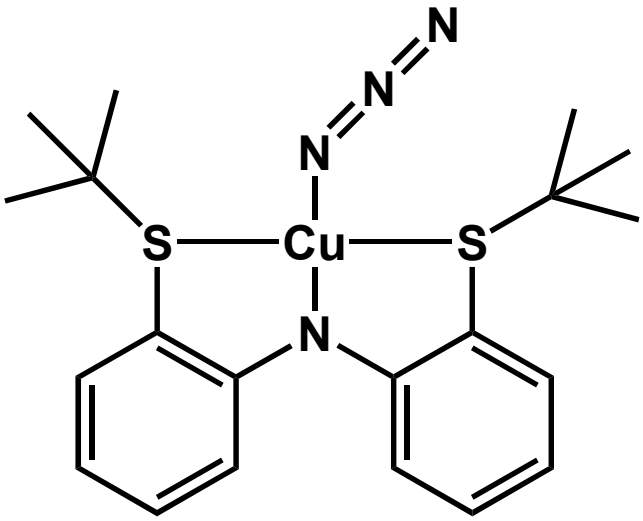


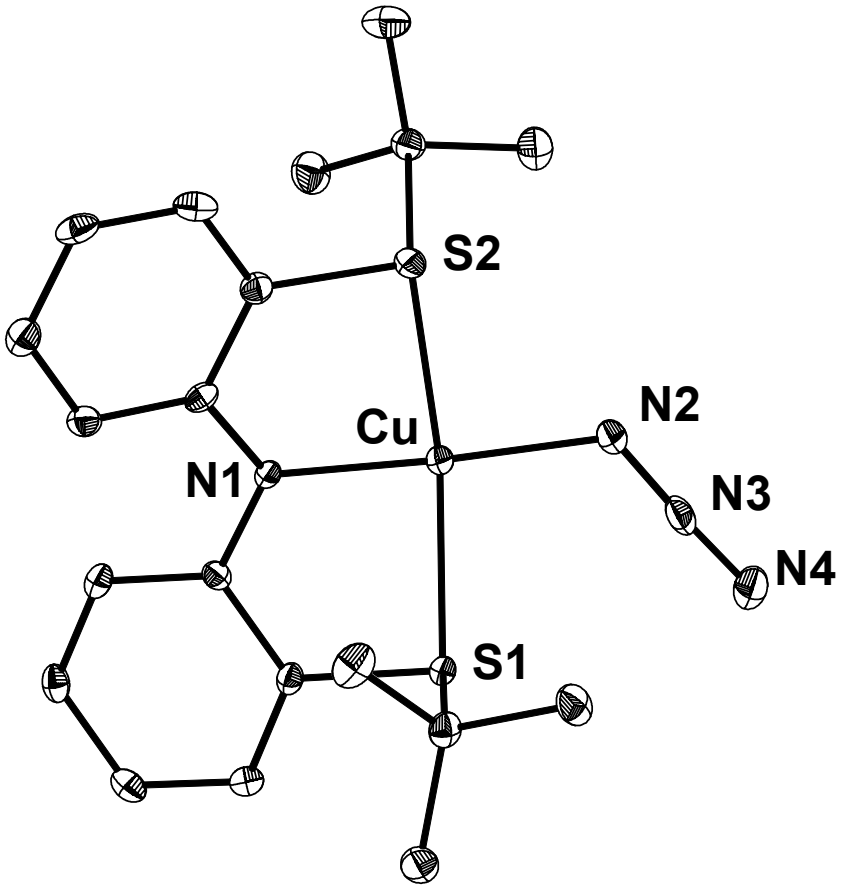


(SNS)CuN$_3$

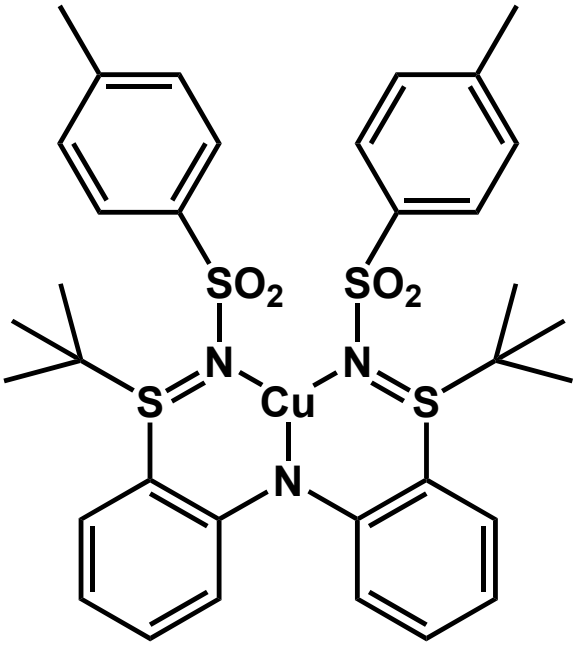
Bond Lengths and Angles

Cu−N1	1.911(2) Å
Cu−S1	2.342(1) Å
Cu−S2	2.370(1) Å
Cu−N2	1.930(2) Å
N2−N3	1.200(2) Å
N3−N4	1.154(2) Å
S1−Cu−N1	86.14(5)°
N1−Cu−S2	85.88(5)°
S2−Cu−N2	93.28(5)°
N2−Cu−S1	96.17(5)°
Cu−N2−N3	123.81(14)°
N2−N3−N4	177.01(19)°
S1−Cu−S2	162.45(2)°
N1−Cu−N2	174.26(7)°



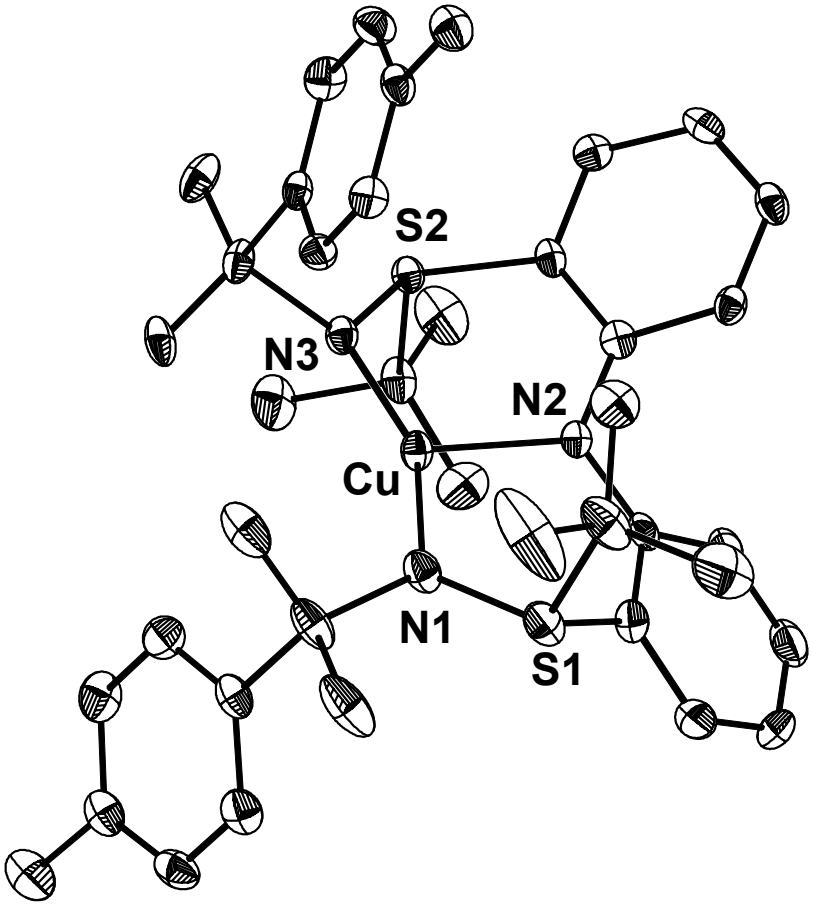


((TosN)$_2$-SNS)Cu



Bond Lengths and Angles

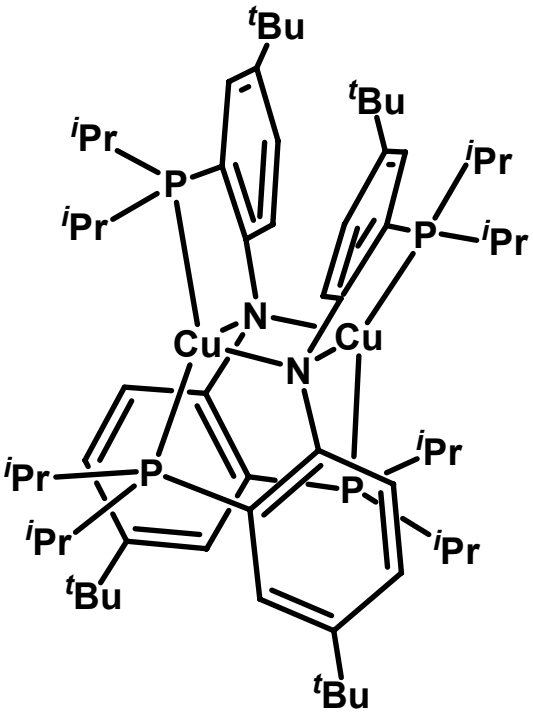
Cu−N1	1.898(18) Å
Cu−N2	2.017(3) Å
Cu−N3	1.903(18) Å
N1−S1	1.649(12) Å
N3−S2	1.652(10) Å
N1−Cu−N2	102.87(12)°
N2−Cu−N3	103.66(12)°
N3−Cu−N1	153.47(14)°
Cu−N1−S1	120.06(19)°
Cu−N3−S2	118.36(17)°

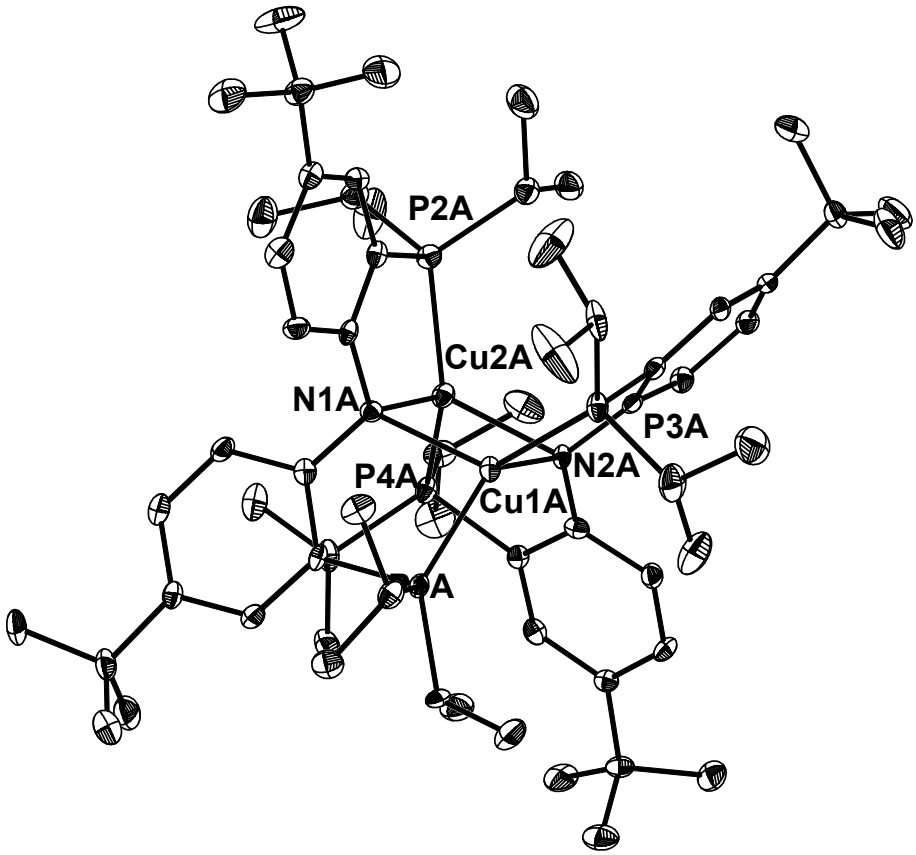


{(^{t}Bu$_2$-^{iPr}PNP)Cu}$_2$

Bond Lengths and Angles

Cu1A-Cu2A	2.7027(6) Å
Cu1A−N1A	2.143(3) Å
Cu1A −N2A	2.171(2) Å
Cu2A −N1A	2.186(2) Å
Cu2A −N2A	2.169(3) Å
Cu1A−P1A	2.237(1) Å
Cu1A −P3A	2.215(1) Å
Cu2A −P2A	2.215(1) Å
Cu2A −P4A	2.221(1) Å
N1A−Cu1A−N2A	103.50(9)°
N1A−Cu2A−N2A	102.17(9)°
Cu1A −N1A−Cu2A	77.26(8)°
Cu1A −N2A−Cu2A	77.04(8)°
P1A− Cu1A −P3A	128.82(4)°
P2A− Cu2A −P4A	137.75(4)°

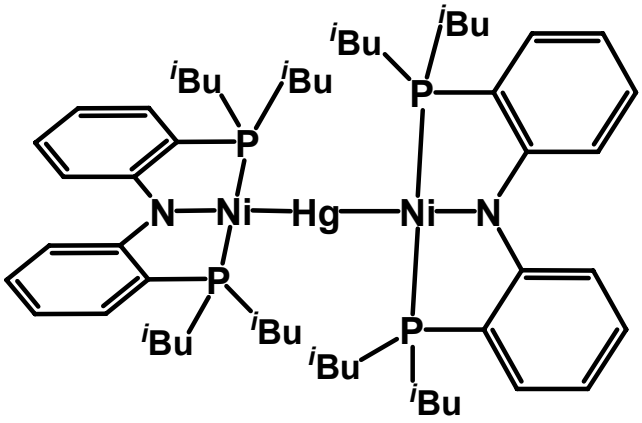


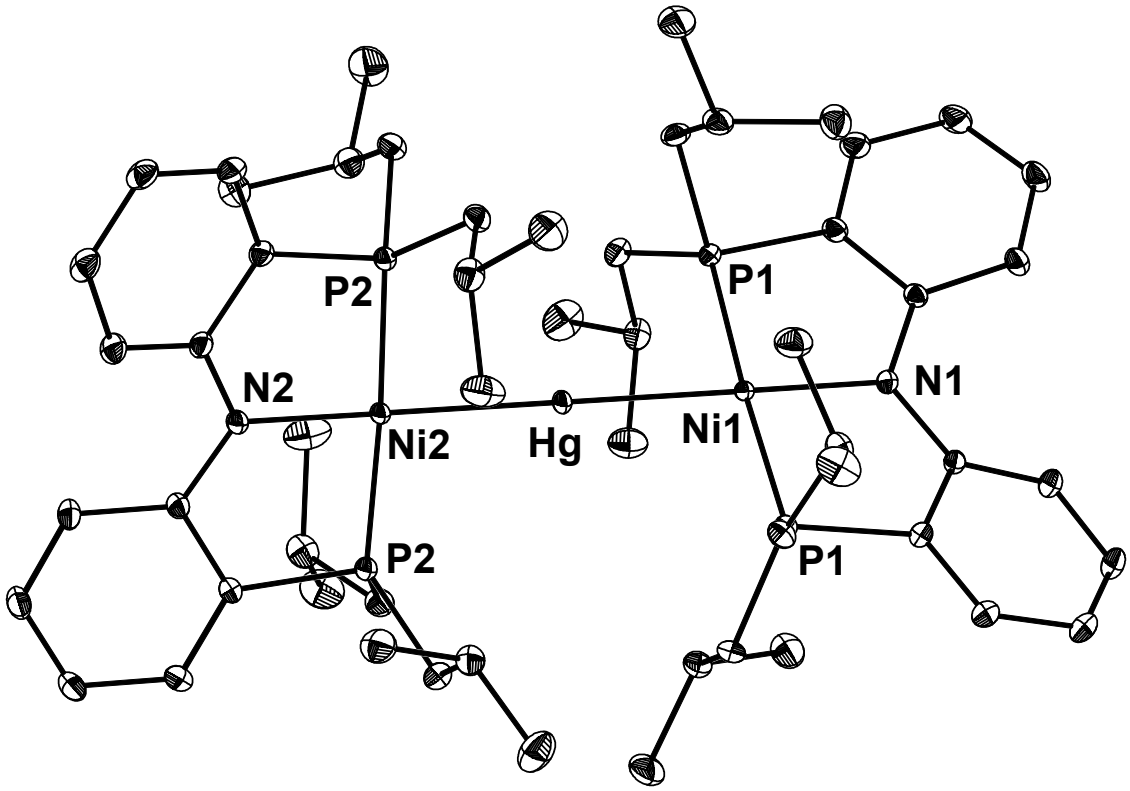


{(PNP)Ni}$_2$Hg

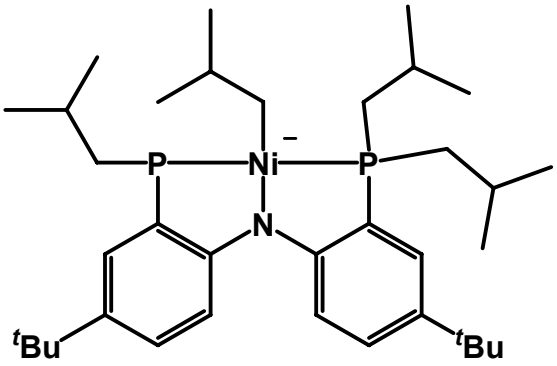
Bond Lengths and Angles

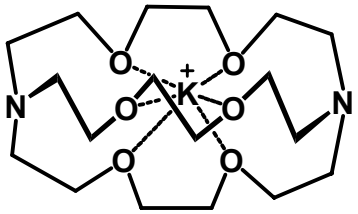
Ni1−P1	2.135(1) Å
Ni1−N1	1.969(2) Å
Ni2−P2	2.141(1) Å
Ni2−N2	1.969(2) Å
Ni2−Hg	2.509(0) Å
Ni1−Hg	2.514(0) Å
P1−Ni1−N1	88.63(1)°
P1−Ni1−P1	177.25(1)°
P2−Ni2−N2	88.25(1)°
P2−Ni2−P2	176.49(1)°
N1−Ni1−Hg	180.00(3)°
Ni1−Hg−Ni2	180.0°
Hg−Ni2−N2	180.00(3)°





[(PNP′)Ni-$CH_2CH(CH_3)_2$][(crypt)K]





Bond Lengths and Angles

N1−Ni	1.960(6)
P1−Ni	2.142(24)
P2−Ni	2.201(15)
C33−Ni	1.964(12)
N1−Ni−P1	86.35(6)°
P1−Ni−C33	95.18(7)°
Ni−P2−C33	40.27(5)°
P2−Ni−N1	87.79(6)°
N1−Ni−C33	170.52(9)°
P1−Ni−P2	162.54(4)°