Tri- and Tetracoordinate Copper(I) Complexes bearing Bidentate Soft/Hard SN and SeN Ligands based on 2-Aminopyridine

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Supporting Information

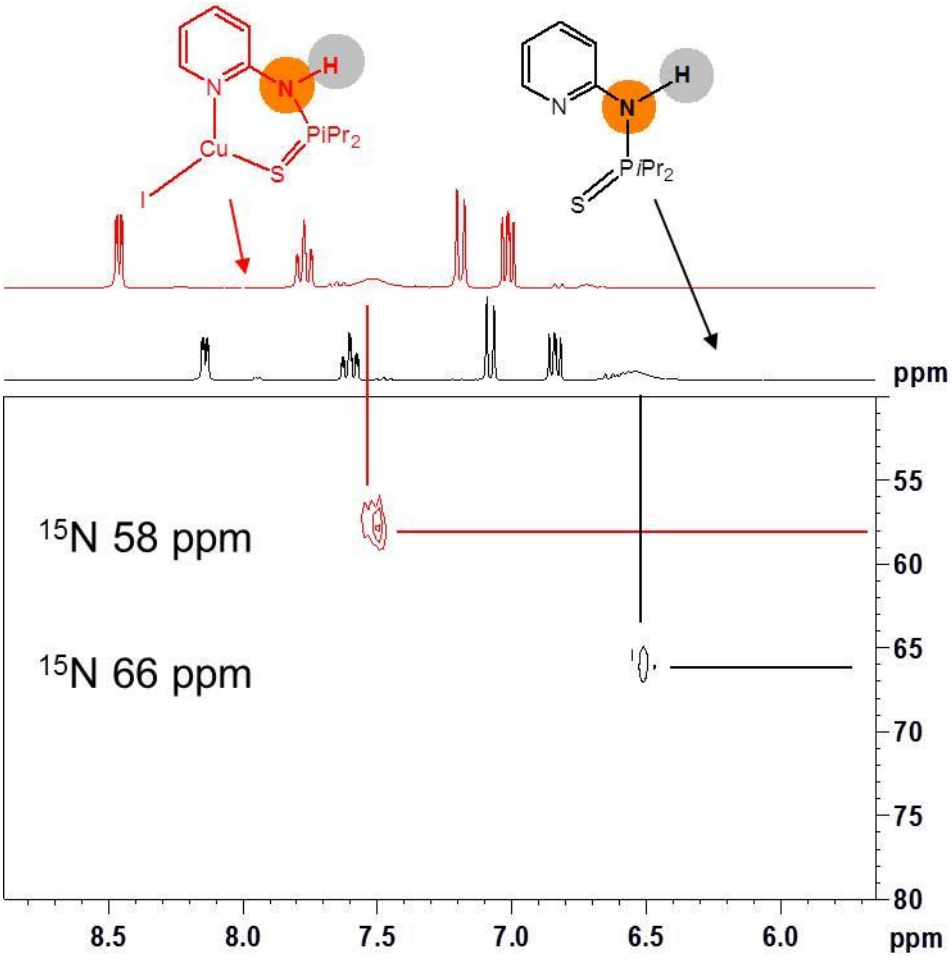

Figure S1. 300 MHz ^{1}H-^{15}N HSQC spectra of SN-*i*Pr (**2b**) and [Cu(SN-*i*Pr)I] (**5b**) in acetone-d_6 at 25^{o}C.

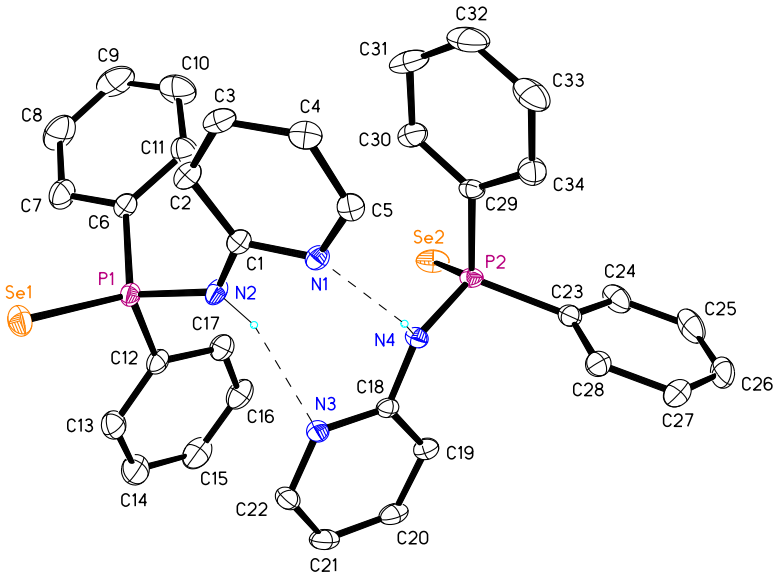

Figure S2. ORTEP diagram of **2a** showing the two independent molecules of the structure with 50% displacement ellipsoids. The compound is isostructural with the S-analogue **1a**. Carbon-bonded H atoms omitted for clarity. Selected distances and angles (Å, °): P1–Se1 2.1004(5), P2–Se2 2.1030(5), P1–N2 1.6692(15), P2–N4 1.6692(14), N2–P1–Se1 116.19(6), N4–P2–Se2 115.53(5), N1-C1–N2–P1 176.0(1), N3–C18–N4–P2 -151.0(12), C1–N2–P1–Se1 -58.7(2), C18–N4–P2–Se2 45.8(2), N2···N3 2.940(2), N4···N1 2.926(2).

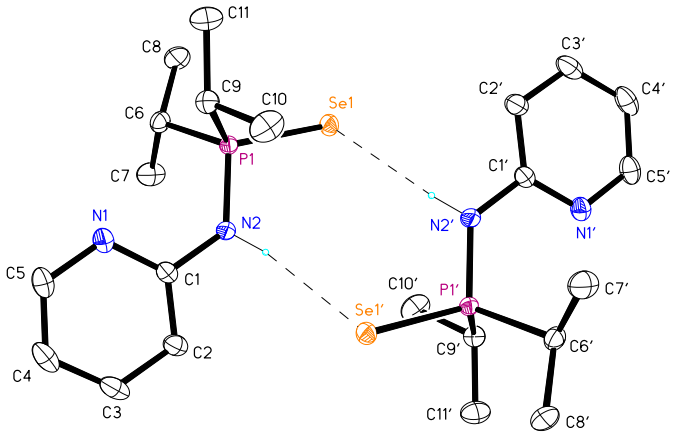

Figure S3. ORTEP diagram of **2b** showing two inversion-related and N-H···Se hydrogen bonded molecules of the structure with 50% displacement ellipsoids. Atoms with primed atom labels are symmetry equivalents of the unprimed atoms. The compound is not isostructural with the S-analogue **1b**. Carbon-bonded H atoms omitted for clarity. Selected distances and angles (Å, °): P1–Se1 2.1136(3), P1–N2 1.6812(9), N2–P1–Se1 105.50(3), N1-C1–N2–P1 -1.61(14), C1–N2–P1–Se1 -177.33(8), N2···Se1' 3.590(1).

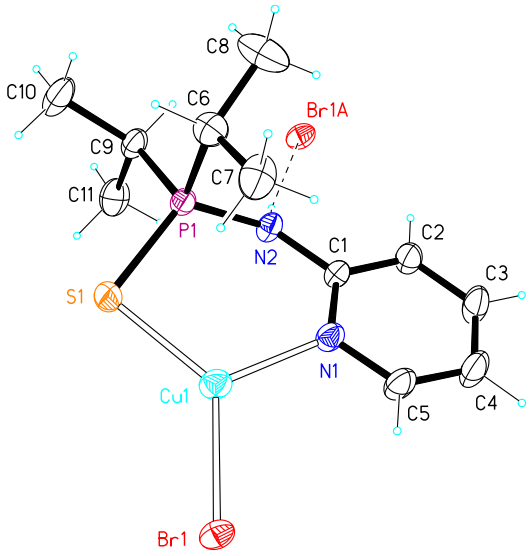

Figure S4. Molecular structure of **3b** showing 30% displacement ellipsoids. The compound is isostructural with **5b** and **6b**. Selected distances and angles (Å, °): Cu1–N1 2.026(2), Cu1–S1 2.2046(7), Cu1–Br1 2.3267(4), P1–S1 1.9892(8), P1–N2 1.674(2), N2–C1 1.390(3), N1–Cu1–S1 115.24(5), N1–Cu1–Br1 113.86(5), S1–Cu1–Br1 130.27(2), P1–S1–Cu1 93.62(3), N2–P1–S1 117.50(7), C1–N2–P1 131.8(2), N1–C1–N2 118.9(2), Cu1–N1–C1 123.3(2); hydrogen bond N2···Br1a 3.447(2).

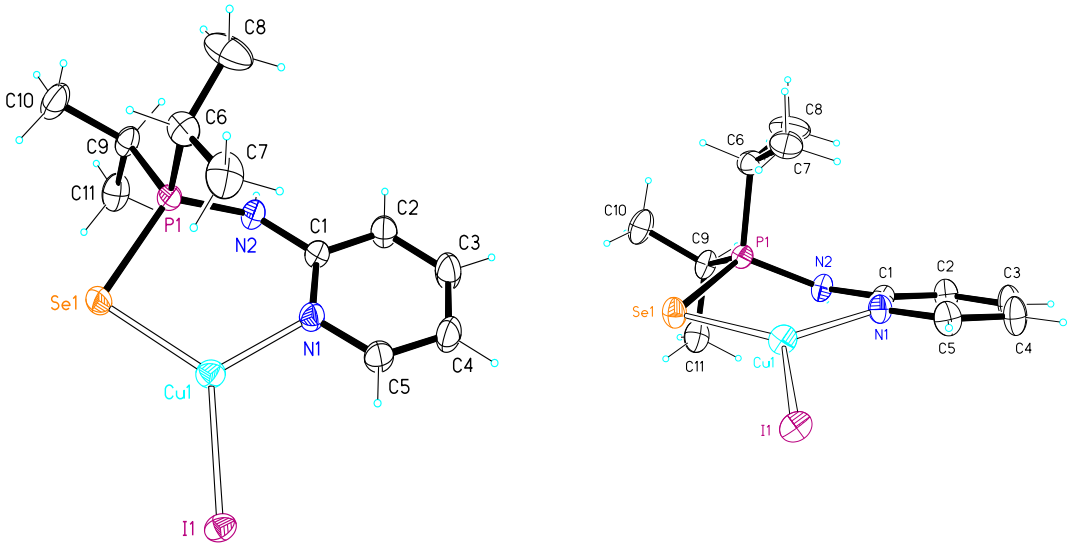

Figure S5. Molecular structure of **6b** showing 30% displacement ellipsoids in top and side view. The compound is isostructural with **3b** and **5b**. Selected distances and angles (Å, °): Cu1–N1 2.017(4), Cu1–Se1 2.3226(8), Cu1–I1 2.4946(6), P1–Se1 2.145(1), P1–N2 1.680(4), N2–C1 1.387(6), N1–Cu1–Se1 117.87(14), N1–Cu1–I1 115.52(11), Se1–Cu1–I1 126.97(3), P1–Se1–Cu1 88.76(4), N2–P1–Se1 117.87(14), C1–N2–P1 132.3(3), N1–C1–N2 118.8(4), Cu1–N1–C1 124.2(3); hydrogen bond N2···I1, 3.721(3) Å, not shown.

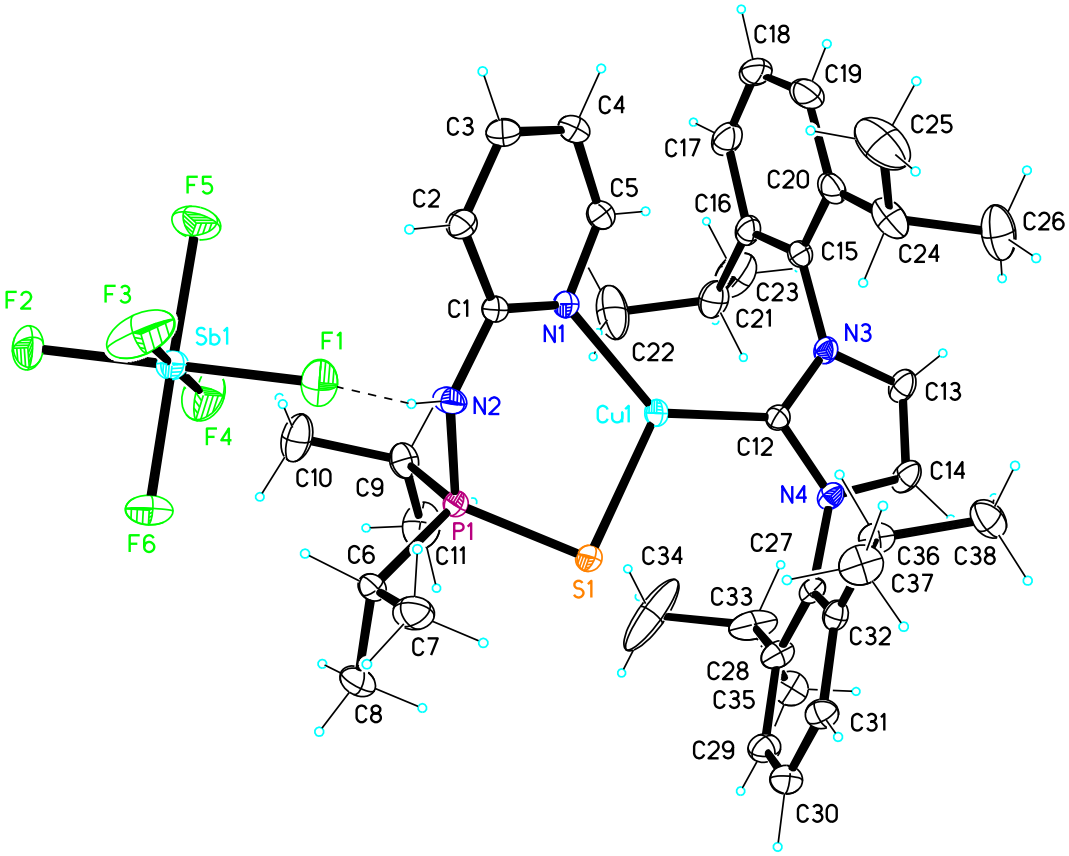

Figure S6. Molecular structure of **7b** showing 50% displacement ellipsoids. Selected distances and angles (Å, °): Cu1–C12 1.935(2), Cu1–N1 2.044(2), Cu1–S1 2.3057(5), P1–S1 1.9746(6), P1–N2 1.672(2), C12–Cu1–N1 135.19(7), C12–Cu1–S1 117.74(5), N1–Cu1–S1 106.91(4), P1–S1–Cu1 94.47(2); hydrogen bond N2···F1 3.023(2).