Supporting Information

Imine-coordinated 2-Aminoazole Complexes of Au(I): Complicating Reactions and Verification of Products by Crystal Structure Determination

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Additional analytical data

2-Amino-4-methylthiazole:

^{1}H NMR ($(CD_3)_2CO$): δ = 6.70 (bs, 2H, NH_2), 6.06 (s, 1H, SCH), 2.10 (s, 3H, CH_3). – ^{13}C NMR ($(CD_3)_2CO$): δ = 170.5 (s, NCS), 149.9 (s, CH_3*C*), 102.6 (s, SC), 18.3 (s, CH_3). – ^{15}N NMR ($(CD_3)_2CO$): δ = –122.5 (N=C), –313.7 (NH_2).

^{1}H NMR (CD_2Cl_2): δ = 6.04 (q, 1H, ^{4}J = 1.74 Hz, SCH), 5.94 (bs, 2H, NH_2), 2.17 (d, 3H, ^{4}J = 1.74 Hz, CH_3). – ^{13}C NMR (CD_2Cl_2): δ = 168.6 (s, NCS), 148.6 (s, CH_3*C*), 102.0 (s, SC), 17.1 (s, CH_3).

2-Aminobenzothiazole:

^{1}H NMR ($(CD_3)_2CO$): δ = 7.63 (d, 1H, ^{3}J = 7.3 Hz, NCCH), 7.41 (d, 1H, ^{3}J = 7.3 Hz, SCCH), 7.24 (dd, 1H, ^{3}J = 7.3 Hz, NCCHC*H*), 7.05 (dd, 1H, ^{3}J = 7.3 Hz, SCCHC*H*), 7.00 (bs, 2H, NH_2). – ^{13}C NMR ($(CD_3)_2CO$): δ = 168.4 (s, NCS), 154.9 (s, N*C*CHCH), 133.5 (s, S*C*CHCH), 127.3 (s, SCCH*C*H), 123.1 (s, NCCH*C*H), 122.5 (s, SC*C*HCH), 120.2 (s, NC*C*HCH). – ^{15}N NMR ($(CD_3)_2CO$): δ = –140.3 (N=C), –309.6 (NH_2).

2-Aminobenzimidazole:

^{1}H NMR ($(CD_3)_2CO$): δ = 7.18 (m, 2H, NCC*H*CH), 6.90 (m, 2H, NCCHC*H*), 6.21 (bs, 2H, NH_2). – ^{13}C NMR ($(CD_3)_2CO$): δ = 157.4 (s, NCN), 140.7 (s, N*C*CHCH), 121.4 (s, NCCH*C*H), 113.7 (s, NC*C*HCH). – ^{15}N NMR (CD_3OH): δ = –200.3 (N=C or NH), –331.8 (NH_2).

2-Aminothiazoline:

^{1}H NMR ($(CD_3)_2CO$): δ = 4.71 (bs, 2H, NH_2), 3.84 (dd, 2H, ^3J = 7.5 Hz, NCH_2), 3.27 (dd, 2H, ^3J = 7.5 Hz, SCH_2). – ^{13}C NMR ($(CD_3)_2CO$): δ = 162.5 (s, NCS), 62.1 (s, NCH_2), 37.1 (s, SCH_2). – ^{15}N NMR ($(CD_3)_2CO$): δ = –164.0 (N=C), –305.9 (NH_2).

Crystal structure determinations

Crystallographic data for **3b**: $C_{53}H_{56}Au_2N_8O_9P_2$, M_r = 1404.94, colorless needle, 0.20 × 0.06 × 0.06 mm^3, monoclinic, space group $P2_1/c$ (no. 14), a = 9.7420(9), b = 13.6773(12), c = 21.0830(19) Å, β = 93.197(2)°, V = 2804.8(4) Å^3, Z = 2, D_c = 1.66 g/cm^3, F_{000} = 1380 e, Bruker APEX CCD area-detector, MoK_α radiation, λ = 0.71073 Å, T = 100(2) K, $2\theta_{max}$ = 52.8º, 16145 reflections collected, 5720 unique (R_{int} = 0.0451). Final *GooF* = 1.052, $R1$ = 0.0415, $wR2$ = 0.0886, R indices based on 4376 reflections with $I > 2\,\sigma(I)$ (refinement on F^2), 385 parameters, 25 restraints. Lp and absorption corrections applied, μ = 5.3 mm^{-1}.

The nitrate anion was found to be disordered over two positions with refined site occupancies of 0.63(1):0.37(1). Some of the anisotropic displacement parameters were restrained in this counter ion.

Crystallographic data for **3c** × solvent: $C_{25}H_{22}AuN_4O_3P$, M_r = 654.40, colorless needle, 0.17 × 0.06 × 0.06 mm^3, monoclinic, space group $P2_1/c$ (no. 14), a = 8.955(5), b = 23.045(12), c = 14.660(8) Å, β = 118.107(9)°, V = 2668(2) Å^3, Z = 4, D_c = 1.63 g/cm^3, F_{000} = 1272 e, Bruker APEX CCD area-detector, MoK_α radiation, λ = 0.71073 Å, T = 100(2) K, $2\theta_{max}$ = 56.8º, 16491 reflections collected, 6252 unique (R_{int} = 0.0339). Final *GooF* = 0.983,

$R1$ = 0.0297, $wR2$ = 0.0671, R indices based on 5247 reflections with $I > 2\sigma(I)$ (refinement on F^2), 314 parameters, 2 restraints. Lp and absorption corrections applied, μ = 5.6 mm^{-1}.

In structure **3c,** the solvent molecules could not be assigned because of diffuse electron density. Therefore, the electron density was subtracted and the SQUEEZE instruction of PLATON was applied. Consequently, the relative molecular mass M, F(000), and absorption coefficient are not correct since, solvent molecules were not taken into account in these calculations.