Electronic Supplementary Material (ESI) for Dalton Transactions.

Coordination Chemistry of Mercury (II) Halide complexes: A Combined Experimental, Theoretical and (ICSD & CSD) Database study on the Relationship between Inorganic and Organic Units

Ali Samie[1], Alireza Salimi*[1], Jered C. Garrison[2]

[1]*Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran*

[2]*Department of Pharmaceutical Sciences, University of Nebraska Medical Center, 985830, Nebraska, United States*

Supporting Information

S0. List of Contents

S1. General Synthesis Procedure

To a solution of 0.1 mmol mercuric (II) halide (HgX_2, X = Cl, Br) in 10 mL acetonitrile, a solution of 0.2 mmol of L in 10 mL acetonitrile was added with stirring. The Metal to Ligand ratio was 1: 2 except complexes 5 and 6 (1: 1). The mixture was stirred for about 24 hours at the ambient situation and then filtered. The same procedure was done for HgI_2 in acetone as a solvent. All of the solutions were dried on the ambient situation and recrystallized at room temperature but in different solvents and situations upon different evaporation times. The crystallization solvent(s), crystallization period, crystalline color, and crystalline shape were presented in S2.

S2. Crystallization Details

Complex	Crystallization Solvent(s)	Crystallization Period	Crystalline Color	Crystalline Shape
1	acetonitrile	2months	yellow	coral-shaped
2	acetonitrile/methanol (ethanol)	2months	white	coral-shaped
3	3 acetone/methanol	2months	amber	block
4	acetonitrile	2months	amber	cubic
5	acetone/methanol	2months	amber	block
6	acetone/methanol (ethanol)	2months	amber	block
7	acetonitrile	2months	amber	prism
8	acetonitrile	2months	amber	cubic
9	acetonitrile/ethanol/methanol	2months	amber	prism
10	acetonitrile	2months	amber	pipe
11	acetonitrile/ethanol	2months	amber	needle

S3. Instrumentation Details

All the reagents and solvents for syntheses and analyses were purchased from either Aldrich or Merck and used without further purification.

Fourier Transform Infrared Spectroscopy (FTIR) spectra (4000 – 400 cm^{-1}) of the solid sample were taken as 1% dispersion in KBr pellets were recorded with an Avatar 370 FTIR Thermal Nicolet spectrometer.

Elemental Analyses for C, H and N were performed using a Thermo Finning Flash EA1112 CHNO-S Microanalyzer.

Differential Scanning Calorimetry (DSC) was recorded on a Mettler Toledo DSC 823e instrument within a range from 25 to 300 °C with a step size of 0.1 °C/min.

Thermal Gravimetric Analysis (TGA) was performed with Mettler Toledo TGA/SDTA 851e within temperature range of 25 to 400 °C with a step size of 0.1 °C/min.

Nuclear Magnetic Resonance (NMR) was gathered in DMSO-d6 as a media by 300MHz Bruker Avance III for both ^{1}H and ^{13}C.

Powder X-Ray Diffraction (PXRD) data were collected on PANalytical X-ray powder diffractometer equipped with a X'cellerator detector using Cu Kα (λ = 1.54184 Å) at room temperature with the scan range 2θ = 5 to 50° and step size of 0.026 °. X'Pert HighScore Plus was used to compare the experimental PXRD pattern with the calculated lines from the crystal structure.

Single Crystal X-ray Diffraction (SCXRD) Single crystal X-ray diffraction (SCXRD) data for complexes 1, 2, 3, 4, 5, 6, 8, 10, and 11 crystals were collected at 100(2) K on an Oxford Diffraction Excalibur PX Ultra diffractometer equipped with an Enhance Ultra (Cu) X-ray source and Onyx CCD detector. Data reduction and analysis for these structures were carried out with the CrysAlisPro program v. 1.171.37.35.[1] Diffraction data for 7 and 9 were collected on a Rigaku Mercury 375/M CCD (XtaLAB mini) diffractometer using graphite monochromatic Mo(K_α) radiation (0.71075 Å) at 140(2) and 293(2) K, respectively. The data were processed with the Rigaku Crystal Clear 2.0 software.[2] The structures were solved by direct methods[3] and subsequent difference Fourier maps were used for refinement on F^2 by a full-matrix least-squares procedure using anisotropic displacement parameters. The structures were checked for higher symmetry with the help of the program PLATON[4, 5] and Mercury 4.0.0 was utilized for molecular representations and packing diagrams. For the title compounds, the non-H atoms were refined anisotropically and H atoms were placed in the ideal positions. The structural resolution

procedure was performed using the WinGX crystallographic software package.[6] Crystallographic data and refinement parameters are shown in table 1.

S4. Theoretical Details

Initially the binding energies of the all molecules pairs (dimer) assessed based on both B3LYP-D3 and M06-2X as a DFT dispersion-corrected method with with 6-311G (d, p) (for C, H, O, and N) and lanl2dz (for Hg, Cl, Br, and I) basis sets.[7, 8] The presence of heavy metal, halide anions, and organic ligands, made the theoretical study time-consuming and in this regard it was cost-effective. Since the results for both of the methods were close to each other the theoretical studies were performed by the second method which was faster than the other one. In fact, the results of these two methods were validated compared to each other.[9-12] The calculation of noncovalent interactions from the DFT-D3 new method is particularly reliable where the dispersion component has a significant contribution.[13] For the Basis Set Superposition Error (BSSE) corrections the counterpoise method was used.[14] For the computational studies, input data has taken directly from the crystal structure and H atoms were normalized at their neutron distances (1.08 Å for C−H). All the calculations were performed in the GAMESS program package.[15]

S5. Characterization for Complexes 1-11

Complex 1: m.p. 194.69^{o}C; IR (KBr disc) vcm^{-1}: 2847.67, 2917.14 (C–H stretching in aromatic rings), 1746.77 (C=O stretching), 1596.22, 1508.84 (two couple of peaks for C=C in aromatic rings), 1274.86, 1099.34 (C–O stretching); Anal. Calcd. for $C_{32}H_{22}Cl_2HgN_2O_4$: C, 49.91;H, 2.88; N, 3.64; Found: C, 49.17; H, 2.91; N, 3.62; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.6 (m, 4H, H_2, H_3, H_4 and H_6), 7.750 (m, 1H, H_9), 7.953 (m, 2H, H_7 and H_8), 8.0575 (d, 1H, H_{15}, ^{3}J = 6.4 Hz with H_{14}), 8.6425 (d, 1H, H_{14}, ^{3}J= 6.6 Hz with H_{15}), 8.981 (s, 1H, H_{16}), 9.438 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.147, 121.481, 124.849, 125.553, 126.236, 126.735, 126.822, 127.245, 127.436, 128.543, 134.673, 138.482, 146.558, 151.100, 154.762, 164.196.

Complex 2: m.p. 191.64^{o}C; IR (KBr disc) vcm^{-1}: 2847.17, 2920.73 (C–H stretching in aromatic rings), 1746.30 (C=O stretching), 1596.28, 1508.99, 1462.40 (two couple of peaks for C=C in aromatic rings), 1274.75, 1099.28 (C–O stretching); Anal. Calcd. for $C_{32}H_{22}Br_2HgN_2O_4$: C, 44.75;H,

2.58; N, 3.26; Found: C, 44.67; H, 2.59; N, 3.19; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.6 (m, 4H, H_2, H_3, H_4 and H_6), 7.7565 (dd, 1H, H_9 ^{3}J = 7.6 Hz with H_8 and ^{4}J = 4.8 Hz with H_7), 7.9535 (m, 2H, H_7 and H_8), 8.058 (d, 1H, H_{15}, ^{3}J = 7.3 Hz with H_{14}), 8.6475 (d, 1H, H_{14}, ^{3}J= 7.9 Hz with H_{15}), 8.983 (s, 1H, H_{16}), 9.438 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.148, 121.489, 124.890, 125.561, 126.238, 126.730, 126.824, 127.250, 127.439, 128.542, 134.670, 138.534, 146.554, 151.080, 154.739, 164.179.

Complex 3: m.p. 157.70^{o}C; IR (KBr disc) vcm^{-1}: 2847.67, 2917.14 (C–H stretching in aromatic rings), 1744.09 (C=O stretching), 1634.05 (C=N in pyrazine ring), 1594.99, 1507.86, 1461.24 (two couple of peaks for C=C in aromatic rings), 1273.92, 1098.46 (C–O stretching); Anal. Calcd. for $C_{32}H_{22}I_2HgN_2O_4$: C, 40.33;H, 2.33; N, 2.94; Found: C, 40.12; H, 2.28; N, 2.95; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.6 (m, 4H, H_2, H_3, H_4 and H_6), 7.753 (m, 1H, H_9), 7.959 (m, 2H, H_7 and H_8), 8.0555 (d, 1H, H_{15}, ^{3}J = 6.8 Hz with H_{14}), 8.6425 (d, 1H, H_{14}, ^{3}J= 6.8 Hz with H_{15}), 8.980 (s, 1H, H_{16}), 9.436 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.144, 121.499, 124.890, 125.592, 126.238, 126.731, 126.821, 127.250, 127.436, 128.542, 134.667, 138.528, 146.553, 151.010, 154.667, 164.168.

Complex 4: m.p. 174.53 ^{o}C; IR (KBr disc) vcm^{-1}: 2850.09, 2920.01 (C–H stretching in aromatic rings), 1743.38 (C=O stretching) 1628.23 (C=N in pyrazine ring), 1595.27, 1582.31, 1507.76 (C=C in aromatic rings), 1281.04, 1157.63 (C–O stretching); Anal. Calcd. for $C_{32}H_{22}Cl_2HgN_2O_4$: C, 49.91; H, 2.88; N, 3.64; Found: C, 49.15; H, 3.73; N, 3.52;

^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.5215 (dd, 1H, H_3, ^{3}J = 8.9 Hz with H_4, ^{4}J = 2.4 Hz with H_1), 7.587 (m, 2H, H_7 and H_8), 7.757 (s, 1H, H_{15}), 7.9025 (d, 1H, H_1, ^{4}J = 2.2 Hz with H_3), 7.9735 (dd, 1H, H_9, ^{3}J = 6 Hz with H_8, ^{4}J = 2.5 Hz with H_7), 8.0145 (dd, 1H, H_6, ^{3}J = 6 Hz with H_7, ^{4}J = 2.5 Hz with H_8), 8.0635 (d, 1H, H_4, ^{3}J= 8.9 Hz with H_3), 8.576 (d, 1H, H_{14}, ^{3}J = 7.9 Hz with H_{15}), 8.991 (s, 1H, H_{16}), 9.399 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.213, 121.967, 124.881, 124.139, 126.524, 127.318, 128.051, 128.253, 129.971, 131.670, 133.776, 138.402, 148.490, 150.967, 154.610, 164.232.

Complex 5: m.p. 183.44 ^{o}C; IR (KBr disc) vcm^{-1}: 2847.67, 2929.40 (C–H stretching in aromatic rings), 1738.20 (C=O stretching), 1625.88 (C=N in pyrazine ring), 1597.92, 1578.77, 1478.77 (C=C in aromatic rings), 1284.20, 1156.22 (C–O stretching); Anal. Calcd. for $C_{16}H_{11}Br_2HgNO_2$: C, 31.52;

H, 1.82; N, 2.30; Found: C, 30.98; H, 1.87; N, 2.51; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.5285 (dd, 1H, H_3, ^{3}J = 8.7 Hz with H_4, ^{4}J = 1.6 Hz with H_1), 7.590 (m, 2H, H_7 and H_8), 7.772 (dd, 1H, H_{15},^{3}J = 6.9 Hz with H_{14}, ^{4}J= 4.4 Hz with H_{16}), 7.905 (s, 1H, H_1, ^{4}J = 2.2 Hz with H_3), 7.9745 (d, 1H, H_9, ^{3}J = 8.7 Hz with H_8), 8.0175 (d, 1H, H_6, ^{3}J = 8.8 Hz with H_7), 8.066 (d, 1H, H_4, ^{3}J= 8.9 Hz with H_3), 8.5975 (d, 1H, H_{14}, ^{3}J = 7.8 Hz with H_{15}), 8.972 (s, 1H, H_{16}), 9.384 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.204, 121.941, 125.101, 126.069, 126.532, 127.321, 128.051, 128.251, 129.976, 131.666, 133.763, 138.717, 148.467, 150.843, 154.427, 164.087.

Complex 6: m.p. 146.35 ^{o}C; IR (KBr disc) vcm^{-1}: 2847.17, 2924.82 (C–H stretching in aromatic rings), 1737.21 (C=O stretching), 1625.22 (C=N in pyrazine ring), 1597.53, 1509.07 (C=C in aromatic rings), 1280.69, 1154.77 (C–O stretching); Anal. Calcd. for $C_{16}H_{11}I_2HgNO_2$: C, 27.31; H, 1.58; N, 2.0; Found: C, 28.24; H, 1.78; N, 3.0; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ:7.566 (dd, 1H, H_3, ^{3}J = 8.9 Hz with H_4, ^{4}J = 2.4 Hz with H_1), 7.616 (m, 2H, H_7 and H_8), 7.778 (dd, 1H, H_{15},^{3}J = 7.4 Hz with H_{14}, ^{4}J= 5.2 Hz with H_{16}), 7.9325 (d, 1H, H_1, ^{4}J = 2.2 Hz with H_3), 8.0015 (dd, 1H, H_9, ^{3}J = 6 Hz with H_8, ^{4}J = 2.5 Hz with H_7), 8.0425 (dd, 1H, H_6, ^{3}J = 6 Hz with H_7, ^{4}J = 2.5 Hz with H_8), 8.092 (d, 1H, H_4, ^{3}J= 8.9 Hz with H_3), 8.608 (d, 1H, H_{14}, ^{3}J = 7.9 Hz with H_{15}), 8.977 (d, 1H, H_{16}, ^{3}J = 2.4 Hz with H_{15}), 9.379 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.216, 121.966, 124.917, 125.899, 126.533, 127.328, 128.054, 128.256, 129.974, 131.664, 133.767, 138.533, 148.476, 150.801, 154.440, 164.140.

Complex 7: m.p. 137.16, 150.23 ^{o}C; IR (KBr disc) vcm^{-1}: 3007.04, 2924.61, 2855.85 (C–H stretching in aromatic rings), 1752.53 (C=O stretching), 1598.62, 1508.02, 1462.43 (two couple of peaks for C=C in aromatic rings), 1306.38, 1136.00 (C–O stretching); Anal. Calcd. for $C_{30}H_{20}Cl_2HgN_4O_4$: C, 46.67; H, 2.61; N, 7.26; Found: C, 45.98; H, 2.74; N, 7.02; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.615 (m, 4H, H_2, H_3, H_4 and H_6), 7.9635 (d, 1H, H_7, ^{4}J= 8 Hz with H_8), 8.016 (d, 1H, H_8, ^{3}J = 7.9 Hz with H_7), 8.0655 (d, 1H, H_9, ^{3}J = 7.5 Hz with H_8), 9.000 (s, 1H, H_{14}), 9.050 (s, 1H, H_{15}), 9.534 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz DMSO, 25^{o}C, ppm): 118.988, 121.559, 126.263, 126.612, 126.890, 127.294, 127.431, 128.524, 134.685, 142.947, 145.589, 146.607, 146.861, 149.179, 163.063.

Complex 8: m.p. 125.85, 135.75 ^{o}C; IR (KBr disc) vcm^{-1}: 3007.04, 2921.23, 2851.76 (C–H stretching in aromatic rings), 1734.54 (C=O stretching), 1599.45, 1507.38 (two couple of peaks for C=C in aromatic rings), 1309.80, 1130.84 (C–O stretching); Anal. Calcd. for $C_{30}H_{20}Br_2HgN_4O_4$: C, 41.85; H,

2.34; N, 6.51; Found: C, 41.57; H, 2.61; N, 5.95; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.615 (m, 4H, H_2, H_3, H_4 and H_6), 7.964 (d, 1H, H_7, ^{4}J= 8 Hz with H_8), 8.0175 (d, 1H, H_8, ^{3}J = 7.6 Hz with H_7), 8.067 (d, 1H, H_9, ^{3}J = 7.8 Hz with H_8), 9.000 (s, 1H, H_{14}), 9.0525 (d, 1H, H_{15}, ^{3}J = 2.2 Hz with H_{14}), 9.535 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm): 118.989, 121.563, 126.264, 126.612, 126.890, 127.296, 127.432, 128.524, 134.684, 142.949, 145.588, 146.607, 146.867, 149.181, 163.061.

Complex 9: m.p. 89.61, 94.65 ^{o}C; IR (KBr disc) vcm^{-1}: 3011.12, 2953.92, 2851.76 (C–H stretching in aromatic rings), 1736.14 (C=O stretching), 1597.92, 1506.78, 1460.72 (two couple of peaks for C=C in aromatic rings), 1312.30, 1128.39 (C–O stretching); Anal. Calcd. for $C_{30}H_{20}I_2HgN_4O_4$: C, 37.73; H, 2.11; N, 5.87; Found: C, 38.29; H, 2.28; N, 5.86; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.614 (m, 4H, H_2, H_3, H_4 and H_6), 7.9625 (d, 1H, H_7, ^{4}J= 8 Hz with H_8), 8.0165 (d, 1H, H_8, ^{3}J = 8 Hz with H_7), 8.0655 (d, 1H, H_9, ^{3}J = 7.5 Hz with H_8), 8.999 (s, 1H, H_{14}), 9.049 (s, 1H, H_{15}), 9.534 (s, 1H, H_{13}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm): 118.987, 121.566, 126.266, 126.613, 126.891, 127.298, 127.433, 128.525, 134.683, 142.949, 145.590, 146.606, 146.868, 149.179, 163.057.

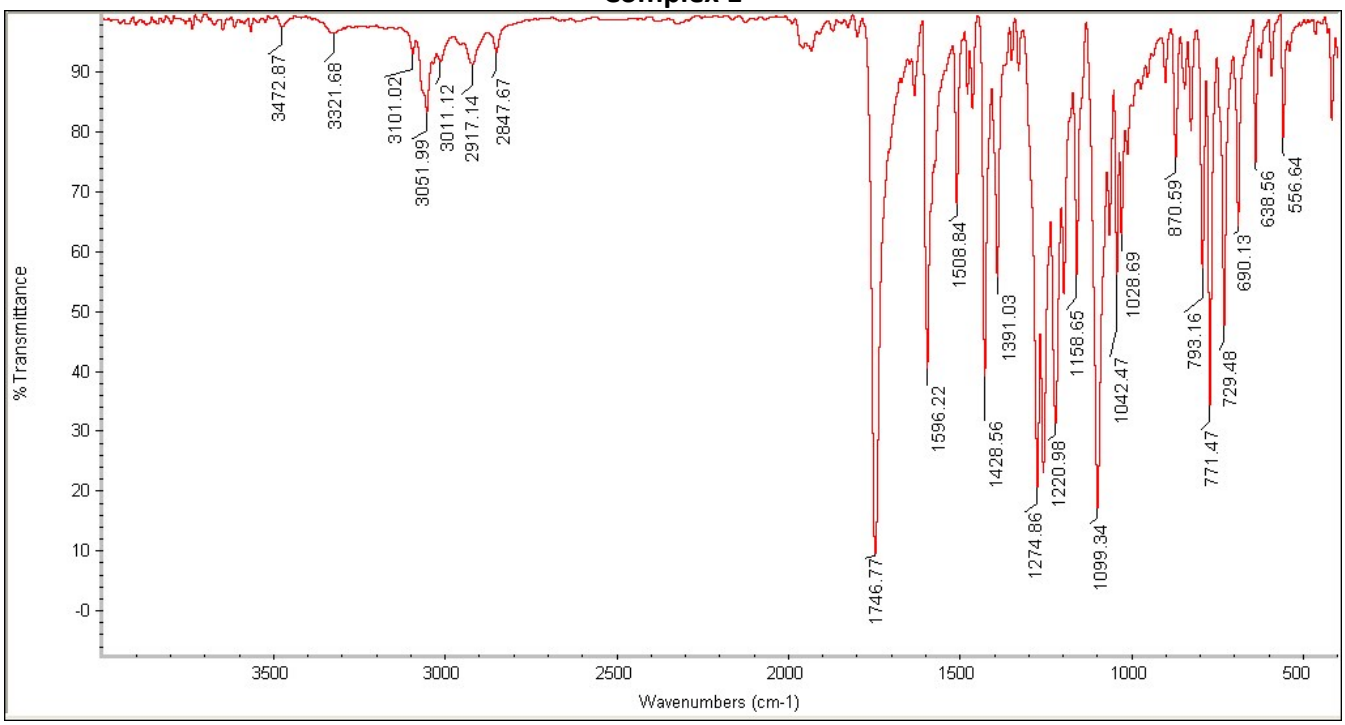
Complex 10: m.p. 167.68 ^{o}C; IR (KBr disc) vcm^{-1}: 2850.45, 2926.80 (C–H stretching in aromatic rings), 1764.48 (C=O stretching), 1627.05 (C=N in pyrazine ring), 1579.78, 1507.61, 1462.43 (two couple of peaks for C=C in aromatic rings), 1303.85, 1156.62 (C–O stretching); Anal. Calcd. for $C_{30}H_{20}Cl_2HgN_4O_4$: C, 46.67; H, 2.61; N, 7.26; Found: C, 47.03; H, 3.08; N, 7.17; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.533 (d, 1H, H_3, ^{4}J= 2.4 Hz with H_1), 7.581 (m, 2H, H_7 and H_8), 7.9115 (d, 1H, H_1, ^{4}J = 2.2 Hz with H_3), 7.975 (dd, 1H, H_9, ^{3}J = 7.3 Hz with H_8, ^{4}J = 3 Hz with H_7), 8.0075 (dd, 1H, H_6, ^{3}J = 7.2 Hz with H_7, ^{4}J = 3.2 Hz with H_8), 8.0665 (d, 1H, H_4, ^{3}J = 8.9 Hz with H_3), 8.9535 (dd, 1H, H_{14}, ^{3}J= 2.4 Hz with H_{15}, ^{4}J = 1.6 Hz with H_{13}), 9.0125 (d, 1H, H_{15}, ^{3}J = 2.4 Hz with H_{14}), 9.461 (d, 1H, H_{13}, ^{4}J = 1.3 Hz with H_{14}); ^{13}C NMR (75.65 MHz, DMSO, 25^{o}C, ppm) δ: 119.101, 121.787, 126.559, 127.333, 128.082, 128.257, 130.055, 131.701, 133.778, 143.045, 145.520, 146.716, 148.522, 149.056, 163.044.

Complex 11: m.p. 163.09 ^{o}C; IR (KBr disc) vcm^{-1}: 2851.76, 2926.71 (C–H stretching in aromatic rings), 1764.23 (C=O stretching) 1626.76 (C=N in pyrazine ring), 1600.93, 1579.67, 1507.55 (two couple of peaks for C=C in aromatic rings), 1303.05, 1155.40 (C–O stretching); Anal. Calcd. for $C_{30}H_{20}Br_2HgN_4O_4$: C, 41.85; H, 2.34; N, 6.51; Found: C, 42.51; H, 2.72; N, 6.38; ^{1}H NMR (300.811 MHz, DMSO, 25^{o}C, ppm) δ: 7.5325 (d, 1H, H_3, ^{4}J= 2.4 Hz with H_1), 7.580 (m, 2H, H_7 and H_8), 7.9105

(d, 1H, H_1, ^4J = 2 Hz with H_3), 7.991 (m, 2H, H_9 and H_6), 8.065 (d, 1H, H_4, ^3J = 9 Hz with H_3), 8.953 (m, 1H, H_{14}), 9.0115 (d, 1H, H_{15}, ^3J = 2.4 Hz with H_{14}), 9.461 (d, 1H, H_{13}, ^4J = 1.1 Hz with H_{14}); ^{13}C NMR (75.65 MHz, DMSO, 25°C, ppm) δ: 119.101, 121.786, 126.560, 127.333, 128.079, 128.255, 130.052, 131.699, 133.777, 143.044, 145.516, 146.720, 148.520, 149.053, 163.039.

S6. FT-IR transmittance plots for compounds 1-11

Complex 1



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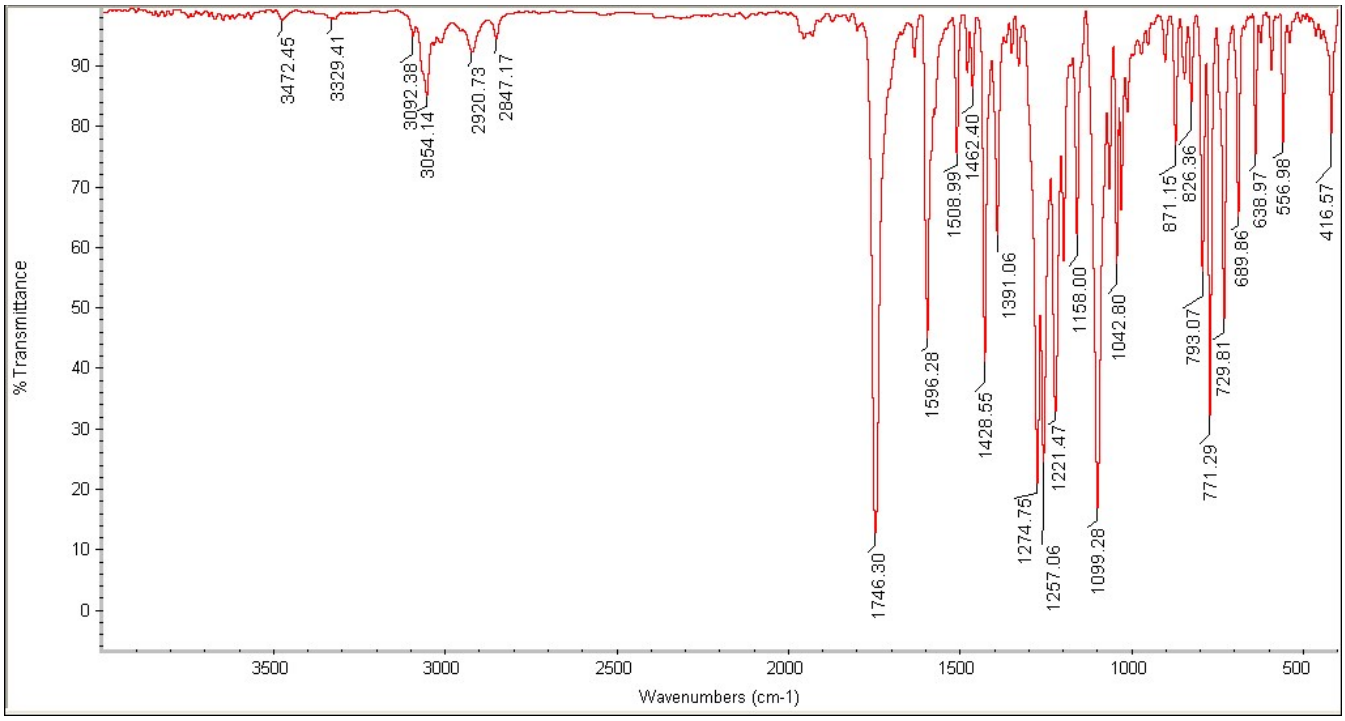

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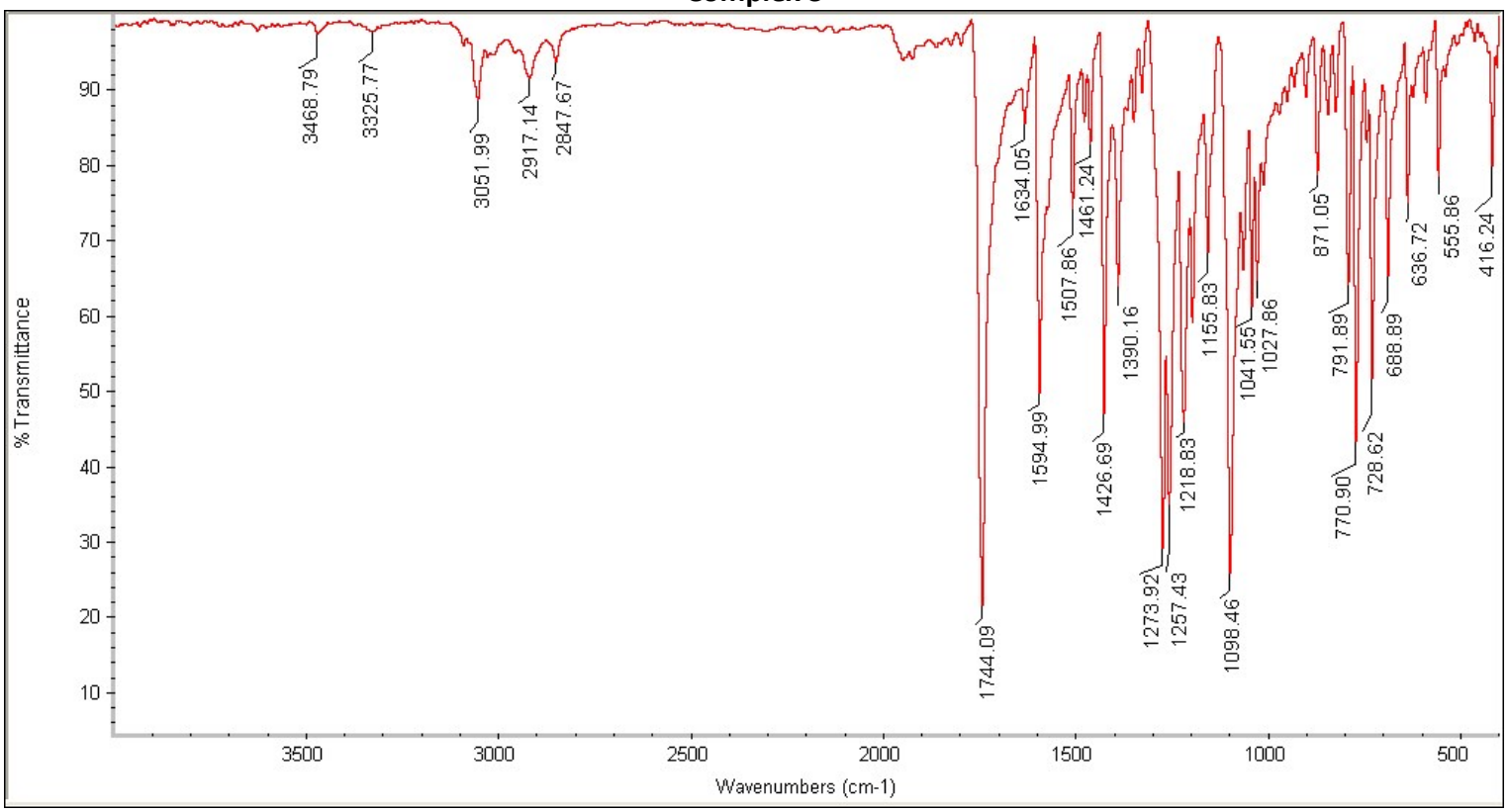

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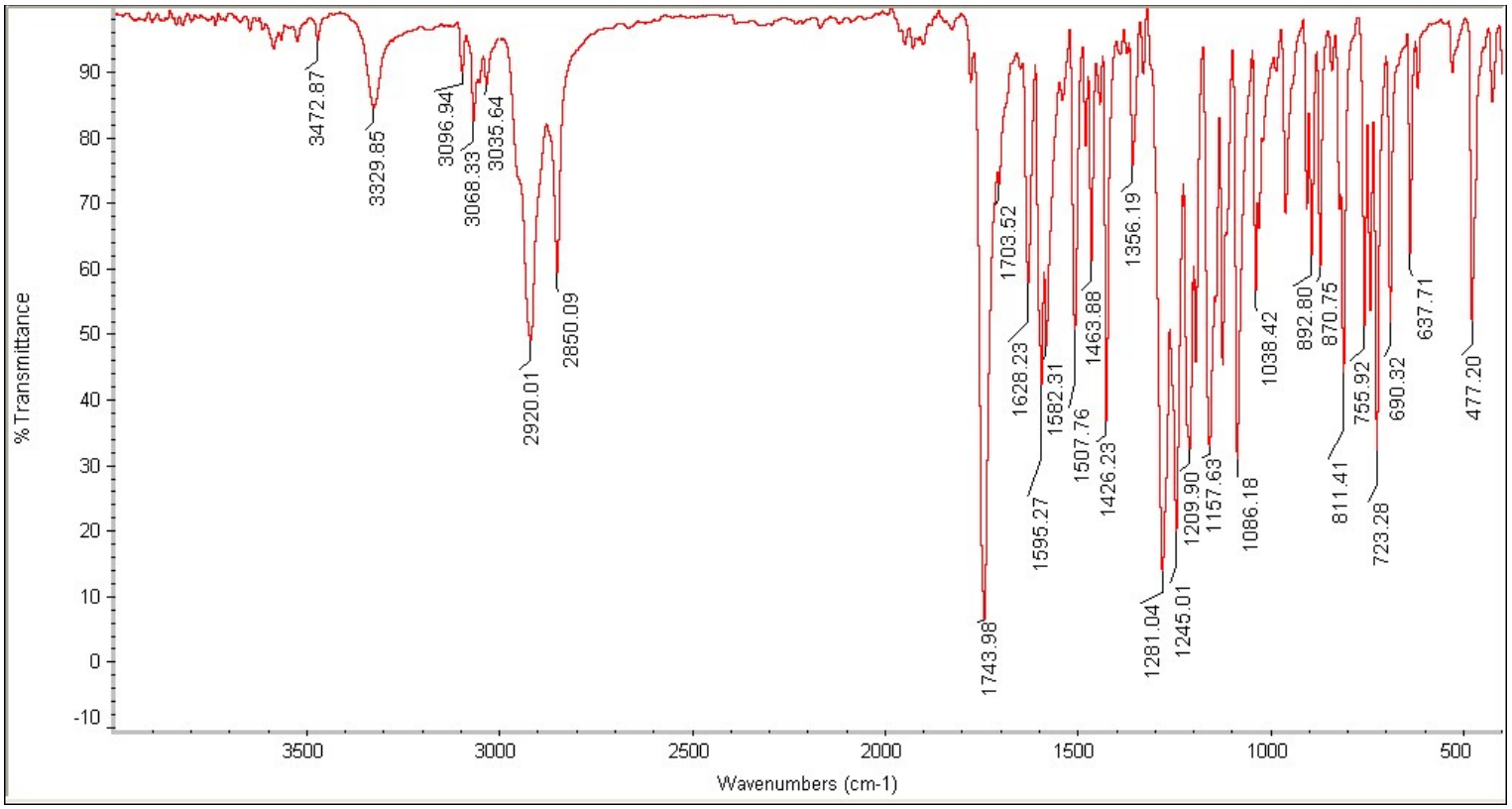
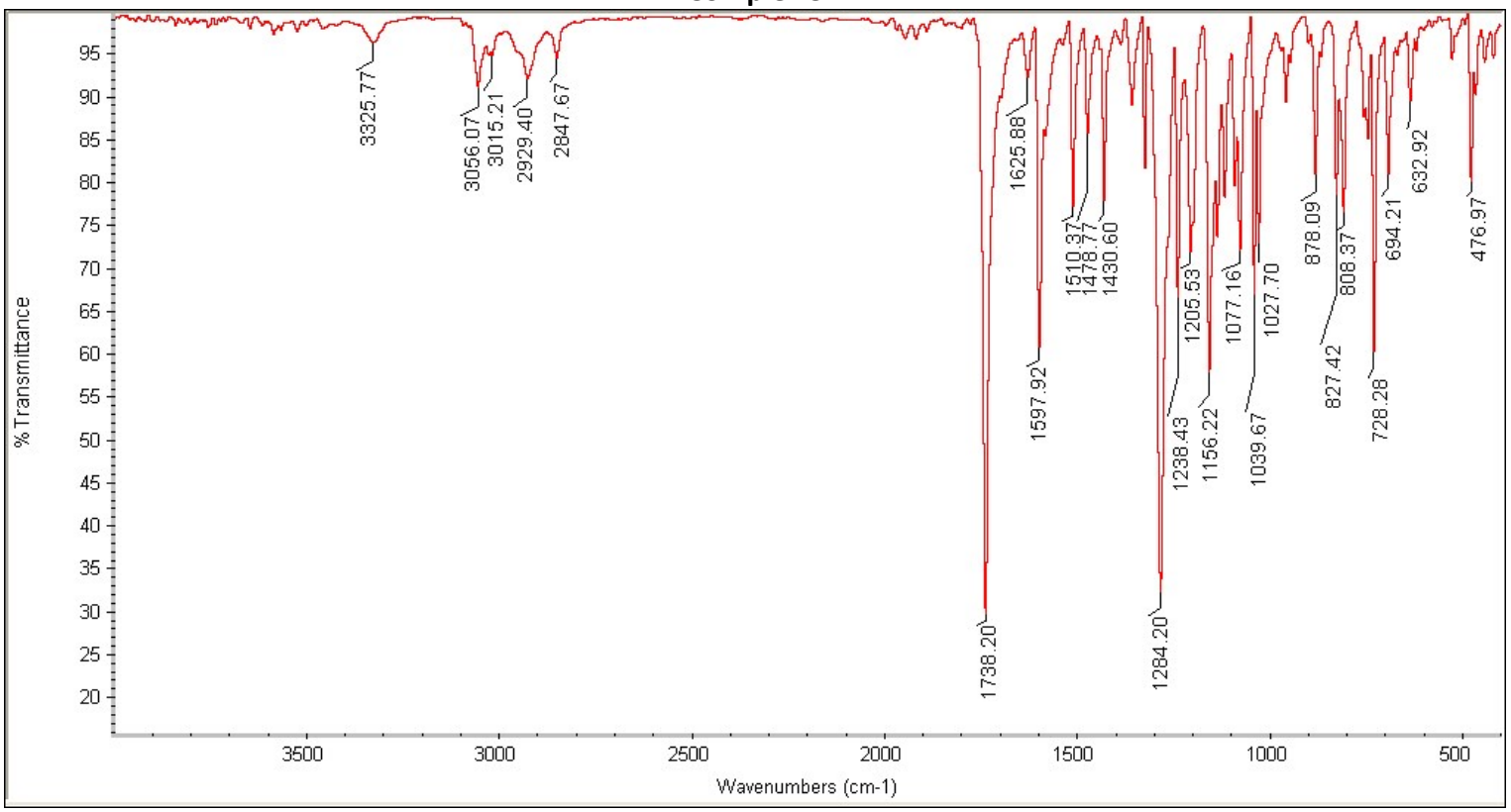
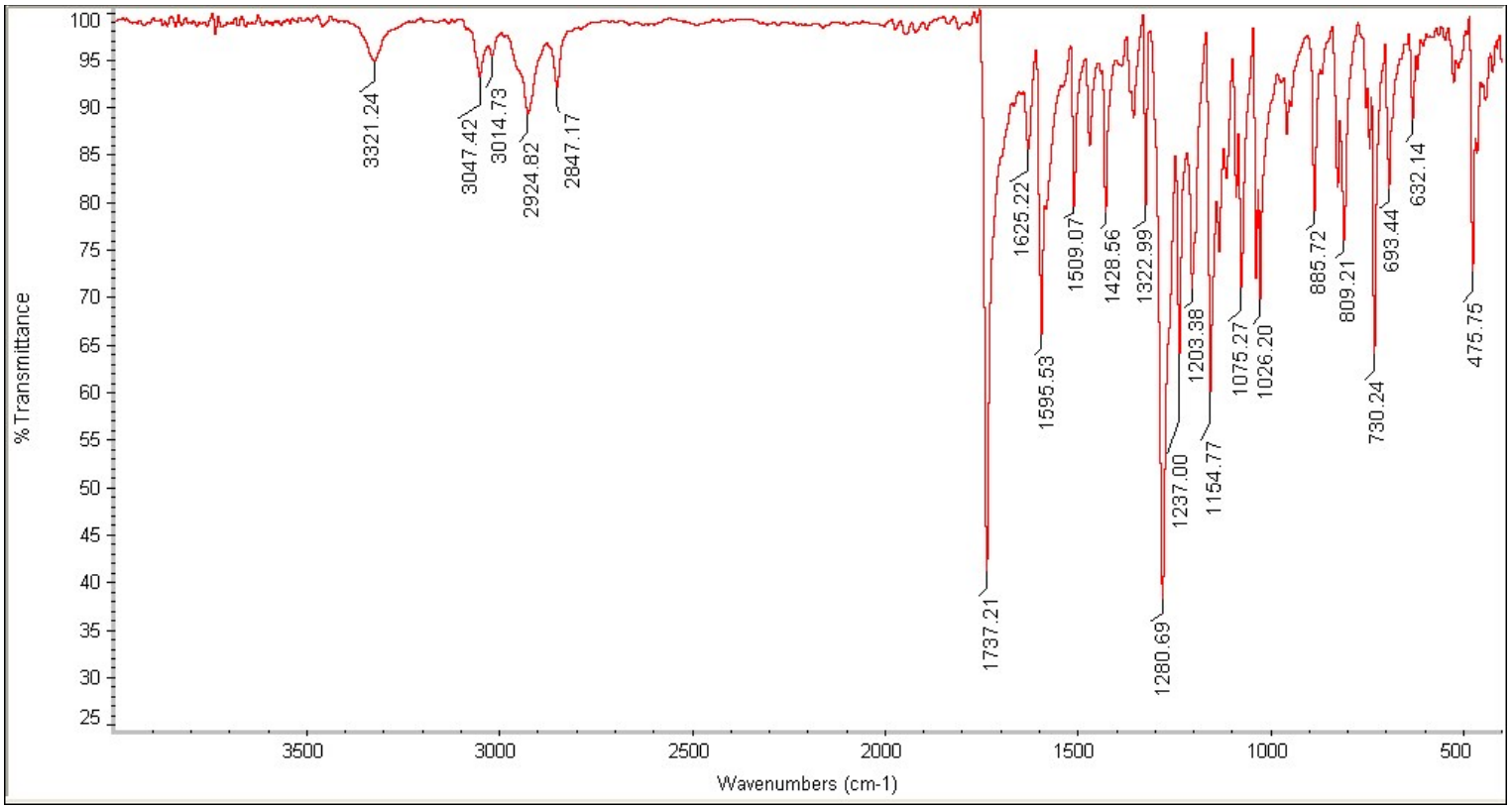


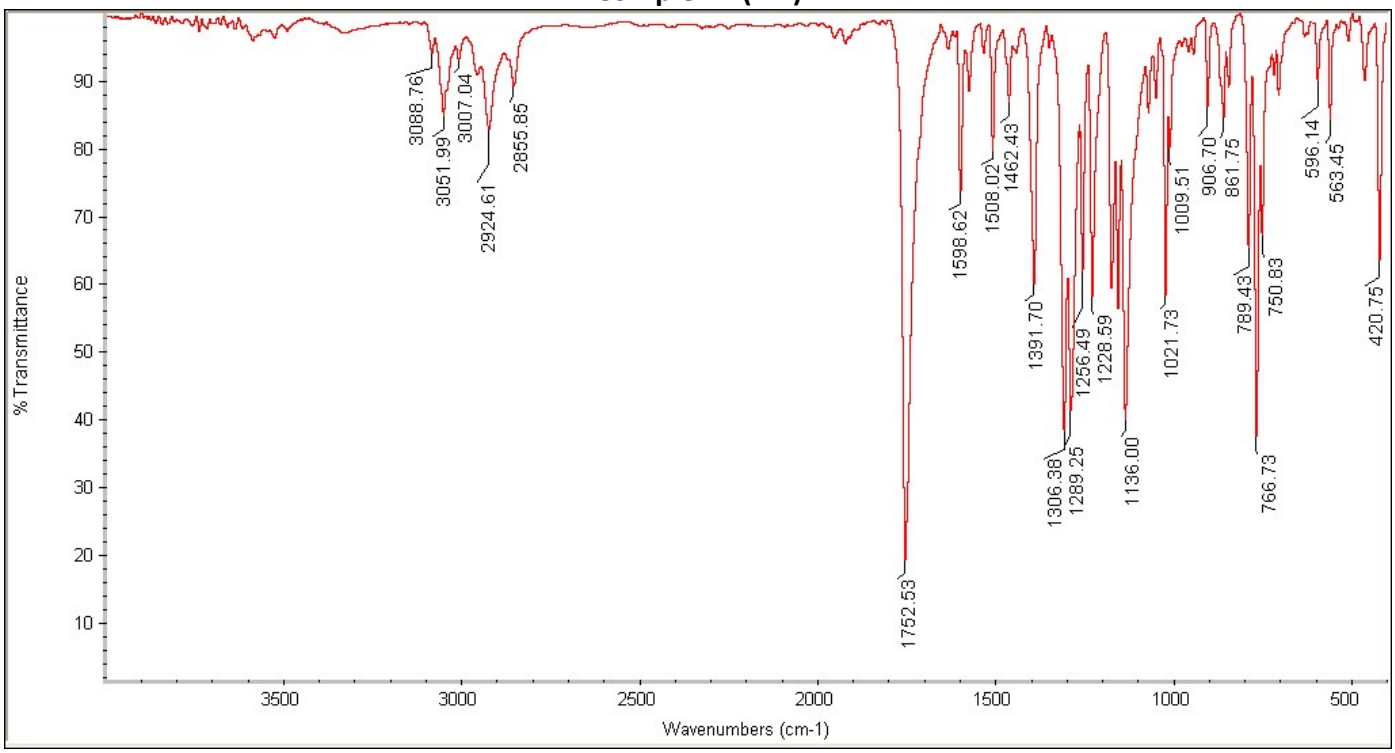
Complex 5



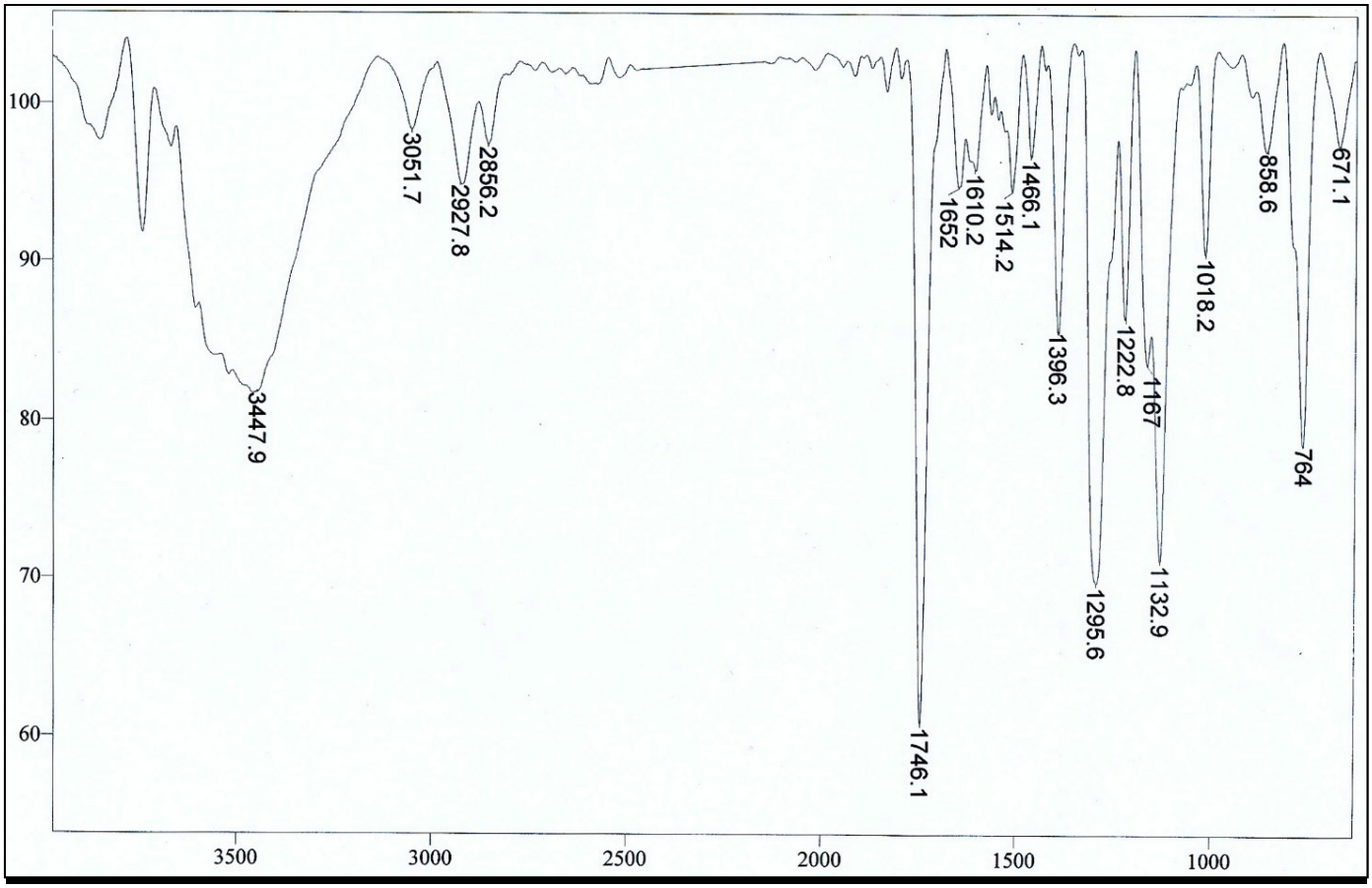
Complex 6



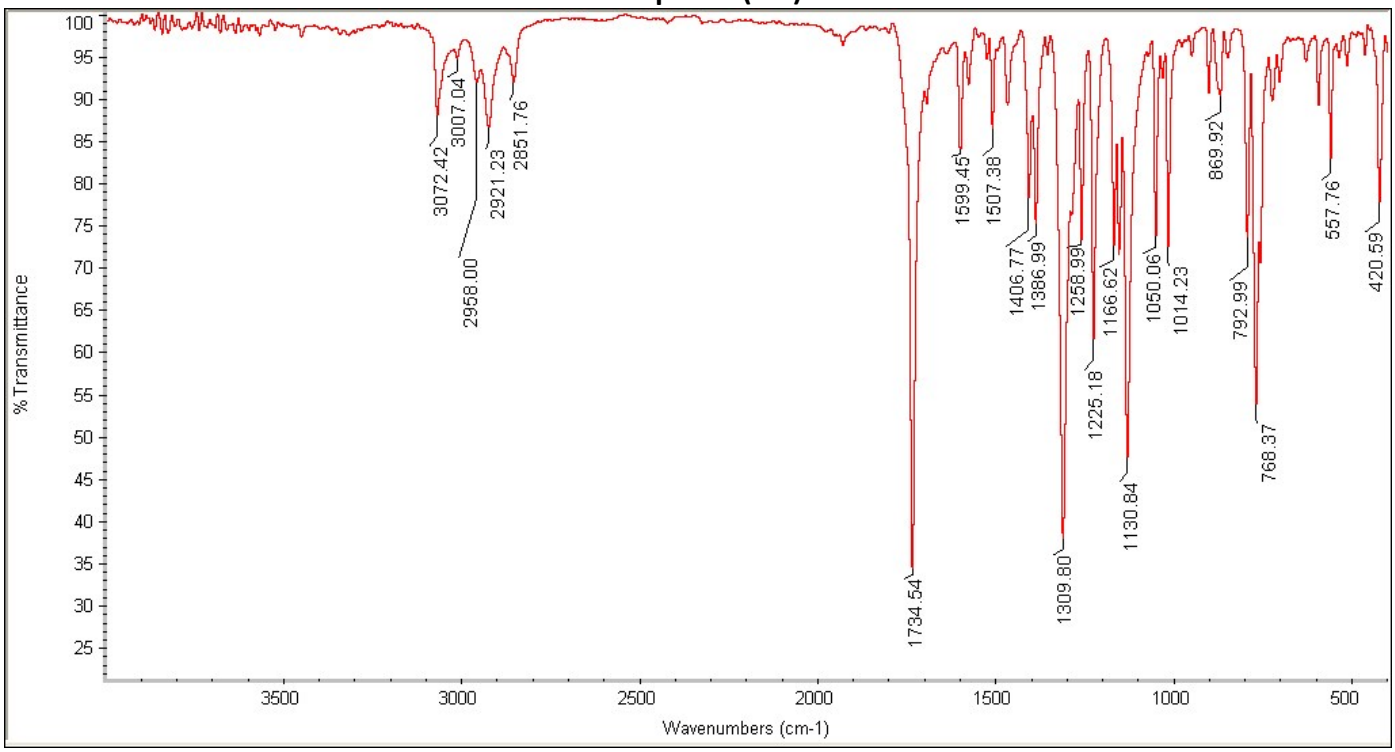
Complex 7 (1:2)



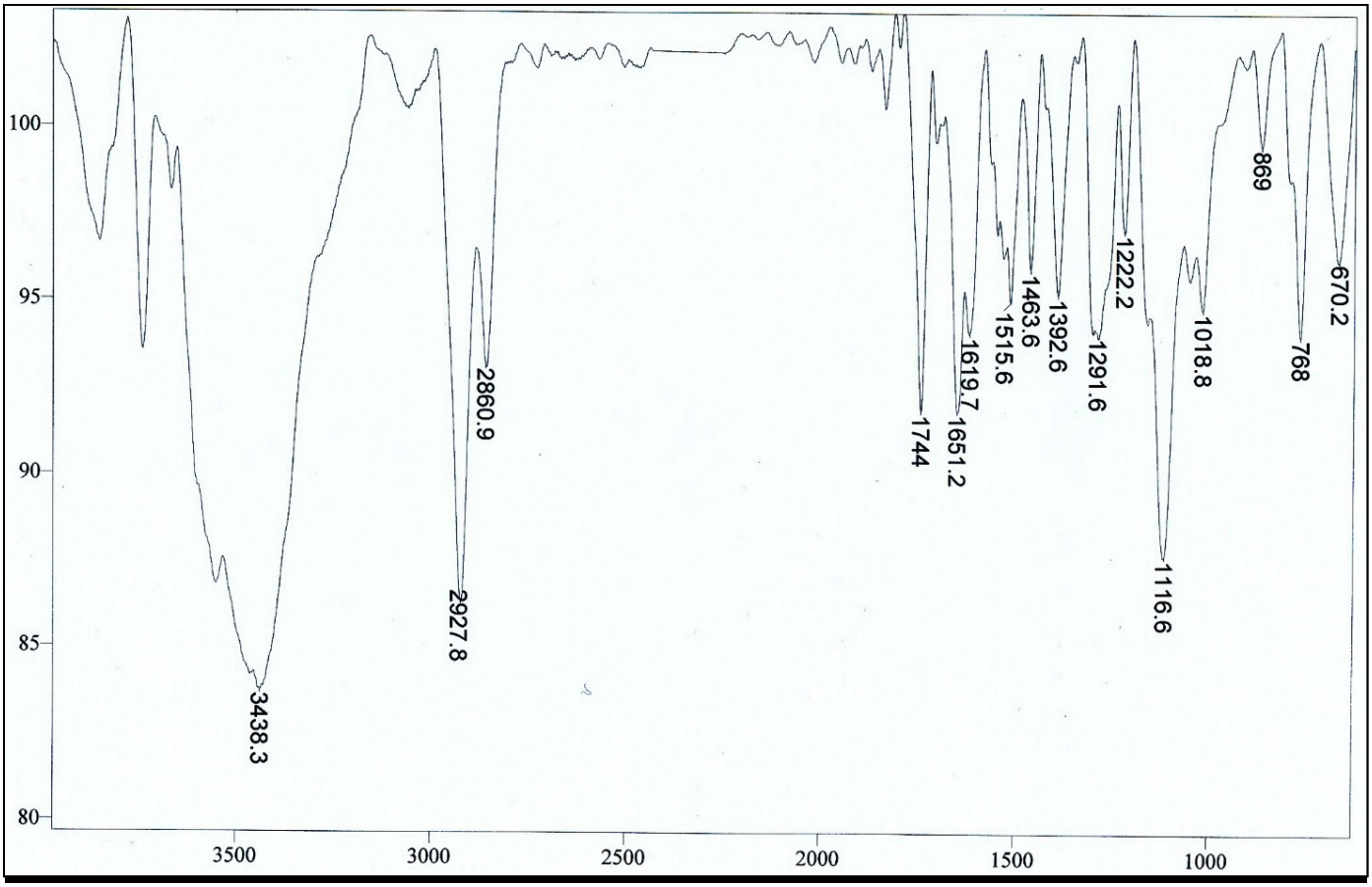
Complex 7' (1:1)



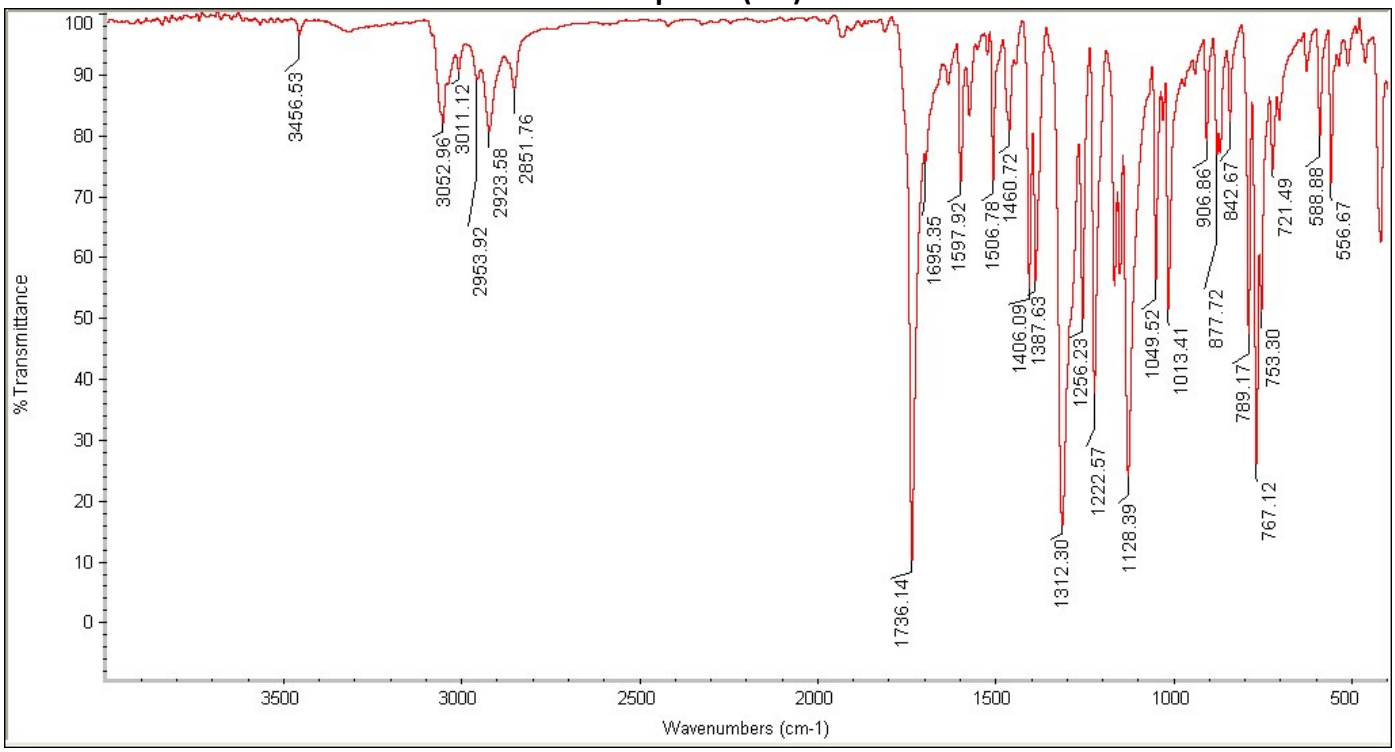
Complex 8 (1:2)



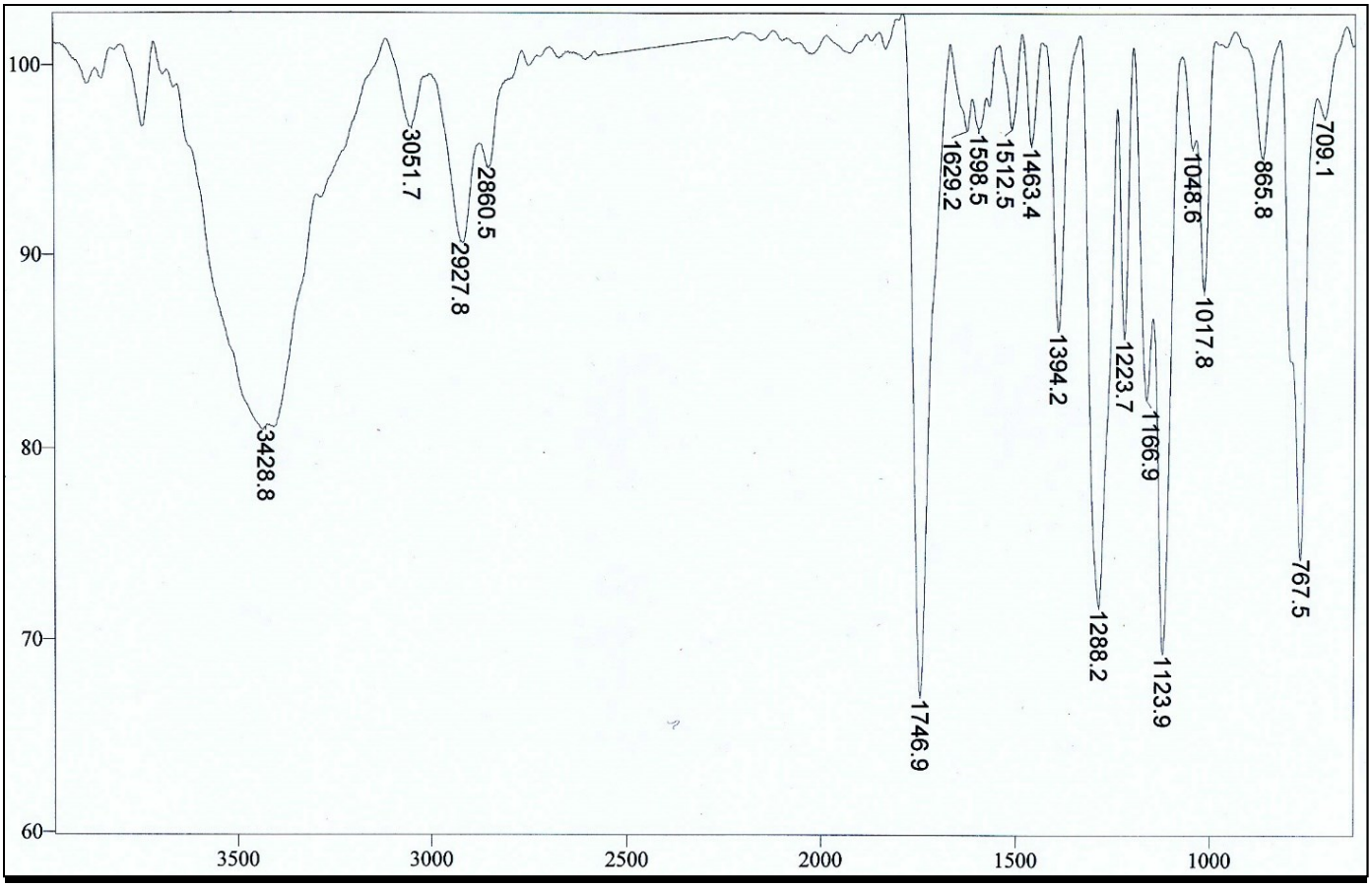
Complex 8' (1:1)



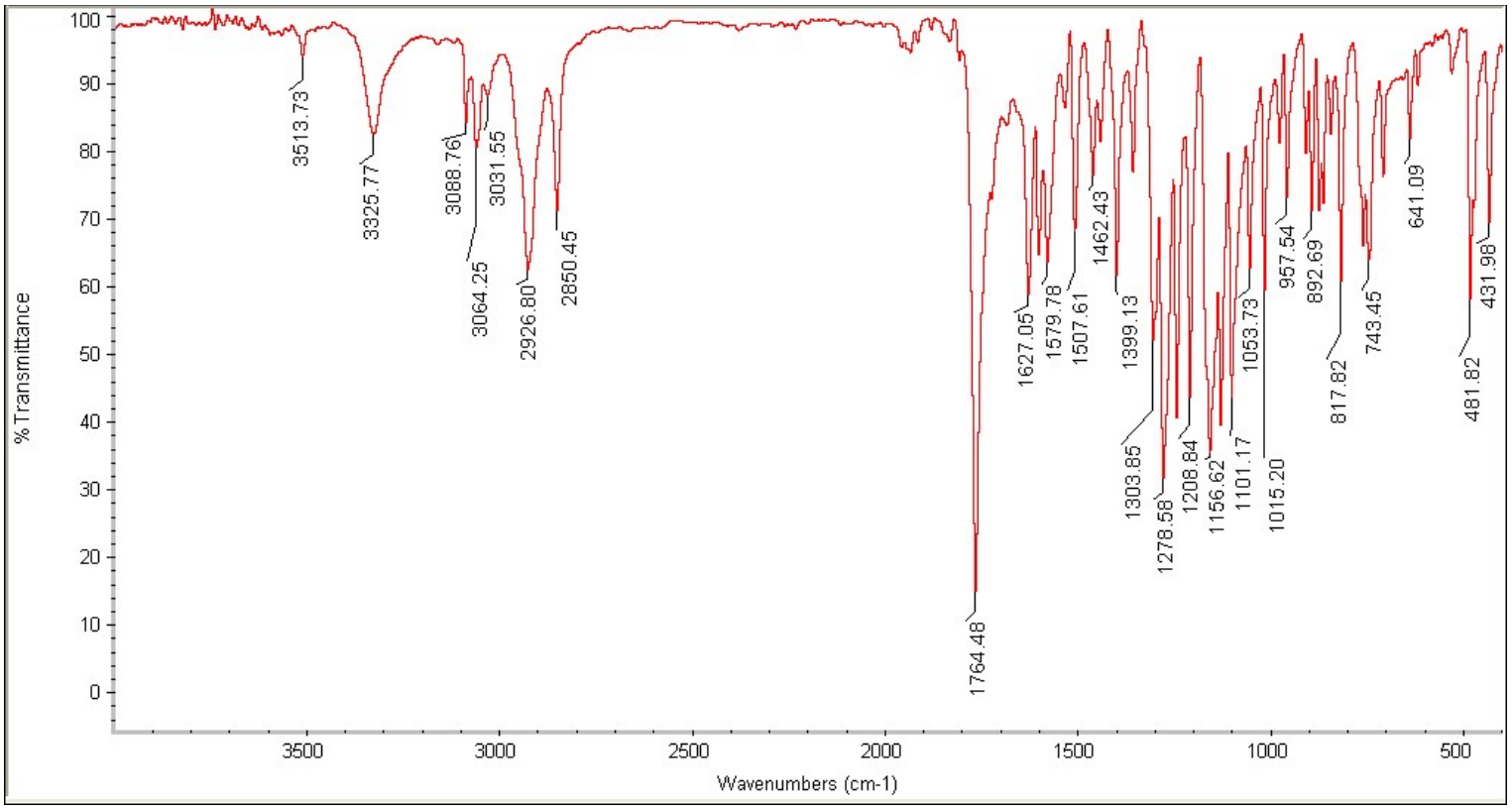
Complex 9 (1:2)



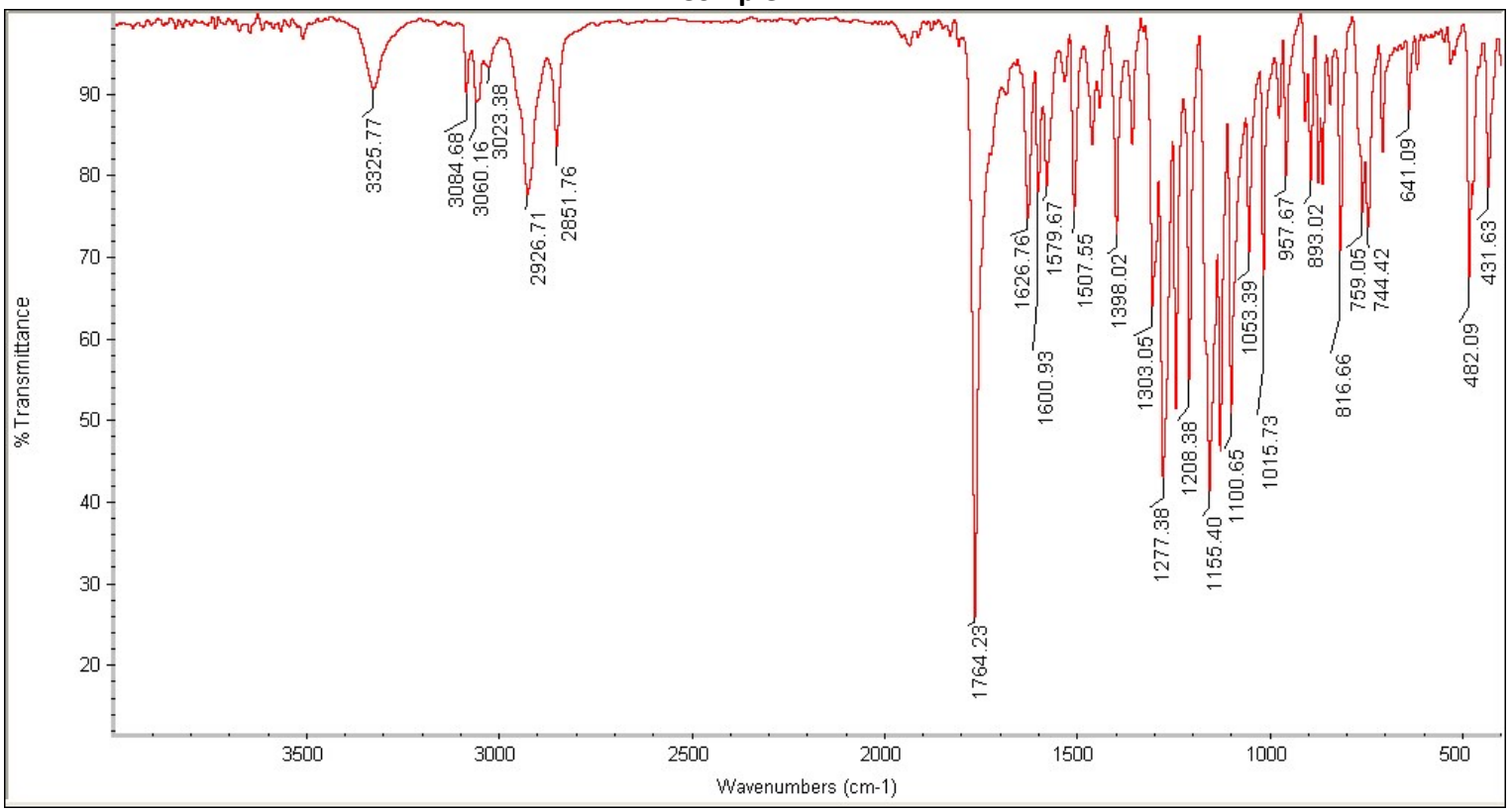
Complex 9' (1:1)


100
90
80
70
60
3500
3000
2500
2000
1500
1000
3428.8
3051.7
2927.8
2860.5
1746.9
1629.2
1598.5
1512.5
1463.4
1394.2
1288.2
1223.7
1166.9
1123.9
1048.6
1017.8
865.8
767.5
709.1

Complex 10



Complex 11



S7. CHN-Elemental Analysis for compounds 1-11

Complex 1

Eager 300 Summarize Results

Date : 22/04/2017 at 11:49:07
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-88		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
88	1	AS8	UNK	1.234	6.25	---	

Component name	Element %
Nitrogen%	3.618430376
Carbon%	49.17246628
Hydrogen%	2.913830519
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.618430376
Carbon%	49.17246628
Hydrogen%	2.913830519
Sulphur%	0

Complex 2

Eager 300 Summarize Results

Date : 22/04/2017 at 11:48:54
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-86		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
86	1	AS21	UNK	1.083	6.25	---	

Component name	Element %
Nitrogen%	3.188761473
Carbon%	44.67723083
Hydrogen%	2.594818592
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.188761473
Carbon%	44.67723083
Hydrogen%	2.594818592
Sulphur%	0

Complex 3

Eager 300 Summarize Results

Date : 22/04/2017 at 11:49:00
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-87		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
87	1	AS13	UNK	1.28	6.25	---	

Component name	Element %
Nitrogen%	2.952723265
Carbon%	40.11894226
Hydrogen%	2.276647568
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	2.952723265
Carbon%	40.11894226
Hydrogen%	2.276647568
Sulphur%	0

Complex 4

Eager 300 Summarize Results

Date : 22/04/2017 at 11:48:29
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-83		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
83	1	AS9	UNK	1.514	6.25	---	

Component name	Element %
Nitrogen%	3.514662981
Carbon%	49.15002823
Hydrogen%	3.730189562
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.514662981
Carbon%	49.15002823
Hydrogen%	3.730189562
Sulphur%	0

Complex 5

Eager 300 Summarize Results

Date : 13/05/2017 at 11:34:18
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-146		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
146	1	AS14a	UNK	1.214	6.25	---	

Component name	Element %
Nitrogen%	2.51397562
Carbon%	30.98172951
Hydrogen%	1.870144248
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	2.51397562
Carbon%	30.98172951
Hydrogen%	1.870144248
Sulphur%	0

Complex 6

Eager 300 Summarize Results

Date : 13/05/2017 at 11:34:24
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-147		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
147	1	AS17	UNK	1.55	6.25	---	

Component name	Element %
Nitrogen%	3.022508144
Carbon%	28.24775696
Hydrogen%	1.781832695
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.022508144
Carbon%	28.24775696
Hydrogen%	1.781832695
Sulphur%	0

Complex 7 (1:2)

Complex 7' (1:1)

Eager 300 Summarize Results

Date : 03/05/2017 at 11:58:21
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-119		

#	Group	Sample Name	Type	Weig.	Pro.F	---
119	1	AS15	UNK	1.299	6.25	---

Component name	Element %
Nitrogen%	7.016540051
Carbon%	45.98410034
Hydrogen%	2.746521711
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	7.016540051
Carbon%	45.98410034
Hydrogen%	2.746521711
Sulphur%	0

Complex 8 (1:2)

Eager 300 Summarize Results

Date : 29/07/2017 at 11:19:43
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-104		

#	Group	Sample Name	Type	Weig.	Pro.F	---
104	1	AS15a	UNK	1.121	6.25	---

Component name	Element %
Nitrogen%	5.185403824
Carbon%	35.33866501
Hydrogen%	2.285821199
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	5.185403824
Carbon%	35.33866501
Hydrogen%	2.285821199
Sulphur%	0

Complex 8' (1:1)

Eager 300 Summarize Results

Date : 22/04/2017 at 11:48:40
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-84		

#	Group	Sample Name	Type	Weig.	Pro.F	---
84	1	AS10	UNK	1.174	6.25	---

Component name	Element %
Nitrogen%	5.948138237
Carbon%	41.56671524
Hydrogen%	2.608825207
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	5.948138237
Carbon%	41.56671524
Hydrogen%	2.608825207
Sulphur%	0

Complex 9 (1:2)

Eager 300 Summarize Results

Date : 03/05/2017 at 11:58:27
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-120		

#	Group	Sample Name	Type	Weig.	Pro.F	---
120	1	AS10a	UNK	1.065	6.25	---

Component name	Element %
Nitrogen%	4.535764417
Carbon%	29.94066550
Hydrogen%	1.603418018
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	4.535764417
Carbon%	29.94066550
Hydrogen%	1.603418018
Sulphur%	0

Complex 9' (1:1)

Eager 300 Summarize Results

Date : 29/04/2017 at 12:19:58
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-105		

#	Group	Sample Name	Type	Weig.	Pro.F	---
105	1	AS19	UNK	1.375	6.25	---

Component name	Element %
Nitrogen%	5.861464977
Carbon%	38.29249573
Hydrogen%	2.280479431
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	5.861464977
Carbon%	38.29249573
Hydrogen%	2.280479431
Sulphur%	0

Complex 10

Eager 300 Summarize Results

Date : 13/05/2017 at 11:34:12
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-145		

#	Group	Sample Name	Type	Weig.	Pro.F	---
145	1	AS19a	UNK	2.075	6.25	---

Component name	Element %
Nitrogen%	3.862572517
Carbon%	25.21708679
Hydrogen%	1.330710745
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.862572517
Carbon%	25.21708679
Hydrogen%	1.330710745
Sulphur%	0

Complex 11

Eager 300 Summarize Results

Date : 22/04/2017 at 11:48:21
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-82		

#	Group	Sample Name	Type	Weig.	Pro.F		
82	1	As11	UNK	1.267	6.25	---	

Component name	Element %
Nitrogen%	7.162701607
Carbon%	47.0364418
Hydrogen%	3.08091712
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	7.162701607
Carbon%	47.0364418
Hydrogen%	3.08091712
Sulphur%	0

Eager 300 Summarize Results

Date : 22/04/2017 at 11:48:47
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
samie-85		

#	Group	Sample Name	Type	Weig.	Pro.F		
85	1	AS20	UNK	0.968	6.25	---	

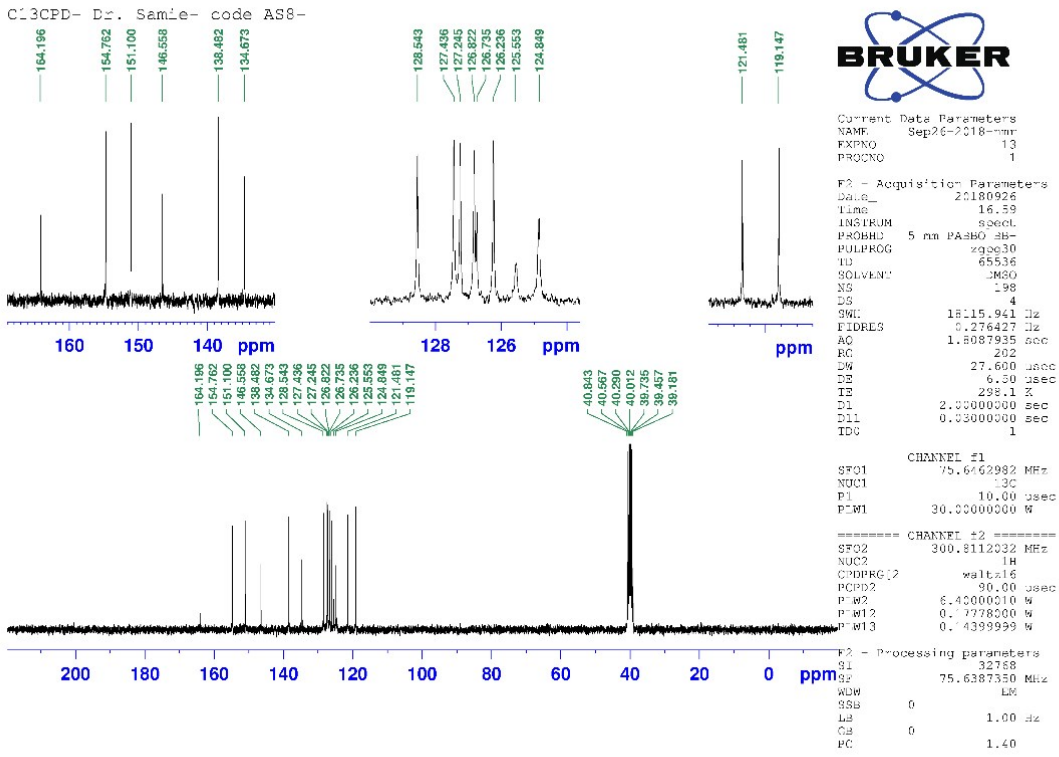
Component name	Element %
Nitrogen%	6.381759167
Carbon%	42.50958633
Hydrogen%	2.7260077
Sulphur%	0

1 Sample(s) in Group No : 1

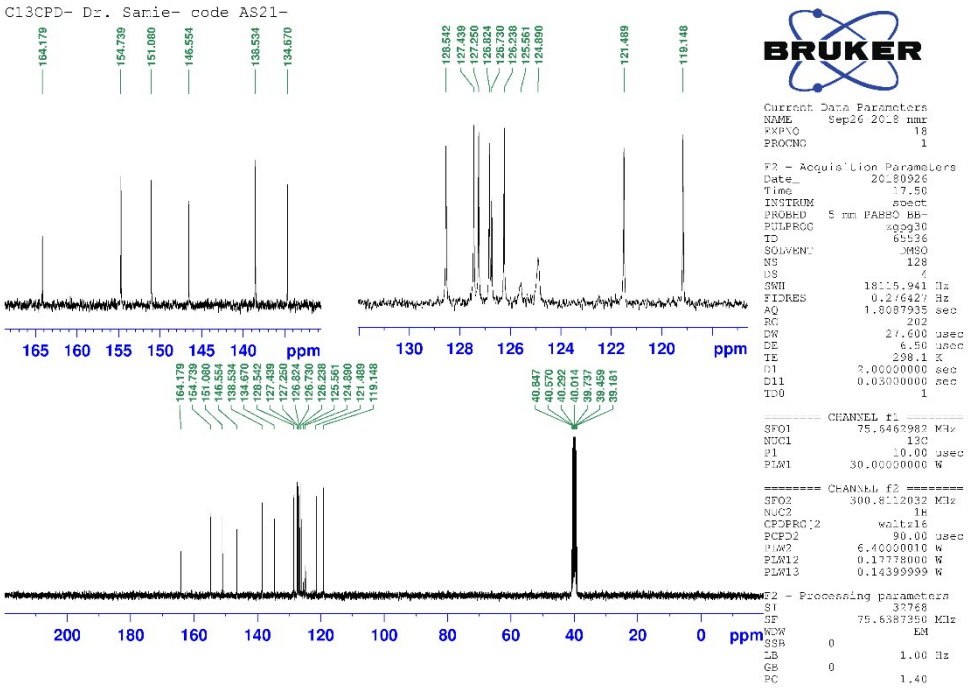
Component Name	Average
Nitrogen%	6.381759167
Carbon%	42.50958633
Hydrogen%	2.7260077
Sulphur%	0

S8. ^{13}C-NMR spectrums for compounds 1-11

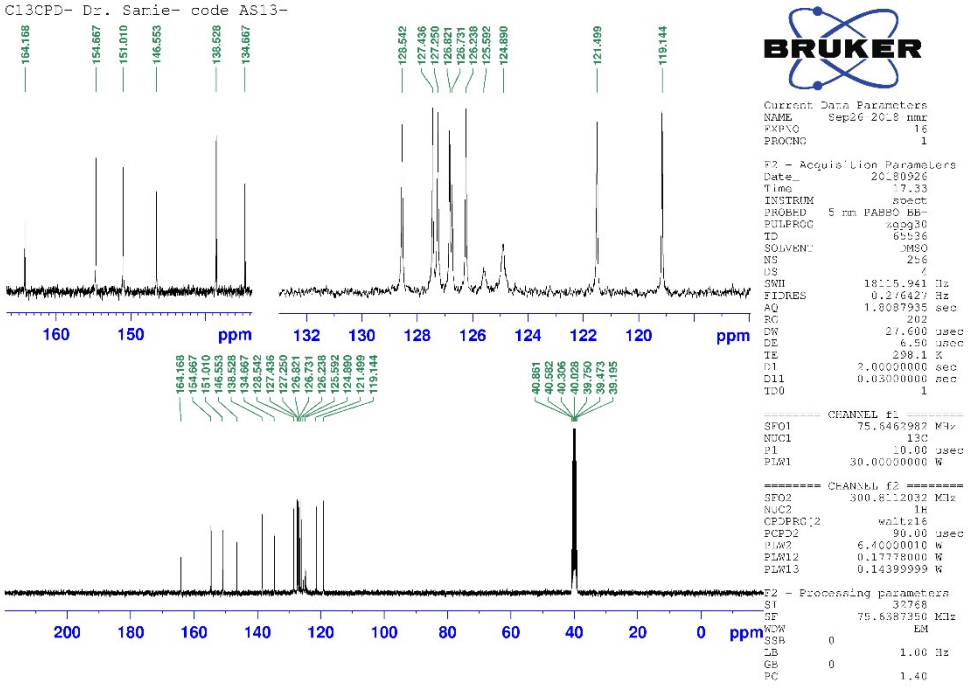
Complex 1



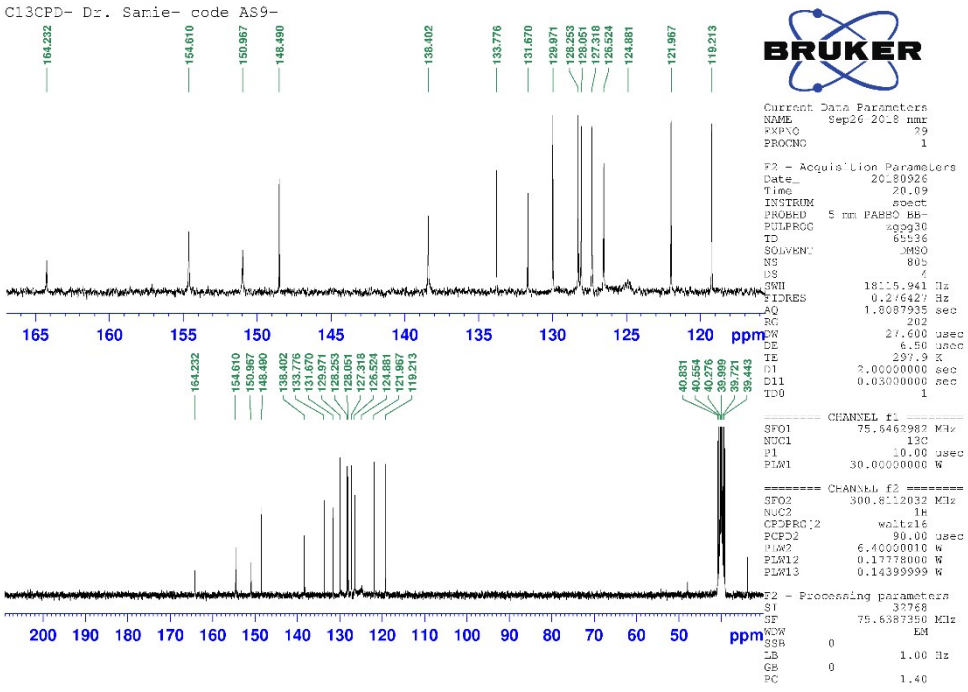
Complex 2



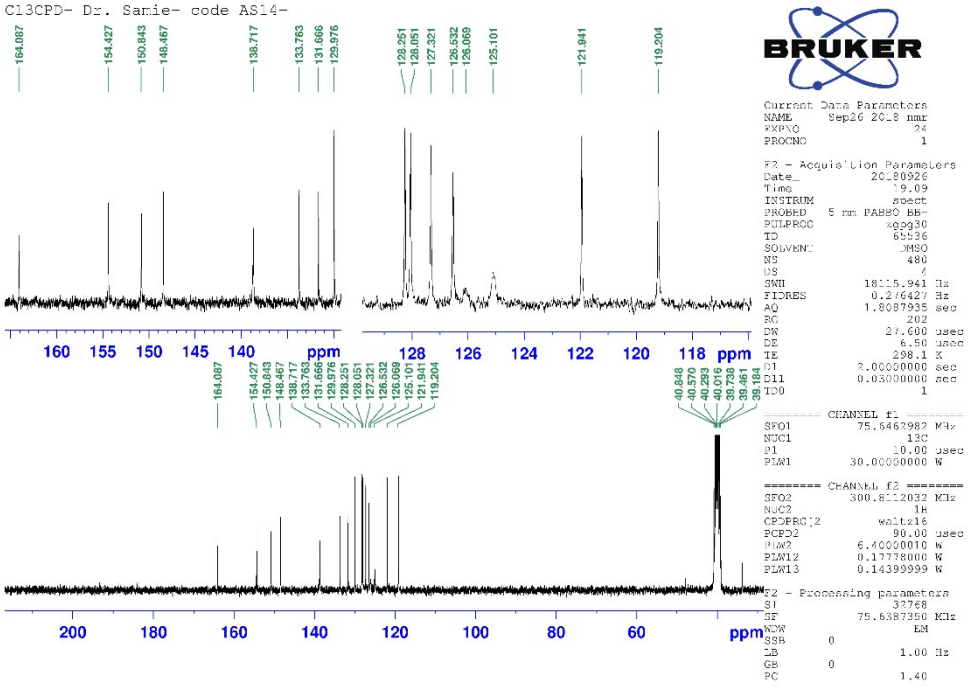
Complex 3



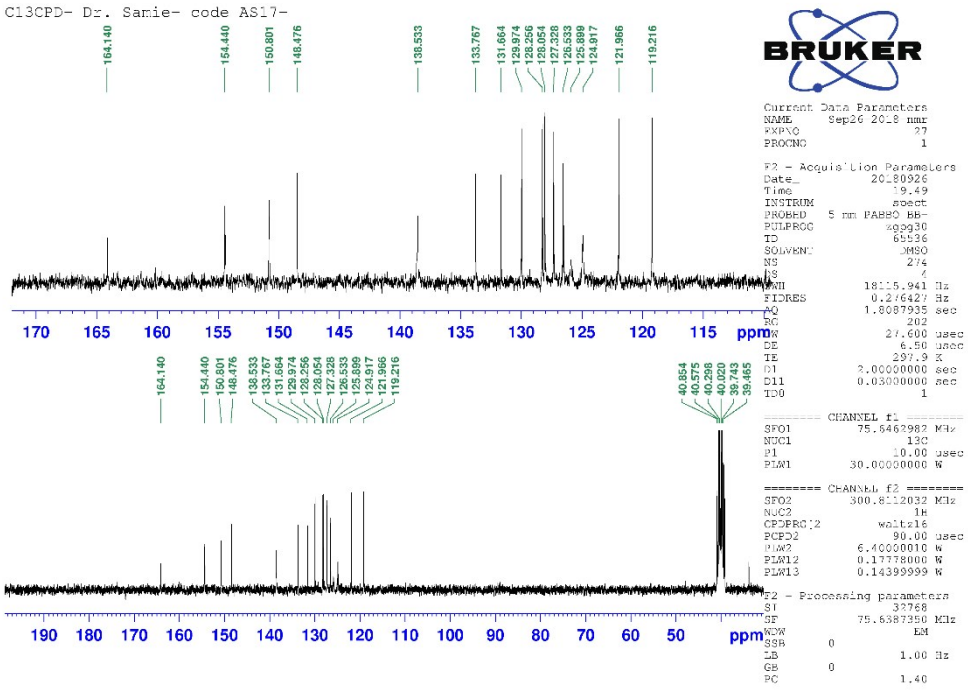
Complex 4



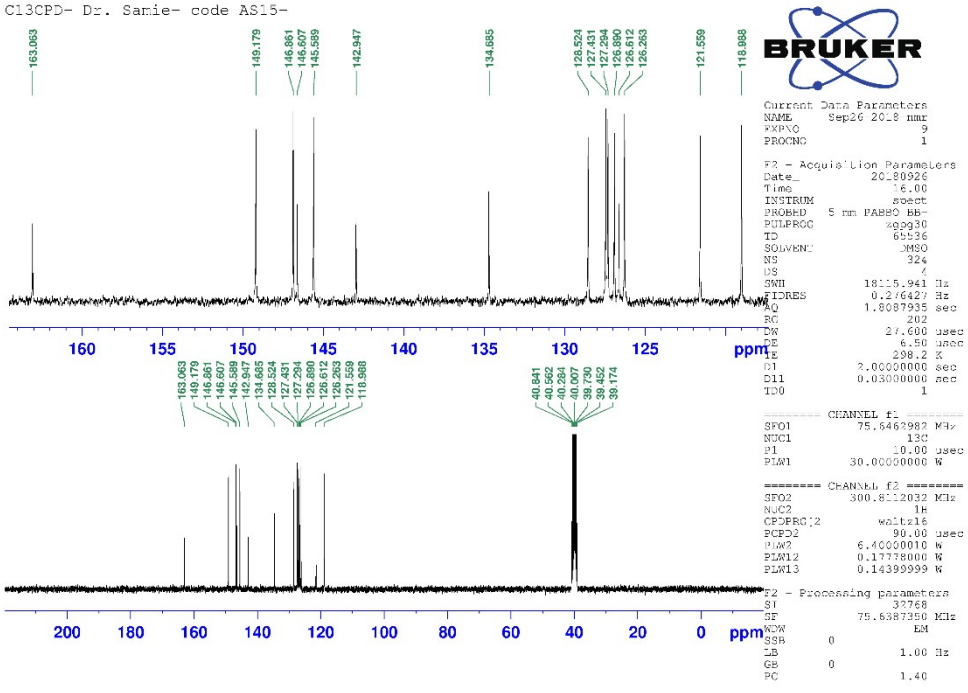
Complex 5



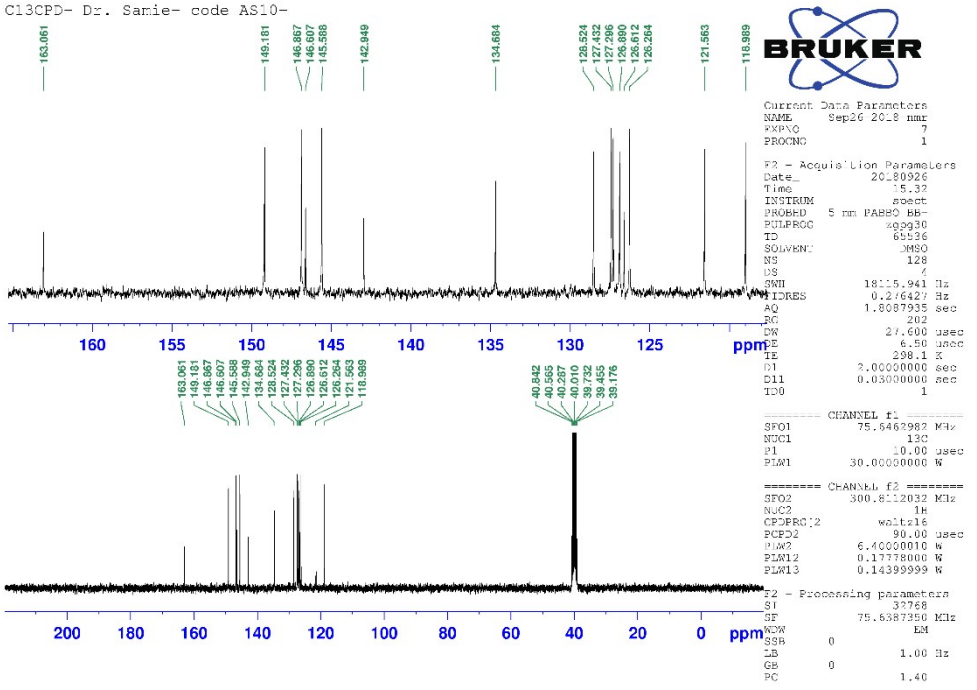
Complex 6



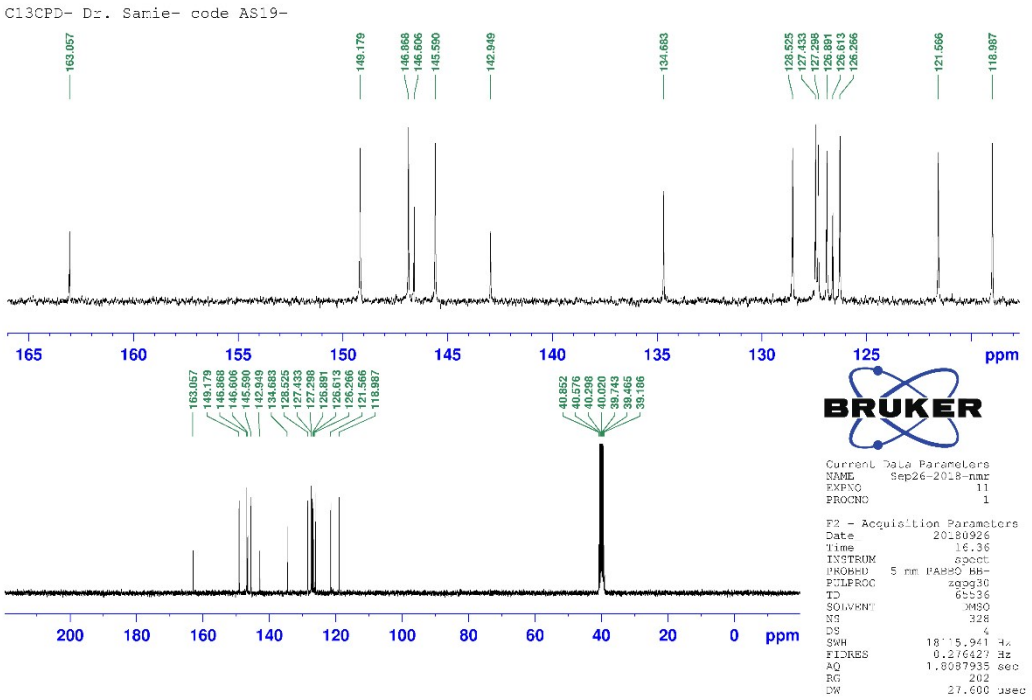
Complex 7



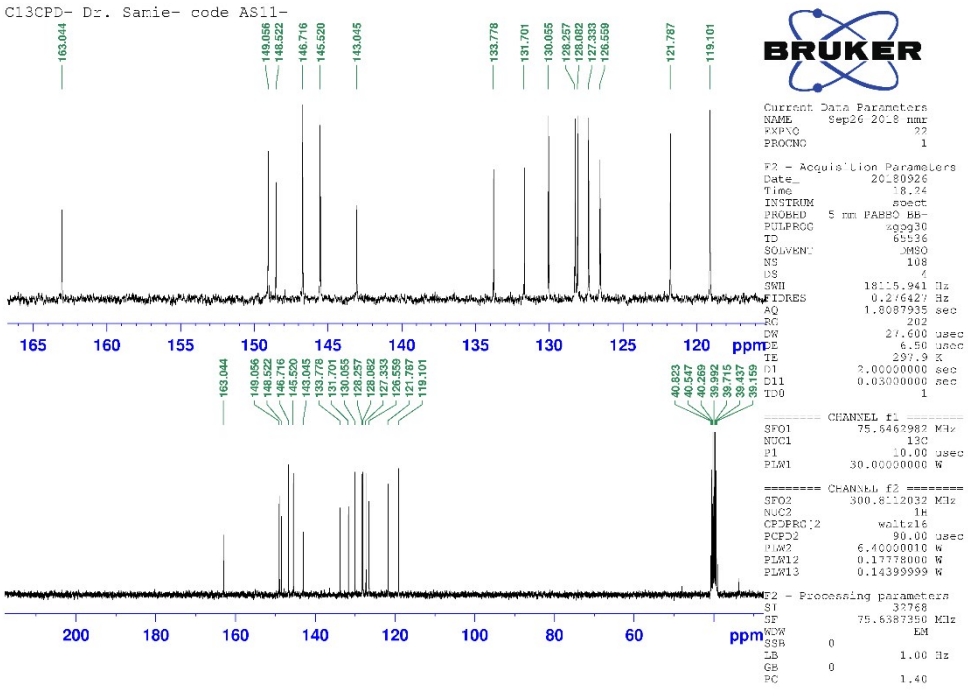
Complex 8



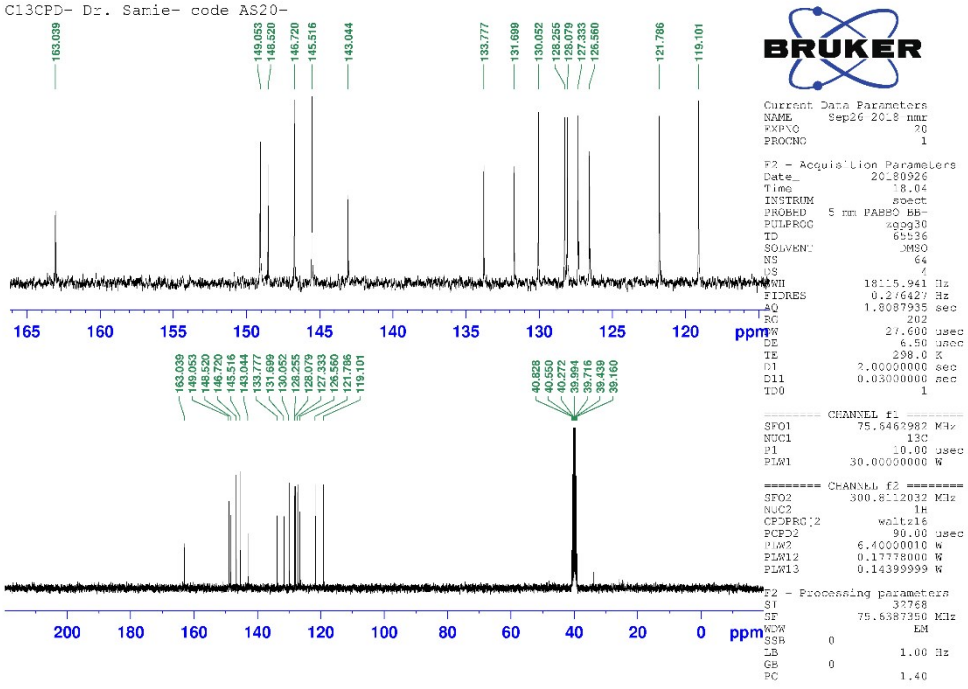
Complex 9



Complex 10

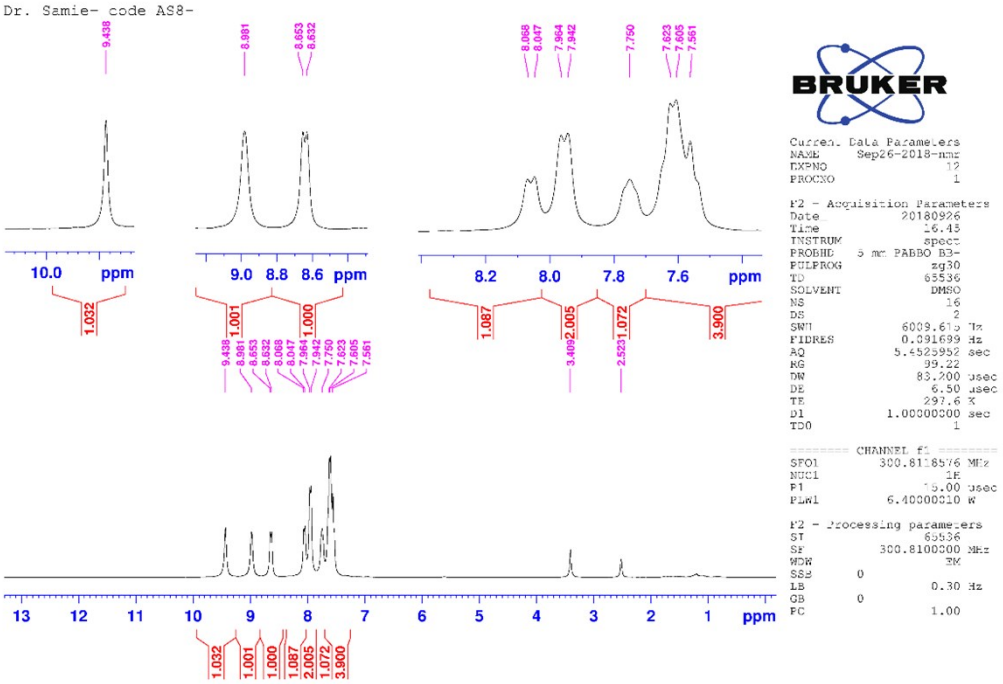


Complex 11

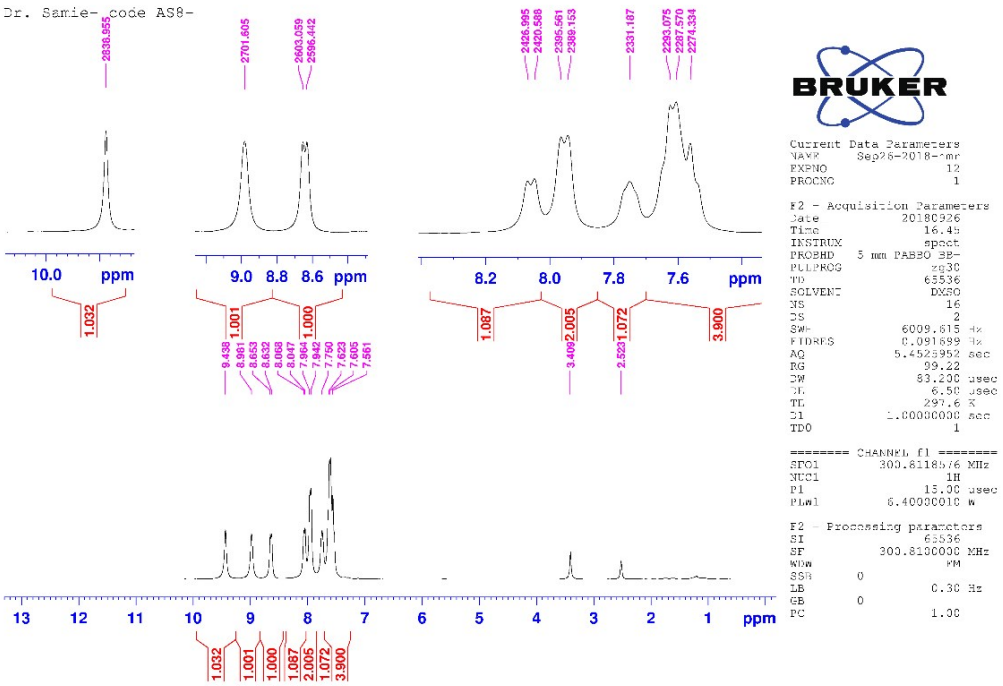


S9. ^{1}H-NMR spectrums for compounds 1-11

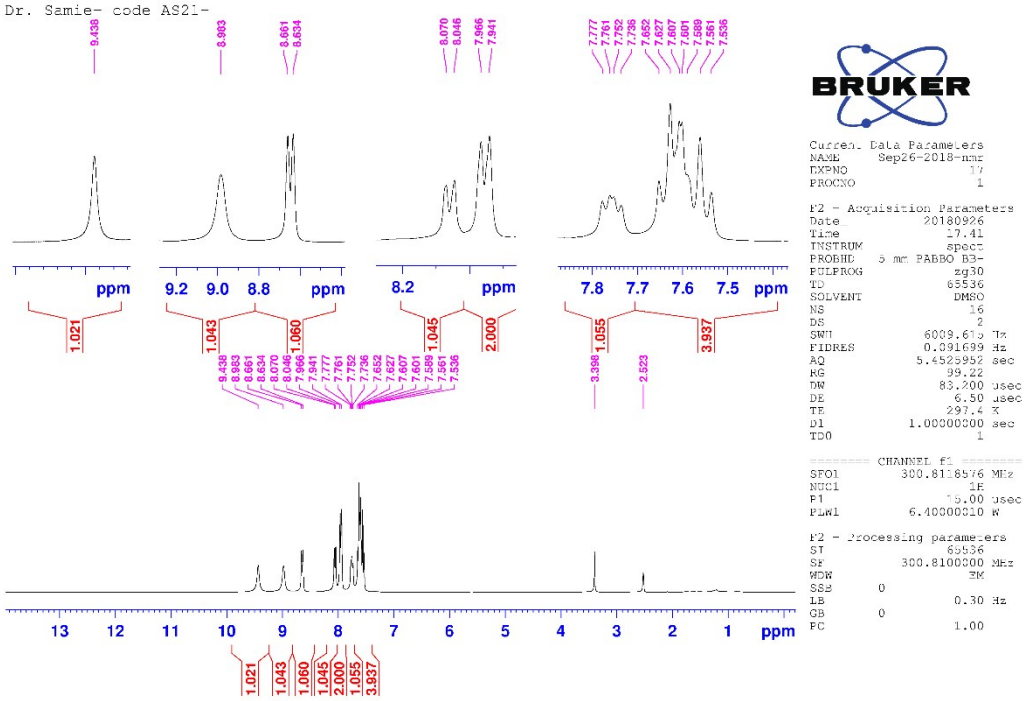
Complex 1



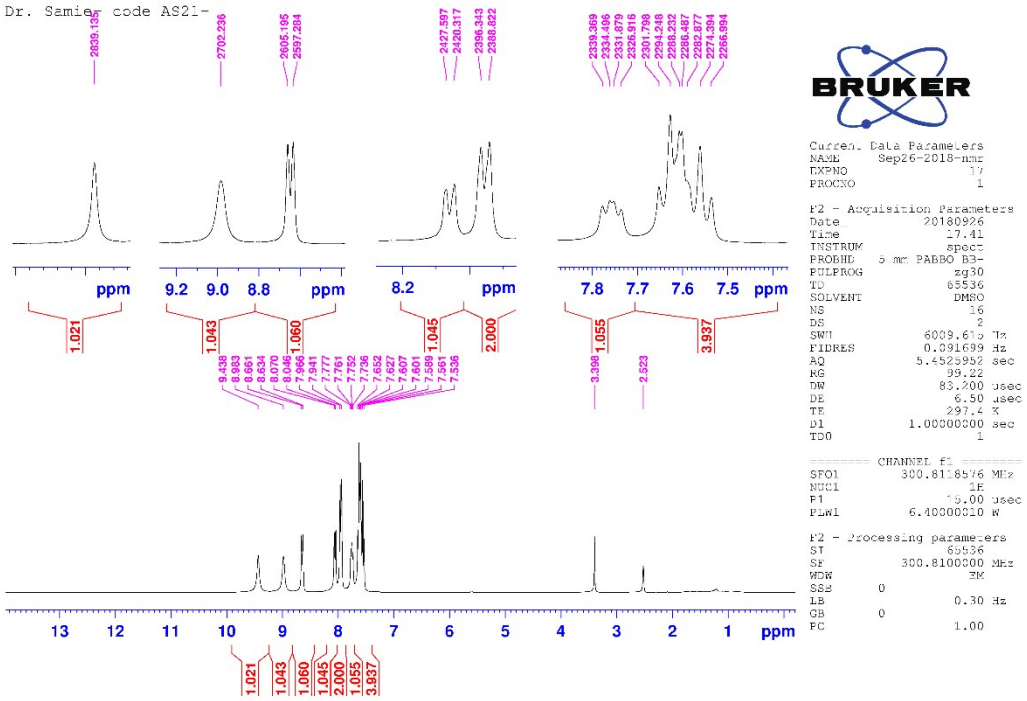
Complex 1



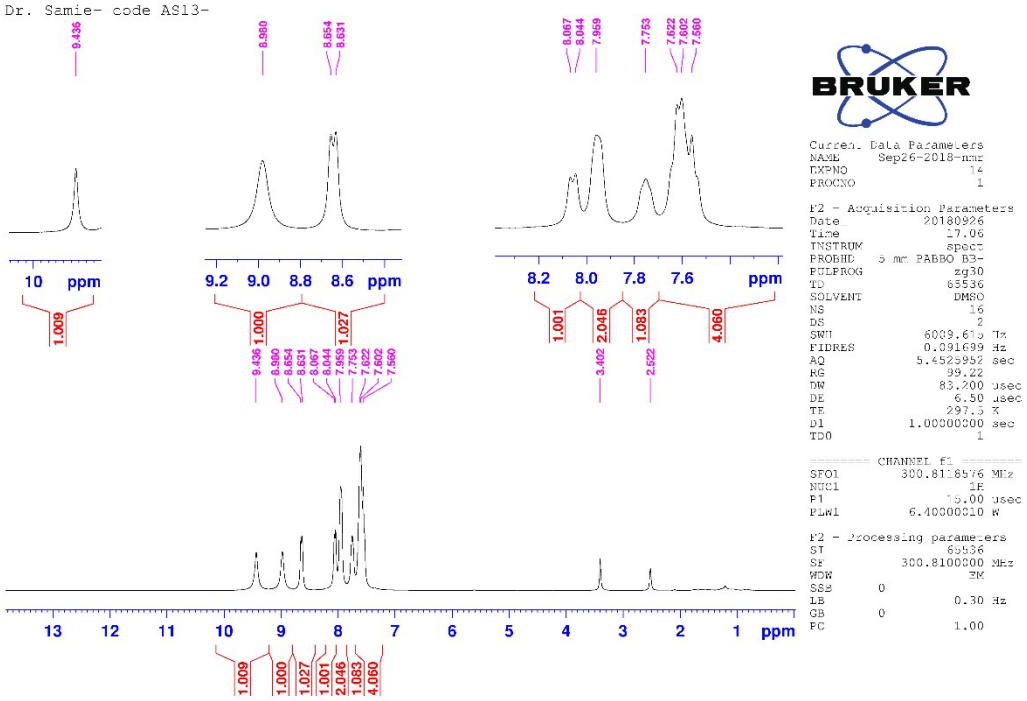
Complex 2



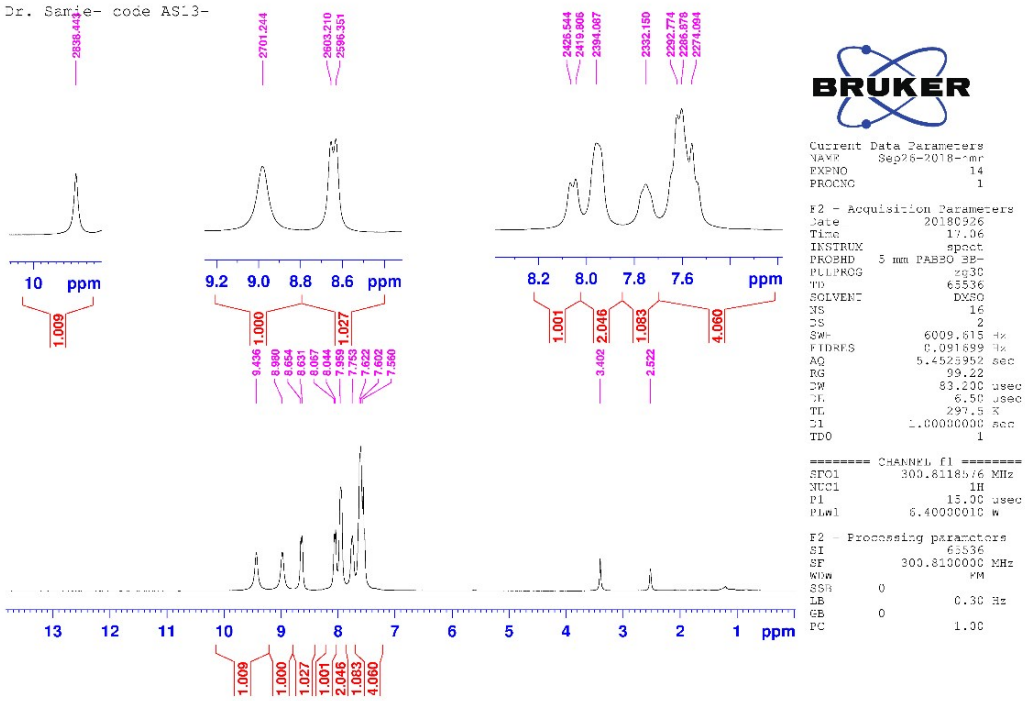
Complex 2



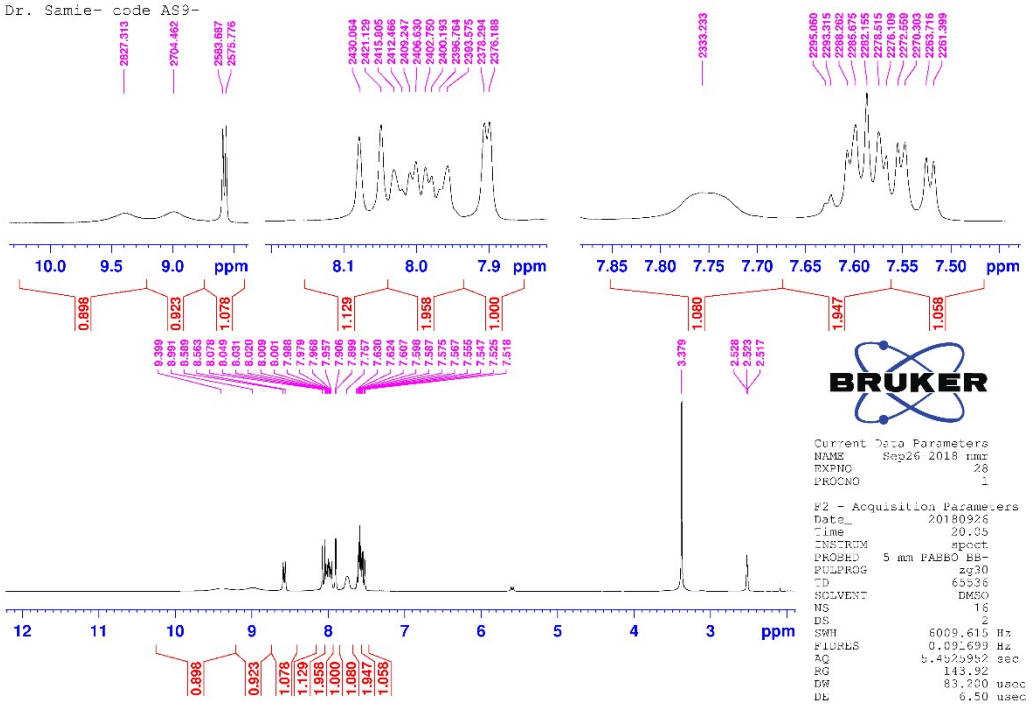
Complex 3



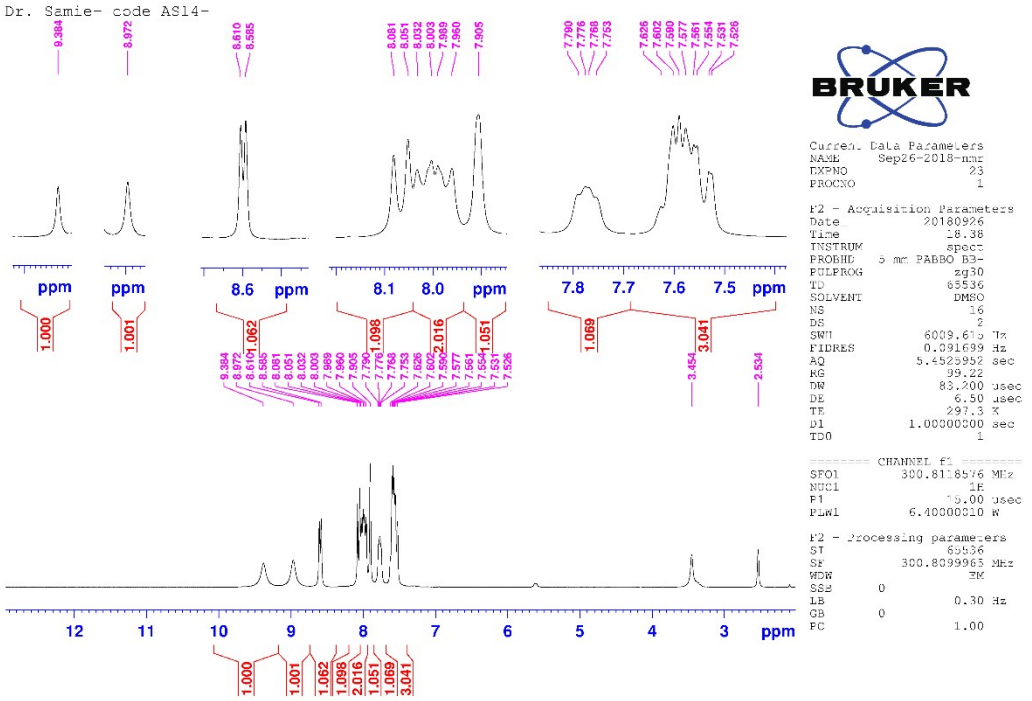
Complex 3



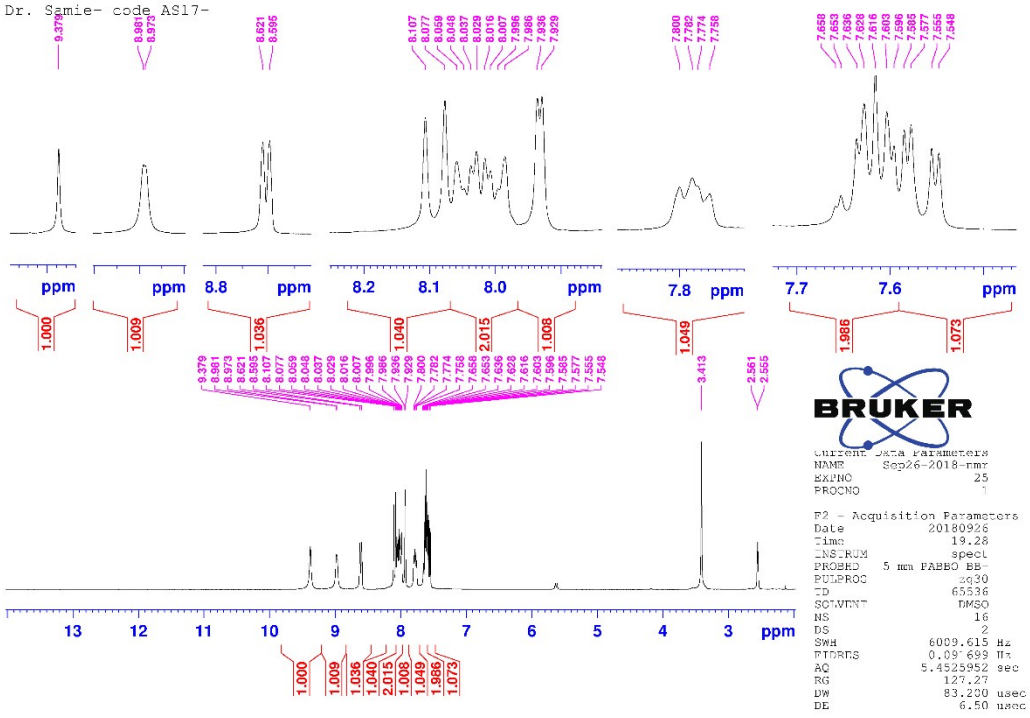
Complex 4



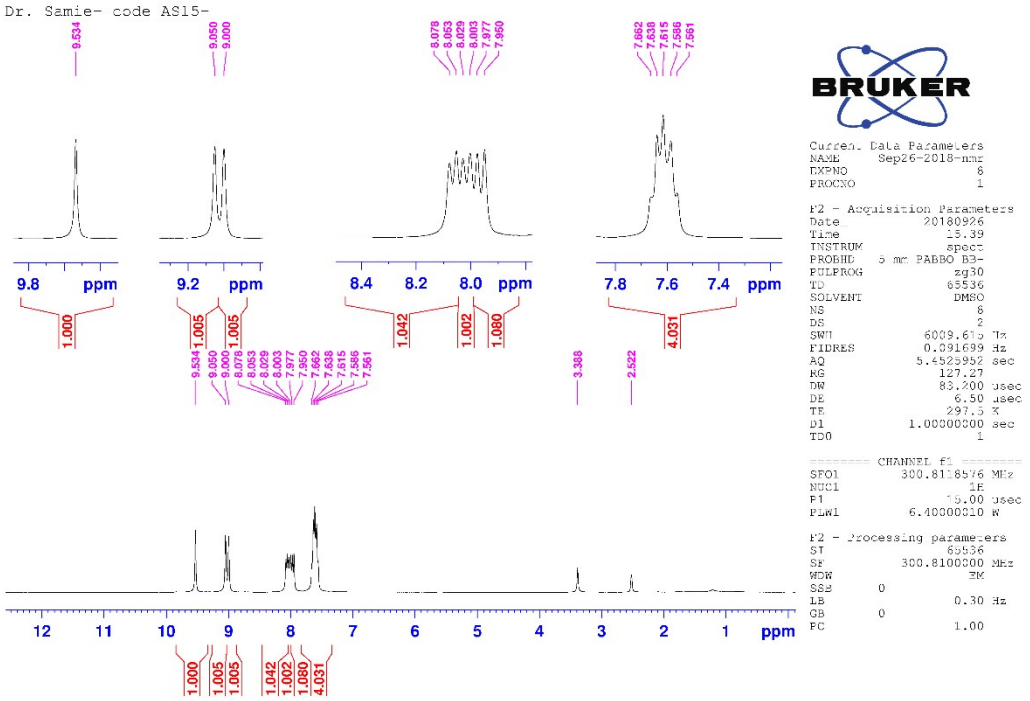
Complex 5



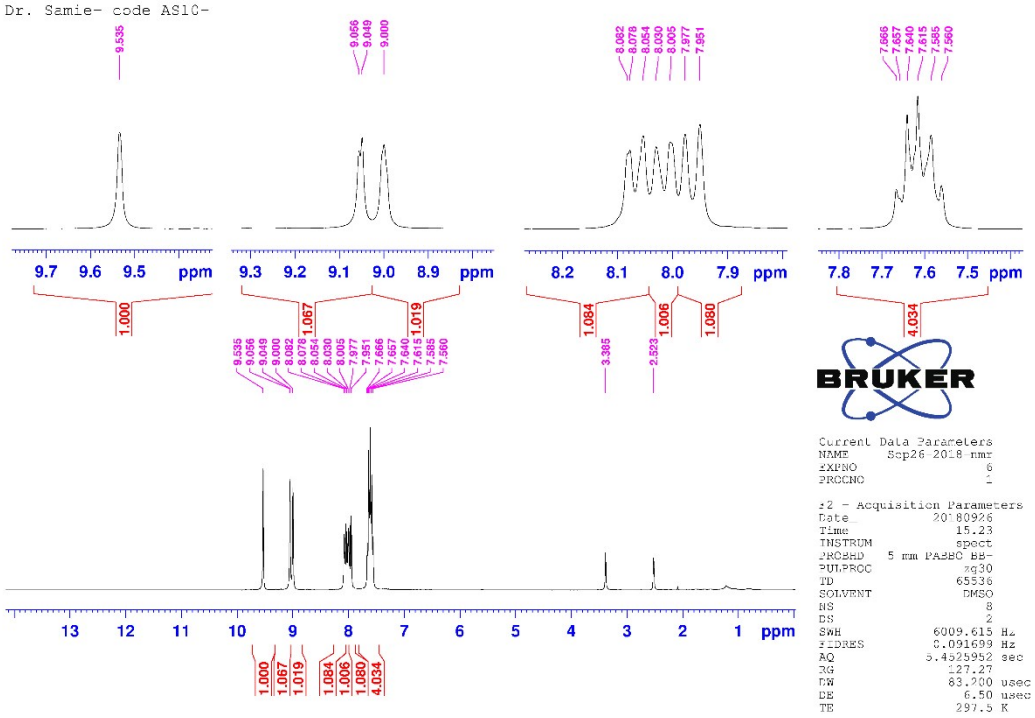
Complex 6



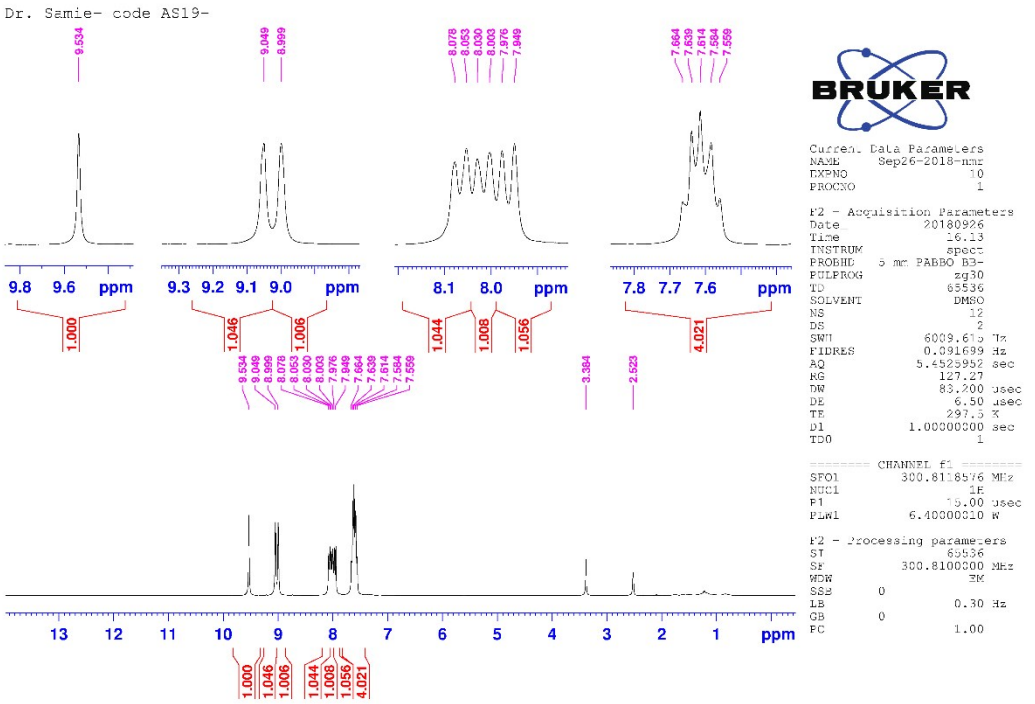
Complex 7



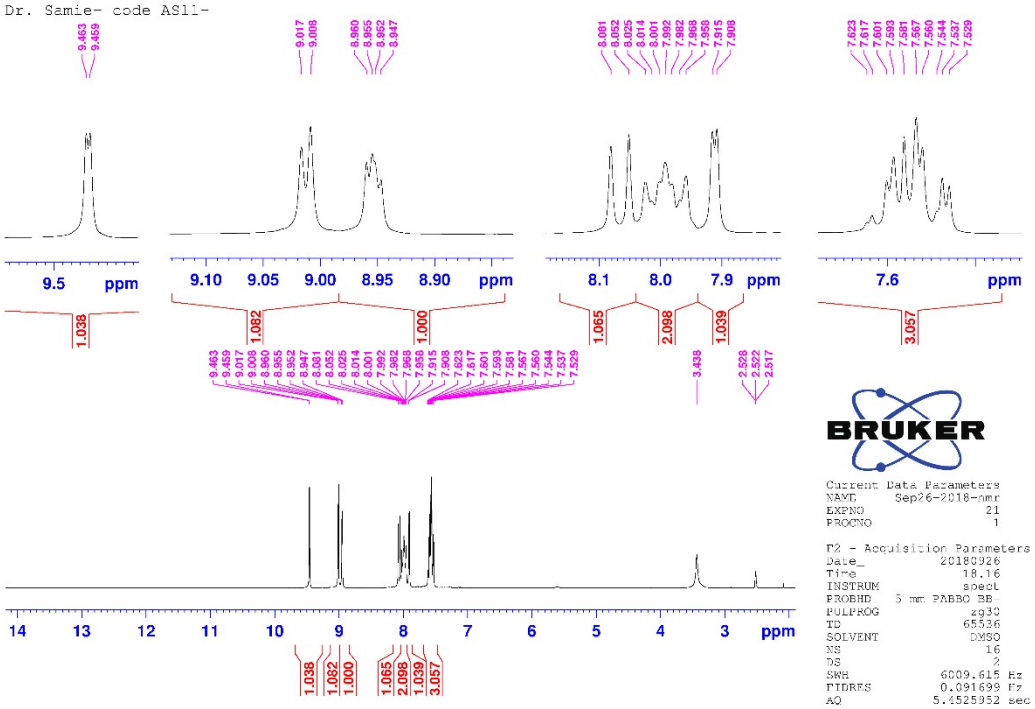
Complex 8



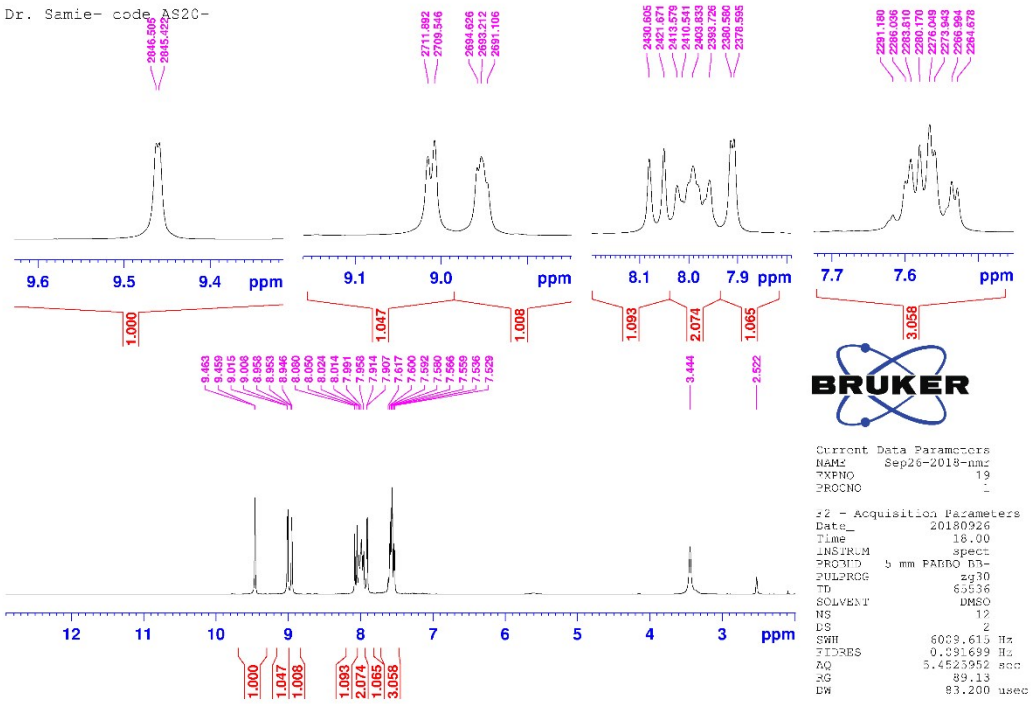
Complex 9



Complex 10

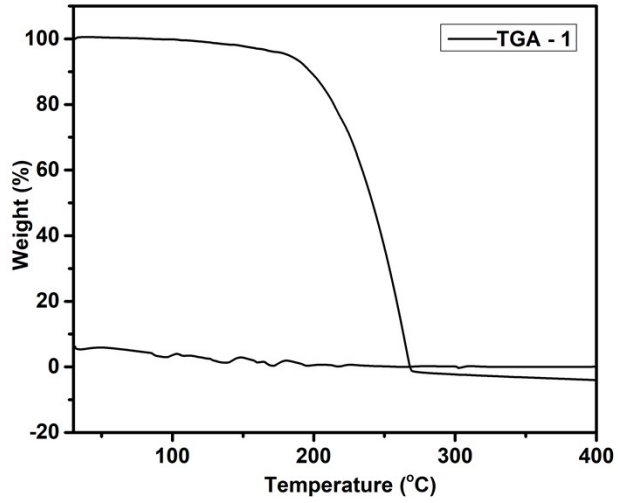


Complex 11

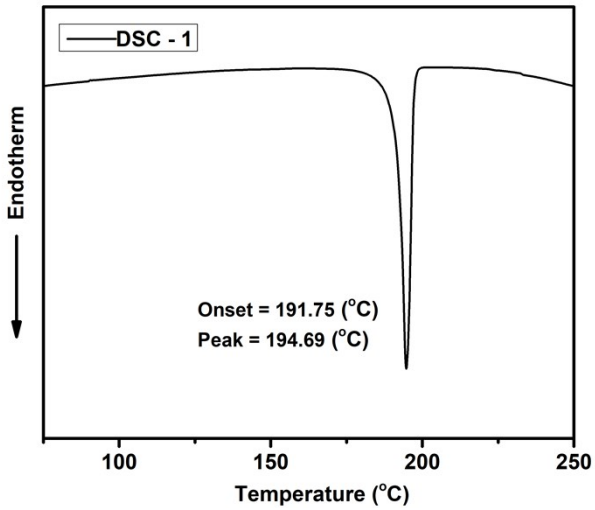


S10. TGA and DSC diagrams for compounds 1-11

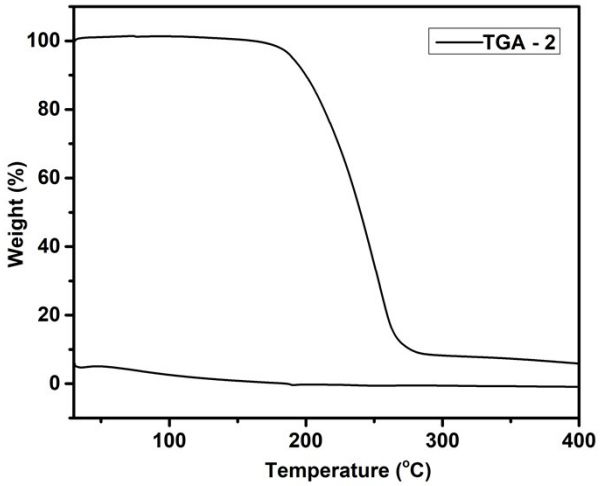
Complex 1



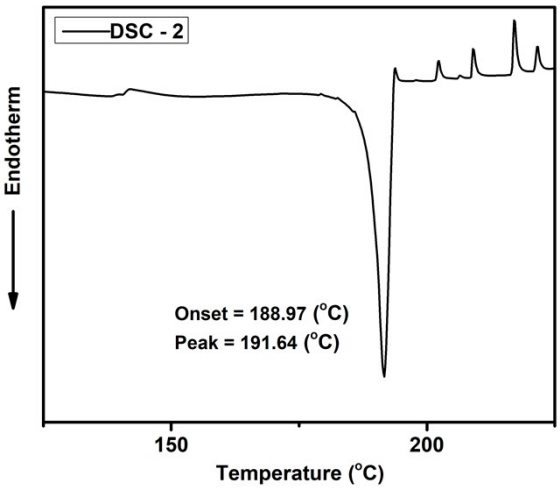
Complex 1



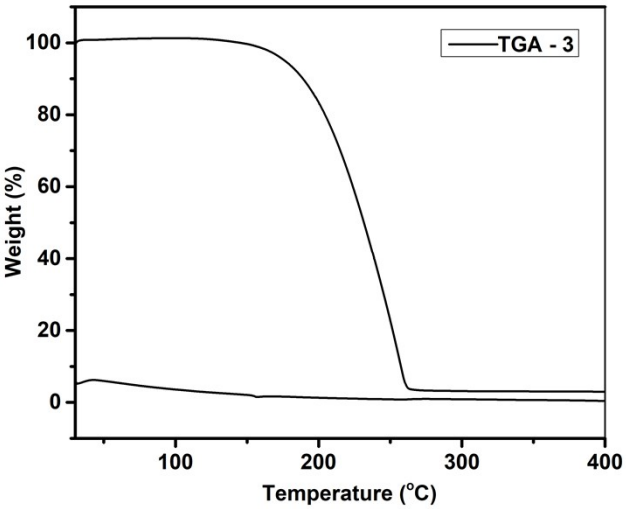
Complex 2



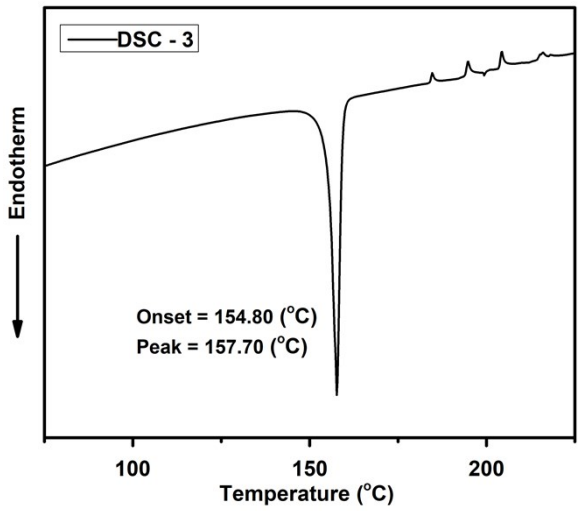
Complex 2



Complex 3

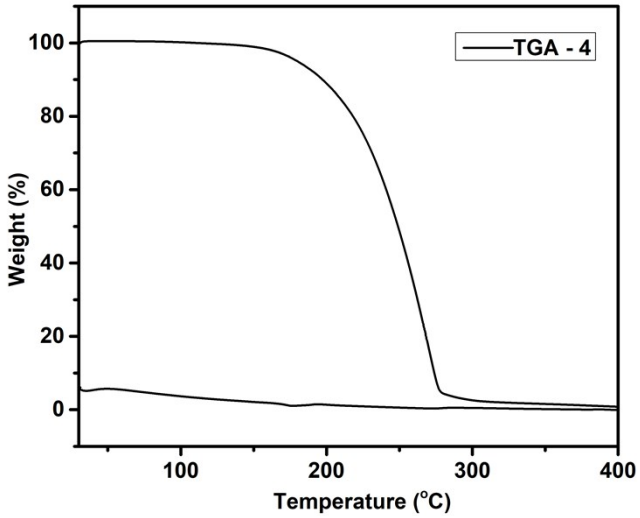


Complex 3

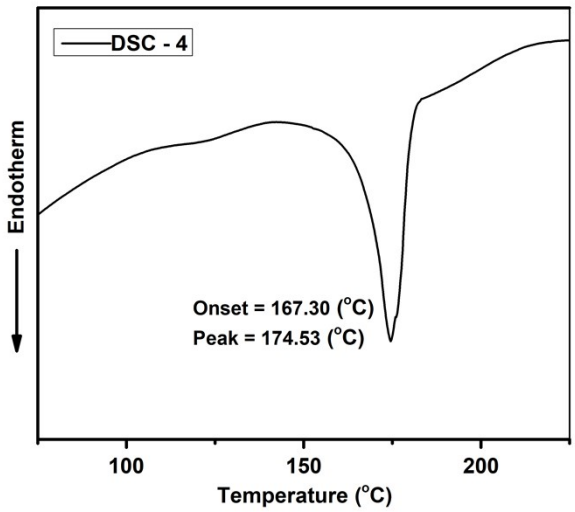


Complex 4

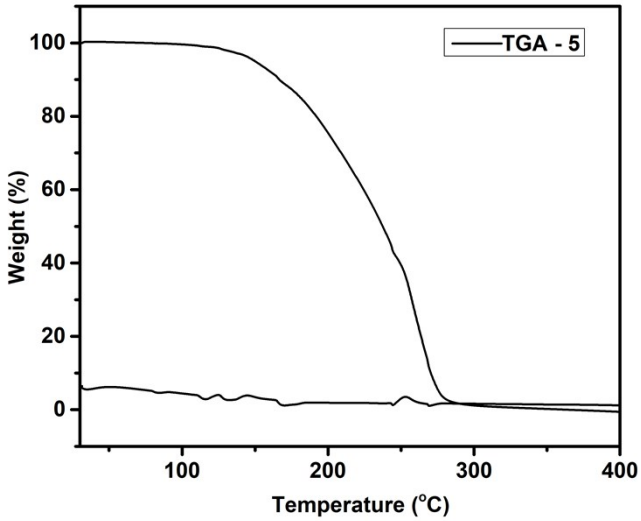
Complex 4



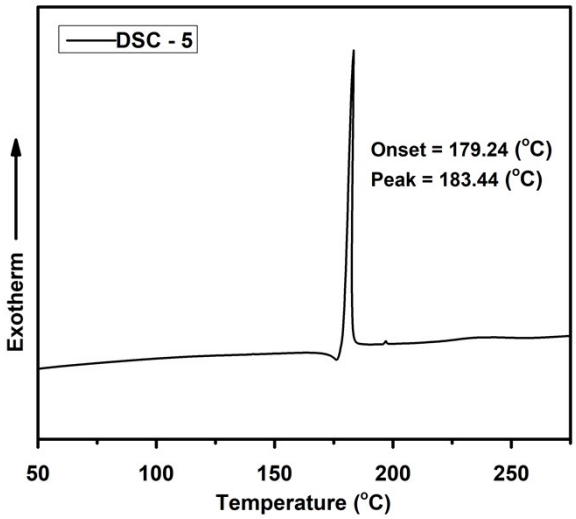
Complex 5



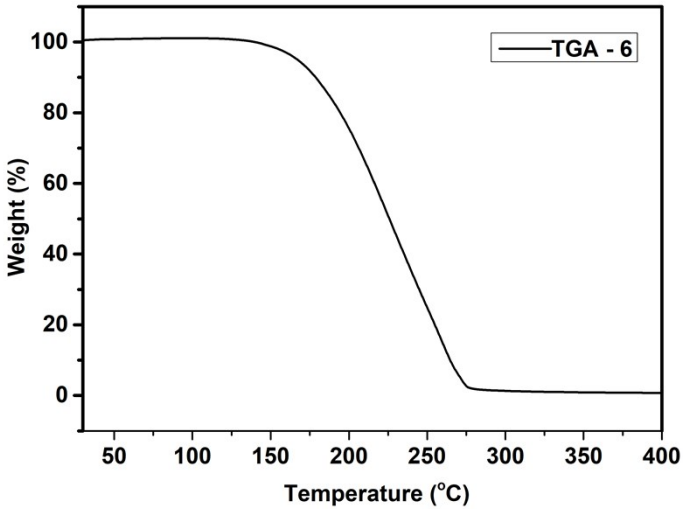
Complex 5



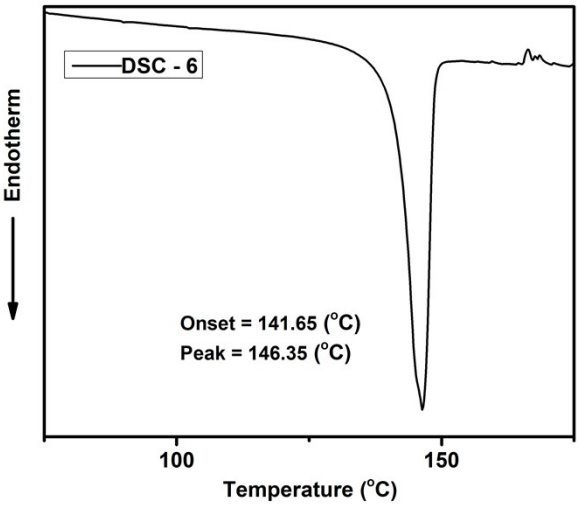
Complex 6



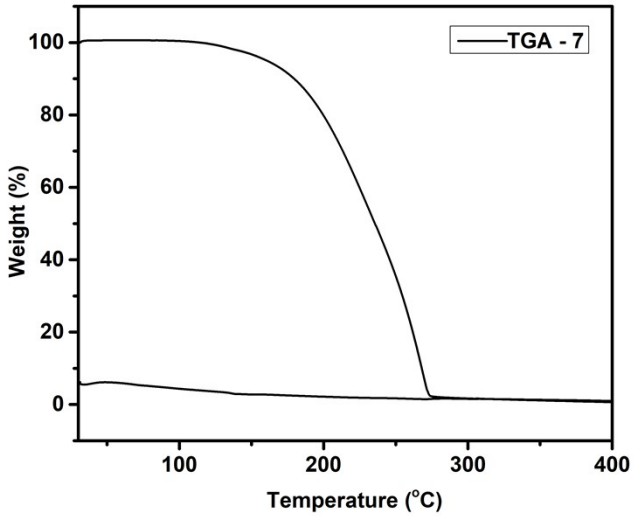
Complex 6



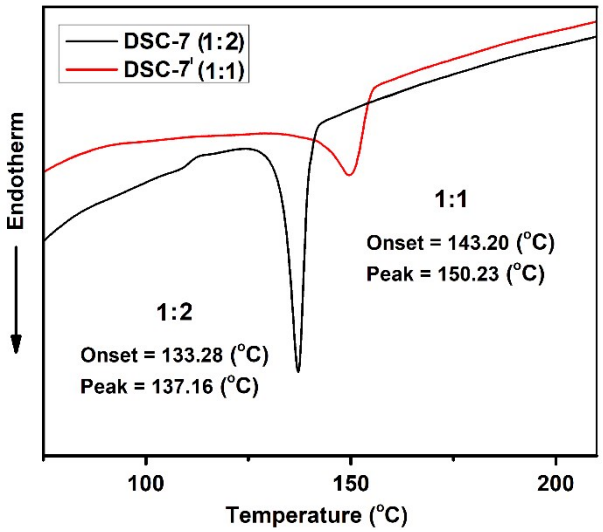
Complex 7



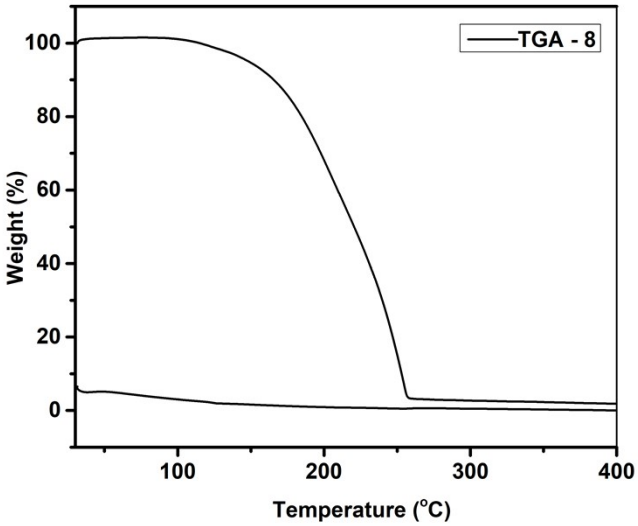
Complexes 7 and 7'



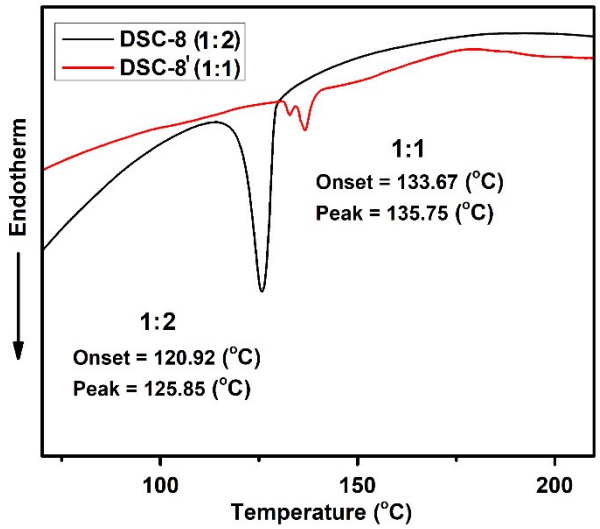
Complex 8



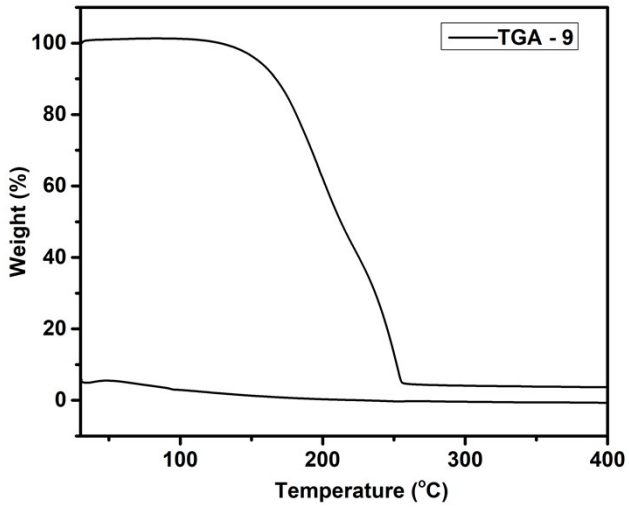
Complexes 8 and 8'



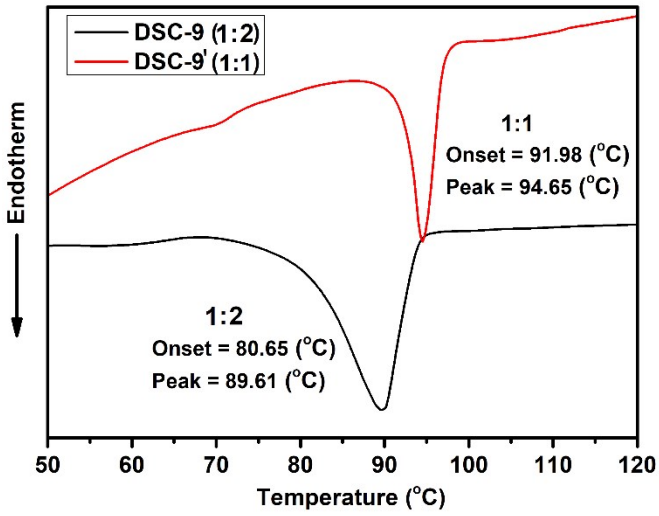
Complex 9



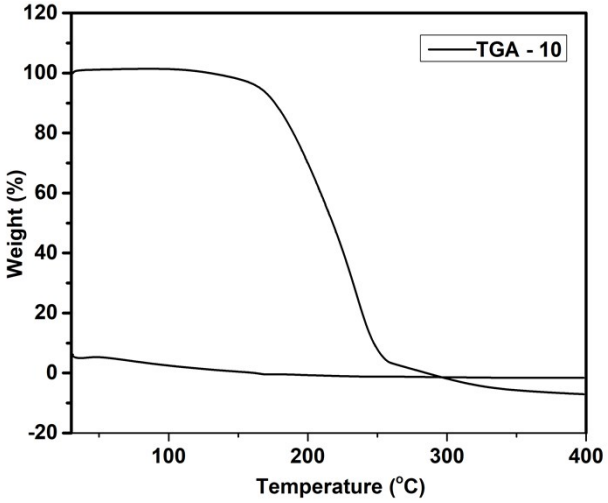
Complexes 9 and 9'

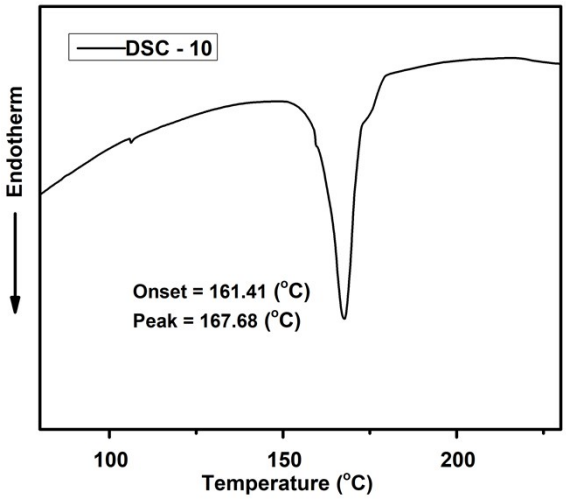


Complex 10

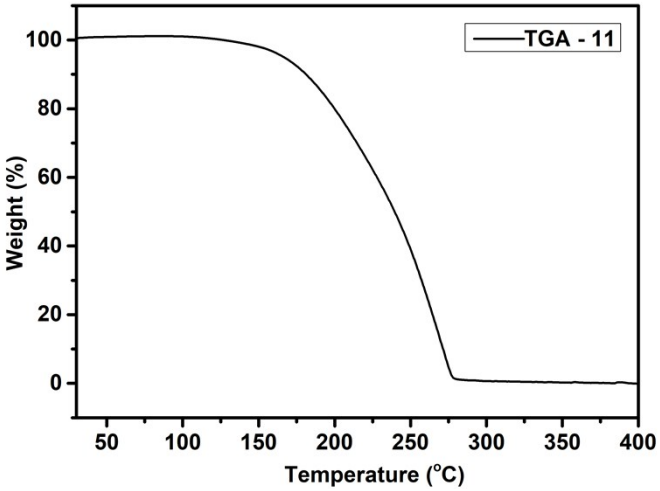


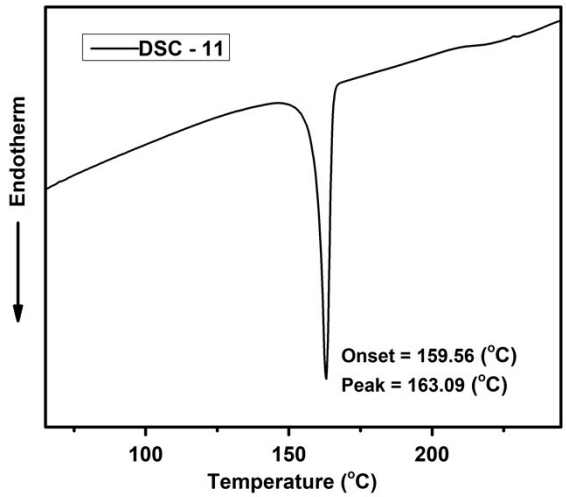
Complex 10





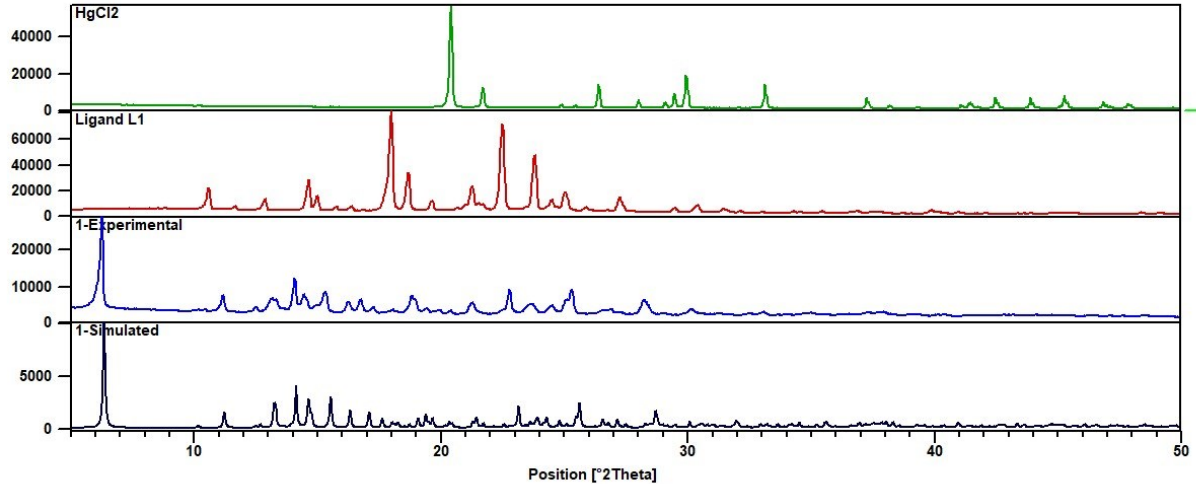
Complex 11 **Complex 11**



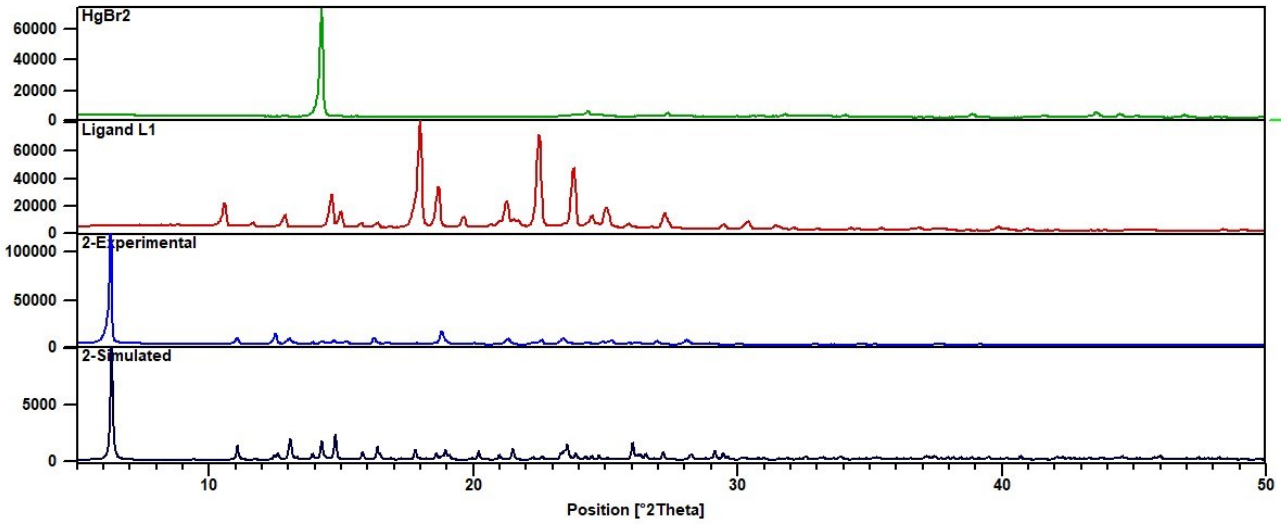


S11. PXRD patterns for compounds 1-11

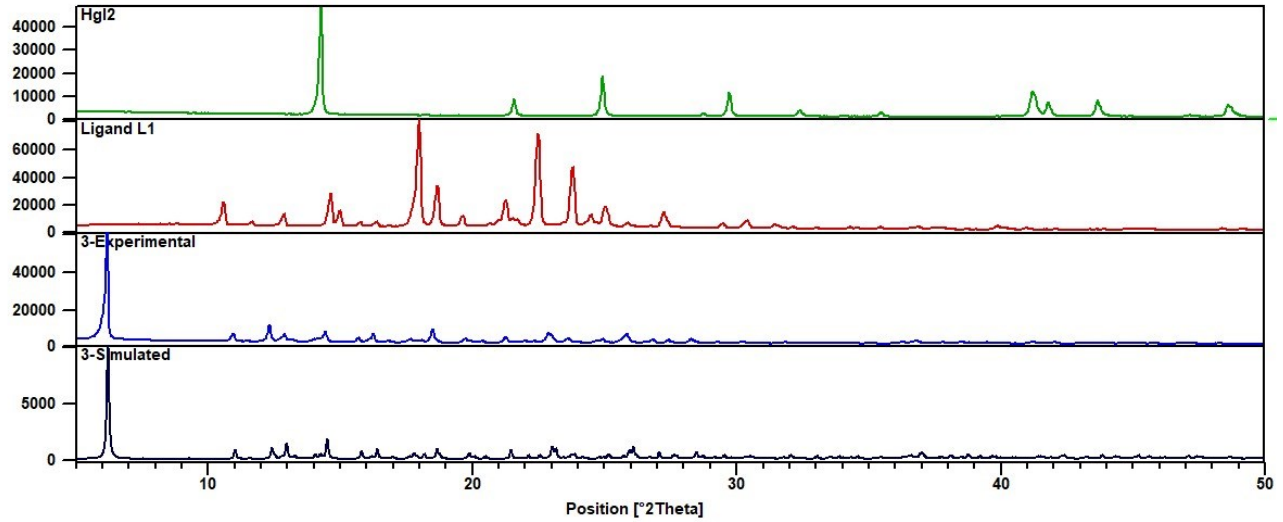
Complex 1



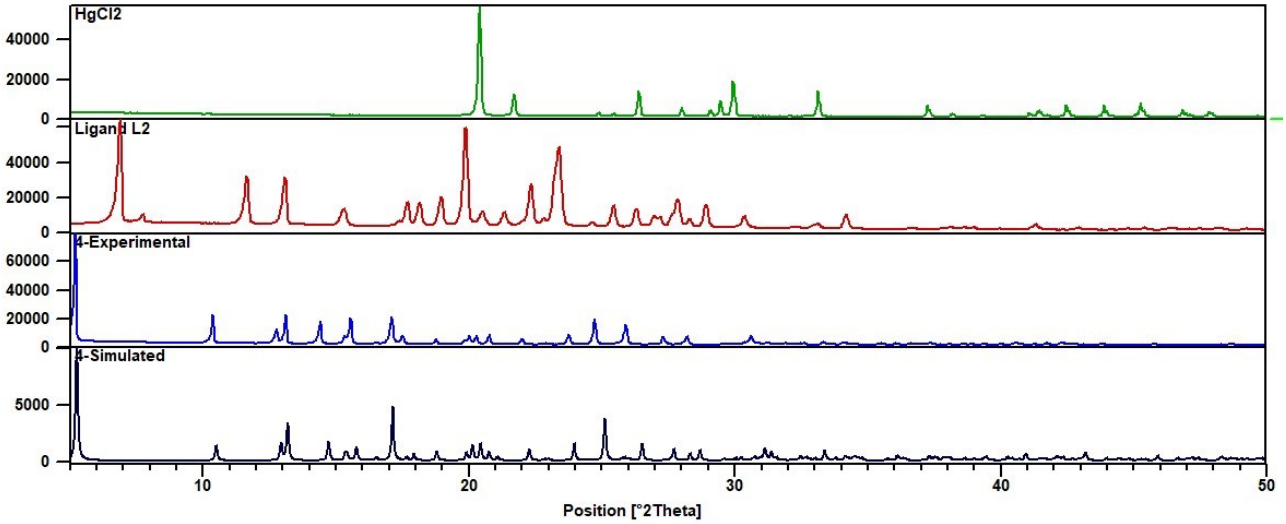
Complex 2



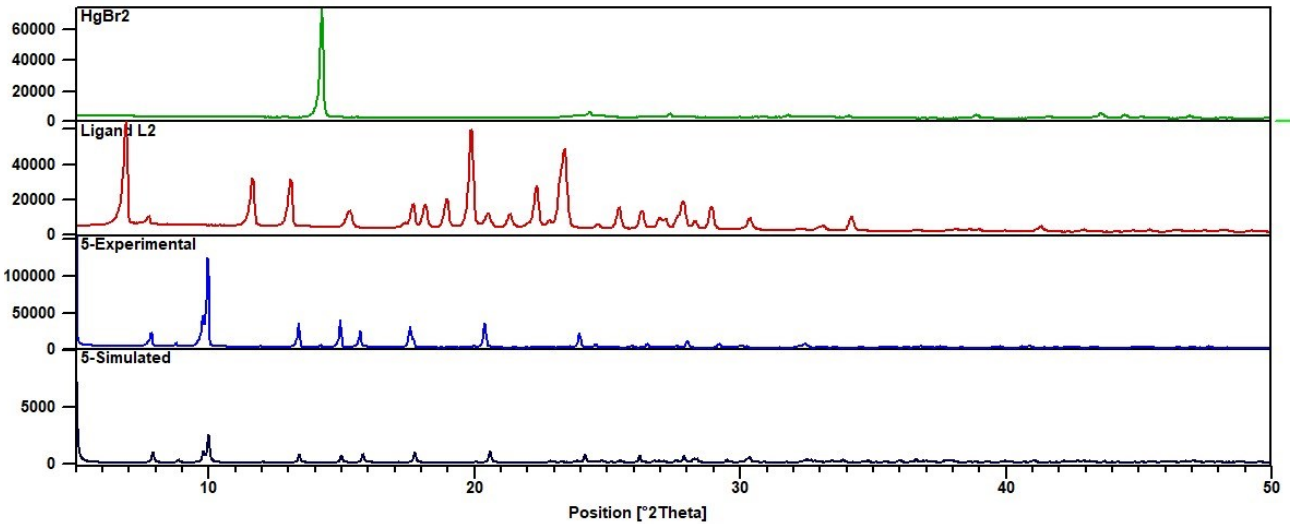
Complex 3



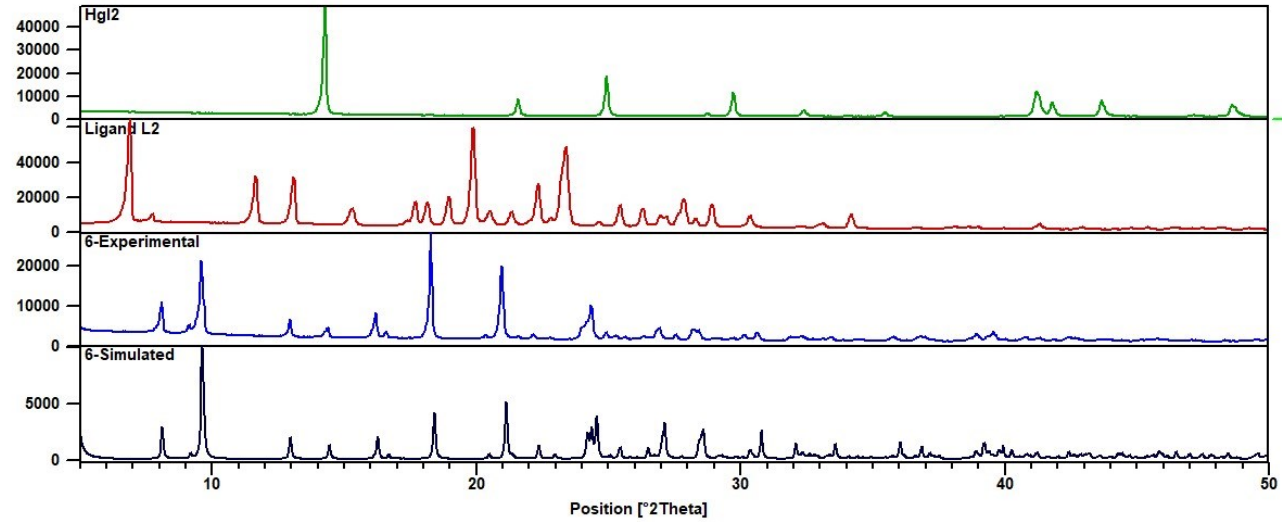
Complex 4



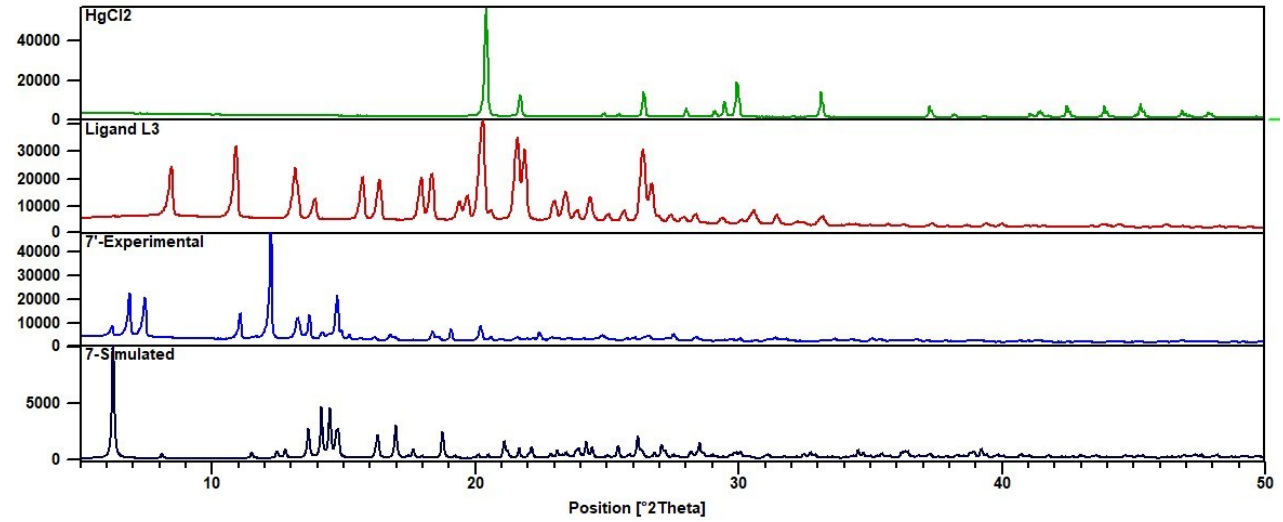
Complex 5



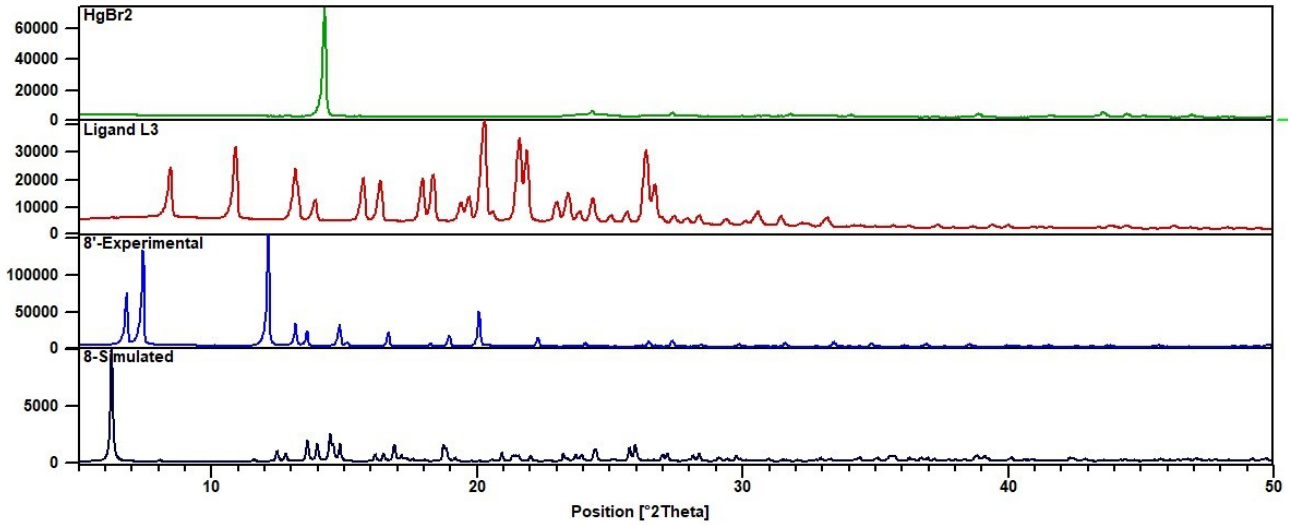
Complex 6



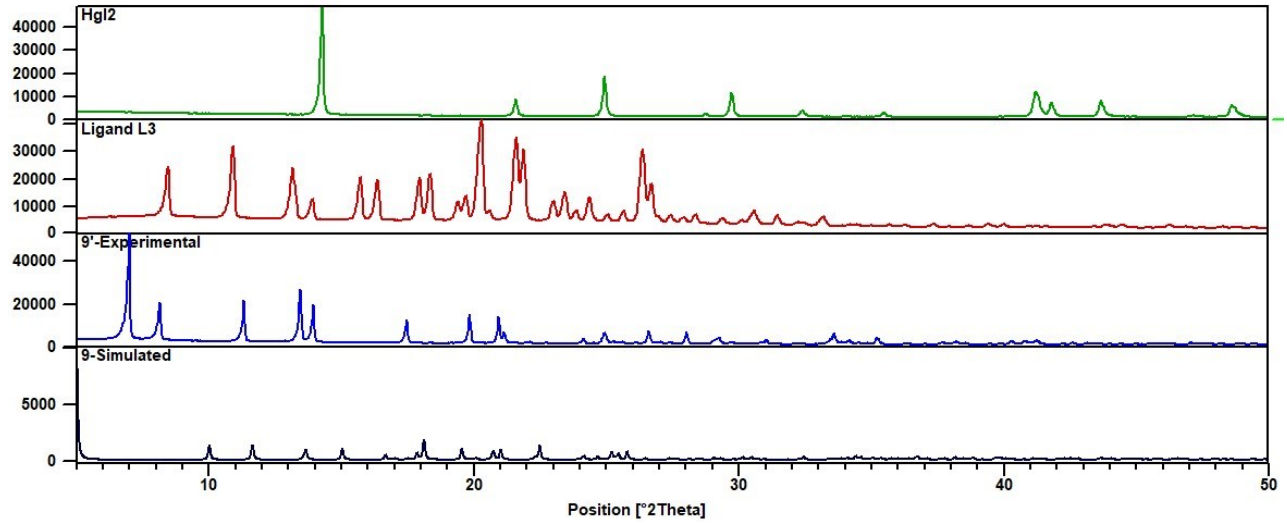
Complexes 7 and 7'



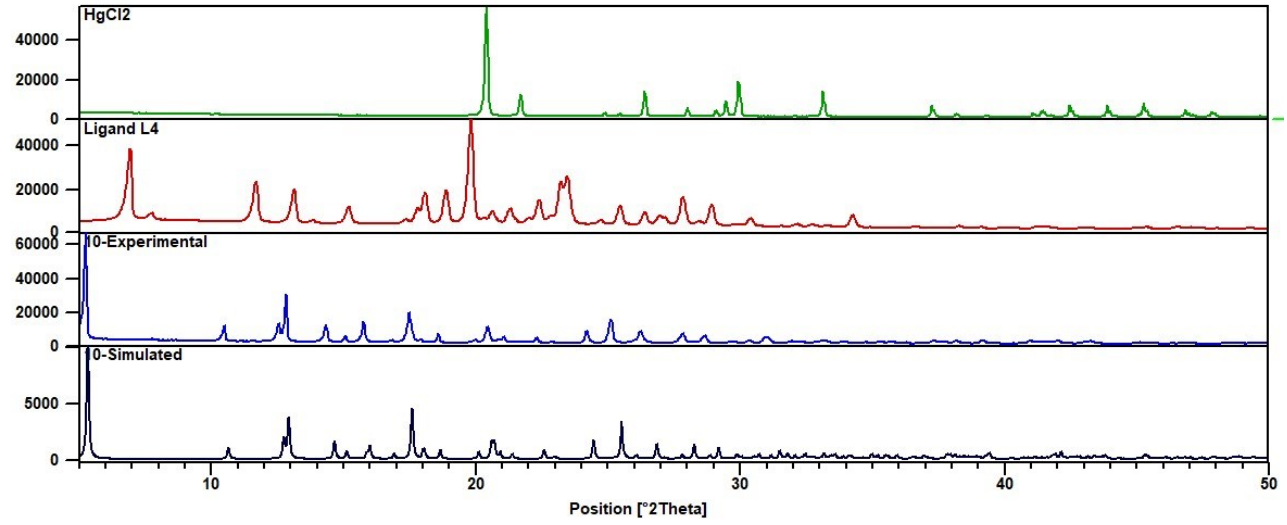
Complexes 8 and 8'



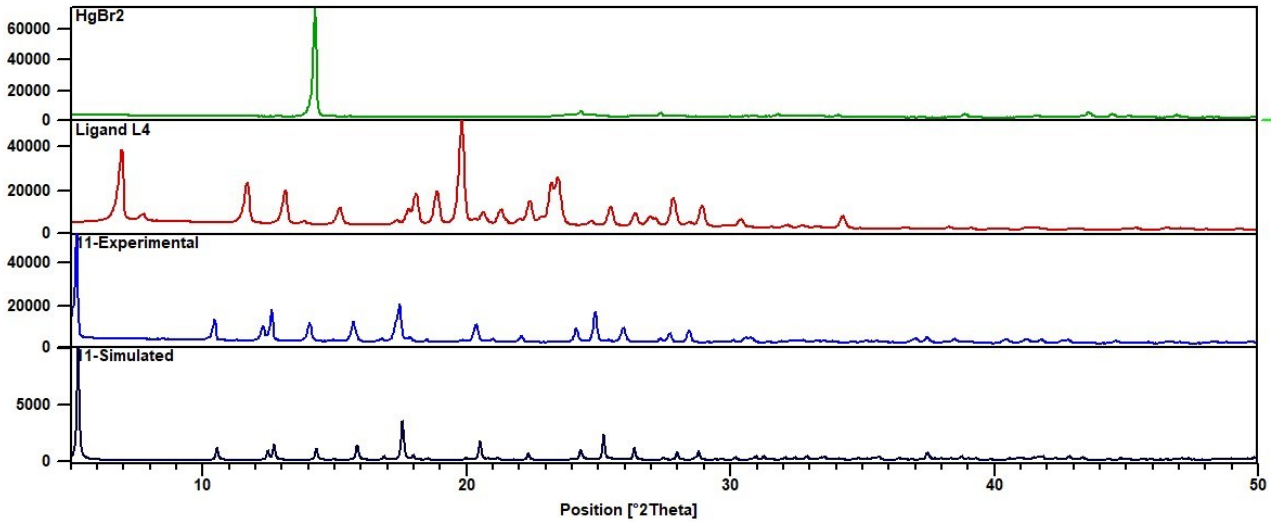
Complexes 9 and 9'



Complex 10



Complex 11



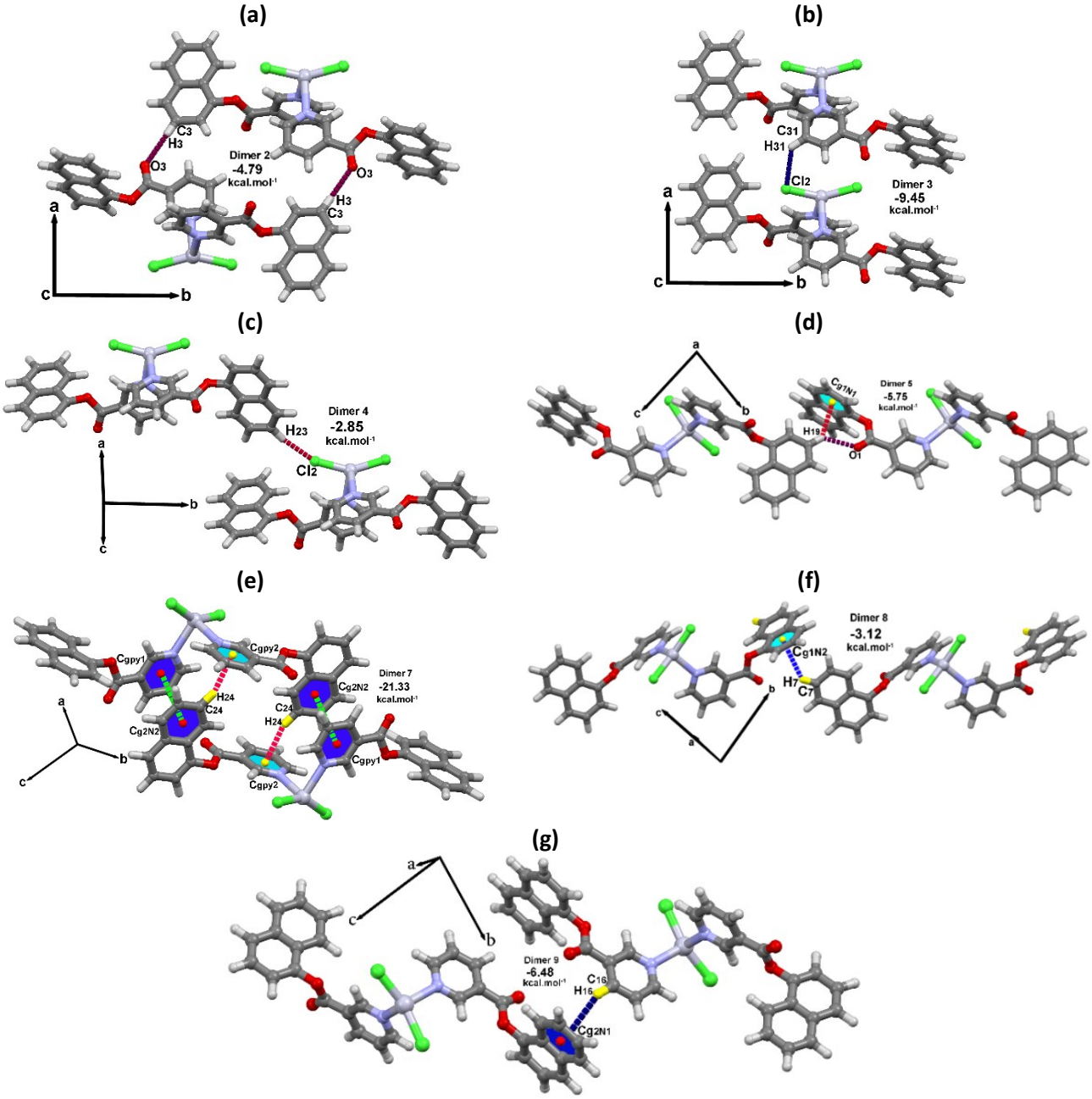
S12. Intermolecular interactions geometrical parameters and energies for complexes 1-11

Complex 1				
Dimers	**Interactions**	**H···A/Å**	**∠D–H···A/°**	**Energy (kcal.mol^{-1})**
Dimer 1	$C_{14}–H_{14}\cdots Cl_1$	2.65	138	-7.40
	$C_{g(py1)}\cdots C_{g(1N2)}$	3.66	8	
Dimer 2	$C_3–H_3\cdots O_3$	2.32	178	-4.79
Dimer 3	$C_{31}–H_{31}\cdots Cl_2$	2.91	124	-9.45
Dimer 4	$C_{23}–H_{23}\cdots Cl_2$	2.59	163	-2.85
Dimer 5	$C_{19}–H_{19}\cdots C_{g(1N1)}$	2.71	137	-5.75
	$C_{19}–H_{19}\cdots O_1$	2.51	132	
Dimer 6	$C_{30}–H_{30}\cdots Cl_2$	2.69	147	-37.06
	$C_{g(py2)}\cdots C_{g(1N1)}$	3.53	2	
Dimer 7	$C_{24}–H_{24}\cdots C_{g(py2)}$	2.67	161	-21.33
	$C_{g(py1)}\cdots C_{g(2N2)}$	3.73	8	
Dimer 8	$C_7–H_7\cdots C_{g(1N2)}$	3.25	128	-3.12
Dimer 9	$C_{16}–H_{16}\cdots C_{g(2N1)}$	3.20	144	-6.48
Total Dimer Biding Energy				**-135.77 kcal.mol^{-1}**
Complex 2				
Dimer 1	$C_{23}–H_{23}\cdots Br_1$	2.64	166	-1.80
Dimer 2	$C_3–H_3\cdots O_3$	2.40	174	-13.72
	$C_{24}–H_{24}\cdots C_{g(py2)}$	2.87	169	
	$C_{g(py1)}\cdots C_{g(2N1)}$	3.82	7	
Dimer 3	$C_{30}–H_{30}\cdots Br_2$	2.91	149	-44.59
	$C_{14}–H_{14}\cdots Br_2$	2.86	144	
	$C_{g(py1)}\cdots C_{g(2N1)}$	3.59	2	
	$C_{g(py2)}\cdots C_{g(1N2)}$	3.64	7	
Dimer 4	$C_7–H_7\cdots C_{g(1N2)}$	3.19	129	-3.21
Dimer 5	$C_{19}–H_{19}\cdots C_{g(1N1)}$	2.64	143	-6.86
	$C_{19}–H_{19}\cdots O_1$	2.55	126	
	$C_{20}–H_{20}\cdots O_1$	2.70	120	
Dimer 6	$C_{16}–H_{16}\cdots C_{g(2N1)}$	3.21	141	-7.46
Total Dimer Biding Energy				**-77.64 kcal.mol^{-1}**
Complex 3				
Dimer 1	$C_{23}–H_{23}\cdots I_1$	2.84	168	-1.24

Dimer 2	$C_3–H_3\cdots O_3$	2.46	168	-12.31
	$C_{24}–H_{24}\cdots C_{g(py2)}$	3.32	170	
	$C_{g(py1)}\cdots C_{g(2N1)}$	3.96	6	
Dimer 3	$C_{30}–H_{30}\cdots I_2$	3.07	138	-43.63
	$C_{14}–H_{14}\cdots I_2$	3.03	148	
	$C_{g(py1)}\cdots C_{g(1N2)}$	3.69	3	
	$C_{g(py2)}\cdots C_{g(1N1)}$	3.63	6	
	$C_9–H_9\cdots I_1$	3.12	126	
Dimer 4	$C_7–H_7\cdots C_{g(1N2)}$	3.00	133	-4.15
Dimer 5	$C_{19}–H_{19}\cdots C_{g(1N1)}$	2.61	141	-7.16
	$C_{19}–H_{19}\cdots O_1$	2.50	126	
	$C_{20}–H_{20}\cdots O_1$	2.69	119	
Dimer 6	$C_{16}–H_{16}\cdots C_{g(2N1)}$	3.27	144	-7.11
Total Dimer Biding Energy				**-75.6 kcal.mol^{-1}**
Complex 4				
Dimer 1	$C_3–H_3\cdots Cl_1$	3.03	138	-33.18
Dimer 2	$C_4–H_4\cdots O_1$	2.55	148	-6.70
	$C_6–H_6\cdots O_1$	2.70	144	
Dimer 3	$C_{14}–H_{14}\cdots Cl_1$	2.77	121	-9.89
Dimer 4	$C_9–H_9\cdots C_{g(2N)}$	2.55	132	-6.69
	$C_8–H_8\cdots C_{g(1N)}$	3.04	121	
Total Dimer Biding Energy				**-56.46 kcal.mol^{-1}**
Complex 5				
Dimer 1	$C_{g(py)}\cdots C_{g(py)}$	3.96	0	-12.34
	$C_{g(1N)}\cdots C_{g(1N)}$	3.96	0	
	$C_{g(2N)}\cdots C_{g(2N)}$	3.96	0	
	$C_{g(1N)}\cdots C_{g(2N)}$	3.79	0	
	$C_3–H_3\cdots O_3$	2.75	132	
Dimer 2	$C_4–H_4\cdots O_1$	2.32	162	-8.58
Dimer 3	$C_{16}–H_{16}\cdots C_{g(2N)}$	3.52	135	-5.82
Dimer 4	$C_9–H_9\cdots O_{2b}$	3.10	173	-3.13
Dimer 5	$C_{15}–H_{15}\cdots Br_2$	2.91	137	-9.10
Total Dimer Biding Energy				**-38.97 kcal.mol^{-1}**
Complex 6				
Dimer 1	$C_{g(1N)}\cdots C_{g(2N)}$	3.87	0	-11.32
	$C_3–H_3\cdots O_1$	2.82	136	
Dimer 2	$C_4–H_4\cdots O_1$	2.35	161	-8.23
	$C_7–H_7\cdots I_1$	3.09	130	
Dimer 3	$C_{16}–H_{16}\cdots C_{g(2N)}$	3.51	130	-6.86
Dimer 4	$C_9–H_9\cdots O_{2b}$	3.02	176	-3.60
	$C_8–H_8\cdots C_{g(py)}$	3.51	139	
Dimer 5	$C_{15}–H_{15}\cdots I_2$	3.15	130	-6.28
Total Dimer Biding Energy				**-36.29 kcal.mol^{-1}**
Complex 7				
Dimer 1	$C_{22}–H_{22}\cdots Cl_1$	2.51	155	-2.49
Dimer 2	$C_{18}–H_{18}\cdots N_2$	2.60	152	-5.24
	$C_{17}–H_{17}\cdots O_1$	2.31	154	
Dimer 3	$C_8–H_8\cdots N_4$	2.72	133	-6.97
	$C_7–H_7\cdots O_3$	2.18	167	
Dimer 4	$C_4–H_4\cdots O_1$	2.46	132	-14.57

	$C_6–H_6\cdots O_1$	2.72	129	
Dimer 5	$C_{14}–H_{14}\cdots Cl_2$	2.51	149	-43.78
Dimer 6	$C_{g(pz)}\cdots C_{g(1N1)}$	3.66	4	-39.61
Dimer 7	$C_{15}–H_{15}\cdots O_3$	2.60	153	-23.76
	$C_{23}–H_{23}\cdots C_{g(Pz2)}$	3.10	174	
Total Dimer Biding Energy				**-136.42 kcal.mol^{-1}**
Complex 8				
Dimer 1	$C_{22}–H_{22}\cdots Br_2$	2.67	148	-2.27
Dimer 2	$C_{18}–H_{18}\cdots N_2$	2.45	147	-5.48
	$C_{17}–H_{17}\cdots O_1$	2.33	157	
Dimer 3	$C_8–H_8\cdots N_4$	2.71	128	-7.22
	$C_7–H_7\cdots O_3$	2.18	169	
Dimer 4	$C_4–H_4\cdots O_1$	2.43	132	-14.87
	$C_6–H_6\cdots O_1$	2.65	128	
Dimer 5	$C_{14}–H_{14}\cdots Br_1$	2.65	146	-43.56
	$C_{24}–H_{24}\cdots Br_1$	3.03	133	
Dimer 6	$C_{g(PZ2)}\cdots C_{g(1N1)}$	3.63	5	-41.63
Dimer 7	$C_{15}–H_{15}\cdots O_3$	2.71	151	-22.40
	$C_{23}–H_{23}\cdots C_{g(PZ2)}$	3.33	175	
	$C_{g(PZ1)}\cdots C_{g(1N2)}$	3.67	2	
Total Dimer Biding Energy				**-137.43 kcal.mol^{-1}**
Complex 9				
Dimer 1	$C_2–H_2\cdots O_2$	2.68	144	-35.35
	$C_9–H_9\cdots I_1$	3.08	148	
	$C_{g(1N)}\cdots C_{g(2N)}$	3.94	2	
Dimer 2	$C_3–H_3\cdots C_{g(1N)}$	2.99	135	-4.60
Dimer 3	$C_8–H_8\cdots N_2$	2.62	138	-8.35
	$C_7–H_7\cdots O_1$	2.38	173	
Total Dimer Biding Energy				**-48.3 kcal.mol^{-1}**
Complex 10				
Dimer 1	$C_3–H_3\cdots Cl_1$	3.06	138	-37.90
Dimer 2	$C_9–H_9\cdots C_{g(2N)}$	2.55	133	-6.48
	$C_8–H_8\cdots C_{g(1N)}$	3.10	120	
Dimer 3	$C_6–H_6\cdots O_1$	2.48	146	-11.74
	$C_4–H_4\cdots O_1$	2.53	144	
	$C_4–H_4\cdots N_2$	2.61	143	
Dimer 4	$C_{g(PZ)}\cdots C_{g(1N)}$	3.60	3	-26.44
Dimer 5	$C_{14}–H_{14}\cdots Cl_1$	2.79	130	-10.29
Total Dimer Biding Energy				**-92.85 kcal.mol^{-1}**
Complex 11				
Dimer 1	$C_3–H_3\cdots Br_1$	3.10	137	-36.32
Dimer 2	$C_9–H_9\cdots C_{g2N}$	2.56	134	-6.53
	$C_8–H_8\cdots C_{g1N}$	3.12	119	
Dimer 3	$C_6–H_6\cdots O_1$	2.48	149	-11.62
	$C_4–H_4\cdots O_1$	2.65	144	
	$C_4–H_4\cdots N_2$	2.57	146	
Dimer 4	$C_{g(PZ)}\cdots C_{g(1N)}$	3.66	5	-25.24
Dimer 5	$C_{14}–H_{14}\cdots Br_1$	2.90	130	-8.66
Total Dimer Biding Energy				**-88.37 kcal.mol^{-1}**

S13. Representation of dimer2 (a), dimer3 (b), dimer4 (c), dimer5 (d), dimer7 (e), dimer8 (f), and dimer9 (g) with calculated binding energy for the dimers in complex 1

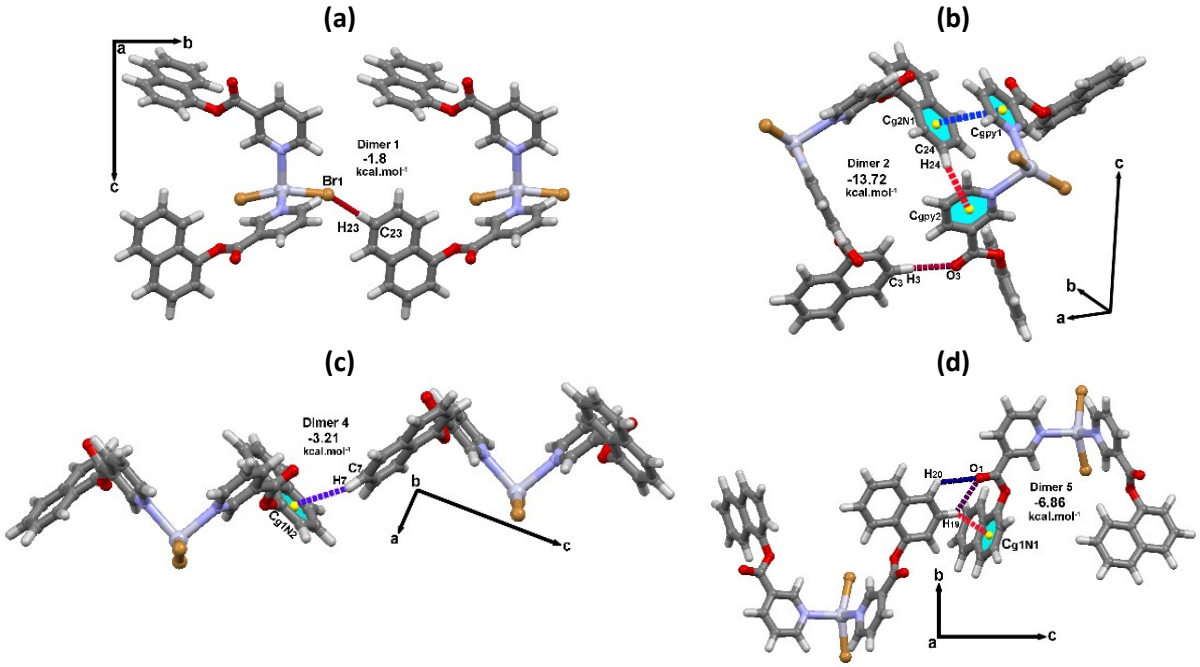


Complex 1

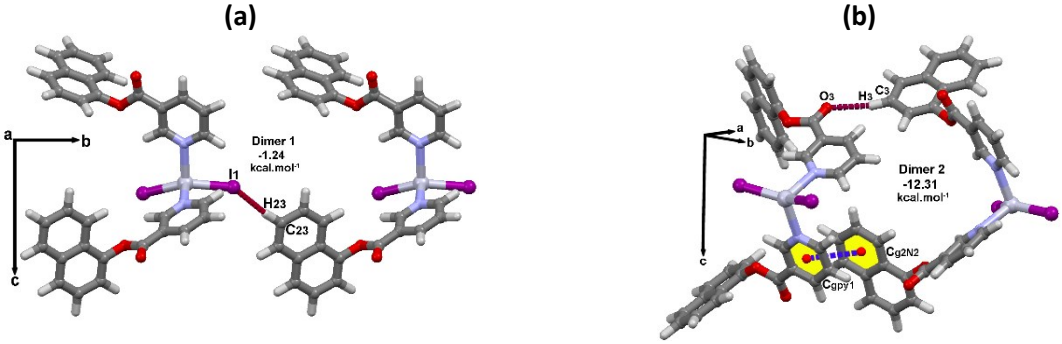
Dimer2 in complex 1 which formed by two symmetric interactions of $C_3–H_3\cdots O_3$ (-4.79 kcal.mol^{-1}) is presented in figure S13a. Dimer3 with binding energy of -9.45 kcal.mol^{-1} contains $C_{31}–H_{31}\cdots Cl_2$ interaction which shaped in fishbone style, figure S13b. Cl_2 as double acceptor engaged in $C_{23}–H_{23}\cdots Cl_2$ interaction to create dimer4 with -2.85 kcal.mol^{-1} energy and staircase style, figure S13c. Bifurcated interactions for H_{19} in dimer5, made $C_{19}–H_{19}\cdots C_{g1N1}$ and $C_{19}–H_{19}\cdots O_1$ in which the

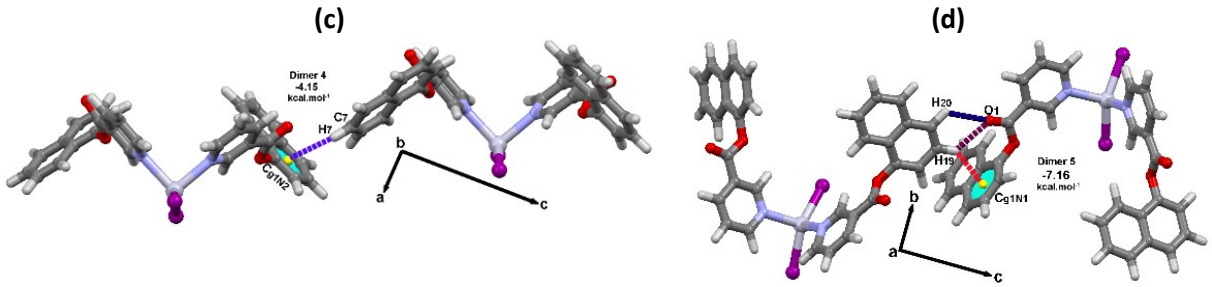
structure enlarged diametrically in *ab*-plane, figure S13d. The total energy for this dimer was calculated as -5.75 kcal.mol^{-1}. There are two C–H···π interactions of C_{24}–H_{24}···C_{gPy2} and two π···π interaction of C_{gPy1}···C_{g2N2} which made dimer7 with the energy of -21.33 kcal.mol^{-1}, figure S13e. C_7–H_7··· C_{g1N2} created dimer8 with the energy of -3.12 kcal.mol^{-1} (figure S13f) and C_{16}–H_{16}··· C_{g2N1} formed dimer9 with the energy of -6.48 kcal.mol^{-1} (figure S13g).

S14. Representation of dimer1 (a), dimer2 (b), dimer4 (c), and dimer5 (d) with calculated binding energy for the dimers in complex 2



S15. Representation of dimer1 (a), dimer2 (b), dimer4 (c), and dimer5 (d) with calculated binding energy for the dimers in complex 3

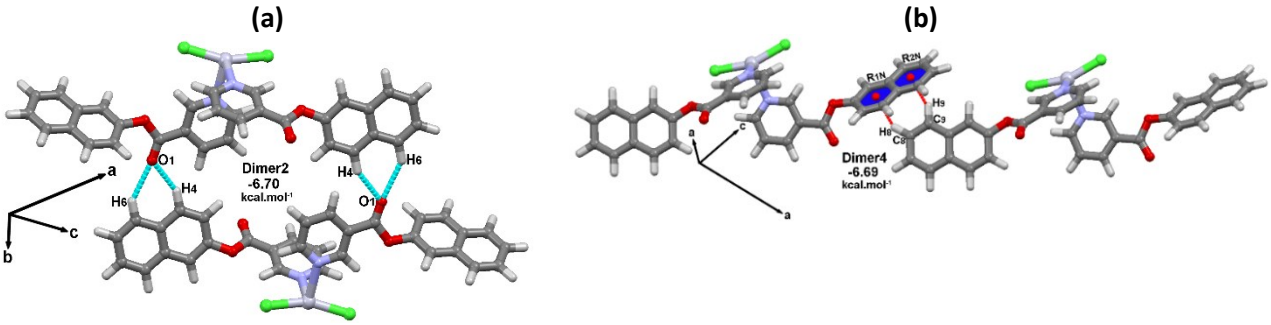




Complexes 2 and 3

As it is shown in the figures S14a and S15a, C_{23}–H_{23}···Br_1/I_1 (dimer1) occurred between two molecules of the complexes via pearl-like region with the energies of -1.8 and -1.24 kcal.mol^{-1}, respectively. C_{gPy1}...C_{g2N1}, C_{24}–H_{24}···C_{gPy2} and C_3–H_3···O_3 (dimer2) exhibited in figure S14b occurred between the ligands of two molecules with the energy of -13.72 kcal.mol^{-1}. C_{gPy1}...C_{g2N2} and C_3–H_3···O_3 with the energy of -12.31 kcal.mol^{-1} happened in complex 3 that are demonstrated as dimer2 in figure S15b as well. C_7–H_7···C_{g1N2} (dimer4) interaction for both of the complexes is depicted in the figures S14c and S15c with the energy of -3.21 and -4.15 kcal.mol^{-1}, respectively. In figures S14d and S15d, bifurcated interactions of O_1 (C_{20}–H_{20}···O_1, C_{19}–H_{19}···O_1) alongside C_{19}–H_{19}···C_{g1N1} made dimer5 with the energy of -6.86 and -7.15 kcal.mol^{-1} for compounds 2 and 3, respectively.

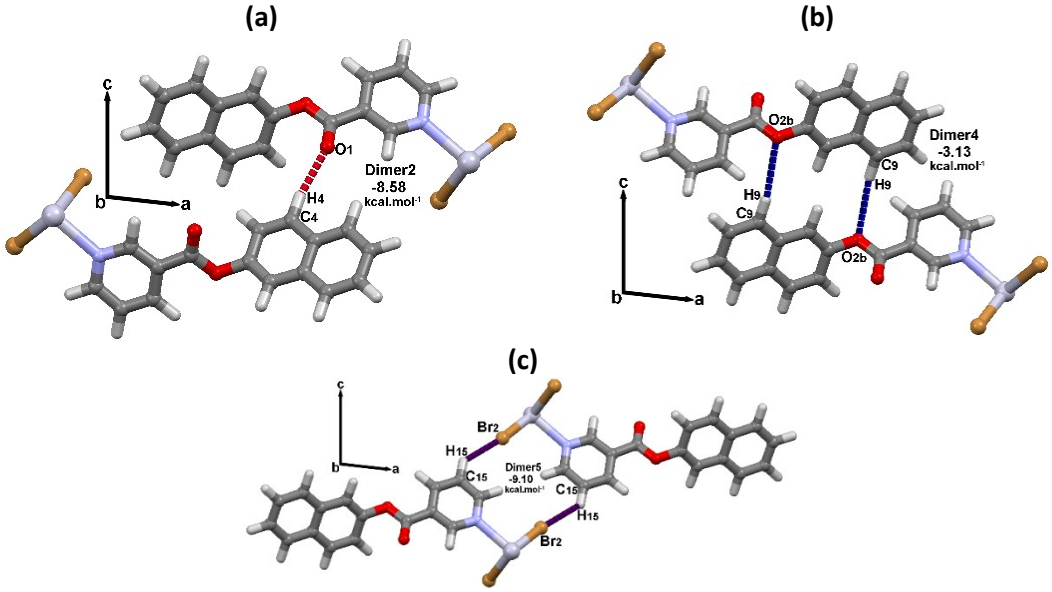
S16. Representation of dimer2 (a) and dimer4 (b) with calculated binding energy for the dimers in complex 4



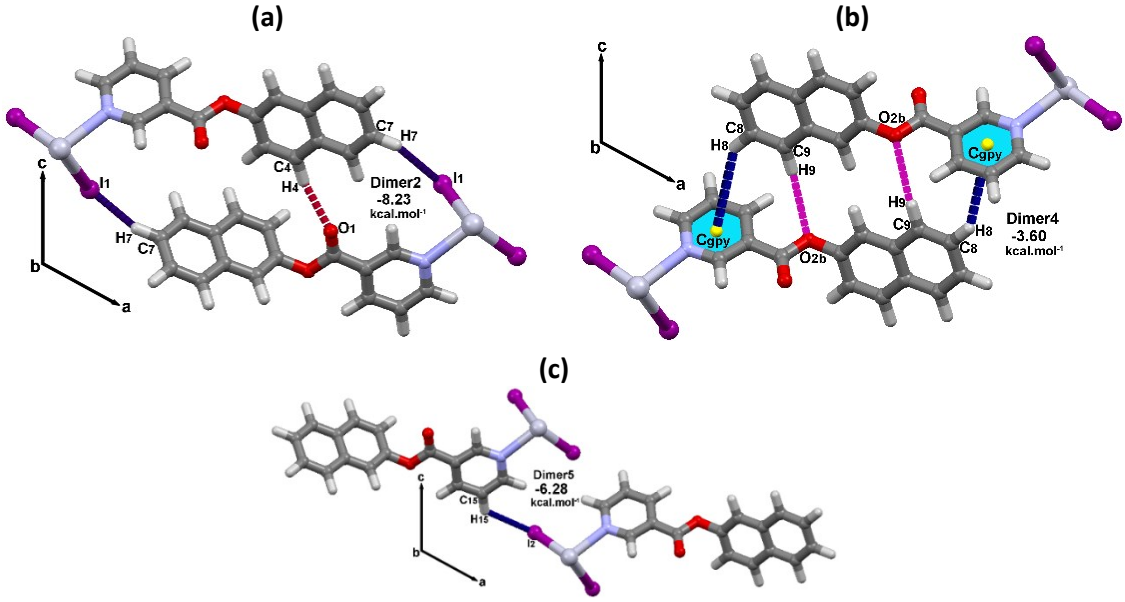
Complex 4

The ligands of complex molecules contacted to each other with two symmetrical bifurcated C_4–H_4···O_1 and C_6–H_6···O_1 interactions to make dimer2 with the energy of -6.69 kcal.mol^{-1}, figure S16a. In the figure S16b, the molecules in dimer4 propagated in linear shape accompanying two C–H···π contacts of C_8–H_8···C_{g1N} and C_9–H_9···C_{g2N}. The contacts in dimer4 presented the energy of -6.69 kcal.mol^{-1}.

S17. Representation of dimer2 (a), dimer4 (b), and dimer5 (c) with calculated binding energy for the dimers in complex 5



S18. Representation of dimer2 (a), dimer4 (b), and dimer5 (c) with calculated binding energy for the dimers in complex 6

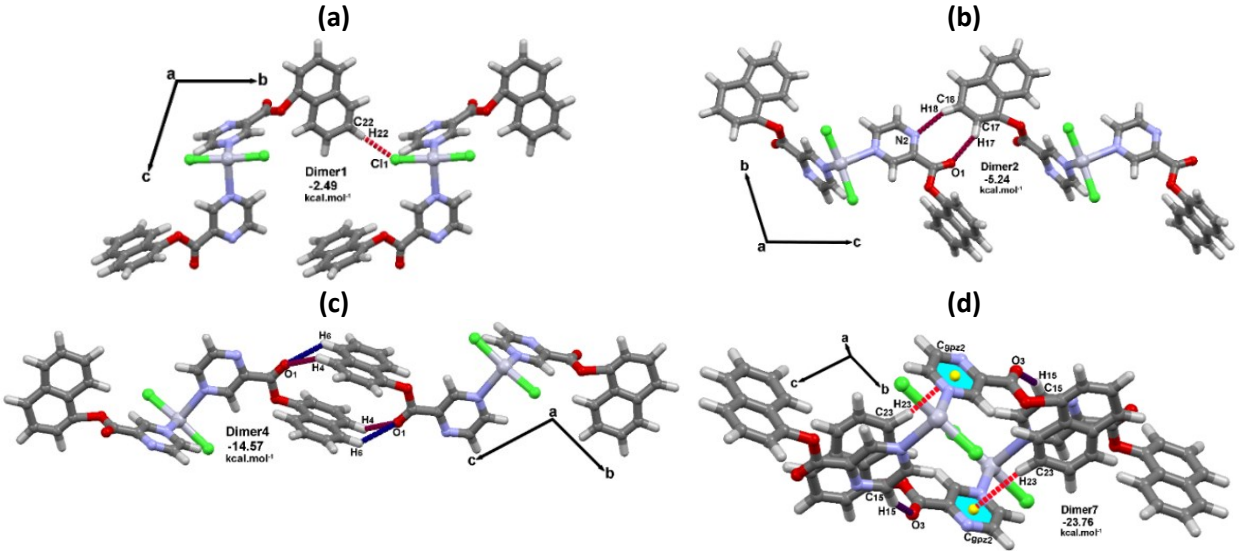


Complexes 5, 6

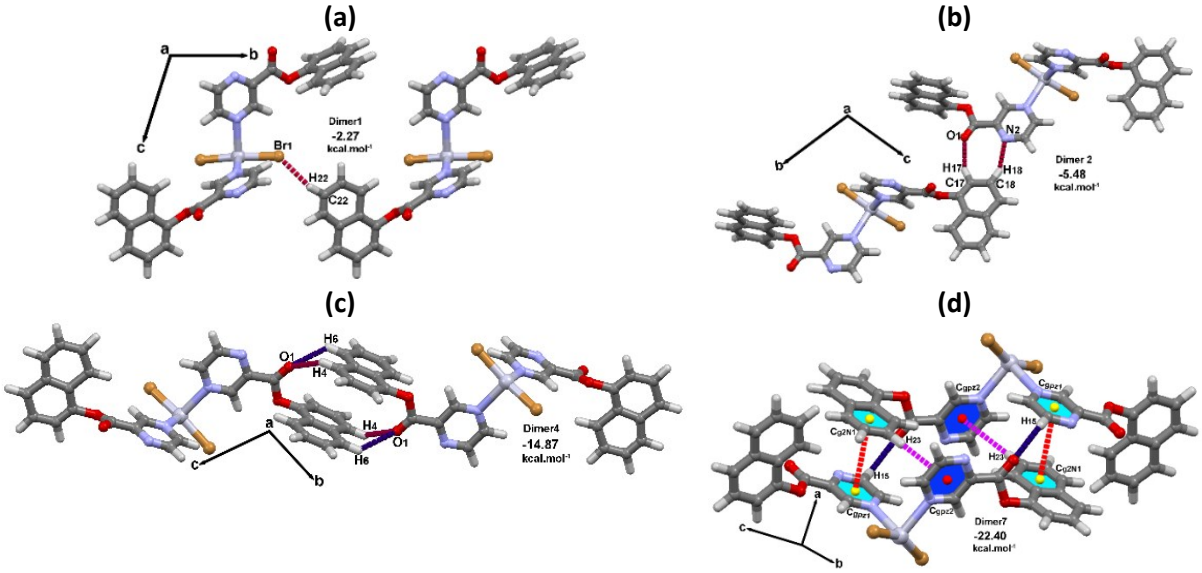
The interconnection among organic parts of these complexes occurred through three interactions of C–H···O, C–H···π and C–H···X. C_4–H_4···O_1 with the energy of -8.58 kcal.mol^{-1} in complex 5 and C_4–H_4···O_1 alongside C_7–H_7···I_1 with the energy of -8.23 kcal.mol^{-1} in complex 6 formed dimer2, (figures S17a, S18a). C_9–H_9···O_{2b} with the energy of -3.13 kcal.mol^{-1} in complex 5 and C_9–H_9···O_{2b} and C_8–H_8···C_{gpy} with the energy of -3.60 kcal.mol^{-1} in complex 6 made dimer4, (figures S17b, S18b). The connection between organic and inorganic parts was formed via two

symmetrical C_{15}–H_{15}···Br_2 interactions (dimer5 with -9.10 kcal.mol^{-1} energy) in the figure S17c. Dimer5 (-6.28 kcal.mol^{-1} energy) for complex 6 which is depicted in figure S18c, is the analogue of dimer5 in complex 5.

S19. Representation of dimer1 (a), dimer2 (b), dimer4 (c), and dimer7 (d) with calculated binding energy for the dimers in complex 7



S20. Representation of dimer1 (a), dimer2 (b), dimer4 (c), and dimer7 (d) with calculated binding energy for the dimers in complex 8

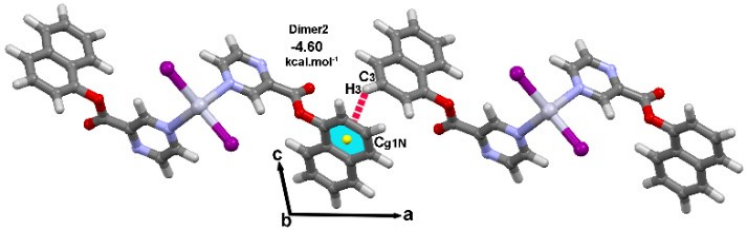


Complexes 7, 8

C_{22}–H_{22}···Cl_1/Br_1 occurred in complexes 7/8 and made dimer1 with -2.49/-2.27 kcal.mol^{-1} energy, (figures S19a, S20a). Bifurcated interactions of oxygen as an acceptor for both of the complexes

are represented in figures S19c and S20c. The bifurcated interactions constituted dimer4 with the energy of -14.57 and -14.78 kcal.mol^{-1}. Since there are not many acceptors in the designed structures, some of the molecules interacted with each other in a bifurcated style. In the dimer7, there were three types of interactions at the plank; 1) $C_{gPz1}\cdots C_{g2N1}$ or π···π; 2) $C_{23}–H_{23}\cdots C_{gPz2}$ or C–H···π; 3) $C_{15}–H_{15}\cdots O_3$, figures S19d and S20d. The interactions produced a tight dimer with the energy of -23.76 and -22.40 kcal.mol^{-1} in order for complexes 7 and 8.

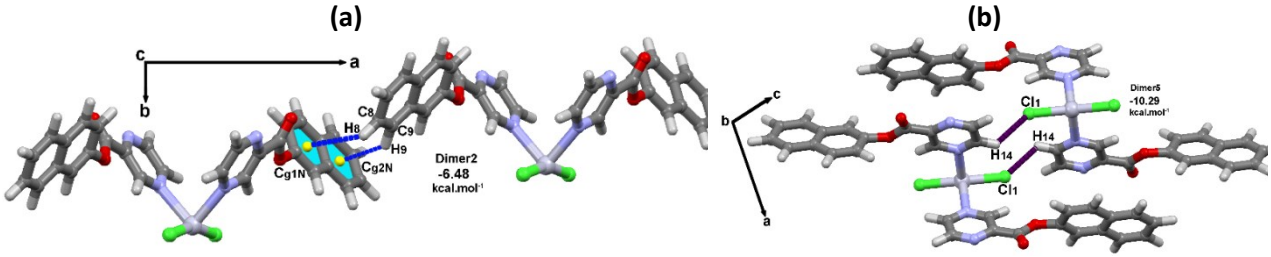
S21. Representation of dimer1 in complex 9 with calculated binding energy



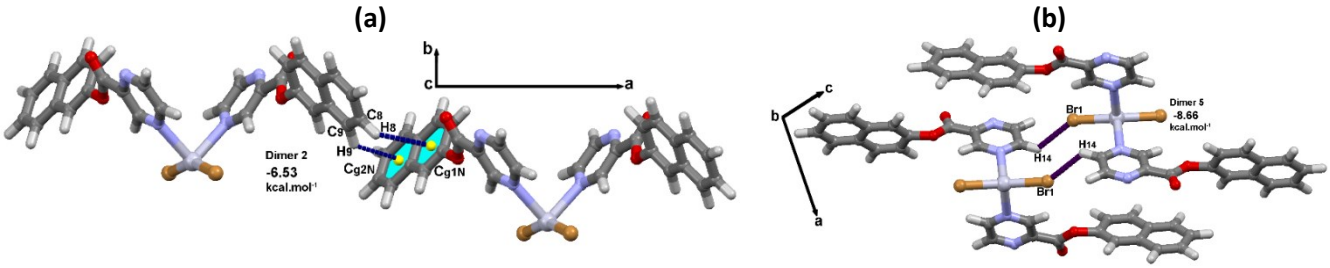
Complex 9

In figure S21, dimer2 was formed for complex 9 by C–H···π interaction between $C_3–H_3$ and C_{gR1N} with -4.60 kcal.mol^{-1} binding energy.

S22. Representation of dimer2 (a) and dimer5 (b) with calculated binding energy for the dimers in complex 10



S23. Representation of dimer2 (a) and dimer5 (b) with calculated binding energy for the dimers in complex 11



Complexes 10, 11

Two C–H···π interactions ($C_9–H_9\cdots C_{g2N}$ and $C_8–H_8\cdots C_{g1N}$) between naphthol rings made dimer2 in diametrical style at ab-plane which is presented in figures S22a and S23a for both of the

complexes 10 and 11. The shaped dimers indicated the energy of -6.48 and -6.53 kcal.mol^{-1} in order for complexes 10 and 11. C_{14}–H_{14}···Cl_1/Br_1 interwove two molecules by 1O/1U (1-Over/ 1-Under) fashion in order to elongate the molecules (via dimer5) through c-axis, figures S22b and S23b. The energy of this dimer for the compounds 10 and 11 was -10.29 and -8.66 kcal.mol^{-1}, respectively.

S24. Dimer binding energy for all of the symmetry operators in complexes 1-11

	Translation (T)	Inversion Center (I)	Screw Axis (S)	Glide Plane (G)	I+S+G
Complex 1	-21.17	-114.6	-	-	-
Complex 2	-1.8	-7.46	-58.31	-10.07	-
Complex 3	-1.24	-7.11	-55.94	-11.31	-
Complex 4	-39.87	-	-	-	-16.59
Complex 5	-12.34	-18.05	-8.58	-	-
Complex 6	-11.32	-10.46	-14.51	-	-
Complex 7	-7.73	-128.69	-	-	-
Complex 8	-7.75	-129.68	-	-	-
Complex 9	-	-	-39.95	-	-8.35
Complex 10	-	-	-44.38	-	-48.47
Complex 11	-	-	-42.85	-	-45.52

S25. References

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S26. Contents of the CSD-Analysis' for the tables S27, S28, 29

The tables are included eight parts from left to right as each part explained below.

I) The number of hits.

II) Ref. Codes for all of the hits.

III) The number of different mercury halide centers which presents in each hit.

IV) Polymerization mode which included three groups. First, the molecules which are formed discrete molecules. Second, the molecules which are expanded through anion or TA (including dimer, trimer, tetramer, pentamer, oligomer, and polymer through anion). Third, the molecules which are expanded through ligand or TL (including dimer, trimer, tetramer, pentamer, oligomer, and polymer through anion). It should be noted that these compounds are included the ligands with more than one donor in their structure and they are mostly acted as a linker between metal centers.

V) Geometry mode which is shown the geometry around metal center and apart from their abundance, it can be classified to 20 modes for mercuric halide (II) in our study as below; Linear, Bent, Trigonal-Planar, Trigonal Pyramid, Tetrahedral, D- Tetrahedral (Seesaw), D-Tetrahedral (Pyramid), Square Planar, Square Pyramid, Trigonal Bipyramid, Pentagonal, T-Shaped, Octahedral, Hexagonal, Pentagonal Pyramid, Trigonal Prismatic, Trigonal Anti-Prismatic, Pentagonal Bipyramid, Hexagonal Bipyramid, and the Distorted (D) forms for any of the mentioned geometries.

VI) Coordination number (C.N.) which is contained C.N. = 2 to C.N. = 8.

VII) Coordination mode of the ligand which is included being chelates, non-chelate, and independent metal halides. In this column metal to metal bond is also assigned as a part of non-chelate complexes with M-M symbol.

VIII) The donor atom of the ligand is represented in this column and for one mercury center it can be contained at most three donor atoms. The represented donors are N, O, S, C, P, Se. In this column metal (in a few cases non-metal) of mentioned M-M is named, as well. X (Cl, Br, and I) as a linked halide into metal center also represented here for independent metal halide cases.

S27. CSD-Analysis for $HgCl_2$ Compounds

Number	Ref. Code	Hits	Polymerization Mode	Geometry	C.N.	Chelation Mode	Donor Atom of Ligand
1	ARIRUQ	1	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor, O-Donor
2	ARISAX	2	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor
		3	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor
3	ASABON	4	Discrete Molecule	T-Shape	5	Chelate	N-Donor
4	ASEDIN	5	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor
5	AVANIW	6	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor
6	AXAWIH	7	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
7	AXAWON	8	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor, O-Donor
8	EREQEZ	9	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
9	EWUDUX	10	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
10	ISOQEO	11	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
11	ISOQIS	12	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
12	ISOQOY	13	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
13	ISOQUE	14	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
14	ISORAL	15	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
15	ISOREP	16	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
16	ISORIT	17	Discrete Molecule	Seesaw	4	Chelate	N-Donor
17	ISOROZ	18	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
18	ISORUF	19	Discrete Molecule	Seesaw	4	Chelate	N-Donor
19	ISOSAM	20	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
20	ISOSEQ	21	Discrete Molecule	Seesaw	4	Chelate	N-Donor
21	ISOSIU	22	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
22	ISOSOA	23	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
23	OJULOW	24	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor
24	OSOGIO	25	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
25	UTENIS	26	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	S-Donor
		27	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine
		28	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
26	UTENOY	29	Dimer Through Anion	D-trigonal Bipyramid	5	Non-Chelate	S-Donor, O-Donor
27	UWOLID	30	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor
28	UXACUT	31	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine
29	ACIWUF	32	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
30	ACIXAM	33	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	N-Donor, O-Donor
31	ACOZOH	34	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
32	ADEJEZ	35	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine
33	ADNCHG10	36	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine
34	ADOJEJ	37	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
35	ADOJIN	38	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
36	ADOJOT	39	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
37	ADOJUZ	40	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
		41	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine
		42	Polymer Through Anion	D-Octahedral	6	Metal Halide Only	Chlorine
38	AGERUA	43	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor

39	**AGOCEG**	44	Tetramer Through Anion	D-Square Pyramid	5	Metal Halide Only	Chlorine	
		45	Tetramer Through Anion	Seesaw	4	Chelate	N-Donor	
40	**AHOJEM**	46	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
41	**AJAJIF**	47	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor	
42	**AKIROB**	48	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
43	**AKIRUH**	49	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		50	Tetramer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
44	**AKIRUH01**	51	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		52	Tetramer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
45	**AKISAO**	53	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
46	**AKISES**	54	Discrete Molecule	D-Octahedral	6	Non-Chelate	C-Donor	O-Donor
47	**AKULIB**	55	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
48	**ALIFOS**	56	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
49	**AMEJUX**	57	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
50	**AMEJUX01**	58	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
51	**AMODAH**	59	Dimer Through Anion	D-Octahedral	6	Chelate	N-Donor	
52	**APEYUR**	60	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	N-Donor	
53	**AQATAN**	61	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
54	**AQAWOG**	62	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		63	Trimer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
55	**AQEFEJ**	64	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
56	**AQEFUZ**	65	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
57	**AQEGIO**	66	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
58	**AQEHAH**	67	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
59	**ARUJEC**	68	Oligomer Through Anion	Trigonal	3	Non-Chelate	P-Donor	
		69	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		70	Oligomer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
60	**ARUJIG**	71	Oligomer Through Anion	Trigonal	3	Non-Chelate	P-Donor	
		72	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		73	Oligomer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
		74	Oligomer Through Anion	Trigonal Pyramid	4	Non-Chelate	P-Donor	
61	**ASOKIC**	75	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-donor	
62	**ASUKII**	76	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
63	**AVISII**	77	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
64	**AWOKAZ**	78	Polymer through ligand	Seesaw	4	Non-Chelate	N-donor	
65	**AXUDON**	79	Tetramer Through Anion	Seesaw	4	Non-Chelate	O-donor	
		80	Tetramer Through Anion	Trigonal	3	Non-Chelate	C-donor	Chlorine
66	**AYIMUR**	81	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-donor	
67	**AZCDHG**	82	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
68	**AZOBIB**	83	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
69	**BABLOH**	84	Oligomer Through Ligand	D-Octahedral	6	Non-Chelate	N-Donor	
		85	Oligomer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
		86	Oligomer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		87	Oligomer Through Ligand	Trigonal	3	Non-Chelate	N-Donor	
		88	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
		89	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
70	**BABLUN**	90	Polymer through ligand	Seesaw	4	Non-Chelate	N-Donor	
71	**BABNAU**	91	Dimer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
		92	Discrete Molecule	Trigonal	3	Non-Chelate	O-Donor	
72	**BABRED**	93	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
73	**BABZUZ**	94	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
74	**BACZUB**	95	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
75	**BAKMEH**	96	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
76	**BAPWAQ**	97	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
77	**BAPWEU**	98	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
78	**BARGUW**	99	Tetramer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
		100	Tetramer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine	
79	**BARYOJ**	101	Polymer Through Anion	Square Planar	4	Non-Chelate	N-Donor	
80	**BASJIP**	102	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
81	**BASJOV**	103	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
82	**BAVKIS**	104	Polymer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
		105	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
83	**BEGREK**	106	Tetramer Through Anion	Seesaw	4	Non-Chelate	Se-Donor	N-Donor

		107	Tetramer Through Anion	Seesaw	4	Non-Chelate	Se-Donor	
84	**BEGZIW**	108	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
85	**BEHLUV**	109	Polymer Through Anion	Trigonal bipyramid	5	Non-Chelate	S-Donor	
86	**BEMTOC**	110	Polymer Through Anion	D-Octahedral	6	Metal Halide Only	Chlorine	
87	**BENGIM**	111	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
88	**BEQNAM**	112	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	
89	**BESNET**	113	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
90	**BETPAR**	114	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
91	**BEVCUC**	115	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
92	**BEVDAJ**	116	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
93	**BEVDEN**	117	Dimer through anion	D-Square Pyramid	5	Chelate	N-Donor	
94	**BEVDIR**	118	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
95	**BEVDOX**	119	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
96	**BIFHOO**	120	Dimer Through Anion	Seesaw	4	Non-Chelate	Iodine	
97	**BIHZEZ**	121	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	O-Donor
98	**BIHZID**	122	Polymer through anion	D-Octahedral	6	Chelate	N-Donor	O-Donor
99	**BIMJAI**	123	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
100	**BITGOA10**	124	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
101	**BITHAN10**	125	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		126	Polymer Through Anion	Octahedral	4	Metal Halide Only	Chlorine	
102	**BITHER10**	127	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
103	**BITHIV10**	128	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		129	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
104	**BITHIV11**	130	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		131	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
105	**BIXCIU**	132	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
106	**BIZVIQ**	133	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
107	**BOCDIG**	134	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
108	**BOCDIG10**	135	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
109	**BOCPOA**	136	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
110	**BOCXIC**	137	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
111	**BOPXIN**	138	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
112	**BOPXIN01**	139	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
113	**BOQTIL**	140	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
114	**BOQTOR**	141	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	Bromine
115	**BOTYEQ**	142	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
116	**BOVNEG**	143	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
117	**BSHGCL**	144	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
118	**BTCHGP**	145	Tetramer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		146	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
119	**BULSOQ**	147	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
120	**BULSOQ01**	148	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
121	**BULZAJ**	149	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
122	**BULZAJ01**	150	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
123	**BULZAJ02**	151	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
124	**BUPSUA**	152	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		153	Dimer Through Anion	D-Octahedral	6	Chelate	N-Donor	
125	**BUPXAL01**	154	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
126	**BURHGC**	155	Discrete Molecule	Square Planar	4	Non-Chelate	O-Donor	
127	**BURVAN**	156	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
128	**BUTYUM**	157	Polymer Through Ligand	D-Square Pyramid	5	Non-Chelate	N-Donor	
		158	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor	
129	**BUVPAL**	159	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
130	**BZACHG**	160	Polymer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
		161	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
131	**BZCRHG**	162	Polymer Through Anion	D-Prism	6	Non-Chelate | M-M	C-Donor	Chromium
		163	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
132	**BZPIHG**	164	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		165	Polymer Through Anion	D-Square Pyramid	5	Metal Halide Only	Chlorine	
133	**CAJPAF**	166	Discrete Molecule	D-Prism	6	Non-Chelate	C-Donor	
134	**CAJPEJ**	167	Discrete Molecule	D-Prism	6	Non-Chelate	C-Donor	
135	**CAJPIN**	168	Discrete Molecule	D-Prism	6	Non-Chelate	C-Donor	
136	**CAJPOT**	169	Discrete Molecule	D-Prism	6	Non-Chelate	C-Donor	

137	**CAJPOT01**	170	Discrete Molecule	D-Prism	6	Non-Chelate		C-Donor	
138	**CAJPUZ**	171	Discrete Molecule	D-Prism	6	Non-Chelate		C-Donor	
139	**CALPAG**	172	Dimer Through Ligand	Seesaw	4	Non-Chelate		O-Donor	
140	**CAVJEO**	173	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
141	**CAVMUH**	174	Discrete Molecule	Seesaw	4	Metal to Metal		Rhodium	
142	**CAYBOT**	175	Discrete Molecule	Seesaw	4	Chelate		P-Donor	
143	**CAYLOD**	176	Dimer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
144	**CECSIN**	177	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
145	**CEDYOB**	178	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate		N-Donor	
146	**CEFLEG**	179	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate		N-Donor	
147	**CEFLOQ**	180	Dimer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
148	**CEGMOQ**	181	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		182	Polymer Through Anion	Octahedral	6	Metal Halide Only		Chlorine	
149	**CEGMUW**	183	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
150	**CEGMUW01**	184	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
151	**CEGMUW02**	185	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
152	**CEGMUW03**	186	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
153	**CEGNAD**	187	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine	
		188	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
154	**CEJXEV**	189	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
155	**CEKHUX**	190	Discrete Molecule	Square Planar	4	Non-Chelate		N-Donor	
156	**CEKJOT**	191	Discrete Molecule	Square Planar	4	Non-Chelate		N-Donor	
		192	Discrete Molecule	Square Pyramid	5	Non-Chelate		O-Donor	
157	**CENWEX**	193	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
158	**CERWIG**	194	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	
159	**CESLAN**	195	Discrete Molecule	Seesaw	4	Non-Chelate	M-M	N-Donor	Iron
160	**CESZOP**	196	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor	
161	**CETCHG01**	197	Polymer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate		S-Donor	
		198	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	
162	**CETYAC**	199	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
163	**CHEXHG**	200	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
164	**CHGIRP**	201	Discrete Molecule	Linear	2	Metal to Metal		Iridium	
165	**CHGMPP**	202	Dimer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		203	Dimer Through Anion	Square Planar	4	Non-Chelate		P-Donor	
166	**CICZAQ**	204	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
167	**CIDFAW**	205	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	
		206	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	
168	**CIDFAW02**	207	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	
		208	Polymer Through Anion	seesaw	4	Non-Chelate		S-Donor	
169	**CIDLOS**	209	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
170	**CIDMEJ**	210	Dimer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
171	**CIDMUZ**	211	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
172	**CIDZUL**	212	Dimer Through Anion	Trigonal	3	Non-Chelate		C-Donor	
173	**CINVOL**	213	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
174	**CITBUD**	214	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
175	**CITNAW**	215	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
176	**CIZNOO**	216	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
177	**CLBHGC**	217	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
178	**CLGUHG**	218	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
179	**CLNCHG**	219	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
180	**CLTCHG10**	220	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
181	**CLTEHG**	221	Discrete Molecule	Seesaw	4	Non-Chelate		P-Donor	
182	**CMCPHG10**	222	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
183	**CMPRTM**	223	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
184	**CMSMOM**	224	Tetramer Through Anion	D-Prism	6	Non-Chelate	M-M	C-Donor	Molybdenum
		225	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
185	**CNONHG**	226	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate		O-Donor	
		227	Polymer Through Anion	Square Planar	4	Non-Chelate		O-Donor	
186	**COCBUR**	228	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
187	**COCGAC**	229	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor	
188	**COCNOY**	230	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
189	**CODYOJ01**	231	Dimer Through Ligand	Seesaw	4	Non-Chelate		O-Donor	N-Donor

190	**COEZIH**	232	Dimer Through Ligand	Seesaw	4	Chelate	M-M	N-Donor	Iridium
191	**COLYOS**	233	Discrete Molecule	Seesaw	4	Metal Halide Only		Chlorine	
192	**CONZEL**	234	Discrete Molecule	Seesaw	4	Non-Chelate		P-Donor	
193	**CORKUQ**	235	Discrete Molecule	Seesaw	4	Metal Halide Only		Chlorine	
194	**COYRAK**	236	Discrete Molecule	T-Shape	5	Chelate		N-Donor	O-Donor
195	**COYWIX**	237	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
196	**COZMAF**	238	Discrete Molecule	D-Square Planar	4	Non-Chelate	M-M	C-Donor	Iron
197	**COZMAF10**	239	Discrete Molecule	D-Square Planar	4	Non-Chelate	M-M	C-Donor	Iron
198	**CPCOHG10**	240	Dimer Through Anion	Square Pyramid	4	Metal to Metal		Cobalt	
199	**CPCOMC**	241	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		242	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		O-Donor	C-Donor
		243	Polymer Through Anion	Trigonal	3	Metal Halide Only		Chlorine	
		244	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
200	**CPEAHG**	245	Discrete Molecule	Seesaw	4	Chelate		P-Donor	N-Donor
201	**CTSCHG**	246	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
202	**CUFCEL10**	247	Oligomer Through Anion	Trigonal	3	Non-Chelate		C-Donor	
203	**CUHMUP**	248	Discrete Molecule	Seesaw	4	Chelate	M-M	S-Donor	Tellurium
204	**CUMGEW**	249	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
205	**CUMGIA**	250	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
206	**CUPXUH**	251	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		252	Polymer Through Anion	Trigonal	3	Metal Halide Only		Chlorine	
		253	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine	
207	**CURJAC**	254	Discrete Molecule	Seesaw	4	Metal to Metal		Palladium	
208	**CUSBEY**	255	Trimer Through Anion	Square Planar	4	Metal Halide Only		Chlorine	
		256	Trimer Through Anion	T-Shape	5	Chelate		N-Donor	
209	**CUSRAK**	257	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
210	**CUSSEP**	258	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
211	**CUTDIE**	259	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
212	**CUTMAG**	260	Polymer Through Ligand	D-Trigonal Bipyramid	5	Chelate		O-Donor	N-Donor
213	**CUYDUW**	261	Discrete Molecule	Square Planar	4	Non-Chelate		O-Donor	
214	**CUYHAG**	262	Discrete Molecule	Trigonal Pyramid	4	Non-Chelate		S-Donor	
215	**DABPEB**	263	Tetramer Through Anion	Seesaw	4	Non-Chelate		P-Donor	
216	**DAGBIX**	264	Discrete molecule	Seesaw	4	Chelate		N-Donor	
217	**DAGHIC**	265	Polymer Through Anion	D-Octahedral	6	Chelate		N-Donor	
		266	Polymer Through Anion	Linear	2	Metal Halide Only		Chlorine	
		267	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
218	**DAVYUU10**	268	Polymer Through Anion	Octahedral	6	Metal Halide Only		Chlorine	
219	**DAXNOH**	269	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
		270	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
220	**DAXPOJ**	271	Polymer Through Anion	Square Pyramid	5	Non-Chelate		S-Donor	
		272	Polymer Through Ligand	Square Pyramid	5	Non-Chelate		S-Donor	
221	**DAYBAH**	273	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
222	**DAYJUK**	274	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
223	**DEBWAJ**	275	Dimer Through Ligand	T-Shape	5	Non-Chelate		O-Donor	
224	**DEBWEN**	276	Discrete Molecule	T-Shape	6	Non-Chelate		O-Donor	
225	**DEKYIB**	277	Discrete Molecule	Trigonal	3	Non-Chelate		O-Donor	
226	**DEPHIQ**	278	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
227	**DEPVOK**	279	Polymer Through Anion	Seesaw	4	Non-Chelate		C-Donor	
228	**DEXJOH**	280	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
229	**DEYMUP**	281	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
230	**DHURHG**	282	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
231	**DICMAE**	283	Dimer Through Anion	Square Pyramid	5	Non-Chelate		S-Donor	
232	**DIFPEN**	284	Discrete Molecule	D-Square Pyramid	5	Chelate		S-Donor	O-Donor
233	**DIQPUQ**	285	Polymer Through Anion	Seesaw	4	Metal Halide Only		Bromine	
234	**DIQQAX**	286	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
235	**DIVJAT**	287	Discrete Molecule	Seesaw	4	Metal to Metal		Tellurium	
236	**DIXNUU**	288	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
237	**DIXPAD**	289	Discrete Molecule	T-Shape	5	Chelate		N-Donor	O-Donor
238	**DIXPIL**	290	Polymer Through Anion	Square Pyramid	5	Chelate		N-Donor	
239	**DIZSIP**	291	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor	
240	**DMSOMC**	292	Dimer Through Ligand	Seesaw	4	Non-Chelate		O-Donor	
		293	Polymer Through Anion	T-Shape	3	Metal Halide Only		Chlorine	
241	**DOBCAZ**	294	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	

		295	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
		296	Polymer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
242	**DOBCIH**	297	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		298	Polymer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
243	**DOBDOO**	299	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		300	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
244	**DOPJAT**	301	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
245	**DORSEI**	302	Polymer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
		303	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
246	**DORSIM**	304	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
247	**DOTLIH**	305	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
248	**DPSOHG**	306	Discrete Molecule	Trigonal	3	Non-Chelate	O-Donor	
249	**DTIZHG01**	307	Discrete Molecule	Trigonal	3	Non-Chelate	S-Donor	
250	**DTIZHG10**	308	Polymer Through Anion	Bent	4	Non-Chelate	S-Donor	
251	**DUCVAY10**	309	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
252	**DUFQIE**	310	Dimer Through Anion	Seesaw	4	Chelate	S-Donor	
253	**DUFREB**	311	Dimer Through Anion	Seesaw	4	Chelate	S-Donor	
254	**DUFSUS**	312	Dimer Through Anion	Seesaw	4	Chelate	S-Donor	
255	**DUHPUS**	313	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
256	**DUKDIY**	314	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
257	**DUKHAU**	315	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
258	**DUKLOL**	316	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor	
259	**DUKLOL01**	317	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor	
260	**DULQIL**	318	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
261	**DURNUA**	319	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
262	**DURWIX**	320	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
263	**DUSFAA**	321	Dimer Through Ligand	Trigonal	3	Non-Chelate	O-Donor	
264	**DUTDEB**	322	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
265	**DUTDIF**	323	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
266	**DUWMIR**	324	Discrete Molecule	Seesaw	4	Chelate	P-Donor	
267	**DUWXAV**	325	Discrete Molecule	Pentagonal Bipyramid	7	Chelate	O-Donor	
		326	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
268	**EAMCHG**	327	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
269	**EBAROP**	328	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
270	**EBARUV**	329	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
271	**EBASAC**	330	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
272	**EBASEG**	331	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
273	**EBASIK**	332	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
274	**EBASOQ**	333	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
		334	Discrete Molecule	Linear	2	Non-Chelate	C-Donor	
275	**EBATAD**	335	Polymer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
276	**EBATEH**	336	Polymer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
277	**ECAWAI**	337	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor	
278	**EFASIN**	338	Discrete Molecule	Seesaw	4	Chelate	O-Donor	
279	**EFOYEF**	339	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
280	**EFUKEX**	340	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
281	**EHIVUN**	341	Discrete Molecule	Square Pyramid	5	Chelate	N-Donor	
282	**EHIWAU**	342	Polymer Through Ligand	T-Shape	5	Chelate	N-Donor	O-Donor
283	**EHUJEX**	343	Dimer Through Anion	Square Pyramid	5	Chelate	N-Donor	
284	**EHXGMC**	344	Discrete Molecule	T-Shape	6	Chelate	O-Donor	
285	**EJOPEZ**	345	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor	
286	**EJOXUY**	346	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
287	**EKAPOX**	347	Discrete Molecule	T-Shape	6	Non-Chelate	N-Donor	O-Donor
288	**ELEXOK**	348	Trimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	N-Donor
		349	Trimer Through Anion	D-Square Planar	4	Non-Chelate	S-Donor	
289	**EMIGAK**	350	Dimer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
290	**EMIPAT**	351	Dimer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
291	**EMOPUT**	352	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
292	**EMSCHG**	353	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
293	**EMUDUN**	354	Discrete molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
294	**ENOREF**	355	Discrete Molecule	Seesaw	4	Chelate	O-Donor	
295	**EQUHUT**	356	Discrete Molecule	T-Shape	5	Chelate	O-Donor	

296	**EQUWUJ**	357	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor	
297	**ERIBAI**	358	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	N-Donor
298	**ETANUI**	359	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
299	**ETAPAQ**	360	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
300	**ETOVEP**	361	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
301	**ETPHGC10**	362	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
302	**ETUMOW**	363	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	O-Donor
		364	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor	O-Donor
303	**ETURHG**	365	Discrete Molecule	Square Planar	4	Non-Chelate		O-Donor	
304	**EWIPIK**	366	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
305	**EWOQUC**	367	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
306	**EWORIR**	368	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	
		369	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
307	**EWORIR01**	370	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	
		371	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
308	**EXUYAY**	372	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
309	**EZIWUG**	373	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
		374	Discrete Molecule	Trigonal Pyramid	3	Metal Halide Only		Chlorine	
310	**FADFAR**	375	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		Se-Donor	
311	**FADWEN**	376	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
312	**FADWIR**	377	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor	
313	**FAHVEP**	378	Discrete Molecule	Square Pyramid	5	Metal Halide Only		Chlorine	
314	**FAHWIW**	379	Discrete Molecule	Seesaw	4	Metal to Metal		Ruthenium	
315	**FAJNUZ**	380	Polymer Through Ligand	Seesaw	4	Non-Chelate		S-Donor	
316	**FAJPAH**	381	Polymer Through Ligand	Seesaw	4	Non-Chelate		S-Donor	
317	**FAJPEL**	382	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
318	**FAJPIP**	383	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
319	**FAQVEY**	384	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
320	**FAQVEY01**	385	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
321	**FATREY**	386	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
		387	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
322	**FATSEY**	388	Discrete Molecule	Seesaw	4	Metal to Metal		Ruthenium	
323	**FAXGIW**	389	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
324	**FAXHET**	390	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
325	**FAXHIX**	391	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
326	**FECHEC**	392	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
327	**FEGDIF**	393	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
328	**FEGLAE**	394	Oligomer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		395	Oligomer Through Anion	Square Planar	4	Metal Halide Only		Chlorine	
		396	Oligomer Through Anion	Trigonal	3	Non-Chelate		O-Donor	
		397	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
329	**FEHDUS**	398	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
330	**FEJBIH**	399	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel
331	**FEJBUT**	400	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel
332	**FEJCAA**	401	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel
333	**FELMIU**	402	Polymer Through Ligand	D-Trigonal Bipyramid	5	Chelate		N-Donor	
334	**FEMSUL10**	403	Oligomer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine	
		404	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
335	**FEMTAS10**	405	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		406	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
336	**FEYCIW**	407	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
337	**FEYDAP**	408	Polymer Through Ligand	Trigonal Bipyramid	5	Chelate		N-Donor	S-Donor
		409	Polymer Through Anion	Trigonal Bipyramid	5	Chelate		N-Donor	S-Donor
338	**FIPMIC**	410	Discrete Molecule	D-Octahedral	6	Chelate		O-Donor	N-Donor
339	**FISBEO**	411	Tetramer Through Anion	Trigonal Pyramid	4	Metal Halide Only		Chlorine	
		412	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
		413	Tetramer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
340	**FISBOY**	414	Polymer Through Anion	Octahedral	6	Metal Halide Only		Chlorine	
		415	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
		416	Polymer Through Anion	Bent	2	Metal Halide Only		Chlorine	
341	**FISBUE**	417	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
		418	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
342	**FISCAL**	419	Polymer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine	

		420	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
343	**FISLEY**	421	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
344	**FOCLEO**	422	Discrete Molecule	Linear	2	Non-Chelate	C-Donor	
		423	Trimer Through Anion	Linear	2	Non-Chelate	C-Donor	
		424	Trimer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
		425	Trimer Through Anion	Tetrahedral	4	Non-Chelate	C-Donor	
345	**FOCLIS**	426	Dimer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
		427	Dimer Through Anion	Trigonal Pyramid	4	Non-Chelate	C-Donor	
346	**FOCLOY**	428	Discrete Molecule	Linear	2	Non-Chelate	C-Donor	
		429	Trimer Through Anion	Linear	2	Non-Chelate	C-Donor	
		430	Trimer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
		431	Trimer Through Anion	Tetrahedral	4	Non-Chelate	C-Donor	
347	**FOGZUX**	432	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor	
348	**FOJZEJ**	433	Discrete Molecule	T-Shape	5	Chelate	S-Donor	N-Donor
349	**FOTMIM**	434	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
350	**FOVFEB10**	435	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
351	**FOWBID**	436	Dimer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
352	**FOWCOL**	437	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	N-Donor
353	**FOZHAE**	438	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
354	**FOZHIM**	439	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
355	**FOZXAV**	440	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
		441	Dimer Through Anion	Seesaw	4	Metal Halide Only	Iodine	
356	**FTFHGC10**	442	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		443	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
357	**FULBOD**	444	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor	
358	**FUYWON**	445	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
359	**GADVEO**	446	Dimer Through Anion	Trigonal Bipyramid	5	Chelate	N-Donor	Fluorine
		447	Dimer Through Ligand	Trigonal Bipyramid	5	Chelate	N-Donor	Fluorine
360	**GAFSAJ**	448	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
361	**GAJGAA**	449	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
362	**GAJGEE**	450	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor	
363	**GANRIY**	451	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
364	**GAVBOV**	452	Dimer Through Ligand	T-Shape	5	Chelate	N-Donor	
365	**GEFTEQ10**	453	Dimer through anion	D-Tetrahedral (Py)	4	Metal to Metal	Ruthenium	
366	**GEFTIU10**	454	Dimer Through Anion	D-Tetrahedral (Py)	4	Metal to Metal	Ruthenium	
367	**GEHNUD**	455	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
368	**GEKTIB**	456	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
369	**GELKIR**	457	Polymer Through Anion	Pentagonal Bipyramid	4	Chelate	N-Donor	
		458	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
370	**GEQXIK**	459	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
371	**GEQXUW**	460	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
372	**GEVJOG**	461	Dimer Through Anion	Seesaw	4	Chelate	P-Donor	
373	**GIFYUP**	462	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
374	**GIWZOB**	463	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	N-Donor	O-Donor
375	**GOKFAN**	464	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
376	**GOKPIG**	465	Pentamer Through Anion	Seesaw	4	Metal to Metal	Tellurium	
377	**GOKVIL**	466	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
378	**GOZROC**	467	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		468	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
379	**GOZRUI**	469	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
380	**GUBFIS**	470	Dimer Through Anion	Seesaw	5	Chelate	O-Donor	
		471	Discrete Molecule	Seesaw	5	Chelate	N-Donor	
381	**GUGZAJ**	472	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
382	**GURKOU**	473	Discrete Molecule	Square Planar	4	Non-Chelate	N-Donor	
383	**GUTLEN**	474	Dimer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
		475	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
384	**HARRAV**	476	Dimer Through Anion	Trigonal Bipyramid	5	Non-Chelate	O-Donor	
		477	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
		478	Discrete Molecule	Trigonal	3	Non-Chelate	N-Donor	
385	**HARREZ**	479	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
386	**HATQUQ**	480	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
387	**HATRAX**	481	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	

388	**HAVCEO**	482	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	O-Donor
389	**HECQEM**	483	Discrete Molecule	T-Shape	5	Non-Chelate	S-Donor	N-Donor
390	**HEDMOS**	484	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
391	**HEHDAB**	485	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
392	**HETYAH**	486	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	S-Donor
393	**HEYDEV**	487	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
394	**HEYVAJ**	488	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		489	Dimer Through Anion	D-Tetrahedral (Py)	4	Metal Halide Only	O-Donor	
395	**HGCBPO10**	490	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
396	**HGCETS**	491	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		492	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
397	**HGCLTU**	493	Polymer Through Anion	Seesaw	4	Non-Chelate	S-donor	
		494	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
398	**HGCPAO**	495	Dimer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
399	**HGCPHO10**	496	Discrete Molecule	Square Planar	4	Non-Chelate	S-Donor	
400	**HGCSCD10**	497	Polymer Through Ligand	Trigonal	3	Metal Halide Only	Chlorine	
		498	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
401	**HGCTHS**	499	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
402	**HGCTHS01**	500	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
403	**HGCTOX**	501	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
404	**HGPARO**	502	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	
405	**HGTPSE**	503	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor	
406	**HGTRIT**	504	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-donor	
407	**HIGQUL**	505	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
408	**HIRWEK**	506	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
409	**HIRWIO**	507	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
410	**HISHGC**	508	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	
411	**HIVREJ**	509	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		510	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
412	**HIVVAL**	511	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
413	**HIXMUY**	512	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
414	**HOCMAN**	513	Discrete Molecule	Seesaw	4	Chelate	N-Donor	S-Donor
415	**HODBUX**	514	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	
		515	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	
416	**HOTBID**	516	Polymer Through Ligand	D-Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
417	**HOXBEB**	517	Oligomer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
418	**HOXBIF**	518	Oligomer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
419	**HOXCEC**	519	Oligomer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
420	**HOXZUP**	520	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	N-Donor
		521	Tetramer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	N-Donor
421	**HUBCUD**	522	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
422	**HUBDAK**	523	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
423	**HUBDEO**	524	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
424	**HUBDIS**	525	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
425	**HUBDOY**	526	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
426	**HUBDUE**	527	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
427	**HUKTAJ**	528	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
428	**HUKTEN**	529	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
429	**HULKUW**	530	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
430	**HUPKEK**	531	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
431	**IBAFEY**	532	Discrete Molecule	Trigonal	3	Non-Chelate	C-Donor	
432	**IBAFIC**	533	Discrete Molecule	Trigonal	3	Non-Chelate	C-Donor	
433	**IBIRIV**	534	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
434	**IBUWEJ**	535	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	O-Donor
435	**ICUWIM**	536	Discrete Molecule	Trigonal	3	Non-Chelate	O-Donor	
436	**IDEFOO**	537	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
437	**IGEFIJ**	538	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		539	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
438	**IGEMOX**	540	Polymer through ligand	Square Pyramid	5	Non-Chelate	N-Donor	
439	**IGOPOJ**	541	Tetramer Through Ligand	Square Pyramid	5	Non-Chelate	O-Donor	
		542	Tetramer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
440	**IGUQUX**	543	Polymer Through Ligand	Seesaw	5	Non-Chelate	N-Donor	

441	**IJEKIS**	544	Polymer Through Anion	Tetrahedral	5	Metal Halide Only	Chlorine	
442	**IJEKOY**	545	Dimer Through Anion	Tetrahedral	5	Metal Halide Only	Chlorine	
443	**IJIRAV**	546	Polymer Through Anion	Tetrahedral	5	Metal Halide Only	Chlorine	
444	**IJIREZ**	547	Dimer Through Anion	Tetrahedral	5	Metal Halide Only	Chlorine	
445	**IJIRID**	548	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
446	**IJIROJ**	549	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
447	**IJIRUP**	550	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
448	**IMATAS**	551	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
449	**INIYAF**	552	Tetramer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor	O-Donor
		553	Tetramer Through Anion	D-Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
450	**IPADUY**	554	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	O-Donor
451	**IPAFAG**	555	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		556	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
452	**IPILID**	557	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
453	**IPOTUD**	558	Polymer Through Anion	Square Planar	4	Non-Chelate	P-Donor	
		559	Polymer Through Anion	Square Pyramid	4	Metal Halide Only	Chlorine	
		560	Polymer Through Anion	Seesaw	5	Metal Halide Only	Chlorine	
454	**IQIHUM**	561	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
455	**IREMEZ**	562	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
456	**IRETOP**	563	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
457	**IRIZOA**	564	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
		565	Trimer Through Anion	Trigonal Pyramid	3	Non-Chelate	N-Donor	
458	**IRUTUK**	566	Discrete Molecule	Seesaw	4	Non-Chelate	Bromine	
459	**ISADEM**	567	Polymer Through Ligand	D-Square Planar	4	Non-Chelate	O-Donor	
460	**ISATOM**	568	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
461	**ISETUW**	569	Discrete Molecule	Square Planar	4	Metal Halide Only	Chlorine	
		570	Trimer Through Anion	Linear	2	Non-Chelate	C-Donor	
462	**ISEVOS**	571	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
463	**JADDEX**	572	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
464	**JADPAF**	573	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		574	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
465	**JADSIT**	575	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
466	**JADTEQ**	576	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
467	**JAGMOU**	577	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
468	**JAGMUA**	578	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
469	**JAHCEA**	579	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	O-Donor	
470	**JAJTEU**	580	Discrete molecule	Seesaw	4	Non-Chelate	S-Donor	
471	**JAMDAC**	581	Discrete molecule	Seesaw	4	Chelate	O-Donor	
472	**JAMJIR**	582	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
473	**JAMJOX**	583	Polymer Through Anion	D-Prism	6	Chelate	N-Donor	
474	**JANDUY**	584	Dimer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
475	**JANFEK**	585	Dimer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
476	**JAPJAM**	586	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
477	**JAPJAM01**	587	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
478	**JAPJUG**	588	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
479	**JATTAZ**	589	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
480	**JATTED**	590	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
481	**JATTIH**	591	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
482	**JATVAB**	592	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		593	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
483	**JENGAK**	594	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
484	**JEPTII**	595	Polymer Through Anion	D-Square Pyramid	5	Metal Halide Only	Chlorine	
		596	Polymer Through Anion	D-Octahedral	6	Non-Chelate	S-Donor	
485	**JEXMOO**	597	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
486	**JIQYAK**	598	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
487	**JIZWEU**	599	Tetramer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
488	**JOGJOE**	600	Discrete Molecule	Trigonal	3	Metal Halide Only	Chlorine	
		601	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		602	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
489	**JOTXIZ**	603	Trimer Through Anion	T-Shape	3	Metal Halide Only	Chlorine	
		604	Trimer Through Ligand	T-Shape	5	Non-Chelate	O-Donor	
490	**JOTXOF**	605	Polymer Through Ligand	Square Planar	4	Non-Chelate	O-Donor	

		606	Polymer Through Ligand	T-Shape	5	Non-Chelate		O-Donor	
491	**JOTXUL**	607	Dimer Through Anion	D-Square Pyramid	5	Non-Chelate		O-Donor	
492	**JOWLEO**	608	Dimer Through Anion	Seesaw	4	Non-Chelate		Se-Donor	P-Donor
493	**JUHYAM**	609	Polymer Through Anion	D-Pentagonal Bipyramid	7	Non-Chelate		O-Donor	N-Donor
		610	Polymer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine	
		611	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine	
494	**JUHYIU**	612	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor	N-Donor
495	**JUHYOA**	613	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor	N-Donor
496	**JUMRIU**	614	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
		615	Polymer Through Anion	Square Planar	4	Metal Halide Only		Chlorine	
497	**JURHUB**	616	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
498	**KABRUC**	617	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor	
499	**KACBUL**	618	Polymer Through Anion	D-Octahedral	6	Chelate		O-Donor	S-Donor
500	**KAMTAT**	619	Dimer Through Anion	D-Tetrahedral (Py)	4	Metal to Metal		Ruthenium	
501	**KAPCUB**	620	Polymer Through Anion	Trigonal Pyramid	4	Non-Chelate		N-Donor	
502	**KASTED**	621	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
503	**KATGET**	622	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
504	**KATGIX**	623	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
505	**KATGOD**	624	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
506	**KATGUJ**	625	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
507	**KEJWAX**	626	Discrete Molecule	Seesaw	4	Chelate		S-Donor	
508	**KEQKEY**	627	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
509	**KEYZUK**	628	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
510	**KEZBAT**	629	Polymer Through Anion	Seesaw	4	Non-Chelate		O-Donor	
		630	Polymer Through Anion	Square Pyramid	5	Non-Chelate		O-Donor	
		631	Polymer Through Anion	Seesaw	4	Non-Chelate		O-Donor	
511	**KEZBEX**	632	Discrete Molecule	Trigonal Pyramid	4	Non-Chelate		N-Donor	
512	**KEZBIB**	633	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
513	**KEZYOF**	634	Discrete Molecule	T-Shape	6	Chelate		O-Donor	
514	**KIBFOR**	635	Polymer Through Ligand	Square Planar	4	Non-Chelate		N-Donor	
515	**KIBVEW**	636	Discrete Molecule	Trigonal Pyramid	4	Non-Chelate		N-Donor	
516	**KICMOA**	637	Polymer Through Anion	Square Pyramid	5	Chelate		N-donor	
517	**KICYOM**	638	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	
518	**KIMXEL**	639	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
		640	Polymer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
519	**KIPTUY**	641	Dimer Through Anion	Seesaw	4	Metal to Metal		Ruthenium	
520	**KIYBIE**	642	Dimer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	
521	**KOPRUC**	643	Discrete Molecule	Seesaw	4	Chelate		S-Donor	
522	**KOWPUH**	644	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-Donor	
523	**KOXRAS**	645	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
524	**KOZREY**	646	Tetramer Through Anion	Trigonal	3	Metal Halide Only		Chlorine	
		647	Tetramer Through Anion	Trigonal Bipyramid	5	Chelate		N-Donor	
525	**KOZRIC**	648	Dimer Through Ligand	Tetrahedral	4	Chelate		N-Donor	
526	**KUCWAI**	649	Polymer Through Anion	T-Shape	6	Non-Chelate		N-Donor	
		650	Polymer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine	
		651	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
527	**KUCWUC**	652	Discrete Molecule	T-Shape	6	Non-Chelate		N-Donor	
528	**KUJVOB**	653	Discrete molecule	T-Shape	5	Chelate		S-Donor	N-Donor
529	**KUJVUI**	654	Dimer Through Anion	Square Pyramid	5	Chelate		N-Donor	
		655	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
530	**KUJWOD**	656	Polymer Through Anion	D-Trigonal Bipyramid	5	Chelate		N-Donor	
		657	Polymer Through Ligand	Square Pyramid	5	Metal Halide Only		Chlorine	
531	**KUKNAF**	658	Dimer Through Anion	Trigonal	3	Metal to Metal		Iridium	
		659	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
532	**KUSMAM**	660	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
533	**LACCUP**	661	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
534	**LACTEQ**	662	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
535	**LACTEQ01**	663	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
536	**LACVAO**	664	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	O-Donor
537	**LAHDOO**	665	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	M-M	S-Donor	Nickel
538	**LAHFOQ**	666	Tetramer Through Ligand	D-Prism	6	Non-Chelate	M-M	S-Donor	Nickel
		667	Tetramer Through Anion	D-Prism	6	Non-Chelate	M-M	S-Donor	Nickel

539	**LAMLAO**	668	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
540	**LANDIP**	669	Polymer Through Anion	Seesaw	4	Metal Halide Only	O-Donor	
541	**LAPKUI**	670	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
542	**LARLAT**	671	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
543	**LATXOV**	672	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
544	**LAYWIR**	673	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
545	**LEBVAQ**	674	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
546	**LEHMAO**	675	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
547	**LEKSEB**	676	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	
548	**LEKSEB01**	677	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
		678	Dimer Through Anion	T-Shape	5	Chelate	N-Donor	
549	**LEKSOL**	679	Dimer Through Anion	Square Pyramid	5	Chelate	N-Donor	
550	**LEKSUR**	680	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	
551	**LEMPIC**	681	Polymer Through Anion	D-Octahedral	6	Non-Chelate	S-Donor	N-Donor
552	**LEQLEA**	682	Dimer Through Anion	Seesaw	4	Metal Halide Only	Iodine	
553	**LEQRIJ**	683	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
554	**LEQROP**	684	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
		685	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
555	**LERFIZ**	686	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		687	Polymer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
556	**LERSUY**	688	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
557	**LEXBIA**	689	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
558	**LEZDOJ**	690	Dimer Through Ligand	T-Shape	6	Chelate	N-Donor	O-Donor
559	**LIDKIS**	691	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
		692	Discrete Molecule	Trigonal	3	chelate	N-Donor	
560	**LILWEI**	693	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
561	**LINXUD**	694	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
562	**LITREL**	695	Discrete Molecule	Square Pyramid	5	Metal Halide Only	Chlorine	
563	**LITRIP**	696	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
564	**LITRUB**	697	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		698	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
565	**LITSAI**	699	Trimer Through Anion	Trigonal Bipyramid	5	Non-Chelate	O-Donor	
		700	Trimer Through Anion	Trigonal Bipyramid	4	Metal Halide Only	Chlorine	
		701	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		702	Dimer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
566	**LITSEM**	703	Tetramer Through Anion	T-Shape	5	Non-Chelate	O-Donor	
		704	Tetramer Through Anion	D-Octahedral	6	Non-Chelate	O-Donor	
		705	Discrete Molecule	Trigonal	3	Metal Halide Only	Chlorine	
		706	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		707	Discrete Molecule	T-Shape	5	Non-Chelate	O-Donor	
567	**LITSOW**	708	Dimer Through anion	D-Tetrahedral (Py)	4	Metal Halide Only	Iodine	
568	**LIVCEY**	709	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	O-Donor
569	**LIYLAG**	710	Discrete Molecule	T-Shape	6	Non-Chelate	S-Donor	O-Donor
570	**LOFFIV**	711	Tetramer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		712	Tetramer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
571	**LOFFOB**	713	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
572	**LOFFUH**	714	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
573	**LOVKAI**	715	Discrete Molecule	D-Prism	4	Non-Chelate	C-Donor	
574	**LOWGIP**	716	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
575	**LOWJUE**	717	Polymer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
		718	Polymer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine	
		719	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
576	**LOWKEP**	720	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
577	**LOWKIT**	721	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
		722	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
578	**LOYBEG**	723	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
579	**LUHDID**	724	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
580	**LUJNIP**	725	Discrete Molecule	T-Shape	5	Non-Chelate | M-M	O-Donor	Nickel
581	**LUKYAS**	726	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
		727	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		728	Polymer Through Anion	T-Shape	3	Metal Halide Only	Chlorine	
582	**MARRAY**	729	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	

583	**MCOLID**	730	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
584	**MCYTHG**	731	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	O-Donor
585	**MEFYEC**	732	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
586	**MEPHGC10**	733	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
		734	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
587	**MEPYHG**	735	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
588	**MESFLV03**	736	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
589	**MESFLV10**	737	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
590	**METHGD**	738	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
		739	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	S-Donor	
591	**MIDZEF**	740	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		741	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
592	**MIHBAH**	742	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
593	**MIHBIP**	743	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
594	**MIHBOV**	744	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
595	**MIMJAT**	745	Dimer Through Anion	Square Pyramid	4	Non-Chelate	C-Donor	N-Donor
		746	Discrete Molecule	Trigonal	3	Non-Chelate	N-Donor	
596	**MIWJEI**	747	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
597	**MIZYOL**	748	Tetramer Through Ligand	Seesaw	4	Non-Chelate M-M	O-Donor	Tellurium
598	**MIZYUR**	749	Tetramer Through Ligand	Trigonal Pyramid	4	Non-Chelate M-M	O-Donor	Tellurium
		750	Tetramer Through Anion	Pentagonal Pyramid	6	Metal to Metal	Tellurium	
599	**MOFXIP**	751	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
600	**MOKTAI**	752	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
601	**MOWFOU**	753	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
602	**MPHGCL10**	754	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
603	**MTEGMC**	755	Discrete Molecule	D-Pentagonal Bipyramid	7	Non-Chelate	O-Donor	
604	**MUKWUM**	756	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
605	**MUKXAT**	757	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
606	**MUMDAB**	758	Discrete Molecule	Trigonal	3	Non-Chelate	O-Donor	
607	**MUSHOZ**	759	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
608	**MUYNAV**	760	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
609	**NACCOK**	761	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
610	**NAKGOX**	762	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
611	**NAQQOL**	763	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
612	**NAVPIK**	764	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	O-Donor	
613	**NAVRIL**	765	Tetramer Through Anion	Seesaw	4	Non-Chelate	Silicon	
		766	Tetramer Through Anion	Trigonal	3	Non-Chelate	Silicon	
614	**NAXVUE**	767	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
615	**NAYJIH**	768	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
616	**NBUPHG10**	769	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
617	**NEBCAA**	770	Discrete Molecule	T-Shape	5	Chelate	N-Donor	S-Donor
618	**NEFKUE**	771	Dimer Through Ligand	T-Shape	5	Chelate	O-Donor	
619	**NEFLEP**	772	Dimer Through Anion	D-Square Pyramid	5	Chelate	O-Donor	
620	**NEHQUM01**	773	Tetramer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
		774	Tetramer Through Ligand	T-Shape	5	Non-Chelate	O-Donor	
621	**NEKNUM**	775	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
622	**NEPFOE**	776	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
		777	Polymer Through Ligand	T-Shape	5	Non-Chelate	N-Donor	
623	**NESWUD**	778	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
624	**NETGOJ**	779	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
625	**NETGUO**	780	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
626	**NETHAW**	781	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
627	**NEVQAH**	782	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
628	**NEWBEX**	783	Discrete Molecule	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
629	**NEWKAC**	784	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
630	**NEWRUE**	785	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
		786	Polymer Through Anion	Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
631	**NIDWIG**	787	Discrete Molecule	Seesaw	4	Chelate	P-Donor	
632	**NIMDUJ**	788	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
633	**NIMFAR**	789	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
634	**NIMFEV**	790	Discrete Molecule	D-Octahedral	6	Non-Chelate	O-Donor	
		791	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
635	**NIMFOF**	792	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	

636	**NINDOE**	793	Tetramer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor		
		794	Tetramer Through Anion	Seesaw	4	Non-Chelate		N-Donor		
637	**NIRQAG**	795	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	O-Donor	
		796	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		S-Donor	O-Donor	
638	**NITZUL**	797	Discrete Molecule	D-Pentagonal Bipyramid	7	Non-Chelate	M-M	N-Donor	C-Donor	Iron
639	**NODZIP**	798	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
640	**NOFPAZ**	799	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
641	**NOJZOD**	800	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
642	**NOKCOF**	801	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-Donor		
643	**NOMSEO**	802	Discrete Molecule	T-Shape	5	Non-Chelate	M-M	Iodine	Platinum	
644	**NOQVUK**	803	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
645	**NUMJUA**	804	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
646	**NUMKAH**	805	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
647	**NUXWEJ**	806	Dimer Through Ligand	Seesaw	4	Chelate		S-Donor		
648	**OCODAM**	807	Discrete Molecule	Seesaw	4	Non-Chelate		P-Donor		
649	**OCODEQ**	808	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor		
650	**ODIPAT**	809	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor		
651	**ODITIF**	810	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
		811	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor		
652	**ODIWEF**	812	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor		
653	**ODUMOQ**	813	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
654	**OFOLAY**	814	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
655	**OGAROF**	815	Discrete Molecule	Seesaw	4	Chelate		S-Donor		
656	**OHURAM**	816	Oligomer Through Anion	Trigonal Pyramid	4	Metal Halide Only		Chlorine		
		817	Oligomer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine		
		818	Oligomer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine		
657	**OKAJOZ**	819	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine		
658	**OKOWUG**	820	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
659	**OLAGAJ**	821	Tetramer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
660	**OLAGEN**	822	Tetramer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
661	**OMEXEL**	823	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
662	**OMIKIG**	824	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
663	**ONINIK**	825	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
664	**ONINUW**	826	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
665	**ONOFAZ**	827	Discrete Molecule	T-Shape	5	Chelate		O-Donor	N-Donor	
666	**OPUYUU**	828	Polymer Through Ligand	Seesaw	4	Chelate		N-Donor		
		829	Polymer Through Anion	Square Planar	4	Metal Halide Only		Chlorine		
667	**OQIDOI**	830	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
668	**OROQOC**	831	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
669	**OROQUI**	832	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor		
		833	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
670	**OTPCHG**	834	Dimer Through Anion	Seesaw	4	Non-Chelate		P-Donor	O-Donor	
671	**OVEFIF**	835	Polymer through ligand	T-Shape	5	Non-Chelate		N-Donor		
672	**OWUGIX**	836	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
673	**OWUGOD**	837	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
674	**OXTETH10**	838	Discrete Molecule	T-Shape	5	Non-Chelate		O-Donor		
675	**PAFRIZ**	839	Tetramer Through Anion	Seesaw	4	Chelate		N-Donor		
		840	Tetramer Through Ligand	T-Shape	5	Chelate		N-Donor		
676	**PAHNUH**	841	Trimer Through Ligand	Trigonal	3	Chelate		O-Donor		
		842	Trimer Through Ligand	Seesaw	4	Chelate		O-Donor		
677	**PANCIR**	843	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
678	**PASCHI**	844	Tetramer Through Anion	Trigonal	3	Metal to Metal		Iron		
		845	Tetramer Through Ligand	D-Tetrahedral (Py)	4	Metal to Metal		Iron		
679	**PATJUP**	846	Tetramer Through Ligand	Seesaw	4	Non-Chelate		S-Donor		
680	**PATJUP10**	847	Tetramer Through Ligand	Seesaw	4	Non-Chelate		S-Donor		
681	**PAVSUA**	848	Oligomer Through Ligand	Seesaw	4	Non-Chelate	M-M	P-Donor	Iron	
682	**PAVTAH**	849	Oligomer Through Ligand	Seesaw	4	Non-Chelate	M-M	P-Donor	Iron	
683	**PAVTOV**	850	Oligomer Through Ligand	Seesaw	4	Non-Chelate	M-M	P-Donor	Iron	
684	**PAVTUB**	851	Oligomer Through Ligand	Seesaw	4	Non-Chelate	M-M	P-Donor	Iron	
685	**PAYCOJ**	852	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
686	**PEHWEE**	853	Discrete Molecule	Trigonal	3	Non-Chelate		O-Donor		
		854	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
687	**PEHYOQ**	855	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		

688	**PEJYEI**	856	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	M-M	N-Donor	Platinum
689	**PEQVIR**	857	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
		858	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
690	**PERLOL**	859	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
691	**PETXOC**	860	Trimer Through Anion	Square Pyramid	5	Metal Halide Only		Chlorine	
		861	Trimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
		862	Trimer Through Anion	Seesaw	4	Chelate		N-Donor	
692	**PETXUI**	863	Polymer Through Anion	Trigonal Bipyramid	5	Chelate		N-Donor	
693	**PEWVAO**	864	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	
694	**PEWVES**	865	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
		866	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
695	**PEYKIP**	867	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
696	**PEYKIP01**	868	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
697	**PIDCIO**	869	Trimer Through Anion	Seesaw	4	Metal Halide Only		Chlorine	
		870	Trimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
698	**PIFXIN**	871	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
699	**PIGQED**	872	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor	
700	**PIHCAL**	873	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
701	**PIHPON**	874	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
702	**PIWGOT**	875	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
703	**PIXWAV**	876	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
704	**PIXWEZ**	877	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
705	**PIZLUH**	878	Oligomer Through Anion	Trigonal Pyramid	3	Non-Chelate		C-donor	
		879	Oligomer Through Anion	Trigonal	3	Non-Chelate		N-Donor	
		880	Oligomer Through Ligand	D-Square Planar	4	Metal Halide Only		Chlorine	
706	**POCVIO**	881	Discrete Molecule	D-Octahedral	6	Non-Chelate		N-Donor	
707	**PODWIO**	882	Discrete Molecule	D-Pentagonal Bipyramid	7	Chelate		O-Donor	
708	**POLLAD**	883	Polymer Through Anion	Trigonal Bipyramid	5	Chelate		O-Donor	
		884	Polymer Through Anion	Seesaw	4	Chelate		O-Donor	
709	**POMCID**	885	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
710	**POMKAE**	886	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
711	**POMKAE01**	887	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
712	**POMKOS**	888	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
713	**POMQOY**	889	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
714	**PONHEG**	890	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
715	**PONWEU**	891	Polymer Through Anion	D-Octahedral	6	Chelate		O-Donor	N-Donor
716	**POPCUS**	892	Polymer Through Anion	Square Pyramid	5	Chelate		O-Donor	N-Donor
717	**POPDON**	893	Dimer Through Anion	Square Pyramid	5	Chelate		O-Donor	N-Donor
718	**POPDUT**	894	Tetramer Through Anion	Square Pyramid	5	Chelate		O-Donor	N-Donor
719	**PORLOY**	895	Discrete Molecule	Seesaw	4	Chelate		P-Donor	C-Donor
720	**POTGAG**	896	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
721	**POWQUO**	897	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
722	**POZWAE**	898	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	M-M	P-Donor	Mercury
723	**POZZEL**	899	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
724	**PTUMHG**	900	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
725	**PUBBIZ**	901	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
726	**PUKJAG**	902	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
727	**PUKZEA**	903	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine	
728	**PUNJEP**	904	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
729	**PURGIS**	905	Dimer Through Ligand	Seesaw	3	Metal to Metal		Iridium	
		906	Dimer Through Ligand	Trigonal	4	Chelate		N-Donor	
730	**PUSWUX**	907	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
731	**PUTKOG**	908	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
732	**PUTKUM**	909	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
733	**PUVLUN**	910	Polymer Through Anion	Octahedral	6	Metal Halide Only		Chlorine	
734	**PUVTEH**	911	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine	
735	**PYDSHG**	912	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
736	**PYNOHG**	913	Dimer Through Ligand	Seesaw	4	Chelate		O-Donor	
737	**QABSUK**	914	Discrete Molecule	D-Trigonal Bipyramid	5	Non-Chelate		N-donor	O-Donor
738	**QAHRIC**	915	Discrete Molecule	Square Pyramid	5	Chelate		N-Donor	
		916	Discrete Molecule	Linear	2	Metal Halide Only		Chlorine	
739	**QAPTEI**	917	Discrete Molecule	T-Shape	5	Non-Chelate		N-Donor	

740	**QARNED**	918	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	N-Donor
741	**QAVVIU**	919	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
742	**QAYTIT**	920	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
743	**QAYZEV**	921	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		922	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
744	**QEJSOP**	923	Trimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		924	Trimer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
745	**QEJZOU**	925	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
746	**QEKJAR**	926	Dimer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor	
747	**QEPTIO**	927	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
748	**QEPYIU**	928	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		929	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
749	**QEPYUG**	930	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		931	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
750	**QEVHUU**	932	Oligomer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
		933	Oligomer Through Anion	Square Pyramid	4	Metal to Metal	Iron	
		934	Oligomer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
751	**QEYBUR**	935	Dimer Through Ligand	T-Shape	5	Non-Chelate	O-Donor	
752	**QEZNIU**	936	Polymer through ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
753	**QEZNOA**	937	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
754	**QEZNUG**	938	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
755	**QEZPAO**	939	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
756	**QIQXAR**	940	Discrete Molecule	Seesaw	4	Chelate	P-Donor	
757	**QIRZIC**	941	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
758	**QISVIX**	942	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
759	**QIVXAV**	943	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		944	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
760	**QIXGUA**	945	Dimer Through Ligand	T-Shape	5	Non-Chelate	N-Donor	
761	**QIZRUO**	946	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
		947	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
762	**QOJMUY**	948	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
763	**QOLGUU**	949	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		950	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
764	**QONGEG**	951	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		952	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
765	**QOPGUY**	953	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
766	**QOQCII**	954	Polymer Through Anion	T-Shape	5	Non-Chelate	S-Donor	
		955	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		956	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
767	**QORKIT**	957	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
768	**QQQBVJ03**	958	Trimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		959	Trimer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
769	**QQQBVJ04**	960	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
770	**QQQBVJ21**	961	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
771	**QQQBVJ31**	962	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
772	**QULQEV**	963	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
773	**QUMSIA**	964	Discrete Molecule	Square Planar	4	Non-Chelate	O-Donor	
774	**QUMVIE**	965	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
775	**QUVWIP**	966	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
776	**QUVXEM**	967	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
777	**QUVZOY**	968	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
778	**QUZDUM**	969	Polymer Through Ligand	D-Octahedral	6	Chelate	N-Donor	
779	**RACYUS**	970	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	N-Donor	O-Donor
780	**RAFJUD**	971	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
		972	Polymer Through Anion	Square Pyramid	5	Non-Chelate	O-Donor	
781	**RAHCOT**	973	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
782	**RAHCUZ**	974	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
783	**RAHDAG**	975	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
784	**RAHDEK**	976	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
785	**RAHDIO**	977	Polymer Through Anion	Seesaw	4	Chelate	C-Donor	
		978	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
786	**RAJMAR**	979	Discrete Molecule	Seesaw	4	Chelate	O-Donor	

787	**RARBET**	980	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	O-Donor
788	**RARZIV**	981	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
789	**RASGIC**	982	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		983	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
790	**RAWSUE**	984	Dimer Through Ligand	Seesaw	4	Metal Halide Only	N-Donor	
791	**RAZDOM**	985	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
792	**RAZDUS**	986	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		987	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
793	**RAZTES**	988	Polymer Through Anion	D-Octahedral	6	Non-Chelate	O-Donor	
794	**RAZTUI**	989	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
795	**RECZUU**	990	Tetramer Through Ligand	D-Octahedral	6	Non-Chelate	S-Donor	O-Donor
		991	Tetramer Through Anion	Seesaw	4	Non-Chelate	S-Donor	O-Donor
		992	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
796	**REDDUZ**	993	Polymer through ligand	Square Planar	4	Non-Chelate	O-Donor	
		994	Polymer through ligand	Seesaw	4	Non-Chelate	O-Donor	
		995	Polymer through ligand	Seesaw	4	Non-Chelate	S-Donor	O-Donor
797	**REDTEB**	996	Dimer Through Anion	T-Shape	5	Chelate	N-Donor	
		997	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
798	**REJTEF**	998	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
799	**REMDUI**	999	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
800	**REXZUP**	1000	Polymer Through Anion	D-Octahedral	4	Non-Chelate	N-Donor	
		1001	Polymer Through Ligand	D-Octahedral	4	Non-Chelate	N-Donor	
801	**REZWEZ**	1002	Polymer through ligand	Square Pyramid	5	Non-Chelate	N-Donor	
802	**RICSEC**	1003	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
803	**RICSIG**	1004	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
804	**RIHGUL**	1005	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
805	**RILHID**	1006	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	
806	**RILHID01**	1007	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	
807	**RINWES**	1008	Discrete Molecule	Seesaw	4	Metal Halide Only	Chlorine	
808	**RINXET**	1009	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	O-Donor
809	**RITLUB**	1010	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		1011	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
810	**RIVMEO**	1012	Dimer Through Ligand	T-Shape	6	Non-Chelate	C-Donor	
811	**RIXGUA**	1013	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	N-Donor	
		1014	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
812	**RIYHOX**	1015	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
813	**ROGVOY**	1016	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
814	**ROKGED**	1017	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
815	**ROKHAA**	1018	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
816	**RUBMUX**	1019	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
817	**RUKFOS**	1020	Discrete Molecule	Hexagonal Bipyramid	8	Chelate	O-Donor	
818	**RUMWOM**	1021	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
819	**RUQNAT**	1022	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
820	**RUSNEZ**	1023	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
821	**RUTSEG**	1024	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
822	**RUXBOD**	1025	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
823	**RUYVUE**	1026	Polymer Through Ligand	Trigonal bipyramid	5	Non-Chelate	O-Donor	N-Donor
		1027	Polymer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
824	**RUYWIT**	1028	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor	O-Donor
825	**SACHOV**	1029	Polymer Through Anion	Linear	2	Non-Chelate	N-Donor	
		1030	Polymer Through Ligand	Square Planar	4	Non-Chelate	N-Donor	
		1031	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
826	**SACPAQ**	1032	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	O-Donor	
		1033	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		1034	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		1035	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		1036	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
		1037	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
827	**SAJVEF**	1038	Discrete molecule	Seesaw	4	Chelate	N-Donor	
828	**SAKBOV**	1039	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
829	**SARPUX**	1040	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
830	**SAVQOV**	1041	Discrete Molecule	T-Shape	5	Chelate	N-Donor	

831	**SAXDOK**	1042	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
832	**SAXFAA**	1043	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
833	**SAYKUY**	1044	Discrete Molecule	D-Tetrahedral (Py)	4	Metal Halide Only	Iodine	Chlorine
834	**SAYLAF**	1045	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
835	**SAYMAI**	1046	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
836	**SAYMIQ**	1047	Tetramer Through Ligand	Tetrahedral	4	Metal Halide Only	Chlorine	
		1048	Tetramer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		1049	Tetramer Through Anion	D-Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
837	**SEBNAP**	1050	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor	
838	**SEPCAS**	1051	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		1052	Trimer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
839	**SEPCEW**	1053	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
840	**SEPCIA**	1054	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		1055	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		1056	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
841	**SERGOL**	1057	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
842	**SETJAD**	1058	Polymer Through Anion	Tetrahedral	4	Metal to Metal	Cupper	
843	**SINHEE**	1059	Polymer Through Ligand	Tetrahedral	4	Non-Chelate	N-Donor	
844	**SIRDEC**	1060	Dimer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
845	**SIRMAH**	1061	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
846	**SISLUB**	1062	Dimer Through Anion	Square Planar	4	Metal to Metal	Ruthenium	
		1063	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
847	**SISLUB10**	1064	Dimer Through Anion	Square Planar	4	Metal to Metal	Ruthenium	
		1065	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
848	**SIWJIT**	1066	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
849	**SODZES**	1067	Discrete Molecule	Trigonal	3	Non-Chelate	N-Donor	
850	**SOHCUP**	1068	Discrete molecule	Square Pyramid	5	Non-Chelate	N-Donor	O-Donor
851	**SOHKEH**	1069	Polymer Through Ligand	D-Trigonal Bipyramid	5	Chelate	N-Donor	O-Donor
852	**SOHMAF**	1070	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
853	**SOPDOQ**	1071	Polymer Through Anion	Seesaw	4	Non-Chelate	Bromine	
854	**SOYPIF**	1072	Discrete Molecule	Trigonal	3	Metal Halide Only	Chlorine	
855	**SUPWIL**	1073	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	
856	**SURHGC**	1074	Discrete Molecule	D-Trigonal Bipyramid	5	Non-Chelate	S-Donor	
857	**SURNOI**	1075	Dimer Through Ligand	T-Shape	5	Chelate	S-Donor	O-Donor
858	**SUSJAR**	1076	Discrete Molecule	Seesaw	4	Chelate	O-Donor	
859	**TACSUM**	1077	Discrete Molecule	Trigonal Bipyramid	5	Chelate	S-Donor	
860	**TACTAT**	1078	Polymer Through Ligand	D-Octahedral	6	Chelate	S-Donor	
861	**TAGCAF**	1079	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
862	**TAJCAJ**	1080	Dimer Through Ligand	Trigonal	3	Chelate	N-Donor	
		1081	Dimer Through Ligand	Square Planar	4	Non-Chelate	N-Donor	
863	**TAKMUP**	1082	Dimer Through Anion	Trigonal Bipyramid	5	Chelate	S-Donor	N-Donor
		1083	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
864	**TAMHGC**	1084	Polymer through anion	D-Octahedral	6	Non-Chelate	S-Donor	
865	**TAZGAC**	1085	Dimer through anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
866	**TBTPHG**	1086	Tetramer Through Anion	Seesaw	4	Non-Chelate	N-Donor	S-Donor
		1087	Tetramer Through Anion	Bent	4	Non-Chelate	S-Donor	
867	**TEBPAS**	1088	Tetramer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
868	**TEBPEW**	1089	Tetramer Through Anion	Trigonal	3	Non-Chelate	C-Donor	
869	**TEDBEJ**	1090	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
870	**TEKXOW**	1091	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
871	**TENNAD**	1092	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
872	**TESTHG**	1093	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	
873	**TESZUM**	1094	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
874	**TEVQIU01**	1095	Polymer Through Anion	Bent	4	Non-Chelate	S-Donor	
		1096	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
875	**TEZTEX**	1097	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
876	**TIBCOY**	1098	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
877	**TIFTOR**	1099	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
878	**TIGGUL**	1100	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
879	**TIGHAS**	1101	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
880	**TIGHEW**	1102	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
881	**TIGHIA**	1103	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	

882	**TIGHOG**	1104	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
883	**TIGHUM**	1105	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
884	**TIKSIQ**	1106	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel	
885	**TIKSIQ01**	1107	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel	
886	**TIKSIQ02**	1108	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Nickel	
887	**TINWOC**	1109	Dimer through anion	Tetrahedral	4	Metal Halide Only		Chlorine		
		1110	Dimer through anion	D-Octahedral	6	Chelate	M-M	N-Donor	C-Donor	Iron
888	**TIZNIB**	1111	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	O-Donor	
889	**TIZYEH**	1112	Polymer Through Anion	Seesaw	4	Non-Chelate		O-Donor		
		1113	Polymer Through Anion	Square Pyramid	5	Non-Chelate		O-Donor		
890	**TMDPHG**	1114	Polymer Through Ligand	Seesaw	4	Non-Chelate		P-Donor		
891	**TMSCHG**	1115	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine		
892	**TODQOS**	1116	Dimer Through Ligand	D-Tetrahedral (Py)	4	Chelate		N-Donor		
893	**TOGMIL**	1117	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
894	**TOLLAI**	1118	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
895	**TOPZOP**	1119	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
896	**TORGUC**	1120	Discrete Molecule	Seesaw	4	Non-Chelate		P-Donor		
897	**TPHGCL10**	1121	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor		
898	**TPHGCL11**	1122	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor		
899	**TRPHGA**	1123	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine		
900	**TTPHGC10**	1124	Dimer Through Ligand	Bent	4	Non-Chelate		S-Donor		
901	**TUBJIJ**	1125	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
902	**TUBXOF**	1126	Dimer Through Anion	Trigonal	3	Metal Halide Only		Chlorine		
		1127	Dimer Through Anion	T-Shape	5	Chelate	M-M	O-Donor	Nickel	
903	**TUBYAS**	1128	Discrete Molecule	D-Octahedral	6	Chelate		O-Donor		
904	**TUBYOG**	1129	Oligomer Through Ligand	T-Shape	8	Chelate	M-M	O-Donor	N-Donor	Nickel
		1130	Oligomer Through Ligand	T-Shape	7	Chelate	M-M	O-Donor	N-Donor	Nickel
905	**TUFJUA**	1131	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor		
906	**TUFKAH**	1132	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor		
		1133	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor		
907	**TUJXOM**	1134	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
908	**UCEYUX**	1135	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
909	**UCEZAE**	1136	Trimer Through Anion	Square Planar	4	Metal Halide Only		Chlorine		
		1137	Trimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
910	**UCIVAF**	1138	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
911	**UCIVOS**	1139	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
912	**UFACIO**	1140	Dimer Through Anion	D-Square Pyramid	5	Chelate		N-Donor		
913	**UGUBOO**	1141	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
914	**UGUPOB**	1142	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
915	**UGUQES**	1143	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
		1144	Tetramer Through Anion	Trigonal	3	Metal Halide Only		Chlorine		
916	**UHUTIA**	1145	Trimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
		1146	Trimer Through Anion	Trigonal	3	Metal Halide Only		Chlorine		
917	**UHUWUP**	1147	Polymer Through Anion	Seesaw	4	Non-Chelate		C-Donor		
		1148	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Chlorine		
918	**UJECER**	1149	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
919	**UJIKEE**	1150	Discrete Molecule	D-Octahedral	6	Chelate		N-Donor	O-Donor	
920	**ULAMEA**	1151	Discrete Molecule	Square Pyramid	5	Chelate		N-Donor		
921	**UQEREO**	1152	Dimer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Chlorine		
922	**UQOXOO**	1153	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
923	**URILHG**	1154	Polymer Through Anion	D-Octahedral	6	Non-Chelate		O-Donor		
924	**USIHOU**	1155	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor		
		1156	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor		
925	**USUXAI**	1157	Discrete Molecule	Seesaw	4	Non-Chelate		P-Donor		
926	**UTIZIH**	1158	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
927	**UYAGOR**	1159	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
928	**UYUSOX**	1160	Polymer Through Ligand	D-Square Pyramid	5	Chelate		O-Donor		
929	**UYUSUD**	1161	Pentamer Through Anion	T-Shape	3	Metal Halide Only		Chlorine		
		1162	Pentamer Through Ligand	T-Shape	3	Non-Chelate		O-Donor		
930	**VAGNID**	1163	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
931	**VAHGIV**	1164	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		
932	**VAHGIV01**	1165	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Chlorine		

933	**VAHGIV02**	1166	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
934	**VALRUX**	1167	Discrete Molecule	D-Octahedral	6	Non-Chelate	O-Donor	
935	**VAQHUQ**	1168	Discrete Molecule	Seesaw	4	Chelate	O-Donor	N-Donor
936	**VARXUJ**	1169	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
937	**VAXGAC**	1170	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
938	**VAXJOT**	1171	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
		1172	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
939	**VAYHOS**	1173	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
940	**VEGROQ**	1174	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
941	**VEHSIL**	1175	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
942	**VEHSOR**	1176	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
943	**VEHSUX**	1177	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
944	**VEKCET**	1178	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		1179	Polymer Through Ligand	D-Tetrahedral (Py)	4	Metal to Metal	Ruthenium	
945	**VEYFAH**	1180	Dimer Through Anion	Trigonal Bipyramid	5	Chelate	N-donor	
946	**VEZLAP**	1181	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
		1182	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
947	**VEZLET**	1183	Tetramer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
948	**VEZLIX**	1184	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
949	**VEZYAC**	1185	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
950	**VEZYEG**	1186	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
951	**VICFIW**	1187	Discrete Molecule	Trigonal	3	Non-Chelate	O-Donor	
		1188	Discrete Molecule	Linear	2	Metal Halide Only	Chlorine	
952	**VINTUJ**	1189	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
953	**VIRKIS**	1190	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
954	**VIWKOC**	1191	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
955	**VIWKOC01**	1192	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	
956	**VOBJOM**	1193	Dimer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
957	**VOBKAZ**	1194	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
		1195	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
958	**VOCPEJ**	1196	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
959	**VOFSEO**	1197	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor	
960	**VOGLOU**	1198	Dimer Through Ligand	T-Shape	5	Non-Chelate	O-Donor	
961	**VOGMOV**	1199	Discrete Molecule	Seesaw	4	Chelate	O-Donor	
962	**VORPAT**	1200	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
963	**VORZOR**	1201	Dimer Through Anion	Seesaw	4	Metal to Metal	Osmium	
964	**VOTXUZ**	1202	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
965	**VOVRUV**	1203	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
966	**VOWKOJ**	1204	Polymer Through Ligand	T-Shape	4	Non-Chelate	N-Donor	
967	**VUDJOT**	1205	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
968	**VUDSET**	1206	Discrete Molecule	Seesaw	4	Metal to Metal	Tellurium	
969	**VUDSIX**	1207	Dimer Through Anion	D-Tetrahedral (Py)	4	Metal to Metal	Tellurium	
970	**VUDSUJ**	1208	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		1209	Polymer Through Anion	Trigonal Bipyramid	5	Metal to Metal	Tellurium	
		1210	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
971	**VUFPAN**	1211	Trimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
972	**VUJZAC**	1212	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
973	**VULLAQ**	1213	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
974	**VULMUM**	1214	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
975	**VUPWOT**	1215	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
976	**VUPXAG**	1216	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	S-Donor	
		1217	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
977	**VUWGEZ**	1218	Discrete Molecule	Seesaw	4	Chelate	O-Donor	N-Donor
978	**VUWVAK**	1219	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
979	**VUWVEO**	1220	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
980	**VUWVIS**	1221	Discrete Molecule	Seesaw	4	Metal Halide Only	Chlorine	
981	**VUWVIS01**	1222	Discrete Molecule	Seesaw	4	Metal Halide Only	Chlorine	
982	**VUWVOY**	1223	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
		1224	Trimer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
983	**VUWVUE**	1225	Dimer Through Anion	Square Pyramid	5	Metal Halide Only	Chlorine	
		1226	Dimer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
984	**VUYDEA**	1227	Discrete Molecule	T-Shape	5	Chelate	O-Donor	
985	**WABCEH**	1228	Polymer Through Anion	Trigonal	3	Metal to Metal	Iridium	

		1229	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
986	**WASGOM**	1230	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
987	**WAXHOU**	1231	Dimer Through Anion	Square Pyramid	5	Chelate	N-Donor	
988	**WAXHUA**	1232	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
989	**WAXJAI**	1233	Polymer Through Anion	T-Shape	5	Chelate	N-Donor	
		1234	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
990	**WAYNUH**	1235	Dimer Through Anion	Seesaw	4	Non-Chelate	Se-Donor	
991	**WAYWOK**	1236	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
992	**WECGAO**	1237	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
993	**WEKPEJ**	1238	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
994	**WEKPOT**	1239	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
995	**WENVIU**	1240	Dimer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		1241	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
996	**WENXIY**	1242	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	
997	**WENXOE**	1243	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	
998	**WEQMEL**	1244	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
		1245	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
999	**WIBJAU**	1246	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1000	**WICWOU**	1247	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	
1001	**WICWOU01**	1248	Discrete Molecule	T-Shape	6	Non-Chelate	O-Donor	
1002	**WIJGAY**	1249	Discrete Molecule	D-Trigonal Bipyramid	5	Non-Chelate	S-Donor	N-Donor
1003	**WILSUG**	1250	Polymer Through Anion	Tetrahedral	4	Non-Chelate	C-Donor	
		1251	Polymer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine	
1004	**WILTAN**	1252	Polymer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
		1253	Polymer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine	
1005	**WIMNUD**	1254	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
		1255	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
1006	**WIMPAL**	1256	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1007	**WIMPEP**	1257	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1008	**WIRJEO**	1258	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1009	**WIRJIS**	1259	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1010	**WIRJOY**	1260	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1011	**WIRKAJ**	1261	Discrete Molecule	T-Shape	4	Chelate	O-Donor	
1012	**WIZLIC**	1262	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Chlorine	
		1263	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
		1264	Polymer Through Anion	Octahedral	6	Metal Halide Only	Chlorine	
1013	**WODCUN**	1265	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
1014	**WOGPUE**	1266	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1015	**WOHQAL**	1267	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1016	**WONKEP**	1268	Dimer Through Anion	Square Pyramid	5	Non-Chelate	P-Donor	O-Donor
1017	**WOPKET**	1269	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1018	**WOVMOJ**	1270	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
1019	**WOVWEL**	1271	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1020	**WOVWOV**	1272	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1021	**WOWGUM**	1273	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1022	**WUNXIO**	1274	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1023	**WUQLEA**	1275	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
1024	**WURPIJ**	1276	Discrete Molecule	Trigonal	3	Metal Halide Only	Chlorine	
1025	**WUSHEZ**	1277	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1026	**WUZHAB**	1278	Polymer Through Anion	Trigonal Bipyramid	5	Chelate	N-Donor	
		1279	Polymer Through Ligand	Trigonal Bipyramid	5	Chelate	N-Donor	
		1280	Polymer Through Anion	T-Shape	5	Chelate	N-Donor	
		1281	Polymer Through Ligand	T-Shape	5	Chelate	N-Donor	
		1282	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1027	**XAFREB**	1283	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1028	**XAHROO**	1284	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1029	**XAHRUU**	1285	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1030	**XAHSOP**	1286	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	N-Donor	
1031	**XAHTAE**	1287	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1032	**XAKMAZ**	1288	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1033	**XAKZOA**	1289	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
1034	**XECPIG**	1290	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	

1035	**XECVUY**	1291	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1036	**XEJDEV**	1292	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1037	**XEKZIX**	1293	Discrete Molecule	T-Shape	6	Chelate	S-Donor	O-Donor
1038	**XELQOV**	1294	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
1039	**XEMTUG**	1295	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1040	**XEMVIW**	1296	Dimer Through Anion	Square Pyramid	4	Chelate	S-Donor	
1041	**XEQZAV**	1297	Trimer Through Anion	Seesaw	4	Chelate	N-Donor	
		1298	Trimer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
1042	**XEZNUL**	1299	Dimer Through Ligand	Seesaw	4	Non-Chelate	P-Donor	
1043	**XIGWUG**	1300	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
1044	**XINLUD**	1301	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1045	**XINVIB**	1302	Discrete Molecule	Tetrahedral	4	Non-Chelate	N-Donor	
1046	**XIPCAB**	1303	Discrete Molecule	T-Shape	5	Chelate	S-Donor	N-Donor
1047	**XISCEI**	1304	Discrete Molecule	Seesaw	4	Chelate	P-Donor	
1048	**XIVKIW**	1305	Dimer Through Ligand	Trigonal	3	Non-Chelate	N-Donor	
1049	**XIVKOC**	1306	Dimer Through Ligand	Trigonal	3	Non-Chelate	N-Donor	
1050	**XIYBOX**	1307	Discrete Molecule	Seesaw	4	Chelate	N-Donor	O-Donor
1051	**XIYBUD**	1308	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1052	**XIYCAK**	1309	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1053	**XIYCEO**	1310	Discrete Molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1054	**XOKYOL**	1311	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1055	**XORPUP**	1312	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
1056	**XOVGOE**	1313	Dimer Through Ligand	T-Shape	5	Non-Chelate	N-Donor	O-Donor
1057	**XOZZUI**	1314	Polymer Through Ligand	Square Planar	4	Non-Chelate	O-Donor	N-Donor
		1315	Polymer Through Anion	Square Planar	4	Non-Chelate	O-Donor	
1058	**XUBLUD**	1316	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
		1317	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
1059	**XUBMAK**	1318	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1060	**XUBMEO**	1319	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
1061	**XUBZEB**	1320	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
		1321	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	N-Donor	
1062	**XUCDEF**	1322	Discrete Molecule	Trigonal Pyramid	3	Metal Halide Only	Chlorine	
		1323	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1063	**XUFDEJ**	1324	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1064	**XUGDUZ**	1325	Discrete Molecule	Trigonal Pyramid	3	Metal Halide Only	Chlorine	
		1326	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Chlorine	
1065	**XUKSAZ**	1327	Discrete Molecule	D-Square Pyramid	5	Metal to Metal	Osmium	
1066	**XULGEQ**	1328	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		1329	Dimer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
1067	**YABCEL**	1330	Trimer Through Anion	Square Planar	4	Metal Halide Only	Chlorine	
		1331	Trimer Through Anion	Seesaw	4	Chelate	N-Donor	
1068	**YACDUD**	1332	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1069	**YACGUF**	1333	Discrete Molecule	T-Shape	5	Chelate	S-Donor	N-Donor
1070	**YATMUD**	1334	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1071	**YATPUG**	1335	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	N-Donor	
		1336	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
1072	**YAVJAI**	1337	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
1073	**YAWNOZ**	1338	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1074	**YAWNUF**	1339	Discrete Molecule	Trigonal	3	Metal Halide Only	Chlorine	
1075	**YEJDOH**	1340	Discrete Molecule	Seesaw	4	Metal to Metal	Tellurium	
1076	**YESROD**	1341	Dimer Through Ligand	Trigonal Pyramid	4	Non-Chelate	N-Donor	S-Donor
1077	**YEXNUK**	1342	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor	
1078	**YEZGEP**	1343	Polymer Through Anion	D-Prism	6	Non-Chelate	O-Donor	
		1344	Polymer Through Ligand	T-Shape	5	Non-Chelate	O-Donor	
		1345	Polymer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine	
		1346	Polymer Through Ligand	T-Shape	3	Metal Halide Only	Chlorine	
1079	**YIJKAE**	1347	Dimer Through Anion	Square Pyramid	5	Non-Chelate	C-Donor	O-Donor
1080	**YIPMOZ**	1348	Discrete Molecule	T-Shape	5	Non-Chelate	O-Donor	
1081	**YIQPAQ**	1349	Dimer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Chlorine	
1082	**YISPOF**	1350	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1083	**YITPOG**	1351	Polymer Through Ligand	T-Shape	6	Non-Chelate	O-Donor	
1084	**YITPUM**	1352	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	

1085	**YITRAU**	1353	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
1086	**YIYWIN**	1354	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	C-Donor
1087	**YIZTUW**	1355	Dimer through anion	Trigonal Bipyramid	5	Chelate	N-Donor	
1088	**YOCYOG**	1356	Discrete molecule	T-Shape	5	Chelate	N-Donor	O-Donor
1089	**YOGJEL**	1357	Discrete Molecule	Tetrahedral	4	Metal Halide Only		
1090	**YOWLUR**	1358	Tetramer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
		1359	Tetramer Through Ligand	D-Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
1091	**YUBYEZ**	1360	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1092	**YUBYID**	1361	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1093	**YUCBAZ**	1362	Dimer Through Ligand	D-Tetrahedral (Py)	4	Chelate	S-Donor	
1094	**YUNLAV**	1363	Polymer through ligand	Seesaw	4	Non-Chelate	N-Donor	
		1364	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
1095	**YUTNIM**	1365	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
		1366	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
1096	**YUTNOS**	1367	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
1097	**YUTNUY**	1368	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
1098	**ZAMHUQ**	1369	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Chlorine	
1099	**ZASLOU**	1370	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		1371	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
1100	**ZEFQUY**	1372	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
1101	**ZEPSEU**	1373	Polymer Through Anion	Square Pyramid	5	Chelate	N-Donor	O-Donor
		1374	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
1102	**ZEPSIY**	1375	Dimer Through Anion	Seesaw	4	Chelate	O-Donor	N-Donor
		1376	Dimer Through Anion	Trigonal	3	Metal Halide Only	Chlorine	
1103	**ZESPOC**	1377	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
1104	**ZIGPIQ**	1378	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor	S-Donor
1105	**ZITSOK**	1379	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
		1380	Tetramer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
1106	**ZOGMIT**	1381	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
1107	**ZUFHUF**	1382	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
1108	**ZUFWEE**	1383	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	C-Donor	O-Donor
		1384	Polymer Through Anion	Square Pyramid	5	Non-Chelate	C-Donor	O-Donor
1109	**ZUNTAF**	1385	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
1110	**ZUPCOC**	1386	Oligomer Through Ligand	Seesaw	4	Chelate	O-Donor	
1111	**ZUPCUI**	1387	Polymer through ligand	Seesaw	4	Chelate	O-Donor	
		1388	polymer through ligand	D-Octahedral	6	Chelate	O-Donor	
1112	**ZZZLCI01**	1389	Polymer through anion	D-Octahedral	6	Non-Chelate	N-Donor	

S28. CSD-Analysis for $HgBr_2$ Compounds

Number	Ref. Code	Hits	Polymerization Mode	Geometry	C.N.	Chelation Mode	Donor Atom of Ligand		
1	**AQOFUJ**	1	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
		2	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	C-Donor	O-Donor	Se-Donor
2	**ASAMEO**	3	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor		
3	**ATAWOJ**	4	Discrete Molecule	T-Shape	5	Chelate	O-Donor	N-Donor	
4	**AVIZAI**	5	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate	N-Donor		
5	**IVOKIP**	6	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor		
6	**ORUYUX**	7	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
7	**ORUZAE**	8	Dimer Through Anion	Seesaw	4	Metal Halide Only	Bromine		
8	**OSOGOU**	9	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
9	**ACNHGB**	10	Discrete Molecule	Linear	2	Metal Halide Only	Bromine		
		11	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor		
10	**ACOZUN**	12	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
11	**ADOKAG**	13	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor		
12	**ADOKEK**	14	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor		
13	**ADOKIO**	15	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor		
14	**AGEWUF**	16	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
15	**AHIMAH**	17	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Bromine		
16	**AHOLUE**	18	Discrete Molecule	Seesaw	4	Non-Chelate	Se-Donor		
17	**AJAJOL**	19	Dimer Through Anion	Seesaw	4	Non-Chelate	Se-Donor		
18	**AJIFIK**	20	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor		

19	**AJIKAG**	21	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
20	**AKULEX**	22	Dimer Through Anion	Seesaw	4	Chelate	P-Donor
21	**AKULOH**	23	Dimer Through Anion	Seesaw	4	Chelate	P-Donor
22	**AMODEL**	24	Discrete Molecule	Seesaw	4	Chelate	N-Donor
23	**APULON**	25	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor
24	**AQAWIA**	26	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor
25	**AQEFAF**	27	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
26	**AQEFOT**	28	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
27	**AQEGEK**	29	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
28	**AQEGUA**	30	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
29	**ARUJOM**	31	Discrete Molecule	T-Shape	3	Chelate	P-Donor
		32	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
30	**ASUROW**	33	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
31	**ASURUC**	34	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
32	**AVISEE**	35	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
33	**AWUCOL**	36	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
34	**AXEDEM**	37	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor
35	**BAHJUR**	38	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
36	**BAKPOS**	39	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
37	**BAXPOG**	40	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
38	**BBPYHG**	41	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
39	**BBPYHG01**	42	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
40	**BDMPHG**	43	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor
41	**BEJLAD**	44	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
42	**BENJOT**	45	Discrete Molecule	Seesaw	4	Chelate	P-Donor
43	**BENLUC**	46	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor / S-Donor
44	**BEVCIQ**	47	Discrete Molecule	Seesaw	4	Chelate	N-Donor
45	**BEVCIQ01**	48	Discrete Molecule	Seesaw	4	Chelate	N-Donor
46	**BEZVOT**	49	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor / C-Donor
47	**BHGETC**	50	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
		51	Discrete Molecule	D-Square Pyramid	5	Non-Chelate	S-Donor
48	**BHGIRP**	52	Dimer Through Anion	T-Shape	3	M-M / Non-Chelate	Iridium
49	**BMTUHG**	53	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor
50	**BONDOX**	54	Discrete Molecule	Seesaw	4	Chelate	O-Donor
51	**BOPGOC11**	55	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
52	**BOQTUX**	56	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor
53	**BOQVAF**	57	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
54	**BPACHG**	58	Polymer Through Ligand	D-Square Pyramid	5	Non-Chelate	O-Donor / N-Donor
		59	Dimer Through Anion	D-Square Pyramid	5	Non-Chelate	O-Donor / N-Donor
55	**BPOHGB**	60	Discrete Molecule	T-Shape	6	Chelate	O-Donor
56	**BRRUHG**	61	Dimer Through Anion	Seesaw	4	M-M / Non-Chelate	Rhodium
57	**BTETHG**	62	Discrete Molecule	Seesaw	4	Chelate	S-Donor
58	**BUKYEN**	63	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
59	**BUKYIR**	64	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
60	**BULZEN01**	65	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
61	**BUTCCU**	66	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
62	**BUTCCU01**	67	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
63	**BUTLOS**	68	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
64	**BUTLUY**	69	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
65	**BUVZOJ**	70	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor
66	**BUWBIE**	71	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
67	**BUWBOK**	72	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
68	**CABFET**	73	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor
69	**CCGBTC**	74	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
70	**CEKJAF**	75	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor
71	**CEKJIN**	76	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
72	**CIBDUN**	77	Polymer Through Anion	Square Pyramid	5	Non-Chelate	O-Donor
73	**CIDLUY**	78	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
74	**CIDMIN**	79	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
75	**CIDNAG**	80	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
76	**CIDNEK**	81	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
77	**CINZEF**	82	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-donor / O-donor

		83	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	N-donor	O-donor
78	**CIZNII**	84	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
79	**COLSAY**	85	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
80	**COTSAH**	86	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
81	**COYLOS**	87	Discrete Molecule	Seesaw	4	Non-Chelate	O-Donor	
82	**COYWET**	88	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
83	**CUMXIT**	89	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
84	**CUSBAU**	90	Discrete Molecule	T-Shape	5	Chelate	N-donor	
85	**CUSBOI**	91	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
86	**CUSREO**	92	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
87	**CUSRUE**	93	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
88	**CUXMEP**	94	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor	
89	**CUYFEI**	95	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	O-Donor
90	**DAHYIW**	96	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
91	**DAXNUN**	97	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
92	**DAXPID**	98	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
		99	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
93	**DAZDAK**	100	Polymer Through Ligand	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-donor	
		101	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-donor	
94	**DEBMAY**	102	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Bromine	
95	**DECFOI**	103	Discrete Molecule	T-Shape	5	Chelate	N-Donor	
96	**DECFUO**	104	Polymer Through Anion	T-Shape	5	Chelate	N-donor	
97	**DEFYET**	105	Dimer Through Ligand	T-Shape	3	Non-Chelate	S-Donor	
98	**DEGJOP**	106	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
99	**DEJZIB**	107	Tetramer Through Ligand	T-Shape	3	Non-Chelate	O-Donor	
		108	Tetramer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
100	**DENLAK**	109	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
101	**DEPFEK**	110	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
102	**DEPVIE**	111	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
103	**DICMEI**	112	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
104	**DIQPUQ**	113	Polymer Through Anion	Seesaw	4	Metal Halide Only	Bromine	
105	**DITCOY**	114	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
106	**DIVZAJ**	115	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor	
107	**DIYVEM**	116	Discrete Molecule	T-Shape	5	Chelate	N-Donor	S-Donor
108	**DIZSOV**	117	Dimer Through Ligand	Seesaw	4	Chelate	N-donor	
109	**DUFHUH10**	118	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
110	**DUKTAF**	119	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
111	**DULWAJ**	120	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
112	**DUWSOE**	121	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
113	**DUWSUK**	122	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
114	**DUWVIC**	123	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
		124	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	C-Donor	O-Donor
		125	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
115	**ECOGUZ**	126	Discrete Molecule	Seesaw	4	Chelate	S-Donor	
116	**EDUFOA**	127	Polymer Through Anion	Octahedral	6	Chelate	N-Donor	
117	**EDUGOB**	128	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
118	**EDUVOP**	129	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
119	**EFIGAD**	130	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
120	**EFIGEH**	131	Tetramer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		132	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor	
121	**ELEWIC**	133	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
		134	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
122	**ELEXIE**	135	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
123	**ELOYEJ**	136	Trimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
124	**ELUQUZ**	137	Polymer Through Ligand	Square Planar	4	Non-Chelate	N-Donor	
		138	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
125	**EMIFUD**	139	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	O-Donor
126	**EMINUL**	140	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
127	**EQUXEU**	141	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
128	**EWIPEG**	142	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
129	**EWORAJ**	143	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	

130	**EWOROX**	144	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
131	**EXERII**	145	Discrete Molecule	D-Square Pyramid	5	Chelate		P-Donor	O-Donor
132	**EYAFOA**	146	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		C-Donor	
133	**EYUWUR**	147	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine	
134	**FAXGOC**	148	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
135	**FAXHOD**	149	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
136	**FAYKAS**	150	Discrete Molecule	Seesaw	4	Chelate		O-Donor	
137	**FEHXOH**	151	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
138	**FELMOA**	152	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor	
		153	Polymer Through Ligand	D-Square Pyramid	5	Chelate		N-Donor	
139	**FIJPEU**	154	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
140	**FIJQOF**	155	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Metal Halide Only		Bromine	
		156	Polymer Through Anion	Seesaw	4	Chelate		S-Donor	
141	**FIPWOR**	157	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine	
		158	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Chelate		N-Donor	S-Donor
142	**FIPXIM**	159	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor	S-Donor
143	**FOTMOS**	160	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
144	**FOWKOS**	161	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine	
145	**FULBUJ**	162	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		S-Donor	
146	**FUNKEF**	163	Discrete Molecule	T-Shape	7	Chelate	M-M	O-Donor	Nickel
147	**FUNKIJ**	164	Discrete Molecule	T-Shape	6	Chelate		O-Donor	
148	**GAKDIF**	165	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor	
149	**GANPAO**	166	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine	
150	**GASEESAWUO**	167	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
151	**GAZTUW01**	168	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine	
		169	Discrete Molecule	Linear	2	Metal Halide Only		Bromine	
152	**GEMPUK**	170	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine	
153	**GEMPUK01**	171	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine	
154	**GIRPUU**	172	Polymer Through Ligand	T-Shape	3	Non-Chelate		S-Donor	
		173	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
155	**GIWZER**	174	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
156	**GIYLUV**	175	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
157	**GODJOY**	176	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		N-Donor	
158	**GOWQIU**	177	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
159	**GOWWUK**	178	Polymer Through M-M	Seesaw	4	Metal Halide Only		Bromine	
160	**GOWXAR**	179	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine	
161	**GUDZIP**	180	Trimer Through Anion	Square Planar	4	Metal Halide Only		Bromine	
		181	Trimer Through Anion	Seesaw	4	Non-Chelate		Tellurium	
162	**GURKUA**	182	Discrete Molecule	Square Planar	4	Non-Chelate		N-Donor	
163	**GUTLIR**	183	Discrete Molecule	D-Octahedral	6	Chelate		N-Donor	S-Donor
164	**HATREB**	184	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine	
165	**HATRIF**	185	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Bromine	
166	**HAYPEE**	186	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine	
167	**HAZSOQ**	187	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
168	**HGBDOX**	188	Polymer Through Ligand	D-Octahedral	6	Non-Chelate		O-Donor	
169	**HIZPIQ**	189	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	P-Donor
170	**HIZQAJ**	190	Dimer Through Ligand	D-Tetrahedral (Pyramid)	4	Non-Chelate		P-Donor	
171	**HOCMER**	191	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Chelate		S-Donor	N-Donor
172	**HOSQAJ**	192	Discrete Molecule	T-Shape	5	Chelate		N-Donor	O-Donor
173	**HOTBUP**	193	Polymer Through Ligand	D-octahedral	6	Non-Chelate		N-Donor	
		194	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		N-Donor	
174	**HOTCAW**	195	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor	
175	**HOXBAX**	196	Oligomer Through Anion	Seesaw	4	M-M	Non-Chelate	Iron	
		197	Oligomer Through Anion	Seesaw	4	Non-Chelate		P-Donor	
176	**HOXBOL**	198	Oligomer Through Anion	Seesaw	4	M-M	Non-Chelate	Iron	
		199	Oligomer Through Anion	Seesaw	4	Non-Chelate		P-Donor	
177	**HOXBUR**	200	Oligomer Through Anion	Seesaw	4	M-M	Non-Chelate	Iron	
		201	Oligomer Through Anion	Seesaw	4	Non-Chelate		P-Donor	
178	**HOXCAY**	202	Oligomer Through Anion	Seesaw	4	M-M	Non-Chelate	Iron	
		203	Oligomer Through Anion	Seesaw	4	Non-Chelate		P-Donor	
179	**HOYBAY**	204	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		N-Donor	
180	**HOYLIS**	205	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor	

181	**HOYLOY**	206	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor		
182	**HOYLUE**	207	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor		
183	**HOYMAL**	208	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor		
184	**HUGBRA10**	209	Discrete Molecule	Pentagonal Pyramid	6	Chelate	N-Donor		
		210	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
185	**HUKSUD**	211	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor		
186	**HULVOA**	212	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
187	**HUPKIO**	213	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	N-donor		
		214	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
188	**ICUWOS**	215	Dimer Through Anion	Seesaw	4	Non-Chelate	O-Donor		
189	**IDOWEE**	216	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor		
190	**IFAWUH**	217	Discrete Molecule	T-Shape	5	Chelate	N-Donor	S-Donor	
191	**IGEFOP**	218	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor		
192	**IGEMUD**	219	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-donor		
193	**IHANIP**	220	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
194	**IJUBEU**	221	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor		
195	**IKAHIN**	222	Discrete Molecule	D-Octahedral	6	Chelate	N-Donor		
196	**IKUVUH**	223	Tetramer Through Anion	Seesaw	4	Non-Chelate	S-Donor	N-Donor	
197	**INIWOR**	224	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
198	**INOHOJ**	225	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
199	**INOHUP**	226	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	O-Donor	
200	**IPILOJ**	227	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor		
		228	Polymer Through Anion	T-Shape	5	Non-Chelate	N-Donor		
		229	Polymer Through Anion	D-Octahedral	6	Metal Halide Only	Bromine		
201	**IQIJAU**	230	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor		
202	**IREXAF**	231	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
203	**IREXEJ**	232	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
204	**IRUTUK**	233	Discrete Molecule	Seesaw	4	Non-Chelate	Chlorine		
205	**IRUVAS**	234	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
		235	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
206	**IRUVEW**	236	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
207	**ISATUS**	237	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
208	**IXIQOV**	238	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
209	**JAGLUZ**	239	Discrete Molecule	T-Shape	5	Non-Chelate	S-Donor	N-Donor	
210	**JAPJEQ**	240	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
211	**JAPKAN**	241	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
212	**JAPKER**	242	Trimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	O-Donor	
		243	Trimer Through Ligand	Square Planar	4	Non-Chelate	N-Donor	O-Donor	
213	**JAVJOG**	244	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor		
214	**JECXUK**	245	Dimer Through Ligand	T-Shape	5	Chelate	S-Donor		
215	**JEQMOI**	246	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
216	**JISFUN01**	247	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		
217	**JIZXUN**	248	Dimer Through Anion	Seesaw	4	Metal Halide Only	Bromine		
		249	Tetramer Through Anion	D-Tetrahedral (Pyramid)	4	Metal Halide Only	Bromine		
		250	Tetramer Through Anion	Pentagonal Bipyramid	7	Non-Chelate	O-Donor	N-Donor	S-Donor
218	**JOBBOT**	251	Discrete Molecule	Seesaw	4	Chelate	S-Donor		
219	**JOWVEW**	252	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate	O-Donor		
220	**JUDJUN**	253	Discrete Molecule	Seesaw	4	Chelate	S-Donor		
221	**KADQOX**	254	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor		
222	**KATHAQ**	255	Tetramer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
223	**KEKFUD**	256	Discrete Molecule	Seesaw	4	Chelate	N-Donor		
224	**KEWWUE**	257	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
225	**KEYZOE**	258	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine		
226	**KIBRUJ**	259	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor		
227	**KIJKOD**	260	Dimer Through Ligand	D-Tetrahedral (Pyramid)	4	Non-Chelate	Tellurium		
228	**KUCWEM**	261	Polymer Through Ligand	D-Octahedral	6	Chelate	N-Donor		
		262	Polymer Through Ligand	Tetrahedral	4	Metal Halide Only	Bromine		
229	**KUCWIQ**	263	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor		
230	**KUCXAJ**	264	Polymer Through Anion	Seesaw	4	Metal Halide Only	Bromine		
		265	Polymer Through Ligand	T-Shape	6	Chelate	N-Donor		
231	**KUDNUT**	266	Discrete Molecule	Square Pyramid	5	Chelate	C-Donor	O-Donor	
		267	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine		

232	**KUDPAB**	268	Polymer Through Ligand	Square Pyramid	5	Chelate	C-Donor	O-Donor
		269	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
233	**KUGPAD**	270	Dimer Through Ligand	Seesaw	4	Chelate	S-Donor	
234	**KUJWAP**	271	Discrete Molecule	T-Shape	6	Chelate	S-Donor	
235	**KUJWUJ**	272	Polymer Through Ligand	D-Trigonal Bipyramid	5	Chelate	N-Donor	
		273	Polymer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	
236	**KUNNAK**	274	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
237	**KUNNAK01**	275	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
238	**KUNYIC**	276	Discrete Molecule	T-Shape	3	Chelate	C-Donor	
		277	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
		278	Discrete Molecule	Seesaw	4	Chelate	C-Donor	
239	**KUNYOI**	279	Discrete Molecule	T-Shape	3	Chelate	C-Donor	
		280	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
		281	Discrete Molecule	Seesaw	4	Chelate	C-Donor	
240	**LACTIU**	282	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor	
241	**LADJOR**	283	Discrete Molecule	Seesaw	4	Chelate	C-Donor	P-Donor
242	**LAQGEP**	284	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
243	**LARLEX**	285	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
244	**LAZMAC**	286	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
245	**LAZTAH**	287	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
246	**LECROC**	288	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
247	**LECRUI**	289	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
248	**LECSAP**	290	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
249	**LECSAP01**	291	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
250	**LEHSAU**	292	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
251	**LEJQOH**	293	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
252	**LEKRUQ**	294	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
253	**LEKTAY**	295	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
254	**LELYAC**	296	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
255	**LEQRUV**	297	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
		298	Polymer Through Anion	Square Planar	4	Metal Halide Only	Bromine	
		299	Polymer Through Anion	T-Shape	3	Metal Halide Only	Bromine	
		300	Polymer Through Anion	Trigonal Pyramid	3	Chelate	N-Donor	
256	**LEXBEW**	301	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor	
257	**LEZDUP**	302	Dimer Through Ligand	T-Shape	6	Chelate	O-Donor	N-Donor
258	**LIFKUG**	303	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor	
259	**LIGRID**	304	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor	
260	**LINYAK**	305	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
261	**LOBYUX**	306	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
262	**LOLFIC**	307	Polymer Through Anion	D-Trigonal Bipyramid	5	Chelate	S-Donor	N-Donor
		308	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
263	**LOLFUO**	309	Polymer Through Ligand	Seesaw	4	Chelate	S-Donor	N-Donor
		310	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Chelate	S-Donor	
264	**LURVOJ**	311	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
265	**LUVKET**	312	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
266	**LUVKET01**	313	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
267	**MAJGUB**	314	Polymer Through Ligand	T-Shape	5	Chelate	N-Donor	O-Donor
268	**MAJHAI**	315	Dimer Through Anion	T-Shape	3	Metal Halide Only	Bromine	
269	**MARREC**	316	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	
270	**MARVAE**	317	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
271	**MATBHG**	318	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
272	**MAWFOF**	319	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	Arsenic	
273	**MECLIQ**	320	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor	
274	**MECLOW**	321	Dimer Through Ligand	Trigonal Pyramid	3	Non-Chelate	P-Donor	O-Donor
275	**MEVBAQ**	322	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
276	**MICCAC**	323	Discrete Molecule	Square Pyramid	5	Chelate | M-M	P-Donor	Mercury
277	**MIDZIJ**	324	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
278	**MIGBUA**	325	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
279	**MIHBAH**	326	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
280	**MIHBEL**	327	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
281	**MILTOQ**	328	Discrete Molecule	Seesaw	4	Chelate	S-Donor	
282	**MIRPUZ**	329	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	

283	**MOJFOI**	330	Dimer Through Anion	Seesaw	4	Chelate		C-Donor		
		331	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
284	**MOJFUO**	332	Dimer Through Anion	Seesaw	4	Chelate		C-Donor		
		333	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
285	**MOLVUE**	334	Polymer Through Anion	Seesaw	4	Metal Halide Only		Bromine		
		335	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
286	**MOWFUA**	336	Discrete Molecule	T-Shape	3	Non-Chelate		N-Donor		
287	**MOWGEL**	337	Polymer Through Anion	D-Octahedral	6	Non-Chelate		N-Donor		
288	**MTBRHG**	338	Polymer Through Anion	Square Pyramid	5	Non-Chelate		S-Donor		
289	**NAQYOT**	339	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only		Bromine		
290	**NAXWAL**	340	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		S-Donor		
		341	Polymer Through Ligand	D-Tetrahedral (Pyramid)	4	Non-Chelate		S-Donor		
291	**NAZLUX**	342	Dimer Through Anion	Seesaw	4	Non-Chelate		N-Donor		
292	**NEBCII**	343	Discrete Molecule	D-Trigonal Bipyramid	5	Chelate		N-Donor	S-Donor	
		344	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine		
293	**NEBYUO**	345	Discrete Molecule	T-Shape	3	Metal Halide Only		Bromine		
		346	Discrete Molecule	Linear	2	Chelate	M-M	C-Donor	Palladium	
294	**NEKJES**	347	Dimer Through Anion	Seesaw	4	Chelate		C-Donor		
		348	Dimer Through Ligand	Tetrahedral	4	Metal Halide Only		Bromine		
295	**NEKWIJ**	349	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
296	**NEPFIY**	350	Polymer Through Ligand	D-Square Pyramid	5	Chelate		N-Donor		
297	**NETGUP**	351	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
298	**NEWROY**	352	Polymer Through Ligand	Square Pyramid	5	Non-Chelate		O-Donor	N-Donor	
		353	Polymer Through Anion	Square Pyramid	5	Non-Chelate		O-Donor	N-Donor	
299	**NIFBAH**	354	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Metal Halide Only		S-Donor		
300	**NIMBAO**	355	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		S-Donor		
301	**NINFEW**	356	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
302	**NIPNIK**	357	Polymer Through Ligand	Seesaw	4	Non-Chelate		O-Donor		
303	**NIVBAV**	358	Discrete Molecule	D-Pentagonal Bipyramid	7	Chelate	M-M	C-Donor	N-Donor	Iron
304	**NIYCUT**	359	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
305	**NIYDAA**	360	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
306	**NOHZOA**	361	Dimer Through Ligand	Tetrahedral	4	Non-Chelate		N-Donor		
307	**NOQVOE**	362	Discrete Molecule	Tetrahedral	4	Non-Chelate		S-Donor		
308	**NUXWIN**	363	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-Donor		
309	**OBOGOD**	364	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
310	**ODESUM**	365	Oligomer Through Anion	Tetrahedral	4	Metal Halide Only		Bromine		
311	**ODETAT**	366	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	N-Donor	
		367	Discrete Molecule	D-Tetrahedral (Pyramid)	4	Non-Chelate		S-Donor	N-Donor	
312	**ODINUL**	368	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate		C-Donor		
313	**ODISIE**	369	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
314	**ODITEB**	370	Polymer Through Anion	D-Trigonal Bipyramid	5	Chelate		N-Donor		
		371	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Chelate		N-Donor		
315	**OFORIM**	372	Polymer Through Ligand	Tetrahedral	4	Chelate		Se-Donor		
		373	Polymer Through Ligand	Seesaw	4	Chelate		Se-Donor		
		374	Polymer Through Ligand	Seesaw	4	Chelate		N-Donor	Se-Donor	
316	**OMEMOI**	375	Discrete Molecule	Trigonal Pyramid	4	Chelate		N-Donor	Tellurium	
317	**OMENAV**	376	Discrete Molecule	Trigonal Pyramid	4	Chelate		N-Donor	Tellurium	
318	**OMILED**	377	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Bromine		
319	**ONEYUD**	378	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
320	**ONEZAK**	379	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
321	**ONEZIS**	380	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
322	**OQAJUM**	381	Discrete Molecule	T-Shape	5	Non-Chelate		N-Donor		
323	**OQIDIC**	382	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor		
324	**OROJIP**	383	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
325	**PAGWID**	384	Discrete Molecule	D- Trigonal Pyramid	4	M-M	Non-Chelate	Platinum		
326	**PASHGB**	385	Discrete Molecule	Seesaw	4	Non-Chelate		Arsenic		
327	**PAYCAT**	386	Discrete Molecule	T-Shape	3	Non-Chelate		N-Donor		
328	**PAYCEX**	387	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor	O-Donor	
329	**PAYCIB**	388	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	O-Donor	
330	**PAYCOH**	389	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	O-Donor	
		390	Polymer Through Anion	Octahedral	6	Metal Halide Only		Bromine		
331	**PEDPIZ**	391	Polymer Through Ligand	D-Trigonal Bipyramid	5	Chelate		N-Donor		
332	**PERGOJ**	392	Dimer Through Anion	Trigonal Bipyramid	5	Non-Chelate		S-Donor	P-Donor	

333	**PEXFEE**	393	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
334	**PIGRIH**	394	Discrete Molecule	Seesaw	4	Metal Halide Only	Bromine
335	**PIHJIA**	395	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
336	**PIHJOG**	396	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
337	**PIHJUM**	397	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
338	**PIMCIZ**	398	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
339	**PIMCIZ01**	399	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
340	**PIQCID**	400	Polymer Through Anion	T-Shape	3	Non-Chelate	C-Donor
		401	Polymer Through Anion	Square Planar	4	Non-Chelate	C-Donor
341	**PIZLIV**	402	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
342	**PODWOU**	403	Tetramer Through Anion	D-Pentagonal Bipyramid	7	Chelate	O-Donor
		404	Tetramer Through Anion	D-Trigonal Bipyramid	5	Chelate	O-Donor
343	**POLKEG**	405	Discrete Molecule	Hexagonal Bipyramid	8	Chelate	O-Donor
344	**POLLEH**	406	Discrete Molecule	T-Shape	6	Chelate	O-Donor
345	**POMGOO**	407	Discrete Molecule	Seesaw	4	Chelate	N-Donor
346	**POMGOO01**	408	Discrete Molecule	Seesaw	4	Chelate	N-Donor
347	**POPHIL**	409	Polymer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Bromine
348	**PORLUE**	410	Discrete Molecule	Seesaw	4	Chelate	P-Donor / S-Donor
349	**PURWEF**	411	Discrete Molecule	Seesaw	4	Chelate	N-Donor
350	**QACFIJ**	412	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
351	**QAHWIH**	413	Discrete Molecule	Tetrahedral	4	Chelate	N-Donor
352	**QAYTOZ**	414	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
353	**QEMDUH**	415	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
		416	Polymer Through Anion	Seesaw	4	Metal Halide Only	Bromine
354	**QEPXAK**	417	Polymer Through Anion	Trigonal Bipyramid	5	M-M / Non-Chelate	Cupper
355	**QEPXEO**	418	Polymer Through Anion	Tetrahedral	4	M-M / Non-Chelate	Cupper
356	**QEPZAN**	419	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
357	**QEVMAG**	420	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
358	**QEVMIO**	421	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
359	**QEVMUA**	422	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
360	**QEZPES**	423	Dimer Through Ligand	Seesaw	4	Non-Chelate	O-Donor / N-Donor
361	**QEZPIW**	424	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
362	**QEZPOC**	425	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
363	**QEZPUI**	426	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
364	**QEZQAP**	427	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
365	**QIQHUT**	428	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
366	**QIVWAU**	429	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
367	**QODHEW**	430	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
368	**QODHEW01**	431	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
369	**QOPNAM**	432	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Bromine
370	**QOQCOO**	433	Polymer Through Anion	D-Octahedral	6	Non-Chelate	S-Donor
		434	Polymer Through Anion	T-Shape	5	Non-Chelate	S-Donor
		435	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
371	**QOTJAL**	436	Discrete Molecule	Seesaw	4	Chelate	N-Donor
372	**QUMREX**	437	Tetramer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Bromine
		438		Seesaw	4	Chelate	N-Donor
373	**QUMSOG**	439	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	O-Donor
374	**QUMTOI**	440	Polymer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor
375	**QUMTUO**	441	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
376	**QUMVEA**	442	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
377	**QUPBOU**	443	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
378	**QUVWAH**	444	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor
379	**QUVWEL**	445	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
380	**QUVWOV**	446	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor
381	**QUVZUE**	447	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
382	**QUZFAU**	448	Polymer Through Anion	Square Planar	4	Non-Chelate	N-Donor
383	**RACQIV**	449	Trimer Through Ligand	Seesaw	4	Non-Chelate	Tellurium
		450	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
384	**RADDOS**	451	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
		452	Polymer Through Ligand	D-Square Pyramid	5	Chelate	N-Donor
385	**RAMJEV**	453	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
386	**RASGEY**	454	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor

		455	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		456	Polymer Through Anion	Trigonal Pyramid	4	Non-Chelate	S-Donor	
387	**RAWTAL**	457	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
388	**REPFEZ**	458	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
389	**REZWOJ**	459	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
390	**REZWUP**	460	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
391	**RIHHAS**	461	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
392	**RITMAI**	462	Discrete Molecule	T-Shape	3	Non-Chelate	P-Donor	
393	**RITYUQ**	463	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
394	**RITZAX**	464	Polymer Through Anion	Square Pyramid	5	Non-Chelate	S-Donor	
395	**RODXEO**	465	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
396	**ROMFIK**	466	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
397	**RORREV**	467	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
398	**ROSDOS**	468	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	P-Donor
399	**RUKGEJ**	469	Discrete Molecule	Hexagonal Bipyramid	8	Chelate	O-Donor	
400	**RUYWAL**	470	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	N-Donor
401	**RUYWOZ**	471	Polymer Through Ligand	Square Pyramid	5	Non-Chelate	O-Donor	N-Donor
402	**SAFBUY**	472	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
403	**SAFCAD**	473	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	S-Donor
404	**SAJVIJ**	474	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
405	**SEDPOI**	475	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
406	**SEGTAA**	476	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
407	**SEMGEY**	477	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
408	**SIFCAL**	478	Discrete Molecule	Trigonal	3	Metal Halide Only	Bromine	
409	**SINHII**	479	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
410	**SIRYIC**	480	Discrete Molecule	Seesaw	4	Chelate	S-Donor	
411	**SOHMEJ**	481	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
412	**SOPDOQ**	482	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
413	**SUSWUY**	483	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor	
414	**SUZCOF**	484	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor	
415	**SUZCOF01**	485	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor	
416	**TABYUS**	486	Dimer Through Ligand	T-Shape	3	Non-Chelate	N-Donor	
417	**TAGKIV**	487	Dimer Through Anion	D-Square Pyramid	5	Non-Chelate	S-Donor	
418	**TENNEH**	488	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor	
419	**TEYFEK**	489	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
420	**THFHGB**	490	Polymer Through Anion	Square Pyramid	5	Non-Chelate	O-Donor	
421	**THLHGA**	491	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
422	**TIPZIC**	492	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
423	**TIRSIY**	493	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
424	**TIZNOH**	494	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	O-Donor
425	**TMAHGB**	495	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
426	**TMAHGB01**	496	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
427	**TOBCOD**	497	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
428	**TRPHGB**	498	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
429	**TSCHGB**	499	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
430	**TUTLOL**	500	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
431	**TUYQAH**	501	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
432	**UGUPAO**	502	Dimer Through Ligand	Seesaw	4	Non-Chelate	C-Donor	
433	**UGUPES**	503	Dimer Through Ligand	Seesaw	4	Non-Chelate	C-Donor	
434	**UGUPUH**	504	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
435	**UGUQAO**	505	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
		506	Discrete Molecule	Linear	2	Metal Halide Only	Bromine	
436	**UHABUA**	507	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
437	**UKOTEU**	508	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
438	**UPEWIW**	509	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor	
		510	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
439	**UPUDEP**	511	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
440	**UQUQED**	512	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
441	**USUWOV**	513	Discrete Molecule	Seesaw	4	Chelate	P-Donor	N-Donor
442	**USUXEM**	514	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
443	**USUYIR**	515	Discrete Molecule	Seesaw	4	Chelate	P-Donor	N-Donor
444	**USUYOX**	516	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor	P-Donor
		517	Polymer Through Ligand	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor	P-Donor

445	**USUYUD**	518	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
446	**USUZEO**	519	Polymer Through Ligand	Seesaw	4	Non-Chelate	P-Donor | N-Donor
447	**VAGNEZ**	520	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
448	**VANDOF**	521	Discrete Molecule	Square Planar	4	Non-Chelate	Se-Donor
449	**VAQHIE**	522	Dimer Through Anion	D-Square Pyramid	5	Chelate	O-Donor | N-Donor
450	**VAXGEG**	523	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor
451	**VAYHIO**	524	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor
		525	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
452	**VAZKIR**	526	Polymer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	S-Donor
453	**VEGRUW**	527	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
454	**VEMWUF**	528	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
455	**VEQDOM**	529	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
456	**VEQJAE**	530	Polymer Through Anion	Square Pyramid	5	Metal Halide Only	Bromine
457	**VEVBAZ**	531	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
458	**VIFPAD**	532	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
459	**VOBKED**	533	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
460	**VOFROX**	534	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
461	**VOPXUT**	535	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor
462	**VOVRIJ**	536	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor
463	**VOVSAC**	537	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor
464	**VOZGEW**	538	Dimer Through Anion	T-Shape	3	M-M | Non-Chelate	Iron
465	**VUHCEG**	539	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
466	**VUJYAB**	540	Polymer Through Ligand	Bent	4	Non-Chelate	N-Donor
467	**VUVNOQ**	541	Discrete Molecule	Trigonal	3	Non-Chelate	P-Donor
468	**VUXLIK**	542	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iron
469	**VUXLOQ**	543	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
470	**WAMYUF**	544	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	S-Donor
471	**WAMZAM**	545	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
472	**WAYPAP**	546	Dimer Through Anion	Bent	4	Non-Chelate	P-Donor | Se-donor
473	**WEBZOS**	547	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
474	**WEBZUY**	548	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor
475	**WEDVOQ**	549	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor
476	**WEQMIP**	550	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	N-Donor
		551	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
477	**WIBJUO**	552	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
478	**WIDZIS**	553	Tetramer Through Anion	Seesaw	4	Metal Halide Only	S-Donor
479	**WIVTAY**	554	Dimer Through Anion	T-Shape	3	Non-Chelate	Boron
480	**WODDAU**	555	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
481	**WOGMUB**	556	Dimer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	N-Donor
482	**WOKNUF**	557	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
483	**WOLLUE**	558	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
484	**WOLMAL**	559	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	P-Donor
485	**WONKIT**	560	Dimer Through Anion	D-Square Pyramid	5	Non-Chelate	P-Donor | O-Donor
486	**WOPTUR**	561	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor
487	**WOPVAZ**	562	Dimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	C-Donor
488	**WOPYAD**	563	Discrete Molecule	Seesaw	4	Chelate	C-Donor | P-Donor
489	**WURPOP**	564	Polymer Through Anion	D-Trigonal Bipyramid	5	Metal Halide Only	Bromine
490	**WURXUC**	565	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine
491	**WUZHEF**	566	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
492	**XAHSAB**	567	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
493	**XAHSUX**	568	Discrete Molecule	T-Shape	5	Chelate	N-Donor | O-Donor
494	**XAKHIA**	569	Trimer Through Anion	Square Planar	4	Metal Halide Only	Bromine
		570	Trimer Through Anion	Trigonal Pyramid	4	M-M | Non-Chelate	Platinum
495	**XAKZUG**	571	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
496	**XECXUA**	572	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor | O-Donor
497	**XELQIP**	573	Polymer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	S-Donor
498	**XEMVAO**	574	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine
499	**XEZPAT**	575	Dimer Through Ligand	Seesaw	4	Non-Chelate	P-Donor
500	**XIPWAV**	576	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
501	**XUDHAG**	577	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
502	**XUDHIO**	578	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
503	**XUFDIN**	579	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor

504	**YACDOX**	580	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
505	**YACHIU**	581	Trimer Through Anion	T-Shape	5	Non-Chelate	N-Donor	S-Donor
		582	Trimer Through Anion	D-Tetrahedral (Pyramid)	4	Non-Chelate	N-Donor	S-Donor
506	**YARNEL**	583	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Bromine	
507	**YEJDIB**	584	Discrete Molecule	Seesaw	4	Non-Chelate	Tellurium	
508	**YEVFIO**	585	Discrete Molecule	T-Shape	6	Non-Chelate	C-Donor	
509	**YEZGAL**	586	Polymer Through Anion	Seesaw	4	Non-Chelate	O-Donor	
		587	Polymer Through Anion	T-Shape	5	Metal Halide Only	Bromine	
		588	Polymer Through Anion	T-Shape	3	Metal Halide Only	Bromine	
510	**YODZUM**	589	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Bromine	
511	**YUDZIG**	590	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	S-Donor	
512	**YUHTUR**	591	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
513	**YUNLEZ**	592	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
514	**ZADMAV**	593	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
515	**ZATJOT**	594	Dimer Through Anion	Seesaw	4	Chelate	N-Donor	
516	**ZEFRAF**	595	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
517	**ZEVMEU**	596	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
518	**ZIVXAF**	597	Polymer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
519	**ZIVXEJ**	598	Polymer Through Anion	Seesaw	4	Metal Halide Only	Bromine	
520	**ZUBMOY**	599	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
521	**ZUFREZ**	600	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor	
522	**ZUWJAC**	601	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	

S29. CSD-Analysis for HgI_2 Compounds

Number	Ref. Code	Hits	Polymerization Mode	Geometry	C.N.	Chelation Mode	Donor Atom of Ligand
1	**ATAHAG**	1	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
2	**ATEQAT**	2	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
3	**AVIYUB**	3	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
4	**AVONIK**	4	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
5	**ORUZEI**	5	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
6	**ORUZIM**	6	Polymer Through Ligand	Seesaw	4	Metal Halide Only	Chlorine
7	**UXAZUQ**	7	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
8	**ABIXAM**	8	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
9	**ACAGOC**	9	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
10	**ADIZES**	10	Discrete Molecule	Seesaw	4	Non-Chelate	Tellurium
11	**ADOKOU**	11	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
12	**ADOKUA**	12	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
13	**ADOLAH**	13	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
14	**ADOLEL**	14	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
15	**AFEYIV**	15	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
16	**AFEYOB**	16	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		17	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
17	**AFEYUH**	18	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
18	**AFEZAO**	19	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
19	**AGOMAM**	20	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
20	**AGOMEQ**	21	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
21	**AGOXOK**	22	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
22	**AHOMAL**	23	Discrete Molecule	Seesaw	4	Chelate	Se-donor
23	**AJAJEB**	24	Discrete Molecule	Seesaw	4	Non-Chelate	Se-Donor
24	**AKULUN**	25	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor
25	**AKUMAU**	26	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor
26	**AQAXEX**	27	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
27	**AQEDUX**	28	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
28	**AQEFIN**	29	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
29	**AQEGAG**	30	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
30	**AQEGOU**	31	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
31	**ARUKAZ**	32	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
32	**ARUKED**	33	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
33	**ATOGUL**	34	Discrete Molecule	Seesaw	4	Chelate	S-Donor
34	**AXEDIQ**	35	Dimer Through Anion	Seesaw	4	Non-Chelate	C-Donor

35	**AZATUQ**	36	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
36	**AZEBIQ**	37	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
37	**AZIWUC**	38	Discrete Molecule	Tetrahedral	4	Chelate	N-Donor	
38	**AZODOJ**	39	Polymer Through Ligand	T-Shape	5	Chelate	N-Donor	
39	**BAHKAY**	40	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
40	**BAKJOM**	41	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
41	**BAKKED**	42	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
42	**BAKNOQ**	43	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
43	**BAKREK01**	44	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
44	**BEJLEH**	45	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
45	**BEJLEH01**	46	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
46	**BEJLEH02**	47	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
47	**BEKDOL**	48	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
48	**BENMAJ**	49	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor	N-Donor
49	**BESJEP**	50	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
50	**BETPEV**	51	Discrete Molecule	Trigonal	3	Metal Halide Only	Iodine	
51	**BEVDUD**	52	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
52	**BIFHOO**	53	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
53	**BIYYIS**	54	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
54	**BOLLET**	55	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
55	**BONJEU**	56	Discrete molecule	Trigonal Pyramid	4	Non-Chelate	C-Donor	O-Donor
56	**BUBWAY**	57	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		58	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
57	**BUBZAB**	59	polymer through ligand	Seesaw	4	Non-Chelate	N-Donor	
58	**BURLUX**	60	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
59	**BUSGEC**	61	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	
60	**BUTZEX**	62	Polymer Through Anion	D-Square Pyramid	5	Non-Chelate	N-Donor	
		63	Polymer Through Ligand	D-Square Pyramid	5	Non-Chelate	N-Donor	
61	**BUVZUP**	64	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
62	**CABFIX**	65	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
63	**CADCEQ**	66	Discrete molecule	Seesaw	4	Chelate	P-Donor	
64	**CAGPIK**	67	Discrete Molecule	D-Tetrahedral (Py)	4	Chelate M-M	N-Donor	Rhodium
65	**CALYOD**	68	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
66	**CALYUJ**	69	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
67	**CAMBIB**	70	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
68	**CAMBOH**	71	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
69	**CAYBIN**	72	Discrete Molecule	Seesaw	4	Chelate	P-Donor	
70	**CECYOZ**	73	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
71	**CECYUF**	74	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
72	**CEKHOR**	75	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor	
73	**CEKJEJ**	76	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
74	**CEKYUO**	77	Discrete Molecule	D-Tetrahedral (Py)	4	Chelate	N-Donor	
75	**CELYAT**	78	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Tellurium	
76	**CETJIV**	79	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		80	Tetramer Through Anion	D-Octahedral	6	Non-Chelate	N-Donor	
77	**CIDLIM**	81	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
78	**CIDMAF**	82	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
79	**CIDMOT**	83	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
80	**CINPAQ**	84	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
81	**CIPTAW**	85	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor	
82	**CIYZOA**	86	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
		87	Polymer Through Ligand	Linear	2	Non-Chelate	N-Donor	
83	**CIZBAP**	88	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
84	**CNPSHG**	89	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
85	**COLRUR**	90	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
86	**CORLAX**	91	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
87	**CORLEB**	92	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only	Iodine	
		93	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
88	**CUDQUN**	94	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
89	**CUDRIC**	95	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
90	**CUDWIH**	96	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
91	**CUGFIT**	97	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	

92	**CUGFIT01**	98	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
93	**CUSBIC**	99	Discrete Molecule	T-Shape	5	Chelate	N-Donor
94	**CUSSAL**	100	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor
95	**CUYFAE**	101	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
96	**DAHYES**	102	Discrete Molecule	Seesaw	4	Chelate	N-Donor
97	**DAKLIM**	103	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
98	**DAXPAV**	104	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
99	**DEBHID**	105	Discrete Molecule	Seesaw	4	Chelate	N-Donor
100	**DEBMEC**	106	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
101	**DEBWIR**	107	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
102	**DENLEO**	108	Tetramer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
103	**DENZUR**	109	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate	O-Donor
104	**DENZUR01**	110	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate	O-Donor
105	**DENZUR02**	111	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate	O-Donor
106	**DENZUR03**	112	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate	O-Donor
107	**DEPDUY**	113	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
108	**DEYTAD**	114	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
109	**DICGOL**	115	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
110	**DILTOH**	116	Discrete Molecule	Trigonal	3	Metal Halide Only	Iodine
111	**DIRCEO**	117	Discrete Molecule	Seesaw	4	Chelate	N-Donor
112	**DISPUR**	118	Discrete Molecule	Seesaw	4	Chelate	Se-Donor
113	**DISQAY**	119	Dimer Through Ligand	Seesaw	4	Chelate	Se-Donor
114	**DITCUE**	120	Discrete Molecule	Seesaw	4	Chelate	N-Donor
115	**DITPHG**	121	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
116	**DODJUC**	122	Polymer Through Ligand	D-Trigonal Bipyramid	5	Non-Chelate	O-Donor / N-Donor
117	**DOHBOR**	123	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
118	**DOXYEU**	124	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
119	**DUFHOB10**	125	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
120	**DUGCEN**	126	Discrete Molecule	D-Square Pyramid	5	Chelate / M-M	N-Donor / C-Donor / Iron
121	**DUGDOY**	127	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
122	**DUKGUM**	128	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
123	**DURROY**	129	Discrete Molecule	Seesaw	4	Chelate	N-Donor
124	**DUWSEU**	130	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
125	**DUWVOI**	131	Tetramer Through Anion	Trigonal Bipyramid	5	Non-Chelate	O-Donor / C-Donor / N-Donor
		132	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
126	**DUWVUO**	133	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
127	**DUWWAV**	134	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
128	**DUXKAI**	135	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
129	**DUZFIN**	136	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
130	**EAHIHG**	137	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
		138	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
131	**ECIYUL**	139	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
		140	Polymer Through Ligand	Tetrahedral	4	Metal Halide Only	Iodine
132	**EDUVOP**	141	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
133	**EFIGIL**	142	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
134	**EFIGOR**	143	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
135	**EIMTIM**	144	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
136	**EJAGUS**	145	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
137	**EJOZIM**	146	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
138	**EJOZUY**	147	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
139	**EJOZUY01**	148	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
140	**EJUBEQ**	149	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
141	**EJUBIU**	150	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
142	**EJUBOA**	151	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
143	**EJUBOA01**	152	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
144	**EJUBUG**	153	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
145	**ELEWAU**	154	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		155	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
146	**ELEWEY**	156	Polymer Through Anion	T-Shape	3	Non-Chelate	N-Donor
		157	Polymer Through Ligand	Trigonal Pyramid	3	Non-Chelate	N-Donor
		158	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
147	**ELURAG**	159	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor
		160	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor

148	**EMIFOX**	161	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
149	**EMINOF**	162	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
150	**ENORUV**	163	Discrete Molecule	T-Shape	5	Chelate	O-Donor	
151	**ENTIHG**	164	Polymer Through Anion	Trigonal Bipyramid	4	Non-Chelate	N-Donor	
		165	Polymer Through Anion	Tetrahedral	4	Non-Chelate	N-Donor	
152	**EROLIG**	166	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
		167	Polymer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
153	**ERUWUK**	168	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
154	**ERUXAR**	169	Dimer Through Anion	Seesaw	4	Non-Chelate	S-Donor	
		170	Dimer Through Anion	T-Shape	3	Non-Chelate	S-Donor	
155	**ERUXEV**	171	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
156	**EWOREN**	172	Dimer Through Ligand	T-Shape	3	Non-Chelate	N-Donor	
157	**EWOREN01**	173	Dimer Through Anion	Seesaw	4	Non-Chelate	N-Donor	
158	**EXEROO**	174	Tetramer Through Anion	Square Pyramid	5	Chelate	O-Donor	P-Donor
		175	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
159	**EYAFUG**	176	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
160	**EYUXAY**	177	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
161	**FAGGUR**	178	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
162	**FAHWES**	179	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
163	**FAHXOE**	180	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
164	**FAQVOJ**	181	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
165	**FARXON**	182	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor	
166	**FAXGUI**	183	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
167	**FAXHUJ**	184	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
168	**FAXKEV**	185	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
169	**FAYKEW**	186	Discrete Molecule	Seesaw	4	Chelate	O-Donor	
170	**FELZEC**	187	Discrete Molecule	Seesaw	4	Chelate	S-Donor	
171	**FIJPAQ**	188	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
172	**FIPWUX**	189	Discrete Molecule	Seesaw	4	Chelate	N-Donor	S-Donor
173	**FIPXOS**	190	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	S-Donor
174	**FOTNEJ**	191	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor	
		192	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
175	**FOVCIE**	193	Tetramer Through Anion	Trigonal Bipyramid	5	Chelate	O-Donor	S-Donor
		194	Tetramer Through Ligand	Tetrahedral	4	Chelate	O-Donor	S-Donor
176	**FOVCUQ**	195	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
177	**FOZXAV**	196	Dimer Through Anion	Seesaw	4	Non-Chelate	Chlorine	
178	**FOZXEZ**	197	Discrete Molecule	Seesaw	4	Chelate	C-Donor	
179	**FOZXID**	198	Discrete Molecule	Seesaw	4	Chelate	C-Donor	
180	**FOZXOJ**	199	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
181	**FUBVOP**	200	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
182	**FULCAQ**	201	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor	
183	**FUZLIW**	202	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor	O-Donor
184	**GAHPIR**	203	Dimer Through Ligand	T-Shape	5	Chelate	N-Donor	
185	**GASTAV**	204	Discrete Molecule	Seesaw	4	Non-Chelate	Se-Donor	
186	**GEHXIC**	205	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
187	**GEHXOI**	206	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
188	**GEQCIP**	207	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
189	**GEQCOV**	208	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
190	**GEZKIH**	209	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
191	**GEZKON**	210	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
192	**GICKAG**	211	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
193	**GIDFAB**	212	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
194	**GIRQAB**	213	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	S-Donor
		214	Polymer Through Anion	Trigonal	3	Metal Halide Only	Iodine	
		215	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
195	**GITJAW**	216	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
196	**GIZNIN**	217	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
197	**GODDUY**	218	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
198	**GODFAG**	219	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
199	**GOFKIW**	220	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
200	**GOGHEQ**	221	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
201	**GOGHUH**	222	Dimer Through Anion	T-Shape	3	Non-Chelate	C-Donor	
202	**GOHZOS**	223	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	S-Donor

203	**GUBBEK**	224	Discrete Molecule	Trigonal	3	Metal Halide Only		Iodine	
		225	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
204	**GUGVEJ**	226	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		Chlorine	
205	**GULKUU**	227	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	
206	**GUTLOX**	228	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
207	**GUTLUD**	229	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	N-Donor
208	**GUVGAG**	230	Polymer Through Ligand	Seesaw	4	Non-Chelate		Se-Donor	
209	**HAGZAR**	231	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
210	**HAVCIS**	232	Discrete Molecule	T-Shape	5	Chelate		O-Donor	N-Donor
211	**HEDTUF**	233	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor	
212	**HEFZIC**	234	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
213	**HGITUR**	235	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
214	**HGTXZO**	236	Discrete Molecule	Hexagonal Bipyramid	8	Chelate		N-Donor	O-Donor
215	**HIGRAS**	237	Polymer Through Anion	Square Planar	4	Metal Halide Only		Iodine	
216	**HIPTUV**	238	Trimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor	
		239	Trimer Through Anion	Tetrahedral	4	Non-Chelate		C-Donor	
217	**HIRTOR**	240	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
218	**HIRTUX**	241	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
219	**HIRVAF**	242	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
220	**HIYMAE**	243	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
221	**HIYMEI**	244	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
222	**HIYMIM**	245	Polymer Through Ligand	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor	
		246	Polymer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor	
223	**HIYMOS**	247	Polymer Through Ligand	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor	
		248	Polymer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate		N-Donor	
224	**HOKTOR**	249	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
225	**HOLHOH**	250	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
226	**HOLHUN**	251	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
227	**HOSPAI**	252	Discrete Molecule	T-Shape	5	Chelate		O-Donor	N-Donor
228	**HOSPEM**	253	Discrete Molecule	T-Shape	5	Chelate		O-Donor	N-Donor
229	**HOSPIQ**	254	Polymer Through Ligand	T-Shape	5	Chelate		O-Donor	N-Donor
		255	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
230	**HOSPOW**	256	Tetramer Through Ligand	T-Shape	5	Chelate		O-Donor	N-Donor
		257	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
231	**HOTBOJ**	258	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
		259	Polymer Through Anion	Linear	2	Metal Halide Only		Iodine	
232	**HOTCEA**	260	Discrete Molecule	T-Shape	3	Non-Chelate		N-Donor	
233	**HOYMEP**	261	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
234	**HOYMIT**	262	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
235	**HOYMOZ**	263	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
236	**HOYMUF**	264	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
237	**HUBCAK**	265	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
238	**HUBMEY**	266	Discrete Molecule	T-Shape	5	Chelate		N-Donor	O-Donor
239	**HUBMIC**	267	Discrete Molecule	Seesaw	4	Non-Chelate		N-donor	
240	**HUCHET**	268	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
241	**HUCZIQ**	269	Dimer Through Anion	Anti-Prism	6	Non-Chelate	M-M	C-Donor	Molybdenum
242	**HUSNUG**	270	Polymer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
243	**IBAFOI**	271	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor	
244	**IBZTHG**	272	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
245	**ICEQUE**	273	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
246	**IDANAE**	274	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
247	**IETHSH**	275	Discrete Molecule	Seesaw	4	Chelate		S-Donor	
248	**IETHSH01**	276	Discrete Molecule	Seesaw	4	Chelate		S-Donor	
249	**IGENAK**	277	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
250	**IHGTUR**	278	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
251	**IMTSHG**	279	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
252	**INOZIU**	280	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
253	**INOZOA**	281	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
254	**IPESHG**	282	Discrete Molecule	Seesaw	4	Chelate		P-Donor	
255	**IQIJEY**	283	Dimer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
256	**IQOGOK**	284	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
257	**IQUJUZ**	285	Discrete Molecule	T-Shape	5	Chelate	M-M	O-Donor	Zinc
258	**IROMIL**	286	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	

259	**ISAVAA**	287	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
260	**ISERUU**	288	Discrete Molecule	T-Shape	5	Non-Chelate	O-Donor
261	**ISOKIL**	289	Discrete Molecule	D-Trigonal Bipyramid	5	Non-Chelate	O-Donor, C-Donor
262	**ISOKOR**	290	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
263	**ISOKUX**	291	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
264	**ISOLAE**	292	Discrete Molecule	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor
265	**ISOLEI**	293	Dimer Through Anion	Anti-Prism	6	Non-Chelate	O-Donor, C-Donor
		294	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
266	**IWEVIP**	295	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
267	**IZIRIS**	296	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
268	**JADLAB10**	297	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor
		298	Dimer Through Anion	Tetrahedral	4	Non-Chelate	P-Donor
269	**JAHCOK**	299	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor
270	**JAHCOK01**	300	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-donor
271	**JAHCOK02**	301	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-donor
272	**JAPHAK**	302	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-donor
273	**JAPHEO**	303	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
274	**JAPJIU**	304	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
275	**JAPJOA**	305	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
276	**JAPKIV**	306	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
277	**JAPKOB**	307	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
278	**JARCAH**	308	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		309	Discrete Molecule	Linear	2	Metal Halide Only	Iodine
279	**JATVEF**	310	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
280	**JETKEY**	311	Dimer Through Ligand	Tetrahedral	4	Metal Halide Only	Iodine
281	**JEWGUN**	312	Dimer Through Anion	D-Trigonal Bipyramid	5	Metal Halide Only	Iodine
		313	Discrete Molecule	Trigonal Pyramid	3	Non-Chelate	O-Donor
282	**JIBHOR**	314	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		315	Discrete Molecule	Linear	2	Metal Halide Only	Iodine
283	**JIBHOR01**	316	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		317	Discrete Molecule	Linear	2	Metal Halide Only	Iodine
284	**JIFNOB**	318	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
285	**JIGXEC**	319	Discrete Molecule	Seesaw	4	Metal Halide Only	Iodine
286	**JINZAH**	320	Polymer Through Anion	D-Octahedral	6	Non-Chelate	P-Donor
		321	Polymer Through Anion	Tetrahedral	4	Non-Chelate	P-Donor
287	**JIQYEO**	322	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
288	**JIQYEO01**	323	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
289	**JIQYIS**	324	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
290	**JIQYIS01**	325	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
291	**JOKHEW**	326	Polymer Through Ligand	Tetrahedral	4	Metal Halide Only	Iodine
292	**JOKHIA**	327	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
293	**JOKHIA01**	328	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
294	**JOMJOK**	329	Tetramer Through Ligand	Seesaw	4	Non-Chelate	C-Donor
		330	Tetramer Through Ligand	T-Shape	3	Non-Chelate	C-Donor
295	**JOMJOK10**	331	Tetramer Through Ligand	Seesaw	4	Non-Chelate	C-Donor
		332	Tetramer Through Ligand	T-Shape	3	Non-Chelate	C-Donor
296	**JOMVEO**	333	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
297	**JOTJIL**	334	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
298	**JOVKOU**	335	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
299	**JULSAM**	336	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
300	**KANLES**	337	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
301	**KEJVOK**	338	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor, S-Donor
302	**KEMVAA**	339	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
303	**KEMVEE**	340	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
304	**KERYOX**	341	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
305	**KEZBOH**	342	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
306	**KIQKUS**	343	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
307	**KOBVUT**	344	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
308	**KOBWAA**	345	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor, O-Donor
309	**KOBWEE**	346	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
310	**KOFXAE**	347	Discrete Molecule	Trigonal	3	M-M, Non-Chelate	Iron
311	**KOPPIO**	348	Dimer Through Anion	D-Tetrahedral (Py)	4	M-M, Non-Chelate	Nickel
312	**KOXROG**	349	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor

313	**KUCWOW**	350	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
314	**KUJWET**	351	Discrete Molecule	Seesaw	6	Chelate	N-Donor	
315	**KUJXAQ**	352	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor	
316	**KULPIR**	353	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
317	**KUNNIS**	354	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
318	**KUNNIS01**	355	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
319	**LACDAW**	356	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
320	**LACTOA**	357	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
321	**LADJIL**	358	Discrete Molecule	Seesaw	4	Chelate	P-Donor	C-Donor
322	**LAMVEC**	359	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
323	**LAQGIT**	360	Discrete Molecule	Trigonal	3	Non-Chelate	S-Donor	
324	**LARLIB**	361	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
325	**LARLOH**	362	Trimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
326	**LECDED**	363	Discrete Molecule	Tetrahedral	4	Non-Chelate	Iodine	
327	**LEHGAI**	364	Discrete Molecule	T-Shape	5	Non-Chelate	O-Donor	N-Donor
328	**LEHZIJ**	365	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
329	**LEKSAX**	366	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
330	**LEKTEC**	367	Discrete Molecule	Seesaw	4	Chelate	N-Donor	
331	**LEQLAW**	368	Polymer Through Ligand	seesaw	4	Non-Chelate	N-Donor	
332	**LEQLEA**	369	Dimer Through Anion	Seesaw	4	Metal Halide Only	Chlorine	
333	**LEQPII**	370	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	Chlorine
334	**LEQRAB**	371	Dimer Through Ligand	T-Shape	3	Non-Chelate	N-Donor	
335	**LEQSAC**	372	Polymer Through Ligand	Seesaw	4	Chelate	N-Donor	
		373	Polymer Through Anion	Seesaw	4	Chelate	N-Donor	
336	**LEXBOG**	374	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor	
337	**LIBNOZ**	375	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
338	**LIGFEO**	376	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
339	**LIGFIS**	377	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
340	**LINYEO**	378	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
341	**LIVKOS**	379	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
342	**LOLFOI**	380	Polymer Through Anion	Square Pyramid	5	Chelate	S-Donor	N-Donor
		381	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
343	**LOMPAG**	382	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor	
344	**LOMPEK**	383	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
345	**LOWKAL**	384	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
346	**LOWKOZ**	385	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
347	**LUHDOJ**	386	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
348	**LUTWON**	387	Polymer Through Anion	Square Planar	4	Non-Chelate	O-Donor	
		388	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor	
349	**LUZVOS**	389	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
350	**MAJHEM**	390	Dimer Through Anion	T-Shape	3	Metal Halide Only	Iodine	
351	**MASYIO**	391	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
352	**MASYIO01**	392	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
353	**MEPFIX**	393	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
354	**MESWEM**	394	Polymer Through Anion	Trigonal Bipyramid	5	Non-Chelate	S-Donor	
355	**MESWIQ**	395	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
356	**MESZEQ**	396	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor	
357	**MIHBOV**	397	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine	
358	**MIQTEN**	398	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor	
		399	Polymer Through Anion	Tetrahedral	4	Non-Chelate	S-Donor	
359	**MIYSIX**	400	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
360	**MOLWAL**	401	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
361	**MOVDIM**	402	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor	
362	**MOWGAH**	403	Dimer Through Ligand	T-Shape	3	Non-Chelate	N-Donor	
363	**NABJAC**	404	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
364	**NABJEG**	405	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
365	**NAZMAE**	406	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor	
366	**NAZRAJ**	407	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor	
367	**NEBZAV**	408	Dimer Through Anion	D-Tetrahedral (Py)	4	M-M	Non-Chelate	Platinum
368	**NEFLAL**	409	Dimer Through Ligand	T-Shape	5	Chelate	O-Donor	
369	**NEJXEF**	410	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
370	**NEJXIJ**	411	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine	
371	**NEPGAR**	412	Dimer Through Ligand	Seesaw	4	Chelate	N-donor	

372	**NETHEA**	413	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-donor	
373	**NEZDUR**	414	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
374	**NIKBUF**	415	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-donor	
375	**NIMBES**	416	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		S-donor	
		417	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-donor	
376	**NIVBEZ**	418	Discrete Molecule	Prism	6	Chelate	M-M	N-Donor	Iron
377	**NOHZAM**	419	Discrete Molecule	Seesaw	4	Chelate		N-donor	
378	**NOMSEO**	420	Discrete Molecule	T-Shape	5	Chelate	M-M	Chlorine	Platinum
379	**NOMSIS**	421	Dimer Through Anion	D-Tetrahedral (Py)	4	Chelate		Chlorine	
380	**NOQVIY**	422	Discrete Molecule	Seesaw	4	Non-Chelate		S-donor	
381	**NUBXOX**	423	Trimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
		424	Trimer Through Anion	T-Shape	3	Metal Halide Only		Iodine	
382	**NUXGAP**	425	Discrete Molecule	Seesaw	4	Non-Chelate		P-donor	
383	**NUXWOT**	426	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-donor	
384	**OBAPUE**	427	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-donor	
385	**OBAQEP**	428	Dimer Through Anion	Tetrahedral	4	Non-Chelate		S-donor	
		429	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-donor	
386	**OBATIU**	430	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
387	**OBATOA**	431	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
388	**OBOZUA**	432	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-donor	
389	**OBUCEU**	433	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-donor	
390	**OBUMAA**	434	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
391	**ODISEA**	435	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
392	**ODISOK**	436	polymer through ligand	seesaw	4	Non-Chelate		n-donor	
393	**ODISUQ**	437	Polymer Through Ligand	seesaw	4	Non-Chelate		N-Donor	
394	**ODITAX**	438	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
395	**OFOROR**	439	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor	
396	**OFORUY**	440	Tetramer Through Anion	Seesaw	4	Non-Chelate		Se-Donor	
397	**OHUTAM**	441	Discrete Molecule	Seesaw	4	Chelate		N-Donor	
398	**OJEPIE**	442	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor	
		443	Polymer Through Anion	D-Octahedral	6	Non-Chelate		S-Donor	
399	**OLAFOY**	444	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Iodine	
400	**OLAFUE**	445	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Iodine	
401	**OMUVEY**	446	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
402	**ONEZEO**	447	Discrete Molecule	Seesaw	4	Non-Chelate		N-Donor	
403	**ONIHUQ**	448	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
404	**ONINOQ**	449	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
405	**ONOZAU**	450	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	
406	**ONOZAU01**	451	Discrete Molecule	Seesaw	4	Non-Chelate		Se-Donor	
407	**OQALOI**	452	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
		453	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
408	**OQALUO**	454	Tetramer Through Anion	Seesaw	4	Non-Chelate		N-Donor	
		455	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
409	**OQAMAV**	456	Trimer Through Anion	Tetrahedral	4	Non-Chelate		N-Donor	
		457	Trimer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor	
410	**PAIOHG**	458	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
411	**PEDPOF**	459	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor	
412	**PEDPOF01**	460	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor	
413	**PEGXUV**	461	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor	
414	**PENNUR**	462	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
415	**PEVYOF**	463	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
416	**PEVYUL**	464	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
417	**PEXHAC**	465	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
418	**PIFWEI**	466	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
419	**PIJRAB**	467	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
420	**PIJVOU**	468	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		P-Donor	
421	**PIRYUL**	469	Trimer Through Anion	T-Shape	3	Metal Halide Only		Iodine	
		470	Trimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine	
422	**PIZLOB**	471	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor	
423	**PODWEK**	472	Discrete Molecule	T-Shape	5	Chelate		N-Donor	
424	**POHXUF**	473	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor	
425	**POLKUW**	474	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor	
426	**PORMAL**	475	Dimer Through Ligand	Seesaw	4	Non-Chelate		P-Donor	C-Donor

427	**POTPAP**	476	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
428	**PPENHG**	477	Polymer Through Ligand	Seesaw	4	Non-Chelate	P-Donor
429	**PUFBOI**	478	Trimer Through Anion	T-Shape	3	Non-Chelate	C-Donor
		479	Trimer Through Anion	Tetrahedral	4	Non-Chelate	C-Donor
430	**PUFBUO**	480	Polymer Through Anion	Square Pyramid	5	Non-Chelate	C-Donor
		481	Polymer Through Anion	Tetrahedral	4	Non-Chelate	C-Donor
431	**PUKLOW**	482	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
432	**QAHNIX**	483	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
433	**QAMXIL**	484	Polymer Through Ligand	Seesaw	4	Non-Chelate	O-Donor
		485	Discrete Molecule	Linear	2	Metal Halide Only	Iodine
434	**QAPTIM**	486	Discrete Molecule	T-Shape	5	Chelate	N-Donor
435	**QAVFEA**	487	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
436	**QAVFEA01**	488	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
437	**QEVMEK**	489	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	
438	**QEZQET**	490	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
439	**QEZQIX**	491	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
440	**QEZQOD**	492	Polymer Through Anion	Square Pyramid	5	Non-Chelate	N-Donor
441	**QIJXIQ**	493	Discrete Molecule	Trigonal	3	Non-Chelate	S-Donor
442	**QIJXIQ01**	494	Discrete Molecule	Trigonal	3	Non-Chelate	S-Donor
443	**QIVWIC**	495	Discrete Molecule	Seesaw	4	Chelate	N-Donor
444	**QOFQEH**	496	Discrete Molecule	Trigonal	3	Metal Halide Only	Iodine
445	**QOKXUJ**	497	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
446	**QOTLOB**	498	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
447	**QUMRIB**	499	Tetramer Through Anion	Seesaw	4	Chelate	N-Donor
		500	Tetramer Through Anion	Trigonal Bipyramid	5	Metal Halide Only	Iodine
448	**QUMSUM**	501	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	O-Donor
449	**QUVWUB**	502	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
450	**QUVXAI**	503	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
451	**QUZFEY**	504	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
		505	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
452	**RACXID**	506	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
453	**RAHDIP**	507	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
454	**RAHDOV**	508	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
455	**RAHDUB**	509	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
456	**RAHPIB**	510	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
457	**RAJJET**	511	Tetramer Through Anion	D-Square Pyramid	5	Non-Chelate	O-Donor, N-Donor
		512	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
458	**RAMJIZ**	513	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
459	**RAMSON**	514	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
460	**RAWTEP**	515	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
461	**REGVUV**	516	Tetramer Through Anion	Seesaw	4	Metal Halide Only	Iodine
		517	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
462	**RESHUT**	518	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
		519	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
463	**REZWID**	520	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
464	**RIPPIQ**	521	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
465	**RIPPOW**	522	Discrete Molecule	Seesaw	4	Non-Chelate	C-Donor
466	**RIZNAP**	523	Dimer Through Anion	Seesaw	4	Non-Chelate	Se-Donor
467	**ROBVUA**	524	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
468	**ROBWEL**	525	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
469	**RODMUT**	526	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
470	**RODNEE**	527	Tetramer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
471	**RODVIQ**	528	Discrete Molecule	Seesaw	4	Chelate	N-Donor
472	**RUMWIG**	529	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
473	**RUQHAM**	530	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor
474	**RUXBUJ**	531	Dimer Through Anion	D-Square Pyramid	5	Chelate	N-Donor
		532	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
475	**RUYWEP**	533	Polymer Through Anion	D-Trigonal Bipyramid	5	Non-Chelate	N-Donor, O-Donor
476	**RUYWUF**	534	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
477	**SARBOC**	535	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
478	**SAYQAK**	536	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
479	**SCPIHG**	537	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
480	**SEGRUT**	538	Discrete Molecule	Seesaw	4	Chelate	N-Donor

481	**SEGSAA**	539	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
482	**SEGTEE**	540	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Iodine		
483	**SESMUZ**	541	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
484	**SINHOO**	542	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
485	**SIRYEY**	543	Tetramer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
486	**SODXOY**	544	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
487	**SUFSAP**	545	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Iodine		
488	**SUVZOZ**	546	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
489	**TACJUC**	547	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
490	**TAHLEV**	548	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
491	**TAHLEV01**	549	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
492	**TAJCEN**	550	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
493	**TAPFUM**	551	Dimer Through Ligand	Seesaw	4	Non-Chelate		S-Donor	N-Donor	
494	**TAWREP**	552	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
495	**TENDAR**	553	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
496	**TEWZOM**	554	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
497	**TIBCUE**	555	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor		
498	**TIBDAL**	556	Dimer Through Ligand	Seesaw	4	Chelate		N-Donor		
499	**TIMXUJ**	557	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
500	**TINWUI**	558	Dimer Through Anion	D-Pentagonal	7	Chelate	M-M	C-Donor	N-Donor	Iron
		559	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
501	**TIPZOI**	560	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
		561	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
502	**TIPZUO**	562	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
		563	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
503	**TIZFUE**	564	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
504	**TIZNUN**	565	Discrete Molecule	Linear	2	Metal Halide Only		Iodine		
505	**TMAIHG10**	566	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
506	**TMAIHG11**	567	Polymer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
507	**TMSHGI**	568	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
508	**TMSHGI01**	569	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
509	**TMSHGI02**	570	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
510	**TOJDAX**	571	Discrete Molecule	Anti-Prism	6	Chelate	M-M	C-Donor	N-Donor	Iron
511	**TORNUK**	572	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate		O-Donor		
512	**TPHGDI10**	573	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		C-Donor		
513	**TUHGIN**	574	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
514	**TUYFUO**	575	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
515	**TUZCAT**	576	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
516	**TUZCEX**	577	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
517	**TUZCIB**	578	Polymer Through Anion	Seesaw	4	Metal Halide Only		Iodine		
		579	Polymer Through Anion	Trigonal Pyramid	4	Metal Halide Only		Iodine		
518	**UCEYIL**	580	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor		
519	**UCEYOR**	581	Dimer Through Anion	Tetrahedral	4	Metal Halide Only		Iodine		
		582	Dimer Through Anion	Linear	2	Metal Halide Only		Iodine		
520	**UFOMEH**	583	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
521	**UHABEK**	584	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
522	**UHABIO**	585	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
523	**UHABIO01**	586	Discrete Molecule	Seesaw	4	Non-Chelate		S-Donor		
524	**UHABOU**	587	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
525	**UJABAK**	588	Polymer Through Anion	Square Pyramid	5	Non-Chelate		N-Donor		
		589	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate		N-Donor		
526	**UJEROQ**	590	Discrete Molecule	T-Shape	5	Non-Chelate		O-Donor	P-Donor	
527	**UJEROQ01**	591	Discrete Molecule	T-Shape	5	Non-Chelate		O-Donor	P-Donor	
528	**UJOQIT**	592	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
529	**UJOQIT01**	593	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
530	**UKOTIY**	594	Discrete Molecule	Tetrahedral	4	Metal Halide Only		Iodine		
531	**ULADUG**	595	Dimer Through Anion	D-Tetrahedral (Py)	4	Chelate		N-Donor		
532	**ULAFAO**	596	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
533	**ULAFES**	597	Polymer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		
534	**ULAWUA**	598	Polymer Through Anion	Seesaw	4	Non-Chelate		S-Donor		
		599	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate		S-Donor		
535	**ULAXIP**	600	Discrete Molecule	Seesaw	4	Chelate		N-Donor		
536	**URITIZ**	601	Dimer Through Ligand	Seesaw	4	Non-Chelate		N-Donor		

537	**USUXIQ**	602	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor
538	**UTUFIZ**	603	Hexamer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
539	**UZEPAR**	604	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
540	**UZEZIJ**	605	discrete molecule	Tetrahedral	4	Metal Halide Only	Iodine
541	**UZEZUV**	606	Polymer Through Ligand	Square Planar	4	Non-Chelate	C-Donor
		607	Polymer Through Ligand	Tetrahedral	4	Non-Chelate	C-Donor
542	**VALSAE**	608	Polymer Through Ligand	D-Octahedral	6	Non-Chelate	O-donor
543	**VANDUL**	609	Discrete Molecule	Square Planar	4	Non-Chelate	Se-Donor
544	**VAQHOK**	610	Dimer Through Anion	Square Pyramid	4	Chelate	N-Donor, O-Donor
545	**VARCIB**	611	Discrete Molecule	Seesaw	4	Chelate	N-Donor
546	**VAXGUW**	612	Discrete Molecule	Trigonal	3	Non-Chelate	P-Donor
547	**VAYHEK**	613	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
548	**VEGSAD**	614	Discrete Molecule	T-Shape	3	Non-Chelate	N-Donor
549	**VEWKOY**	615	Trimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	Se-Donor
		616	Trimer Through Anion	Tetrahedral	4	Non-Chelate	Se-Donor
550	**VIQSOF**	617	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
551	**VOBJUS**	618	Discrete Molecule	Seesaw	4	Chelate	S-Donor
552	**VOBKIH**	619	Polymer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
553	**VOSZAG**	620	Dimer Through Anion	Seesaw	4	M-M, Non-Chelate	Rhenium
554	**VOVROP**	621	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
555	**VOVSEG**	622	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
556	**VUJXUU**	623	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
557	**VUJYUV**	624	Polymer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
558	**VUPWUZ**	625	Dimer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
		626	Discrete Molecule	T-Shape	3	Non-Chelate	S-Donor
559	**VUPXEK**	627	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
560	**VUVNIK**	628	Discrete Molecule	Seesaw	4	Chelate	P-Donor
561	**WAHJIB**	629	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor
562	**WAPKII**	630	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
563	**WAXROC**	631	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
564	**WECBAH**	632	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	P-Donor
565	**WECBEL**	633	Dimer Through Anion	Tetrahedral	4	Non-Chelate	P-Donor
		634	Dimer Through Anion	Seesaw	4	Non-Chelate	P-Donor
566	**WEFREF**	635	Discrete Molecule	T-Shape	5	Non-Chelate	N-Donor, O-Donor
567	**WENSAK**	636	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
		637	Polymer Through Anion	Seesaw	4	Metal Halide Only	Iodine
568	**WEQMOV**	638	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
569	**WIDZOY**	639	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
570	**WIFZOB**	640	Dimer Through Ligand	Seesaw	4	Non-Chelate	Se-Donor
571	**WIHLAB**	641	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
572	**WODDEY**	642	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
573	**WONKOZ**	643	Discrete Molecule	Seesaw	4	Non-Chelate	P-Donor, O-Donor
574	**WOPCEJ**	644	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
575	**WOPCIN**	645	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
576	**WUNXOU**	646	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
577	**WURPUV**	647	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
578	**WURXOW**	648	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
579	**WUZHIJ**	649	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
580	**XAHSEF**	650	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
581	**XAHSUV**	651	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
582	**XAHWAF**	652	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
583	**XALBAP**	653	Dimer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
584	**XANBIX**	654	Polymer Through Ligand	D-Square Pyramid	5	Chelate	N-Donor, O-Donor
		655	Polymer Through Anion	D-Square Pyramid	5	Chelate	N-Donor, O-Donor
585	**XAQCID**	656	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
586	**XAQCOJ**	657	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
587	**XEHWOY**	658	Polymer Through Ligand	D-Tetrahedral (Py)	4	Chelate	N-Donor
		659	Polymer Through Ligand	T-Shape	5	Chelate	N-Donor, O-Donor
588	**XEHWUE**	660	Discrete Molecule	T-Shape	5	Chelate	N-Donor, O-Donor
589	**XEHXAL**	661	Discrete Molecule	T-Shape	5	Chelate	N-Donor, O-Donor
590	**XELQEL**	662	Polymer Through Ligand	D-Tetrahedral (Py)	4	Non-Chelate	S-Donor
591	**XEMVES**	663	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine

592	**XENFAZ**	664	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
593	**XEWKIU**	665	Discrete Molecule	Linear	2	Metal Halide Only	Iodine
594	**XEWKOA**	666	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
595	**XEWKUG**	667	Dimer Through Anion	D-Trigonal Bipyramid	5	Chelate	N-Donor
596	**XIDDOF**	668	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
		669	Trimer Through Anion	T-Shape	3	Chelate	C-Donor / N-Donor
597	**XIHZOE**	670	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
598	**XIPNER**	671	Discrete Molecule	Seesaw	4	Non-Chelate	N-Donor
599	**XIPVUO**	672	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor
		673	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
600	**XITLUI**	674	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
601	**XOGKIN**	675	Discrete Molecule	Trigonal Pyramid	4	Metal Halide Only	Chlorine
		676	Discrete Molecule	Trigonal	3	Metal Halide Only	Iodine
602	**XORVIK**	677	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	N-Donor
603	**XOYHAW**	678	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
		679	Dimer Through Anion	Trigonal Bipyramid	5	Chelate	N-Donor
604	**XOYHEA**	680	Dimer Through Ligand	Seesaw	4	Chelate	N-Donor
		681	Dimer Through Ligand	T-Shape	5	Chelate	N-Donor
605	**XUCWEY**	682	Discrete Molecule	Seesaw	4	Chelate	N-Donor
606	**XUKRUS**	683	Tetramer Through Anion	Square Pyramid	5	M-M / Non-Chelate	Osmium
607	**XUVRIQ**	684	Discrete Molecule	Trigonal	3	Metal Halide Only	Iodine
		685	Discrete Molecule	D-Tetrahedral (Py)	4	Metal Halide Only	Chlorine
608	**XUZLIO**	686	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
609	**YACFAL**	687	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
610	**YAWKIQ**	688	Tetramer Through Anion	T-Shape	3	Non-Chelate	C-Donor
		689	Tetramer Through Anion	Seesaw	4	Non-Chelate	C-Donor
611	**YIJREQ**	690	Discrete Molecule	Seesaw	4	Chelate	C-Donor / P-Donor
612	**YIVJES**	691	Trimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
613	**YIYSUV**	692	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
614	**YIYWOT**	693	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
615	**YOCZUM**	694	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
616	**YOGSES**	695	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
617	**YOLMES**	696	Discrete Molecule	Tetrahedral	4	Metal Halide Only	Iodine
618	**YOWYEQ**	697	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
619	**YOZDUO**	698	Dimer Through Ligand	Seesaw	4	Non-Chelate	S-Donor
620	**YOZFAW**	699	Discrete Molecule	Seesaw	4	Non-Chelate	S-Donor
621	**YUMCEO**	700	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
622	**YUNFOD**	701	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
623	**YUNGIY**	702	Discrete Molecule	Seesaw	4	Chelate	N-Donor
624	**YUPBUH**	703	Polymer Through Anion	Seesaw	4	Non-Chelate	N-Donor
		704	Polymer Through Ligand	Trigonal Bipyramid	5	Non-Chelate	N-Donor
		705	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
625	**YUQNEF**	706	Polymer Through Ligand	Tetrahedral	4	Metal Halide Only	Iodine
		707	Polymer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
626	**YUYVUK**	708	Polymer Through Ligand	Seesaw	4	Non-Chelate	P-Donor
627	**ZECBAK**	709	Dimer Through Anion	Tetrahedral	4	Metal Halide Only	Iodine
628	**ZEFREJ**	710	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
629	**ZESPIW**	711	Dimer Through Anion	D-Tetrahedral (Py)	4	Non-Chelate	C-Donor
630	**ZEVMAQ**	712	Polymer Through Anion	Seesaw	4	Chelate	N-Donor
		713	Polymer Through Anion	Seesaw	4	Metal Halide Only	Iodine
		714	Polymer Through Anion	Octahedral	6	Metal Halide Only	Iodine
631	**ZEXJER**	715	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
632	**ZINWIE**	716	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
633	**ZIYXEK**	717	Discrete Molecule	Hexagonal Bipyramid	8	Non-Chelate	O-Donor
634	**ZOGWIB**	718	Dimer Through Anion	Square Pyramid	5	Chelate	N-Donor
635	**ZOZRUD**	719	Polymer Through Ligand	Seesaw	4	Non-Chelate	N-Donor
636	**ZUBMAK**	720	Tetramer Through Anion	T-Shape	3	Chelate	C-Donor
		721	Tetramer Through Anion	Seesaw	4	Chelate	C-Donor
637	**ZUBMEO**	722	Tetramer Through Anion	Seesaw	4	Chelate	C-Donor