Hydrogen bonds

Ligand				
D-H…A	**D-H [Å]**	**H…A [Å]**	**D…A [Å]**	**∠D-H…A [°]**
O1-H1...N1	0.82	1.87	2.595	147
O2-H2...N2	0.82	1.89	2.615	147
C4"-H4"...O1[-1/2+x,1/2-y,1-z]	0.93	2.49	2.947	111
Complex				
O1W-H2D...O2W	0.87	0.75	1.323	109
C1'A-H1'A…O1B	1.00	2.52	3.305	135
C4AA-H4AA...O3W[1/2+x,1/2+y,z]	0.95	2.46	3.377	162
C1"B-H1"B…O1A	1.00	2.58	3.468	148
C1'B-H1'B…O2A[x,-1+y,z]	1.00	2.50	3.430	155

Ring Puckering Analysis

Ligand

Cg1: C1-C9(naph1) Cg2: C1'-C2' Cg3: C1a-C6a(phenyl)
Cg4: C5-C10(naph2) Cg5: C1-C7(naph)

Complex

Cg6: Cu1-N2a-O2a Cg7: C1aa-C6aa(phenyl) Cg8: Cu1-N1a-O1a
Cg9: C1a-C9a(naph) Cg10: C1a-C9a(naph1) Cg11: C5a-c10a(naph2)
Cg13: Cu2-N2b-O2b Cg14: C1ab-C6ab(phenyl) Cg15: Cu2-O1b-N1b
Cg16: C1b-C9b(naph) Cg17: C1b-C9b(naph1) Cg18: C5b-C10b(naph2)

Ligand				
Cg(I) -> Cg(J)	**Cg-Cg [Å]**	**Alpha [°]**	**CgI_Perp [Å]**	**CgJ_Perp [Å]**
Cg1 -> Cg3	4.170	18.31	4.0736	3.8544
Cg3 -> Cg3[1-X,-1/2+Y,1/2-Z]	5.923	83	2.4299	-4.4832
Cg3 -> Cg4	4.115	16.7	3.8823	3.7798
Cg3 -> Cg4[1-X,-1/2+Y,1/2-Z]	5.763	80.4	2.8182	-4.9974
Cg4 -> Cg3[-1+X,Y,Z]	5.816	16.7	-1.6023	-2.9626
Complex				
Cg6 -> Cg13	5.349	4.2	3.131	-3.480
Cg6 -> Cg13[X,1+Y,Z]	4.679	4.2	-3.434	2.815
Cg6 -> Cg15	3.321	6.8	3.436	-3.621(4)
Cg6 -> Cg15[X,1+Y,Z]	4.566	6.8	-3.221	2.674
Cg6 -> Cg17	3.860	5.1	3.418	-3.944
Cg6 -> Cg18	5.037	34.8	1.321	-3.801
Cg7 -> Cg15	4.561	5.4	3.656	-3.597
Cg7 -> Cg15[X,1+Y,Z]	4.799	5.4	-3.001	2.786
Cg7 -> Cg17	4.227	3.7	3.675	-3.889
Cg7 -> Cg18	4.015	34.4	0.222	-3.772
Cg8 -> Cg11[3/2-X,1/2+Y,2-Z]	5.825	67.1	5.397	4.890
Cg8 -> Cg13	3.449	5.5	3.336	-3.461
Cg8 -> Cg13[X,1+Y,Z]	4.428	5.5	-3.228	2.751
Cg8 -> Cg14	4.408	17.7	3.372	-3.516
Cg8 -> Cg14[X,1+Y,Z]	4.851	17.7	-3.758	2.696
Cg8 -> Cg15	4.676	8.0	3.705	-3.610
Cg10 -> Cg10[3/2-X,1/2+Y,2-Z]	5.531	51.0	1.414	8.286
Cg10 -> Cg11[3/2-X,1/2+Y,2-Z]	4.886	59.1	3.213	8.014
Cg10 -> Cg13	3.846	5.5	3.408	-0.002
Cg10 -> Cg14	3.836	6.8	3.134	0.061
Cg10 -> Cg14[X,1+Y,Z]	5.943	6.8	-3.996	6.934

Cg11 -> Cg10[3/2-X,1/2+Y,2-Z]	5.005	59.1	1.142	9.465
Cg11 -> Cg11[3/2-X,1/2+Y,2-Z]	5.511	70.0	2.391	8.642
Cg11 -> Cg13	5.180	14.9	3.473	0.467
Cg11 -> Cg14	3.807	14.9	3.399	1.123
Cg15 -> Cg18[3/2-X,-1/2+Y,1-Z]	5.795	79.4	-5.770	-4.570
Cg17 -> Cg17[3/2-X,-1/2+Y,1-Z]	5.564	60.0	1.565	-5.018
Cg17 -> Cg18[3/2-X,-1/2+Y,1-Z]	4.674	79.8	-3.386	-4.630
Cg18 -> Cg15	4.313	33.1	-0.002	-1.071
Cg18 -> Cg17[3/2-X,-1/2+Y,1-Z]	5.055	79.8	1.953	-7.831
Cg18 -> Cg18[3/2-X,-1/2+Y,1-Z]	5.320	71.0	-1.850	-6.296

Cg(I) = Plane number I (= ring number in () above); Cg-Cg = Distance between ring Centroids (Ang.); Alpha = Dihedral Angle between Planes I and J (Deg); CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.); CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

X-H...π Interactions (H...π < 3.0 Å and Gamma < 30.0 Deg)

Ligand					
X-H…Cg	**H…Cg [Å]**	**Gamma [°]**	**X-H...Cg [Å]**	**X...Cg [Å]**	**X-H,π [°]**
C1'-H1'…Cg1[1/2+X,1/2-Y,1-Z]	2.84	2.20	176	3.813	88
C2"-H2"B...Cg4[1/2+X,1/2-Y,1-Z]	2.80	2.56	177	3.774	89
Complex					
C1"A -H1"A [1] -> Cg13[X,1+Y,Z]	2.36	8.88	158	3.312	69
C4A-H4A -> Cg11[3/2-X,-1/2+Y,2-Z]	2.88	18.52	149	3.722	59
C5A-H5A -> Cg10[3/2-X,-1/2+Y,2-Z]	2.72	3.70	148	3.561	57
C5B-H5B -> Cg17[3/2-X,1/2+Y,1-Z]	2.62	9.07	142	3.419	60
C2"B-H2"3 -> Cg7[X,-1+Y,Z]	2.96	7.17	160	3.907	66
C1'B-H1'B -> Cg6 [X,-1+Y,Z]	2.47	9.29	160	3.429	68

Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg);

Ring-Metal Interactions with Cg-Me < 4.0 Å

Complex			
Cg(I) -> Me(J)	**Cg(I)-Me(J) [Å]**	**Me(J)_Perp [Å]**	**Beta [°]**
Cg8 -> Cu2	3.647	-3.530	23.62
Cg15 -> Cu1	3.545	3.518	20.38

Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg);