

MERCURY COMPLEX LOG FILE

```
1|1|UNPC-CARLO-HP|SP|RwB97XD TD-FC|SDD|C56H54Hg1N4O4|CARLO|20-Nov-2014
|0||#p td=(50-50,nstates=20,direct) wb97xd/sdd scrf=(solvent=methanol)
geom=connectivity|CSD ENTRY c65h76n4o8||0,1|H,0,-4.574426,-0.140086,
0.210346|O,0,1.112413,0.853911,0.390346|O,0,-0.312542,4.020605,1.50534
6|N,0,-2.910716,4.111635,0.553346|N,0,-2.491658,1.341672,1.198346|C,0,
-0.927326,4.646259,-0.745654|C,0,0.,4.061668,0.175346|C,0,1.214444,3.5
48297,-0.236654|C,0,2.742317,3.011219,-2.129654|C,0,3.032252,3.030171,
-3.465654|C,0,2.128293,3.608599,-4.384654|C,0,0.958124,4.153856,-3.938
654|C,0,-0.606832,4.670417,-2.076654|C,0,1.538567,3.569016,-1.626654|C
,0,0.626575,4.141003,-2.563654|C,0,2.894911,0.971887,2.025346|C,0,2.05
2636,1.587196,1.047346|C,0,2.14022,2.937067,0.770346|C,0,3.26664,5.120
202,1.197346|C,0,4.240759,5.845059,1.839346|C,0,5.123978,5.227595,2.75
1346|C,0,4.994231,3.898944,3.027346|C,0,3.844255,1.729043,2.659346|C,0
,3.993041,3.11267,2.389346|C,0,3.120183,3.728856,1.446346|C,0,-2.24047
8,5.179335,-0.221654|C,0,-3.479329,3.036899,-0.282654|C,0,-4.747585,3.
473139,-1.030654|C,0,-5.330329,2.350348,-1.890654|C,0,-5.611842,1.1206
19,-1.036654|C,0,-4.353232,0.66955,-0.296654|C,0,-3.74926,1.786827,0.5
60346|C,0,-2.680439,0.478721,2.385346|H,0,3.348477,2.591035,-1.504654|
H,0,3.852542,2.633272,-3.771654|H,0,2.394991,3.597219,-5.347654|H,0,0.
371199,4.574274,-4.557654|H,0,-1.20816,5.026502,-2.713654|H,0,2.700898
,5.547271,0.576346|H,0,4.340536,6.771973,1.675346|H,0,5.790684,5.80980
9,3.220346|H,0,5.560666,3.46185,3.657346|H,0,4.438244,1.356491,3.34234
6|H,0,-2.816367,2.777536,-0.974654|H,0,-4.414948,2.026452,1.246346|H,0
,-1.877655,0.565753,2.952346|H,0,-2.133639,5.969492,0.387346|H,0,-4.68
6644,2.102917,-2.652654|H,0,-2.085562,2.072232,1.461346|H,0,-3.539463,
4.503627,1.023346|H,0,-1.166025,4.135933,1.557346|H,0,-4.625746,4.2526
64,-1.553654|H,0,-6.176327,2.67186,-2.355654|H,0,-5.912977,0.369389,-1
.608654|H,0,-3.69081,0.377633,-1.015654|H,0,-2.799542,5.531461,-1.0116
54|H,0,-5.443079,3.726961,-0.355654|H,0,-6.297331,1.381218,-0.381654|H
,0,-3.427812,0.804859,2.909346|H,0,4.574426,0.140086,0.210346|O,0,-1.1
12413,-0.853911,0.390346|O,0,0.312542,-4.020605,1.505346|N,0,2.910716,
-4.111635,0.553346|N,0,2.491658,-1.341672,1.198346|C,0,0.927326,-4.646
259,-0.745654|C,0,0.,-4.061668,0.175346|C,0,-1.214444,-3.548297,-0.236
654|C,0,-2.742317,-3.011219,-2.129654|C,0,-3.032252,-3.030171,-3.46565
4|C,0,-2.128293,-3.608599,-4.384654|C,0,-0.958124,-4.153856,-3.938654|
C,0,0.606832,-4.670417,-2.076654|C,0,-1.538567,-3.569016,-1.626654|C,0
,-0.626575,-4.141003,-2.563654|C,0,-2.894911,-0.971887,2.025346|C,0,-2
.052636,-1.587196,1.047346|C,0,-2.14022,-2.937067,0.770346|C,0,-3.2666
4,-5.120202,1.197346|C,0,-4.240759,-5.845059,1.839346|C,0,-5.123978,-5
.227595,2.751346|C,0,-4.994231,-3.898944,3.027346|C,0,-3.844255,-1.729
043,2.659346|C,0,-3.993041,-3.11267,2.389346|C,0,-3.120183,-3.728856,1
.446346|C,0,2.240478,-5.179335,-0.221654|C,0,3.479329,-3.036899,-0.282
654|C,0,4.747585,-3.473139,-1.030654|C,0,5.330329,-2.350348,-1.890654|
C,0,5.611842,-1.120619,-1.036654|C,0,4.353232,-0.66955,-0.296654|C,0,3
.74926,-1.786827,0.560346|C,0,2.680439,-0.478721,2.385346|H,0,-3.34847
7,-2.591035,-1.504654|H,0,-3.852542,-2.633272,-3.771654|H,0,-2.394991,
-3.597219,-5.347654|H,0,-0.371199,-4.574274,-4.557654|H,0,1.20816,-5.0
26502,-2.713654|H,0,-2.700898,-5.547271,0.576346|H,0,-4.340536,-6.7719
73,1.675346|H,0,-5.790684,-5.809809,3.220346|H,0,-5.560666,-3.46185,3.
657346|H,0,-4.438244,-1.356491,3.342346|H,0,2.816367,-2.777536,-0.9746
54|H,0,4.414948,-2.026452,1.246346|H,0,1.877655,-0.565753,2.952346|H,0
,2.133639,-5.969492,0.387346|H,0,4.686644,-2.102917,-2.652654|H,0,2.08
5562,-2.072232,1.461346|H,0,3.539463,-4.503627,1.023346|H,0,1.166025,-
4.135933,1.557346|H,0,4.625746,-4.252664,-1.553654|H,0,6.176327,-2.671
86,-2.355654|H,0,5.912977,-0.369389,-1.608654|H,0,3.69081,-0.377633,-1
.015654|H,0,2.799542,-5.531461,-1.011654|H,0,5.443079,-3.726961,-0.355
654|H,0,6.297331,-1.381218,-0.381654|H,0,3.427812,-0.804859,2.909346|H
g,0,0.,0.,0.001802||Version=EM64W-G09RevD.01|State=1-A|HF=-2837.539995
7|RMSD=8.035e-009|PG=C02 [C2(Hg1),X(C56H54N4O4)]||@
```

CADMIUM COMPLEX LOG FILE

```
1|1|UNPC-CARLO-HP|SP|RwB97XD TD-FC|SDD|C56H54Cd1N4O4|CARLO|22-Nov-2014
|0||#p td=(50-50,nstates=20,direct) rwb97xd/sdd scrf=(solvent=methanol
) geom=connectivity||CSD ENTRY c65h76n4o8||0,1|H,0,-4.574426,-0.140086
,0.210538|O,0,1.112413,0.853911,0.390538|O,0,-0.312542,4.020605,1.5055
38|N,0,-2.910716,4.111635,0.553538|N,0,-2.491658,1.341672,1.198538|C,0
,-0.927326,4.646259,-0.745462|C,0,0.,4.061668,0.175538|C,0,1.214444,3.
548297,-0.236462|C,0,2.742317,3.011219,-2.129462|C,0,3.032252,3.030171
,-3.465462|C,0,2.128293,3.608599,-4.384462|C,0,0.958124,4.153856,-3.93
8462|C,0,-0.606832,4.670417,-2.076462|C,0,1.538567,3.569016,-1.626462|
C,0,0.626575,4.141003,-2.563462|C,0,2.894911,0.971887,2.025538|C,0,2.0
52636,1.587196,1.047538|C,0,2.14022,2.937067,0.770538|C,0,3.26664,5.12
0202,1.197538|C,0,4.240759,5.845059,1.839538|C,0,5.123978,5.227595,2.7
51538|C,0,4.994231,3.898944,3.027538|C,0,3.844255,1.729043,2.659538|C,
0,3.993041,3.11267,2.389538|C,0,3.120183,3.728856,1.446538|C,0,-2.2404
78,5.179335,-0.221462|C,0,-3.479329,3.036899,-0.282462|C,0,-4.747585,3
.473139,-1.030462|C,0,-5.330329,2.350348,-1.890462|C,0,-5.611842,1.120
619,-1.036462|C,0,-4.353232,0.66955,-0.296462|C,0,-3.74926,1.786827,0.
560538|C,0,-2.680439,0.478721,2.385538|H,0,3.348477,2.591035,-1.504462
|H,0,3.852542,2.633272,-3.771462|H,0,2.394991,3.597219,-5.347462|H,0,0
.371199,4.574274,-4.250759,5.845059,1.839538|H,0,-1.20816,5.026502,-2.713462|H,0,2.70089
8,5.547271,0.576538|H,0,4.340536,6.771973,1.675538|H,0,5.790684,5.8098
09,3.220538|H,0,5.560666,3.46185,3.657538|H,0,4.438244,1.356491,3.3425
38|H,0,-2.816367,2.777536,-0.974462|H,0,-4.414948,2.026452,1.246538|H,
0,-1.877655,0.565753,2.952538|H,0,-2.133639,5.969492,0.387538|H,0,-4.6
86644,2.102917,-2.652462|H,0,-2.085562,2.072232,1.461538|H,0,-3.539463
,4.503627,1.023538|H,0,-1.166025,4.135933,1.557538|H,0,-4.625746,4.252
664,-1.553462|H,0,-6.176327,2.67186,-2.355462|H,0,-5.912977,0.369389,-
1.608462|H,0,-3.69081,0.377633,-1.015462|H,0,-2.799542,5.531461,-1.011
462|H,0,-5.443079,3.726961,-0.355462|H,0,-6.297331,1.381218,-0.381462|
H,0,-3.427812,0.804859,2.909538|H,0,4.574426,0.140086,0.210538|O,0,-1.
112413,-0.853911,0.390538|O,0,0.312542,-4.020605,1.505538|N,0,2.910716
,-4.111635,0.553538|N,0,2.491658,-1.341672,1.198538|C,0,0.927326,-4.64
6259,-0.745462|C,0,0.,-4.061668,0.175538|C,0,-1.214444,-3.548297,-0.23
6462|C,0,-2.742317,-3.011219,-2.129462|C,0,-3.032252,-3.030171,-3.4654
62|C,0,-2.128293,-3.608599,-4.384462|C,0,-0.958124,-4.153856,-3.938462
|C,0,0.606832,-4.670417,-2.076462|C,0,-1.538567,-3.569016,-1.626462|C,
0,-0.626575,-4.141003,-2.563462|C,0,-2.894911,-0.971887,2.025538|C,0,-
2.052636,-1.587196,1.047538|C,0,-2.14022,-2.937067,0.770538|C,0,-3.266
64,-5.120202,1.197538|C,0,-4.240759,-5.845059,1.839538|C,0,-5.123978,-
5.227595,2.751538|C,0,-4.994231,-3.898944,3.027538|C,0,-3.844255,-1.72
9043,2.659538|C,0,-3.993041,-3.11267,2.389538|C,0,-3.120183,-3.728856,
1.446538|C,0,2.240478,-5.179335,-0.221462|C,0,3.479329,-3.036899,-0.28
2462|C,0,4.747585,-3.473139,-1.030462|C,0,5.330329,-2.350348,-1.890462
|C,0,5.611842,-1.120619,-1.036462|C,0,4.353232,-0.66955,-0.296462|C,0,
3.74926,-1.786827,0.560538|C,0,2.680439,-0.478721,2.385538|H,0,-3.3484
77,-2.591035,-1.504462|H,0,-3.852542,-2.633272,-3.771462|H,0,-2.394991
,-3.597219,-5.347462|H,0,-0.371199,-4.574274,-4.557462|H,0,1.20816,-5.
026502,-2.713462|H,0,-2.700898,-5.547271,0.576538|H,0,-4.340536,-6.771
973,1.675538|H,0,-5.790684,-5.809809,3.220538|H,0,-5.560666,-3.46185,3
.657538|H,0,-4.438244,-1.356491,3.342538|H,0,2.816367,-2.777536,-0.974
462|H,0,4.414948,-2.026452,1.246538|H,0,1.877655,-0.565753,2.952538|H,
0,2.133639,-5.969492,0.387538|H,0,4.686644,-2.102917,-2.652462|H,0,2.0
85562,-2.072232,1.461538|H,0,3.539463,-4.503627,1.023538|H,0,1.166025,
-4.135933,1.557538|H,0,4.625746,-4.252664,-1.553462|H,0,6.176327,-2.67
186,-2.355462|H,0,5.912977,-0.369389,-1.608462|H,0,3.69081,-0.377633,-
1.015462|H,0,2.799542,-5.531461,-1.011462|H,0,5.443079,-3.726961,-0.35
5462|H,0,6.297331,-1.381218,-0.381462|H,0,3.427812,-0.804859,2.909538|
Cd,0,0.,0.001994||Version=EM64W-G09RevD.01|State=1-A|HF=-2851.93464
8|RMSD=1.942e-009|PG=C02 [C2(Cd1),X(C56H54N4O4)]||@
```

ZINC COMPLEX LOG FILE

```
1|1|UNPC-HP8-DESKTOP2013|SP|RwB97XD TD-FC|SDD|C56H54N4O4Zn1|CARL|22-No
v-2014|0||#p td=(50-50,nstates=20,direct) wb97xd/sdd scrf=(solvent=met
hanol) geom=connectivity||CSD ENTRY c65h76n4o8||0,1|H,0,-2.707257,-3.6
93306,-0.16442|O,0,1.299677,0.462702,-0.345094|O,0,3.127352,-2.491822,
-1.455084|N,0,1.747605,-4.694783,-0.502005|N,0,-0.312624,-2.797816,-1.
```

151082|C,0,3.299527,-3.349005,0.797026|C,0,3.335027,-2.254349,-0.12514
2|C,0,3.588961,-0.960168,0.285686|C,0,3.997247,0.608639,2.177364|C,0,4
.17394,0.839759,3.513283|C,0,4.146414,-0.232085,4.433434|C,0,3.943719,
-1.507461,3.988635|C,0,3.497644,-3.095479,2.127941|C,0,3.786202,-0.701
647,1.675596|C,0,3.748824,-1.776522,2.613739|C,0,2.396732,1.871994,-1.
980578|C,0,2.434236,0.830688,-1.001398|C,0,3.601602,0.148019,-0.722518
|C,0,6.041617,-0.140958,-1.146836|C,0,7.18815,0.259853,-1.788165|C,0,7
.171713,1.336366,-2.701362|C,0,5.998333,1.97222,-2.979198|C,0,3.556156
,2.234205,-2.613851|C,0,4.785756,1.58335,-2.341946|C,0,4.806904,0.5161
71,-1.397754|C,0,3.006782,-4.736136,0.274263|C,0,0.537918,-4.56351,0.3
3268|C,0,0.188823,-5.857841,1.081762|C,0,-1.06862,-5.711356,1.940384|C
,0,-2.244411,-5.257269,1.084745|C,0,-1.913012,-3.962623,0.343646|C,0,-
0.648261,-4.088429,-0.511992|C,0,-1.132248,-2.472543,-2.339235|H,0,3.9
88936,1.345455,1.551547|H,0,4.303878,1.742006,3.818421|H,0,4.285327,-0
.003652,5.396319|H,0,3.962994,-2.228473,4.608445|H,0,3.455531,-3.79239
9,2.765666|H,0,6.078259,-0.848135,-0.525025|H,0,8.011953,-0.176099,-1.
622888|H,0,8.027806,1.56246,-3.169781|H,0,5.95378,2.685576,-3.610023|H
,0,3.580561,2.934209,-3.297596|H,0,0.693394,-3.868197,1.024069|H,0,-0.
821624,-4.774946,-1.197407|H,0,-0.61024,-1.856628,-2.906405|H,0,3.7219
61,-5.090537,-0.333656|H,0,-0.914113,-5.038618,2.701797|H,0,0.520332,-
2.870492,-1.413195|H,0,1.720972,-5.435734,-0.971219|H,0,2.745258,-3.26
3695,-1.506608|H,0,0.902489,-6.192621,1.605821|H,0,-1.276163,-6.591864
,2.406148|H,0,-3.036046,-5.085706,1.65579|H,0,-1.784842,-3.249507,1.06
1989|H,0,2.984895,-5.395648,1.064966|H,0,0.01053,-6.576994,0.407376|H,
0,-2.411507,-5.971902,0.430365|H,0,-1.279798,-3.274997,-2.862499|H,0,2
.645741,3.731342,-0.167372|O,0,-1.360845,-0.425061,-0.346699|O,0,-3.18
6357,2.527018,-1.466707|N,0,-1.808457,4.732066,-0.515788|N,0,0.253024,
2.833685,-1.156708|C,0,-3.362897,3.389136,0.783181|C,0,-3.396611,2.292
462,-0.136651|C,0,-3.651344,0.999184,0.276521|C,0,-4.0633,-0.565473,2.
170839|C,0,-4.242583,-0.793663,3.506917|C,0,-4.216838,0.280196,4.42476
5|C,0,-4.013278,1.554595,3.977565|C,0,-3.563595,3.13853,2.114262|C,0,-
3.851279,0.338562|C,0,0.587423,4.125697,-0.5198|C,0,1.074948,2.505809,-
2.342554|H,0,-4.053778,-1.303657,1.546657|H,0,-4.373114,-1.695239,3.81
3779|H,0,-4.357617,0.053876,5.387879|H,0,-4.033754,2.276964,4.595754|H
,0,-3.522714,3.836846,2.750537|H,0,-6.139067,0.885369,-0.538767|H,0,-8
.07063,0.210921,-1.638901|H,0,-8.083488,-1.531025,-3.182006|H,0,-6.008
614,-2.655099,-3.615763|H,0,-3.636006,-2.903041,-3.298191|H,0,-0.75720
7,3.908831,1.014136|H,0,0.762115,4.81071,-1.206383|H,0,0.554038,1.8886
5,-2.909382|H,0,-3.783134,5.128184,-0.352135|H,0,0.847046,5.082933,2.6
92406|H,0,-0.579424,2.905783,-1.420595|H,0,-1.780912,5.471987,-0.98657
2|H,0,-2.804163,3.298776,-1.519182|H,0,-0.967425,6.234524,1.590383|H,0
,1.209673,6.635527,2.394055|H,0,2.971003,5.12773,1.650414|H,0,1.720949
,3.290232,1.058217|H,0,-3.04878,5.436363,1.04724|H,0,-0.073144,6.61627
,0.39283|H,0,2.348844,6.011235,0.421841|H,0,1.223513,3.307115,-2.86728
9|Zn,0,0.174163,-0.108274,-0.251833||Version=EM64W-G09RevD.01|State=1-
A|HF=-2911.5258648|RMSD=5.912e-009|PG=C01 [X(C56H54N4O4Zn1)]||@