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COMMENTS
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> This file contains 300 systems computed in the work Rulisek, L.; Havlas, Z.:
> Theoretical Studies of Metal Ion Selectivity. 3. A Theoretical Design of the
> Most Specific Metal-Binding Sites for Selected Transition Metal Ions (Co²⁺,
> Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, Hg²⁺), submitted for publication in J. Am. Chem. Soc.
>
> The ordering of the information is as follows:
> First, 60 optimized geometries (at the B3LYP/BS1 level), molecular energies
> (at the B3LYP/BS2 level), dipoles, and S**2 projections are listed for
> ten candidates for the most specific Co²⁺-sites (Co,Ni,Cu,Zn,Cd,Hg complexed
> in the sites). Then, the same is repeated for ten candidates for most
> specific Ni²⁺-sites (60 complexes), Cu²⁺-sites (60 complexes), Zn²⁺-sites
> (60 complexes), Cd²⁺-sites (60). Each geometry is preceded by the title name
> of the complex, which is MXXStN, where M is the metal ion, XX is XX²⁺-site,
> and N is the number of the candidate 1-10. Thus NiCOST6 means the candidate
> No. 6 for Co²⁺-specific site with the nickel ion complexed in the site, and
> corresponds to the second column and sixth row of Table 2 in the article.
>
> Then follows 300 hundred lines with the molecular energies of ligands
> and only ghost atom corresponding to metal ion - Bq[M]- left in its place.
> These energies are in the same order as the above 300 hundred complexes.
> Each of six sections is preceded by the keyword, which may be used for
> the faster orientation in the file:
>
> 1. Co²⁺-specific sites
> 2. Ni²⁺-specific sites
> 3. Cu²⁺-specific sites
> 4. Zn²⁺-specific sites
> 5. Cd²⁺-specific sites
> 6. ENERGIES OF LIGANDS

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SUPPORTING INFORMATION
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1. Co²⁺-specific sites

CoCOST1

2,4
Co
0,1,2.1731909573
0,1,2.1639882855,2,90.
N,1,2.2119603875,3,90.,2,180.
N,1,2.2115056511,2,90.,3,180.
0,1,2.1760678644,2,90.,3,90.
N,1,2.2084631739,2,90.,3,-90.
C,2,1.22563,1,136.949,3,249.382
H,8,1.09962,2,120.13,1,182.469
H,8,1.10082,2,121.623,9,179.847
C,3,1.2249,1,137.193,2,315.826
H,11,1.09973,3,120.118,1,180.217

H, 11, 1.10088, 3, 121.647, 12, 179.844
 C, 4, 1.47396, 1, 118.382, 3, 4.196
 C, 4, 1.27526, 1, 124.614, 3, 182.286
 H, 15, 1.09333, 4, 122.064, 14, -0.811
 H, 15, 1.08639, 4, 120.211, 14, 179.198
 H, 14, 1.09473, 4, 112.002, 15, 0.745
 H, 14, 1.09316, 4, 109.525, 15, 122.047
 H, 14, 1.09359, 4, 109.341, 15, -120.475
 C, 5, 1.47204, 1, 121.374, 2, 81.903
 C, 5, 1.27902, 1, 121.311, 2, -93.574
 H, 22, 1.09378, 5, 122.113, 21, 1.449
 H, 22, 1.08739, 5, 119.831, 21, 181.145
 H, 21, 1.09488, 5, 111.675, 22, -4.615
 H, 21, 1.09345, 5, 109.266, 22, 116.088
 H, 21, 1.09293, 5, 109.759, 22, -125.747
 C, 6, 1.22596, 1, 136.985, 2, -108.33
 H, 28, 1.09968, 6, 120.083, 1, 185.133
 H, 28, 1.1006, 6, 121.526, 29, 180.
 C, 7, 1.47174, 1, 121.445, 2, -181.642
 C, 7, 1.27841, 1, 121.56, 2, 0.242
 H, 32, 1.0937, 7, 122.161, 31, 0.718
 H, 32, 1.08777, 7, 119.842, 31, 180.336
 H, 31, 1.09474, 7, 111.708, 32, 0.98
 H, 31, 1.09301, 7, 109.479, 32, 121.848
 H, 31, 1.09296, 7, 109.639, 32, -120.033

 HF=-2127.9807543
 S2=3.757337
 S2-1=0.
 S2A=3.750022
 RMSD=4.857e-09
 Dipole=0.5979789, -0.7915747, 0.8618682
 PG=C01 [X(C9H21Co1N3O3)]

CoC0St2

2, 4
 Co
 S, 1, 2.7716572087
 O, 1, 2.1625734658, 2, 90.
 S, 1, 2.6093855813, 3, 90., 2, 180.
 N, 1, 2.1562097738, 2, 90., 3, 180.
 O, 1, 2.1092057596, 2, 90., 3, 90.
 N, 1, 2.2216298273, 2, 90., 3, -90.
 H, 2, 1.34881534, 1, 111.20788624, 3, 61.2915949
 H, 2, 1.34861006, 1, 107.49069874, 3, 163.5405823
 C, 3, 1.22560306, 1, 142.43197169, 2, 302.68298071
 H, 10, 1.09955355, 3, 120.17127698, 1, 181.69337721
 H, 10, 1.10159815, 3, 121.60901186, 11, 179.75946607
 H, 4, 1.35045104, 1, 105.14887431, 3, 10.37095801
 H, 4, 1.35026859, 1, 102.01129132, 3, 108.20415772
 C, 5, 1.47541626, 1, 121.40210603, 2, 120.2007734
 C, 5, 1.27926166, 1, 120.96882623, 2, -66.38785063
 H, 16, 1.09316049, 5, 122.12210288, 15, -0.71313089
 H, 16, 1.08766881, 5, 120.14378718, 15, 179.01279474
 H, 15, 1.09415924, 5, 111.36363942, 16, -9.85551017
 H, 15, 1.09263789, 5, 109.63251317, 16, 110.65043795

H, 15, 1.0930845, 5, 109.65595131, 16, -130.78642095
C, 6, 1.22824825, 1, 137.52229166, 2, -75.85500261
H, 22, 1.09883147, 6, 119.6745348, 1, 182.88353651
H, 22, 1.09960211, 6, 121.71729987, 23, 179.82994699
C, 7, 1.47525075, 1, 119.10749415, 2, -209.0210721
C, 7, 1.27562776, 1, 123.90650675, 2, -30.12547504
H, 26, 1.09339102, 7, 122.36429896, 25, -0.43198012
H, 26, 1.08710168, 7, 119.97505591, 25, 178.79557796
H, 25, 1.09466079, 7, 111.9860476, 26, 9.35085384
H, 25, 1.09364797, 7, 109.65836177, 26, 130.50197671
H, 25, 1.09418879, 7, 109.37387053, 26, -111.12204448

HF=-2678.2564574

S2=3.757517

S2-1=0.

S2A=3.750024

RMSD=3.026e-09

Dipole=0.894263, -0.1565031, 0.5359196

PG=C01 [X(C6H18Co1N2O2S2)]

CoC0St3

1, 4

Co

O, 1, 1.8975598924

O, 1, 2.2586290951, 2, 90.

N, 1, 2.2181901414, 3, 90., 2, 180.

N, 1, 2.3696910952, 2, 90., 3, 180.

N, 1, 2.3369707605, 2, 90., 3, 90.

N, 1, 2.275085779, 2, 90., 3, -90.

H, 2, 0.96627448, 1, 115.09828913, 3, 215.8203581

C, 3, 1.22454354, 1, 116.46145005, 2, 361.26004049

H, 9, 1.10240447, 3, 119.66332571, 1, 181.54688342

H, 9, 1.10088477, 3, 120.09542621, 10, 179.97113302

C, 4, 1.46923838, 1, 117.96167271, 3, 3.12756334

C, 4, 1.27412375, 1, 123.86102839, 3, 186.19223285

H, 13, 1.09425947, 4, 121.88254721, 12, 0.31745774

H, 13, 1.08645203, 4, 119.41284487, 12, 180.50509806

H, 12, 1.09603075, 4, 111.82785769, 13, -2.09116397

H, 12, 1.09289123, 4, 109.0796288, 13, 119.61981881

H, 12, 1.09315219, 4, 109.24331875, 13, -124.02075863

C, 5, 1.46247329, 1, 115.87826411, 2, 63.30865168

C, 5, 1.27337158, 1, 123.16390978, 2, -96.14764789

H, 20, 1.09666532, 5, 122.90235324, 19, 0.71556026

H, 20, 1.08987433, 5, 119.45867798, 19, 180.93558282

H, 19, 1.0979733, 5, 112.64801852, 20, -2.75598921

H, 19, 1.09375054, 5, 108.46137891, 20, 118.80842699

H, 19, 1.09493196, 5, 109.13843137, 20, -124.29095746

C, 6, 1.4630784, 1, 115.52811899, 2, 0.47785178

C, 6, 1.27274341, 1, 126.33297373, 2, 187.51408193

H, 27, 1.09628576, 6, 122.96986823, 26, -0.27243325

H, 27, 1.08957929, 6, 119.69407245, 26, 179.52900171

H, 26, 1.09766485, 6, 112.41864083, 27, 4.39015409

H, 26, 1.09238419, 6, 108.97476193, 27, 127.10211137

H, 26, 1.09558699, 6, 108.80031235, 27, -116.51101369

C, 7, 1.46227381, 1, 127.08372369, 2, -180.15300864

C, 7, 1.27599861, 1, 114.47439894, 2, 3.15281942

H, 34, 1.09638881, 7, 121.85955006, 33, 0.43791297
H, 34, 1.08996653, 7, 117.80389912, 33, 180.14619721
H, 33, 1.09753436, 7, 112.51329733, 34, -1.44399391
H, 33, 1.09523785, 7, 109.38244789, 34, 119.62095564
H, 33, 1.09534211, 7, 109.45250392, 34, -122.71126756

HF=-2109.0568068

S2=3.759414

S2-1=0.

S2A=3.750038

RMSD=1.976e-09

Dipole=-0.3738997, -0.3882785, -0.9476392

PG=C01 [X(C9H23Co1N4O2)]

CoC0St4

1, 4

Co

O, 1, 2.0030341376

O, 1, 2.1956043857, 2, 90.

N, 1, 2.1699353632, 3, 90., 2, 180.

N, 1, 2.3013254352, 2, 90., 3, 180.

O, 1, 2.2038822585, 2, 90., 3, 90.

N, 1, 2.2734959295, 2, 90., 3, -90.

C, 2, 1.30015511, 1, 143.19201849, 3, 162.11730012

H, 8, 1.10791216, 2, 113.45597863, 1, 153.70210836

O, 8, 1.22880248, 2, 127.12128069, 9, 178.59002058

C, 3, 1.22402662, 1, 122.7321684, 2, 349.7625523

H, 11, 1.1010666, 3, 119.79552245, 1, 183.47912394

H, 11, 1.09981386, 3, 120.73162218, 12, 180.14881842

C, 4, 1.46877182, 1, 118.82704478, 3, 30.37822449

C, 4, 1.27299136, 1, 122.59083029, 3, 207.44654072

H, 15, 1.09381616, 4, 121.97111058, 14, -1.01009888

H, 15, 1.08687774, 4, 119.74948496, 14, 178.89572087

H, 14, 1.09573869, 4, 111.8832565, 15, 0.34585208

H, 14, 1.09275478, 4, 109.06416327, 15, 122.13557513

H, 14, 1.09432971, 4, 108.59502615, 15, -120.6759747

C, 5, 1.46627047, 1, 123.35223933, 2, 74.53630973

C, 5, 1.27450958, 1, 119.15847625, 2, -99.62546017

H, 22, 1.0954148, 5, 122.45839718, 21, 0.0794399

H, 22, 1.08870471, 5, 119.96893438, 21, 180.04608476

H, 21, 1.09701953, 5, 111.7972798, 22, -6.86211989

H, 21, 1.09306218, 5, 108.0047378, 22, 113.99285702

H, 21, 1.09461636, 5, 109.316376, 22, -128.01983287

C, 6, 1.22296412, 1, 124.30345751, 2, 349.23234657

H, 28, 1.10102012, 6, 119.96107241, 1, 179.62638331

H, 28, 1.10018313, 6, 120.81009768, 29, 180.42238221

C, 7, 1.46744922, 1, 120.52302577, 2, -209.04717175

C, 7, 1.27620831, 1, 121.56838792, 2, -20.35756173

H, 32, 1.09620608, 7, 121.40606762, 31, 0.74792834

H, 32, 1.08910626, 7, 119.85144773, 31, 179.93034655

H, 31, 1.09701255, 7, 112.28940998, 32, 5.14470273

H, 31, 1.09503955, 7, 109.4746132, 32, 126.51209993

H, 31, 1.0946892, 7, 109.70689371, 32, -115.74858328

HF=-2202.9934488

S2=3.757643

S2-1=0.
S2A=3.750024
RMSD=1.952e-09
Dipole=1.155008, -0.8713004, -1.6542486
PG=C01 [X(C9H20Co1N3O4)]

CoC0St5

1, 4
Co
0, 1, 2.1931881664
0, 1, 2.2291849223, 2, 90.
0, 1, 2.2044724837, 3, 90., 2, 180.
0, 1, 2.1908631643, 2, 90., 3, 180.
0, 1, 1.8918841377, 2, 90., 3, 90.
0, 1, 2.1263699043, 2, 90., 3, -90.
H, 2, 0.9720149, 1, 123.97643821, 3, 30.70208825
H, 2, 0.97373627, 1, 100.3773561, 3, 272.09837541
H, 3, 0.97164996, 1, 111.16296615, 2, 119.06258038
H, 3, 0.97276639, 1, 126.03498844, 2, -109.7637634
C, 4, 1.22445531, 1, 120.15335199, 3, 93.20263009
H, 12, 1.10053206, 4, 120.12141936, 1, -0.56768575
H, 12, 1.10125446, 4, 119.62016625, 13, 180.15036259
C, 5, 1.22589589, 1, 119.33780051, 2, 280.0637351
H, 15, 1.09992094, 5, 120.11509397, 1, -1.67343225
H, 15, 1.1008052, 5, 119.55602214, 16, 180.35285688
H, 6, 0.96713251, 1, 121.05157668, 2, -61.60025127
C, 7, 1.22510616, 1, 128.829406, 5, -15.62138707
H, 19, 1.09869018, 7, 121.45757107, 1, 0.60806461
H, 19, 1.099019, 7, 119.46160896, 1, 180.37329962

HF=-1955.0789143
S2=3.757071
S2-1=0.
S2A=3.750022
RMSD=4.767e-09
Dipole=0.2755607, 0.3025495, -0.11645
PG=C01 [X(C3H11Co106)]

CoC0St6

0, 4
27 0.309241 -0.211474 -0.234987
8 -1.237279 -1.577721 -0.633697
8 1.776359 -1.989710 0.167773
7 1.938345 1.227732 0.185013
7 -1.220931 1.643187 -0.655057
8 0.802393 -0.226325 -2.096943
7 -0.264656 -0.194191 1.931827
6 -2.515082 -1.629728 -0.665794
1 -2.922291 -2.457187 -1.287358
8 -3.328731 -0.884575 -0.087084
6 1.751343 -2.765440 -0.773198

1	2.301849	-3.722270	-0.715002
1	1.199075	-2.517487	-1.689690
6	3.160468	0.907977	-0.546290
6	1.781544	2.395313	0.658330
1	2.544378	3.178644	0.565312
1	0.852710	2.646381	1.169955
1	3.856573	1.757742	-0.592255
1	3.648140	0.057780	-0.057655
1	2.862923	0.590984	-1.551633
6	-2.360402	2.145606	0.103542
6	-1.027226	2.101060	-1.826866
1	-1.679075	2.868139	-2.269646
1	-0.199813	1.692039	-2.408349
1	-2.861728	2.988965	-0.396179
1	-3.068818	1.320507	0.230835
1	-2.024258	2.468433	1.096422
1	0.057589	-0.664460	-2.537162
6	0.787009	-0.227893	2.949364
6	-1.477161	-0.314794	2.306022
1	-1.729394	-0.405810	3.370443
1	-2.274729	-0.358896	1.560292
1	0.376318	-0.346398	3.961235
1	1.460570	-1.062281	2.728675
1	1.376281	0.691937	2.902887

HF=-2164.48789781
S2=3.7581
S2-1=0.
S2A=3.750037
RMSD=1.575e-08

CoC0St7

0,4
Co
0,1,2.1043635984
0,1,2.3475172344,2,90.
N,1,2.2103610287,3,90.,2,180.
N,1,2.3136201576,2,90.,3,180.
0,1,2.2156044938,2,90.,3,90.
0,1,1.9221991671,2,90.,3,-90.
C,2,1.28512113,1,132.4833235,3,113.15801594
H,8,1.11267675,2,113.71051297,1,183.98285741
O,8,1.23931276,2,128.04409112,9,179.90487409
C,3,1.22374177,1,109.60458532,2,281.53153682
H,11,1.10639136,3,119.25177869,1,176.8030791
H,11,1.10526152,3,119.17725213,12,179.14009744
C,4,1.4585547,1,126.34067226,3,81.98896457
C,4,1.27475584,1,113.81398476,3,263.68927834
H,15,1.09819287,4,121.24591122,14,0.52012724
H,15,1.09255565,4,117.30070407,14,181.07893926
H,14,1.09937234,4,112.41865489,15,-0.15888386
H,14,1.09533075,4,108.94725468,15,121.27846475
H,14,1.09506993,4,109.22201792,15,-121.77956847
C,5,1.45824323,1,114.61249078,2,76.96852908
C,5,1.27058069,1,126.53746045,2,-102.17068816
H,22,1.0983786,5,122.81105298,21,0.24317589

H, 22, 1.09062295, 5, 119.68247559, 21, 180.36622633
H, 21, 1.10023651, 5, 111.92600434, 22, -2.05585188
H, 21, 1.09453342, 5, 108.43630078, 22, 120.46801482
H, 21, 1.09306121, 5, 108.39554244, 22, -124.63010712
C, 6, 1.22467958, 1, 116.27830033, 2, 344.85453428
H, 28, 1.10344602, 6, 119.41487377, 1, 181.36113942
H, 28, 1.10021369, 6, 120.54746606, 29, 180.9089484
H, 7, 0.97351221, 1, 106.16199891, 2, -20.16209972

HF=-2145.0398449

S2=3.760996

S2-1=0.

S2A=3.750049

RMSD=8.129e-09

Dipole=0.1832907, -2.3228606, -1.8216728

PG=C01 [X(C7H16Co1N2O5)]

CoC0St8

O, 4

Co

O, 1, 1.9242005521

O, 1, 2.2214515757, 2, 90.

O, 1, 2.2101823762, 3, 90., 2, 180.

N, 1, 2.2863998126, 2, 90., 3, 180.

O, 1, 2.1683330903, 2, 90., 3, 90.

N, 1, 2.2097705841, 2, 90., 3, -90.

H, 2, 0.96865023, 1, 108.08842339, 3, -100.29361099

H, 3, 0.97866159, 1, 101.65493542, 2, 121.00783634

H, 3, 0.97775904, 1, 88.18104588, 2, 13.52134073

H, 4, 1.00509417, 1, 94.31150347, 3, 54.43527047

H, 4, 0.96992155, 1, 110.30996541, 3, -196.44300049

C, 5, 1.45704791, 1, 116.65955457, 2, 53.67455915

C, 5, 1.27167149, 1, 120.49985338, 2, -103.14971942

H, 14, 1.09801744, 5, 122.60800744, 13, 1.81880405

H, 14, 1.08913776, 5, 119.37397259, 13, 183.84860425

H, 13, 1.09974551, 5, 112.52766715, 14, -3.59844165

H, 13, 1.094505, 5, 107.37448232, 14, 117.60643689

H, 13, 1.09500495, 5, 109.28713862, 14, -125.33350659

C, 6, 1.26777603, 1, 117.58161599, 2, -135.87622175

H, 20, 1.10701777, 6, 116.42743509, 1, 169.82760765

O, 20, 1.26474324, 6, 126.1975142, 21, 180.73463792

C, 7, 1.45735134, 1, 123.98823491, 2, -181.58160825

C, 7, 1.27352477, 1, 115.64192328, 2, 7.35602023

H, 24, 1.09812166, 7, 121.67267369, 23, 1.1914942

H, 24, 1.09036744, 7, 117.9562185, 23, 181.53167357

H, 23, 1.09946743, 7, 112.44619419, 24, -1.84934157

H, 23, 1.09419978, 7, 108.69976593, 24, 119.99245608

H, 23, 1.09561948, 7, 109.17741582, 24, -123.51701581

HF=-2068.8936412

S2=3.757164

S2-1=0.

S2A=3.750023

RMSD=4.575e-09

Dipole=-1.7116309, 1.12188, -0.2854224

PG=C01 [X(C5H16Co1N2O5)]

CoCOST9

-1,4
Co
O,1,2.069779662
O,1,2.0725022525,2,90.
N,1,2.2751045491,3,90.,2,180.
N,1,2.3253195559,2,90.,3,180.
O,1,2.0751375005,2,90.,3,90.
N,1,2.3349751075,2,90.,3,-90.
C,2,1.26698348,1,151.74721092,3,152.91832679
H,8,1.11491431,2,114.27702106,1,156.87029317
O,8,1.25374582,2,128.51197908,9,178.89523078
C,3,1.26962476,1,144.36454032,2,235.17735019
H,11,1.11601646,3,113.78267072,1,163.93956421
O,11,1.25161406,3,129.08020178,12,178.87001174
C,4,1.45596772,1,116.03396096,3,26.75593066
C,4,1.26773489,1,124.53550702,3,198.11378645
H,15,1.0984643,4,122.51258335,14,0.37503423
H,15,1.08916411,4,119.55957835,14,179.41493309
H,14,1.10086651,4,111.79744517,15,-2.59706684
H,14,1.09441306,4,108.0642583,15,119.55830925
H,14,1.09273847,4,108.15610291,15,-123.44427438
C,5,1.45818128,1,120.68752974,2,56.02377856
C,5,1.2728032,1,119.56629975,2,-113.0492404
H,22,1.10136311,5,120.9977843,21,0.04957576
H,22,1.09215424,5,119.89489707,21,179.95110997
H,21,1.102136,5,111.93509753,22,-0.89946811
H,21,1.09671317,5,108.93988567,22,121.23771347
H,21,1.09654632,5,108.861694,22,-121.7126668
C,6,1.27106117,1,141.64447214,2,-200.85075891
H,28,1.1160048,6,113.76601057,1,161.01916041
O,28,1.25081271,6,128.85576052,29,179.13499975
C,7,1.4590207,1,119.95315544,2,-201.87526524
C,7,1.27247731,1,120.13848855,2,-8.12719526
H,32,1.10088491,7,121.0380667,31,0.79142917
H,32,1.09013271,7,120.15158129,31,180.31446035
H,31,1.10202188,7,111.89833208,32,-1.69652346
H,31,1.09704443,7,108.2765996,32,119.64524295
H,31,1.09622687,7,109.14650328,32,-122.54610875

HF=-2352.65773
S2=3.756757
S2-1=0.
S2A=3.75002
RMSD=1.271e-09
Dipole=-1.8671767,1.6054715,-1.7119077
PG=C01 [X(C9H18Co1N3O6)]

CoCOST10

-1,4

Co

S,1,3.1515837284
N,1,2.1871492136,2,90.
O,1,1.9382204064,3,90.,2,180.
O,1,2.1435825723,2,90.,3,180.
N,1,2.1677862495,2,90.,3,90.
O,1,2.1294912195,2,90.,3,-90.
H,2,1.37137084,1,68.98737662,3,60.13152301
H,2,1.34995954,1,68.87600307,3,163.38684742
H,3,1.01649383,1,125.54886593,2,73.55205756
H,3,1.02262177,1,91.87096883,2,190.06213232
H,3,1.02214414,1,107.23171868,2,-58.23756144
H,4,0.96789674,1,105.45799613,3,-135.33034611
C,5,1.26991852,1,131.60725745,2,-80.06634025
H,14,1.1160537,5,114.15912931,1,192.02989006
O,14,1.2545012,5,129.03165872,15,179.64749292
H,6,1.03342131,1,103.76270075,2,73.09849173
H,6,1.02173048,1,95.44332656,2,183.37055709
H,6,1.01715252,1,126.67645371,2,-56.00776351
C,7,1.26589241,1,125.4355857,2,46.92957952
H,20,1.11381724,7,114.91970239,1,-188.27084693
O,20,1.2603282,7,128.02959413,21,180.64311568

HF=-2349.8911677

S2=3.756616

S2-1=0.

S2A=3.75002

RMSD=7.318e-09

Dipole=1.6782172,-0.6546464,0.3467135

PG=C01 [X(C2H11Co1N2O5S1)]

NiCOST1

2,3

Ni

O,1,2.1410806777
O,1,2.1365393601,2,90.
N,1,2.1679441982,3,90.,2,180.
N,1,2.1695747862,2,90.,3,180.
O,1,2.1368201015,2,90.,3,90.
N,1,2.170374636,2,90.,3,-90.
C,2,1.22563,1,136.949,3,249.382
H,8,1.09962,2,120.13,1,182.469
H,8,1.10082,2,121.623,9,179.847
C,3,1.2249,1,137.193,2,315.826
H,11,1.09973,3,120.118,1,180.217
H,11,1.10088,3,121.647,12,179.844
C,4,1.47396,1,118.382,3,4.196
C,4,1.27526,1,124.614,3,182.286
H,15,1.09333,4,122.064,14,-0.811
H,15,1.08639,4,120.211,14,179.198
H,14,1.09473,4,112.002,15,0.745
H,14,1.09316,4,109.525,15,122.047
H,14,1.09359,4,109.341,15,-120.475
C,5,1.47204,1,121.374,2,81.903
C,5,1.27902,1,121.311,2,-93.574
H,22,1.09378,5,122.113,21,1.449

H, 22, 1.08739, 5, 119.831, 21, 181.145
H, 21, 1.09488, 5, 111.675, 22, -4.615
H, 21, 1.09345, 5, 109.266, 22, 116.088
H, 21, 1.09293, 5, 109.759, 22, -125.747
C, 6, 1.22596, 1, 136.985, 2, -108.33
H, 28, 1.09968, 6, 120.083, 1, 185.133
H, 28, 1.1006, 6, 121.526, 29, 180.
C, 7, 1.47174, 1, 121.445, 2, -181.642
C, 7, 1.27841, 1, 121.56, 2, 0.242
H, 32, 1.0937, 7, 122.161, 31, 0.718
H, 32, 1.08777, 7, 119.842, 31, 180.336
H, 31, 1.09474, 7, 111.708, 32, 0.98
H, 31, 1.09301, 7, 109.479, 32, 121.848
H, 31, 1.09296, 7, 109.639, 32, -120.033

HF=-2253.5205007
S2=2.004797
S2-1=0.
S2A=2.000015
RMSD=4.891e-10
Dipole=0.5623945, -0.7505237, 0.8285888
PG=C01 [X(C9H21N3Ni103)]

NiCOST2

2, 3
Ni
S, 1, 2.6695818991
O, 1, 2.1469829729, 2, 90.
S, 1, 2.5297674617, 3, 90., 2, 180.
N, 1, 2.1256705191, 2, 90., 3, 180.
O, 1, 2.0958456195, 2, 90., 3, 90.
N, 1, 2.2028247488, 2, 90., 3, -90.
H, 2, 1.34881534, 1, 111.20788624, 3, 61.2915949
H, 2, 1.34861006, 1, 107.49069874, 3, 163.5405823
C, 3, 1.22560306, 1, 142.43197169, 2, 302.68298071
H, 10, 1.09955355, 3, 120.17127698, 1, 181.69337721
H, 10, 1.10159815, 3, 121.60901186, 11, 179.75946607
H, 4, 1.35045104, 1, 105.14887431, 3, 10.37095801
H, 4, 1.35026859, 1, 102.01129132, 3, 108.20415772
C, 5, 1.47541626, 1, 121.40210603, 2, 120.2007734
C, 5, 1.27926166, 1, 120.96882623, 2, -66.38785063
H, 16, 1.09316049, 5, 122.12210288, 15, -0.71313089
H, 16, 1.08766881, 5, 120.14378718, 15, 179.01279474
H, 15, 1.09415924, 5, 111.36363942, 16, -9.85551017
H, 15, 1.09263789, 5, 109.63251317, 16, 110.65043795
H, 15, 1.0930845, 5, 109.65595131, 16, -130.78642095
C, 6, 1.22824825, 1, 137.52229166, 2, -75.85500261
H, 22, 1.09883147, 6, 119.6745348, 1, 182.88353651
H, 22, 1.09960211, 6, 121.71729987, 23, 179.82994699
C, 7, 1.47525075, 1, 119.10749415, 2, -209.0210721
C, 7, 1.27562776, 1, 123.90650675, 2, -30.12547504
H, 26, 1.09339102, 7, 122.36429896, 25, -0.43198012
H, 26, 1.08710168, 7, 119.97505591, 25, 178.79557796
H, 25, 1.09466079, 7, 111.9860476, 26, 9.35085384
H, 25, 1.09364797, 7, 109.65836177, 26, 130.50197671
H, 25, 1.09418879, 7, 109.37387053, 26, -111.12204448

HF=-2803.795011
S2=2.005411
S2-1=0.
S2A=2.000019
RMSD=2.804e-09
Dipole=0.873375, -0.1094586, 0.5336327
PG=C01 [X(C6H18N2Ni10S2)]

NiCOST3

1, 3
Ni
O, 1, 1.9361736389
O, 1, 2.1891227395, 2, 90.
N, 1, 2.1937262402, 3, 90., 2, 180.
N, 1, 2.2896782289, 2, 90., 3, 180.
N, 1, 2.2781967529, 2, 90., 3, 90.
N, 1, 2.2129304935, 2, 90., 3, -90.
H, 2, 0.96627448, 1, 115.09828913, 3, 215.8203581
C, 3, 1.22454354, 1, 116.46145005, 2, 361.26004049
H, 9, 1.10240447, 3, 119.66332571, 1, 181.54688342
H, 9, 1.10088477, 3, 120.09542621, 10, 179.97113302
C, 4, 1.46923838, 1, 117.96167271, 3, 3.12756334
C, 4, 1.27412375, 1, 123.86102839, 3, 186.19223285
H, 13, 1.09425947, 4, 121.88254721, 12, 0.31745774
H, 13, 1.08645203, 4, 119.41284487, 12, 180.50509806
H, 12, 1.09603075, 4, 111.82785769, 13, -2.09116397
H, 12, 1.09289123, 4, 109.0796288, 13, 119.61981881
H, 12, 1.09315219, 4, 109.24331875, 13, -124.02075863
C, 5, 1.46247329, 1, 115.87826411, 2, 63.30865168
C, 5, 1.27337158, 1, 123.16390978, 2, -96.14764789
H, 20, 1.09666532, 5, 122.90235324, 19, 0.71556026
H, 20, 1.08987433, 5, 119.45867798, 19, 180.93558282
H, 19, 1.0979733, 5, 112.64801852, 20, -2.75598921
H, 19, 1.09375054, 5, 108.46137891, 20, 118.80842699
H, 19, 1.09493196, 5, 109.13843137, 20, -124.29095746
C, 6, 1.4630784, 1, 115.52811899, 2, 0.47785178
C, 6, 1.27274341, 1, 126.33297373, 2, 187.51408193
H, 27, 1.09628576, 6, 122.96986823, 26, -0.27243325
H, 27, 1.08957929, 6, 119.69407245, 26, 179.52900171
H, 26, 1.09766485, 6, 112.41864083, 27, 4.39015409
H, 26, 1.09238419, 6, 108.97476193, 27, 127.10211137
H, 26, 1.09558699, 6, 108.80031235, 27, -116.51101369
C, 7, 1.46227381, 1, 127.08372369, 2, -180.15300864
C, 7, 1.27599861, 1, 114.47439894, 2, 3.15281942
H, 34, 1.09638881, 7, 121.85955006, 33, 0.43791297
H, 34, 1.08996653, 7, 117.80389912, 33, 180.14619721
H, 33, 1.09753436, 7, 112.51329733, 34, -1.44399391
H, 33, 1.09523785, 7, 109.38244789, 34, 119.62095564
H, 33, 1.09534211, 7, 109.45250392, 34, -122.71126756

HF=-2234.5912375
S2=2.004935
S2-1=0.
S2A=2.000016
RMSD=1.877e-09

Dipole=-0.3838258, -0.3883409, -1.062131
PG=C01 [X(C9H23N4Ni102)]

NiC0St4

1, 3
Ni
O, 1, 2.0115364363
O, 1, 2.1450709822, 2, 90.
N, 1, 2.1284457081, 3, 90., 2, 180.
N, 1, 2.247130424, 2, 90., 3, 180.
O, 1, 2.1621567894, 2, 90., 3, 90.
N, 1, 2.2217168253, 2, 90., 3, -90.
C, 2, 1.30015511, 1, 143.19201849, 3, 162.11730012
H, 8, 1.10791216, 2, 113.45597863, 1, 153.70210836
O, 8, 1.22880248, 2, 127.12128069, 9, 178.59002058
C, 3, 1.22402662, 1, 122.7321684, 2, 349.7625523
H, 11, 1.1010666, 3, 119.79552245, 1, 183.47912394
H, 11, 1.09981386, 3, 120.73162218, 12, 180.14881842
C, 4, 1.46877182, 1, 118.82704478, 3, 30.37822449
C, 4, 1.27299136, 1, 122.59083029, 3, 207.44654072
H, 15, 1.09381616, 4, 121.97111058, 14, -1.01009888
H, 15, 1.08687774, 4, 119.74948496, 14, 178.89572087
H, 14, 1.09573869, 4, 111.8832565, 15, 0.34585208
H, 14, 1.09275478, 4, 109.06416327, 15, 122.13557513
H, 14, 1.09432971, 4, 108.59502615, 15, -120.6759747
C, 5, 1.46627047, 1, 123.35223933, 2, 74.53630973
C, 5, 1.27450958, 1, 119.15847625, 2, -99.62546017
H, 22, 1.0954148, 5, 122.45839718, 21, 0.0794399
H, 22, 1.08870471, 5, 119.96893438, 21, 180.04608476
H, 21, 1.09701953, 5, 111.7972798, 22, -6.86211989
H, 21, 1.09306218, 5, 108.0047378, 22, 113.99285702
H, 21, 1.09461636, 5, 109.316376, 22, -128.01983287
C, 6, 1.22296412, 1, 124.30345751, 2, 349.23234657
H, 28, 1.10102012, 6, 119.96107241, 1, 179.62638331
H, 28, 1.10018313, 6, 120.81009768, 29, 180.42238221
C, 7, 1.46744922, 1, 120.52302577, 2, -209.04717175
C, 7, 1.27620831, 1, 121.56838792, 2, -20.35756173
H, 32, 1.09620608, 7, 121.40606762, 31, 0.74792834
H, 32, 1.08910626, 7, 119.85144773, 31, 179.93034655
H, 31, 1.09701255, 7, 112.28940998, 32, 5.14470273
H, 31, 1.09503955, 7, 109.4746132, 32, 126.51209993
H, 31, 1.0946892, 7, 109.70689371, 32, -115.74858328

HF=-2328.5319218
S2=2.004799
S2-1=0.
S2A=2.000015
RMSD=1.069e-09
Dipole=1.1584993, -0.8684576, -1.6821999
PG=C01 [X(C9H20N3Ni104)]

NiC0St5

1, 3
Ni
O, 1, 2.1164461569
O, 1, 2.1459492484, 2, 90.
O, 1, 2.148381045, 3, 90., 2, 180.
O, 1, 2.1286978143, 2, 90., 3, 180.
O, 1, 1.9225622267, 2, 90., 3, 90.
O, 1, 2.0889275597, 2, 90., 3, -90.
H, 2, 0.9720149, 1, 123.97643821, 3, 30.70208825
H, 2, 0.97373627, 1, 100.3773561, 3, 272.09837541
H, 3, 0.97164996, 1, 111.16296615, 2, 119.06258038
H, 3, 0.97276639, 1, 126.03498844, 2, -109.7637634
C, 4, 1.22445531, 1, 120.15335199, 3, 93.20263009
H, 12, 1.10053206, 4, 120.12141936, 1, -0.56768575
H, 12, 1.10125446, 4, 119.62016625, 13, 180.15036259
C, 5, 1.22589589, 1, 119.33780051, 2, 280.0637351
H, 15, 1.09992094, 5, 120.11509397, 1, -1.67343225
H, 15, 1.1008052, 5, 119.55602214, 16, 180.35285688
H, 6, 0.96713251, 1, 121.05157668, 2, -61.60025127
C, 7, 1.22510616, 1, 128.829406, 5, -15.62138707
H, 19, 1.09869018, 7, 121.45757107, 1, 0.60806461
H, 19, 1.099019, 7, 119.46160896, 1, 180.37329962

HF=-2080.6133014
S2=2.003832
S2-1=0.
S2A=2.000009
RMSD=8.364e-09
Dipole=0.256148, 0.3786163, -0.1404166
PG=C01 [X(C3H11Ni106)]

NiCOSt6

0, 3
Ni
O, 1, 2.0794503498
O, 1, 2.2522082777, 2, 90.
N, 1, 2.1615184502, 3, 90., 2, 180.
N, 1, 2.3656089013, 2, 90., 3, 180.
O, 1, 1.9468484747, 2, 90., 3, 90.
N, 1, 2.2101150806, 2, 90., 3, -90.
C, 2, 1.27926373, 1, 140.01153609, 3, 158.91753185
H, 8, 1.11213731, 2, 114.20495445, 1, 158.39893196
O, 8, 1.24586635, 2, 128.05105561, 9, 179.42167699
C, 3, 1.21975734, 1, 109.7318329, 2, 412.35906254
H, 11, 1.10542665, 3, 119.97711754, 1, 186.40362895
H, 11, 1.09838034, 3, 120.69301685, 12, 180.99916318
C, 4, 1.45966893, 1, 112.24918192, 3, 49.17204886
C, 4, 1.26959053, 1, 125.28674879, 3, 209.26906449
H, 15, 1.09734956, 4, 122.61736972, 14, -1.71107483
H, 15, 1.08973739, 4, 119.48414781, 14, 177.58305455
H, 14, 1.09944257, 4, 112.44143128, 15, 1.10522857
H, 14, 1.09518227, 4, 108.62343641, 15, 122.68180522
H, 14, 1.09532307, 4, 107.20573804, 15, -121.07510976
C, 5, 1.45818152, 1, 131.46476303, 2, 70.32236976
C, 5, 1.27291172, 1, 109.65490124, 2, -100.47203764

H, 22, 1.09971516, 5, 122.09708986, 21, 1.02464264
H, 22, 1.09088635, 5, 118.115603, 21, 182.6052029
H, 21, 1.10104631, 5, 112.5568363, 22, -7.7293838
H, 21, 1.09491783, 5, 107.84407541, 22, 113.2834034
H, 21, 1.0968229, 5, 109.44245134, 22, -129.04585391
H, 6, 0.96978719, 1, 104.22008938, 2, 12.89356028
C, 7, 1.46373305, 1, 119.19940733, 2, -222.30562795
C, 7, 1.27465099, 1, 121.77483158, 2, -33.88141964
H, 30, 1.09767865, 7, 120.73722199, 29, 2.15485323
H, 30, 1.09278223, 7, 119.8513587, 29, 184.02227532
H, 29, 1.09845059, 7, 111.9766943, 30, -0.75701878
H, 29, 1.09480257, 7, 108.62978978, 30, 120.27757257
H, 29, 1.09338376, 7, 109.77338818, 30, -122.41555046

HF=-2290.0239163

S2=2.004963

S2-1=0.

S2A=2.000016

RMSD=5.009e-09

Dipole=0.5821201, 0.6945258, -2.3305714

PG=C01 [X(C8H19N3Ni104)]

NiC0St7

O, 3

Ni

O, 1, 2.0782368493

O, 1, 2.2787863872, 2, 90.

N, 1, 2.1492053165, 3, 90., 2, 180.

N, 1, 2.2356592778, 2, 90., 3, 180.

O, 1, 2.2025384307, 2, 90., 3, 90.

O, 1, 1.9559163212, 2, 90., 3, -90.

C, 2, 1.28512113, 1, 132.4833235, 3, 113.15801594

H, 8, 1.11267675, 2, 113.71051297, 1, 183.98285741

O, 8, 1.23931276, 2, 128.04409112, 9, 179.90487409

C, 3, 1.22374177, 1, 109.60458532, 2, 281.53153682

H, 11, 1.10639136, 3, 119.25177869, 1, 176.8030791

H, 11, 1.10526152, 3, 119.17725213, 12, 179.14009744

C, 4, 1.4585547, 1, 126.34067226, 3, 81.98896457

C, 4, 1.27475584, 1, 113.81398476, 3, 263.68927834

H, 15, 1.09819287, 4, 121.24591122, 14, 0.52012724

H, 15, 1.09255565, 4, 117.30070407, 14, 181.07893926

H, 14, 1.09937234, 4, 112.41865489, 15, -0.15888386

H, 14, 1.09533075, 4, 108.94725468, 15, 121.27846475

H, 14, 1.09506993, 4, 109.22201792, 15, -121.77956847

C, 5, 1.45824323, 1, 114.61249078, 2, 76.96852908

C, 5, 1.27058069, 1, 126.53746045, 2, -102.17068816

H, 22, 1.0983786, 5, 122.81105298, 21, 0.24317589

H, 22, 1.09062295, 5, 119.68247559, 21, 180.36622633

H, 21, 1.10023651, 5, 111.92600434, 22, -2.05585188

H, 21, 1.09453342, 5, 108.43630078, 22, 120.46801482

H, 21, 1.09306121, 5, 108.39554244, 22, -124.63010712

C, 6, 1.22467958, 1, 116.27830033, 2, 344.85453428

H, 28, 1.10344602, 6, 119.41487377, 1, 181.36113942

H, 28, 1.10021369, 6, 120.54746606, 29, 180.9089484

H, 7, 0.97351221, 1, 106.16199891, 2, -20.16209972

HF=-2270.576602
S2=2.004891
S2-1=0.
S2A=2.000015
RMSD=5.090e-09
Dipole=0.1446506, -2.388103, -1.7663208
PG=C01 [X(C7H16N2Ni105)]

NiC0St8

0, 3
Ni
0, 1, 1.9439821071
0, 1, 2.1484750772, 2, 90.
0, 1, 2.1784890826, 3, 90., 2, 180.
N, 1, 2.2165439709, 2, 90., 3, 180.
0, 1, 2.1458253137, 2, 90., 3, 90.
N, 1, 2.1540294307, 2, 90., 3, -90.
H, 2, 0.96865023, 1, 108.08842339, 3, -100.29361099
H, 3, 0.97866159, 1, 101.65493542, 2, 121.00783634
H, 3, 0.97775904, 1, 88.18104588, 2, 13.52134073
H, 4, 1.00509417, 1, 94.31150347, 3, 54.43527047
H, 4, 0.96992155, 1, 110.30996541, 3, -196.44300049
C, 5, 1.45704791, 1, 116.65955457, 2, 53.67455915
C, 5, 1.27167149, 1, 120.49985338, 2, -103.14971942
H, 14, 1.09801744, 5, 122.60800744, 13, 1.81880405
H, 14, 1.08913776, 5, 119.37397259, 13, 183.84860425
H, 13, 1.09974551, 5, 112.52766715, 14, -3.59844165
H, 13, 1.094505, 5, 107.37448232, 14, 117.60643689
H, 13, 1.09500495, 5, 109.28713862, 14, -125.33350659
C, 6, 1.26777603, 1, 117.58161599, 2, -135.87622175
H, 20, 1.10701777, 6, 116.42743509, 1, 169.82760765
O, 20, 1.26474324, 6, 126.1975142, 21, 180.73463792
C, 7, 1.45735134, 1, 123.98823491, 2, -181.58160825
C, 7, 1.27352477, 1, 115.64192328, 2, 7.35602023
H, 24, 1.09812166, 7, 121.67267369, 23, 1.1914942
H, 24, 1.09036744, 7, 117.9562185, 23, 181.53167357
H, 23, 1.09946743, 7, 112.44619419, 24, -1.84934157
H, 23, 1.09419978, 7, 108.69976593, 24, 119.99245608
H, 23, 1.09561948, 7, 109.17741582, 24, -123.51701581

HF=-2194.4324899
S2=2.00424
S2-1=0.
S2A=2.000012
RMSD=3.448e-09
Dipole=-1.7006278, 1.0878819, -0.3762108
PG=C01 [X(C5H16N2Ni105)]

NiC0St9

-1, 3
Ni

O,1,2.0690326982
 O,1,2.0645247514,2,90.
 N,1,2.2101209681,3,90.,2,180.
 N,1,2.2694754952,2,90.,3,180.
 O,1,2.064388686,2,90.,3,90.
 N,1,2.2750085256,2,90.,3,-90.
 C,2,1.26698348,1,151.74721092,3,152.91832679
 H,8,1.11491431,2,114.27702106,1,156.87029317
 O,8,1.25374582,2,128.51197908,9,178.89523078
 C,3,1.26962476,1,144.36454032,2,235.17735019
 H,11,1.11601646,3,113.78267072,1,163.93956421
 O,11,1.25161406,3,129.08020178,12,178.87001174
 C,4,1.45596772,1,116.03396096,3,26.75593066
 C,4,1.26773489,1,124.53550702,3,198.11378645
 H,15,1.0984643,4,122.51258335,14,0.37503423
 H,15,1.08916411,4,119.55957835,14,179.41493309
 H,14,1.10086651,4,111.79744517,15,-2.59706684
 H,14,1.09441306,4,108.0642583,15,119.55830925
 H,14,1.09273847,4,108.15610291,15,-123.44427438
 C,5,1.45818128,1,120.68752974,2,56.02377856
 C,5,1.2728032,1,119.56629975,2,-113.0492404
 H,22,1.10136311,5,120.9977843,21,0.04957576
 H,22,1.09215424,5,119.89489707,21,179.95110997
 H,21,1.102136,5,111.93509753,22,-0.89946811
 H,21,1.09671317,5,108.93988567,22,121.23771347
 H,21,1.09654632,5,108.861694,22,-121.7126668
 C,6,1.27106117,1,141.64447214,2,-200.85075891
 H,28,1.1160048,6,113.76601057,1,161.01916041
 O,28,1.25081271,6,128.85576052,29,179.13499975
 C,7,1.4590207,1,119.95315544,2,-201.87526524
 C,7,1.27247731,1,120.13848855,2,-8.12719526
 H,32,1.10088491,7,121.0380667,31,0.79142917
 H,32,1.09013271,7,120.15158129,31,180.31446035
 H,31,1.10202188,7,111.89833208,32,-1.69652346
 H,31,1.09704443,7,108.2765996,32,119.64524295
 H,31,1.09622687,7,109.14650328,32,-122.54610875

HF=-2478.1912878

S2=2.00417

S2-1=0.

S2A=2.000011

RMSD=1.472e-09

Dipole=-1.8760905,1.6093641,-1.7661588

PG=C01 [X(C9H18N3Ni106)]

NiCOST10

-1,3

Ni

S,1,3.125403921

N,1,2.1258325607,2,90.

O,1,1.9589036079,3,90.,2,180.

O,1,2.1070404776,2,90.,3,180.

N,1,2.1113922578,2,90.,3,90.

O,1,2.0944006865,2,90.,3,-90.

H,2,1.37137084,1,68.98737662,3,60.13152301

H,2,1.34995954,1,68.87600307,3,163.38684742

H, 3, 1.01649383, 1, 125.54886593, 2, 73.55205756
H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232
H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144
H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611
C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025
H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006
O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292
H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173
H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709
H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351
C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952
H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-2475.4280898

S2=2.004348

S2-1=0.

S2A=2.000012

RMSD=8.988e-09

Dipole=1.621995, -0.6110249, 0.431221

PG=C01 [X(C2H11N2Ni10S1)]

CuCOSt1

2, 2

Cu

O, 1, 2.5229945057

O, 1, 2.080104327, 2, 90.

N, 1, 2.4727441497, 3, 90., 2, 180.

N, 1, 2.1169677042, 2, 90., 3, 180.

O, 1, 2.0578076536, 2, 90., 3, 90.

N, 1, 2.0742365456, 2, 90., 3, -90.

C, 2, 1.22563, 1, 136.949, 3, 249.382

H, 8, 1.09962, 2, 120.13, 1, 182.469

H, 8, 1.10082, 2, 121.623, 9, 179.847

C, 3, 1.2249, 1, 137.193, 2, 315.826

H, 11, 1.09973, 3, 120.118, 1, 180.217

H, 11, 1.10088, 3, 121.647, 12, 179.844

C, 4, 1.47396, 1, 118.382, 3, 4.196

C, 4, 1.27526, 1, 124.614, 3, 182.286

H, 15, 1.09333, 4, 122.064, 14, -0.811

H, 15, 1.08639, 4, 120.211, 14, 179.198

H, 14, 1.09473, 4, 112.002, 15, 0.745

H, 14, 1.09316, 4, 109.525, 15, 122.047

H, 14, 1.09359, 4, 109.341, 15, -120.475

C, 5, 1.47204, 1, 121.374, 2, 81.903

C, 5, 1.27902, 1, 121.311, 2, -93.574

H, 22, 1.09378, 5, 122.113, 21, 1.449

H, 22, 1.08739, 5, 119.831, 21, 181.145

H, 21, 1.09488, 5, 111.675, 22, -4.615

H, 21, 1.09345, 5, 109.266, 22, 116.088

H, 21, 1.09293, 5, 109.759, 22, -125.747

C, 6, 1.22596, 1, 136.985, 2, -108.33

H, 28, 1.09968, 6, 120.083, 1, 185.133

H, 28, 1.1006, 6, 121.526, 29, 180.

C, 7, 1.47174, 1, 121.445, 2, -181.642

C, 7, 1.27841, 1, 121.56, 2, 0.242

H, 32, 1.0937, 7, 122.161, 31, 0.718
H, 32, 1.08777, 7, 119.842, 31, 180.336
H, 31, 1.09474, 7, 111.708, 32, 0.98
H, 31, 1.09301, 7, 109.479, 32, 121.848
H, 31, 1.09296, 7, 109.639, 32, -120.033

HF=-2385.6633499

S2=0.752626

S2-1=0.

S2A=0.750007

RMSD=3.701e-09

Dipole=0.5475951, -0.5831857, 0.9245389

PG=C01 [X(C9H21Cu1N3O3)]

CuCOSt2

2, 2

Cu

S, 1, 3.3718364758

O, 1, 2.0686222793, 2, 90.

S, 1, 2.970545376, 3, 90., 2, 180.

N, 1, 2.0679752767, 2, 90., 3, 180.

O, 1, 2.0305456776, 2, 90., 3, 90.

N, 1, 2.0706266717, 2, 90., 3, -90.

H, 2, 1.34881534, 1, 111.20788624, 3, 61.2915949

H, 2, 1.34861006, 1, 107.49069874, 3, 163.5405823

C, 3, 1.22560306, 1, 142.43197169, 2, 302.68298071

H, 10, 1.09955355, 3, 120.17127698, 1, 181.69337721

H, 10, 1.10159815, 3, 121.60901186, 11, 179.75946607

H, 4, 1.35045104, 1, 105.14887431, 3, 10.37095801

H, 4, 1.35026859, 1, 102.01129132, 3, 108.20415772

C, 5, 1.47541626, 1, 121.40210603, 2, 120.2007734

C, 5, 1.27926166, 1, 120.96882623, 2, -66.38785063

H, 16, 1.09316049, 5, 122.12210288, 15, -0.71313089

H, 16, 1.08766881, 5, 120.14378718, 15, 179.01279474

H, 15, 1.09415924, 5, 111.36363942, 16, -9.85551017

H, 15, 1.09263789, 5, 109.63251317, 16, 110.65043795

H, 15, 1.0930845, 5, 109.65595131, 16, -130.78642095

C, 6, 1.22824825, 1, 137.52229166, 2, -75.85500261

H, 22, 1.09883147, 6, 119.6745348, 1, 182.88353651

H, 22, 1.09960211, 6, 121.71729987, 23, 179.82994699

C, 7, 1.47525075, 1, 119.10749415, 2, -209.0210721

C, 7, 1.27562776, 1, 123.90650675, 2, -30.12547504

H, 26, 1.09339102, 7, 122.36429896, 25, -0.43198012

H, 26, 1.08710168, 7, 119.97505591, 25, 178.79557796

H, 25, 1.09466079, 7, 111.9860476, 26, 9.35085384

H, 25, 1.09364797, 7, 109.65836177, 26, 130.50197671

H, 25, 1.09418879, 7, 109.37387053, 26, -111.12204448

HF=-2935.9484655

S2=0.752968

S2-1=0.

S2A=0.750008

RMSD=7.264e-09

Dipole=0.7744408, 0.013634, 0.457288

PG=C01 [X(C6H18Cu1N2O2S2)]

CuCOSt3

1, 2

Cu

O, 1, 1.8624895844

O, 1, 2.5035790687, 2, 90.

N, 1, 2.0722000549, 3, 90., 2, 180.

N, 1, 2.8509841225, 2, 90., 3, 180.

N, 1, 2.2369631022, 2, 90., 3, 90.

N, 1, 2.1872768468, 2, 90., 3, -90.

H, 2, 0.96627448, 1, 115.09828913, 3, 215.8203581

C, 3, 1.22454354, 1, 116.46145005, 2, 361.26004049

H, 9, 1.10240447, 3, 119.66332571, 1, 181.54688342

H, 9, 1.10088477, 3, 120.09542621, 10, 179.97113302

C, 4, 1.46923838, 1, 117.96167271, 3, 3.12756334

C, 4, 1.27412375, 1, 123.86102839, 3, 186.19223285

H, 13, 1.09425947, 4, 121.88254721, 12, 0.31745774

H, 13, 1.08645203, 4, 119.41284487, 12, 180.50509806

H, 12, 1.09603075, 4, 111.82785769, 13, -2.09116397

H, 12, 1.09289123, 4, 109.0796288, 13, 119.61981881

H, 12, 1.09315219, 4, 109.24331875, 13, -124.02075863

C, 5, 1.46247329, 1, 115.87826411, 2, 63.30865168

C, 5, 1.27337158, 1, 123.16390978, 2, -96.14764789

H, 20, 1.09666532, 5, 122.90235324, 19, 0.71556026

H, 20, 1.08987433, 5, 119.45867798, 19, 180.93558282

H, 19, 1.0979733, 5, 112.64801852, 20, -2.75598921

H, 19, 1.09375054, 5, 108.46137891, 20, 118.80842699

H, 19, 1.09493196, 5, 109.13843137, 20, -124.29095746

C, 6, 1.4630784, 1, 115.52811899, 2, 0.47785178

C, 6, 1.27274341, 1, 126.33297373, 2, 187.51408193

H, 27, 1.09628576, 6, 122.96986823, 26, -0.27243325

H, 27, 1.08957929, 6, 119.69407245, 26, 179.52900171

H, 26, 1.09766485, 6, 112.41864083, 27, 4.39015409

H, 26, 1.09238419, 6, 108.97476193, 27, 127.10211137

H, 26, 1.09558699, 6, 108.80031235, 27, -116.51101369

C, 7, 1.46227381, 1, 127.08372369, 2, -180.15300864

C, 7, 1.27599861, 1, 114.47439894, 2, 3.15281942

H, 34, 1.09638881, 7, 121.85955006, 33, 0.43791297

H, 34, 1.08996653, 7, 117.80389912, 33, 180.14619721

H, 33, 1.09753436, 7, 112.51329733, 34, -1.44399391

H, 33, 1.09523785, 7, 109.38244789, 34, 119.62095564

H, 33, 1.09534211, 7, 109.45250392, 34, -122.71126756

HF=-2366.7506447

S2=0.752722

S2-1=0.

S2A=0.750007

RMSD=6.315e-09

Dipole=-0.2139585, -0.3573963, -1.0153205

PG=C01 [X(C9H23Cu1N4O2)]

CuCOSt4

1,2
Cu
O,1,1.9092603586
O,1,2.2911964761,2,90.
N,1,2.0247770762,3,90.,2,180.
N,1,2.3975746697,2,90.,3,180.
O,1,2.3053129641,2,90.,3,90.
N,1,2.3690641344,2,90.,3,-90.
C,2,1.30015511,1,143.19201849,3,162.11730012
H,8,1.10791216,2,113.45597863,1,153.70210836
O,8,1.22880248,2,127.12128069,9,178.59002058
C,3,1.22402662,1,122.7321684,2,349.7625523
H,11,1.1010666,3,119.79552245,1,183.47912394
H,11,1.09981386,3,120.73162218,12,180.14881842
C,4,1.46877182,1,118.82704478,3,30.37822449
C,4,1.27299136,1,122.59083029,3,207.44654072
H,15,1.09381616,4,121.97111058,14,-1.01009888
H,15,1.08687774,4,119.74948496,14,178.89572087
H,14,1.09573869,4,111.8832565,15,0.34585208
H,14,1.09275478,4,109.06416327,15,122.13557513
H,14,1.09432971,4,108.59502615,15,-120.6759747
C,5,1.46627047,1,123.35223933,2,74.53630973
C,5,1.27450958,1,119.15847625,2,-99.62546017
H,22,1.0954148,5,122.45839718,21,0.0794399
H,22,1.08870471,5,119.96893438,21,180.04608476
H,21,1.09701953,5,111.7972798,22,-6.86211989
H,21,1.09306218,5,108.0047378,22,113.99285702
H,21,1.09461636,5,109.316376,22,-128.01983287
C,6,1.22296412,1,124.30345751,2,349.23234657
H,28,1.10102012,6,119.96107241,1,179.62638331
H,28,1.10018313,6,120.81009768,29,180.42238221
C,7,1.46744922,1,120.52302577,2,-209.04717175
C,7,1.27620831,1,121.56838792,2,-20.35756173
H,32,1.09620608,7,121.40606762,31,0.74792834
H,32,1.08910626,7,119.85144773,31,179.93034655
H,31,1.09701255,7,112.28940998,32,5.14470273
H,31,1.09503955,7,109.4746132,32,126.51209993
H,31,1.0946892,7,109.70689371,32,-115.74858328

HF=-2460.6805953

S2=0.752205

S2-1=0.

S2A=0.750004

RMSD=8.282e-09

Dipole=1.1062975,-0.8327282,-1.5526684

PG=C01 [X(C9H20Cu1N3O4)]

CuCOSt5

1,2
Cu
O,1,2.1645712528
O,1,2.3663068701,2,90.
O,1,2.198680821,3,90.,2,180.
O,1,2.3250482804,2,90.,3,180.
O,1,1.8496997073,2,90.,3,90.
O,1,2.006384348,2,90.,3,-90.

H, 2, 0.9720149, 1, 123.97643821, 3, 30.70208825
H, 2, 0.97373627, 1, 100.3773561, 3, 272.09837541
H, 3, 0.97164996, 1, 111.16296615, 2, 119.06258038
H, 3, 0.97276639, 1, 126.03498844, 2, -109.7637634
C, 4, 1.22445531, 1, 120.15335199, 3, 93.20263009
H, 12, 1.10053206, 4, 120.12141936, 1, -0.56768575
H, 12, 1.10125446, 4, 119.62016625, 13, 180.15036259
C, 5, 1.22589589, 1, 119.33780051, 2, 280.0637351
H, 15, 1.09992094, 5, 120.11509397, 1, -1.67343225
H, 15, 1.1008052, 5, 119.55602214, 16, 180.35285688
H, 6, 0.96713251, 1, 121.05157668, 2, -61.60025127
C, 7, 1.22510616, 1, 128.829406, 5, -15.62138707
H, 19, 1.09869018, 7, 121.45757107, 1, 0.60806461
H, 19, 1.099019, 7, 119.46160896, 1, 180.37329962

HF=-2212.76807

S2=0.751976

S2-1=0.

S2A=0.750003

RMSD=6.272e-09

Dipole=0.2295656, 0.2308449, -0.159469

PG=C01 [X(C3H11Cu106)]

CuCOSt6

O, 2

Cu

O, 1, 2.0320820683

O, 1, 2.6353800022, 2, 90.

N, 1, 2.1179218731, 3, 90., 2, 180.

N, 1, 2.7820563649, 2, 90., 3, 180.

O, 1, 1.8762493974, 2, 90., 3, 90.

N, 1, 2.1382558872, 2, 90., 3, -90.

C, 2, 1.27926373, 1, 140.01153609, 3, 158.91753185

H, 8, 1.11213731, 2, 114.20495445, 1, 158.39893196

O, 8, 1.24586635, 2, 128.05105561, 9, 179.42167699

C, 3, 1.21975734, 1, 109.7318329, 2, 412.35906254

H, 11, 1.10542665, 3, 119.97711754, 1, 186.40362895

H, 11, 1.09838034, 3, 120.69301685, 12, 180.99916318

C, 4, 1.45966893, 1, 112.24918192, 3, 49.17204886

C, 4, 1.26959053, 1, 125.28674879, 3, 209.26906449

H, 15, 1.09734956, 4, 122.61736972, 14, -1.71107483

H, 15, 1.08973739, 4, 119.48414781, 14, 177.58305455

H, 14, 1.09944257, 4, 112.44143128, 15, 1.10522857

H, 14, 1.09518227, 4, 108.62343641, 15, 122.68180522

H, 14, 1.09532307, 4, 107.20573804, 15, -121.07510976

C, 5, 1.45818152, 1, 131.46476303, 2, 70.32236976

C, 5, 1.27291172, 1, 109.65490124, 2, -100.47203764

H, 22, 1.09971516, 5, 122.09708986, 21, 1.02464264

H, 22, 1.09088635, 5, 118.115603, 21, 182.6052029

H, 21, 1.10104631, 5, 112.5568363, 22, -7.7293838

H, 21, 1.09491783, 5, 107.84407541, 22, 113.2834034

H, 21, 1.0968229, 5, 109.44245134, 22, -129.04585391

H, 6, 0.96978719, 1, 104.22008938, 2, 12.89356028

C, 7, 1.46373305, 1, 119.19940733, 2, -222.30562795

C, 7, 1.27465099, 1, 121.77483158, 2, -33.88141964

H, 30, 1.09767865, 7, 120.73722199, 29, 2.15485323

H, 30, 1.09278223, 7, 119.8513587, 29, 184.02227532
H, 29, 1.09845059, 7, 111.9766943, 30, -0.75701878
H, 29, 1.09480257, 7, 108.62978978, 30, 120.27757257
H, 29, 1.09338376, 7, 109.77338818, 30, -122.41555046

HF=-2422.1855556
S2=0.752678
S2-1=0.
S2A=0.750006
RMSD=4.415e-09
Dipole=0.6064538, 0.6621942, -2.2592332
PG=C01 [X(C8H19Cu1N3O4)]

CuCOSt7

O, 2
Cu
O, 1, 2.0090270242
O, 1, 2.6059043335, 2, 90.
N, 1, 2.1141300274, 3, 90., 2, 180.
N, 1, 2.6893414553, 2, 90., 3, 180.
O, 1, 2.1520174611, 2, 90., 3, 90.
O, 1, 1.8953352305, 2, 90., 3, -90.
C, 2, 1.28512113, 1, 132.4833235, 3, 113.15801594
H, 8, 1.11267675, 2, 113.71051297, 1, 183.98285741
O, 8, 1.23931276, 2, 128.04409112, 9, 179.90487409
C, 3, 1.22374177, 1, 109.60458532, 2, 281.53153682
H, 11, 1.10639136, 3, 119.25177869, 1, 176.8030791
H, 11, 1.10526152, 3, 119.17725213, 12, 179.14009744
C, 4, 1.4585547, 1, 126.34067226, 3, 81.98896457
C, 4, 1.27475584, 1, 113.81398476, 3, 263.68927834
H, 15, 1.09819287, 4, 121.24591122, 14, 0.52012724
H, 15, 1.09255565, 4, 117.30070407, 14, 181.07893926
H, 14, 1.09937234, 4, 112.41865489, 15, -0.15888386
H, 14, 1.09533075, 4, 108.94725468, 15, 121.27846475
H, 14, 1.09506993, 4, 109.22201792, 15, -121.77956847
C, 5, 1.45824323, 1, 114.61249078, 2, 76.96852908
C, 5, 1.27058069, 1, 126.53746045, 2, -102.17068816
H, 22, 1.0983786, 5, 122.81105298, 21, 0.24317589
H, 22, 1.09062295, 5, 119.68247559, 21, 180.36622633
H, 21, 1.10023651, 5, 111.92600434, 22, -2.05585188
H, 21, 1.09453342, 5, 108.43630078, 22, 120.46801482
H, 21, 1.09306121, 5, 108.39554244, 22, -124.63010712
C, 6, 1.22467958, 1, 116.27830033, 2, 344.85453428
H, 28, 1.10344602, 6, 119.41487377, 1, 181.36113942
H, 28, 1.10021369, 6, 120.54746606, 29, 180.9089484
H, 7, 0.97351221, 1, 106.16199891, 2, -20.16209972

HF=-2402.736115
S2=0.753197
S2-1=0.
S2A=0.750008
RMSD=5.224e-09
Dipole=0.2743659, -2.152871, -1.5856933
PG=C01 [X(C7H16Cu1N2O5)]

CuCOSt8

O, 2
Cu
O, 1, 1.877833437
O, 1, 2.4441094961, 2, 90.
O, 1, 2.0780152109, 3, 90., 2, 180.
N, 1, 2.6311759288, 2, 90., 3, 180.
O, 1, 2.1072510354, 2, 90., 3, 90.
N, 1, 2.1248508301, 2, 90., 3, -90.
H, 2, 0.96865023, 1, 108.08842339, 3, -100.29361099
H, 3, 0.97866159, 1, 101.65493542, 2, 121.00783634
H, 3, 0.97775904, 1, 88.18104588, 2, 13.52134073
H, 4, 1.00509417, 1, 94.31150347, 3, 54.43527047
H, 4, 0.96992155, 1, 110.30996541, 3, -196.44300049
C, 5, 1.45704791, 1, 116.65955457, 2, 53.67455915
C, 5, 1.27167149, 1, 120.49985338, 2, -103.14971942
H, 14, 1.09801744, 5, 122.60800744, 13, 1.81880405
H, 14, 1.08913776, 5, 119.37397259, 13, 183.84860425
H, 13, 1.09974551, 5, 112.52766715, 14, -3.59844165
H, 13, 1.094505, 5, 107.37448232, 14, 117.60643689
H, 13, 1.09500495, 5, 109.28713862, 14, -125.33350659
C, 6, 1.26777603, 1, 117.58161599, 2, -135.87622175
H, 20, 1.10701777, 6, 116.42743509, 1, 169.82760765
O, 20, 1.26474324, 6, 126.1975142, 21, 180.73463792
C, 7, 1.45735134, 1, 123.98823491, 2, -181.58160825
C, 7, 1.27352477, 1, 115.64192328, 2, 7.35602023
H, 24, 1.09812166, 7, 121.67267369, 23, 1.1914942
H, 24, 1.09036744, 7, 117.9562185, 23, 181.53167357
H, 23, 1.09946743, 7, 112.44619419, 24, -1.84934157
H, 23, 1.09419978, 7, 108.69976593, 24, 119.99245608
H, 23, 1.09561948, 7, 109.17741582, 24, -123.51701581

HF=-2326.587559

S2=0.75236

S2-1=0.

S2A=0.750005

RMSD=8.382e-09

Dipole=-1.5668953, 1.0808063, -0.1898267

PG=C01 [X(C5H16Cu1N2O5)]

CuCOSt9

-1, 2
Cu
O, 1, 2.0057309956
O, 1, 1.9748599687, 2, 90.
N, 1, 2.1618291808, 3, 90., 2, 180.
N, 1, 2.1258926122, 2, 90., 3, 180.
O, 1, 2.3038395072, 2, 90., 3, 90.
N, 1, 2.7345715179, 2, 90., 3, -90.
C, 2, 1.26698348, 1, 151.74721092, 3, 152.91832679
H, 8, 1.11491431, 2, 114.27702106, 1, 156.87029317
O, 8, 1.25374582, 2, 128.51197908, 9, 178.89523078

C, 3, 1.26962476, 1, 144.36454032, 2, 235.17735019
 H, 11, 1.11601646, 3, 113.78267072, 1, 163.93956421
 O, 11, 1.25161406, 3, 129.08020178, 12, 178.87001174
 C, 4, 1.45596772, 1, 116.03396096, 3, 26.75593066
 C, 4, 1.26773489, 1, 124.53550702, 3, 198.11378645
 H, 15, 1.0984643, 4, 122.51258335, 14, 0.37503423
 H, 15, 1.08916411, 4, 119.55957835, 14, 179.41493309
 H, 14, 1.10086651, 4, 111.79744517, 15, -2.59706684
 H, 14, 1.09441306, 4, 108.0642583, 15, 119.55830925
 H, 14, 1.09273847, 4, 108.15610291, 15, -123.44427438
 C, 5, 1.45818128, 1, 120.68752974, 2, 56.02377856
 C, 5, 1.2728032, 1, 119.56629975, 2, -113.0492404
 H, 22, 1.10136311, 5, 120.9977843, 21, 0.04957576
 H, 22, 1.09215424, 5, 119.89489707, 21, 179.95110997
 H, 21, 1.102136, 5, 111.93509753, 22, -0.89946811
 H, 21, 1.09671317, 5, 108.93988567, 22, 121.23771347
 H, 21, 1.09654632, 5, 108.861694, 22, -121.7126668
 C, 6, 1.27106117, 1, 141.64447214, 2, -200.85075891
 H, 28, 1.1160048, 6, 113.76601057, 1, 161.01916041
 O, 28, 1.25081271, 6, 128.85576052, 29, 179.13499975
 C, 7, 1.4590207, 1, 119.95315544, 2, -201.87526524
 C, 7, 1.27247731, 1, 120.13848855, 2, -8.12719526
 H, 32, 1.10088491, 7, 121.0380667, 31, 0.79142917
 H, 32, 1.09013271, 7, 120.15158129, 31, 180.31446035
 H, 31, 1.10202188, 7, 111.89833208, 32, -1.69652346
 H, 31, 1.09704443, 7, 108.2765996, 32, 119.64524295
 H, 31, 1.09622687, 7, 109.14650328, 32, -122.54610875

HF=-2610.3356208

S2=0.752215

S2-1=0.

S2A=0.750004

RMSD=5.024e-09

Dipole=-1.7039778, 2.1367989, -1.6207444

PG=C01 [X(C9H18Cu1N3O6)]

CuCOSt10

-1, 2

Cu

S, 1, 3.0153639174

N, 1, 2.4704268111, 2, 90.

O, 1, 1.9245094481, 3, 90., 2, 180.

O, 1, 2.2806585769, 2, 90., 3, 180.

N, 1, 2.0421394449, 2, 90., 3, 90.

O, 1, 2.0417008789, 2, 90., 3, -90.

H, 2, 1.37137084, 1, 68.98737662, 3, 60.13152301

H, 2, 1.34995954, 1, 68.87600307, 3, 163.38684742

H, 3, 1.01649383, 1, 125.54886593, 2, 73.55205756

H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232

H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144

H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611

C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025

H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006

O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292

H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173

H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709

H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351
C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952
H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-2607.5730804
S2=0.753189
S2-1=0.
S2A=0.750006
RMSD=4.934e-09
Dipole=2.0296438, -0.4018361, 0.1649226
PG=C01 [X(C2H11Cu1N2O5S1)]

ZnCOSt1

2, 1
Zn
O, 1, 2.203586
O, 1, 2.198484, 2, 90.
N, 1, 2.232777, 3, 90., 2, 180.
N, 1, 2.232284, 2, 90., 3, 180.
O, 1, 2.198086, 2, 90., 3, 90.
N, 1, 2.237162, 2, 90., 3, -90.
C, 2, 1.225629, 1, 136.949, 3, 249.382
H, 8, 1.099618, 2, 120.13, 1, 182.469
H, 8, 1.10082, 2, 121.623, 9, 179.847
C, 3, 1.224904, 1, 137.193, 2, 315.826
H, 11, 1.099728, 3, 120.118, 1, 180.217
H, 11, 1.100878, 3, 121.647, 12, 179.844
C, 4, 1.473957, 1, 118.382, 3, 4.196
C, 4, 1.275256, 1, 124.614, 3, 182.286
H, 15, 1.093325, 4, 122.064, 14, -0.811
H, 15, 1.086391, 4, 120.211, 14, 179.198
H, 14, 1.094732, 4, 112.002, 15, 0.745
H, 14, 1.093161, 4, 109.525, 15, 122.047
H, 14, 1.093589, 4, 109.341, 15, -120.475
C, 5, 1.472042, 1, 121.374, 2, 81.903
C, 5, 1.279023, 1, 121.311, 2, -93.574
H, 22, 1.093777, 5, 122.113, 21, 1.449
H, 22, 1.087392, 5, 119.831, 21, 181.145
H, 21, 1.094877, 5, 111.675, 22, -4.615
H, 21, 1.093446, 5, 109.266, 22, 116.088
H, 21, 1.092933, 5, 109.759, 22, -125.747
C, 6, 1.225955, 1, 136.985, 2, -108.33
H, 28, 1.099683, 6, 120.083, 1, 185.133
H, 28, 1.100604, 6, 121.526, 29, 180.
C, 7, 1.471737, 1, 121.445, 2, -181.642
C, 7, 1.278414, 1, 121.56, 2, 0.242
H, 32, 1.093696, 7, 122.161, 31, 0.718
H, 32, 1.087772, 7, 119.842, 31, 180.336
H, 31, 1.094741, 7, 111.708, 32, 0.98
H, 31, 1.093014, 7, 109.479, 32, 121.848
H, 31, 1.092958, 7, 109.639, 32, -120.033

HF=-2524.5488036
RMSD=1.885e-09
Dipole=0.5954516, -0.7896927, 0.8622276

PG=C01 [X(C9H21N3O3Zn1)]

ZnC0St2

2,1

Zn

S,1,2.8230761944

O,1,2.2075984136,2,90.

S,1,2.650082889,3,90.,2,180.

N,1,2.1789155066,2,90.,3,180.

O,1,2.1435803994,2,90.,3,90.

N,1,2.2508059252,2,90.,3,-90.

H,2,1.3488153391,1,111.20788624,3,61.2915949

H,2,1.3486100625,1,107.49069874,3,163.5405823

C,3,1.2256030587,1,142.43197169,2,302.68298071

H,10,1.0995535473,3,120.17127698,1,181.69337721

H,10,1.1015981546,3,121.60901186,11,179.75946607

H,4,1.3504510383,1,105.14887431,3,10.37095801

H,4,1.3502685868,1,102.01129132,3,108.20415772

C,5,1.4754162608,1,121.40210603,2,120.2007734

C,5,1.2792616599,1,120.96882623,2,-66.38785063

H,16,1.0931604851,5,122.12210288,15,-0.71313089

H,16,1.0876688061,5,120.14378718,15,179.01279474

H,15,1.0941592365,5,111.36363942,16,-9.85551017

H,15,1.0926378935,5,109.63251317,16,110.65043795

H,15,1.0930844971,5,109.65595131,16,-130.78642095

C,6,1.2282482452,1,137.52229166,2,-75.85500261

H,22,1.0988314716,6,119.6745348,1,182.88353651

H,22,1.0996021125,6,121.71729987,23,179.82994699

C,7,1.4752507527,1,119.10749415,2,-209.0210721

C,7,1.2756277642,1,123.90650675,2,-30.12547504

H,26,1.0933910152,7,122.36429896,25,-0.43198012

H,26,1.0871016803,7,119.97505591,25,178.79557796

H,25,1.0946607875,7,111.9860476,26,9.35085384

H,25,1.0936479667,7,109.65836177,26,130.50197671

H,25,1.0941887936,7,109.37387053,26,-111.12204448

HF=-3074.8246277

RMSD=5.591e-09

Dipole=0.8937542,-0.1601473,0.5120326

PG=C01 [X(C6H18N2O2S2Zn1)]

ZnC0St3

1,1

Zn

O,1,1.9056140082

O,1,2.2975763948,2,90.

N,1,2.1585976156,3,90.,2,180.

N,1,2.4964194811,2,90.,3,180.

N,1,2.4417092941,2,90.,3,90.

N,1,2.3188375133,2,90.,3,-90.

H,2,0.9662744843,1,115.09828913,3,215.8203581

C, 3, 1.2245435354, 1, 116.46145005, 2, 361.26004049
 H, 9, 1.1024044682, 3, 119.66332571, 1, 181.54688342
 H, 9, 1.1008847713, 3, 120.09542621, 10, 179.97113302
 C, 4, 1.4692383779, 1, 117.96167271, 3, 3.12756334
 C, 4, 1.274123751, 1, 123.86102839, 3, 186.19223285
 H, 13, 1.0942594713, 4, 121.88254721, 12, 0.31745774
 H, 13, 1.0864520257, 4, 119.41284487, 12, 180.50509806
 H, 12, 1.0960307462, 4, 111.82785769, 13, -2.09116397
 H, 12, 1.0928912293, 4, 109.0796288, 13, 119.61981881
 H, 12, 1.093152188, 4, 109.24331875, 13, -124.02075863
 C, 5, 1.4624732934, 1, 115.87826411, 2, 63.30865168
 C, 5, 1.2733715762, 1, 123.16390978, 2, -96.14764789
 H, 20, 1.096665321, 5, 122.90235324, 19, 0.71556026
 H, 20, 1.0898743264, 5, 119.45867798, 19, 180.93558282
 H, 19, 1.0979732972, 5, 112.64801852, 20, -2.75598921
 H, 19, 1.0937505356, 5, 108.46137891, 20, 118.80842699
 H, 19, 1.0949319575, 5, 109.13843137, 20, -124.29095746
 C, 6, 1.4630783952, 1, 115.52811899, 2, 0.47785178
 C, 6, 1.272743414, 1, 126.33297373, 2, 187.51408193
 H, 27, 1.0962857642, 6, 122.96986823, 26, -0.27243325
 H, 27, 1.0895792909, 6, 119.69407245, 26, 179.52900171
 H, 26, 1.0976648507, 6, 112.41864083, 27, 4.39015409
 H, 26, 1.0923841912, 6, 108.97476193, 27, 127.10211137
 H, 26, 1.095586987, 6, 108.80031235, 27, -116.51101369
 C, 7, 1.4622738053, 1, 127.08372369, 2, -180.15300864
 C, 7, 1.2759986135, 1, 114.47439894, 2, 3.15281942
 H, 34, 1.0963888088, 7, 121.85955006, 33, 0.43791297
 H, 34, 1.0899665258, 7, 117.80389912, 33, 180.14619721
 H, 33, 1.0975343602, 7, 112.51329733, 34, -1.44399391
 H, 33, 1.095237847, 7, 109.38244789, 34, 119.62095564
 H, 33, 1.0953421093, 7, 109.45250392, 34, -122.71126756

 HF=-2505.6232141
 RMSD=2.611e-09
 Dipole=-0.3113694, -0.3127024, -1.1933169
 PG=C01 [X(C9H23N4O2Zn1)]

ZnC0St4

1, 1
 Zn
 O, 1, 1.9900539812
 O, 1, 2.2347970369, 2, 90.
 N, 1, 2.143790602, 3, 90., 2, 180.
 N, 1, 2.3704151927, 2, 90., 3, 180.
 O, 1, 2.2517001657, 2, 90., 3, 90.
 N, 1, 2.3327292107, 2, 90., 3, -90.
 C, 2, 1.3001551118, 1, 143.19201849, 3, 162.11730012
 H, 8, 1.1079121627, 2, 113.45597863, 1, 153.70210836
 O, 8, 1.2288024806, 2, 127.12128069, 9, 178.59002058
 C, 3, 1.2240266219, 1, 122.7321684, 2, 349.7625523
 H, 11, 1.1010665991, 3, 119.79552245, 1, 183.47912394
 H, 11, 1.0998138634, 3, 120.73162218, 12, 180.14881842
 C, 4, 1.4687718233, 1, 118.82704478, 3, 30.37822449
 C, 4, 1.2729913578, 1, 122.59083029, 3, 207.44654072
 H, 15, 1.0938161601, 4, 121.97111058, 14, -1.01009888
 H, 15, 1.0868777419, 4, 119.74948496, 14, 178.89572087

H, 14, 1.0957386871, 4, 111.8832565, 15, 0.34585208
H, 14, 1.0927547824, 4, 109.06416327, 15, 122.13557513
H, 14, 1.0943297145, 4, 108.59502615, 15, -120.6759747
C, 5, 1.4662704733, 1, 123.35223933, 2, 74.53630973
C, 5, 1.274509582, 1, 119.15847625, 2, -99.62546017
H, 22, 1.0954148037, 5, 122.45839718, 21, 0.0794399
H, 22, 1.0887047104, 5, 119.96893438, 21, 180.04608476
H, 21, 1.0970195307, 5, 111.7972798, 22, -6.86211989
H, 21, 1.0930621764, 5, 108.0047378, 22, 113.99285702
H, 21, 1.0946163572, 5, 109.316376, 22, -128.01983287
C, 6, 1.2229641198, 1, 124.30345751, 2, 349.23234657
H, 28, 1.101020123, 6, 119.96107241, 1, 179.62638331
H, 28, 1.1001831256, 6, 120.81009768, 29, 180.42238221
C, 7, 1.4674492238, 1, 120.52302577, 2, -209.04717175
C, 7, 1.2762083092, 1, 121.56838792, 2, -20.35756173
H, 32, 1.0962060849, 7, 121.40606762, 31, 0.74792834
H, 32, 1.0891062579, 7, 119.85144773, 31, 179.93034655
H, 31, 1.0970125481, 7, 112.28940998, 32, 5.14470273
H, 31, 1.0950395545, 7, 109.4746132, 32, 126.51209993
H, 31, 1.0946892012, 7, 109.70689371, 32, -115.74858328

HF=-2599.5616647

RMSD=1.131e-09

Dipole=1.2311171, -0.9099567, -1.7548254

PG=C01 [X(C9H20N3O4Zn1)]

ZnC0St5

1, 1

Zn

O, 1, 2.2202446695

O, 1, 2.2652562477, 2, 90.

O, 1, 2.2493718234, 3, 90., 2, 180.

O, 1, 2.2242968981, 2, 90., 3, 180.

O, 1, 1.9063688524, 2, 90., 3, 90.

O, 1, 2.0817535405, 2, 90., 3, -90.

H, 2, 0.9720148954, 1, 123.97643821, 3, 30.70208825

H, 2, 0.9737362719, 1, 100.3773561, 3, 272.09837541

H, 3, 0.97164996, 1, 111.16296615, 2, 119.06258038

H, 3, 0.9727663905, 1, 126.03498844, 2, -109.7637634

C, 4, 1.2244553127, 1, 120.15335199, 3, 93.20263009

H, 12, 1.1005320597, 4, 120.12141936, 1, -0.56768575

H, 12, 1.1012544621, 4, 119.62016625, 13, 180.15036259

C, 5, 1.2258958944, 1, 119.33780051, 2, 280.0637351

H, 15, 1.0999209442, 5, 120.11509397, 1, -1.67343225

H, 15, 1.1008052024, 5, 119.55602214, 16, 180.35285688

H, 6, 0.9671325106, 1, 121.05157668, 2, -61.60025127

C, 7, 1.2251061583, 1, 128.829406, 5, -15.62138707

H, 19, 1.0986901799, 7, 121.45757107, 1, 0.60806461

H, 19, 1.0990190041, 7, 119.46160896, 1, 180.37329962

HF=-2351.6454207

RMSD=1.058e-09

Dipole=0.205237, 0.5484239, -0.1358703

PG=C01 [X(C3H11O6Zn1)]

ZnC0St6

O,1
 Zn
 O,1,2.1322170944
 O,1,2.3935854353,2,90.
 N,1,2.2846787206,3,90.,2,180.
 N,1,2.5251267991,2,90.,3,180.
 O,1,1.9249945492,2,90.,3,90.
 N,1,2.1878996033,2,90.,3,-90.
 C,2,1.2792637312,1,140.01153609,3,158.91753185
 H,8,1.112137311,2,114.20495445,1,158.39893196
 O,8,1.2458663547,2,128.05105561,9,179.42167699
 C,3,1.2197573361,1,109.7318329,2,412.35906254
 H,11,1.1054266465,3,119.97711754,1,186.40362895
 H,11,1.0983803414,3,120.69301685,12,180.99916318
 C,4,1.4596689255,1,112.24918192,3,49.17204886
 C,4,1.2695905271,1,125.28674879,3,209.26906449
 H,15,1.0973495553,4,122.61736972,14,-1.71107483
 H,15,1.0897373857,4,119.48414781,14,177.58305455
 H,14,1.0994425714,4,112.44143128,15,1.10522857
 H,14,1.0951822671,4,108.62343641,15,122.68180522
 H,14,1.0953230741,4,107.20573804,15,-121.07510976
 C,5,1.458181524,1,131.46476303,2,70.32236976
 C,5,1.2729117186,1,109.65490124,2,-100.47203764
 H,22,1.0997151587,5,122.09708986,21,1.02464264
 H,22,1.0908863518,5,118.115603,21,182.6052029
 H,21,1.1010463128,5,112.5568363,22,-7.7293838
 H,21,1.0949178345,5,107.84407541,22,113.2834034
 H,21,1.0968229003,5,109.44245134,22,-129.04585391
 H,6,0.9697871876,1,104.22008938,2,12.89356028
 C,7,1.4637330509,1,119.19940733,2,-222.30562795
 C,7,1.2746509922,1,121.77483158,2,-33.88141964
 H,30,1.0976786498,7,120.73722199,29,2.15485323
 H,30,1.0927822268,7,119.8513587,29,184.02227532
 H,29,1.098450587,7,111.9766943,30,-0.75701878
 H,29,1.0948025663,7,108.62978978,30,120.27757257
 H,29,1.0933837556,7,109.77338818,30,-122.41555046

HF=-2561.0573306

RMSD=2.703e-09

Dipole=0.6490717,0.8354509,-2.4919082

PG=C01 [X(C8H19N3O4Zn1)]

ZnC0St7

O,1
 Zn
 O,1,2.1214747851
 O,1,2.3658838132,2,90.
 N,1,2.212833203,3,90.,2,180.
 N,1,2.3890547164,2,90.,3,180.
 O,1,2.2096194417,2,90.,3,90.
 O,1,1.9557904469,2,90.,3,-90.

C, 2, 1.2851211265, 1, 132.4833235, 3, 113.15801594
 H, 8, 1.1126767535, 2, 113.71051297, 1, 183.98285741
 O, 8, 1.2393127624, 2, 128.04409112, 9, 179.90487409
 C, 3, 1.2237417677, 1, 109.60458532, 2, 281.53153682
 H, 11, 1.106391358, 3, 119.25177869, 1, 176.8030791
 H, 11, 1.1052615191, 3, 119.17725213, 12, 179.14009744
 C, 4, 1.4585546961, 1, 126.34067226, 3, 81.98896457
 C, 4, 1.2747558373, 1, 113.81398476, 3, 263.68927834
 H, 15, 1.0981928746, 4, 121.24591122, 14, 0.52012724
 H, 15, 1.0925556543, 4, 117.30070407, 14, 181.07893926
 H, 14, 1.0993723388, 4, 112.41865489, 15, -0.15888386
 H, 14, 1.095330747, 4, 108.94725468, 15, 121.27846475
 H, 14, 1.095069933, 4, 109.22201792, 15, -121.77956847
 C, 5, 1.4582432328, 1, 114.61249078, 2, 76.96852908
 C, 5, 1.2705806944, 1, 126.53746045, 2, -102.17068816
 H, 22, 1.0983785973, 5, 122.81105298, 21, 0.24317589
 H, 22, 1.0906229483, 5, 119.68247559, 21, 180.36622633
 H, 21, 1.1002365139, 5, 111.92600434, 22, -2.05585188
 H, 21, 1.0945334215, 5, 108.43630078, 22, 120.46801482
 H, 21, 1.0930612131, 5, 108.39554244, 22, -124.63010712
 C, 6, 1.2246795808, 1, 116.27830033, 2, 344.85453428
 H, 28, 1.1034460195, 6, 119.41487377, 1, 181.36113942
 H, 28, 1.1002136891, 6, 120.54746606, 29, 180.9089484
 H, 7, 0.9735122093, 1, 106.16199891, 2, -20.16209972

HF=-2541.6043587

RMSD=2.301e-09

Dipole=0.2019253, -2.5794463, -1.9262507

PG=C01 [X(C7H16N2O5Zn1)]

ZnCOSt8

O, 1

Zn

O, 1, 1.9414969746

O, 1, 2.2397507779, 2, 90.

O, 1, 2.1685222646, 3, 90., 2, 180.

N, 1, 2.3650825337, 2, 90., 3, 180.

O, 1, 2.1809070098, 2, 90., 3, 90.

N, 1, 2.2373964697, 2, 90., 3, -90.

H, 2, 0.9686502252, 1, 108.08842339, 3, -100.29361099

H, 3, 0.9786615901, 1, 101.65493542, 2, 121.00783634

H, 3, 0.9777590376, 1, 88.18104588, 2, 13.52134073

H, 4, 1.0050941743, 1, 94.31150347, 3, 54.43527047

H, 4, 0.9699215461, 1, 110.30996541, 3, -196.44300049

C, 5, 1.4570479127, 1, 116.65955457, 2, 53.67455915

C, 5, 1.2716714907, 1, 120.49985338, 2, -103.14971942

H, 14, 1.0980174421, 5, 122.60800744, 13, 1.81880405

H, 14, 1.0891377631, 5, 119.37397259, 13, 183.84860425

H, 13, 1.0997455127, 5, 112.52766715, 14, -3.59844165

H, 13, 1.0945050043, 5, 107.37448232, 14, 117.60643689

H, 13, 1.0950049546, 5, 109.28713862, 14, -125.33350659

C, 6, 1.2677760267, 1, 117.58161599, 2, -135.87622175

H, 20, 1.1070177747, 6, 116.42743509, 1, 169.82760765

O, 20, 1.2647432408, 6, 126.1975142, 21, 180.73463792

C, 7, 1.4573513384, 1, 123.98823491, 2, -181.58160825

C, 7, 1.2735247747, 1, 115.64192328, 2, 7.35602023

H, 24, 1.0981216643, 7, 121.67267369, 23, 1.1914942
H, 24, 1.0903674434, 7, 117.9562185, 23, 181.53167357
H, 23, 1.09946743, 7, 112.44619419, 24, -1.84934157
H, 23, 1.0941997758, 7, 108.69976593, 24, 119.99245608
H, 23, 1.0956194766, 7, 109.17741582, 24, -123.51701581

HF=-2465.4628103

RMSD=4.499e-09

Dipole=-1.6867614, 1.2063948, -0.4469437

PG=C01 [X(C5H16N2O5Zn1)]

ZnC0St9

-1, 1

Zn

O, 1, 2.0778314807

O, 1, 2.0796936597, 2, 90.

N, 1, 2.3197415407, 3, 90., 2, 180.

N, 1, 2.3518520862, 2, 90., 3, 180.

O, 1, 2.0821044015, 2, 90., 3, 90.

N, 1, 2.3553351481, 2, 90., 3, -90.

C, 2, 1.2669834768, 1, 151.74721092, 3, 152.91832679

H, 8, 1.1149143112, 2, 114.27702106, 1, 156.87029317

O, 8, 1.2537458166, 2, 128.51197908, 9, 178.89523078

C, 3, 1.2696247598, 1, 144.36454032, 2, 235.17735019

H, 11, 1.1160164641, 3, 113.78267072, 1, 163.93956421

O, 11, 1.2516140631, 3, 129.08020178, 12, 178.87001174

C, 4, 1.4559677228, 1, 116.03396096, 3, 26.75593066

C, 4, 1.2677348885, 1, 124.53550702, 3, 198.11378645

H, 15, 1.0984642981, 4, 122.51258335, 14, 0.37503423

H, 15, 1.0891641113, 4, 119.55957835, 14, 179.41493309

H, 14, 1.1008665105, 4, 111.79744517, 15, -2.59706684

H, 14, 1.0944130627, 4, 108.0642583, 15, 119.55830925

H, 14, 1.092738467, 4, 108.15610291, 15, -123.44427438

C, 5, 1.4581812806, 1, 120.68752974, 2, 56.02377856

C, 5, 1.2728031959, 1, 119.56629975, 2, -113.0492404

H, 22, 1.1013631058, 5, 120.9977843, 21, 0.04957576

H, 22, 1.0921542433, 5, 119.89489707, 21, 179.95110997

H, 21, 1.1021359983, 5, 111.93509753, 22, -0.89946811

H, 21, 1.0967131688, 5, 108.93988567, 22, 121.23771347

H, 21, 1.0965463226, 5, 108.861694, 22, -121.7126668

C, 6, 1.2710611722, 1, 141.64447214, 2, -200.85075891

H, 28, 1.1160048003, 6, 113.76601057, 1, 161.01916041

O, 28, 1.2508127094, 6, 128.85576052, 29, 179.13499975

C, 7, 1.4590206982, 1, 119.95315544, 2, -201.87526524

C, 7, 1.272477307, 1, 120.13848855, 2, -8.12719526

H, 32, 1.1008849135, 7, 121.0380667, 31, 0.79142917

H, 32, 1.0901327091, 7, 120.15158129, 31, 180.31446035

H, 31, 1.1020218772, 7, 111.89833208, 32, -1.69652346

H, 31, 1.0970444317, 7, 108.2765996, 32, 119.64524295

H, 31, 1.0962268691, 7, 109.14650328, 32, -122.54610875

HF=-2749.2259851

RMSD=1.620e-09

Dipole=-1.9188596, 1.6466577, -1.76584

PG=C01 [X(C9H18N3O6Zn1)]

ZnC0St10

-1,1
Zn
S,1,3.1748589582
N,1,2.205374015,2,90.
O,1,1.9848737912,3,90.,2,180.
O,1,2.1491404684,2,90.,3,180.
N,1,2.1709906538,2,90.,3,90.
O,1,2.1252327102,2,90.,3,-90.
H,2,1.3713708366,1,68.98737662,3,60.13152301
H,2,1.3499595351,1,68.87600307,3,163.38684742
H,3,1.0164938269,1,125.54886593,2,73.55205756
H,3,1.0226217719,1,91.87096883,2,190.06213232
H,3,1.0221441382,1,107.23171868,2,-58.23756144
H,4,0.9678967352,1,105.45799613,3,-135.33034611
C,5,1.2699185166,1,131.60725745,2,-80.06634025
H,14,1.1160536964,5,114.15912931,1,192.02989006
O,14,1.2545011961,5,129.03165872,15,179.64749292
H,6,1.0334213139,1,103.76270075,2,73.09849173
H,6,1.021730479,1,95.44332656,2,183.37055709
H,6,1.0171525222,1,126.67645371,2,-56.00776351
C,7,1.2658924071,1,125.4355857,2,46.92957952
H,20,1.1138172356,7,114.91970239,1,-188.27084693
O,20,1.2603282004,7,128.02959413,21,180.64311568

HF=-2746.4578078
RMSD=6.969e-09
Dipole=1.7135546,-0.6576052,0.6232451
PG=C01 [X(C2H11N205S1Zn1)]

CdC0St1

2,1
Cd
O,1,2.4242505982
O,1,2.422251454,2,90.
N,1,2.4114246964,3,90.,2,180.
N,1,2.4107000134,2,90.,3,180.
O,1,2.4202869799,2,90.,3,90.
N,1,2.4096429953,2,90.,3,-90.
C,2,1.22563,1,136.949,3,249.382
H,8,1.09962,2,120.13,1,182.469
H,8,1.10082,2,121.623,9,179.847
C,3,1.2249,1,137.193,2,315.826
H,11,1.09973,3,120.118,1,180.217
H,11,1.10088,3,121.647,12,179.844
C,4,1.47396,1,118.382,3,4.196
C,4,1.27526,1,124.614,3,182.286
H,15,1.09333,4,122.064,14,-0.811
H,15,1.08639,4,120.211,14,179.198
H,14,1.09473,4,112.002,15,0.745
H,14,1.09316,4,109.525,15,122.047

H, 14, 1.09359, 4, 109.341, 15, -120.475
 C, 5, 1.47204, 1, 121.374, 2, 81.903
 C, 5, 1.27902, 1, 121.311, 2, -93.574
 H, 22, 1.09378, 5, 122.113, 21, 1.449
 H, 22, 1.08739, 5, 119.831, 21, 181.145
 H, 21, 1.09488, 5, 111.675, 22, -4.615
 H, 21, 1.09345, 5, 109.266, 22, 116.088
 H, 21, 1.09293, 5, 109.759, 22, -125.747
 C, 6, 1.22596, 1, 136.985, 2, -108.33
 H, 28, 1.09968, 6, 120.083, 1, 185.133
 H, 28, 1.1006, 6, 121.526, 29, 180.
 C, 7, 1.47174, 1, 121.445, 2, -181.642
 C, 7, 1.27841, 1, 121.56, 2, 0.242
 H, 32, 1.0937, 7, 122.161, 31, 0.718
 H, 32, 1.08777, 7, 119.842, 31, 180.336
 H, 31, 1.09474, 7, 111.708, 32, 0.98
 H, 31, 1.09301, 7, 109.479, 32, 121.848
 H, 31, 1.09296, 7, 109.639, 32, -120.033

 HF=-912.1097553
 RMSD=3.808e-09
 Dipole=0.5650198, -0.7654328, 0.8447301
 PG=C01 [X(C9H21Cd1N3O3)]

CdC0St2

2, 1
 Cd
 S, 1, 2.9032821844
 O, 1, 2.4489367637, 2, 90.
 S, 1, 2.7957089447, 3, 90., 2, 180.
 N, 1, 2.384539927, 2, 90., 3, 180.
 O, 1, 2.3845555896, 2, 90., 3, 90.
 N, 1, 2.4365728158, 2, 90., 3, -90.
 H, 2, 1.34881534, 1, 111.20788624, 3, 61.2915949
 H, 2, 1.34861006, 1, 107.49069874, 3, 163.5405823
 C, 3, 1.22560306, 1, 142.43197169, 2, 302.68298071
 H, 10, 1.09955355, 3, 120.17127698, 1, 181.69337721
 H, 10, 1.10159815, 3, 121.60901186, 11, 179.75946607
 H, 4, 1.35045104, 1, 105.14887431, 3, 10.37095801
 H, 4, 1.35026859, 1, 102.01129132, 3, 108.20415772
 C, 5, 1.47541626, 1, 121.40210603, 2, 120.2007734
 C, 5, 1.27926166, 1, 120.96882623, 2, -66.38785063
 H, 16, 1.09316049, 5, 122.12210288, 15, -0.71313089
 H, 16, 1.08766881, 5, 120.14378718, 15, 179.01279474
 H, 15, 1.09415924, 5, 111.36363942, 16, -9.85551017
 H, 15, 1.09263789, 5, 109.63251317, 16, 110.65043795
 H, 15, 1.0930845, 5, 109.65595131, 16, -130.78642095
 C, 6, 1.22824825, 1, 137.52229166, 2, -75.85500261
 H, 22, 1.09883147, 6, 119.6745348, 1, 182.88353651
 H, 22, 1.09960211, 6, 121.71729987, 23, 179.82994699
 C, 7, 1.47525075, 1, 119.10749415, 2, -209.0210721
 C, 7, 1.27562776, 1, 123.90650675, 2, -30.12547504
 H, 26, 1.09339102, 7, 122.36429896, 25, -0.43198012
 H, 26, 1.08710168, 7, 119.97505591, 25, 178.79557796
 H, 25, 1.09466079, 7, 111.9860476, 26, 9.35085384
 H, 25, 1.09364797, 7, 109.65836177, 26, 130.50197671

H, 25, 1.09418879, 7, 109.37387053, 26, -111.12204448

HF=-1462.3913341

RMSD=2.932e-09

Dipole=0.8671894, -0.1781334, 0.533777

PG=C01 [X(C6H18Cd1N202S2)]

CdC0St3

1, 1

Cd

O, 1, 2.1158298952

O, 1, 2.4895359968, 2, 90.

N, 1, 2.381806193, 3, 90., 2, 180.

N, 1, 2.6274189417, 2, 90., 3, 180.

N, 1, 2.587091594, 2, 90., 3, 90.

N, 1, 2.4700793435, 2, 90., 3, -90.

H, 2, 0.96627448, 1, 115.09828913, 3, 215.8203581

C, 3, 1.22454354, 1, 116.46145005, 2, 361.26004049

H, 9, 1.10240447, 3, 119.66332571, 1, 181.54688342

H, 9, 1.10088477, 3, 120.09542621, 10, 179.97113302

C, 4, 1.46923838, 1, 117.96167271, 3, 3.12756334

C, 4, 1.27412375, 1, 123.86102839, 3, 186.19223285

H, 13, 1.09425947, 4, 121.88254721, 12, 0.31745774

H, 13, 1.08645203, 4, 119.41284487, 12, 180.50509806

H, 12, 1.09603075, 4, 111.82785769, 13, -2.09116397

H, 12, 1.09289123, 4, 109.0796288, 13, 119.61981881

H, 12, 1.09315219, 4, 109.24331875, 13, -124.02075863

C, 5, 1.46247329, 1, 115.87826411, 2, 63.30865168

C, 5, 1.27337158, 1, 123.16390978, 2, -96.14764789

H, 20, 1.09666532, 5, 122.90235324, 19, 0.71556026

H, 20, 1.08987433, 5, 119.45867798, 19, 180.93558282

H, 19, 1.0979733, 5, 112.64801852, 20, -2.75598921

H, 19, 1.09375054, 5, 108.46137891, 20, 118.80842699

H, 19, 1.09493196, 5, 109.13843137, 20, -124.29095746

C, 6, 1.4630784, 1, 115.52811899, 2, 0.47785178

C, 6, 1.27274341, 1, 126.33297373, 2, 187.51408193

H, 27, 1.09628576, 6, 122.96986823, 26, -0.27243325

H, 27, 1.08957929, 6, 119.69407245, 26, 179.52900171

H, 26, 1.09766485, 6, 112.41864083, 27, 4.39015409

H, 26, 1.09238419, 6, 108.97476193, 27, 127.10211137

H, 26, 1.09558699, 6, 108.80031235, 27, -116.51101369

C, 7, 1.46227381, 1, 127.08372369, 2, -180.15300864

C, 7, 1.27599861, 1, 114.47439894, 2, 3.15281942

H, 34, 1.09638881, 7, 121.85955006, 33, 0.43791297

H, 34, 1.08996653, 7, 117.80389912, 33, 180.14619721

H, 33, 1.09753436, 7, 112.51329733, 34, -1.44399391

H, 33, 1.09523785, 7, 109.38244789, 34, 119.62095564

H, 33, 1.09534211, 7, 109.45250392, 34, -122.71126756

HF=-893.1747349

RMSD=6.156e-09

Dipole=-0.3623814, -0.2857929, -1.4909961

PG=C01 [X(C9H23Cd1N402)]

CdC0St4

1,1
Cd
O,1,2.1636535339
O,1,2.4538471172,2,90.
N,1,2.3614945687,3,90.,2,180.
N,1,2.5031962256,2,90.,3,180.
O,1,2.4686817907,2,90.,3,90.
N,1,2.4729754785,2,90.,3,-90.
C,2,1.30015511,1,143.19201849,3,162.11730012
H,8,1.10791216,2,113.45597863,1,153.70210836
O,8,1.22880248,2,127.12128069,9,178.59002058
C,3,1.22402662,1,122.7321684,2,349.7625523
H,11,1.1010666,3,119.79552245,1,183.47912394
H,11,1.09981386,3,120.73162218,12,180.14881842
C,4,1.46877182,1,118.82704478,3,30.37822449
C,4,1.27299136,1,122.59083029,3,207.44654072
H,15,1.09381616,4,121.97111058,14,-1.01009888
H,15,1.08687774,4,119.74948496,14,178.89572087
H,14,1.09573869,4,111.8832565,15,0.34585208
H,14,1.09275478,4,109.06416327,15,122.13557513
H,14,1.09432971,4,108.59502615,15,-120.6759747
C,5,1.46627047,1,123.35223933,2,74.53630973
C,5,1.27450958,1,119.15847625,2,-99.62546017
H,22,1.0954148,5,122.45839718,21,0.0794399
H,22,1.08870471,5,119.96893438,21,180.04608476
H,21,1.09701953,5,111.7972798,22,-6.86211989
H,21,1.09306218,5,108.0047378,22,113.99285702
H,21,1.09461636,5,109.316376,22,-128.01983287
C,6,1.22296412,1,124.30345751,2,349.23234657
H,28,1.10102012,6,119.96107241,1,179.62638331
H,28,1.10018313,6,120.81009768,29,180.42238221
C,7,1.46744922,1,120.52302577,2,-209.04717175
C,7,1.27620831,1,121.56838792,2,-20.35756173
H,32,1.09620608,7,121.40606762,31,0.74792834
H,32,1.08910626,7,119.85144773,31,179.93034655
H,31,1.09701255,7,112.28940998,32,5.14470273
H,31,1.09503955,7,109.4746132,32,126.51209993
H,31,1.0946892,7,109.70689371,32,-115.74858328

HF=-987.1156546

RMSD=3.883e-09

Dipole=1.1452797,-0.8014489,-2.0953187

PG=C01 [X(C9H20Cd1N3O4)]

CdC0St5

1,1
Cd
O,1,2.427098984
O,1,2.457882719,2,90.
O,1,2.4396273111,3,90.,2,180.
O,1,2.4175260659,2,90.,3,180.
O,1,2.0971577914,2,90.,3,90.

O,1,2.3193167217,2,90.,3,-90.
H,2,0.9720149,1,123.97643821,3,30.70208825
H,2,0.97373627,1,100.3773561,3,272.09837541
H,3,0.97164996,1,111.16296615,2,119.06258038
H,3,0.97276639,1,126.03498844,2,-109.7637634
C,4,1.22445531,1,120.15335199,3,93.20263009
H,12,1.10053206,4,120.12141936,1,-0.56768575
H,12,1.10125446,4,119.62016625,13,180.15036259
C,5,1.22589589,1,119.33780051,2,280.0637351
H,15,1.09992094,5,120.11509397,1,-1.67343225
H,15,1.1008052,5,119.55602214,16,180.35285688
H,6,0.96713251,1,121.05157668,2,-61.60025127
C,7,1.22510616,1,128.829406,5,-15.62138707
H,19,1.09869018,7,121.45757107,1,0.60806461
H,19,1.099019,7,119.46160896,1,180.37329962

HF=-739.1919343

RMSD=5.643e-09

Dipole=0.1544446,0.7269294,-0.1826098

PG=C01 [X(C3H11Cd106)]

CdC0St6

O,1

Cd

O,1,2.2785303621

O,1,2.5832870711,2,90.

N,1,2.4954170414,3,90.,2,180.

N,1,2.5941100121,2,90.,3,180.

O,1,2.1395835293,2,90.,3,90.

N,1,2.3860973673,2,90.,3,-90.

C,2,1.27926373,1,140.01153609,3,158.91753185

H,8,1.11213731,2,114.20495445,1,158.39893196

O,8,1.24586635,2,128.05105561,9,179.42167699

C,3,1.21975734,1,109.7318329,2,412.35906254

H,11,1.10542665,3,119.97711754,1,186.40362895

H,11,1.09838034,3,120.69301685,12,180.99916318

C,4,1.45966893,1,112.24918192,3,49.17204886

C,4,1.26959053,1,125.28674879,3,209.26906449

H,15,1.09734956,4,122.61736972,14,-1.71107483

H,15,1.08973739,4,119.48414781,14,177.58305455

H,14,1.09944257,4,112.44143128,15,1.10522857

H,14,1.09518227,4,108.62343641,15,122.68180522

H,14,1.09532307,4,107.20573804,15,-121.07510976

C,5,1.45818152,1,131.46476303,2,70.32236976

C,5,1.27291172,1,109.65490124,2,-100.47203764

H,22,1.09971516,5,122.09708986,21,1.02464264

H,22,1.09088635,5,118.115603,21,182.6052029

H,21,1.10104631,5,112.5568363,22,-7.7293838

H,21,1.09491783,5,107.84407541,22,113.2834034

H,21,1.0968229,5,109.44245134,22,-129.04585391

H,6,0.96978719,1,104.22008938,2,12.89356028

C,7,1.46373305,1,119.19940733,2,-222.30562795

C,7,1.27465099,1,121.77483158,2,-33.88141964

H,30,1.09767865,7,120.73722199,29,2.15485323

H,30,1.09278223,7,119.8513587,29,184.02227532

H,29,1.09845059,7,111.9766943,30,-0.75701878

H, 29, 1.09480257, 7, 108.62978978, 30, 120.27757257
H, 29, 1.09338376, 7, 109.77338818, 30, -122.41555046

HF=-948.6059801
RMSD=5.673e-09
Dipole=0.6132449, 1.1438274, -2.8284288
PG=C01 [X(C8H19Cd1N3O4)]

CdC0St7

0, 1
Cd
O, 1, 2.2746800866
O, 1, 2.5178541169, 2, 90.
N, 1, 2.3991322465, 3, 90., 2, 180.
N, 1, 2.5411756381, 2, 90., 3, 180.
O, 1, 2.4493220048, 2, 90., 3, 90.
O, 1, 2.1562339841, 2, 90., 3, -90.
C, 2, 1.28512113, 1, 132.4833235, 3, 113.15801594
H, 8, 1.11267675, 2, 113.71051297, 1, 183.98285741
O, 8, 1.23931276, 2, 128.04409112, 9, 179.90487409
C, 3, 1.22374177, 1, 109.60458532, 2, 281.53153682
H, 11, 1.10639136, 3, 119.25177869, 1, 176.8030791
H, 11, 1.10526152, 3, 119.17725213, 12, 179.14009744
C, 4, 1.4585547, 1, 126.34067226, 3, 81.98896457
C, 4, 1.27475584, 1, 113.81398476, 3, 263.68927834
H, 15, 1.09819287, 4, 121.24591122, 14, 0.52012724
H, 15, 1.09255565, 4, 117.30070407, 14, 181.07893926
H, 14, 1.09937234, 4, 112.41865489, 15, -0.15888386
H, 14, 1.09533075, 4, 108.94725468, 15, 121.27846475
H, 14, 1.09506993, 4, 109.22201792, 15, -121.77956847
C, 5, 1.45824323, 1, 114.61249078, 2, 76.96852908
C, 5, 1.27058069, 1, 126.53746045, 2, -102.17068816
H, 22, 1.0983786, 5, 122.81105298, 21, 0.24317589
H, 22, 1.09062295, 5, 119.68247559, 21, 180.36622633
H, 21, 1.10023651, 5, 111.92600434, 22, -2.05585188
H, 21, 1.09453342, 5, 108.43630078, 22, 120.46801482
H, 21, 1.09306121, 5, 108.39554244, 22, -124.63010712
C, 6, 1.22467958, 1, 116.27830033, 2, 344.85453428
H, 28, 1.10344602, 6, 119.41487377, 1, 181.36113942
H, 28, 1.10021369, 6, 120.54746606, 29, 180.9089484
H, 7, 0.97351221, 1, 106.16199891, 2, -20.16209972

HF=-929.1516124
RMSD=6.268e-09
Dipole=0.1890814, -2.8503405, -2.3100202
PG=C01 [X(C7H16Cd1N2O5)]

CdC0St8

0, 1
Cd
O, 1, 2.145545235

O,1,2.4617448049,2,90.
O,1,2.3874959241,3,90.,2,180.
N,1,2.5432661624,2,90.,3,180.
O,1,2.3037308367,2,90.,3,90.
N,1,2.4155165023,2,90.,3,-90.
H,2,0.96865023,1,108.08842339,3,-100.29361099
H,3,0.97866159,1,101.65493542,2,121.00783634
H,3,0.97775904,1,88.18104588,2,13.52134073
H,4,1.00509417,1,94.31150347,3,54.43527047
H,4,0.96992155,1,110.30996541,3,-196.44300049
C,5,1.45704791,1,116.65955457,2,53.67455915
C,5,1.27167149,1,120.49985338,2,-103.14971942
H,14,1.09801744,5,122.60800744,13,1.81880405
H,14,1.08913776,5,119.37397259,13,183.84860425
H,13,1.09974551,5,112.52766715,14,-3.59844165
H,13,1.094505,5,107.37448232,14,117.60643689
H,13,1.09500495,5,109.28713862,14,-125.33350659
C,6,1.26777603,1,117.58161599,2,-135.87622175
H,20,1.10701777,6,116.42743509,1,169.82760765
O,20,1.26474324,6,126.1975142,21,180.73463792
C,7,1.45735134,1,123.98823491,2,-181.58160825
C,7,1.27352477,1,115.64192328,2,7.35602023
H,24,1.09812166,7,121.67267369,23,1.1914942
H,24,1.09036744,7,117.9562185,23,181.53167357
H,23,1.09946743,7,112.44619419,24,-1.84934157
H,23,1.09419978,7,108.69976593,24,119.99245608
H,23,1.09561948,7,109.17741582,24,-123.51701581

HF=-853.005734

RMSD=5.028e-09

Dipole=-1.7522597,1.5238665,-0.7012097

PG=C01 [X(C5H16Cd1N2O5)]

CdC0St9

-1,1

Cd

O,1,2.2614439288

O,1,2.2593130551,2,90.

N,1,2.5091066792,3,90.,2,180.

N,1,2.4826341741,2,90.,3,180.

O,1,2.2691308266,2,90.,3,90.

N,1,2.4884568193,2,90.,3,-90.

C,2,1.26698348,1,151.74721092,3,152.91832679

H,8,1.11491431,2,114.27702106,1,156.87029317

O,8,1.25374582,2,128.51197908,9,178.89523078

C,3,1.26962476,1,144.36454032,2,235.17735019

H,11,1.11601646,3,113.78267072,1,163.93956421

O,11,1.25161406,3,129.08020178,12,178.87001174

C,4,1.45596772,1,116.03396096,3,26.75593066

C,4,1.26773489,1,124.53550702,3,198.11378645

H,15,1.0984643,4,122.51258335,14,0.37503423

H,15,1.08916411,4,119.55957835,14,179.41493309

H,14,1.10086651,4,111.79744517,15,-2.59706684

H,14,1.09441306,4,108.0642583,15,119.55830925

H,14,1.09273847,4,108.15610291,15,-123.44427438

C,5,1.45818128,1,120.68752974,2,56.02377856

C, 5, 1.2728032, 1, 119.56629975, 2, -113.0492404
H, 22, 1.10136311, 5, 120.9977843, 21, 0.04957576
H, 22, 1.09215424, 5, 119.89489707, 21, 179.95110997
H, 21, 1.102136, 5, 111.93509753, 22, -0.89946811
H, 21, 1.09671317, 5, 108.93988567, 22, 121.23771347
H, 21, 1.09654632, 5, 108.861694, 22, -121.7126668
C, 6, 1.27106117, 1, 141.64447214, 2, -200.85075891
H, 28, 1.1160048, 6, 113.76601057, 1, 161.01916041
O, 28, 1.25081271, 6, 128.85576052, 29, 179.13499975
C, 7, 1.4590207, 1, 119.95315544, 2, -201.87526524
C, 7, 1.27247731, 1, 120.13848855, 2, -8.12719526
H, 32, 1.10088491, 7, 121.0380667, 31, 0.79142917
H, 32, 1.09013271, 7, 120.15158129, 31, 180.31446035
H, 31, 1.10202188, 7, 111.89833208, 32, -1.69652346
H, 31, 1.09704443, 7, 108.2765996, 32, 119.64524295
H, 31, 1.09622687, 7, 109.14650328, 32, -122.54610875

HF=-1136.7817256

RMSD=7.796e-09

Dipole=-2.274377, 1.9946688, -2.0882565

PG=C01 [X(C9H18Cd1N3O6)]

CdC0St10

-1, 1

Cd

S, 1, 3.1841635439

N, 1, 2.431745547, 2, 90.

O, 1, 2.1847867053, 3, 90., 2, 180.

O, 1, 2.3095119282, 2, 90., 3, 180.

N, 1, 2.3918279318, 2, 90., 3, 90.

O, 1, 2.3034110813, 2, 90., 3, -90.

H, 2, 1.37137084, 1, 68.98737662, 3, 60.13152301

H, 2, 1.34995954, 1, 68.87600307, 3, 163.38684742

H, 3, 1.01649383, 1, 125.54886593, 2, 73.55205756

H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232

H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144

H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611

C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025

H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006

O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292

H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173

H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709

H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351

C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952

H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693

O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-1134.0048892

RMSD=5.884e-09

Dipole=2.0280847, -1.003025, 0.8479618

PG=C01 [X(C2H11Cd1N2O5S1)]

HgC0St1

2,1

Hg

O,1,2.5339492657
 O,1,2.5313838865,2,90.
 N,1,2.4534402821,3,90.,2,180.
 N,1,2.4531471336,2,90.,3,180.
 O,1,2.5295537444,2,90.,3,90.
 N,1,2.4568649573,2,90.,3,-90.
 C,2,1.22563,1,136.949,3,249.382
 H,8,1.09962,2,120.13,1,182.469
 H,8,1.10082,2,121.623,9,179.847
 C,3,1.2249,1,137.193,2,315.826
 H,11,1.09973,3,120.118,1,180.217
 H,11,1.10088,3,121.647,12,179.844
 C,4,1.47396,1,118.382,3,4.196
 C,4,1.27526,1,124.614,3,182.286
 H,15,1.09333,4,122.064,14,-0.811
 H,15,1.08639,4,120.211,14,179.198
 H,14,1.09473,4,112.002,15,0.745
 H,14,1.09316,4,109.525,15,122.047
 H,14,1.09359,4,109.341,15,-120.475
 C,5,1.47204,1,121.374,2,81.903
 C,5,1.27902,1,121.311,2,-93.574
 H,22,1.09378,5,122.113,21,1.449
 H,22,1.08739,5,119.831,21,181.145
 H,21,1.09488,5,111.675,22,-4.615
 H,21,1.09345,5,109.266,22,116.088
 H,21,1.09293,5,109.759,22,-125.747
 C,6,1.22596,1,136.985,2,-108.33
 H,28,1.09968,6,120.083,1,185.133
 H,28,1.1006,6,121.526,29,180.
 C,7,1.47174,1,121.445,2,-181.642
 C,7,1.27841,1,121.56,2,0.242
 H,32,1.0937,7,122.161,31,0.718
 H,32,1.08777,7,119.842,31,180.336
 H,31,1.09474,7,111.708,32,0.98
 H,31,1.09301,7,109.479,32,121.848
 H,31,1.09296,7,109.639,32,-120.033

HF=-898.9096758

RMSD=5.387e-10

Dipole=0.3821131,-0.5975467,0.6697563

PG=C01 [X(C9H21Hg1N3O3)]

HgC0St2

2,1

Hg

S,1,2.9245366538
 O,1,2.5864196538,2,90.
 S,1,2.8069119813,3,90.,2,180.
 N,1,2.4446841418,2,90.,3,180.
 O,1,2.4942356034,2,90.,3,90.
 N,1,2.4910403025,2,90.,3,-90.
 H,2,1.34881534,1,111.20788624,3,61.2915949

H, 2, 1.34861006, 1, 107.49069874, 3, 163.5405823
C, 3, 1.22560306, 1, 142.43197169, 2, 302.68298071
H, 10, 1.09955355, 3, 120.17127698, 1, 181.69337721
H, 10, 1.10159815, 3, 121.60901186, 11, 179.75946607
H, 4, 1.35045104, 1, 105.14887431, 3, 10.37095801
H, 4, 1.35026859, 1, 102.01129132, 3, 108.20415772
C, 5, 1.47541626, 1, 121.40210603, 2, 120.2007734
C, 5, 1.27926166, 1, 120.96882623, 2, -66.38785063
H, 16, 1.09316049, 5, 122.12210288, 15, -0.71313089
H, 16, 1.08766881, 5, 120.14378718, 15, 179.01279474
H, 15, 1.09415924, 5, 111.36363942, 16, -9.85551017
H, 15, 1.09263789, 5, 109.63251317, 16, 110.65043795
H, 15, 1.0930845, 5, 109.65595131, 16, -130.78642095
C, 6, 1.22824825, 1, 137.52229166, 2, -75.85500261
H, 22, 1.09883147, 6, 119.6745348, 1, 182.88353651
H, 22, 1.09960211, 6, 121.71729987, 23, 179.82994699
C, 7, 1.47525075, 1, 119.10749415, 2, -209.0210721
C, 7, 1.27562776, 1, 123.90650675, 2, -30.12547504
H, 26, 1.09339102, 7, 122.36429896, 25, -0.43198012
H, 26, 1.08710168, 7, 119.97505591, 25, 178.79557796
H, 25, 1.09466079, 7, 111.9860476, 26, 9.35085384
H, 25, 1.09364797, 7, 109.65836177, 26, 130.50197671
H, 25, 1.09418879, 7, 109.37387053, 26, -111.12204448

HF=-1449.1983655

RMSD=4.162e-09

Dipole=0.6587178, -0.0596966, 0.4706724

PG=C01 [X(C6H18Hg1N2O2S2)]

HgCOSt3

1,1

Hg

O, 1, 2.0661890612

O, 1, 2.7403911078, 2, 90.

N, 1, 2.2279903601, 3, 90., 2, 180.

N, 1, 2.9027317324, 2, 90., 3, 180.

N, 1, 2.8869147037, 2, 90., 3, 90.

N, 1, 2.6897902555, 2, 90., 3, -90.

H, 2, 0.96627448, 1, 115.09828913, 3, 215.8203581

C, 3, 1.22454354, 1, 116.46145005, 2, 361.26004049

H, 9, 1.10240447, 3, 119.66332571, 1, 181.54688342

H, 9, 1.10088477, 3, 120.09542621, 10, 179.97113302

C, 4, 1.46923838, 1, 117.96167271, 3, 3.12756334

C, 4, 1.27412375, 1, 123.86102839, 3, 186.19223285

H, 13, 1.09425947, 4, 121.88254721, 12, 0.31745774

H, 13, 1.08645203, 4, 119.41284487, 12, 180.50509806

H, 12, 1.09603075, 4, 111.82785769, 13, -2.09116397

H, 12, 1.09289123, 4, 109.0796288, 13, 119.61981881

H, 12, 1.09315219, 4, 109.24331875, 13, -124.02075863

C, 5, 1.46247329, 1, 115.87826411, 2, 63.30865168

C, 5, 1.27337158, 1, 123.16390978, 2, -96.14764789

H, 20, 1.09666532, 5, 122.90235324, 19, 0.71556026

H, 20, 1.08987433, 5, 119.45867798, 19, 180.93558282

H, 19, 1.0979733, 5, 112.64801852, 20, -2.75598921

H, 19, 1.09375054, 5, 108.46137891, 20, 118.80842699

H, 19, 1.09493196, 5, 109.13843137, 20, -124.29095746

C, 6, 1.4630784, 1, 115.52811899, 2, 0.47785178
C, 6, 1.27274341, 1, 126.33297373, 2, 187.51408193
H, 27, 1.09628576, 6, 122.96986823, 26, -0.27243325
H, 27, 1.08957929, 6, 119.69407245, 26, 179.52900171
H, 26, 1.09766485, 6, 112.41864083, 27, 4.39015409
H, 26, 1.09238419, 6, 108.97476193, 27, 127.10211137
H, 26, 1.09558699, 6, 108.80031235, 27, -116.51101369
C, 7, 1.46227381, 1, 127.08372369, 2, -180.15300864
C, 7, 1.27599861, 1, 114.47439894, 2, 3.15281942
H, 34, 1.09638881, 7, 121.85955006, 33, 0.43791297
H, 34, 1.08996653, 7, 117.80389912, 33, 180.14619721
H, 33, 1.09753436, 7, 112.51329733, 34, -1.44399391
H, 33, 1.09523785, 7, 109.38244789, 34, 119.62095564
H, 33, 1.09534211, 7, 109.45250392, 34, -122.71126756

HF=-879.9859808

RMSD=2.913e-09

Dipole=-0.2961811, -0.1674615, -1.3895413

PG=C01 [X(C9H23Hg1N4O2)]

HgC0St4

1, 1

Hg

O, 1, 2.1367615363

O, 1, 2.6632845885, 2, 90.

N, 1, 2.2766050064, 3, 90., 2, 180.

N, 1, 2.6557389024, 2, 90., 3, 180.

O, 1, 2.6829366827, 2, 90., 3, 90.

N, 1, 2.6186989708, 2, 90., 3, -90.

C, 2, 1.30015511, 1, 143.19201849, 3, 162.11730012

H, 8, 1.10791216, 2, 113.45597863, 1, 153.70210836

O, 8, 1.22880248, 2, 127.12128069, 9, 178.59002058

C, 3, 1.22402662, 1, 122.7321684, 2, 349.7625523

H, 11, 1.1010666, 3, 119.79552245, 1, 183.47912394

H, 11, 1.09981386, 3, 120.73162218, 12, 180.14881842

C, 4, 1.46877182, 1, 118.82704478, 3, 30.37822449

C, 4, 1.27299136, 1, 122.59083029, 3, 207.44654072

H, 15, 1.09381616, 4, 121.97111058, 14, -1.01009888

H, 15, 1.08687774, 4, 119.74948496, 14, 178.89572087

H, 14, 1.09573869, 4, 111.8832565, 15, 0.34585208

H, 14, 1.09275478, 4, 109.06416327, 15, 122.13557513

H, 14, 1.09432971, 4, 108.59502615, 15, -120.6759747

C, 5, 1.46627047, 1, 123.35223933, 2, 74.53630973

C, 5, 1.27450958, 1, 119.15847625, 2, -99.62546017

H, 22, 1.0954148, 5, 122.45839718, 21, 0.0794399

H, 22, 1.08870471, 5, 119.96893438, 21, 180.04608476

H, 21, 1.09701953, 5, 111.7972798, 22, -6.86211989

H, 21, 1.09306218, 5, 108.0047378, 22, 113.99285702

H, 21, 1.09461636, 5, 109.316376, 22, -128.01983287

C, 6, 1.22296412, 1, 124.30345751, 2, 349.23234657

H, 28, 1.10102012, 6, 119.96107241, 1, 179.62638331

H, 28, 1.10018313, 6, 120.81009768, 29, 180.42238221

C, 7, 1.46744922, 1, 120.52302577, 2, -209.04717175

C, 7, 1.27620831, 1, 121.56838792, 2, -20.35756173

H, 32, 1.09620608, 7, 121.40606762, 31, 0.74792834

H, 32, 1.08910626, 7, 119.85144773, 31, 179.93034655

H, 31, 1.09701255, 7, 112.28940998, 32, 5.14470273
H, 31, 1.09503955, 7, 109.4746132, 32, 126.51209993
H, 31, 1.0946892, 7, 109.70689371, 32, -115.74858328

HF=-973.9172244
RMSD=1.547e-09
Dipole=1.1007706, -0.7602453, -2.1616634
PG=C01 [X(C9H20Hg1N3O4)]

HgC0St5

1, 1
Hg
O, 1, 2.6369079286
O, 1, 2.6756118176, 2, 90.
O, 1, 2.6348844459, 3, 90., 2, 180.
O, 1, 2.6085841509, 2, 90., 3, 180.
O, 1, 2.0707653991, 2, 90., 3, 90.
O, 1, 2.2696467329, 2, 90., 3, -90.
H, 2, 0.9720149, 1, 123.97643821, 3, 30.70208825
H, 2, 0.97373627, 1, 100.3773561, 3, 272.09837541
H, 3, 0.97164996, 1, 111.16296615, 2, 119.06258038
H, 3, 0.97276639, 1, 126.03498844, 2, -109.7637634
C, 4, 1.22445531, 1, 120.15335199, 3, 93.20263009
H, 12, 1.10053206, 4, 120.12141936, 1, -0.56768575
H, 12, 1.10125446, 4, 119.62016625, 13, 180.15036259
C, 5, 1.22589589, 1, 119.33780051, 2, 280.0637351
H, 15, 1.09992094, 5, 120.11509397, 1, -1.67343225
H, 15, 1.1008052, 5, 119.55602214, 16, 180.35285688
H, 6, 0.96713251, 1, 121.05157668, 2, -61.60025127
C, 7, 1.22510616, 1, 128.829406, 5, -15.62138707
H, 19, 1.09869018, 7, 121.45757107, 1, 0.60806461
H, 19, 1.099019, 7, 119.46160896, 1, 180.37329962

HF=-725.9941134
RMSD=3.955e-09
Dipole=0.2186977, 0.5366605, -0.0872426
PG=C01 [X(C3H11Hg1O6)]

HgC0St6

0, 1
Hg
O, 1, 2.4208569601
O, 1, 2.8680226281, 2, 90.
N, 1, 2.8277388799, 3, 90., 2, 180.
N, 1, 2.8045313466, 2, 90., 3, 180.
O, 1, 2.0889424132, 2, 90., 3, 90.
N, 1, 2.2374427074, 2, 90., 3, -90.
C, 2, 1.27926373, 1, 140.01153609, 3, 158.91753185
H, 8, 1.11213731, 2, 114.20495445, 1, 158.39893196
O, 8, 1.24586635, 2, 128.05105561, 9, 179.42167699
C, 3, 1.21975734, 1, 109.7318329, 2, 412.35906254

H, 11, 1.10542665, 3, 119.97711754, 1, 186.40362895
 H, 11, 1.09838034, 3, 120.69301685, 12, 180.99916318
 C, 4, 1.45966893, 1, 112.24918192, 3, 49.17204886
 C, 4, 1.26959053, 1, 125.28674879, 3, 209.26906449
 H, 15, 1.09734956, 4, 122.61736972, 14, -1.71107483
 H, 15, 1.08973739, 4, 119.48414781, 14, 177.58305455
 H, 14, 1.09944257, 4, 112.44143128, 15, 1.10522857
 H, 14, 1.09518227, 4, 108.62343641, 15, 122.68180522
 H, 14, 1.09532307, 4, 107.20573804, 15, -121.07510976
 C, 5, 1.45818152, 1, 131.46476303, 2, 70.32236976
 C, 5, 1.27291172, 1, 109.65490124, 2, -100.47203764
 H, 22, 1.09971516, 5, 122.09708986, 21, 1.02464264
 H, 22, 1.09088635, 5, 118.115603, 21, 182.6052029
 H, 21, 1.10104631, 5, 112.5568363, 22, -7.7293838
 H, 21, 1.09491783, 5, 107.84407541, 22, 113.2834034
 H, 21, 1.0968229, 5, 109.44245134, 22, -129.04585391
 H, 6, 0.96978719, 1, 104.22008938, 2, 12.89356028
 C, 7, 1.46373305, 1, 119.19940733, 2, -222.30562795
 C, 7, 1.27465099, 1, 121.77483158, 2, -33.88141964
 H, 30, 1.09767865, 7, 120.73722199, 29, 2.15485323
 H, 30, 1.09278223, 7, 119.8513587, 29, 184.02227532
 H, 29, 1.09845059, 7, 111.9766943, 30, -0.75701878
 H, 29, 1.09480257, 7, 108.62978978, 30, 120.27757257
 H, 29, 1.09338376, 7, 109.77338818, 30, -122.41555046

HF=-935.413974

RMSD=1.639e-09

Dipole=0.6017895, 1.0767836, -2.927544

PG=C01 [X(C8H19Hg1N3O4)]

HgC0St7

O, 1

Hg

O, 1, 2.3368677669

O, 1, 2.6995121714, 2, 90.

N, 1, 2.4698453402, 3, 90., 2, 180.

N, 1, 2.6721025969, 2, 90., 3, 180.

O, 1, 2.5262442834, 2, 90., 3, 90.

O, 1, 2.180181153, 2, 90., 3, -90.

C, 2, 1.28512113, 1, 132.4833235, 3, 113.15801594

H, 8, 1.11267675, 2, 113.71051297, 1, 183.98285741

O, 8, 1.23931276, 2, 128.04409112, 9, 179.90487409

C, 3, 1.22374177, 1, 109.60458532, 2, 281.53153682

H, 11, 1.10639136, 3, 119.25177869, 1, 176.8030791

H, 11, 1.10526152, 3, 119.17725213, 12, 179.14009744

C, 4, 1.4585547, 1, 126.34067226, 3, 81.98896457

C, 4, 1.27475584, 1, 113.81398476, 3, 263.68927834

H, 15, 1.09819287, 4, 121.24591122, 14, 0.52012724

H, 15, 1.09255565, 4, 117.30070407, 14, 181.07893926

H, 14, 1.09937234, 4, 112.41865489, 15, -0.15888386

H, 14, 1.09533075, 4, 108.94725468, 15, 121.27846475

H, 14, 1.09506993, 4, 109.22201792, 15, -121.77956847

C, 5, 1.45824323, 1, 114.61249078, 2, 76.96852908

C, 5, 1.27058069, 1, 126.53746045, 2, -102.17068816

H, 22, 1.0983786, 5, 122.81105298, 21, 0.24317589

H, 22, 1.09062295, 5, 119.68247559, 21, 180.36622633

H, 21, 1.10023651, 5, 111.92600434, 22, -2.05585188
H, 21, 1.09453342, 5, 108.43630078, 22, 120.46801482
H, 21, 1.09306121, 5, 108.39554244, 22, -124.63010712
C, 6, 1.22467958, 1, 116.27830033, 2, 344.85453428
H, 28, 1.10344602, 6, 119.41487377, 1, 181.36113942
H, 28, 1.10021369, 6, 120.54746606, 29, 180.9089484
H, 7, 0.97351221, 1, 106.16199891, 2, -20.16209972

HF=-915.9520187

RMSD=3.278e-09

Dipole=0.1589366, -2.6432589, -2.3868455

PG=C01 [X(C7H16Hg1N2O5)]

HgC0St8

O, 1

Hg

O, 1, 2.1658267756

O, 1, 2.6292277613, 2, 90.

O, 1, 2.4220326819, 3, 90., 2, 180.

N, 1, 2.6999333727, 2, 90., 3, 180.

O, 1, 2.370273907, 2, 90., 3, 90.

N, 1, 2.4983967102, 2, 90., 3, -90.

H, 2, 0.96865023, 1, 108.08842339, 3, -100.29361099

H, 3, 0.97866159, 1, 101.65493542, 2, 121.00783634

H, 3, 0.97775904, 1, 88.18104588, 2, 13.52134073

H, 4, 1.00509417, 1, 94.31150347, 3, 54.43527047

H, 4, 0.96992155, 1, 110.30996541, 3, -196.44300049

C, 5, 1.45704791, 1, 116.65955457, 2, 53.67455915

C, 5, 1.27167149, 1, 120.49985338, 2, -103.14971942

H, 14, 1.09801744, 5, 122.60800744, 13, 1.81880405

H, 14, 1.08913776, 5, 119.37397259, 13, 183.84860425

H, 13, 1.09974551, 5, 112.52766715, 14, -3.59844165

H, 13, 1.094505, 5, 107.37448232, 14, 117.60643689

H, 13, 1.09500495, 5, 109.28713862, 14, -125.33350659

C, 6, 1.26777603, 1, 117.58161599, 2, -135.87622175

H, 20, 1.10701777, 6, 116.42743509, 1, 169.82760765

O, 20, 1.26474324, 6, 126.1975142, 21, 180.73463792

C, 7, 1.45735134, 1, 123.98823491, 2, -181.58160825

C, 7, 1.27352477, 1, 115.64192328, 2, 7.35602023

H, 24, 1.09812166, 7, 121.67267369, 23, 1.1914942

H, 24, 1.09036744, 7, 117.9562185, 23, 181.53167357

H, 23, 1.09946743, 7, 112.44619419, 24, -1.84934157

H, 23, 1.09419978, 7, 108.69976593, 24, 119.99245608

H, 23, 1.09561948, 7, 109.17741582, 24, -123.51701581

HF=-839.8042335

RMSD=3.193e-09

Dipole=-1.7395823, 1.6234264, -0.517191

PG=C01 [X(C5H16Hg1N2O5)]

HgC0St9

-1,1
Hg
O,1,2.3356036506
O,1,2.3160183497,2,90.
N,1,2.600784096,3,90.,2,180.
N,1,2.5303516043,2,90.,3,180.
O,1,2.3256419958,2,90.,3,90.
N,1,2.533986812,2,90.,3,-90.
C,2,1.26698348,1,151.74721092,3,152.91832679
H,8,1.11491431,2,114.27702106,1,156.87029317
O,8,1.25374582,2,128.51197908,9,178.89523078
C,3,1.26962476,1,144.36454032,2,235.17735019
H,11,1.11601646,3,113.78267072,1,163.93956421
O,11,1.25161406,3,129.08020178,12,178.87001174
C,4,1.45596772,1,116.03396096,3,26.75593066
C,4,1.26773489,1,124.53550702,3,198.11378645
H,15,1.0984643,4,122.51258335,14,0.37503423
H,15,1.08916411,4,119.55957835,14,179.41493309
H,14,1.10086651,4,111.79744517,15,-2.59706684
H,14,1.09441306,4,108.0642583,15,119.55830925
H,14,1.09273847,4,108.15610291,15,-123.44427438
C,5,1.45818128,1,120.68752974,2,56.02377856
C,5,1.2728032,1,119.56629975,2,-113.0492404
H,22,1.10136311,5,120.9977843,21,0.04957576
H,22,1.09215424,5,119.89489707,21,179.95110997
H,21,1.102136,5,111.93509753,22,-0.89946811
H,21,1.09671317,5,108.93988567,22,121.23771347
H,21,1.09654632,5,108.861694,22,-121.7126668
C,6,1.27106117,1,141.64447214,2,-200.85075891
H,28,1.1160048,6,113.76601057,1,161.01916041
O,28,1.25081271,6,128.85576052,29,179.13499975
C,7,1.4590207,1,119.95315544,2,-201.87526524
C,7,1.27247731,1,120.13848855,2,-8.12719526
H,32,1.10088491,7,121.0380667,31,0.79142917
H,32,1.09013271,7,120.15158129,31,180.31446035
H,31,1.10202188,7,111.89833208,32,-1.69652346
H,31,1.09704443,7,108.2765996,32,119.64524295
H,31,1.09622687,7,109.14650328,32,-122.54610875

HF=-1123.5745778

RMSD=1.720e-09

Dipole=-2.3650091,2.0969926,-2.2449365

PG=C01 [X(C9H18Hg1N3O6)]

HgC0St10

-1,1
Hg
S,1,3.2206981502
N,1,2.5405329486,2,90.
O,1,2.2327523777,3,90.,2,180.
O,1,2.3879172369,2,90.,3,180.
N,1,2.4521418209,2,90.,3,90.
O,1,2.3681999491,2,90.,3,-90.
H,2,1.37137084,1,68.98737662,3,60.13152301
H,2,1.34995954,1,68.87600307,3,163.38684742
H,3,1.01649383,1,125.54886593,2,73.55205756

H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232
H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144
H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611
C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025
H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006
O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292
H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173
H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709
H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351
C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952
H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-1120.8040229

RMSD=8.029e-09

Dipole=2.1711486, -1.146605, 0.5171689

PG=C01 [X(C2H11Hg1N2O5S1)]

2. Ni2+-specific sites

CoNIST1

2, 4

Co

N, 1, 2.2415863576
N, 1, 2.2179821387, 2, 90.
N, 1, 2.3052585208, 3, 90., 2, 180.
N, 1, 2.2159442765, 2, 90., 3, 180.
N, 1, 2.2458333733, 2, 90., 3, 90.
N, 1, 2.2844220643, 2, 90., 3, -90.
H, 2, 1.02218632, 1, 112.22230275, 3, 223.49426626
H, 2, 1.0223562, 1, 111.8622484, 3, 105.85354145
H, 2, 1.021818, 1, 116.66392317, 3, -15.64697026
H, 3, 1.02157842, 1, 115.99569948, 2, 1.61642018
H, 3, 1.02137034, 1, 112.23907909, 2, 122.68064921
H, 3, 1.02193552, 1, 111.60215044, 2, -119.10354552
C, 4, 1.47270364, 1, 117.52363247, 3, 24.2182394
C, 4, 1.27594969, 1, 126.02316009, 3, 204.07467814
H, 15, 1.09405058, 4, 122.79020236, 14, 0.71683646
H, 15, 1.08865738, 4, 120.40794031, 14, 181.53214421
H, 14, 1.09521435, 4, 112.407814, 15, -7.93615567
H, 14, 1.09501518, 4, 109.11434803, 15, 112.16320819
H, 14, 1.09398096, 4, 109.52210655, 15, -129.09331387
H, 5, 1.02228651, 1, 110.38060153, 2, -54.50224095
H, 5, 1.02200185, 1, 113.73948656, 2, 63.81666447
H, 5, 1.02065328, 1, 115.84669011, 2, -173.41596908
C, 6, 1.47183093, 1, 120.70414207, 2, -35.22193953
C, 6, 1.27692234, 1, 122.08757902, 2, 145.00490064
H, 25, 1.09393523, 6, 122.68385326, 24, -0.12880028
H, 25, 1.08906056, 6, 119.77860924, 24, 180.19261198
H, 24, 1.09511836, 6, 112.30949882, 25, 5.39598009
H, 24, 1.09442174, 6, 109.64543793, 25, 126.40186077
H, 24, 1.0947024, 6, 109.57076216, 25, -115.19184781
C, 7, 1.4711703, 1, 122.97107907, 2, -137.17289098
C, 7, 1.2766656, 1, 120.32224335, 2, 43.68852151

H, 32, 1.09382253, 7, 122.9400758, 31, 0.7819722
H, 32, 1.09020783, 7, 120.06708854, 31, 180.98587137
H, 31, 1.09507839, 7, 112.21123533, 32, -6.50137934
H, 31, 1.09339785, 7, 109.01854692, 32, 114.14383787
H, 31, 1.09427919, 7, 109.76786183, 32, -127.41503691

HF=-1954.1157771
S2=3.755364
S2-1=0.
S2A=3.750012
RMSD=2.148e-09
Dipole=-0.1285186, 0.0288582, 0.7322767
PG=C01 [X(C6H24Co1N6)]

CoNIST2

2, 4
Co
O, 1, 2.241689036
N, 1, 2.172114722, 2, 90.
N, 1, 2.2880111489, 3, 90., 2, 180.
N, 1, 2.2039374143, 2, 90., 3, 180.
O, 1, 2.2266772254, 2, 90., 3, 90.
N, 1, 2.2340494106, 2, 90., 3, -90.
H, 2, 0.97368841, 1, 130.97482456, 3, -5.85841175
H, 2, 0.97377175, 1, 121.64169799, 3, -168.78459624
H, 3, 1.02259906, 1, 114.99280011, 2, 46.33872299
H, 3, 1.0203905, 1, 112.24954558, 2, 166.67549256
H, 3, 1.02244685, 1, 111.41493789, 2, -74.5015318
C, 4, 1.47372514, 1, 121.36166483, 3, -2.5807896
C, 4, 1.27722263, 1, 122.38153411, 3, 175.53958192
H, 14, 1.09374558, 4, 122.50146252, 13, -1.57757251
H, 14, 1.08684747, 4, 120.05126423, 13, 178.44793197
H, 13, 1.09505735, 4, 112.31112933, 14, 6.28671479
H, 13, 1.09423462, 4, 109.9342315, 14, 126.9771068
H, 13, 1.09642623, 4, 109.38470904, 14, -113.58881233
C, 5, 1.47423005, 1, 120.94283352, 2, 93.91801668
C, 5, 1.27996526, 1, 121.98914058, 2, -84.26213118
H, 21, 1.0932691, 5, 121.96356757, 20, 1.2043501
H, 21, 1.08657457, 5, 119.6884568, 20, 180.78222839
H, 20, 1.09438215, 5, 111.4461756, 21, -5.65142706
H, 20, 1.09254592, 5, 109.35013667, 21, 115.0842733
H, 20, 1.09232612, 5, 109.70068599, 21, -126.76119399
H, 6, 0.97356595, 1, 127.48132716, 2, -14.42430135
H, 6, 0.97331821, 1, 123.90588551, 2, 185.95183484
C, 7, 1.47210171, 1, 121.5669719, 2, -184.35958277
C, 7, 1.27801685, 1, 121.52287562, 2, -0.67349326
H, 30, 1.09385171, 7, 122.39397313, 29, 0.94674555
H, 30, 1.08786263, 7, 119.6913342, 29, 180.61054521
H, 29, 1.09496735, 7, 111.98562445, 30, -4.37422902
H, 29, 1.0941034, 7, 109.43167124, 30, 116.18306956
H, 29, 1.09255731, 7, 109.74392265, 30, -125.7230154

HF=-1993.8505686
S2=3.755517
S2-1=0.
S2A=3.750013

RMSD=4.125e-09
Dipole=0.6498694, -1.0556081, 0.9100571
PG=C01 [X(C6H22Co1N402)]

CoNISt3

1,4
Co
N,1,2.2587332894
N,1,2.1962691323,2,90.
O,1,2.0375917478,3,90.,2,180.
N,1,2.2047056834,2,90.,3,180.
N,1,2.2689943099,2,90.,3,90.
N,1,2.2758573371,2,90.,3,-90.
H,2,1.02041823,1,116.3434121,3,214.69712301
H,2,1.02109528,1,109.08667667,3,94.79719124
H,2,1.02013228,1,112.09711674,3,-22.76966693
H,3,1.02090032,1,111.03814971,2,99.73078353
H,3,1.03904471,1,97.63041354,2,210.23649954
H,3,1.0202815,1,126.0560228,2,-30.76114288
C,4,1.29527034,1,128.6974004,3,-34.38404821
H,14,1.10566777,4,114.08923242,1,188.20398973
O,14,1.23806142,4,126.75699776,15,180.07538558
H,5,1.02029618,1,114.32986053,2,-72.48741888
H,5,1.01968023,1,118.82592358,2,55.47735735
H,5,1.02256008,1,102.44537934,2,-186.89870823
C,6,1.46382906,1,124.32364829,2,-6.18359127
C,6,1.27649808,1,117.53570753,2,176.68167292
H,21,1.09579235,6,122.14479204,20,0.052042
H,21,1.0885834,6,118.71905982,20,180.39386403
H,20,1.09707672,6,112.63394322,21,0.92231435
H,20,1.09565663,6,109.40817419,21,121.94664764
H,20,1.0959373,6,109.52019072,21,-120.03495471
C,7,1.46503907,1,117.88951861,2,-131.67946192
C,7,1.27239396,1,123.24611285,2,61.64017731
H,28,1.09477306,7,122.95479491,27,0.14739501
H,28,1.08978219,7,119.84919829,27,180.81757135
H,27,1.09651842,7,112.49786868,28,2.62776433
H,27,1.09306345,7,108.79383548,28,124.00272794
H,27,1.09600334,7,109.20152576,28,-118.09623287

HF=-2009.6867795
S2=3.756144
S2-1=0.
S2A=3.750016
RMSD=3.167e-09
Dipole=-1.3155429, -0.682969, 2.8949096
PG=C01 [X(C5H20Co1N502)]

CoNISt4

1,4
Co

O,1,2.1003574704
 S,1,2.718020309,2,90.
 N,1,2.1564946965,3,90.,2,180.
 O,1,2.0370055068,2,90.,3,180.
 O,1,2.2321917657,2,90.,3,90.
 N,1,2.1903687084,2,90.,3,-90.
 H,2,0.97054617,1,127.22203423,3,-43.94365587
 H,2,1.03126791,1,101.53728323,3,-168.77839308
 H,3,1.34990657,1,104.6956663,2,116.94024125
 H,3,1.34884165,1,102.87555698,2,214.65018774
 H,4,1.02141578,1,113.63452577,3,72.84309743
 H,4,1.02267896,1,104.60430397,3,188.5406777
 H,4,1.01882045,1,116.97407739,3,-52.69609427
 C,5,1.28168243,1,128.42333822,2,-9.95926201
 H,15,1.10167561,5,115.65029181,1,177.7621724
 O,15,1.2514157,5,126.05829288,16,179.39579074
 C,6,1.22306023,1,127.95418031,2,54.38684708
 H,18,1.10103871,6,119.96608833,1,174.76860011
 H,18,1.10063637,6,121.5411447,19,179.76799675
 C,7,1.4663415,1,119.7003069,2,-143.88818255
 C,7,1.27541028,1,120.89208142,2,23.45582206
 H,22,1.09452207,7,122.20163832,21,-1.3820998
 H,22,1.08767527,7,119.5382759,21,177.44209351
 H,21,1.09610171,7,112.10980723,22,-2.4053076
 H,21,1.09576433,7,109.7047724,22,118.03891377
 H,21,1.09406806,7,108.63112368,22,-123.41484564

HF=-2352.939966

S2=3.756161

S2-1=0.

S2A=3.750017

RMSD=5.938e-09

Dipole=1.4154061, -0.2196366, -1.6437564

PG=C01 [X(C4H15Co1N2O4S1)]

CoNIST5

1,4

Co

O,1,2.2446187308
 O,1,2.1321749272,2,90.
 O,1,2.0786569769,3,90.,2,180.
 N,1,2.2010985889,2,90.,3,180.
 N,1,2.2107780724,2,90.,3,90.
 N,1,2.2056905393,2,90.,3,-90.
 H,2,0.97296023,1,112.16865729,3,-6.80686301
 H,2,0.97197859,1,115.61478673,3,-246.06419016
 H,3,0.97057074,1,118.43936251,2,85.72796264
 H,3,1.0330723,1,97.43694776,2,-161.76364113
 C,4,1.28370719,1,125.14944826,3,-23.39579163
 H,12,1.10302426,4,115.62431868,1,190.23720759
 O,12,1.24939379,4,126.36133311,13,180.27015948
 C,5,1.46483012,1,122.25565863,2,4.79421932
 C,5,1.27542205,1,119.22790851,2,-172.1882213
 H,16,1.09511258,5,121.87993726,15,0.14738443
 H,16,1.08803585,5,118.8937645,15,179.7497631
 H,15,1.0965316,5,112.35556676,16,1.34137805

H, 15, 1.09400843, 5, 109.29029594, 16, 122.94856457
H, 15, 1.09648123, 5, 109.19328629, 16, -119.28821791
C, 6, 1.46643399, 1, 121.99423945, 2, -2.30944573
C, 6, 1.27518632, 1, 119.75349617, 2, -183.52228528
H, 23, 1.09481, 6, 121.90235038, 22, 0.05148818
H, 23, 1.08732197, 6, 119.02051155, 22, 180.05030546
H, 22, 1.09646026, 6, 112.28205752, 23, -1.34805213
H, 22, 1.09565074, 6, 109.28667184, 23, 119.50746083
H, 22, 1.09357065, 6, 109.29529017, 23, -123.0985196
C, 7, 1.46546877, 1, 120.2559771, 2, -121.27358117
C, 7, 1.27598575, 1, 120.63253081, 2, 70.26653624
H, 30, 1.09449754, 7, 122.20123209, 29, 0.97097733
H, 30, 1.08823337, 7, 119.61644432, 29, 182.32574445
H, 29, 1.09609776, 7, 111.94502789, 30, -0.7837748
H, 29, 1.09346675, 7, 108.69717189, 30, 120.28177774
H, 29, 1.09399338, 7, 109.45380317, 30, -122.03589325

HF=-2126.8450061

S2=3.756828

S2-1=0.

S2A=3.750019

RMSD=5.082e-09

Dipole=-1.3036484, -0.3504627, 1.92439

PG=C01 [X(C7H20Co1N3O4)]

CoNIST6

O, 4

Co

N, 1, 2.1871385382

O, 1, 2.1691816997, 2, 90.

O, 1, 2.0776313827, 3, 90., 2, 180.

O, 1, 2.0905201932, 2, 90., 3, 180.

O, 1, 2.1805705239, 2, 90., 3, 90.

N, 1, 2.2000164269, 2, 90., 3, -90.

H, 2, 1.01908318, 1, 115.5621522, 3, -14.96344912

H, 2, 1.01849089, 1, 111.26121655, 3, 108.4424075

H, 2, 1.02323815, 1, 105.8404396, 3, -134.75467573

H, 3, 0.97112394, 1, 108.28761455, 2, 81.6646543

H, 3, 1.02304661, 1, 97.80392418, 2, -168.95716576

C, 4, 1.2742347, 1, 127.82099865, 3, -14.12880404

H, 13, 1.10612313, 4, 115.29564313, 1, 185.68264568

O, 13, 1.25528257, 4, 127.37705979, 14, 179.99772

C, 5, 1.27123034, 1, 122.3007382, 2, -55.12433709

H, 16, 1.10668905, 5, 115.686955, 1, 174.24881814

O, 16, 1.25921146, 5, 126.78984261, 17, 180.17200808

H, 6, 1.00599966, 1, 95.59832954, 2, 61.71032057

H, 6, 0.97189607, 1, 103.7317423, 2, 169.88928881

C, 7, 1.4601769, 1, 116.99232253, 2, -114.11575284

C, 7, 1.27201034, 1, 122.86053587, 2, 74.62011213

H, 22, 1.0967847, 7, 122.27117519, 21, 1.10542599

H, 22, 1.08908345, 7, 119.22225123, 21, 182.20151921

H, 21, 1.09878261, 7, 112.20757437, 22, -1.38175132

H, 21, 1.09397861, 7, 108.13863684, 22, 120.4332478

H, 21, 1.09322508, 7, 108.90709937, 22, -123.99727428

HF=-2104.9039295

S2=3.755881
S2-1=0.
S2A=3.750014
RMSD=6.903e-09
Dipole=0.3241375,1.3595689,1.490036
PG=C01 [X(C4H14Co1N206)]

CoNISt7

0,4
Co
N,1,2.1876896371
O,1,2.1764299093,2,90.
O,1,2.0697839431,3,90.,2,180.
N,1,2.1976150563,2,90.,3,180.
O,1,2.082105909,2,90.,3,90.
N,1,2.3234750187,2,90.,3,-90.
H,2,1.02898128,1,100.93861993,3,-125.72297767
H,2,1.0184998,1,118.8740048,3,-244.72562218
H,2,1.01936669,1,111.78985893,3,-10.53215645
H,3,0.97272908,1,102.24011537,2,81.683871
H,3,1.0178043,1,98.41575201,2,-171.58021223
C,4,1.27234602,1,129.29559016,3,-4.45491891
H,13,1.10607734,4,115.34101058,1,173.68242238
O,13,1.25528522,4,127.15300857,14,179.45785389
H,5,1.01777801,1,127.55451684,2,69.26807101
H,5,1.02102012,1,102.7068079,2,193.20851145
H,5,1.02771264,1,101.29207317,2,-55.24041314
C,6,1.27626236,1,123.9387555,2,44.96125971
H,19,1.10812486,6,115.04782625,1,178.95271958
O,19,1.25478665,6,126.90331622,20,180.24079754
C,7,1.4609659,1,115.43336081,2,-244.03545366
C,7,1.26935867,1,126.12677613,2,-65.86852803
H,23,1.09712882,7,122.89262562,22,0.54298214
H,23,1.08978492,7,119.77638238,22,180.59388516
H,22,1.09907263,7,112.51641284,23,-1.30804604
H,22,1.09441114,7,108.43090638,23,120.46210531
H,22,1.09340227,7,108.87930888,23,-123.58816988

HF=-2085.0217975
S2=3.755155
S2-1=0.
S2A=3.750012
RMSD=2.942e-09
Dipole=-0.9745666,2.284818,1.369608
PG=C01 [X(C4H15Co1N305)]

CoNISt8

0,4
Co
O,1,2.2471071054
O,1,2.3348326813,2,90.

N, 1, 2.2161619765, 3, 90., 2, 180.
N, 1, 2.1840643241, 2, 90., 3, 180.
O, 1, 1.9236596532, 2, 90., 3, 90.
O, 1, 2.0750587613, 2, 90., 3, -90.
H, 2, 0.98214527, 1, 98.03740504, 3, 41.23140709
H, 2, 0.97303739, 1, 95.55627717, 3, 291.16967905
H, 3, 0.96938221, 1, 109.05225919, 2, 56.26983926
H, 3, 0.98936737, 1, 92.40867582, 2, -52.33589396
H, 4, 1.01857229, 1, 104.27730482, 3, 114.08554484
H, 4, 1.01867956, 1, 120.12431911, 3, -122.86529826
H, 4, 1.01969088, 1, 107.16574374, 3, 0.09642521
H, 5, 1.01738507, 1, 118.93736461, 2, 140.77093849
H, 5, 1.0191144, 1, 109.57910585, 2, 16.1650075
H, 5, 1.02021522, 1, 102.53365938, 2, -98.35376445
H, 6, 0.96787022, 1, 116.01791444, 2, -116.07779375
C, 7, 1.27379513, 1, 119.27103665, 2, -314.62134876
H, 19, 1.10566353, 7, 115.51957561, 1, -176.02088516
O, 19, 1.25889972, 7, 126.63707658, 20, 179.96043374

HF=-1914.0878235
S2=3.755784
S2-1=0.
S2A=3.750015
RMSD=9.744e-09
Dipole=-0.7252213, -0.4135582, -1.1596297
PG=C01 [X(C1H12Co1N2O5)]

CoNIst9

-1, 4
Co
O, 1, 2.1973104459
O, 1, 2.1691646733, 2, 90.
O, 1, 2.1012877007, 3, 90., 2, 180.
O, 1, 2.1208601439, 2, 90., 3, 180.
O, 1, 2.163517991, 2, 90., 3, 90.
O, 1, 2.0959090951, 2, 90., 3, -90.
H, 2, 0.97175182, 1, 99.52841139, 3, 104.51642737
H, 2, 0.99881877, 1, 94.29456214, 3, 211.68565945
H, 3, 1.00910859, 1, 98.68960825, 2, -94.09939069
H, 3, 0.97099223, 1, 101.38789902, 2, -201.97750436
C, 4, 1.26878383, 1, 127.01843031, 3, 111.33200025
H, 12, 1.11133539, 4, 114.97633126, 1, 165.77026947
O, 12, 1.2568272, 4, 128.2325859, 13, 179.4719588
C, 5, 1.26286828, 1, 120.82600369, 2, -40.62039042
H, 15, 1.11032012, 5, 115.80738502, 1, 188.1673724
O, 15, 1.26542938, 5, 127.21421399, 16, 179.78233688
H, 6, 0.97558209, 1, 102.4577341, 2, 53.67963108
H, 6, 1.00806546, 1, 98.4646123, 2, 163.90836736
C, 7, 1.26868733, 1, 129.00837508, 2, -260.68082653
H, 20, 1.11121701, 7, 114.90604985, 1, -189.63994372
O, 20, 1.2562652, 7, 128.27473249, 21, 179.68083534

HF=-2180.1178886
S2=3.754517
S2-1=0.
S2A=3.750009

RMSD=6.127e-09
Dipole=-0.2868869,0.3165835,0.2861447
PG=C01 [X(C3H9Co109)]

CoNISt10

-1,4
Co
S,1,3.1515837284
N,1,2.1871492136,2,90.
O,1,1.9382204064,3,90.,2,180.
O,1,2.1435825723,2,90.,3,180.
N,1,2.1677862495,2,90.,3,90.
O,1,2.1294912195,2,90.,3,-90.
H,2,1.37137084,1,68.98737662,3,60.13152301
H,2,1.34995954,1,68.87600307,3,163.38684742
H,3,1.01649383,1,125.54886593,2,73.55205756
H,3,1.02262177,1,91.87096883,2,190.06213232
H,3,1.02214414,1,107.23171868,2,-58.23756144
H,4,0.96789674,1,105.45799613,3,-135.33034611
C,5,1.26991852,1,131.60725745,2,-80.06634025
H,14,1.1160537,5,114.15912931,1,192.02989006
O,14,1.2545012,5,129.03165872,15,179.64749292
H,6,1.03342131,1,103.76270075,2,73.09849173
H,6,1.02173048,1,95.44332656,2,183.37055709
H,6,1.01715252,1,126.67645371,2,-56.00776351
C,7,1.26589241,1,125.4355857,2,46.92957952
H,20,1.11381724,7,114.91970239,1,-188.27084693
O,20,1.2603282,7,128.02959413,21,180.64311568

HF=-2349.8911677
S2=3.756616
S2-1=0.
S2A=3.75002
RMSD=7.318e-09
Dipole=1.6782172,-0.6546464,0.3467135
PG=C01 [X(C2H11Co1N205S1)]

NiNISt1

2,3
Ni
N,1,2.190343649
N,1,2.1652298423,2,90.
N,1,2.266320026,3,90.,2,180.
N,1,2.1621467483,2,90.,3,180.
N,1,2.2019244751,2,90.,3,90.
N,1,2.2454766212,2,90.,3,-90.
H,2,1.02218632,1,112.22230275,3,223.49426626
H,2,1.0223562,1,111.8622484,3,105.85354145
H,2,1.021818,1,116.66392317,3,-15.64697026
H,3,1.02157842,1,115.99569948,2,1.61642018
H,3,1.02137034,1,112.23907909,2,122.68064921

H, 3, 1.02193552, 1, 111.60215044, 2, -119.10354552
 C, 4, 1.47270364, 1, 117.52363247, 3, 24.2182394
 C, 4, 1.27594969, 1, 126.02316009, 3, 204.07467814
 H, 15, 1.09405058, 4, 122.79020236, 14, 0.71683646
 H, 15, 1.08865738, 4, 120.40794031, 14, 181.53214421
 H, 14, 1.09521435, 4, 112.407814, 15, -7.93615567
 H, 14, 1.09501518, 4, 109.11434803, 15, 112.16320819
 H, 14, 1.09398096, 4, 109.52210655, 15, -129.09331387
 H, 5, 1.02228651, 1, 110.38060153, 2, -54.50224095
 H, 5, 1.02200185, 1, 113.73948656, 2, 63.81666447
 H, 5, 1.02065328, 1, 115.84669011, 2, -173.41596908
 C, 6, 1.47183093, 1, 120.70414207, 2, -35.22193953
 C, 6, 1.27692234, 1, 122.08757902, 2, 145.00490064
 H, 25, 1.09393523, 6, 122.68385326, 24, -0.12880028
 H, 25, 1.08906056, 6, 119.77860924, 24, 180.19261198
 H, 24, 1.09511836, 6, 112.30949882, 25, 5.39598009
 H, 24, 1.09442174, 6, 109.64543793, 25, 126.40186077
 H, 24, 1.0947024, 6, 109.57076216, 25, -115.19184781
 C, 7, 1.4711703, 1, 122.97107907, 2, -137.17289098
 C, 7, 1.2766656, 1, 120.32224335, 2, 43.68852151
 H, 32, 1.09382253, 7, 122.9400758, 31, 0.7819722
 H, 32, 1.09020783, 7, 120.06708854, 31, 180.98587137
 H, 31, 1.09507839, 7, 112.21123533, 32, -6.50137934
 H, 31, 1.09339785, 7, 109.01854692, 32, 114.14383787
 H, 31, 1.09427919, 7, 109.76786183, 32, -127.41503691

HF=-2079.6581053

S2=2.004477

S2-1=0.

S2A=2.000013

RMSD=2.338e-09

Dipole=-0.1224582, 0.0282199, 0.6995412

PG=C01 [X(C6H24N6Ni1)]

NiNIST2

2, 3

Ni

O, 1, 2.1977801507

N, 1, 2.1199611128, 2, 90.

N, 1, 2.2468798404, 3, 90., 2, 180.

N, 1, 2.1651396521, 2, 90., 3, 180.

O, 1, 2.1969693582, 2, 90., 3, 90.

N, 1, 2.1960298935, 2, 90., 3, -90.

H, 2, 0.97368841, 1, 130.97482456, 3, -5.85841175

H, 2, 0.97377175, 1, 121.64169799, 3, -168.78459624

H, 3, 1.02259906, 1, 114.99280011, 2, 46.33872299

H, 3, 1.0203905, 1, 112.24954558, 2, 166.67549256

H, 3, 1.02244685, 1, 111.41493789, 2, -74.5015318

C, 4, 1.47372514, 1, 121.36166483, 3, -2.5807896

C, 4, 1.27722263, 1, 122.38153411, 3, 175.53958192

H, 14, 1.09374558, 4, 122.50146252, 13, -1.57757251

H, 14, 1.08684747, 4, 120.05126423, 13, 178.44793197

H, 13, 1.09505735, 4, 112.31112933, 14, 6.28671479

H, 13, 1.09423462, 4, 109.9342315, 14, 126.9771068

H, 13, 1.09642623, 4, 109.38470904, 14, -113.58881233

C, 5, 1.47423005, 1, 120.94283352, 2, 93.91801668

C, 5, 1.27996526, 1, 121.98914058, 2, -84.26213118
H, 21, 1.0932691, 5, 121.96356757, 20, 1.2043501
H, 21, 1.08657457, 5, 119.6884568, 20, 180.78222839
H, 20, 1.09438215, 5, 111.4461756, 21, -5.65142706
H, 20, 1.09254592, 5, 109.35013667, 21, 115.0842733
H, 20, 1.09232612, 5, 109.70068599, 21, -126.76119399
H, 6, 0.97356595, 1, 127.48132716, 2, -14.42430135
H, 6, 0.97331821, 1, 123.90588551, 2, 185.95183484
C, 7, 1.47210171, 1, 121.5669719, 2, -184.35958277
C, 7, 1.27801685, 1, 121.52287562, 2, -0.67349326
H, 30, 1.09385171, 7, 122.39397313, 29, 0.94674555
H, 30, 1.08786263, 7, 119.6913342, 29, 180.61054521
H, 29, 1.09496735, 7, 111.98562445, 30, -4.37422902
H, 29, 1.0941034, 7, 109.43167124, 30, 116.18306956
H, 29, 1.09255731, 7, 109.74392265, 30, -125.7230154

HF=-2119.3905059

S2=2.004145

S2-1=0.

S2A=2.000011

RMSD=4.745e-09

Dipole=0.6230124, -0.9978617, 0.8345434

PG=C01 [X(C6H22N4Ni102)]

NiNIST3

1, 3

Ni

N, 1, 2.2100227226

N, 1, 2.1552572986, 2, 90.

O, 1, 2.0265685581, 3, 90., 2, 180.

N, 1, 2.1495024822, 2, 90., 3, 180.

N, 1, 2.2146004343, 2, 90., 3, 90.

N, 1, 2.2294441351, 2, 90., 3, -90.

H, 2, 1.02041823, 1, 116.3434121, 3, 214.69712301

H, 2, 1.02109528, 1, 109.08667667, 3, 94.79719124

H, 2, 1.02013228, 1, 112.09711674, 3, -22.76966693

H, 3, 1.02090032, 1, 111.03814971, 2, 99.73078353

H, 3, 1.03904471, 1, 97.63041354, 2, 210.23649954

H, 3, 1.0202815, 1, 126.0560228, 2, -30.76114288

C, 4, 1.29527034, 1, 128.6974004, 3, -34.38404821

H, 14, 1.10566777, 4, 114.08923242, 1, 188.20398973

O, 14, 1.23806142, 4, 126.75699776, 15, 180.07538558

H, 5, 1.02029618, 1, 114.32986053, 2, -72.48741888

H, 5, 1.01968023, 1, 118.82592358, 2, 55.47735735

H, 5, 1.02256008, 1, 102.44537934, 2, -186.89870823

C, 6, 1.46382906, 1, 124.32364829, 2, -6.18359127

C, 6, 1.27649808, 1, 117.53570753, 2, 176.68167292

H, 21, 1.09579235, 6, 122.14479204, 20, 0.052042

H, 21, 1.0885834, 6, 118.71905982, 20, 180.39386403

H, 20, 1.09707672, 6, 112.63394322, 21, 0.92231435

H, 20, 1.09565663, 6, 109.40817419, 21, 121.94664764

H, 20, 1.0959373, 6, 109.52019072, 21, -120.03495471

C, 7, 1.46503907, 1, 117.88951861, 2, -131.67946192

C, 7, 1.27239396, 1, 123.24611285, 2, 61.64017731

H, 28, 1.09477306, 7, 122.95479491, 27, 0.14739501

H, 28, 1.08978219, 7, 119.84919829, 27, 180.81757135

H, 27, 1.09651842, 7, 112.49786868, 28, 2.62776433
H, 27, 1.09306345, 7, 108.79383548, 28, 124.00272794
H, 27, 1.09600334, 7, 109.20152576, 28, -118.09623287

HF=-2135.2296727
S2=2.004314
S2-1=0.
S2A=2.000012
RMSD=6.753e-10
Dipole=-1.3038424, -0.682181, 2.8675597
PG=C01 [X(C5H20N5Ni102)]

NiNIST4

1, 3
Ni
O, 1, 2.0814084435
S, 1, 2.6399550889, 2, 90.
N, 1, 2.104319181, 3, 90., 2, 180.
O, 1, 2.0291749923, 2, 90., 3, 180.
O, 1, 2.1751481132, 2, 90., 3, 90.
N, 1, 2.1362046771, 2, 90., 3, -90.
H, 2, 0.97054617, 1, 127.22203423, 3, -43.94365587
H, 2, 1.03126791, 1, 101.53728323, 3, -168.77839308
H, 3, 1.34990657, 1, 104.6956663, 2, 116.94024125
H, 3, 1.34884165, 1, 102.87555698, 2, 214.65018774
H, 4, 1.02141578, 1, 113.63452577, 3, 72.84309743
H, 4, 1.02267896, 1, 104.60430397, 3, 188.5406777
H, 4, 1.01882045, 1, 116.97407739, 3, -52.69609427
C, 5, 1.28168243, 1, 128.42333822, 2, -9.95926201
H, 15, 1.10167561, 5, 115.65029181, 1, 177.7621724
O, 15, 1.2514157, 5, 126.05829288, 16, 179.39579074
C, 6, 1.22306023, 1, 127.95418031, 2, 54.38684708
H, 18, 1.10103871, 6, 119.96608833, 1, 174.76860011
H, 18, 1.10063637, 6, 121.5411447, 19, 179.76799675
C, 7, 1.4663415, 1, 119.7003069, 2, -143.88818255
C, 7, 1.27541028, 1, 120.89208142, 2, 23.45582206
H, 22, 1.09452207, 7, 122.20163832, 21, -1.3820998
H, 22, 1.08767527, 7, 119.5382759, 21, 177.44209351
H, 21, 1.09610171, 7, 112.10980723, 22, -2.4053076
H, 21, 1.09576433, 7, 109.7047724, 22, 118.03891377
H, 21, 1.09406806, 7, 108.63112368, 22, -123.41484564

HF=-2478.4809051
S2=2.004391
S2-1=0.
S2A=2.000012
RMSD=2.551e-09
Dipole=1.4450576, -0.171122, -1.6584436
PG=C01 [X(C4H15N2Ni104S1)]

NiNIST5

1,3
 Ni
 O,1,2.2055478901
 O,1,2.1102734587,2,90.
 O,1,2.0667398802,3,90.,2,180.
 N,1,2.1531280478,2,90.,3,180.
 N,1,2.1622551494,2,90.,3,90.
 N,1,2.153164167,2,90.,3,-90.
 H,2,0.97296023,1,112.16865729,3,-6.80686301
 H,2,0.97197859,1,115.61478673,3,-246.06419016
 H,3,0.97057074,1,118.43936251,2,85.72796264
 H,3,1.0330723,1,97.43694776,2,-161.76364113
 C,4,1.28370719,1,125.14944826,3,-23.39579163
 H,12,1.10302426,4,115.62431868,1,190.23720759
 O,12,1.24939379,4,126.36133311,13,180.27015948
 C,5,1.46483012,1,122.25565863,2,4.79421932
 C,5,1.27542205,1,119.22790851,2,-172.1882213
 H,16,1.09511258,5,121.87993726,15,0.14738443
 H,16,1.08803585,5,118.8937645,15,179.7497631
 H,15,1.0965316,5,112.35556676,16,1.34137805
 H,15,1.09400843,5,109.29029594,16,122.94856457
 H,15,1.09648123,5,109.19328629,16,-119.28821791
 C,6,1.46643399,1,121.99423945,2,-2.30944573
 C,6,1.27518632,1,119.75349617,2,-183.52228528
 H,23,1.09481,6,121.90235038,22,0.05148818
 H,23,1.08732197,6,119.02051155,22,180.05030546
 H,22,1.09646026,6,112.28205752,23,-1.34805213
 H,22,1.09565074,6,109.28667184,23,119.50746083
 H,22,1.09357065,6,109.29529017,23,-123.0985196
 C,7,1.46546877,1,120.2559771,2,-121.27358117
 C,7,1.27598575,1,120.63253081,2,70.26653624
 H,30,1.09449754,7,122.20123209,29,0.97097733
 H,30,1.08823337,7,119.61644432,29,182.32574445
 H,29,1.09609776,7,111.94502789,30,-0.7837748
 H,29,1.09346675,7,108.69717189,30,120.28177774
 H,29,1.09399338,7,109.45380317,30,-122.03589325

HF=-2252.386074
 S2=2.004424
 S2-1=0.
 S2A=2.000013
 RMSD=1.639e-09
 Dipole=-1.3237879,-0.331607,1.8768633
 PG=C01 [X(C7H20N3Ni104)]

NiNIST6

O,3
 Ni
 N,1,2.1308771991
 O,1,2.1473326202,2,90.
 O,1,2.0624488944,3,90.,2,180.
 O,1,2.0785572379,2,90.,3,180.
 O,1,2.1354407636,2,90.,3,90.
 N,1,2.1378961986,2,90.,3,-90.
 H,2,1.01908318,1,115.5621522,3,-14.96344912
 H,2,1.01849089,1,111.26121655,3,108.4424075

H, 2, 1.02323815, 1, 105.8404396, 3, -134.75467573
H, 3, 0.97112394, 1, 108.28761455, 2, 81.6646543
H, 3, 1.02304661, 1, 97.80392418, 2, -168.95716576
C, 4, 1.2742347, 1, 127.82099865, 3, -14.12880404
H, 13, 1.10612313, 4, 115.29564313, 1, 185.68264568
O, 13, 1.25528257, 4, 127.37705979, 14, 179.99772
C, 5, 1.27123034, 1, 122.3007382, 2, -55.12433709
H, 16, 1.10668905, 5, 115.686955, 1, 174.24881814
O, 16, 1.25921146, 5, 126.78984261, 17, 180.17200808
H, 6, 1.00599966, 1, 95.59832954, 2, 61.71032057
H, 6, 0.97189607, 1, 103.7317423, 2, 169.88928881
C, 7, 1.4601769, 1, 116.99232253, 2, -114.11575284
C, 7, 1.27201034, 1, 122.86053587, 2, 74.62011213
H, 22, 1.0967847, 7, 122.27117519, 21, 1.10542599
H, 22, 1.08908345, 7, 119.22225123, 21, 182.20151921
H, 21, 1.09878261, 7, 112.20757437, 22, -1.38175132
H, 21, 1.09397861, 7, 108.13863684, 22, 120.4332478
H, 21, 1.09322508, 7, 108.90709937, 22, -123.99727428

HF=-2230.4451979

S2=2.003813

S2-1=0.

S2A=2.000009

RMSD=2.064e-09

Dipole=0.3194257, 1.4000758, 1.4647902

PG=C01 [X(C4H14N2Ni106)]

NiNIST7

O, 3

Ni

N, 1, 2.1374088817

O, 1, 2.1378922042, 2, 90.

O, 1, 2.0581320418, 3, 90., 2, 180.

N, 1, 2.1381186219, 2, 90., 3, 180.

O, 1, 2.066448168, 2, 90., 3, 90.

N, 1, 2.2685225264, 2, 90., 3, -90.

H, 2, 1.02898128, 1, 100.93861993, 3, -125.72297767

H, 2, 1.0184998, 1, 118.8740048, 3, -244.72562218

H, 2, 1.01936669, 1, 111.78985893, 3, -10.53215645

H, 3, 0.97272908, 1, 102.24011537, 2, 81.683871

H, 3, 1.0178043, 1, 98.41575201, 2, -171.58021223

C, 4, 1.27234602, 1, 129.29559016, 3, -4.45491891

H, 13, 1.10607734, 4, 115.34101058, 1, 173.68242238

O, 13, 1.25528522, 4, 127.15300857, 14, 179.45785389

H, 5, 1.01777801, 1, 127.55451684, 2, 69.26807101

H, 5, 1.02102012, 1, 102.7068079, 2, 193.20851145

H, 5, 1.02771264, 1, 101.29207317, 2, -55.24041314

C, 6, 1.27626236, 1, 123.9387555, 2, 44.96125971

H, 19, 1.10812486, 6, 115.04782625, 1, 178.95271958

O, 19, 1.25478665, 6, 126.90331622, 20, 180.24079754

C, 7, 1.4609659, 1, 115.43336081, 2, -244.03545366

C, 7, 1.26935867, 1, 126.12677613, 2, -65.86852803

H, 23, 1.09712882, 7, 122.89262562, 22, 0.54298214

H, 23, 1.08978492, 7, 119.77638238, 22, 180.59388516

H, 22, 1.09907263, 7, 112.51641284, 23, -1.30804604

H, 22, 1.09441114, 7, 108.43090638, 23, 120.46210531

H, 22, 1.09340227, 7, 108.87930888, 23, -123.58816988

HF=-2210.5626718

S2=2.003821

S2-1=0.

S2A=2.000009

RMSD=1.101e-09

Dipole=-0.9718579, 2.2666706, 1.3736404

PG=C01 [X(C4H15N3Ni105)]

NiNiSt8

0, 3

Ni

0, 1, 2.1740399232

0, 1, 2.2544603744, 2, 90.

N, 1, 2.1344079332, 3, 90., 2, 180.

N, 1, 2.1097747687, 2, 90., 3, 180.

O, 1, 1.9526449136, 2, 90., 3, 90.

O, 1, 2.0689841144, 2, 90., 3, -90.

H, 2, 0.98214527, 1, 98.03740504, 3, 41.23140709

H, 2, 0.97303739, 1, 95.55627717, 3, 291.16967905

H, 3, 0.96938221, 1, 109.05225919, 2, 56.26983926

H, 3, 0.98936737, 1, 92.40867582, 2, -52.33589396

H, 4, 1.01857229, 1, 104.27730482, 3, 114.08554484

H, 4, 1.01867956, 1, 120.12431911, 3, -122.86529826

H, 4, 1.01969088, 1, 107.16574374, 3, 0.09642521

H, 5, 1.01738507, 1, 118.93736461, 2, 140.77093849

H, 5, 1.0191144, 1, 109.57910585, 2, 16.1650075

H, 5, 1.02021522, 1, 102.53365938, 2, -98.35376445

H, 6, 0.96787022, 1, 116.01791444, 2, -116.07779375

C, 7, 1.27379513, 1, 119.27103665, 2, -314.62134876

H, 19, 1.10566353, 7, 115.51957561, 1, -176.02088516

O, 19, 1.25889972, 7, 126.63707658, 20, 179.96043374

HF=-2039.625607

S2=2.003456

S2-1=0.

S2A=2.000008

RMSD=4.461e-09

Dipole=-0.7346304, -0.2393808, -1.1522809

PG=C01 [X(C1H12N2Ni105)]

NiNiSt9

-1, 3

Ni

0, 1, 2.1497254287

0, 1, 2.1282729703, 2, 90.

0, 1, 2.0818982686, 3, 90., 2, 180.

0, 1, 2.0979379845, 2, 90., 3, 180.

0, 1, 2.1256410837, 2, 90., 3, 90.

0, 1, 2.0785115294, 2, 90., 3, -90.

H, 2, 0.97175182, 1, 99.52841139, 3, 104.51642737
H, 2, 0.99881877, 1, 94.29456214, 3, 211.68565945
H, 3, 1.00910859, 1, 98.68960825, 2, -94.09939069
H, 3, 0.97099223, 1, 101.38789902, 2, -201.97750436
C, 4, 1.26878383, 1, 127.01843031, 3, 111.33200025
H, 12, 1.11133539, 4, 114.97633126, 1, 165.77026947
O, 12, 1.2568272, 4, 128.2325859, 13, 179.4719588
C, 5, 1.26286828, 1, 120.82600369, 2, -40.62039042
H, 15, 1.11032012, 5, 115.80738502, 1, 188.1673724
O, 15, 1.26542938, 5, 127.21421399, 16, 179.78233688
H, 6, 0.97558209, 1, 102.4577341, 2, 53.67963108
H, 6, 1.00806546, 1, 98.4646123, 2, 163.90836736
C, 7, 1.26868733, 1, 129.00837508, 2, -260.68082653
H, 20, 1.11121701, 7, 114.90604985, 1, -189.63994372
O, 20, 1.2562652, 7, 128.27473249, 21, 179.68083534

HF=-2305.6550755

S2=2.003091

S2-1=0.

S2A=2.000006

RMSD=1.846e-09

Dipole=-0.3328019, 0.3250539, 0.2699733

PG=C01 [X(C3H9Ni109)]

NiNIST10

-1, 3

Ni

S, 1, 3.125403921

N, 1, 2.1258325607, 2, 90.

O, 1, 1.9589036079, 3, 90., 2, 180.

O, 1, 2.1070404776, 2, 90., 3, 180.

N, 1, 2.1113922578, 2, 90., 3, 90.

O, 1, 2.0944006865, 2, 90., 3, -90.

H, 2, 1.37137084, 1, 68.98737662, 3, 60.13152301

H, 2, 1.34995954, 1, 68.87600307, 3, 163.38684742

H, 3, 1.01649383, 1, 125.54886593, 2, 73.55205756

H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232

H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144

H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611

C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025

H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006

O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292

H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173

H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709

H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351

C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952

H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693

O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-2475.4280898

S2=2.004348

S2-1=0.

S2A=2.000012

RMSD=8.988e-09

Dipole=1.621995, -0.6110249, 0.431221

PG=C01 [X(C2H11N2Ni105S1)]

CuNIST1

2,2

Cu

N,1,2.6873113614
N,1,2.0668386754,2,90.
N,1,2.755317991,3,90.,2,180.
N,1,2.0642848749,2,90.,3,180.
N,1,2.1080234725,2,90.,3,90.
N,1,2.1298925145,2,90.,3,-90.
H,2,1.02218632,1,112.22230275,3,223.49426626
H,2,1.0223562,1,111.8622484,3,105.85354145
H,2,1.021818,1,116.66392317,3,-15.64697026
H,3,1.02157842,1,115.99569948,2,1.61642018
H,3,1.02137034,1,112.23907909,2,122.68064921
H,3,1.02193552,1,111.60215044,2,-119.10354552
C,4,1.47270364,1,117.52363247,3,24.2182394
C,4,1.27594969,1,126.02316009,3,204.07467814
H,15,1.09405058,4,122.79020236,14,0.71683646
H,15,1.08865738,4,120.40794031,14,181.53214421
H,14,1.09521435,4,112.407814,15,-7.93615567
H,14,1.09501518,4,109.11434803,15,112.16320819
H,14,1.09398096,4,109.52210655,15,-129.09331387
H,5,1.02228651,1,110.38060153,2,-54.50224095
H,5,1.02200185,1,113.73948656,2,63.81666447
H,5,1.02065328,1,115.84669011,2,-173.41596908
C,6,1.47183093,1,120.70414207,2,-35.22193953
C,6,1.27692234,1,122.08757902,2,145.00490064
H,25,1.09393523,6,122.68385326,24,-0.12880028
H,25,1.08906056,6,119.77860924,24,180.19261198
H,24,1.09511836,6,112.30949882,25,5.39598009
H,24,1.09442174,6,109.64543793,25,126.40186077
H,24,1.0947024,6,109.57076216,25,-115.19184781
C,7,1.4711703,1,122.97107907,2,-137.17289098
C,7,1.2766656,1,120.32224335,2,43.68852151
H,32,1.09382253,7,122.9400758,31,0.7819722
H,32,1.09020783,7,120.06708854,31,180.98587137
H,31,1.09507839,7,112.21123533,32,-6.50137934
H,31,1.09339785,7,109.01854692,32,114.14383787
H,31,1.09427919,7,109.76786183,32,-127.41503691

HF=-2211.8049812

S2=0.752516

S2-1=0.

S2A=0.750006

RMSD=3.589e-09

Dipole=-0.1020696,0.0350675,0.9701809

PG=C01 [X(C6H24Cu1N6)]

CuNIST2

2,2

Cu
O, 1, 2.5819892418
N, 1, 2.0324314826, 2, 90.
N, 1, 2.5877999866, 3, 90., 2, 180.
N, 1, 2.0901265021, 2, 90., 3, 180.
O, 1, 2.1443105965, 2, 90., 3, 90.
N, 1, 2.1208725174, 2, 90., 3, -90.
H, 2, 0.97368841, 1, 130.97482456, 3, -5.85841175
H, 2, 0.97377175, 1, 121.64169799, 3, -168.78459624
H, 3, 1.02259906, 1, 114.99280011, 2, 46.33872299
H, 3, 1.0203905, 1, 112.24954558, 2, 166.67549256
H, 3, 1.02244685, 1, 111.41493789, 2, -74.5015318
C, 4, 1.47372514, 1, 121.36166483, 3, -2.5807896
C, 4, 1.27722263, 1, 122.38153411, 3, 175.53958192
H, 14, 1.09374558, 4, 122.50146252, 13, -1.57757251
H, 14, 1.08684747, 4, 120.05126423, 13, 178.44793197
H, 13, 1.09505735, 4, 112.31112933, 14, 6.28671479
H, 13, 1.09423462, 4, 109.9342315, 14, 126.9771068
H, 13, 1.09642623, 4, 109.38470904, 14, -113.58881233
C, 5, 1.47423005, 1, 120.94283352, 2, 93.91801668
C, 5, 1.27996526, 1, 121.98914058, 2, -84.26213118
H, 21, 1.0932691, 5, 121.96356757, 20, 1.2043501
H, 21, 1.08657457, 5, 119.6884568, 20, 180.78222839
H, 20, 1.09438215, 5, 111.4461756, 21, -5.65142706
H, 20, 1.09254592, 5, 109.35013667, 21, 115.0842733
H, 20, 1.09232612, 5, 109.70068599, 21, -126.76119399
H, 6, 0.97356595, 1, 127.48132716, 2, -14.42430135
H, 6, 0.97331821, 1, 123.90588551, 2, 185.95183484
C, 7, 1.47210171, 1, 121.5669719, 2, -184.35958277
C, 7, 1.27801685, 1, 121.52287562, 2, -0.67349326
H, 30, 1.09385171, 7, 122.39397313, 29, 0.94674555
H, 30, 1.08786263, 7, 119.6913342, 29, 180.61054521
H, 29, 1.09496735, 7, 111.98562445, 30, -4.37422902
H, 29, 1.0941034, 7, 109.43167124, 30, 116.18306956
H, 29, 1.09255731, 7, 109.74392265, 30, -125.7230154

HF=-2251.5409226
S2=0.752503
S2-1=0.
S2A=0.750006
RMSD=8.059e-09
Dipole=0.5657105, -0.8470571, 1.0776162
PG=C01 [X(C6H22Cu1N4O2)]

CuNIST3

1, 2
Cu
N, 1, 2.1082490249
N, 1, 2.0719627623, 2, 90.
O, 1, 1.9709091461, 3, 90., 2, 180.
N, 1, 2.0695428127, 2, 90., 3, 180.
N, 1, 2.5986245488, 2, 90., 3, 90.
N, 1, 2.6653203724, 2, 90., 3, -90.
H, 2, 1.02041823, 1, 116.3434121, 3, 214.69712301
H, 2, 1.02109528, 1, 109.08667667, 3, 94.79719124
H, 2, 1.02013228, 1, 112.09711674, 3, -22.76966693

H, 3, 1.02090032, 1, 111.03814971, 2, 99.73078353
 H, 3, 1.03904471, 1, 97.63041354, 2, 210.23649954
 H, 3, 1.0202815, 1, 126.0560228, 2, -30.76114288
 C, 4, 1.29527034, 1, 128.6974004, 3, -34.38404821
 H, 14, 1.10566777, 4, 114.08923242, 1, 188.20398973
 O, 14, 1.23806142, 4, 126.75699776, 15, 180.07538558
 H, 5, 1.02029618, 1, 114.32986053, 2, -72.48741888
 H, 5, 1.01968023, 1, 118.82592358, 2, 55.47735735
 H, 5, 1.02256008, 1, 102.44537934, 2, -186.89870823
 C, 6, 1.46382906, 1, 124.32364829, 2, -6.18359127
 C, 6, 1.27649808, 1, 117.53570753, 2, 176.68167292
 H, 21, 1.09579235, 6, 122.14479204, 20, 0.052042
 H, 21, 1.0885834, 6, 118.71905982, 20, 180.39386403
 H, 20, 1.09707672, 6, 112.63394322, 21, 0.92231435
 H, 20, 1.09565663, 6, 109.40817419, 21, 121.94664764
 H, 20, 1.0959373, 6, 109.52019072, 21, -120.03495471
 C, 7, 1.46503907, 1, 117.88951861, 2, -131.67946192
 C, 7, 1.27239396, 1, 123.24611285, 2, 61.64017731
 H, 28, 1.09477306, 7, 122.95479491, 27, 0.14739501
 H, 28, 1.08978219, 7, 119.84919829, 27, 180.81757135
 H, 27, 1.09651842, 7, 112.49786868, 28, 2.62776433
 H, 27, 1.09306345, 7, 108.79383548, 28, 124.00272794
 H, 27, 1.09600334, 7, 109.20152576, 28, -118.09623287

HF=-2267.3778308

S2=0.752137

S2-1=0.

S2A=0.750004

RMSD=5.188e-09

Dipole=-1.2570913, -0.6863594, 2.7446191

PG=C01 [X(C5H20Cu1N5O2)]

CuNIST4

1, 2

Cu

O, 1, 1.9994163858

S, 1, 2.5685104798, 2, 90.

N, 1, 2.0228844795, 3, 90., 2, 180.

O, 1, 2.0007768985, 2, 90., 3, 180.

O, 1, 2.5327534314, 2, 90., 3, 90.

N, 1, 2.4229291617, 2, 90., 3, -90.

H, 2, 0.97054617, 1, 127.22203423, 3, -43.94365587

H, 2, 1.03126791, 1, 101.53728323, 3, -168.77839308

H, 3, 1.34990657, 1, 104.6956663, 2, 116.94024125

H, 3, 1.34884165, 1, 102.87555698, 2, 214.65018774

H, 4, 1.02141578, 1, 113.63452577, 3, 72.84309743

H, 4, 1.02267896, 1, 104.60430397, 3, 188.5406777

H, 4, 1.01882045, 1, 116.97407739, 3, -52.69609427

C, 5, 1.28168243, 1, 128.42333822, 2, -9.95926201

H, 15, 1.10167561, 5, 115.65029181, 1, 177.7621724

O, 15, 1.2514157, 5, 126.05829288, 16, 179.39579074

C, 6, 1.22306023, 1, 127.95418031, 2, 54.38684708

H, 18, 1.10103871, 6, 119.96608833, 1, 174.76860011

H, 18, 1.10063637, 6, 121.5411447, 19, 179.76799675

C, 7, 1.4663415, 1, 119.7003069, 2, -143.88818255

C, 7, 1.27541028, 1, 120.89208142, 2, 23.45582206

H, 22, 1.09452207, 7, 122.20163832, 21, -1.3820998
H, 22, 1.08767527, 7, 119.5382759, 21, 177.44209351
H, 21, 1.09610171, 7, 112.10980723, 22, -2.4053076
H, 21, 1.09576433, 7, 109.7047724, 22, 118.03891377
H, 21, 1.09406806, 7, 108.63112368, 22, -123.41484564

HF=-2610.6264108

S2=0.752377

S2-1=0.

S2A=0.750005

RMSD=8.861e-09

Dipole=1.4547099, -0.2403403, -1.7071525

PG=C01 [X(C4H15Cu1N2O4S1)]

CuNIST5

1, 2

Cu

O, 1, 2.6305675323

O, 1, 2.0861367082, 2, 90.

O, 1, 2.1800054895, 3, 90., 2, 180.

N, 1, 2.1101119254, 2, 90., 3, 180.

N, 1, 2.0823730766, 2, 90., 3, 90.

N, 1, 2.0801167499, 2, 90., 3, -90.

H, 2, 0.97296023, 1, 112.16865729, 3, -6.80686301

H, 2, 0.97197859, 1, 115.61478673, 3, -246.06419016

H, 3, 0.97057074, 1, 118.43936251, 2, 85.72796264

H, 3, 1.0330723, 1, 97.43694776, 2, -161.76364113

C, 4, 1.28370719, 1, 125.14944826, 3, -23.39579163

H, 12, 1.10302426, 4, 115.62431868, 1, 190.23720759

O, 12, 1.24939379, 4, 126.36133311, 13, 180.27015948

C, 5, 1.46483012, 1, 122.25565863, 2, 4.79421932

C, 5, 1.27542205, 1, 119.22790851, 2, -172.1882213

H, 16, 1.09511258, 5, 121.87993726, 15, 0.14738443

H, 16, 1.08803585, 5, 118.8937645, 15, 179.7497631

H, 15, 1.0965316, 5, 112.35556676, 16, 1.34137805

H, 15, 1.09400843, 5, 109.29029594, 16, 122.94856457

H, 15, 1.09648123, 5, 109.19328629, 16, -119.28821791

C, 6, 1.46643399, 1, 121.99423945, 2, -2.30944573

C, 6, 1.27518632, 1, 119.75349617, 2, -183.52228528

H, 23, 1.09481, 6, 121.90235038, 22, 0.05148818

H, 23, 1.08732197, 6, 119.02051155, 22, 180.05030546

H, 22, 1.09646026, 6, 112.28205752, 23, -1.34805213

H, 22, 1.09565074, 6, 109.28667184, 23, 119.50746083

H, 22, 1.09357065, 6, 109.29529017, 23, -123.0985196

C, 7, 1.46546877, 1, 120.2559771, 2, -121.27358117

C, 7, 1.27598575, 1, 120.63253081, 2, 70.26653624

H, 30, 1.09449754, 7, 122.20123209, 29, 0.97097733

H, 30, 1.08823337, 7, 119.61644432, 29, 182.32574445

H, 29, 1.09609776, 7, 111.94502789, 30, -0.7837748

H, 29, 1.09346675, 7, 108.69717189, 30, 120.28177774

H, 29, 1.09399338, 7, 109.45380317, 30, -122.03589325

HF=-2384.5297568

S2=0.752552

S2-1=0.

S2A=0.750006

RMSD=8.934e-09
Dipole=-1.441677, -0.3872955, 2.0539573
PG=C01 [X(C7H20Cu1N304)]

CuNIST6

0, 2
Cu
N, 1, 2.0379827913
O, 1, 2.0975129449, 2, 90.
O, 1, 2.0129851019, 3, 90., 2, 180.
O, 1, 2.0450065516, 2, 90., 3, 180.
O, 1, 2.3929596681, 2, 90., 3, 90.
N, 1, 2.4614266049, 2, 90., 3, -90.
H, 2, 1.01908318, 1, 115.5621522, 3, -14.96344912
H, 2, 1.01849089, 1, 111.26121655, 3, 108.4424075
H, 2, 1.02323815, 1, 105.8404396, 3, -134.75467573
H, 3, 0.97112394, 1, 108.28761455, 2, 81.6646543
H, 3, 1.02304661, 1, 97.80392418, 2, -168.95716576
C, 4, 1.2742347, 1, 127.82099865, 3, -14.12880404
H, 13, 1.10612313, 4, 115.29564313, 1, 185.68264568
O, 13, 1.25528257, 4, 127.37705979, 14, 179.99772
C, 5, 1.27123034, 1, 122.3007382, 2, -55.12433709
H, 16, 1.10668905, 5, 115.686955, 1, 174.24881814
O, 16, 1.25921146, 5, 126.78984261, 17, 180.17200808
H, 6, 1.00599966, 1, 95.59832954, 2, 61.71032057
H, 6, 0.97189607, 1, 103.7317423, 2, 169.88928881
C, 7, 1.4601769, 1, 116.99232253, 2, -114.11575284
C, 7, 1.27201034, 1, 122.86053587, 2, 74.62011213
H, 22, 1.0967847, 7, 122.27117519, 21, 1.10542599
H, 22, 1.08908345, 7, 119.22225123, 21, 182.20151921
H, 21, 1.09878261, 7, 112.20757437, 22, -1.38175132
H, 21, 1.09397861, 7, 108.13863684, 22, 120.4332478
H, 21, 1.09322508, 7, 108.90709937, 22, -123.99727428

HF=-2362.5886832
S2=0.751881
S2-1=0.
S2A=0.750003
RMSD=4.954e-09
Dipole=0.2930292, 1.3545079, 1.3394599
PG=C01 [X(C4H14Cu1N206)]

CuNIST7

0, 2
Cu
N, 1, 2.0506516095
O, 1, 2.0905930479, 2, 90.
O, 1, 2.0055902046, 3, 90., 2, 180.
N, 1, 2.0779417805, 2, 90., 3, 180.
O, 1, 2.2030284227, 2, 90., 3, 90.
N, 1, 2.7322801587, 2, 90., 3, -90.

H, 2, 1.02898128, 1, 100.93861993, 3, -125.72297767
H, 2, 1.0184998, 1, 118.8740048, 3, -244.72562218
H, 2, 1.01936669, 1, 111.78985893, 3, -10.53215645
H, 3, 0.97272908, 1, 102.24011537, 2, 81.683871
H, 3, 1.0178043, 1, 98.41575201, 2, -171.58021223
C, 4, 1.27234602, 1, 129.29559016, 3, -4.45491891
H, 13, 1.10607734, 4, 115.34101058, 1, 173.68242238
O, 13, 1.25528522, 4, 127.15300857, 14, 179.45785389
H, 5, 1.01777801, 1, 127.55451684, 2, 69.26807101
H, 5, 1.02102012, 1, 102.7068079, 2, 193.20851145
H, 5, 1.02771264, 1, 101.29207317, 2, -55.24041314
C, 6, 1.27626236, 1, 123.9387555, 2, 44.96125971
H, 19, 1.10812486, 6, 115.04782625, 1, 178.95271958
O, 19, 1.25478665, 6, 126.90331622, 20, 180.24079754
C, 7, 1.4609659, 1, 115.43336081, 2, -244.03545366
C, 7, 1.26935867, 1, 126.12677613, 2, -65.86852803
H, 23, 1.09712882, 7, 122.89262562, 22, 0.54298214
H, 23, 1.08978492, 7, 119.77638238, 22, 180.59388516
H, 22, 1.09907263, 7, 112.51641284, 23, -1.30804604
H, 22, 1.09441114, 7, 108.43090638, 23, 120.46210531
H, 22, 1.09340227, 7, 108.87930888, 23, -123.58816988

HF=-2342.705225

S2=0.75186

S2-1=0.

S2A=0.750003

RMSD=6.608e-09

Dipole=-0.8685775, 2.4539284, 1.1608531

PG=C01 [X(C4H15Cu1N3O5)]

CuNIST8

O, 2

Cu

O, 1, 2.1354290125

O, 1, 2.5807240739, 2, 90.

N, 1, 2.099152986, 3, 90., 2, 180.

N, 1, 2.4012834804, 2, 90., 3, 180.

O, 1, 1.8871826389, 2, 90., 3, 90.

O, 1, 2.0077463643, 2, 90., 3, -90.

H, 2, 0.98214527, 1, 98.03740504, 3, 41.23140709

H, 2, 0.97303739, 1, 95.55627717, 3, 291.16967905

H, 3, 0.96938221, 1, 109.05225919, 2, 56.26983926

H, 3, 0.98936737, 1, 92.40867582, 2, -52.33589396

H, 4, 1.01857229, 1, 104.27730482, 3, 114.08554484

H, 4, 1.01867956, 1, 120.12431911, 3, -122.86529826

H, 4, 1.01969088, 1, 107.16574374, 3, 0.09642521

H, 5, 1.01738507, 1, 118.93736461, 2, 140.77093849

H, 5, 1.0191144, 1, 109.57910585, 2, 16.1650075

H, 5, 1.02021522, 1, 102.53365938, 2, -98.35376445

H, 6, 0.96787022, 1, 116.01791444, 2, -116.07779375

C, 7, 1.27379513, 1, 119.27103665, 2, -314.62134876

H, 19, 1.10566353, 7, 115.51957561, 1, -176.02088516

O, 19, 1.25889972, 7, 126.63707658, 20, 179.96043374

HF=-2171.7792052

S2=0.751933

S2-1=0.
S2A=0.750003
RMSD=5.767e-09
Dipole=-0.6474458, -0.3810134, -1.1793696
PG=C01 [X(C1H12Cu1N2O5)]

CuNIST9

-1,2
Cu
O,1,2.4181124418
O,1,2.0716720103,2,90.
O,1,2.2074817801,3,90.,2,180.
O,1,2.0515622412,2,90.,3,180.
O,1,2.0717021398,2,90.,3,90.
O,1,2.0401500247,2,90.,3,-90.
H,2,0.97175182,1,99.52841139,3,104.51642737
H,2,0.99881877,1,94.29456214,3,211.68565945
H,3,1.00910859,1,98.68960825,2,-94.09939069
H,3,0.97099223,1,101.38789902,2,-201.97750436
C,4,1.26878383,1,127.01843031,3,111.33200025
H,12,1.11133539,4,114.97633126,1,165.77026947
O,12,1.2568272,4,128.2325859,13,179.4719588
C,5,1.26286828,1,120.82600369,2,-40.62039042
H,15,1.11032012,5,115.80738502,1,188.1673724
O,15,1.26542938,5,127.21421399,16,179.78233688
H,6,0.97558209,1,102.4577341,2,53.67963108
H,6,1.00806546,1,98.4646123,2,163.90836736
C,7,1.26868733,1,129.00837508,2,-260.68082653
H,20,1.11121701,7,114.90604985,1,-189.63994372
O,20,1.2562652,7,128.27473249,21,179.68083534

HF=-2437.7954264
S2=0.751692
S2-1=0.
S2A=0.750003
RMSD=8.946e-09
Dipole=-0.3270433,0.5247071,0.5661628
PG=C01 [X(C3H9Cu1O9)]

CuNIST10

-1,2
Cu
S,1,3.0153639174
N,1,2.4704268111,2,90.
O,1,1.9245094481,3,90.,2,180.
O,1,2.2806585769,2,90.,3,180.
N,1,2.0421394449,2,90.,3,90.
O,1,2.0417008789,2,90.,3,-90.
H,2,1.37137084,1,68.98737662,3,60.13152301
H,2,1.34995954,1,68.87600307,3,163.38684742
H,3,1.01649383,1,125.54886593,2,73.55205756

H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232
H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144
H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611
C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025
H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006
O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292
H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173
H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709
H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351
C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952
H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-2607.5730804

S2=0.753189

S2-1=0.

S2A=0.750006

RMSD=4.934e-09

Dipole=2.0296438, -0.4018361, 0.1649226

PG=C01 [X(C2H11Cu1N2O5S1)]

ZnNIST1

2, 1

Zn

N, 1, 2.2718922204

N, 1, 2.2290488638, 2, 90.

N, 1, 2.3449409937, 3, 90., 2, 180.

N, 1, 2.2286298461, 2, 90., 3, 180.

N, 1, 2.2789598555, 2, 90., 3, 90.

N, 1, 2.3202449428, 2, 90., 3, -90.

H, 2, 1.0221863213, 1, 112.22230275, 3, 223.49426626

H, 2, 1.0223562047, 1, 111.8622484, 3, 105.85354145

H, 2, 1.0218180033, 1, 116.66392317, 3, -15.64697026

H, 3, 1.0215784199, 1, 115.99569948, 2, 1.61642018

H, 3, 1.021370344, 1, 112.23907909, 2, 122.68064921

H, 3, 1.0219355197, 1, 111.60215044, 2, -119.10354552

C, 4, 1.4727036358, 1, 117.52363247, 3, 24.2182394

C, 4, 1.275949695, 1, 126.02316009, 3, 204.07467814

H, 15, 1.0940505808, 4, 122.79020236, 14, 0.71683646

H, 15, 1.0886573811, 4, 120.40794031, 14, 181.53214421

H, 14, 1.0952143456, 4, 112.407814, 15, -7.93615567

H, 14, 1.0950151766, 4, 109.11434803, 15, 112.16320819

H, 14, 1.0939809576, 4, 109.52210655, 15, -129.09331387

H, 5, 1.0222865102, 1, 110.38060153, 2, -54.50224095

H, 5, 1.0220018507, 1, 113.73948656, 2, 63.81666447

H, 5, 1.0206532761, 1, 115.84669011, 2, -173.41596908

C, 6, 1.4718309315, 1, 120.70414207, 2, -35.22193953

C, 6, 1.276922338, 1, 122.08757902, 2, 145.00490064

H, 25, 1.0939352276, 6, 122.68385326, 24, -0.12880028

H, 25, 1.0890605647, 6, 119.77860924, 24, 180.19261198

H, 24, 1.0951183628, 6, 112.30949882, 25, 5.39598009

H, 24, 1.0944217352, 6, 109.64543793, 25, 126.40186077

H, 24, 1.0947023983, 6, 109.57076216, 25, -115.19184781

C, 7, 1.4711702952, 1, 122.97107907, 2, -137.17289098

C, 7, 1.2766655955, 1, 120.32224335, 2, 43.68852151

H, 32, 1.0938225267, 7, 122.9400758, 31, 0.7819722

H, 32, 1.0902078287, 7, 120.06708854, 31, 180.98587137
H, 31, 1.0950783866, 7, 112.21123533, 32, -6.50137934
H, 31, 1.0933978466, 7, 109.01854692, 32, 114.14383787
H, 31, 1.0942791931, 7, 109.76786183, 32, -127.41503691

HF=-2350.6848635
RMSD=3.834e-10
Dipole=-0.1228006, 0.0223279, 0.7380986
PG=C01 [X(C6H24N6Zn1)]

ZnNIst2

2, 1
Zn
O, 1, 2.2813616209
N, 1, 2.1374123159, 2, 90.
N, 1, 2.3399186059, 3, 90., 2, 180.
N, 1, 2.181218696, 2, 90., 3, 180.
O, 1, 2.2807270984, 2, 90., 3, 90.
N, 1, 2.293418703, 2, 90., 3, -90.
H, 2, 0.9736884092, 1, 130.97482456, 3, -5.85841175
H, 2, 0.9737717502, 1, 121.64169799, 3, -168.78459624
H, 3, 1.0225990585, 1, 114.99280011, 2, 46.33872299
H, 3, 1.0203904953, 1, 112.24954558, 2, 166.67549256
H, 3, 1.0224468548, 1, 111.41493789, 2, -74.5015318
C, 4, 1.4737251407, 1, 121.36166483, 3, -2.5807896
C, 4, 1.277222627, 1, 122.38153411, 3, 175.53958192
H, 14, 1.0937455773, 4, 122.50146252, 13, -1.57757251
H, 14, 1.0868474732, 4, 120.05126423, 13, 178.44793197
H, 13, 1.0950573517, 4, 112.31112933, 14, 6.28671479
H, 13, 1.0942346166, 4, 109.9342315, 14, 126.9771068
H, 13, 1.0964262289, 4, 109.38470904, 14, -113.58881233
C, 5, 1.4742300484, 1, 120.94283352, 2, 93.91801668
C, 5, 1.2799652632, 1, 121.98914058, 2, -84.26213118
H, 21, 1.093269104, 5, 121.96356757, 20, 1.2043501
H, 21, 1.0865745686, 5, 119.6884568, 20, 180.78222839
H, 20, 1.0943821526, 5, 111.4461756, 21, -5.65142706
H, 20, 1.0925459175, 5, 109.35013667, 21, 115.0842733
H, 20, 1.0923261241, 5, 109.70068599, 21, -126.76119399
H, 6, 0.9735659537, 1, 127.48132716, 2, -14.42430135
H, 6, 0.9733182144, 1, 123.90588551, 2, 185.95183484
C, 7, 1.4721017139, 1, 121.5669719, 2, -184.35958277
C, 7, 1.2780168483, 1, 121.52287562, 2, -0.67349326
H, 30, 1.0938517109, 7, 122.39397313, 29, 0.94674555
H, 30, 1.0878626265, 7, 119.6913342, 29, 180.61054521
H, 29, 1.0949673459, 7, 111.98562445, 30, -4.37422902
H, 29, 1.0941033995, 7, 109.43167124, 30, 116.18306956
H, 29, 1.092557306, 7, 109.74392265, 30, -125.7230154

HF=-2390.4219702
RMSD=1.301e-09
Dipole=0.6132601, -1.0794477, 0.8974815
PG=C01 [X(C6H22N4O2Zn1)]

ZnNIST3

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1,1
Zn
N,1,2.2844324149
N,1,2.2104245983,2,90.
O,1,2.0400445179,3,90.,2,180.
N,1,2.2026823462,2,90.,3,180.
N,1,2.314103763,2,90.,3,90.
N,1,2.3459035821,2,90.,3,-90.
H,2,1.0204182342,1,116.3434121,3,214.69712301
H,2,1.0210952814,1,109.08667667,3,94.79719124
H,2,1.0201322774,1,112.09711674,3,-22.76966693
H,3,1.020900324,1,111.03814971,2,99.73078353
H,3,1.0390447075,1,97.63041354,2,210.23649954
H,3,1.0202814968,1,126.0560228,2,-30.76114288
C,4,1.2952703387,1,128.6974004,3,-34.38404821
H,14,1.105667774,4,114.08923242,1,188.20398973
O,14,1.2380614185,4,126.75699776,15,180.07538558
H,5,1.0202961841,1,114.32986053,2,-72.48741888
H,5,1.0196802334,1,118.82592358,2,55.47735735
H,5,1.0225600815,1,102.44537934,2,-186.89870823
C,6,1.4638290611,1,124.32364829,2,-6.18359127
C,6,1.2764980775,1,117.53570753,2,176.68167292
H,21,1.0957923528,6,122.14479204,20,0.052042
H,21,1.0885834028,6,118.71905982,20,180.39386403
H,20,1.0970767176,6,112.63394322,21,0.92231435
H,20,1.0956566254,6,109.40817419,21,121.94664764
H,20,1.0959372979,6,109.52019072,21,-120.03495471
C,7,1.4650390695,1,117.88951861,2,-131.67946192
C,7,1.2723939646,1,123.24611285,2,61.64017731
H,28,1.0947730563,7,122.95479491,27,0.14739501
H,28,1.0897821885,7,119.84919829,27,180.81757135
H,27,1.0965184242,7,112.49786868,28,2.62776433
H,27,1.0930634472,7,108.79383548,28,124.00272794
H,27,1.0960033424,7,109.20152576,28,-118.09623287

HF=-2406.256014
RMSD=2.764e-09
Dipole=-1.3384541,-0.7079984,2.9215976
PG=C01 [X(C5H20N5O2Zn1)]

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ZnNIST4

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1,1
Zn
O,1,2.1005550338
S,1,2.7884392032,2,90.
N,1,2.1419427368,3,90.,2,180.
O,1,2.0483241969,2,90.,3,180.
O,1,2.275652276,2,90.,3,90.
N,1,2.2277781553,2,90.,3,-90.
H,2,0.9705461677,1,127.22203423,3,-43.94365587
H,2,1.0312679133,1,101.53728323,3,-168.77839308
H,3,1.349906566,1,104.6956663,2,116.94024125
H,3,1.3488416533,1,102.87555698,2,214.65018774

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H, 4, 1.0214157752, 1, 113.63452577, 3, 72.84309743
H, 4, 1.0226789571, 1, 104.60430397, 3, 188.5406777
H, 4, 1.0188204547, 1, 116.97407739, 3, -52.69609427
C, 5, 1.2816824316, 1, 128.42333822, 2, -9.95926201
H, 15, 1.1016756118, 5, 115.65029181, 1, 177.7621724
O, 15, 1.2514156962, 5, 126.05829288, 16, 179.39579074
C, 6, 1.2230602313, 1, 127.95418031, 2, 54.38684708
H, 18, 1.1010387055, 6, 119.96608833, 1, 174.76860011
H, 18, 1.1006363715, 6, 121.5411447, 19, 179.76799675
C, 7, 1.4663415037, 1, 119.7003069, 2, -143.88818255
C, 7, 1.2754102763, 1, 120.89208142, 2, 23.45582206
H, 22, 1.0945220717, 7, 122.20163832, 21, -1.3820998
H, 22, 1.087675268, 7, 119.5382759, 21, 177.44209351
H, 21, 1.0961017051, 7, 112.10980723, 22, -2.4053076
H, 21, 1.0957643267, 7, 109.7047724, 22, 118.03891377
H, 21, 1.0940680582, 7, 108.63112368, 22, -123.41484564

HF=-2749.5096766

RMSD=1.257e-09

Dipole=1.4835323, -0.1729534, -1.6988723

PG=C01 [X(C4H15N2O4S1Zn1)]

ZnNIST5

1, 1

Zn

O, 1, 2.2753942907

O, 1, 2.1506152924, 2, 90.

O, 1, 2.0916542284, 3, 90., 2, 180.

N, 1, 2.228089933, 2, 90., 3, 180.

N, 1, 2.233216298, 2, 90., 3, 90.

N, 1, 2.2212263345, 2, 90., 3, -90.

H, 2, 0.9729602312, 1, 112.16865729, 3, -6.80686301

H, 2, 0.9719785926, 1, 115.61478673, 3, -246.06419016

H, 3, 0.9705707382, 1, 118.43936251, 2, 85.72796264

H, 3, 1.0330723046, 1, 97.43694776, 2, -161.76364113

C, 4, 1.2837071939, 1, 125.14944826, 3, -23.39579163

H, 12, 1.1030242588, 4, 115.62431868, 1, 190.23720759

O, 12, 1.2493937864, 4, 126.36133311, 13, 180.27015948

C, 5, 1.4648301164, 1, 122.25565863, 2, 4.79421932

C, 5, 1.2754220525, 1, 119.22790851, 2, -172.1882213

H, 16, 1.0951125816, 5, 121.87993726, 15, 0.14738443

H, 16, 1.0880358526, 5, 118.8937645, 15, 179.7497631

H, 15, 1.096531598, 5, 112.35556676, 16, 1.34137805

H, 15, 1.0940084324, 5, 109.29029594, 16, 122.94856457

H, 15, 1.0964812293, 5, 109.19328629, 16, -119.28821791

C, 6, 1.4664339913, 1, 121.99423945, 2, -2.30944573

C, 6, 1.2751863169, 1, 119.75349617, 2, -183.52228528

H, 23, 1.0948100034, 6, 121.90235038, 22, 0.05148818

H, 23, 1.0873219743, 6, 119.02051155, 22, 180.05030546

H, 22, 1.0964602584, 6, 112.28205752, 23, -1.34805213

H, 22, 1.0956507435, 6, 109.28667184, 23, 119.50746083

H, 22, 1.0935706499, 6, 109.29529017, 23, -123.0985196

C, 7, 1.4654687677, 1, 120.2559771, 2, -121.27358117

C, 7, 1.2759857504, 1, 120.63253081, 2, 70.26653624

H, 30, 1.0944975364, 7, 122.20123209, 29, 0.97097733

H, 30, 1.0882333729, 7, 119.61644432, 29, 182.32574445

H, 29, 1.0960977596, 7, 111.94502789, 30, -0.7837748
H, 29, 1.0934667473, 7, 108.69717189, 30, 120.28177774
H, 29, 1.0939933765, 7, 109.45380317, 30, -122.03589325

HF=-2523.4133954
RMSD=1.113e-09
Dipole=-1.3516994, -0.3372681, 1.9685181
PG=C01 [X(C7H20N3O4Zn1)]

ZnNIST6

O, 1
Zn
N, 1, 2.1883477314
O, 1, 2.1963639303, 2, 90.
O, 1, 2.0812749442, 3, 90., 2, 180.
O, 1, 2.1034539754, 2, 90., 3, 180.
O, 1, 2.199089824, 2, 90., 3, 90.
N, 1, 2.2431275537, 2, 90., 3, -90.
H, 2, 1.0190831789, 1, 115.5621522, 3, -14.96344912
H, 2, 1.0184908855, 1, 111.26121655, 3, 108.4424075
H, 2, 1.0232381479, 1, 105.8404396, 3, -134.75467573
H, 3, 0.9711239377, 1, 108.28761455, 2, 81.6646543
H, 3, 1.0230466135, 1, 97.80392418, 2, -168.95716576
C, 4, 1.2742346969, 1, 127.82099865, 3, -14.12880404
H, 13, 1.1061231295, 4, 115.29564313, 1, 185.68264568
O, 13, 1.2552825679, 4, 127.37705979, 14, 179.99772
C, 5, 1.2712303373, 1, 122.3007382, 2, -55.12433709
H, 16, 1.1066890479, 5, 115.686955, 1, 174.24881814
O, 16, 1.2592114638, 5, 126.78984261, 17, 180.17200808
H, 6, 1.0059996638, 1, 95.59832954, 2, 61.71032057
H, 6, 0.971896069, 1, 103.7317423, 2, 169.88928881
C, 7, 1.4601768951, 1, 116.99232253, 2, -114.11575284
C, 7, 1.2720103352, 1, 122.86053587, 2, 74.62011213
H, 22, 1.096784703, 7, 122.27117519, 21, 1.10542599
H, 22, 1.0890834513, 7, 119.22225123, 21, 182.20151921
H, 21, 1.0987826115, 7, 112.20757437, 22, -1.38175132
H, 21, 1.0939786114, 7, 108.13863684, 22, 120.4332478
H, 21, 1.0932250816, 7, 108.90709937, 22, -123.99727428

HF=-2501.4735511
RMSD=1.090e-09
Dipole=0.3740413, 1.4296997, 1.5120943
PG=C01 [X(C4H14N2O6Zn1)]

ZnNIST7

O, 1
Zn
N, 1, 2.1912736665
O, 1, 2.1893010267, 2, 90.
O, 1, 2.0731904839, 3, 90., 2, 180.
N, 1, 2.2070313326, 2, 90., 3, 180.

O,1,2.1006803109,2,90.,3,90.
N,1,2.3824941935,2,90.,3,-90.
H,2,1.0289812804,1,100.93861993,3,-125.72297767
H,2,1.0184998023,1,118.8740048,3,-244.72562218
H,2,1.0193666944,1,111.78985893,3,-10.53215645
H,3,0.9727290768,1,102.24011537,2,81.683871
H,3,1.0178042998,1,98.41575201,2,-171.58021223
C,4,1.2723460186,1,129.29559016,3,-4.45491891
H,13,1.1060773352,4,115.34101058,1,173.68242238
O,13,1.2552852224,4,127.15300857,14,179.45785389
H,5,1.0177780128,1,127.55451684,2,69.26807101
H,5,1.0210201174,1,102.7068079,2,193.20851145
H,5,1.027712636,1,101.29207317,2,-55.24041314
C,6,1.2762623567,1,123.9387555,2,44.96125971
H,19,1.1081248613,6,115.04782625,1,178.95271958
O,19,1.254786655,6,126.90331622,20,180.24079754
C,7,1.4609659011,1,115.43336081,2,-244.03545366
C,7,1.2693586669,1,126.12677613,2,-65.86852803
H,23,1.0971288227,7,122.89262562,22,0.54298214
H,23,1.089784922,7,119.77638238,22,180.59388516
H,22,1.0990726305,7,112.51641284,23,-1.30804604
H,22,1.094411136,7,108.43090638,23,120.46210531
H,22,1.0934022655,7,108.87930888,23,-123.58816988

HF=-2481.5911349

RMSD=3.222e-09

Dipole=-0.9809751,2.3592234,1.3921792

PG=C01 [X(C4H15N3O5Zn1)]

ZnNIST8

O,1

Zn

O,1,2.2650061669

O,1,2.3917443525,2,90.

N,1,2.2768954239,3,90.,2,180.

N,1,2.2166604002,2,90.,3,180.

O,1,1.9354591399,2,90.,3,90.

O,1,2.0510886244,2,90.,3,-90.

H,2,0.982145268,1,98.03740504,3,41.23140709

H,2,0.9730373887,1,95.55627717,3,291.16967905

H,3,0.9693822146,1,109.05225919,2,56.26983926

H,3,0.9893673701,1,92.40867582,2,-52.33589396

H,4,1.0185722936,1,104.27730482,3,114.08554484

H,4,1.0186795601,1,120.12431911,3,-122.86529826

H,4,1.0196908848,1,107.16574374,3,0.09642521

H,5,1.0173850687,1,118.93736461,2,140.77093849

H,5,1.0191144034,1,109.57910585,2,16.1650075

H,5,1.0202152198,1,102.53365938,2,-98.35376445

H,6,0.9678702191,1,116.01791444,2,-116.07779375

C,7,1.2737951297,1,119.27103665,2,-314.62134876

H,19,1.105663528,7,115.51957561,1,-176.02088516

O,19,1.2588997249,7,126.63707658,20,179.96043374

HF=-2310.6576675

RMSD=6.365e-09

Dipole=-0.7500728,-0.2081448,-1.1130858

PG=C01 [X(C1H12N2O5Zn1)]

ZnNIST9

-1,1
Zn
O,1,2.2047794303
O,1,2.1807828988,2,90.
O,1,2.1151556183,3,90.,2,180.
O,1,2.1290582544,2,90.,3,180.
O,1,2.1722435782,2,90.,3,90.
O,1,2.1056807225,2,90.,3,-90.
H,2,0.971751819,1,99.52841139,3,104.51642737
H,2,0.9988187748,1,94.29456214,3,211.68565945
H,3,1.0091085906,1,98.68960825,2,-94.09939069
H,3,0.9709922327,1,101.38789902,2,-201.97750436
C,4,1.2687838319,1,127.01843031,3,111.33200025
H,12,1.1113353908,4,114.97633126,1,165.77026947
O,12,1.2568272029,4,128.2325859,13,179.4719588
C,5,1.2628682811,1,120.82600369,2,-40.62039042
H,15,1.1103201205,5,115.80738502,1,188.1673724
O,15,1.2654293763,5,127.21421399,16,179.78233688
H,6,0.9755820852,1,102.4577341,2,53.67963108
H,6,1.0080654616,1,98.4646123,2,163.90836736
C,7,1.2686873251,1,129.00837508,2,-260.68082653
H,20,1.1112170075,7,114.90604985,1,-189.63994372
O,20,1.2562651997,7,128.27473249,21,179.68083534

HF=-2576.6877223
RMSD=7.442e-09
Dipole=-0.275339,0.3072265,0.3429093
PG=C01 [X(C3H9O9Zn1)]

ZnNIST10

-1,1
Zn
S,1,3.1748589582
N,1,2.205374015,2,90.
O,1,1.9848737912,3,90.,2,180.
O,1,2.1491404684,2,90.,3,180.
N,1,2.1709906538,2,90.,3,90.
O,1,2.1252327102,2,90.,3,-90.
H,2,1.3713708366,1,68.98737662,3,60.13152301
H,2,1.3499595351,1,68.87600307,3,163.38684742
H,3,1.0164938269,1,125.54886593,2,73.55205756
H,3,1.0226217719,1,91.87096883,2,190.06213232
H,3,1.0221441382,1,107.23171868,2,-58.23756144
H,4,0.9678967352,1,105.45799613,3,-135.33034611
C,5,1.2699185166,1,131.60725745,2,-80.06634025
H,14,1.1160536964,5,114.15912931,1,192.02989006
O,14,1.2545011961,5,129.03165872,15,179.64749292
H,6,1.0334213139,1,103.76270075,2,73.09849173

H, 6, 1.021730479, 1, 95.44332656, 2, 183.37055709
H, 6, 1.0171525222, 1, 126.67645371, 2, -56.00776351
C, 7, 1.2658924071, 1, 125.4355857, 2, 46.92957952
H, 20, 1.1138172356, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282004, 7, 128.02959413, 21, 180.64311568

HF=-2746.4578078

RMSD=6.969e-09

Dipole=1.7135546, -0.6576052, 0.6232451

PG=C01 [X(C2H11N2O5S1Zn1)]

CdNIST1

2, 1

Cd

N, 1, 2.4725278052

N, 1, 2.4499865956, 2, 90.

N, 1, 2.4979317898, 3, 90., 2, 180.

N, 1, 2.4529453766, 2, 90., 3, 180.

N, 1, 2.4662031512, 2, 90., 3, 90.

N, 1, 2.4856508653, 2, 90., 3, -90.

H, 2, 1.02218632, 1, 112.22230275, 3, 223.49426626

H, 2, 1.0223562, 1, 111.8622484, 3, 105.85354145

H, 2, 1.021818, 1, 116.66392317, 3, -15.64697026

H, 3, 1.02157842, 1, 115.99569948, 2, 1.61642018

H, 3, 1.02137034, 1, 112.23907909, 2, 122.68064921

H, 3, 1.02193552, 1, 111.60215044, 2, -119.10354552

C, 4, 1.47270364, 1, 117.52363247, 3, 24.2182394

C, 4, 1.27594969, 1, 126.02316009, 3, 204.07467814

H, 15, 1.09405058, 4, 122.79020236, 14, 0.71683646

H, 15, 1.08865738, 4, 120.40794031, 14, 181.53214421

H, 14, 1.09521435, 4, 112.407814, 15, -7.93615567

H, 14, 1.09501518, 4, 109.11434803, 15, 112.16320819

H, 14, 1.09398096, 4, 109.52210655, 15, -129.09331387

H, 5, 1.02228651, 1, 110.38060153, 2, -54.50224095

H, 5, 1.02200185, 1, 113.73948656, 2, 63.81666447

H, 5, 1.02065328, 1, 115.84669011, 2, -173.41596908

C, 6, 1.47183093, 1, 120.70414207, 2, -35.22193953

C, 6, 1.27692234, 1, 122.08757902, 2, 145.00490064

H, 25, 1.09393523, 6, 122.68385326, 24, -0.12880028

H, 25, 1.08906056, 6, 119.77860924, 24, 180.19261198

H, 24, 1.09511836, 6, 112.30949882, 25, 5.39598009

H, 24, 1.09442174, 6, 109.64543793, 25, 126.40186077

H, 24, 1.0947024, 6, 109.57076216, 25, -115.19184781

C, 7, 1.4711703, 1, 122.97107907, 2, -137.17289098

C, 7, 1.2766656, 1, 120.32224335, 2, 43.68852151

H, 32, 1.09382253, 7, 122.9400758, 31, 0.7819722

H, 32, 1.09020783, 7, 120.06708854, 31, 180.98587137

H, 31, 1.09507839, 7, 112.21123533, 32, -6.50137934

H, 31, 1.09339785, 7, 109.01854692, 32, 114.14383787

H, 31, 1.09427919, 7, 109.76786183, 32, -127.41503691

HF=-738.2470472

RMSD=4.487e-09

Dipole=-0.1145901, 0.0327097, 0.6545928

PG=C01 [X(C6H24Cd1N6)]

CdNIST2

2,1

Cd

O,1,2.461149771

N,1,2.3745925127,2,90.

N,1,2.4844841942,3,90.,2,180.

N,1,2.380002092,2,90.,3,180.

O,1,2.4539073821,2,90.,3,90.

N,1,2.4561845968,2,90.,3,-90.

H,2,0.97368841,1,130.97482456,3,-5.85841175

H,2,0.97377175,1,121.64169799,3,-168.78459624

H,3,1.02259906,1,114.99280011,2,46.33872299

H,3,1.0203905,1,112.24954558,2,166.67549256

H,3,1.02244685,1,111.41493789,2,-74.5015318

C,4,1.47372514,1,121.36166483,3,-2.5807896

C,4,1.27722263,1,122.38153411,3,175.53958192

H,14,1.09374558,4,122.50146252,13,-1.57757251

H,14,1.08684747,4,120.05126423,13,178.44793197

H,13,1.09505735,4,112.31112933,14,6.28671479

H,13,1.09423462,4,109.9342315,14,126.9771068

H,13,1.09642623,4,109.38470904,14,-113.58881233

C,5,1.47423005,1,120.94283352,2,93.91801668

C,5,1.27996526,1,121.98914058,2,-84.26213118

H,21,1.0932691,5,121.96356757,20,1.2043501

H,21,1.08657457,5,119.6884568,20,180.78222839

H,20,1.09438215,5,111.4461756,21,-5.65142706

H,20,1.09254592,5,109.35013667,21,115.0842733

H,20,1.09232612,5,109.70068599,21,-126.76119399

H,6,0.97356595,1,127.48132716,2,-14.42430135

H,6,0.97331821,1,123.90588551,2,185.95183484

C,7,1.47210171,1,121.5669719,2,-184.35958277

C,7,1.27801685,1,121.52287562,2,-0.67349326

H,30,1.09385171,7,122.39397313,29,0.94674555

H,30,1.08786263,7,119.6913342,29,180.61054521

H,29,1.09496735,7,111.98562445,30,-4.37422902

H,29,1.0941034,7,109.43167124,30,116.18306956

H,29,1.09255731,7,109.74392265,30,-125.7230154

HF=-777.9847271

RMSD=8.131e-09

Dipole=0.5534473,-0.9254691,0.7530846

PG=C01 [X(C6H22Cd1N4O2)]

CdNIST3

1,1

Cd

N,1,2.4825819807

N,1,2.4214851933,2,90.

O,1,2.1996816639,3,90.,2,180.

N,1,2.4351976781,2,90.,3,180.

N,1,2.4862157433,2,90.,3,90.

N, 1, 2.5222162597, 2, 90., 3, -90.
 H, 2, 1.02041823, 1, 116.3434121, 3, 214.69712301
 H, 2, 1.02109528, 1, 109.08667667, 3, 94.79719124
 H, 2, 1.02013228, 1, 112.09711674, 3, -22.76966693
 H, 3, 1.02090032, 1, 111.03814971, 2, 99.73078353
 H, 3, 1.03904471, 1, 97.63041354, 2, 210.23649954
 H, 3, 1.0202815, 1, 126.0560228, 2, -30.76114288
 C, 4, 1.29527034, 1, 128.6974004, 3, -34.38404821
 H, 14, 1.10566777, 4, 114.08923242, 1, 188.20398973
 O, 14, 1.23806142, 4, 126.75699776, 15, 180.07538558
 H, 5, 1.02029618, 1, 114.32986053, 2, -72.48741888
 H, 5, 1.01968023, 1, 118.82592358, 2, 55.47735735
 H, 5, 1.02256008, 1, 102.44537934, 2, -186.89870823
 C, 6, 1.46382906, 1, 124.32364829, 2, -6.18359127
 C, 6, 1.27649808, 1, 117.53570753, 2, 176.68167292
 H, 21, 1.09579235, 6, 122.14479204, 20, 0.052042
 H, 21, 1.0885834, 6, 118.71905982, 20, 180.39386403
 H, 20, 1.09707672, 6, 112.63394322, 21, 0.92231435
 H, 20, 1.09565663, 6, 109.40817419, 21, 121.94664764
 H, 20, 1.0959373, 6, 109.52019072, 21, -120.03495471
 C, 7, 1.46503907, 1, 117.88951861, 2, -131.67946192
 C, 7, 1.27239396, 1, 123.24611285, 2, 61.64017731
 H, 28, 1.09477306, 7, 122.95479491, 27, 0.14739501
 H, 28, 1.08978219, 7, 119.84919829, 27, 180.81757135
 H, 27, 1.09651842, 7, 112.49786868, 28, 2.62776433
 H, 27, 1.09306345, 7, 108.79383548, 28, 124.00272794
 H, 27, 1.09600334, 7, 109.20152576, 28, -118.09623287

HF=-793.8080369

RMSD=8.586e-09

Dipole=-1.3159516, -0.7354605, 3.2092725

PG=C01 [X(C5H20Cd1N5O2)]

CdNIST4

1, 1

Cd

O, 1, 2.3123657906

S, 1, 2.89835146, 2, 90.

N, 1, 2.3861800418, 3, 90., 2, 180.

O, 1, 2.1855103204, 2, 90., 3, 180.

O, 1, 2.4776320288, 2, 90., 3, 90.

N, 1, 2.4252468556, 2, 90., 3, -90.

H, 2, 0.97054617, 1, 127.22203423, 3, -43.94365587

H, 2, 1.03126791, 1, 101.53728323, 3, -168.77839308

H, 3, 1.34990657, 1, 104.6956663, 2, 116.94024125

H, 3, 1.34884165, 1, 102.87555698, 2, 214.65018774

H, 4, 1.02141578, 1, 113.63452577, 3, 72.84309743

H, 4, 1.02267896, 1, 104.60430397, 3, 188.5406777

H, 4, 1.01882045, 1, 116.97407739, 3, -52.69609427

C, 5, 1.28168243, 1, 128.42333822, 2, -9.95926201

H, 15, 1.10167561, 5, 115.65029181, 1, 177.7621724

O, 15, 1.2514157, 5, 126.05829288, 16, 179.39579074

C, 6, 1.22306023, 1, 127.95418031, 2, 54.38684708

H, 18, 1.10103871, 6, 119.96608833, 1, 174.76860011

H, 18, 1.10063637, 6, 121.5411447, 19, 179.76799675

C, 7, 1.4663415, 1, 119.7003069, 2, -143.88818255

C, 7, 1.27541028, 1, 120.89208142, 2, 23.45582206
H, 22, 1.09452207, 7, 122.20163832, 21, -1.3820998
H, 22, 1.08767527, 7, 119.5382759, 21, 177.44209351
H, 21, 1.09610171, 7, 112.10980723, 22, -2.4053076
H, 21, 1.09576433, 7, 109.7047724, 22, 118.03891377
H, 21, 1.09406806, 7, 108.63112368, 22, -123.41484564

HF=-1137.0605046

RMSD=7.424e-09

Dipole=1.8254639, -0.1138156, -1.7389804

PG=C01 [X(C4H15Cd1N2O4S1)]

CdNIST5

1, 1

Cd

O, 1, 2.4766163954

O, 1, 2.3469895274, 2, 90.

O, 1, 2.2228539415, 3, 90., 2, 180.

N, 1, 2.4222666886, 2, 90., 3, 180.

N, 1, 2.4231017196, 2, 90., 3, 90.

N, 1, 2.4223629355, 2, 90., 3, -90.

H, 2, 0.97296023, 1, 112.16865729, 3, -6.80686301

H, 2, 0.97197859, 1, 115.61478673, 3, -246.06419016

H, 3, 0.97057074, 1, 118.43936251, 2, 85.72796264

H, 3, 1.0330723, 1, 97.43694776, 2, -161.76364113

C, 4, 1.28370719, 1, 125.14944826, 3, -23.39579163

H, 12, 1.10302426, 4, 115.62431868, 1, 190.23720759

O, 12, 1.24939379, 4, 126.36133311, 13, 180.27015948

C, 5, 1.46483012, 1, 122.25565863, 2, 4.79421932

C, 5, 1.27542205, 1, 119.22790851, 2, -172.1882213

H, 16, 1.09511258, 5, 121.87993726, 15, 0.14738443

H, 16, 1.08803585, 5, 118.8937645, 15, 179.7497631

H, 15, 1.0965316, 5, 112.35556676, 16, 1.34137805

H, 15, 1.09400843, 5, 109.29029594, 16, 122.94856457

H, 15, 1.09648123, 5, 109.19328629, 16, -119.28821791

C, 6, 1.46643399, 1, 121.99423945, 2, -2.30944573

C, 6, 1.27518632, 1, 119.75349617, 2, -183.52228528

H, 23, 1.09481, 6, 121.90235038, 22, 0.05148818

H, 23, 1.08732197, 6, 119.02051155, 22, 180.05030546

H, 22, 1.09646026, 6, 112.28205752, 23, -1.34805213

H, 22, 1.09565074, 6, 109.28667184, 23, 119.50746083

H, 22, 1.09357065, 6, 109.29529017, 23, -123.0985196

C, 7, 1.46546877, 1, 120.2559771, 2, -121.27358117

C, 7, 1.27598575, 1, 120.63253081, 2, 70.26653624

H, 30, 1.09449754, 7, 122.20123209, 29, 0.97097733

H, 30, 1.08823337, 7, 119.61644432, 29, 182.32574445

H, 29, 1.09609776, 7, 111.94502789, 30, -0.7837748

H, 29, 1.09346675, 7, 108.69717189, 30, 120.28177774

H, 29, 1.09399338, 7, 109.45380317, 30, -122.03589325

HF=-910.9636744

RMSD=5.241e-09

Dipole=-1.4236092, -0.3644657, 2.2083123

PG=C01 [X(C7H20Cd1N3O4)]

CdNIST6

0,1
Cd
N,1,2.4015559931
O,1,2.3882184555,2,90.
O,1,2.2216847424,3,90.,2,180.
O,1,2.2482108821,2,90.,3,180.
O,1,2.4069308172,2,90.,3,90.
N,1,2.4531261056,2,90.,3,-90.
H,2,1.01908318,1,115.5621522,3,-14.96344912
H,2,1.01849089,1,111.26121655,3,108.4424075
H,2,1.02323815,1,105.8404396,3,-134.75467573
H,3,0.97112394,1,108.28761455,2,81.6646543
H,3,1.02304661,1,97.80392418,2,-168.95716576
C,4,1.2742347,1,127.82099865,3,-14.12880404
H,13,1.10612313,4,115.29564313,1,185.68264568
O,13,1.25528257,4,127.37705979,14,179.99772
C,5,1.27123034,1,122.3007382,2,-55.12433709
H,16,1.10668905,5,115.686955,1,174.24881814
O,16,1.25921146,5,126.78984261,17,180.17200808
H,6,1.00599966,1,95.59832954,2,61.71032057
H,6,0.97189607,1,103.7317423,2,169.88928881
C,7,1.4601769,1,116.99232253,2,-114.11575284
C,7,1.27201034,1,122.86053587,2,74.62011213
H,22,1.0967847,7,122.27117519,21,1.10542599
H,22,1.08908345,7,119.22225123,21,182.20151921
H,21,1.09878261,7,112.20757437,22,-1.38175132
H,21,1.09397861,7,108.13863684,22,120.4332478
H,21,1.09322508,7,108.90709937,22,-123.99727428

HF=-889.0172028
RMSD=7.611e-09
Dipole=0.6169326,1.4571188,1.7857217
PG=C01 [X(C4H14Cd1N2O6)]

CdNIST7

0,1
Cd
N,1,2.4025846218
O,1,2.3991801821,2,90.
O,1,2.2185786216,3,90.,2,180.
N,1,2.430174951,2,90.,3,180.
O,1,2.2545995499,2,90.,3,90.
N,1,2.5385374658,2,90.,3,-90.
H,2,1.02898128,1,100.93861993,3,-125.72297767
H,2,1.0184998,1,118.8740048,3,-244.72562218
H,2,1.01936669,1,111.78985893,3,-10.53215645
H,3,0.97272908,1,102.24011537,2,81.683871
H,3,1.0178043,1,98.41575201,2,-171.58021223
C,4,1.27234602,1,129.29559016,3,-4.45491891
H,13,1.10607734,4,115.34101058,1,173.68242238
O,13,1.25528522,4,127.15300857,14,179.45785389

H, 5, 1.01777801, 1, 127.55451684, 2, 69.26807101
H, 5, 1.02102012, 1, 102.7068079, 2, 193.20851145
H, 5, 1.02771264, 1, 101.29207317, 2, -55.24041314
C, 6, 1.27626236, 1, 123.9387555, 2, 44.96125971
H, 19, 1.10812486, 6, 115.04782625, 1, 178.95271958
O, 19, 1.25478665, 6, 126.90331622, 20, 180.24079754
C, 7, 1.4609659, 1, 115.43336081, 2, -244.03545366
C, 7, 1.26935867, 1, 126.12677613, 2, -65.86852803
H, 23, 1.09712882, 7, 122.89262562, 22, 0.54298214
H, 23, 1.08978492, 7, 119.77638238, 22, 180.59388516
H, 22, 1.09907263, 7, 112.51641284, 23, -1.30804604
H, 22, 1.09441114, 7, 108.43090638, 23, 120.46210531
H, 22, 1.09340227, 7, 108.87930888, 23, -123.58816988

HF=-869.13703
RMSD=6.698e-09
Dipole=-1.024978, 2.6704468, 1.7038099
PG=C01 [X(C4H15Cd1N3O5)]

CdNIST8

O, 1
Cd
O, 1, 2.4803591166
O, 1, 2.5608829137, 2, 90.
N, 1, 2.4921975051, 3, 90., 2, 180.
N, 1, 2.4427245004, 2, 90., 3, 180.
O, 1, 2.1287328465, 2, 90., 3, 90.
O, 1, 2.2054668765, 2, 90., 3, -90.
H, 2, 0.98214527, 1, 98.03740504, 3, 41.23140709
H, 2, 0.97303739, 1, 95.55627717, 3, 291.16967905
H, 3, 0.96938221, 1, 109.05225919, 2, 56.26983926
H, 3, 0.98936737, 1, 92.40867582, 2, -52.33589396
H, 4, 1.01857229, 1, 104.27730482, 3, 114.08554484
H, 4, 1.01867956, 1, 120.12431911, 3, -122.86529826
H, 4, 1.01969088, 1, 107.16574374, 3, 0.09642521
H, 5, 1.01738507, 1, 118.93736461, 2, 140.77093849
H, 5, 1.0191144, 1, 109.57910585, 2, 16.1650075
H, 5, 1.02021522, 1, 102.53365938, 2, -98.35376445
H, 6, 0.96787022, 1, 116.01791444, 2, -116.07779375
C, 7, 1.27379513, 1, 119.27103665, 2, -314.62134876
H, 19, 1.10566353, 7, 115.51957561, 1, -176.02088516
O, 19, 1.25889972, 7, 126.63707658, 20, 179.96043374

HF=-698.2001821
RMSD=4.942e-09
Dipole=-0.7852415, -0.2663382, -1.137117
PG=C01 [X(C1H12Cd1N2O5)]

CdNIST9

-1, 1
Cd

O,1,2.4179092972
O,1,2.3886287031,2,90.
O,1,2.2606850823,3,90.,2,180.
O,1,2.2786950032,2,90.,3,180.
O,1,2.3722297433,2,90.,3,90.
O,1,2.2514604968,2,90.,3,-90.
H,2,0.97175182,1,99.52841139,3,104.51642737
H,2,0.99881877,1,94.29456214,3,211.68565945
H,3,1.00910859,1,98.68960825,2,-94.09939069
H,3,0.97099223,1,101.38789902,2,-201.97750436
C,4,1.26878383,1,127.01843031,3,111.33200025
H,12,1.11133539,4,114.97633126,1,165.77026947
O,12,1.2568272,4,128.2325859,13,179.4719588
C,5,1.26286828,1,120.82600369,2,-40.62039042
H,15,1.11032012,5,115.80738502,1,188.1673724
O,15,1.26542938,5,127.21421399,16,179.78233688
H,6,0.97558209,1,102.4577341,2,53.67963108
H,6,1.00806546,1,98.4646123,2,163.90836736
C,7,1.26868733,1,129.00837508,2,-260.68082653
H,20,1.11121701,7,114.90604985,1,-189.63994372
O,20,1.2562652,7,128.27473249,21,179.68083534

HF=-964.2331058
RMSD=7.570e-09
Dipole=0.0123332,0.0911708,0.631638
PG=C01 [X(C3H9Cd109)]

CdNIST10

-1,1
Cd
S,1,3.1841635439
N,1,2.431745547,2,90.
O,1,2.1847867053,3,90.,2,180.
O,1,2.3095119282,2,90.,3,180.
N,1,2.3918279318,2,90.,3,90.
O,1,2.3034110813,2,90.,3,-90.
H,2,1.37137084,1,68.98737662,3,60.13152301
H,2,1.34995954,1,68.87600307,3,163.38684742
H,3,1.01649383,1,125.54886593,2,73.55205756
H,3,1.02262177,1,91.87096883,2,190.06213232
H,3,1.02214414,1,107.23171868,2,-58.23756144
H,4,0.96789674,1,105.45799613,3,-135.33034611
C,5,1.26991852,1,131.60725745,2,-80.06634025
H,14,1.1160537,5,114.15912931,1,192.02989006
O,14,1.2545012,5,129.03165872,15,179.64749292
H,6,1.03342131,1,103.76270075,2,73.09849173
H,6,1.02173048,1,95.44332656,2,183.37055709
H,6,1.01715252,1,126.67645371,2,-56.00776351
C,7,1.26589241,1,125.4355857,2,46.92957952
H,20,1.11381724,7,114.91970239,1,-188.27084693
O,20,1.2603282,7,128.02959413,21,180.64311568

HF=-1134.0048892
RMSD=5.884e-09
Dipole=2.0280847,-1.003025,0.8479618
PG=C01 [X(C2H11Cd1N205S1)]

HgNIST1

2,1

Hg

N,1,2.5489794853
 N,1,2.5123386548,2,90.
 N,1,2.562410056,3,90.,2,180.
 N,1,2.518028366,2,90.,3,180.
 N,1,2.5118971617,2,90.,3,90.
 N,1,2.5312812884,2,90.,3,-90.
 H,2,1.02218632,1,112.22230275,3,223.49426626
 H,2,1.0223562,1,111.8622484,3,105.85354145
 H,2,1.021818,1,116.66392317,3,-15.64697026
 H,3,1.02157842,1,115.99569948,2,1.61642018
 H,3,1.02137034,1,112.23907909,2,122.68064921
 H,3,1.02193552,1,111.60215044,2,-119.10354552
 C,4,1.47270364,1,117.52363247,3,24.2182394
 C,4,1.27594969,1,126.02316009,3,204.07467814
 H,15,1.09405058,4,122.79020236,14,0.71683646
 H,15,1.08865738,4,120.40794031,14,181.53214421
 H,14,1.09521435,4,112.407814,15,-7.93615567
 H,14,1.09501518,4,109.11434803,15,112.16320819
 H,14,1.09398096,4,109.52210655,15,-129.09331387
 H,5,1.02228651,1,110.38060153,2,-54.50224095
 H,5,1.02200185,1,113.73948656,2,63.81666447
 H,5,1.02065328,1,115.84669011,2,-173.41596908
 C,6,1.47183093,1,120.70414207,2,-35.22193953
 C,6,1.27692234,1,122.08757902,2,145.00490064
 H,25,1.09393523,6,122.68385326,24,-0.12880028
 H,25,1.08906056,6,119.77860924,24,180.19261198
 H,24,1.09511836,6,112.30949882,25,5.39598009
 H,24,1.09442174,6,109.64543793,25,126.40186077
 H,24,1.0947024,6,109.57076216,25,-115.19184781
 C,7,1.4711703,1,122.97107907,2,-137.17289098
 C,7,1.2766656,1,120.32224335,2,43.68852151
 H,32,1.09382253,7,122.9400758,31,0.7819722
 H,32,1.09020783,7,120.06708854,31,180.98587137
 H,31,1.09507839,7,112.21123533,32,-6.50137934
 H,31,1.09339785,7,109.01854692,32,114.14383787
 H,31,1.09427919,7,109.76786183,32,-127.41503691

HF=-725.0500509

RMSD=3.638e-09

Dipole=-0.0977244,0.0225736,0.4587859

PG=C01 [X(C6H24Hg1N6)]

HgNIST2

2,1

Hg

O,1,2.6657938161
 N,1,2.3078777723,2,90.

N,1,2.61891271,3,90.,2,180.
 N,1,2.3040852603,2,90.,3,180.
 O,1,2.6555816966,2,90.,3,90.
 N,1,2.5723672567,2,90.,3,-90.
 H,2,0.97368841,1,130.97482456,3,-5.85841175
 H,2,0.97377175,1,121.64169799,3,-168.78459624
 H,3,1.02259906,1,114.99280011,2,46.33872299
 H,3,1.0203905,1,112.24954558,2,166.67549256
 H,3,1.02244685,1,111.41493789,2,-74.5015318
 C,4,1.47372514,1,121.36166483,3,-2.5807896
 C,4,1.27722263,1,122.38153411,3,175.53958192
 H,14,1.09374558,4,122.50146252,13,-1.57757251
 H,14,1.08684747,4,120.05126423,13,178.44793197
 H,13,1.09505735,4,112.31112933,14,6.28671479
 H,13,1.09423462,4,109.9342315,14,126.9771068
 H,13,1.09642623,4,109.38470904,14,-113.58881233
 C,5,1.47423005,1,120.94283352,2,93.91801668
 C,5,1.27996526,1,121.98914058,2,-84.26213118
 H,21,1.0932691,5,121.96356757,20,1.2043501
 H,21,1.08657457,5,119.6884568,20,180.78222839
 H,20,1.09438215,5,111.4461756,21,-5.65142706
 H,20,1.09254592,5,109.35013667,21,115.0842733
 H,20,1.09232612,5,109.70068599,21,-126.76119399
 H,6,0.97356595,1,127.48132716,2,-14.42430135
 H,6,0.97331821,1,123.90588551,2,185.95183484
 C,7,1.47210171,1,121.5669719,2,-184.35958277
 C,7,1.27801685,1,121.52287562,2,-0.67349326
 H,30,1.09385171,7,122.39397313,29,0.94674555
 H,30,1.08786263,7,119.6913342,29,180.61054521
 H,29,1.09496735,7,111.98562445,30,-4.37422902
 H,29,1.0941034,7,109.43167124,30,116.18306956
 H,29,1.09255731,7,109.74392265,30,-125.7230154

HF=-764.7893765

RMSD=4.738e-09

Dipole=0.2871052,-0.6427769,0.459231

PG=C01 [X(C6H22Hg1N4O2)]

HgNIST3

1,1

Hg

N,1,2.5093598169

N,1,2.4842893745,2,90.

O,1,2.2376891365,3,90.,2,180.

N,1,2.5007326114,2,90.,3,180.

N,1,2.5903445492,2,90.,3,90.

N,1,2.6336103252,2,90.,3,-90.

H,2,1.02041823,1,116.3434121,3,214.69712301

H,2,1.02109528,1,109.08667667,3,94.79719124

H,2,1.02013228,1,112.09711674,3,-22.76966693

H,3,1.02090032,1,111.03814971,2,99.73078353

H,3,1.03904471,1,97.63041354,2,210.23649954

H,3,1.0202815,1,126.0560228,2,-30.76114288

C,4,1.29527034,1,128.6974004,3,-34.38404821

H,14,1.10566777,4,114.08923242,1,188.20398973

O,14,1.23806142,4,126.75699776,15,180.07538558

H, 5, 1.02029618, 1, 114.32986053, 2, -72.48741888
H, 5, 1.01968023, 1, 118.82592358, 2, 55.47735735
H, 5, 1.02256008, 1, 102.44537934, 2, -186.89870823
C, 6, 1.46382906, 1, 124.32364829, 2, -6.18359127
C, 6, 1.27649808, 1, 117.53570753, 2, 176.68167292
H, 21, 1.09579235, 6, 122.14479204, 20, 0.052042
H, 21, 1.0885834, 6, 118.71905982, 20, 180.39386403
H, 20, 1.09707672, 6, 112.63394322, 21, 0.92231435
H, 20, 1.09565663, 6, 109.40817419, 21, 121.94664764
H, 20, 1.0959373, 6, 109.52019072, 21, -120.03495471
C, 7, 1.46503907, 1, 117.88951861, 2, -131.67946192
C, 7, 1.27239396, 1, 123.24611285, 2, 61.64017731
H, 28, 1.09477306, 7, 122.95479491, 27, 0.14739501
H, 28, 1.08978219, 7, 119.84919829, 27, 180.81757135
H, 27, 1.09651842, 7, 112.49786868, 28, 2.62776433
H, 27, 1.09306345, 7, 108.79383548, 28, 124.00272794
H, 27, 1.09600334, 7, 109.20152576, 28, -118.09623287

HF=-780.6070498

RMSD=7.765e-09

Dipole=-1.2311256, -0.7116754, 3.0961472

PG=C01 [X(C5H20Hg1N5O2)]

HgNISt4

1, 1

Hg

O, 1, 2.3994779429

S, 1, 2.8716490148, 2, 90.

N, 1, 2.4551267705, 3, 90., 2, 180.

O, 1, 2.2204989006, 2, 90., 3, 180.

O, 1, 2.6336697141, 2, 90., 3, 90.

N, 1, 2.5142258497, 2, 90., 3, -90.

H, 2, 0.97054617, 1, 127.22203423, 3, -43.94365587

H, 2, 1.03126791, 1, 101.53728323, 3, -168.77839308

H, 3, 1.34990657, 1, 104.6956663, 2, 116.94024125

H, 3, 1.34884165, 1, 102.87555698, 2, 214.65018774

H, 4, 1.02141578, 1, 113.63452577, 3, 72.84309743

H, 4, 1.02267896, 1, 104.60430397, 3, 188.5406777

H, 4, 1.01882045, 1, 116.97407739, 3, -52.69609427

C, 5, 1.28168243, 1, 128.42333822, 2, -9.95926201

H, 15, 1.10167561, 5, 115.65029181, 1, 177.7621724

O, 15, 1.2514157, 5, 126.05829288, 16, 179.39579074

C, 6, 1.22306023, 1, 127.95418031, 2, 54.38684708

H, 18, 1.10103871, 6, 119.96608833, 1, 174.76860011

H, 18, 1.10063637, 6, 121.5411447, 19, 179.76799675

C, 7, 1.4663415, 1, 119.7003069, 2, -143.88818255

C, 7, 1.27541028, 1, 120.89208142, 2, 23.45582206

H, 22, 1.09452207, 7, 122.20163832, 21, -1.3820998

H, 22, 1.08767527, 7, 119.5382759, 21, 177.44209351

H, 21, 1.09610171, 7, 112.10980723, 22, -2.4053076

H, 21, 1.09576433, 7, 109.7047724, 22, 118.03891377

H, 21, 1.09406806, 7, 108.63112368, 22, -123.41484564

HF=-1123.8590822

RMSD=8.149e-09

Dipole=1.7898623, 0.0349325, -1.7223381

PG=C01 [X(C4H15Hg1N2O4S1)]

HgNIST5

1,1
Hg
O,1,2.6210044624
O,1,2.4462223344,2,90.
O,1,2.282369455,3,90.,2,180.
N,1,2.4898328892,2,90.,3,180.
N,1,2.4450408047,2,90.,3,90.
N,1,2.4464997775,2,90.,3,-90.
H,2,0.97296023,1,112.16865729,3,-6.80686301
H,2,0.97197859,1,115.61478673,3,-246.06419016
H,3,0.97057074,1,118.43936251,2,85.72796264
H,3,1.0330723,1,97.43694776,2,-161.76364113
C,4,1.28370719,1,125.14944826,3,-23.39579163
H,12,1.10302426,4,115.62431868,1,190.23720759
O,12,1.24939379,4,126.36133311,13,180.27015948
C,5,1.46483012,1,122.25565863,2,4.79421932
C,5,1.27542205,1,119.22790851,2,-172.1882213
H,16,1.09511258,5,121.87993726,15,0.14738443
H,16,1.08803585,5,118.8937645,15,179.7497631
H,15,1.0965316,5,112.35556676,16,1.34137805
H,15,1.09400843,5,109.29029594,16,122.94856457
H,15,1.09648123,5,109.19328629,16,-119.28821791
C,6,1.46643399,1,121.99423945,2,-2.30944573
C,6,1.27518632,1,119.75349617,2,-183.52228528
H,23,1.09481,6,121.90235038,22,0.05148818
H,23,1.08732197,6,119.02051155,22,180.05030546
H,22,1.09646026,6,112.28205752,23,-1.34805213
H,22,1.09565074,6,109.28667184,23,119.50746083
H,22,1.09357065,6,109.29529017,23,-123.0985196
C,7,1.46546877,1,120.2559771,2,-121.27358117
C,7,1.27598575,1,120.63253081,2,70.26653624
H,30,1.09449754,7,122.20123209,29,0.97097733
H,30,1.08823337,7,119.61644432,29,182.32574445
H,29,1.09609776,7,111.94502789,30,-0.7837748
H,29,1.09346675,7,108.69717189,30,120.28177774
H,29,1.09399338,7,109.45380317,30,-122.03589325

HF=-897.7601873

RMSD=3.745e-09

Dipole=-1.4935727,-0.3541311,2.103078

PG=C01 [X(C7H20Hg1N3O4)]

HgNIST6

0,1
Hg
N,1,2.4176295311
O,1,2.4854006508,2,90.
O,1,2.2522623795,3,90.,2,180.

O,1,2.3056785809,2,90.,3,180.
 O,1,2.5359694235,2,90.,3,90.
 N,1,2.561695079,2,90.,3,-90.
 H,2,1.01908318,1,115.5621522,3,-14.96344912
 H,2,1.01849089,1,111.26121655,3,108.4424075
 H,2,1.02323815,1,105.8404396,3,-134.75467573
 H,3,0.97112394,1,108.28761455,2,81.6646543
 H,3,1.02304661,1,97.80392418,2,-168.95716576
 C,4,1.2742347,1,127.82099865,3,-14.12880404
 H,13,1.10612313,4,115.29564313,1,185.68264568
 O,13,1.25528257,4,127.37705979,14,179.99772
 C,5,1.27123034,1,122.3007382,2,-55.12433709
 H,16,1.10668905,5,115.686955,1,174.24881814
 O,16,1.25921146,5,126.78984261,17,180.17200808
 H,6,1.00599966,1,95.59832954,2,61.71032057
 H,6,0.97189607,1,103.7317423,2,169.88928881
 C,7,1.4601769,1,116.99232253,2,-114.11575284
 C,7,1.27201034,1,122.86053587,2,74.62011213
 H,22,1.0967847,7,122.27117519,21,1.10542599
 H,22,1.08908345,7,119.22225123,21,182.20151921
 H,21,1.09878261,7,112.20757437,22,-1.38175132
 H,21,1.09397861,7,108.13863684,22,120.4332478
 H,21,1.09322508,7,108.90709937,22,-123.99727428

HF=-875.8101524

RMSD=7.615e-09

Dipole=0.6498172,1.4681727,1.7847365

PG=C01 [X(C4H14Hg1N2O6)]

HgNIST7

O,1
 Hg
 N,1,2.4144116046
 O,1,2.5170305531,2,90.
 O,1,2.2508735198,3,90.,2,180.
 N,1,2.5303396231,2,90.,3,180.
 O,1,2.3184800104,2,90.,3,90.
 N,1,2.633656763,2,90.,3,-90.
 H,2,1.02898128,1,100.93861993,3,-125.72297767
 H,2,1.0184998,1,118.8740048,3,-244.72562218
 H,2,1.01936669,1,111.78985893,3,-10.53215645
 H,3,0.97272908,1,102.24011537,2,81.683871
 H,3,1.0178043,1,98.41575201,2,-171.58021223
 C,4,1.27234602,1,129.29559016,3,-4.45491891
 H,13,1.10607734,4,115.34101058,1,173.68242238
 O,13,1.25528522,4,127.15300857,14,179.45785389
 H,5,1.01777801,1,127.55451684,2,69.26807101
 H,5,1.02102012,1,102.7068079,2,193.20851145
 H,5,1.02771264,1,101.29207317,2,-55.24041314
 C,6,1.27626236,1,123.9387555,2,44.96125971
 H,19,1.10812486,6,115.04782625,1,178.95271958
 O,19,1.25478665,6,126.90331622,20,180.24079754
 C,7,1.4609659,1,115.43336081,2,-244.03545366
 C,7,1.26935867,1,126.12677613,2,-65.86852803
 H,23,1.09712882,7,122.89262562,22,0.54298214
 H,23,1.08978492,7,119.77638238,22,180.59388516

H, 22, 1.09907263, 7, 112.51641284, 23, -1.30804604
H, 22, 1.09441114, 7, 108.43090638, 23, 120.46210531
H, 22, 1.09340227, 7, 108.87930888, 23, -123.58816988

HF=-855.9314196
RMSD=7.047e-09
Dipole=-1.0416332, 2.6684833, 1.7273912
PG=C01 [X(C4H15Hg1N3O5)]

HgNIST8

0, 1
Hg
O, 1, 2.7052684433
O, 1, 2.7914988817, 2, 90.
N, 1, 2.7160815348, 3, 90., 2, 180.
N, 1, 2.6120600455, 2, 90., 3, 180.
O, 1, 2.0950793619, 2, 90., 3, 90.
O, 1, 2.1719419401, 2, 90., 3, -90.
H, 2, 0.98214527, 1, 98.03740504, 3, 41.23140709
H, 2, 0.97303739, 1, 95.55627717, 3, 291.16967905
H, 3, 0.96938221, 1, 109.05225919, 2, 56.26983926
H, 3, 0.98936737, 1, 92.40867582, 2, -52.33589396
H, 4, 1.01857229, 1, 104.27730482, 3, 114.08554484
H, 4, 1.01867956, 1, 120.12431911, 3, -122.86529826
H, 4, 1.01969088, 1, 107.16574374, 3, 0.09642521
H, 5, 1.01738507, 1, 118.93736461, 2, 140.77093849
H, 5, 1.0191144, 1, 109.57910585, 2, 16.1650075
H, 5, 1.02021522, 1, 102.53365938, 2, -98.35376445
H, 6, 0.96787022, 1, 116.01791444, 2, -116.07779375
C, 7, 1.27379513, 1, 119.27103665, 2, -314.62134876
H, 19, 1.10566353, 7, 115.51957561, 1, -176.02088516
O, 19, 1.25889972, 7, 126.63707658, 20, 179.96043374

HF=-685.0068109
RMSD=4.454e-09
Dipole=-0.7549184, -0.4068074, -1.0828656
PG=C01 [X(C1H12Hg1N2O5)]

HgNIST9

-1, 1
Hg
O, 1, 2.5201861984
O, 1, 2.4740800858, 2, 90.
O, 1, 2.3171918309, 3, 90., 2, 180.
O, 1, 2.3341480582, 2, 90., 3, 180.
O, 1, 2.4505423144, 2, 90., 3, 90.
O, 1, 2.3005723041, 2, 90., 3, -90.
H, 2, 0.97175182, 1, 99.52841139, 3, 104.51642737
H, 2, 0.99881877, 1, 94.29456214, 3, 211.68565945
H, 3, 1.00910859, 1, 98.68960825, 2, -94.09939069
H, 3, 0.97099223, 1, 101.38789902, 2, -201.97750436

C, 4, 1.26878383, 1, 127.01843031, 3, 111.33200025
H, 12, 1.11133539, 4, 114.97633126, 1, 165.77026947
O, 12, 1.2568272, 4, 128.2325859, 13, 179.4719588
C, 5, 1.26286828, 1, 120.82600369, 2, -40.62039042
H, 15, 1.11032012, 5, 115.80738502, 1, 188.1673724
O, 15, 1.26542938, 5, 127.21421399, 16, 179.78233688
H, 6, 0.97558209, 1, 102.4577341, 2, 53.67963108
H, 6, 1.00806546, 1, 98.4646123, 2, 163.90836736
C, 7, 1.26868733, 1, 129.00837508, 2, -260.68082653
H, 20, 1.11121701, 7, 114.90604985, 1, -189.63994372
O, 20, 1.2562652, 7, 128.27473249, 21, 179.68083534

HF=-951.021924
RMSD=8.296e-09
Dipole=0.0822157, 0.0773487, 0.6878735
PG=C01 [X(C3H9Hg109)]

HgNIST10

-1, 1
Hg
S, 1, 3.2206981502
N, 1, 2.5405329486, 2, 90.
O, 1, 2.2327523777, 3, 90., 2, 180.
O, 1, 2.3879172369, 2, 90., 3, 180.
N, 1, 2.4521418209, 2, 90., 3, 90.
O, 1, 2.3681999491, 2, 90., 3, -90.
H, 2, 1.37137084, 1, 68.98737662, 3, 60.13152301
H, 2, 1.34995954, 1, 68.87600307, 3, 163.38684742
H, 3, 1.01649383, 1, 125.54886593, 2, 73.55205756
H, 3, 1.02262177, 1, 91.87096883, 2, 190.06213232
H, 3, 1.02214414, 1, 107.23171868, 2, -58.23756144
H, 4, 0.96789674, 1, 105.45799613, 3, -135.33034611
C, 5, 1.26991852, 1, 131.60725745, 2, -80.06634025
H, 14, 1.1160537, 5, 114.15912931, 1, 192.02989006
O, 14, 1.2545012, 5, 129.03165872, 15, 179.64749292
H, 6, 1.03342131, 1, 103.76270075, 2, 73.09849173
H, 6, 1.02173048, 1, 95.44332656, 2, 183.37055709
H, 6, 1.01715252, 1, 126.67645371, 2, -56.00776351
C, 7, 1.26589241, 1, 125.4355857, 2, 46.92957952
H, 20, 1.11381724, 7, 114.91970239, 1, -188.27084693
O, 20, 1.2603282, 7, 128.02959413, 21, 180.64311568

HF=-1120.8040229
RMSD=8.029e-09
Dipole=2.1711486, -1.146605, 0.5171689
PG=C01 [X(C2H11Hg1N205S1)]

3. Cu²⁺-specific sites

CoCUST1

2,4			
27	0.027359	-0.403081	-0.001591
7	0.092411	-2.545557	-0.115932
7	2.146401	-0.340230	0.026311
7	-0.036708	1.706961	0.111019
7	-2.083786	-0.465698	-0.029390
1	0.829089	-2.893222	-0.736186
1	0.273555	-2.986285	0.791081
1	-0.780734	-2.963812	-0.446507
6	2.815853	0.249083	-1.150424
6	2.868013	-0.754542	0.997912
1	3.958303	-0.677563	0.983299
1	2.407757	-1.200366	1.879865
1	3.903291	0.265831	-1.030040
1	2.564953	-0.338877	-2.039907
1	2.454170	1.270762	-1.297310
6	-0.767936	2.465986	-0.922437
6	0.511088	2.354520	1.068092
1	0.446442	3.443017	1.142958
1	1.066441	1.827862	1.843065
1	-0.711944	3.544144	-0.744528
1	-0.338995	2.242929	-1.904948
1	-1.816833	2.158008	-0.926192
6	-2.779604	-0.133998	1.229531
6	-2.783100	-0.748404	-1.062379
1	-3.876012	-0.747793	-1.039077
1	-2.300191	-0.997771	-2.007565
1	-3.867021	-0.162420	1.110829
1	-2.486754	-0.851818	2.003264
1	-2.478310	0.866380	1.555052

HF=-1840.87292695
RMSD=5.370e-08
S2=3.7556

CoCUST2

1,4
Co
O,1,1.8216664515
N,1,2.2074426844,2,90.
N,1,2.1572690694,3,90.,2,180.
N,1,2.1569611161,2,90.,3,180.
H,2,0.96776564,1,116.01388195,3,4.20087126
C,3,1.46689181,1,116.2410609,2,81.55885397
C,3,1.27464135,1,123.34508973,2,-82.52741438
H,8,1.09537508,3,122.60019491,7,0.21419141
H,8,1.09027943,3,119.94434526,7,180.91481208
H,7,1.09676294,3,112.51492937,8,-0.0073659
H,7,1.09510531,3,108.89489592,8,121.37344792
H,7,1.09575243,3,109.164399,8,-121.16026048
H,4,1.02185352,1,111.55007023,3,-144.80870749
H,4,1.02193947,1,111.3534806,3,-24.70127
H,4,1.02235954,1,113.23385648,3,94.85559242
C,5,1.46939563,1,113.08012484,2,38.0247252
C,5,1.27390069,1,126.69331004,2,-127.98646699

H, 18, 1.09416378, 5, 122.52374938, 17, 1.06437447
H, 18, 1.09073157, 5, 120.28930861, 17, 181.64645934
H, 17, 1.09592129, 5, 111.85941973, 18, -0.6852935
H, 17, 1.09301112, 5, 107.70565458, 18, 121.68460219
H, 17, 1.0952264, 5, 108.75843567, 18, -121.77155425

HF=-1783.0657781

S2=3.758541

S2-1=0.

S2A=3.750033

RMSD=7.673e-09

Dipole=0.5451367, 0.0368182, -2.2085569

PG=C01 [X(C4H14Co1N3O1)]

CoCUST3

1, 4

Co

S, 1, 2.6069980034

N, 1, 2.1105609709, 2, 90.

O, 1, 1.8250015663, 3, 90., 2, 180.

N, 1, 2.153145274, 2, 90., 3, 180.

H, 2, 1.34864404, 1, 103.94650884, 3, 37.73074991

H, 2, 1.3497036, 1, 103.50423764, 3, 136.03001804

C, 3, 1.47075285, 1, 112.65261797, 2, 129.12999126

C, 3, 1.27386661, 1, 126.05179656, 2, -67.63737041

H, 9, 1.09332782, 3, 122.16196784, 8, -1.67421019

H, 9, 1.08998815, 3, 120.31718054, 8, 177.60138886

H, 8, 1.09533619, 3, 111.61167356, 9, 3.67689696

H, 8, 1.09501349, 3, 108.88657348, 9, 124.66775928

H, 8, 1.09368888, 3, 107.37040282, 9, -117.98476755

H, 4, 0.96749334, 1, 117.91793751, 3, -190.46291701

C, 5, 1.46850125, 1, 115.15949974, 2, 108.44979984

C, 5, 1.27526192, 1, 124.14237216, 2, -86.42875031

H, 17, 1.09444972, 5, 122.26760265, 16, 0.42072497

H, 17, 1.08968207, 5, 120.09063675, 16, 179.82351569

H, 16, 1.09594159, 5, 112.11521785, 17, -1.35053771

H, 16, 1.09559967, 5, 108.98225503, 17, 119.54981327

H, 16, 1.09405243, 5, 108.86886628, 17, -122.99088151

HF=-2125.8873146

S2=3.75908

S2-1=0.

S2A=3.750037

RMSD=8.164e-09

Dipole=-0.4780141, 0.3044968, 1.2936317

PG=C01 [X(C4H13Co1N2O1S1)]

CoCUST4

1, 4

Co

N, 1, 2.1292155342

N,1,2.1709809109,2,90.
N,1,2.140225259,3,90.,2,180.
O,1,1.9131012672,2,90.,3,180.
H,2,1.02199844,1,121.52939236,3,36.93452109
H,2,1.04526066,1,99.85686561,3,155.26463367
H,2,1.023163,1,113.89679045,3,-92.16340639
H,3,1.02264408,1,110.47588004,2,50.21997289
H,3,1.02177674,1,116.92216272,2,171.86463527
H,3,1.0231178,1,110.78518368,2,-66.51641069
H,4,1.02492923,1,102.25176218,3,-183.49142
H,4,1.0221355,1,115.5257596,3,-68.37416037
H,4,1.02176647,1,118.06494296,3,59.76859701
C,5,1.30847706,1,132.95336155,2,25.08575529
H,15,1.1013715,5,113.29104417,1,176.57418561
O,15,1.23052883,5,126.3197477,16,179.85627183

HF=-1741.6401414
S2=3.755958
S2-1=0.
S2A=3.750016
RMSD=6.183e-09
Dipole=3.3563483,-0.5476914,-1.5698474
PG=C01 [X(C1H10Co1N3O2)]

CoCUST5

O,4
Co
O,1,1.8607023914
S,1,2.4192560716,2,90.
N,1,2.1994682967,3,90.,2,180.
N,1,2.2144674668,2,90.,3,180.
H,2,0.97000392,1,103.01546702,3,6.34470537
H,3,1.35332324,1,90.78864053,2,71.43476946
H,4,1.0205681,1,119.00696529,3,-250.97208963
H,4,1.02099594,1,118.15947633,3,-117.29589491
H,4,1.0262128,1,94.44194697,3,-3.2888737
C,5,1.46375877,1,112.17873659,2,26.00570283
C,5,1.27121488,1,126.61661011,2,-138.55669575
H,12,1.09589899,5,122.58502702,11,0.74640693
H,12,1.08984468,5,119.84541668,11,181.11075781
H,11,1.09820789,5,111.98682258,12,3.42804526
H,11,1.09455443,5,107.42785704,12,127.08296681
H,11,1.09555611,5,108.34124662,12,-117.76686106

HF=-2048.0970894
S2=3.760877
S2-1=0.
S2A=3.750052
RMSD=7.396e-09
Dipole=-2.8318153,-0.1729257,-2.2386188
PG=C01 [X(C2H10Co1N2O1S1)]

CoCUST6

0,4

27	-0.116835	-0.495467	-0.018814
8	0.219014	-2.348949	0.000071
16	-2.431648	-0.915589	-0.085677
7	-0.507316	1.659524	-0.040772
7	2.077690	-0.097176	0.044573
1	-0.589437	-2.767015	0.326334
1	-2.231257	-2.049343	-0.787582
6	-1.284170	2.155550	1.093689
6	-0.469404	2.350765	-1.107628
1	-0.986927	3.311806	-1.206817
1	0.076717	1.978871	-1.974433
1	-1.699748	3.155190	0.910035
1	-2.099729	1.451568	1.287245
1	-0.641990	2.183732	1.980835
6	2.754683	1.197189	0.019733
6	2.772298	-1.164891	0.145485
1	3.866746	-1.123390	0.209845
1	2.234444	-2.115740	0.169033
1	3.839668	1.097002	0.156092
1	2.559835	1.692909	-0.937030
1	2.347419	1.834908	0.810407

HF=-2125.50419941

RMSD=7.932e-08

S2=3.7628

CoCUST7

0,4

Co

N,1,2.1212077203
N,1,2.2429906861,2,90.
S,1,2.2499082377,3,90.,2,180.
O,1,2.0739870843,2,90.,3,180.
H,2,1.02076199,1,114.62081313,3,61.94109434
H,2,1.05565578,1,103.19666511,3,179.88714098
H,2,1.02077146,1,114.5878313,3,-62.20681888
H,3,1.02014795,1,128.44110609,2,-0.12325603
H,3,1.02055565,1,102.94939723,2,124.93213289
H,3,1.02055681,1,102.91764206,2,-125.14690284
H,4,1.34866762,1,90.39534618,3,-179.98192431
C,5,1.27968899,1,131.2491159,2,0.12537354
H,13,1.10677125,5,114.86180463,1,179.93855336
O,13,1.25175277,5,127.3190162,14,179.9981024

HF=-2084.0960676

S2=3.759273

S2-1=0.

S2A=3.750037

RMSD=4.490e-09

Dipole=2.7875431,-0.0018644,1.3353776

PG=C01 [X(C1H8Co1N2O2S1)]

CoCUST8

```
-1,4
27 -0.088708 0.108684 -0.000314
8 0.253106 -1.751680 0.000977
16 -2.508250 -0.335873 -0.002220
8 -0.424802 1.937912 -0.001584
8 2.764894 0.632992 0.001933
1 -0.661768 -2.072399 0.014660
1 -2.716878 0.998621 0.028002
1 0.393327 2.462317 0.004840
6 3.058481 -0.550157 -0.001327
1 2.288255 -1.342961 0.003492
1 4.127712 -0.858920 -0.009630
```

HF=-2047.98272477
RMSD=1.424e-08
S2=3.7641

CoCUST9

```
-1,4
27 -0.230252 -0.252193 -0.013335
8 -0.231969 -2.142742 -0.012578
16 -2.825849 -0.249851 -0.052846
16 -0.228125 2.089309 -0.014271
7 2.077424 -0.254275 0.021794
1 -1.190355 -2.310770 -0.027880
1 -2.907273 -0.099839 1.292988
1 -1.575807 2.077389 -0.111768
6 2.951340 0.903487 0.027314
6 2.562700 -1.428666 -0.000420
1 3.649971 -1.614419 -0.015623
1 1.864954 -2.267817 -0.006221
1 4.020963 0.632324 0.006688
1 2.709437 1.531341 -0.836684
1 2.738061 1.502602 0.919118
```

HF=-2390.41829051
RMSD=7.836e-08
S2=3.7605

CoCUST10

```
-1,4
Co
S,1,2.3710177975
0,1,1.9212200575,2,90.
N,1,2.1976226426,3,90.,2,180.
0,1,2.0809212489,2,90.,3,180.
```

H, 2, 1.35130204, 1, 89.20207647, 3, 0.01118615
H, 3, 0.9713541, 1, 115.55122185, 2, 180.17203255
H, 4, 1.03641779, 1, 105.02484417, 3, -180.03432624
H, 4, 1.01800855, 1, 111.55517233, 3, -60.53899077
H, 4, 1.0180085, 1, 111.51248837, 3, 60.48237958
C, 5, 1.27260626, 1, 133.11918609, 2, 179.98357198
H, 11, 1.1139699, 5, 114.01374319, 1, 180.06492356
O, 11, 1.2549452, 5, 129.14978069, 12, 179.99573206

HF=-2103.4320001

S2=3.758587

S2-1=0.

S2A=3.750032

RMSD=9.092e-09

Dipole=0.1380346, 0.0017365, -2.5252071

PG=C01 [X(C1H6Co1N103S1)]

NiCUST1

2, 3

28	0.028582	-0.395290	-0.002165
7	0.088941	-2.486855	-0.118199
7	2.126083	-0.336274	0.025122
7	-0.031153	1.674657	0.112670
7	-2.071048	-0.454366	-0.029480
1	0.824964	-2.834319	-0.739342
1	0.269622	-2.929756	0.787848
1	-0.784900	-2.903111	-0.449459
6	2.796161	0.254506	-1.150521
6	2.847285	-0.753702	0.995693
1	3.937686	-0.678322	0.981003
1	2.386554	-1.200687	1.876810
1	3.883649	0.269376	-1.030340
1	2.544189	-0.331211	-2.041180
1	2.435974	1.277030	-1.295183
6	-0.761469	2.436941	-0.919030
6	0.517817	2.319387	1.070980
1	0.454815	3.407820	1.148143
1	1.072550	1.790275	1.844724
1	-0.703827	3.514639	-0.738872
1	-0.333075	2.215306	-1.902102
1	-1.810826	2.130540	-0.923202
6	-2.766097	-0.124269	1.230287
6	-2.771008	-0.733858	-1.062907
1	-3.863912	-0.731663	-1.039363
1	-2.288676	-0.981963	-2.008720
1	-3.853580	-0.150816	1.111764
1	-2.474153	-0.844148	2.002448
1	-2.463237	0.874972	1.557840

HF=-1966.40125619

RMSD=5.566e-08

S2=2.0044

NiCUST2

1,3

Ni

O,1,1.8060669309
 N,1,2.1404586646,2,90.
 N,1,2.1196466306,3,90.,2,180.
 N,1,2.122053219,2,90.,3,180.
 H,2,0.96776564,1,116.01388195,3,4.20087126
 C,3,1.46689181,1,116.2410609,2,81.55885397
 C,3,1.27464135,1,123.34508973,2,-82.52741438
 H,8,1.09537508,3,122.60019491,7,0.21419141
 H,8,1.09027943,3,119.94434526,7,180.91481208
 H,7,1.09676294,3,112.51492937,8,-0.0073659
 H,7,1.09510531,3,108.89489592,8,121.37344792
 H,7,1.09575243,3,109.164399,8,-121.16026048
 H,4,1.02185352,1,111.55007023,3,-144.80870749
 H,4,1.02193947,1,111.3534806,3,-24.70127
 H,4,1.02235954,1,113.23385648,3,94.85559242
 C,5,1.46939563,1,113.08012484,2,38.0247252
 C,5,1.27390069,1,126.69331004,2,-127.98646699
 H,18,1.09416378,5,122.52374938,17,1.06437447
 H,18,1.09073157,5,120.28930861,17,181.64645934
 H,17,1.09592129,5,111.85941973,18,-0.6852935
 H,17,1.09301112,5,107.70565458,18,121.68460219
 H,17,1.0952264,5,108.75843567,18,-121.77155425

HF=-1908.6022786

S2=2.007731

S2-1=0.

S2A=2.000035

RMSD=7.284e-09

Dipole=0.5461813,0.0335432,-2.0907661

PG=C01 [X(C4H14N3Ni101)]

NiCUST3

1,3

Ni

S,1,2.5572752703
 N,1,2.078990899,2,90.
 O,1,1.812374573,3,90.,2,180.
 N,1,2.0913773892,2,90.,3,180.
 H,2,1.34864404,1,103.94650884,3,37.73074991
 H,2,1.3497036,1,103.50423764,3,136.03001804
 C,3,1.47075285,1,112.65261797,2,129.12999126
 C,3,1.27386661,1,126.05179656,2,-67.63737041
 H,9,1.09332782,3,122.16196784,8,-1.67421019
 H,9,1.08998815,3,120.31718054,8,177.60138886
 H,8,1.09533619,3,111.61167356,9,3.67689696
 H,8,1.09501349,3,108.88657348,9,124.66775928
 H,8,1.09368888,3,107.37040282,9,-117.98476755
 H,4,0.96749334,1,117.91793751,3,-190.46291701
 C,5,1.46850125,1,115.15949974,2,108.44979984
 C,5,1.27526192,1,124.14237216,2,-86.42875031
 H,17,1.09444972,5,122.26760265,16,0.42072497

H, 17, 1.08968207, 5, 120.09063675, 16, 179.82351569
H, 16, 1.09594159, 5, 112.11521785, 17, -1.35053771
H, 16, 1.09559967, 5, 108.98225503, 17, 119.54981327
H, 16, 1.09405243, 5, 108.86886628, 17, -122.99088151

HF=-2251.4233152

S2=2.008678

S2-1=0.

S2A=2.000044

RMSD=1.482e-09

Dipole=-0.4909074, 0.3098557, 1.2067642

PG=C01 [X(C4H13N2Ni10I5S1)]

NiCUST4

1, 3

28	-0.512346	-0.016770	-0.056958
7	0.532738	1.782289	-0.198135
7	-2.350695	1.068443	0.163566
7	-1.559133	-1.818761	0.084449
8	1.124982	-0.983316	-0.253368
1	0.268445	2.598850	0.356714
1	1.476569	1.466489	0.121275
1	0.655834	2.115930	-1.157507
1	-2.440397	1.773384	-0.571833
1	-3.214804	0.523494	0.144217
1	-2.362872	1.586564	1.045707
1	-0.819271	-2.512318	-0.064085
1	-1.965689	-2.021285	1.000123
1	-2.284625	-2.008984	-0.609440
6	2.373286	-0.683257	-0.000755
1	3.067566	-1.518396	-0.183884
8	2.795626	0.401013	0.399482

HF=-1867.17109753

RMSD=2.368e-08

S2=2.0040

NiCUST5

0, 3

Ni

O, 1, 1.8284786444

S, 1, 2.3956918783, 2, 90.

N, 1, 2.155067277, 3, 90., 2, 180.

N, 1, 2.1963331257, 2, 90., 3, 180.

H, 2, 0.97000392, 1, 103.01546702, 3, 6.34470537

H, 3, 1.35332324, 1, 90.78864053, 2, 71.43476946

H, 4, 1.0205681, 1, 119.00696529, 3, -250.97208963

H, 4, 1.02099594, 1, 118.15947633, 3, -117.29589491

H, 4, 1.0262128, 1, 94.44194697, 3, -3.2888737

C, 5, 1.46375877, 1, 112.17873659, 2, 26.00570283

C, 5, 1.27121488, 1, 126.61661011, 2, -138.55669575

H, 12, 1.09589899, 5, 122.58502702, 11, 0.74640693
H, 12, 1.08984468, 5, 119.84541668, 11, 181.11075781
H, 11, 1.09820789, 5, 111.98682258, 12, 3.42804526
H, 11, 1.09455443, 5, 107.42785704, 12, 127.08296681
H, 11, 1.09555611, 5, 108.34124662, 12, -117.76686106

HF=-2173.6334931
S2=2.008931
S2-1=0.
S2A=2.000047
RMSD=1.772e-09
Dipole=-2.8196025, -0.2088958, -2.121588
PG=C01 [X(C2H10N2Ni101S1)]

NiCUST6

O, 3
Ni
O, 1, 1.8436348376
S, 1, 2.3634047232, 2, 90.
N, 1, 2.1447544372, 3, 90., 2, 180.
N, 1, 2.2129728356, 2, 90., 3, 180.
H, 2, 0.96686071, 1, 106.24541341, 3, -22.02823764
H, 3, 1.34841604, 1, 91.0720979, 2, -31.92770671
C, 4, 1.46169306, 1, 114.88951439, 3, 60.97717081
C, 4, 1.271783, 1, 122.53949353, 3, -96.9842452
H, 9, 1.09602395, 4, 122.57642342, 8, 0.77484264
H, 9, 1.08991055, 4, 119.77720569, 8, 182.11077562
H, 8, 1.09804987, 4, 112.35056376, 9, -4.7736256
H, 8, 1.09461981, 4, 108.35926631, 9, 116.28415926
H, 8, 1.09554402, 4, 109.00692435, 9, -126.33662916
C, 5, 1.46093008, 1, 127.83830725, 2, 178.07494722
C, 5, 1.27776331, 1, 112.81410643, 2, -3.65519979
H, 16, 1.0971243, 5, 121.01823175, 15, -0.2242183
H, 16, 1.09268279, 5, 117.46881387, 15, 179.53471262
H, 15, 1.09810001, 5, 112.01931152, 16, -3.44820062
H, 15, 1.0950338, 5, 109.48042413, 16, 117.59051011
H, 15, 1.09440286, 5, 109.36241568, 16, -124.82926089

HF=-2251.0373905
S2=2.008961
S2-1=0.
S2A=2.000049
RMSD=5.819e-09
Dipole=-2.6581918, 0.0561001, -2.1045999
PG=C01 [X(C4H12N2Ni101S1)]

NiCUST7

O, 3
Ni
N, 1, 2.0912712806
N, 1, 2.1886131092, 2, 90.

S,1,2.2172435429,3,90.,2,180.
O,1,2.0654803898,2,90.,3,180.
H,2,1.02076199,1,114.62081313,3,61.94109434
H,2,1.05565578,1,103.19666511,3,179.88714098
H,2,1.02077146,1,114.5878313,3,-62.20681888
H,3,1.02014795,1,128.44110609,2,-0.12325603
H,3,1.02055565,1,102.94939723,2,124.93213289
H,3,1.02055681,1,102.91764206,2,-125.14690284
H,4,1.34866762,1,90.39534618,3,-179.98192431
C,5,1.27968899,1,131.2491159,2,0.12537354
H,13,1.10677125,5,114.86180463,1,179.93855336
O,13,1.25175277,5,127.3190162,14,179.9981024

HF=-2209.6320698
S2=2.008053
S2-1=0.
S2A=2.000036
RMSD=7.717e-09
Dipole=2.8069255,-0.0019484,1.0441099
PG=C01 [X(C1H8N2Ni102S1)]

NiCUST8

-1,3
Ni
O,1,1.8517673245
S,1,2.4784473918,2,90.
O,1,1.8235189041,3,90.,2,180.
O,1,2.9102770544,2,90.,3,180.
H,2,0.96955756,1,98.90718518,3,-0.8567508
H,3,1.35104116,1,88.47364311,2,178.67982072
H,4,0.97179126,1,112.24719263,3,-180.38086767
C,5,1.21903454,1,93.52462369,2,0.19540385
H,9,1.10535489,5,121.89044862,1,-0.44347487
H,9,1.11295051,5,120.04341931,10,179.98443711

HF=-2173.5182841
S2=2.010448
S2-1=0.
S2A=2.000051
RMSD=8.730e-09
Dipole=-2.7927717,-0.0089142,0.7035838
PG=C01 [X(C1H5Ni103S1)]

NiCUST9

-1,3
Ni
O,1,1.8640570804
S,1,2.5457237912,2,90.
S,1,2.3095022579,3,90.,2,180.
N,1,2.2636904698,2,90.,3,180.
H,2,0.97312465,1,99.99469007,3,0.04675989

H, 3, 1.35661386, 1, 92.57994496, 2, 96.32907025
H, 4, 1.35125573, 1, 89.44430573, 3, -3.26595382
C, 5, 1.45057706, 1, 126.99384177, 2, 179.63888886
C, 5, 1.27089809, 1, 112.47997224, 2, 1.46793926
H, 10, 1.10312928, 5, 122.153547, 9, 0.03372208
H, 10, 1.0913558, 5, 117.8066371, 9, 180.15301385
H, 9, 1.10365194, 5, 112.81233586, 10, 0.21958219
H, 9, 1.09508514, 5, 108.75472937, 10, 122.40040101
H, 9, 1.09532607, 5, 108.80507337, 10, -121.85050305

HF=-2515.9569179

S2=2.008728

S2-1=0.

S2A=2.000047

RMSD=8.573e-09

Dipole=-3.3694208, -0.1464996, 0.3696288

PG=C01 [X(C2H8N1Ni101S2)]

NiCUST10

-1, 3

Ni

S, 1, 2.2770260854

O, 1, 1.930516989, 2, 90.

N, 1, 2.161747489, 3, 90., 2, 180.

O, 1, 2.0894095459, 2, 90., 3, 180.

H, 2, 1.35130204, 1, 89.20207647, 3, 0.01118615

H, 3, 0.9713541, 1, 115.55122185, 2, 180.17203255

H, 4, 1.03641779, 1, 105.02484417, 3, -180.03432624

H, 4, 1.01800855, 1, 111.55517233, 3, -60.53899077

H, 4, 1.0180085, 1, 111.51248837, 3, 60.48237958

C, 5, 1.27260626, 1, 133.11918609, 2, 179.98357198

H, 11, 1.1139699, 5, 114.01374319, 1, 180.06492356

O, 11, 1.2549452, 5, 129.14978069, 12, 179.99573206

HF=-2228.9616947

S2=2.007637

S2-1=0.

S2A=2.000034

RMSD=7.309e-09

Dipole=0.1829364, 0.0012603, -2.0768549

PG=C01 [X(C1H6N1Ni103S1)]

CuCUST1

2, 2

Cu

N, 1, 2.0720116327

N, 1, 2.0450908948, 2, 90.

N, 1, 2.0547507801, 3, 90., 2, 180.

N, 1, 2.0459355847, 2, 90., 3, 180.

H, 2, 1.02385586, 1, 113.14143639, 3, -40.3198499

H, 2, 1.02456229, 1, 112.80244485, 3, 79.01833637

H, 2, 1.02303422, 1, 113.54172653, 3, -161.50286868
C, 3, 1.47653715, 1, 117.03264534, 2, 112.59061505
C, 3, 1.27921293, 1, 124.34699924, 2, -68.70036628
H, 10, 1.09310214, 3, 121.98471852, 9, 0.46394224
H, 10, 1.09015416, 3, 120.58152646, 9, 180.35839494
H, 9, 1.09420969, 3, 111.65491951, 10, -0.58510284
H, 9, 1.09536656, 3, 109.21255142, 10, 120.00454837
H, 9, 1.09371708, 3, 109.26439008, 10, -121.50793333
C, 4, 1.47609074, 1, 119.40401794, 3, 124.15354916
C, 4, 1.27882861, 1, 122.16106764, 3, -57.64925753
H, 17, 1.092982, 4, 122.0201926, 16, 0.41898074
H, 17, 1.08920536, 4, 120.40126501, 16, 180.56859201
H, 16, 1.09417169, 4, 111.56144014, 17, 2.17424248
H, 16, 1.09502211, 4, 109.23219579, 17, 122.82109779
H, 16, 1.09318302, 4, 109.44188698, 17, -118.66570006
C, 5, 1.4761667, 1, 116.95142627, 2, 108.57817191
C, 5, 1.279074, 1, 124.3070414, 2, -72.59690188
H, 24, 1.09316028, 5, 121.95622579, 23, 0.20449724
H, 24, 1.0903036, 5, 120.56472847, 23, 180.00011204
H, 23, 1.09424543, 5, 111.72032168, 24, -0.67587349
H, 23, 1.09530387, 5, 109.21759746, 24, 119.96760872
H, 23, 1.09430238, 5, 109.22793286, 24, -121.65462817

HF=-2098.5947017

S2=0.753477

S2-1=0.

S2A=0.750012

RMSD=7.945e-09

Dipole=0.1309514, 0.1971829, 0.8206918

PG=C01 [X(C6H18Cu1N4)]

CuCUST2

1, 2

Cu

O, 1, 1.8349353534

N, 1, 2.0840520718, 2, 90.

N, 1, 2.0963758121, 3, 90., 2, 180.

N, 1, 2.0884091174, 2, 90., 3, 180.

H, 2, 0.96776564, 1, 116.01388195, 3, 4.20087126

C, 3, 1.46689181, 1, 116.2410609, 2, 81.55885397

C, 3, 1.27464135, 1, 123.34508973, 2, -82.52741438

H, 8, 1.09537508, 3, 122.60019491, 7, 0.21419141

H, 8, 1.09027943, 3, 119.94434526, 7, 180.91481208

H, 7, 1.09676294, 3, 112.51492937, 8, -0.0073659

H, 7, 1.09510531, 3, 108.89489592, 8, 121.37344792

H, 7, 1.09575243, 3, 109.164399, 8, -121.16026048

H, 4, 1.02185352, 1, 111.55007023, 3, -144.80870749

H, 4, 1.02193947, 1, 111.3534806, 3, -24.70127

H, 4, 1.02235954, 1, 113.23385648, 3, 94.85559242

C, 5, 1.46939563, 1, 113.08012484, 2, 38.0247252

C, 5, 1.27390069, 1, 126.69331004, 2, -127.98646699

H, 18, 1.09416378, 5, 122.52374938, 17, 1.06437447

H, 18, 1.09073157, 5, 120.28930861, 17, 181.64645934

H, 17, 1.09592129, 5, 111.85941973, 18, -0.6852935

H, 17, 1.09301112, 5, 107.70565458, 18, 121.68460219

H, 17, 1.0952264, 5, 108.75843567, 18, -121.77155425

HF=-2040.7797318
S2=0.753412
S2-1=0.
S2A=0.75001
RMSD=6.625e-09
Dipole=0.5794021,0.0363056,-2.2218276
PG=C01 [X(C4H14Cu1N3O1)]

CuCUST3

1,2
Cu
S,1,2.5565223585
N,1,2.0443113844,2,90.
O,1,1.8492801591,3,90.,2,180.
N,1,2.0354756303,2,90.,3,180.
H,2,1.34864404,1,103.94650884,3,37.73074991
H,2,1.3497036,1,103.50423764,3,136.03001804
C,3,1.47075285,1,112.65261797,2,129.12999126
C,3,1.27386661,1,126.05179656,2,-67.63737041
H,9,1.09332782,3,122.16196784,8,-1.67421019
H,9,1.08998815,3,120.31718054,8,177.60138886
H,8,1.09533619,3,111.61167356,9,3.67689696
H,8,1.09501349,3,108.88657348,9,124.66775928
H,8,1.09368888,3,107.37040282,9,-117.98476755
H,4,0.96749334,1,117.91793751,3,-190.46291701
C,5,1.46850125,1,115.15949974,2,108.44979984
C,5,1.27526192,1,124.14237216,2,-86.42875031
H,17,1.09444972,5,122.26760265,16,0.42072497
H,17,1.08968207,5,120.09063675,16,179.82351569
H,16,1.09594159,5,112.11521785,17,-1.35053771
H,16,1.09559967,5,108.98225503,17,119.54981327
H,16,1.09405243,5,108.86886628,17,-122.99088151

HF=-2383.601271
S2=0.754406
S2-1=0.
S2A=0.750015
RMSD=5.651e-09
Dipole=-0.5293705,0.3127003,1.2921526
PG=C01 [X(C4H13Cu1N2O1S1)]

CuCUST4

1,2
Cu
N,1,2.0444944592
N,1,2.1001510531,2,90.
N,1,2.0533222504,3,90.,2,180.
O,1,1.9092819803,2,90.,3,180.
H,2,1.02199844,1,121.52939236,3,36.93452109
H,2,1.04526066,1,99.85686561,3,155.26463367

H, 2, 1.023163, 1, 113.89679045, 3, -92.16340639
H, 3, 1.02264408, 1, 110.47588004, 2, 50.21997289
H, 3, 1.02177674, 1, 116.92216272, 2, 171.86463527
H, 3, 1.0231178, 1, 110.78518368, 2, -66.51641069
H, 4, 1.02492923, 1, 102.25176218, 3, -183.49142
H, 4, 1.0221355, 1, 115.5257596, 3, -68.37416037
H, 4, 1.02176647, 1, 118.06494296, 3, 59.76859701
C, 5, 1.30847706, 1, 132.95336155, 2, 25.08575529
H, 15, 1.1013715, 5, 113.29104417, 1, 176.57418561
O, 15, 1.23052883, 5, 126.3197477, 16, 179.85627183

HF=-1999.3560076

S2=0.752682

S2-1=0.

S2A=0.750006

RMSD=6.542e-09

Dipole=3.3550776, -0.5536248, -1.5314853

PG=C01 [X(C1H10Cu1N3O2)]

CuCUST5

O, 2

Cu

O, 1, 1.8601901145

S, 1, 2.3709884393, 2, 90.

N, 1, 2.1148887427, 3, 90., 2, 180.

N, 1, 2.1919258064, 2, 90., 3, 180.

H, 2, 0.97000392, 1, 103.01546702, 3, 6.34470537

H, 3, 1.35332324, 1, 90.78864053, 2, 71.43476946

H, 4, 1.0205681, 1, 119.00696529, 3, -250.97208963

H, 4, 1.02099594, 1, 118.15947633, 3, -117.29589491

H, 4, 1.0262128, 1, 94.44194697, 3, -3.2888737

C, 5, 1.46375877, 1, 112.17873659, 2, 26.00570283

C, 5, 1.27121488, 1, 126.61661011, 2, -138.55669575

H, 12, 1.09589899, 5, 122.58502702, 11, 0.74640693

H, 12, 1.08984468, 5, 119.84541668, 11, 181.11075781

H, 11, 1.09820789, 5, 111.98682258, 12, 3.42804526

H, 11, 1.09455443, 5, 107.42785704, 12, 127.08296681

H, 11, 1.09555611, 5, 108.34124662, 12, -117.76686106

HF=-2305.8191623

S2=0.755303

S2-1=0.

S2A=0.750019

RMSD=6.994e-09

Dipole=-2.5066174, -0.2248676, -2.2105714

PG=C01 [X(C2H10Cu1N2O1S1)]

CuCUST6

O, 2

Cu

O, 1, 1.8756222525

S,1,2.3441958682,2,90.
N,1,2.1056431225,3,90.,2,180.
N,1,2.2003990724,2,90.,3,180.
H,2,0.96686071,1,106.24541341,3,-22.02823764
H,3,1.34841604,1,91.0720979,2,-31.92770671
C,4,1.46169306,1,114.88951439,3,60.97717081
C,4,1.271783,1,122.53949353,3,-96.9842452
H,9,1.09602395,4,122.57642342,8,0.77484264
H,9,1.08991055,4,119.77720569,8,182.11077562
H,8,1.09804987,4,112.35056376,9,-4.7736256
H,8,1.09461981,4,108.35926631,9,116.28415926
H,8,1.09554402,4,109.00692435,9,-126.33662916
C,5,1.46093008,1,127.83830725,2,178.07494722
C,5,1.27776331,1,112.81410643,2,-3.65519979
H,16,1.0971243,5,121.01823175,15,-0.2242183
H,16,1.09268279,5,117.46881387,15,179.53471262
H,15,1.09810001,5,112.01931152,16,-3.44820062
H,15,1.0950338,5,109.48042413,16,117.59051011
H,15,1.09440286,5,109.36241568,16,-124.82926089

HF=-2383.2238665
S2=0.755259
S2-1=0.
S2A=0.75002
RMSD=9.133e-09
Dipole=-2.4313281,0.0607594,-2.1990264
PG=C01 [X(C4H12Cu1N2O1S1)]

CuCUST7

O,2
Cu
N,1,2.068383106
N,1,2.1287461883,2,90.
S,1,2.253621913,3,90.,2,180.
O,1,2.0427479574,2,90.,3,180.
H,2,1.02076199,1,114.62081313,3,61.94109434
H,2,1.05565578,1,103.19666511,3,179.88714098
H,2,1.02077146,1,114.5878313,3,-62.20681888
H,3,1.02014795,1,128.44110609,2,-0.12325603
H,3,1.02055565,1,102.94939723,2,124.93213289
H,3,1.02055681,1,102.91764206,2,-125.14690284
H,4,1.34866762,1,90.39534618,3,-179.98192431
C,5,1.27968899,1,131.2491159,2,0.12537354
H,13,1.10677125,5,114.86180463,1,179.93855336
O,13,1.25175277,5,127.3190162,14,179.9981024

HF=-2341.8136258
S2=0.753606
S2-1=0.
S2A=0.75001
RMSD=3.208e-09
Dipole=2.718195,-0.0018515,1.3053607
PG=C01 [X(C1H8Cu1N2O2S1)]

CuCUST8

-1,2
Cu
O,1,1.8722931136
S,1,2.4443627679,2,90.
O,1,1.8454553977,3,90.,2,180.
O,1,2.8854082933,2,90.,3,180.
H,2,0.96955756,1,98.90718518,3,-0.8567508
H,3,1.35104116,1,88.47364311,2,178.67982072
H,4,0.97179126,1,112.24719263,3,-180.38086767
C,5,1.21903454,1,93.52462369,2,0.19540385
H,9,1.10535489,5,121.89044862,1,-0.44347487
H,9,1.11295051,5,120.04341931,10,179.98443711

HF=-2305.6937547
S2=0.757649
S2-1=0.
S2A=0.75002
RMSD=8.141e-09
Dipole=-2.301272,-0.0098057,0.7510511
PG=C01 [X(C1H5Cu103S1)]

CuCUST9

-1,2
Cu
O,1,1.9007963806
S,1,2.4820973816,2,90.
S,1,2.3428121019,3,90.,2,180.
N,1,2.2260596813,2,90.,3,180.
H,2,0.97312465,1,99.99469007,3,0.04675989
H,3,1.35661386,1,92.57994496,2,96.32907025
H,4,1.35125573,1,89.44430573,3,-3.26595382
C,5,1.45057706,1,126.99384177,2,179.63888886
C,5,1.27089809,1,112.47997224,2,1.46793926
H,10,1.10312928,5,122.153547,9,0.03372208
H,10,1.0913558,5,117.8066371,9,180.15301385
H,9,1.10365194,5,112.81233586,10,0.21958219
H,9,1.09508514,5,108.75472937,10,122.40040101
H,9,1.09532607,5,108.80507337,10,-121.85050305

HF=-2648.1371395
S2=0.75493
S2-1=0.
S2A=0.750017
RMSD=8.795e-09
Dipole=-2.97153,-0.1598653,0.3813765
PG=C01 [X(C2H8Cu1N101S2)]

CuCUST10

-1,2
Cu
S,1,2.3112209531
O,1,1.9083360822,2,90.
N,1,2.121718584,3,90.,2,180.
O,1,2.0606488579,2,90.,3,180.
H,2,1.35130204,1,89.20207647,3,0.01118615
H,3,0.9713541,1,115.55122185,2,180.17203255
H,4,1.03641779,1,105.02484417,3,-180.03432624
H,4,1.01800855,1,111.55517233,3,-60.53899077
H,4,1.0180085,1,111.51248837,3,60.48237958
C,5,1.27260626,1,133.11918609,2,179.98357198
H,11,1.1139699,5,114.01374319,1,180.06492356
O,11,1.2549452,5,129.14978069,12,179.99573206

HF=-2361.1476197
S2=0.754242
S2-1=0.
S2A=0.750013
RMSD=5.475e-09
Dipole=0.1763254,0.0017207,-2.2613995
PG=C01 [X(C1H6Cu1N103S1)]

ZnCUSt1

2,1
Zn
N,1,2.1672165302
N,1,2.133845062,2,90.
N,1,2.1485238345,3,90.,2,180.
N,1,2.1341756959,2,90.,3,180.
H,2,1.0238558595,1,113.14143639,3,-40.3198499
H,2,1.0245622913,1,112.80244485,3,79.01833637
H,2,1.023034223,1,113.54172653,3,-161.50286868
C,3,1.4765371533,1,117.03264534,2,112.59061505
C,3,1.2792129264,1,124.34699924,2,-68.70036628
H,10,1.0931021414,3,121.98471852,9,0.46394224
H,10,1.090154159,3,120.58152646,9,180.35839494
H,9,1.094209694,3,111.65491951,10,-0.58510284
H,9,1.095366558,3,109.21255142,10,120.00454837
H,9,1.0937170781,3,109.26439008,10,-121.50793333
C,4,1.4760907382,1,119.40401794,3,124.15354916
C,4,1.278828607,1,122.16106764,3,-57.64925753
H,17,1.0929819979,4,122.0201926,16,0.41898074
H,17,1.0892053579,4,120.40126501,16,180.56859201
H,16,1.0941716929,4,111.56144014,17,2.17424248
H,16,1.0950221099,4,109.23219579,17,122.82109779
H,16,1.0931830233,4,109.44188698,17,-118.66570006
C,5,1.4761666967,1,116.95142627,2,108.57817191
C,5,1.279074002,1,124.3070414,2,-72.59690188
H,24,1.0931602775,5,121.95622579,23,0.20449724
H,24,1.0903036034,5,120.56472847,23,180.00011204
H,23,1.0942454308,5,111.72032168,24,-0.67587349
H,23,1.0953038683,5,109.21759746,24,119.96760872
H,23,1.094302378,5,109.22793286,24,-121.65462817

HF=-2237.4459098
RMSD=9.525e-09
Dipole=0.1267453,0.1938213,0.9136211
PG=C01 [X(C6H18N4Zn1)]

ZnCUSt2

1,1
Zn
O,1,1.8267979994
N,1,2.3597436427,2,90.
N,1,2.08195728,3,90.,2,180.
N,1,2.2339168077,2,90.,3,180.
H,2,0.9677656391,1,116.01388195,3,4.20087126
C,3,1.4668918057,1,116.2410609,2,81.55885397
C,3,1.2746413462,1,123.34508973,2,-82.52741438
H,8,1.0953750765,3,122.60019491,7,0.21419141
H,8,1.0902794281,3,119.94434526,7,180.91481208
H,7,1.0967629445,3,112.51492937,8,-0.0073659
H,7,1.0951053149,3,108.89489592,8,121.37344792
H,7,1.0957524299,3,109.164399,8,-121.16026048
H,4,1.0218535204,1,111.55007023,3,-144.80870749
H,4,1.0219394652,1,111.3534806,3,-24.70127
H,4,1.0223595358,1,113.23385648,3,94.85559242
C,5,1.4693956293,1,113.08012484,2,38.0247252
C,5,1.2739006924,1,126.69331004,2,-127.98646699
H,18,1.0941637831,5,122.52374938,17,1.06437447
H,18,1.090731569,5,120.28930861,17,181.64645934
H,17,1.0959212902,5,111.85941973,18,-0.6852935
H,17,1.0930111223,5,107.70565458,18,121.68460219
H,17,1.0952264028,5,108.75843567,18,-121.77155425

HF=-2179.6346069
RMSD=7.221e-09
Dipole=0.3660972,0.0319065,-2.492888
PG=C01 [X(C4H14N3O1Zn1)]

ZnCUSt3

1,1
Zn
S,1,2.580872368
N,1,2.149367641,2,90.
O,1,1.8466609847,3,90.,2,180.
N,1,2.2329893705,2,90.,3,180.
H,2,1.3486440382,1,103.94650884,3,37.73074991
H,2,1.3497036016,1,103.50423764,3,136.03001804
C,3,1.4707528487,1,112.65261797,2,129.12999126
C,3,1.2738666139,1,126.05179656,2,-67.63737041
H,9,1.0933278179,3,122.16196784,8,-1.67421019
H,9,1.089988152,3,120.31718054,8,177.60138886
H,8,1.0953361894,3,111.61167356,9,3.67689696
H,8,1.0950134917,3,108.88657348,9,124.66775928

H, 8, 1.0936888801, 3, 107.37040282, 9, -117.98476755
H, 4, 0.9674933419, 1, 117.91793751, 3, -190.46291701
C, 5, 1.4685012461, 1, 115.15949974, 2, 108.44979984
C, 5, 1.2752619218, 1, 124.14237216, 2, -86.42875031
H, 17, 1.0944497165, 5, 122.26760265, 16, 0.42072497
H, 17, 1.0896820686, 5, 120.09063675, 16, 179.82351569
H, 16, 1.0959415891, 5, 112.11521785, 17, -1.35053771
H, 16, 1.0955996735, 5, 108.98225503, 17, 119.54981327
H, 16, 1.0940524285, 5, 108.86886628, 17, -122.99088151

HF=-2522.4534011

RMSD=7.457e-09

Dipole=-0.3442818, 0.3286536, 1.6716931

PG=C01 [X(C4H13N2O1S1Zn1)]

ZnCUSt4

1, 1

Zn

N, 1, 2.1394712135

N, 1, 2.2013349473, 2, 90.

N, 1, 2.1290134747, 3, 90., 2, 180.

O, 1, 1.9390739397, 2, 90., 3, 180.

H, 2, 1.0219984449, 1, 121.52939236, 3, 36.93452109

H, 2, 1.0452606571, 1, 99.85686561, 3, 155.26463367

H, 2, 1.0231630026, 1, 113.89679045, 3, -92.16340639

H, 3, 1.0226440831, 1, 110.47588004, 2, 50.21997289

H, 3, 1.0217767371, 1, 116.92216272, 2, 171.86463527

H, 3, 1.0231177957, 1, 110.78518368, 2, -66.51641069

H, 4, 1.0249292274, 1, 102.25176218, 3, -183.49142

H, 4, 1.0221354983, 1, 115.5257596, 3, -68.37416037

H, 4, 1.0217664726, 1, 118.06494296, 3, 59.76859701

C, 5, 1.3084770585, 1, 132.95336155, 2, 25.08575529

H, 15, 1.1013715027, 5, 113.29104417, 1, 176.57418561

O, 15, 1.2305288265, 5, 126.3197477, 16, 179.85627183

HF=-2138.2110739

RMSD=2.322e-09

Dipole=3.5739648, -0.5763331, -1.6701339

PG=C01 [X(C1H10N3O2Zn1)]

ZnCUSt5

0, 1

Zn

O, 1, 1.889154828

S, 1, 2.4659340568, 2, 90.

N, 1, 2.2032447486, 3, 90., 2, 180.

N, 1, 2.2429222944, 2, 90., 3, 180.

H, 2, 0.9700039211, 1, 103.01546702, 3, 6.34470537

H, 3, 1.3533232394, 1, 90.78864053, 2, 71.43476946

H, 4, 1.0205681011, 1, 119.00696529, 3, -250.97208963

H, 4, 1.0209959397, 1, 118.15947633, 3, -117.29589491

H, 4, 1.0262128042, 1, 94.44194697, 3, -3.2888737
C, 5, 1.4637587685, 1, 112.17873659, 2, 26.00570283
C, 5, 1.2712148768, 1, 126.61661011, 2, -138.55669575
H, 12, 1.0958989914, 5, 122.58502702, 11, 0.74640693
H, 12, 1.0898446839, 5, 119.84541668, 11, 181.11075781
H, 11, 1.0982078851, 5, 111.98682258, 12, 3.42804526
H, 11, 1.094554435, 5, 107.42785704, 12, 127.08296681
H, 11, 1.0955561131, 5, 108.34124662, 12, -117.76686106

HF=-2444.664776
RMSD=6.065e-09
Dipole=-3.1132307, -0.2000031, -2.4864835
PG=C01 [X(C2H10N2O1S1Zn1)]

ZnCUSt6

O, 1
Zn
O, 1, 1.9296293026
S, 1, 2.3948300264, 2, 90.
N, 1, 2.2828657416, 3, 90., 2, 180.
N, 1, 2.1949327923, 2, 90., 3, 180.
H, 2, 0.9668607102, 1, 106.24541341, 3, -22.02823764
H, 3, 1.3484160404, 1, 91.0720979, 2, -31.92770671
C, 4, 1.4616930562, 1, 114.88951439, 3, 60.97717081
C, 4, 1.271783003, 1, 122.53949353, 3, -96.9842452
H, 9, 1.0960239487, 4, 122.57642342, 8, 0.77484264
H, 9, 1.0899105537, 4, 119.77720569, 8, 182.11077562
H, 8, 1.0980498747, 4, 112.35056376, 9, -4.7736256
H, 8, 1.0946198097, 4, 108.35926631, 9, 116.28415926
H, 8, 1.0955440238, 4, 109.00692435, 9, -126.33662916
C, 5, 1.4609300827, 1, 127.83830725, 2, 178.07494722
C, 5, 1.2777633127, 1, 112.81410643, 2, -3.65519979
H, 16, 1.0971242968, 5, 121.01823175, 15, -0.2242183
H, 16, 1.0926827878, 5, 117.46881387, 15, 179.53471262
H, 15, 1.0981000119, 5, 112.01931152, 16, -3.44820062
H, 15, 1.0950337985, 5, 109.48042413, 16, 117.59051011
H, 15, 1.0944028586, 5, 109.36241568, 16, -124.82926089

HF=-2522.0705859
RMSD=8.658e-09
Dipole=-2.9018788, 0.0406571, -2.464776
PG=C01 [X(C4H12N2O1S1Zn1)]

ZnCUSt7

O, 1
Zn
N, 1, 2.0547175126
N, 1, 2.4315774529, 2, 90.
S, 1, 2.244492931, 3, 90., 2, 180.
O, 1, 2.1221061315, 2, 90., 3, 180.
H, 2, 1.0207619887, 1, 114.62081313, 3, 61.94109434

H, 2, 1.0556557826, 1, 103.19666511, 3, 179.88714098
H, 2, 1.0207714626, 1, 114.5878313, 3, -62.20681888
H, 3, 1.0201479517, 1, 128.44110609, 2, -0.12325603
H, 3, 1.0205556491, 1, 102.94939723, 2, 124.93213289
H, 3, 1.0205568061, 1, 102.91764206, 2, -125.14690284
H, 4, 1.3486676244, 1, 90.39534618, 3, -179.98192431
C, 5, 1.2796889936, 1, 131.2491159, 2, 0.12537354
H, 13, 1.1067712489, 5, 114.86180463, 1, 179.93855336
O, 13, 1.2517527677, 5, 127.3190162, 14, 179.9981024

HF=-2480.6738969

RMSD=8.106e-09

Dipole=2.8697818, -0.0019999, 1.4216862

PG=C01 [X(C1H8N2O2S1Zn1)]

ZnCUSt8

-1, 1

Zn

O, 1, 1.8724912254

S, 1, 2.6212703346, 2, 90.

O, 1, 1.8464740711, 3, 90., 2, 180.

O, 1, 2.9162482232, 2, 90., 3, 180.

H, 2, 0.9695575559, 1, 98.90718518, 3, -0.8567508

H, 3, 1.3510411558, 1, 88.47364311, 2, 178.67982072

H, 4, 0.9717912615, 1, 112.24719263, 3, -180.38086767

C, 5, 1.2190345424, 1, 93.52462369, 2, 0.19540385

H, 9, 1.1053548872, 5, 121.89044862, 1, -0.44347487

H, 9, 1.1129505131, 5, 120.04341931, 10, 179.98443711

HF=-2444.5570406

RMSD=8.463e-09

Dipole=-3.4479749, -0.0082924, 0.7202754

PG=C01 [X(C1H5O3S1Zn1)]

ZnCUSt9

-1, 1

Zn

O, 1, 1.8739579956

S, 1, 2.7679875061, 2, 90.

S, 1, 2.2967904212, 3, 90., 2, 180.

N, 1, 2.4366850498, 2, 90., 3, 180.

H, 2, 0.9731246479, 1, 99.99469007, 3, 0.04675989

H, 3, 1.3566138642, 1, 92.57994496, 2, 96.32907025

H, 4, 1.3512557349, 1, 89.44430573, 3, -3.26595382

C, 5, 1.450577058, 1, 126.99384177, 2, 179.63888886

C, 5, 1.2708980929, 1, 112.47997224, 2, 1.46793926

H, 10, 1.1031292838, 5, 122.153547, 9, 0.03372208

H, 10, 1.0913557953, 5, 117.8066371, 9, 180.15301385

H, 9, 1.1036519439, 5, 112.81233586, 10, 0.21958219

H, 9, 1.0950851429, 5, 108.75472937, 10, 122.40040101

H, 9, 1.0953260742, 5, 108.80507337, 10, -121.85050305

HF=-2786.9950983
RMSD=7.077e-09
Dipole=-4.0669478, -0.1312886, 0.1656796
PG=C01 [X(C2H8N101S2Zn1)]

ZnCUSt10

-1,1
Zn
S,1,2.3620922501
O,1,1.9591337245,2,90.
N,1,2.2129711479,3,90.,2,180.
O,1,2.1197221556,2,90.,3,180.
H,2,1.3513020392,1,89.20207647,3,0.01118615
H,3,0.9713541017,1,115.55122185,2,180.17203255
H,4,1.0364177858,1,105.02484417,3,-180.03432624
H,4,1.018008555,1,111.55517233,3,-60.53899077
H,4,1.0180085001,1,111.51248837,3,60.48237958
C,5,1.2726062564,1,133.11918609,2,179.98357198
H,11,1.1139699019,5,114.01374319,1,180.06492356
O,11,1.2549451959,5,129.14978069,12,179.99573206

HF=-2500.0042187
RMSD=6.572e-09
Dipole=0.0713346, 0.0017511, -2.5383632
PG=C01 [X(C1H6N103S1Zn1)]

CdCUSt1

2,1
Cd
N,1,2.3717400687
N,1,2.3484671096,2,90.
N,1,2.3522860683,3,90.,2,180.
N,1,2.3478915735,2,90.,3,180.
H,2,1.02385586,1,113.14143639,3,-40.3198499
H,2,1.02456229,1,112.80244485,3,79.01833637
H,2,1.02303422,1,113.54172653,3,-161.50286868
C,3,1.47653715,1,117.03264534,2,112.59061505
C,3,1.27921293,1,124.34699924,2,-68.70036628
H,10,1.09310214,3,121.98471852,9,0.46394224
H,10,1.09015416,3,120.58152646,9,180.35839494
H,9,1.09420969,3,111.65491951,10,-0.58510284
H,9,1.09536656,3,109.21255142,10,120.00454837
H,9,1.09371708,3,109.26439008,10,-121.50793333
C,4,1.47609074,1,119.40401794,3,124.15354916
C,4,1.27882861,1,122.16106764,3,-57.64925753
H,17,1.092982,4,122.0201926,16,0.41898074
H,17,1.08920536,4,120.40126501,16,180.56859201
H,16,1.09417169,4,111.56144014,17,2.17424248
H,16,1.09502211,4,109.23219579,17,122.82109779
H,16,1.09318302,4,109.44188698,17,-118.66570006

C, 5, 1.4761667, 1, 116.95142627, 2, 108.57817191
C, 5, 1.279074, 1, 124.3070414, 2, -72.59690188
H, 24, 1.09316028, 5, 121.95622579, 23, 0.20449724
H, 24, 1.0903036, 5, 120.56472847, 23, 180.00011204
H, 23, 1.09424543, 5, 111.72032168, 24, -0.67587349
H, 23, 1.09530387, 5, 109.21759746, 24, 119.96760872
H, 23, 1.09430238, 5, 109.22793286, 24, -121.65462817

HF=-625.0066229
RMSD=5.429e-09
Dipole=0.113003, 0.1813845, 0.7976913
PG=C01 [X(C6H18Cd1N4)]

CdCUST2

1, 1
Cd
O, 1, 2.0350739239
N, 1, 2.5553399506, 2, 90.
N, 1, 2.3059717252, 3, 90., 2, 180.
N, 1, 2.4318286707, 2, 90., 3, 180.
H, 2, 0.96776564, 1, 116.01388195, 3, 4.20087126
C, 3, 1.46689181, 1, 116.2410609, 2, 81.55885397
C, 3, 1.27464135, 1, 123.34508973, 2, -82.52741438
H, 8, 1.09537508, 3, 122.60019491, 7, 0.21419141
H, 8, 1.09027943, 3, 119.94434526, 7, 180.91481208
H, 7, 1.09676294, 3, 112.51492937, 8, -0.0073659
H, 7, 1.09510531, 3, 108.89489592, 8, 121.37344792
H, 7, 1.09575243, 3, 109.164399, 8, -121.16026048
H, 4, 1.02185352, 1, 111.55007023, 3, -144.80870749
H, 4, 1.02193947, 1, 111.3534806, 3, -24.70127
H, 4, 1.02235954, 1, 113.23385648, 3, 94.85559242
C, 5, 1.46939563, 1, 113.08012484, 2, 38.0247252
C, 5, 1.27390069, 1, 126.69331004, 2, -127.98646699
H, 18, 1.09416378, 5, 122.52374938, 17, 1.06437447
H, 18, 1.09073157, 5, 120.28930861, 17, 181.64645934
H, 17, 1.09592129, 5, 111.85941973, 18, -0.6852935
H, 17, 1.09301112, 5, 107.70565458, 18, 121.68460219
H, 17, 1.0952264, 5, 108.75843567, 18, -121.77155425

HF=-567.1829276
RMSD=4.925e-09
Dipole=0.3273931, 0.0276192, -2.7075676
PG=C01 [X(C4H14Cd1N301)]

CdCUST3

1, 1
Cd
S, 1, 2.7311022947
N, 1, 2.384753421, 2, 90.
O, 1, 2.04653236, 3, 90., 2, 180.
N, 1, 2.479856757, 2, 90., 3, 180.

H, 2, 1.34864404, 1, 103.94650884, 3, 37.73074991
H, 2, 1.3497036, 1, 103.50423764, 3, 136.03001804
C, 3, 1.47075285, 1, 112.65261797, 2, 129.12999126
C, 3, 1.27386661, 1, 126.05179656, 2, -67.63737041
H, 9, 1.09332782, 3, 122.16196784, 8, -1.67421019
H, 9, 1.08998815, 3, 120.31718054, 8, 177.60138886
H, 8, 1.09533619, 3, 111.61167356, 9, 3.67689696
H, 8, 1.09501349, 3, 108.88657348, 9, 124.66775928
H, 8, 1.09368888, 3, 107.37040282, 9, -117.98476755
H, 4, 0.96749334, 1, 117.91793751, 3, -190.46291701
C, 5, 1.46850125, 1, 115.15949974, 2, 108.44979984
C, 5, 1.27526192, 1, 124.14237216, 2, -86.42875031
H, 17, 1.09444972, 5, 122.26760265, 16, 0.42072497
H, 17, 1.08968207, 5, 120.09063675, 16, 179.82351569
H, 16, 1.09594159, 5, 112.11521785, 17, -1.35053771
H, 16, 1.09559967, 5, 108.98225503, 17, 119.54981327
H, 16, 1.09405243, 5, 108.86886628, 17, -122.99088151

HF=-910.0050353

RMSD=5.340e-09

Dipole=-0.2989981, 0.3359658, 1.9592111

PG=C01 [X(C4H13Cd1N201S1)]

CdCUST4

1, 1

Cd

N, 1, 2.3565057692

N, 1, 2.390217927, 2, 90.

N, 1, 2.3622539602, 3, 90., 2, 180.

O, 1, 2.1069718194, 2, 90., 3, 180.

H, 2, 1.02199844, 1, 121.52939236, 3, 36.93452109

H, 2, 1.04526066, 1, 99.85686561, 3, 155.26463367

H, 2, 1.023163, 1, 113.89679045, 3, -92.16340639

H, 3, 1.02264408, 1, 110.47588004, 2, 50.21997289

H, 3, 1.02177674, 1, 116.92216272, 2, 171.86463527

H, 3, 1.0231178, 1, 110.78518368, 2, -66.51641069

H, 4, 1.02492923, 1, 102.25176218, 3, -183.49142

H, 4, 1.0221355, 1, 115.5257596, 3, -68.37416037

H, 4, 1.02176647, 1, 118.06494296, 3, 59.76859701

C, 5, 1.30847706, 1, 132.95336155, 2, 25.08575529

H, 15, 1.1013715, 5, 113.29104417, 1, 176.57418561

O, 15, 1.23052883, 5, 126.3197477, 16, 179.85627183

HF=-525.7628417

RMSD=6.931e-09

Dipole=3.7786655, -0.5694451, -1.5865081

PG=C01 [X(C1H10Cd1N302)]

CdCUST5

0, 1

Cd

O,1,2.1128512876
S,1,2.5930310692,2,90.
N,1,2.4577535471,3,90.,2,180.
N,1,2.418905144,2,90.,3,180.
H,2,0.97000392,1,103.01546702,3,6.34470537
H,3,1.35332324,1,90.78864053,2,71.43476946
H,4,1.0205681,1,119.00696529,3,-250.97208963
H,4,1.02099594,1,118.15947633,3,-117.29589491
H,4,1.0262128,1,94.44194697,3,-3.2888737
C,5,1.46375877,1,112.17873659,2,26.00570283
C,5,1.27121488,1,126.61661011,2,-138.55669575
H,12,1.09589899,5,122.58502702,11,0.74640693
H,12,1.08984468,5,119.84541668,11,181.11075781
H,11,1.09820789,5,111.98682258,12,3.42804526
H,11,1.09455443,5,107.42785704,12,127.08296681
H,11,1.09555611,5,108.34124662,12,-117.76686106

HF=-832.2164935
RMSD=9.134e-09
Dipole=-3.2146201,-0.2013092,-2.7463115
PG=C01 [X(C2H10Cd1N2O1S1)]

CdCUST6

O,1
Cd
O,1,2.1500386701
S,1,2.5375752675,2,90.
N,1,2.5601897038,3,90.,2,180.
N,1,2.3512722344,2,90.,3,180.
H,2,0.96686071,1,106.24541341,3,-22.02823764
H,3,1.34841604,1,91.0720979,2,-31.92770671
C,4,1.46169306,1,114.88951439,3,60.97717081
C,4,1.271783,1,122.53949353,3,-96.9842452
H,9,1.09602395,4,122.57642342,8,0.77484264
H,9,1.08991055,4,119.77720569,8,182.11077562
H,8,1.09804987,4,112.35056376,9,-4.7736256
H,8,1.09461981,4,108.35926631,9,116.28415926
H,8,1.09554402,4,109.00692435,9,-126.33662916
C,5,1.46093008,1,127.83830725,2,178.07494722
C,5,1.27776331,1,112.81410643,2,-3.65519979
H,16,1.0971243,5,121.01823175,15,-0.2242183
H,16,1.09268279,5,117.46881387,15,179.53471262
H,15,1.09810001,5,112.01931152,16,-3.44820062
H,15,1.0950338,5,109.48042413,16,117.59051011
H,15,1.09440286,5,109.36241568,16,-124.82926089

HF=-909.6237931
RMSD=7.934e-09
Dipole=-3.0414707,0.0305462,-2.7312066
PG=C01 [X(C4H12Cd1N2O1S1)]

CdCUST7

0,1
Cd
N,1,2.2770030487
N,1,2.6244365032,2,90.
S,1,2.4335199643,3,90.,2,180.
O,1,2.2583491531,2,90.,3,180.
H,2,1.02076199,1,114.62081313,3,61.94109434
H,2,1.05565578,1,103.19666511,3,179.88714098
H,2,1.02077146,1,114.5878313,3,-62.20681888
H,3,1.02014795,1,128.44110609,2,-0.12325603
H,3,1.02055565,1,102.94939723,2,124.93213289
H,3,1.02055681,1,102.91764206,2,-125.14690284
H,4,1.34866762,1,90.39534618,3,-179.98192431
C,5,1.27968899,1,131.2491159,2,0.12537354
H,13,1.10677125,5,114.86180463,1,179.93855336
O,13,1.25175277,5,127.3190162,14,179.9981024

HF=-868.2289257
RMSD=7.633e-09
Dipole=3.1448495,-0.0020835,1.5639627
PG=C01 [X(C1H8Cd1N2O2S1)]

CdCUST8

-1,1
Cd
O,1,2.1080409049
S,1,2.7132279741,2,90.
O,1,2.0804995023,3,90.,2,180.
O,1,2.9620024859,2,90.,3,180.
H,2,0.96955756,1,98.90718518,3,-0.8567508
H,3,1.35104116,1,88.47364311,2,178.67982072
H,4,0.97179126,1,112.24719263,3,-180.38086767
C,5,1.21903454,1,93.52462369,2,0.19540385
H,9,1.10535489,5,121.89044862,1,-0.44347487
H,9,1.11295051,5,120.04341931,10,179.98443711

HF=-832.1049535
RMSD=8.548e-09
Dipole=-3.3921023,-0.0081192,0.701078
PG=C01 [X(C1H5Cd1O3S1)]

CdCUST9

-1,1
Cd
O,1,2.1100022443
S,1,2.8212194663,2,90.
S,1,2.5073491048,3,90.,2,180.
N,1,2.5979459462,2,90.,3,180.
H,2,0.97312465,1,99.99469007,3,0.04675989
H,3,1.35661386,1,92.57994496,2,96.32907025

H, 4, 1.35125573, 1, 89.44430573, 3, -3.26595382
C, 5, 1.45057706, 1, 126.99384177, 2, 179.63888886
C, 5, 1.27089809, 1, 112.47997224, 2, 1.46793926
H, 10, 1.10312928, 5, 122.153547, 9, 0.03372208
H, 10, 1.0913558, 5, 117.8066371, 9, 180.15301385
H, 9, 1.10365194, 5, 112.81233586, 10, 0.21958219
H, 9, 1.09508514, 5, 108.75472937, 10, 122.40040101
H, 9, 1.09532607, 5, 108.80507337, 10, -121.85050305

HF=-1174.5507377

RMSD=6.480e-09

Dipole=-4.0544896, -0.1270459, 0.2012265

PG=C01 [X(C2H8Cd1N101S2)]

CdCUST10

-1, 1

Cd

S, 1, 2.541507384

O, 1, 2.1719028409, 2, 90.

N, 1, 2.4207210464, 3, 90., 2, 180.

O, 1, 2.2856398568, 2, 90., 3, 180.

H, 2, 1.35130204, 1, 89.20207647, 3, 0.01118615

H, 3, 0.9713541, 1, 115.55122185, 2, 180.17203255

H, 4, 1.03641779, 1, 105.02484417, 3, -180.03432624

H, 4, 1.01800855, 1, 111.55517233, 3, -60.53899077

H, 4, 1.0180085, 1, 111.51248837, 3, 60.48237958

C, 5, 1.27260626, 1, 133.11918609, 2, 179.98357198

H, 11, 1.1139699, 5, 114.01374319, 1, 180.06492356

O, 11, 1.2549452, 5, 129.14978069, 12, 179.99573206

HF=-887.5575367

RMSD=8.759e-09

Dipole=0.2279684, 0.0017106, -2.6006689

PG=C01 [X(C1H6Cd1N103S1)]

HgCUST1

2, 1

Hg

N, 1, 2.4592198791

N, 1, 2.3620684106, 2, 90.

N, 1, 2.4315789033, 3, 90., 2, 180.

N, 1, 2.3605611815, 2, 90., 3, 180.

H, 2, 1.02385586, 1, 113.14143639, 3, -40.3198499

H, 2, 1.02456229, 1, 112.80244485, 3, 79.01833637

H, 2, 1.02303422, 1, 113.54172653, 3, -161.50286868

C, 3, 1.47653715, 1, 117.03264534, 2, 112.59061505

C, 3, 1.27921293, 1, 124.34699924, 2, -68.70036628

H, 10, 1.09310214, 3, 121.98471852, 9, 0.46394224

H, 10, 1.09015416, 3, 120.58152646, 9, 180.35839494

H, 9, 1.09420969, 3, 111.65491951, 10, -0.58510284

H, 9, 1.09536656, 3, 109.21255142, 10, 120.00454837

H, 9, 1.09371708, 3, 109.26439008, 10, -121.50793333
C, 4, 1.47609074, 1, 119.40401794, 3, 124.15354916
C, 4, 1.27882861, 1, 122.16106764, 3, -57.64925753
H, 17, 1.092982, 4, 122.0201926, 16, 0.41898074
H, 17, 1.08920536, 4, 120.40126501, 16, 180.56859201
H, 16, 1.09417169, 4, 111.56144014, 17, 2.17424248
H, 16, 1.09502211, 4, 109.23219579, 17, 122.82109779
H, 16, 1.09318302, 4, 109.44188698, 17, -118.66570006
C, 5, 1.4761667, 1, 116.95142627, 2, 108.57817191
C, 5, 1.279074, 1, 124.3070414, 2, -72.59690188
H, 24, 1.09316028, 5, 121.95622579, 23, 0.20449724
H, 24, 1.0903036, 5, 120.56472847, 23, 180.00011204
H, 23, 1.09424543, 5, 111.72032168, 24, -0.67587349
H, 23, 1.09530387, 5, 109.21759746, 24, 119.96760872
H, 23, 1.09430238, 5, 109.22793286, 24, -121.65462817

HF=-611.8236605

RMSD=5.354e-09

Dipole=0.1006511, 0.1669235, 0.5183857

PG=C01 [X(C6H18Hg1N4)]

HgCUST2

1, 1

Hg

O, 1, 2.0138742104

N, 1, 2.8428419509, 2, 90.

N, 1, 2.2150022903, 3, 90., 2, 180.

N, 1, 2.6430792064, 2, 90., 3, 180.

H, 2, 0.96776564, 1, 116.01388195, 3, 4.20087126

C, 3, 1.46689181, 1, 116.2410609, 2, 81.55885397

C, 3, 1.27464135, 1, 123.34508973, 2, -82.52741438

H, 8, 1.09537508, 3, 122.60019491, 7, 0.21419141

H, 8, 1.09027943, 3, 119.94434526, 7, 180.91481208

H, 7, 1.09676294, 3, 112.51492937, 8, -0.0073659

H, 7, 1.09510531, 3, 108.89489592, 8, 121.37344792

H, 7, 1.09575243, 3, 109.164399, 8, -121.16026048

H, 4, 1.02185352, 1, 111.55007023, 3, -144.80870749

H, 4, 1.02193947, 1, 111.3534806, 3, -24.70127

H, 4, 1.02235954, 1, 113.23385648, 3, 94.85559242

C, 5, 1.46939563, 1, 113.08012484, 2, 38.0247252

C, 5, 1.27390069, 1, 126.69331004, 2, -127.98646699

H, 18, 1.09416378, 5, 122.52374938, 17, 1.06437447

H, 18, 1.09073157, 5, 120.28930861, 17, 181.64645934

H, 17, 1.09592129, 5, 111.85941973, 18, -0.6852935

H, 17, 1.09301112, 5, 107.70565458, 18, 121.68460219

H, 17, 1.0952264, 5, 108.75843567, 18, -121.77155425

HF=-554.0066056

RMSD=9.536e-09

Dipole=0.250376, 0.0222235, -2.5516287

PG=C01 [X(C4H14Hg1N3O1)]

HgCUST3

1,1
Hg
S,1,2.5882916106
N,1,2.5696321019,2,90.
O,1,2.0402599078,3,90.,2,180.
N,1,2.7352258392,2,90.,3,180.
H,2,1.34864404,1,103.94650884,3,37.73074991
H,2,1.3497036,1,103.50423764,3,136.03001804
C,3,1.47075285,1,112.65261797,2,129.12999126
C,3,1.27386661,1,126.05179656,2,-67.63737041
H,9,1.09332782,3,122.16196784,8,-1.67421019
H,9,1.08998815,3,120.31718054,8,177.60138886
H,8,1.09533619,3,111.61167356,9,3.67689696
H,8,1.09501349,3,108.88657348,9,124.66775928
H,8,1.09368888,3,107.37040282,9,-117.98476755
H,4,0.96749334,1,117.91793751,3,-190.46291701
C,5,1.46850125,1,115.15949974,2,108.44979984
C,5,1.27526192,1,124.14237216,2,-86.42875031
H,17,1.09444972,5,122.26760265,16,0.42072497
H,17,1.08968207,5,120.09063675,16,179.82351569
H,16,1.09594159,5,112.11521785,17,-1.35053771
H,16,1.09559967,5,108.98225503,17,119.54981327
H,16,1.09405243,5,108.86886628,17,-122.99088151

HF=-896.8277481

RMSD=6.731e-09

Dipole=-0.2147406,0.3647959,1.9607972

PG=C01 [X(C4H13Hg1N201S1)]

HgCUST4

1,1
Hg
N,1,2.4722342548
N,1,2.3650627918,2,90.
N,1,2.480180804,3,90.,2,180.
O,1,2.1299948122,2,90.,3,180.
H,2,1.02199844,1,121.52939236,3,36.93452109
H,2,1.04526066,1,99.85686561,3,155.26463367
H,2,1.023163,1,113.89679045,3,-92.16340639
H,3,1.02264408,1,110.47588004,2,50.21997289
H,3,1.02177674,1,116.92216272,2,171.86463527
H,3,1.0231178,1,110.78518368,2,-66.51641069
H,4,1.02492923,1,102.25176218,3,-183.49142
H,4,1.0221355,1,115.5257596,3,-68.37416037
H,4,1.02176647,1,118.06494296,3,59.76859701
C,5,1.30847706,1,132.95336155,2,25.08575529
H,15,1.1013715,5,113.29104417,1,176.57418561
O,15,1.23052883,5,126.3197477,16,179.85627183

HF=-512.57491

RMSD=9.053e-09

Dipole=3.5056685,-0.5009055,-1.4069833

PG=C01 [X(C1H10Hg1N302)]

HgCUST5

O,1
Hg
O,1,2.1759984359
S,1,2.6046230323,2,90.
N,1,2.5743997281,3,90.,2,180.
N,1,2.4751559202,2,90.,3,180.
H,2,0.97000392,1,103.01546702,3,6.34470537
H,3,1.35332324,1,90.78864053,2,71.43476946
H,4,1.0205681,1,119.00696529,3,-250.97208963
H,4,1.02099594,1,118.15947633,3,-117.29589491
H,4,1.0262128,1,94.44194697,3,-3.2888737
C,5,1.46375877,1,112.17873659,2,26.00570283
C,5,1.27121488,1,126.61661011,2,-138.55669575
H,12,1.09589899,5,122.58502702,11,0.74640693
H,12,1.08984468,5,119.84541668,11,181.11075781
H,11,1.09820789,5,111.98682258,12,3.42804526
H,11,1.09455443,5,107.42785704,12,127.08296681
H,11,1.09555611,5,108.34124662,12,-117.76686106

HF=-819.038809
RMSD=7.672e-09
Dipole=-2.920334,-0.2145352,-2.6077298
PG=C01 [X(C2H10Hg1N2O1S1)]

HgCUST6

O,1
Hg
O,1,2.2630509897
S,1,2.4679632155,2,90.
N,1,3.0187682644,3,90.,2,180.
N,1,2.2860131725,2,90.,3,180.
H,2,0.96686071,1,106.24541341,3,-22.02823764
H,3,1.34841604,1,91.0720979,2,-31.92770671
C,4,1.46169306,1,114.88951439,3,60.97717081
C,4,1.271783,1,122.53949353,3,-96.9842452
H,9,1.09602395,4,122.57642342,8,0.77484264
H,9,1.08991055,4,119.77720569,8,182.11077562
H,8,1.09804987,4,112.35056376,9,-4.7736256
H,8,1.09461981,4,108.35926631,9,116.28415926
H,8,1.09554402,4,109.00692435,9,-126.33662916
C,5,1.46093008,1,127.83830725,2,178.07494722
C,5,1.27776331,1,112.81410643,2,-3.65519979
H,16,1.0971243,5,121.01823175,15,-0.2242183
H,16,1.09268279,5,117.46881387,15,179.53471262
H,15,1.09810001,5,112.01931152,16,-3.44820062
H,15,1.0950338,5,109.48042413,16,117.59051011
H,15,1.09440286,5,109.36241568,16,-124.82926089

HF=-896.4491455
RMSD=8.088e-09

Dipole=-2.6171975,0.0130814,-2.4387849
PG=C01 [X(C4H12Hg1N2O1S1)]

HgCUST7

O,1
Hg
N,1,2.2358815687
N,1,2.97784419,2,90.
S,1,2.3891956774,3,90.,2,180.
O,1,2.3578063678,2,90.,3,180.
H,2,1.02076199,1,114.62081313,3,61.94109434
H,2,1.05565578,1,103.19666511,3,179.88714098
H,2,1.02077146,1,114.5878313,3,-62.20681888
H,3,1.02014795,1,128.44110609,2,-0.12325603
H,3,1.02055565,1,102.94939723,2,124.93213289
H,3,1.02055681,1,102.91764206,2,-125.14690284
H,4,1.34866762,1,90.39534618,3,-179.98192431
C,5,1.27968899,1,131.2491159,2,0.12537354
H,13,1.10677125,5,114.86180463,1,179.93855336
O,13,1.25175277,5,127.3190162,14,179.9981024

HF=-855.0585732
RMSD=8.407e-09
Dipole=3.1010553,-0.0021572,1.1788801
PG=C01 [X(C1H8Hg1N2O2S1)]

HgCUST8

-1,1
Hg
O,1,2.0936167903
S,1,2.8475118461,2,90.
O,1,2.0687687388,3,90.,2,180.
O,1,3.2579248979,2,90.,3,180.
H,2,0.96955756,1,98.90718518,3,-0.8567508
H,3,1.35104116,1,88.47364311,2,178.67982072
H,4,0.97179126,1,112.24719263,3,-180.38086767
C,5,1.21903454,1,93.52462369,2,0.19540385
H,9,1.10535489,5,121.89044862,1,-0.44347487
H,9,1.11295051,5,120.04341931,10,179.98443711

HF=-818.9365073
RMSD=7.835e-09
Dipole=-3.6128803,-0.0082232,0.6332278
PG=C01 [X(C1H5Hg1O3S1)]

HgCUST9

-1,1
Hg
O,1,2.0985250337
S,1,2.9811779372,2,90.
S,1,2.4305285966,3,90.,2,180.
N,1,3.0211565466,2,90.,3,180.
H,2,0.97312465,1,99.99469007,3,0.04675989
H,3,1.35661386,1,92.57994496,2,96.32907025
H,4,1.35125573,1,89.44430573,3,-3.26595382
C,5,1.45057706,1,126.99384177,2,179.63888886
C,5,1.27089809,1,112.47997224,2,1.46793926
H,10,1.10312928,5,122.153547,9,0.03372208
H,10,1.0913558,5,117.8066371,9,180.15301385
H,9,1.10365194,5,112.81233586,10,0.21958219
H,9,1.09508514,5,108.75472937,10,122.40040101
H,9,1.09532607,5,108.80507337,10,-121.85050305

HF=-1161.3854196
RMSD=8.024e-09
Dipole=-4.1669628,-0.1159058,-0.0056892
PG=C01 [X(C2H8Hg1N101S2)]

HgCUST10

-1,1
Hg
S,1,2.5435866453
O,1,2.2456793219,2,90.
N,1,2.4753932947,3,90.,2,180.
O,1,2.3721239354,2,90.,3,180.
H,2,1.35130204,1,89.20207647,3,0.01118615
H,3,0.9713541,1,115.55122185,2,180.17203255
H,4,1.03641779,1,105.02484417,3,-180.03432624
H,4,1.01800855,1,111.55517233,3,-60.53899077
H,4,1.0180085,1,111.51248837,3,60.48237958
C,5,1.27260626,1,133.11918609,2,179.98357198
H,11,1.1139699,5,114.01374319,1,180.06492356
O,11,1.2549452,5,129.14978069,12,179.99573206

HF=-874.3753479
RMSD=6.237e-09
Dipole=0.599328,0.0017083,-2.2321393
PG=C01 [X(C1H6Hg1N103S1)]

4. Zn²⁺-specific sites

CoZNSt1

2,4
Co
N,1,2.0888660356

N, 1, 2.10207213, 2, 109.47122063
N, 1, 2.0485504321, 2, 109.47122063, 3, 120.
N, 1, 2.0492092669, 2, 109.47122063, 3, -120.
H, 2, 1.02442568, 1, 114.16934879, 3, 56.11134187
H, 2, 1.02431536, 1, 112.8222358, 3, 176.39093265
H, 2, 1.02473646, 1, 112.87129375, 3, -64.39651998
H, 3, 1.0243902, 1, 114.36800519, 2, 17.4943823
H, 3, 1.0236021, 1, 114.33682581, 2, 139.14615199
H, 3, 1.02467028, 1, 111.47340786, 2, -101.97330702
C, 4, 1.4796565, 1, 116.67325199, 2, 62.28172377
C, 4, 1.2796595, 1, 125.07331685, 2, -116.13359339
H, 13, 1.09239633, 4, 121.87066204, 12, 0.76224853
H, 13, 1.0885295, 4, 120.70028833, 12, 180.93768548
H, 12, 1.09367396, 4, 111.56535168, 13, -4.41811074
H, 12, 1.09488936, 4, 109.08722872, 13, 115.90157689
H, 12, 1.09376459, 4, 109.44005502, 13, -125.49229753
C, 5, 1.47809496, 1, 119.14155561, 2, 24.95557376
C, 5, 1.28032309, 1, 122.28376136, 2, -156.29573288
H, 20, 1.0924549, 5, 121.79979793, 19, -0.16485867
H, 20, 1.0892177, 5, 120.36358217, 19, 179.80396526
H, 19, 1.09375511, 5, 111.53355688, 20, -0.19500588
H, 19, 1.09456055, 5, 109.22816531, 20, 120.2261824
H, 19, 1.09487607, 5, 109.33291293, 20, -120.79393302

HF=-1763.4873759

S2=3.756394

S2-1=0.

S2A=3.750019

RMSD=9.712e-09

Dipole=1.0093965, -0.1907673, 0.3041439

PG=C01 [X(C4H16Co1N4)]

CoZNSt2

1, 4

Co

O, 1, 2.0173302721

N, 1, 2.0929634481, 2, 109.47122063

N, 1, 2.0870686981, 2, 109.47122063, 3, 120.

O, 1, 1.9124617749, 2, 109.47122063, 3, -120.

H, 2, 0.97094331, 1, 131.12865202, 3, -3.64011648

H, 2, 1.01922353, 1, 95.25479326, 3, 119.23132056

H, 3, 1.02320618, 1, 109.53177164, 2, -57.35520837

H, 3, 1.02208298, 1, 116.72419391, 2, 63.64557027

H, 3, 1.02309517, 1, 111.10269384, 2, 186.38114572

H, 4, 1.02333954, 1, 110.89531971, 2, 11.3646775

H, 4, 1.02346664, 1, 108.67023837, 2, 127.85337058

H, 4, 1.02156219, 1, 117.17428168, 2, -111.15252971

C, 5, 1.30044135, 1, 115.69395984, 2, -0.50983559

H, 14, 1.09865482, 5, 114.56874068, 1, 179.95696067

O, 14, 1.24152592, 5, 125.74621316, 15, 180.11380172

HF=-1761.5317986

S2=3.755249

S2-1=0.

S2A=3.750013

RMSD=8.197e-09

Dipole=1.8451535, -2.4213155, -1.038354
PG=C01 [X(C1H9Co1N2O3)]

CoZNSt3

1, 4
Co
O, 1, 2.0750638018
O, 1, 2.0084429425, 2, 109.47122063
N, 1, 2.0724608496, 2, 109.47122063, 3, 120.
O, 1, 1.9057098267, 2, 109.47122063, 3, -120.
H, 2, 0.97288446, 1, 127.54275879, 3, -23.7998906
H, 2, 0.97476752, 1, 117.45730466, 3, 121.55527263
H, 3, 1.02174299, 1, 95.11256783, 2, -116.54027415
H, 3, 0.9714419, 1, 131.17702724, 2, 5.82100624
H, 4, 1.02239336, 1, 115.9542546, 2, -2.86083153
H, 4, 1.02355354, 1, 108.38008344, 2, 117.06740093
H, 4, 1.02307434, 1, 111.79049427, 2, -125.7053997
C, 5, 1.30261568, 1, 115.78749587, 2, 117.54782126
H, 13, 1.09837764, 5, 114.42672255, 1, 180.15927516
O, 13, 1.24018073, 5, 125.69063459, 14, 180.21663432

HF=-1781.3908651
S2=3.754855
S2-1=0.
S2A=3.750011
RMSD=9.938e-09
Dipole=-0.1960301, -2.2160193, 1.8626384
PG=C01 [X(C1H8Co1N104)]

CoZNSt4

1, 4
Co
S, 1, 2.4746001721
N, 1, 2.0864179643, 2, 109.47122063
O, 1, 1.9309905091, 2, 109.47122063, 3, 120.
N, 1, 2.045586354, 2, 109.47122063, 3, -120.
H, 2, 1.35149394, 1, 96.06934422, 3, -164.94456095
H, 2, 1.35467569, 1, 88.2239449, 3, -71.08183872
H, 3, 1.02190648, 1, 113.71655382, 2, -173.66547546
H, 3, 1.02131928, 1, 119.41618834, 2, -45.91989102
H, 3, 1.02599938, 1, 101.35131407, 2, 71.81553998
C, 4, 1.29847211, 1, 106.5027002, 2, -63.35172768
H, 11, 1.09977995, 4, 115.32467539, 1, 180.37163733
O, 11, 1.24157909, 4, 123.4649005, 12, 180.07592545
C, 5, 1.4690867, 1, 122.63723218, 2, 60.79705265
C, 5, 1.27887392, 1, 117.63054214, 2, -119.66829617
H, 15, 1.09319261, 5, 121.64432207, 14, 0.11169967
H, 15, 1.0893423, 5, 119.6099667, 14, 180.05190168
H, 14, 1.09481644, 5, 111.68339335, 15, 0.10004536
H, 14, 1.09449096, 5, 109.19650247, 15, 121.1377848
H, 14, 1.094641, 5, 109.13960632, 15, -120.77218499

HF=-2161.8999745
S2=3.757422
S2-1=0.
S2A=3.750025
RMSD=6.692e-09
Dipole=0.1339537, 2.0587145, -0.541332
PG=C01 [X(C3H11Co1N2O2S1)]

CoZNSt5

O, 4
Co
N, 1, 2.0843247817
N, 1, 2.0844381425, 2, 109.47122063
O, 1, 1.9493795555, 2, 109.47122063, 3, 120.
O, 1, 1.9494378847, 2, 109.47122063, 3, -120.
H, 2, 1.03559668, 1, 97.90476108, 3, -115.14245465
H, 2, 1.01993366, 1, 112.72120504, 3, 130.45588264
H, 2, 1.01865135, 1, 119.43529174, 3, 2.31701294
H, 3, 1.03564876, 1, 97.87339203, 2, -115.48224333
H, 3, 1.01865842, 1, 119.38861174, 2, 1.88142499
H, 3, 1.01991003, 1, 112.80130674, 2, 130.07502773
C, 4, 1.29121875, 1, 119.93758563, 2, -5.27307776
H, 12, 1.10502965, 4, 113.75768691, 1, 179.01057226
O, 12, 1.24171014, 4, 127.14734682, 1, -0.99609502
C, 5, 1.2912072, 1, 119.94848738, 2, 115.17722342
H, 15, 1.10502592, 5, 113.75785918, 1, 178.75595529
O, 15, 1.24171186, 5, 127.1502969, 16, 180.02850844

HF=-1874.5429701
S2=3.755616
S2-1=0.
S2A=3.750015
RMSD=7.469e-09
Dipole=1.5278116, 0.002767, 1.0846353
PG=C01 [X(C2H8Co1N2O4)]

CoZNSt6

O, 4
Co
S, 1, 2.4394280074
S, 1, 2.4391906711, 2, 109.47122063
O, 1, 1.9314603917, 2, 109.47122063, 3, 120.
O, 1, 1.9299000316, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135

C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-2560.188402
S2=3.757318
S2-1=0.
S2A=3.750025
RMSD=7.993e-09
Dipole=0.8587331, -0.3385929, 0.2344246
PG=C01 [X(C2H6Co104S2)]

CoZNSt7

O, 4
Co
O, 1, 1.8876004334
O, 1, 1.893152587, 2, 109.47122063
N, 1, 2.1362457851, 2, 109.47122063, 3, 120.
N, 1, 2.092299542, 2, 109.47122063, 3, -120.
H, 2, 0.96815058, 1, 119.91367715, 3, -187.8588022
H, 3, 0.96956331, 1, 105.18571038, 2, -1.18865874
H, 4, 1.01872976, 1, 123.15206419, 2, 119.40326087
H, 4, 1.02097799, 1, 103.73336664, 2, 242.10408529
H, 4, 1.01998215, 1, 105.14868295, 2, -5.13877245
C, 5, 1.45694664, 1, 125.09840467, 2, -51.66180786
C, 5, 1.27438729, 1, 113.40578598, 2, -244.60748781
H, 12, 1.09664822, 5, 121.98192453, 11, -1.03244758
H, 12, 1.09090322, 5, 118.36094952, 11, 177.63866126
H, 11, 1.09847407, 5, 112.43955543, 12, 1.35375125
H, 11, 1.09571246, 5, 109.24073316, 12, 122.82551499
H, 11, 1.09498189, 5, 108.46902993, 12, -119.85343973

HF=-1725.1335377
S2=3.759758
S2-1=0.
S2A=3.750038
RMSD=2.788e-09
Dipole=-2.697824, 0.1869475, -1.3602897
PG=C01 [X(C2H10Co1N202)]

CoZNSt8

O, 4
Co
S, 1, 2.4399643671
N, 1, 2.0754898644, 2, 109.47122063
O, 1, 1.9492751575, 2, 109.47122063, 3, 120.
O, 1, 1.9344392157, 2, 109.47122063, 3, -120.
H, 2, 1.43163488, 1, 77.13840245, 3, -128.17504082
H, 2, 1.35163013, 1, 96.95911806, 3, -36.83805
H, 3, 1.03733852, 1, 97.54654413, 2, -117.5808632
H, 3, 1.01882487, 1, 118.39594959, 2, -1.21840977

H, 3, 1.02010264, 1, 114.05013256, 2, 127.60097468
C, 4, 1.28452295, 1, 121.96223347, 2, 9.38528353
H, 11, 1.10296596, 4, 114.55752691, 1, 175.96518785
O, 11, 1.24907245, 4, 127.39697748, 1, -4.15863711
C, 5, 1.29262228, 1, 120.08902168, 2, 116.69524133
H, 14, 1.10425989, 5, 113.61980985, 1, 180.03422492
O, 14, 1.24083007, 5, 127.11559119, 15, 180.10715411

HF=-2217.3656853

S2=3.756453

S2-1=0.

S2A=3.750019

RMSD=7.860e-09

Dipole=1.5738177, -0.7300202, 0.3019276

PG=C01 [X(C2H7Co1N104S1)]

CoZNSt9

-1, 4

Co

O, 1, 1.9266650602

O, 1, 1.9236338198, 2, 109.47122063

S, 1, 2.4106127425, 2, 109.47122063, 3, 120.

N, 1, 2.0730435963, 2, 109.47122063, 3, -120.

H, 2, 0.96969148, 1, 103.66933231, 3, -116.44634523

H, 3, 0.97083858, 1, 101.51299369, 2, 7.32444724

H, 4, 1.3520271, 1, 89.8894525, 2, -124.8992094

C, 5, 1.45162008, 1, 115.84667301, 2, 51.06091492

C, 5, 1.26881885, 1, 122.67778355, 2, -128.38208859

H, 10, 1.09992247, 5, 122.15918362, 9, 0.12338099

H, 10, 1.09099503, 5, 118.29662417, 9, 180.26177816

H, 9, 1.10195253, 5, 112.73836302, 10, 1.03010974

H, 9, 1.09537352, 5, 107.9883618, 10, 123.23161644

H, 9, 1.09539491, 5, 108.05158913, 10, -120.95295109

HF=-2067.445471

S2=3.765845

S2-1=0.

S2A=3.750088

RMSD=8.603e-09

Dipole=-1.2822427, 2.8627177, -0.6698372

PG=C01 [X(C2H8Co1N102S1)]

CoZNSt10

-1, 4

Co

O, 1, 1.9586734996

O, 1, 1.9578908546, 2, 109.47122063

O, 1, 1.9495420827, 2, 109.47122063, 3, 120.

N, 1, 2.3358226567, 2, 109.47122063, 3, -120.

H, 2, 0.97076301, 1, 103.56159834, 3, -137.21919961

H, 3, 0.97077605, 1, 103.88683657, 2, -221.1634143

H, 4, 0.96973292, 1, 102.21060079, 2, -62.11264818
H, 5, 1.01763487, 1, 107.56225512, 2, 118.74546329
H, 5, 1.01763892, 1, 107.62403392, 2, 0.46922129
H, 5, 1.01729358, 1, 111.96105841, 2, 239.57953692

HF=-1667.0191786

S2=3.761053

S2-1=0.

S2A=3.750049

RMSD=4.150e-09

Dipole=-1.5430125, 1.5635648, -1.1215986

PG=C01 [X(Co1H6N103)]

NiZNSt1

2, 3

Ni

N, 1, 2.1934379865

N, 1, 2.0710723226, 2, 109.47122063

N, 1, 2.0184626863, 2, 109.47122063, 3, 120.

N, 1, 2.0073801038, 2, 109.47122063, 3, -120.

H, 2, 1.02442568, 1, 114.16934879, 3, 56.11134187

H, 2, 1.02431536, 1, 112.8222358, 3, 176.39093265

H, 2, 1.02473646, 1, 112.87129375, 3, -64.39651998

H, 3, 1.0243902, 1, 114.36800519, 2, 17.4943823

H, 3, 1.0236021, 1, 114.33682581, 2, 139.14615199

H, 3, 1.02467028, 1, 111.47340786, 2, -101.97330702

C, 4, 1.4796565, 1, 116.67325199, 2, 62.28172377

C, 4, 1.2796595, 1, 125.07331685, 2, -116.13359339

H, 13, 1.09239633, 4, 121.87066204, 12, 0.76224853

H, 13, 1.0885295, 4, 120.70028833, 12, 180.93768548

H, 12, 1.09367396, 4, 111.56535168, 13, -4.41811074

H, 12, 1.09488936, 4, 109.08722872, 13, 115.90157689

H, 12, 1.09376459, 4, 109.44005502, 13, -125.49229753

C, 5, 1.47809496, 1, 119.14155561, 2, 24.95557376

C, 5, 1.28032309, 1, 122.28376136, 2, -156.29573288

H, 20, 1.0924549, 5, 121.79979793, 19, -0.16485867

H, 20, 1.0892177, 5, 120.36358217, 19, 179.80396526

H, 19, 1.09375511, 5, 111.53355688, 20, -0.19500588

H, 19, 1.09456055, 5, 109.22816531, 20, 120.2261824

H, 19, 1.09487607, 5, 109.33291293, 20, -120.79393302

HF=-1889.0024428

S2=2.0045

S2-1=0.

S2A=2.000013

RMSD=7.971e-09

Dipole=0.9401377, -0.1772593, 0.1735283

PG=C01 [X(C4H16N4Ni1)]

NiZNSt2

1, 3

Ni
O, 1, 2.0822307453
N, 1, 2.039274314, 2, 109.47122063
N, 1, 2.080630311, 2, 109.47122063, 3, 120.
O, 1, 1.9004052461, 2, 109.47122063, 3, -120.
H, 2, 0.97094331, 1, 131.12865202, 3, -3.64011648
H, 2, 1.01922353, 1, 95.25479326, 3, 119.23132056
H, 3, 1.02320618, 1, 109.53177164, 2, -57.35520837
H, 3, 1.02208298, 1, 116.72419391, 2, 63.64557027
H, 3, 1.02309517, 1, 111.10269384, 2, 186.38114572
H, 4, 1.02333954, 1, 110.89531971, 2, 11.3646775
H, 4, 1.02346664, 1, 108.67023837, 2, 127.85337058
H, 4, 1.02156219, 1, 117.17428168, 2, -111.15252971
C, 5, 1.30044135, 1, 115.69395984, 2, -0.50983559
H, 14, 1.09865482, 5, 114.56874068, 1, 179.95696067
O, 14, 1.24152592, 5, 125.74621316, 15, 180.11380172

HF=-1887.046669
S2=2.003584
S2-1=0.
S2A=2.000008
RMSD=8.343e-09
Dipole=1.8595016, -2.4110008, -1.0629977
PG=C01 [X(C1H9N2Ni103)]

NiZNSt3

1, 3
Ni
O, 1, 2.2034566525
O, 1, 1.9769670043, 2, 109.47122063
N, 1, 2.0216482229, 2, 109.47122063, 3, 120.
O, 1, 1.8918807135, 2, 109.47122063, 3, -120.
H, 2, 0.97288446, 1, 127.54275879, 3, -23.7998906
H, 2, 0.97476752, 1, 117.45730466, 3, 121.55527263
H, 3, 1.02174299, 1, 95.11256783, 2, -116.54027415
H, 3, 0.9714419, 1, 131.17702724, 2, 5.82100624
H, 4, 1.02239336, 1, 115.9542546, 2, -2.86083153
H, 4, 1.02355354, 1, 108.38008344, 2, 117.06740093
H, 4, 1.02307434, 1, 111.79049427, 2, -125.7053997
C, 5, 1.30261568, 1, 115.78749587, 2, 117.54782126
H, 13, 1.09837764, 5, 114.42672255, 1, 180.15927516
O, 13, 1.24018073, 5, 125.69063459, 14, 180.21663432

HF=-1906.9084599
S2=2.003749
S2-1=0.
S2A=2.000009
RMSD=3.307e-09
Dipole=-0.2384756, -2.1365595, 1.7051476
PG=C01 [X(C1H8N1Ni104)]

NiZNSt4

1,3
Ni
S,1,2.6311631729
N,1,2.041017069,2,109.47122063
O,1,1.9181625763,2,109.47122063,3,120.
N,1,2.0025320051,2,109.47122063,3,-120.
H,2,1.35149394,1,96.06934422,3,-164.94456095
H,2,1.35467569,1,88.2239449,3,-71.08183872
H,3,1.02190648,1,113.71655382,2,-173.66547546
H,3,1.02131928,1,119.41618834,2,-45.91989102
H,3,1.02599938,1,101.35131407,2,71.81553998
C,4,1.29847211,1,106.5027002,2,-63.35172768
H,11,1.09977995,4,115.32467539,1,180.37163733
O,11,1.24157909,4,123.4649005,12,180.07592545
C,5,1.4690867,1,122.63723218,2,60.79705265
C,5,1.27887392,1,117.63054214,2,-119.66829617
H,15,1.09319261,5,121.64432207,14,0.11169967
H,15,1.0893423,5,119.6099667,14,180.05190168
H,14,1.09481644,5,111.68339335,15,0.10004536
H,14,1.09449096,5,109.19650247,15,121.1377848
H,14,1.094641,5,109.13960632,15,-120.77218499

HF=-2287.4189081
S2=2.004751
S2-1=0.
S2A=2.000014
RMSD=4.929e-09
Dipole=0.1288012,2.0635759,-0.7361696
PG=C01 [X(C3H11N2Ni102S1)]

NiZNSt5

0,3
Ni
N,1,2.0326032337
N,1,2.0326771662,2,109.47122063
O,1,1.9710420075,2,109.47122063,3,120.
O,1,1.9712737403,2,109.47122063,3,-120.
H,2,1.03559668,1,97.90476108,3,-115.14245465
H,2,1.01993366,1,112.72120504,3,130.45588264
H,2,1.01865135,1,119.43529174,3,2.31701294
H,3,1.03564876,1,97.87339203,2,-115.48224333
H,3,1.01865842,1,119.38861174,2,1.88142499
H,3,1.01991003,1,112.80130674,2,130.07502773
C,4,1.29121875,1,119.93758563,2,-5.27307776
H,12,1.10502965,4,113.75768691,1,179.01057226
O,12,1.24171014,4,127.14734682,1,-0.99609502
C,5,1.2912072,1,119.94848738,2,115.17722342
H,15,1.10502592,5,113.75785918,1,178.75595529
O,15,1.24171186,5,127.1502969,16,180.02850844

HF=-2000.0588658
S2=2.004046
S2-1=0.
S2A=2.00001
RMSD=6.597e-09

Dipole=1.5622744,0.0021901,1.1091831
PG=C01 [X(C2H8N2Ni104)]

NiZNSt6

O,3
Ni
S,1,2.5573416994
S,1,2.3952064792,2,109.47122063
O,1,1.9134791979,2,109.47122063,3,120.
O,1,1.9145248764,2,109.47122063,3,-120.
H,2,1.38163488,1,79.86205016,3,-125.74009116
H,2,1.35163013,1,96.26799792,3,-33.30594799
H,3,1.3816,1,79.76133275,2,-117.48390186
H,3,1.3516,1,93.30923331,2,148.57920331
C,4,1.29071169,1,123.55601327,2,6.09180548
H,10,1.10336764,4,113.85514644,1,177.31743037
O,10,1.24276687,4,127.38248639,1,-2.71399135
C,5,1.28915861,1,123.41582602,2,116.90915221
H,13,1.10314255,5,113.94759476,1,179.92846939
O,13,1.24429984,5,127.38196656,14,180.09132496

HF=-2685.7044773
S2=2.005206
S2-1=0.
S2A=2.000016
RMSD=4.314e-09
Dipole=0.9234086,-0.1943949,0.0448965
PG=C01 [X(C2H6Ni104S2)]

NiZNSt7

O,3
Ni
O,1,1.8752263374
O,1,1.8742319576,2,109.47122063
N,1,2.3121538336,2,109.47122063,3,120.
N,1,2.0303324091,2,109.47122063,3,-120.
H,2,0.96815058,1,119.91367715,3,-187.8588022
H,3,0.96956331,1,105.18571038,2,-1.18865874
H,4,1.01872976,1,123.15206419,2,119.40326087
H,4,1.02097799,1,103.73336664,2,242.10408529
H,4,1.01998215,1,105.14868295,2,-5.13877245
C,5,1.45694664,1,125.09840467,2,-51.66180786
C,5,1.27438729,1,113.40578598,2,-244.60748781
H,12,1.09664822,5,121.98192453,11,-1.03244758
H,12,1.09090322,5,118.36094952,11,177.63866126
H,11,1.09847407,5,112.43955543,12,1.35375125
H,11,1.09571246,5,109.24073316,12,122.82551499
H,11,1.09498189,5,108.46902993,12,-119.85343973

HF=-1850.6503124
S2=2.005954

S2-1=0.
S2A=2.000021
RMSD=9.294e-09
Dipole=-2.5843841, 0.3416481, -1.3495851
PG=C01 [X(C2H10N2Ni102)]

NiZNSt8

0, 3
Ni
S, 1, 2.5515444231
N, 1, 2.0223603973, 2, 109.47122063
O, 1, 1.9334269093, 2, 109.47122063, 3, 120.
O, 1, 1.9222283036, 2, 109.47122063, 3, -120.
H, 2, 1.43163488, 1, 77.13840245, 3, -128.17504082
H, 2, 1.35163013, 1, 96.95911806, 3, -36.83805
H, 3, 1.03733852, 1, 97.54654413, 2, -117.5808632
H, 3, 1.01882487, 1, 118.39594959, 2, -1.21840977
H, 3, 1.02010264, 1, 114.05013256, 2, 127.60097468
C, 4, 1.28452295, 1, 121.96223347, 2, 9.38528353
H, 11, 1.10296596, 4, 114.55752691, 1, 175.96518785
O, 11, 1.24907245, 4, 127.39697748, 1, -4.15863711
C, 5, 1.29262228, 1, 120.08902168, 2, 116.69524133
H, 14, 1.10425989, 5, 113.61980985, 1, 180.03422492
O, 14, 1.24083007, 5, 127.11559119, 15, 180.10715411

HF=-2342.8822163
S2=2.004371
S2-1=0.
S2A=2.000012
RMSD=6.081e-09
Dipole=1.6124091, -0.5930015, 0.1658329
PG=C01 [X(C2H7N1Ni104S1)]

NiZNSt9

-1, 3
Ni
O, 1, 1.9052257878
O, 1, 1.8994989278, 2, 109.47122063
S, 1, 2.3476741874, 2, 109.47122063, 3, 120.
N, 1, 2.3562062716, 2, 109.47122063, 3, -120.
H, 2, 0.96969148, 1, 103.66933231, 3, -116.44634523
H, 3, 0.97083858, 1, 101.51299369, 2, 7.32444724
H, 4, 1.3520271, 1, 89.8894525, 2, -124.8992094
C, 5, 1.45162008, 1, 115.84667301, 2, 51.06091492
C, 5, 1.26881885, 1, 122.67778355, 2, -128.38208859
H, 10, 1.09992247, 5, 122.15918362, 9, 0.12338099
H, 10, 1.09099503, 5, 118.29662417, 9, 180.26177816
H, 9, 1.10195253, 5, 112.73836302, 10, 1.03010974
H, 9, 1.09537352, 5, 107.9883618, 10, 123.23161644
H, 9, 1.09539491, 5, 108.05158913, 10, -120.95295109

HF=-2192.962544
S2=2.006851
S2-1=0.
S2A=2.000027
RMSD=4.121e-09
Dipole=-1.3520898,2.8098255,-0.7354677
PG=C01 [X(C2H8N1Ni102S1)]

NiZnSt10

-1,3
Ni
O,1,1.9204692116
O,1,1.9214557773,2,109.47122063
O,1,1.9283778351,2,109.47122063,3,120.
N,1,2.3939622373,2,109.47122063,3,-120.
H,2,0.97076301,1,103.56159834,3,-137.21919961
H,3,0.97077605,1,103.88683657,2,-221.1634143
H,4,0.96973292,1,102.21060079,2,-62.11264818
H,5,1.01763487,1,107.56225512,2,118.74546329
H,5,1.01763892,1,107.62403392,2,0.46922129
H,5,1.01729358,1,111.96105841,2,239.57953692

HF=-1792.5552747
S2=2.00537
S2-1=0.
S2A=2.000018
RMSD=7.656e-09
Dipole=-1.4959264,1.5469875,-1.083403
PG=C01 [X(H6N1Ni103)]

CuZnSt1

2,2
Cu
N,1,2.1338878428
N,1,2.1600284349,2,109.47122063
N,1,2.0352559909,2,109.47122063,3,120.
N,1,1.9668447677,2,109.47122063,3,-120.
H,2,1.02442568,1,114.16934879,3,56.11134187
H,2,1.02431536,1,112.8222358,3,176.39093265
H,2,1.02473646,1,112.87129375,3,-64.39651998
H,3,1.0243902,1,114.36800519,2,17.4943823
H,3,1.0236021,1,114.33682581,2,139.14615199
H,3,1.02467028,1,111.47340786,2,-101.97330702
C,4,1.4796565,1,116.67325199,2,62.28172377
C,4,1.2796595,1,125.07331685,2,-116.13359339
H,13,1.09239633,4,121.87066204,12,0.76224853
H,13,1.0885295,4,120.70028833,12,180.93768548
H,12,1.09367396,4,111.56535168,13,-4.41811074
H,12,1.09488936,4,109.08722872,13,115.90157689
H,12,1.09376459,4,109.44005502,13,-125.49229753
C,5,1.47809496,1,119.14155561,2,24.95557376

C, 5, 1.28032309, 1, 122.28376136, 2, -156.29573288
H, 20, 1.0924549, 5, 121.79979793, 19, -0.16485867
H, 20, 1.0892177, 5, 120.36358217, 19, 179.80396526
H, 19, 1.09375511, 5, 111.53355688, 20, -0.19500588
H, 19, 1.09456055, 5, 109.22816531, 20, 120.2261824
H, 19, 1.09487607, 5, 109.33291293, 20, -120.79393302

HF=-2021.161927
S2=0.752686
S2-1=0.
S2A=0.750006
RMSD=4.959e-09
Dipole=0.655634, 0.0152202, 0.0678144
PG=C01 [X(C4H16Cu1N4)]

CuZNSt2

1, 2
Cu
O, 1, 2.0478367698
N, 1, 2.1483890239, 2, 109.47122063
N, 1, 2.0891065733, 2, 109.47122063, 3, 120.
O, 1, 1.8829710177, 2, 109.47122063, 3, -120.
H, 2, 0.97094331, 1, 131.12865202, 3, -3.64011648
H, 2, 1.01922353, 1, 95.25479326, 3, 119.23132056
H, 3, 1.02320618, 1, 109.53177164, 2, -57.35520837
H, 3, 1.02208298, 1, 116.72419391, 2, 63.64557027
H, 3, 1.02309517, 1, 111.10269384, 2, 186.38114572
H, 4, 1.02333954, 1, 110.89531971, 2, 11.3646775
H, 4, 1.02346664, 1, 108.67023837, 2, 127.85337058
H, 4, 1.02156219, 1, 117.17428168, 2, -111.15252971
C, 5, 1.30044135, 1, 115.69395984, 2, -0.50983559
H, 14, 1.09865482, 5, 114.56874068, 1, 179.95696067
O, 14, 1.24152592, 5, 125.74621316, 15, 180.11380172

HF=-2019.2093986
S2=0.752525
S2-1=0.
S2A=0.750004
RMSD=8.801e-09
Dipole=1.5327456, -1.985975, -1.0573048
PG=C01 [X(C1H9Cu1N2O3)]

CuZNSt3

1, 2
Cu
O, 1, 2.1585140491
O, 1, 2.0422319955, 2, 109.47122063
N, 1, 2.0481883316, 2, 109.47122063, 3, 120.
O, 1, 1.8785818971, 2, 109.47122063, 3, -120.
H, 2, 0.97288446, 1, 127.54275879, 3, -23.7998906
H, 2, 0.97476752, 1, 117.45730466, 3, 121.55527263

H, 3, 1.02174299, 1, 95.11256783, 2, -116.54027415
H, 3, 0.9714419, 1, 131.17702724, 2, 5.82100624
H, 4, 1.02239336, 1, 115.9542546, 2, -2.86083153
H, 4, 1.02355354, 1, 108.38008344, 2, 117.06740093
H, 4, 1.02307434, 1, 111.79049427, 2, -125.7053997
C, 5, 1.30261568, 1, 115.78749587, 2, 117.54782126
H, 13, 1.09837764, 5, 114.42672255, 1, 180.15927516
O, 13, 1.24018073, 5, 125.69063459, 14, 180.21663432

HF=-2039.0710964

S2=0.752596

S2-1=0.

S2A=0.750004

RMSD=8.255e-09

Dipole=-0.3288854, -1.8148128, 1.5424282

PG=C01 [X(C1H8Cu1N104)]

CuZNSt4

1, 2

Cu

S, 1, 2.5719713659

N, 1, 2.1533898687, 2, 109.47122063

O, 1, 1.9155008005, 2, 109.47122063, 3, 120.

N, 1, 2.001829345, 2, 109.47122063, 3, -120.

H, 2, 1.35149394, 1, 96.06934422, 3, -164.94456095

H, 2, 1.35467569, 1, 88.2239449, 3, -71.08183872

H, 3, 1.02190648, 1, 113.71655382, 2, -173.66547546

H, 3, 1.02131928, 1, 119.41618834, 2, -45.91989102

H, 3, 1.02599938, 1, 101.35131407, 2, 71.81553998

C, 4, 1.29847211, 1, 106.5027002, 2, -63.35172768

H, 11, 1.09977995, 4, 115.32467539, 1, 180.37163733

O, 11, 1.24157909, 4, 123.4649005, 12, 180.07592545

C, 5, 1.4690867, 1, 122.63723218, 2, 60.79705265

C, 5, 1.27887392, 1, 117.63054214, 2, -119.66829617

H, 15, 1.09319261, 5, 121.64432207, 14, 0.11169967

H, 15, 1.0893423, 5, 119.6099667, 14, 180.05190168

H, 14, 1.09481644, 5, 111.68339335, 15, 0.10004536

H, 14, 1.09449096, 5, 109.19650247, 15, 121.1377848

H, 14, 1.094641, 5, 109.13960632, 15, -120.77218499

HF=-2419.5774296

S2=0.753023

S2-1=0.

S2A=0.750007

RMSD=9.457e-09

Dipole=-0.0620238, 1.853011, -0.7661595

PG=C01 [X(C3H11Cu1N202S1)]

CuZNSt5

0, 2

Cu

N, 1, 2.0701209174
N, 1, 2.0989079433, 2, 109.47122063
O, 1, 1.9393211067, 2, 109.47122063, 3, 120.
O, 1, 1.9533760066, 2, 109.47122063, 3, -120.
H, 2, 1.03559668, 1, 97.90476108, 3, -115.14245465
H, 2, 1.01993366, 1, 112.72120504, 3, 130.45588264
H, 2, 1.01865135, 1, 119.43529174, 3, 2.31701294
H, 3, 1.03564876, 1, 97.87339203, 2, -115.48224333
H, 3, 1.01865842, 1, 119.38861174, 2, 1.88142499
H, 3, 1.01991003, 1, 112.80130674, 2, 130.07502773
C, 4, 1.29121875, 1, 119.93758563, 2, -5.27307776
H, 12, 1.10502965, 4, 113.75768691, 1, 179.01057226
O, 12, 1.24171014, 4, 127.14734682, 1, -0.99609502
C, 5, 1.2912072, 1, 119.94848738, 2, 115.17722342
H, 15, 1.10502592, 5, 113.75785918, 1, 178.75595529
O, 15, 1.24171186, 5, 127.1502969, 16, 180.02850844

HF=-2132.2158524
S2=0.752604
S2-1=0.
S2A=0.750005
RMSD=2.900e-09
Dipole=1.3693593, -0.0973119, 1.0415751
PG=C01 [X(C2H8Cu1N2O4)]

CuZNSt6

O, 2
Cu
S, 1, 2.4955993025
S, 1, 2.4148136711, 2, 109.47122063
O, 1, 1.9583105179, 2, 109.47122063, 3, 120.
O, 1, 1.8970449954, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135
C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-2817.8676241
S2=0.753088
S2-1=0.
S2A=0.750008
RMSD=8.814e-09
Dipole=0.901348, 0.1378658, -0.0793716
PG=C01 [X(C2H6Cu1O4S2)]

CuZNSt7

0,2
 Cu
 0,1,1.8617665684
 0,1,1.8611693571,2,109.47122063
 N,1,2.2309705046,2,109.47122063,3,120.
 N,1,2.2231462908,2,109.47122063,3,-120.
 H,2,0.96815058,1,119.91367715,3,-187.8588022
 H,3,0.96956331,1,105.18571038,2,-1.18865874
 H,4,1.01872976,1,123.15206419,2,119.40326087
 H,4,1.02097799,1,103.73336664,2,242.10408529
 H,4,1.01998215,1,105.14868295,2,-5.13877245
 C,5,1.45694664,1,125.09840467,2,-51.66180786
 C,5,1.27438729,1,113.40578598,2,-244.60748781
 H,12,1.09664822,5,121.98192453,11,-1.03244758
 H,12,1.09090322,5,118.36094952,11,177.63866126
 H,11,1.09847407,5,112.43955543,12,1.35375125
 H,11,1.09571246,5,109.24073316,12,122.82551499
 H,11,1.09498189,5,108.46902993,12,-119.85343973

HF=-1982.8127108
 S2=0.753596
 S2-1=0.
 S2A=0.750009
 RMSD=9.237e-09
 Dipole=-2.404135,0.2043151,-1.3001448
 PG=C01 [X(C2H10Cu1N2O2)]

CuZNSt8

0,2

29	0.139428	-0.070543	0.136380
16	-1.212178	2.006228	-0.277361
7	1.166631	0.123875	1.891772
8	-1.068585	-1.631419	0.249148
8	1.365217	-0.321474	-1.288947
1	-2.181462	0.961991	-0.417494
1	-1.551306	2.240080	1.009965
1	2.124019	0.070184	1.496049
1	1.072839	0.993471	2.414275
1	1.030694	-0.651112	2.541022
6	-2.314316	-1.550406	-0.053490
1	-2.858904	-2.508737	-0.014012
8	-2.951541	-0.525668	-0.376039
6	2.637510	-0.282936	-1.063874
1	3.251721	-0.441335	-1.967779
8	3.199689	-0.094627	0.026151

HF=-2475.04260043
 RMSD=1.875e-08
 S2=0.7528

CuZNSt9

-1,2
Cu
0,1,1.8932332319
0,1,1.8952541632,2,109.47122063
S,1,2.4641074828,2,109.47122063,3,120.
N,1,2.2348636352,2,109.47122063,3,-120.
H,2,0.96969148,1,103.66933231,3,-116.44634523
H,3,0.97083858,1,101.51299369,2,7.32444724
H,4,1.3520271,1,89.8894525,2,-124.8992094
C,5,1.45162008,1,115.84667301,2,51.06091492
C,5,1.26881885,1,122.67778355,2,-128.38208859
H,10,1.09992247,5,122.15918362,9,0.12338099
H,10,1.09099503,5,118.29662417,9,180.26177816
H,9,1.10195253,5,112.73836302,10,1.03010974
H,9,1.09537352,5,107.9883618,10,123.23161644
H,9,1.09539491,5,108.05158913,10,-120.95295109

HF=-2325.1253825
S2=0.754337
S2-1=0.
S2A=0.750014
RMSD=5.427e-09
Dipole=-1.0481586,3.1131707,-0.4692711
PG=C01 [X(C2H8Cu1N102S1)]

CuZNSt10

-1,2
29 0.067169 -0.009220 -0.029033
8 0.727434 1.781743 -0.635713
8 0.524428 -1.316221 -1.312243
8 0.888803 -0.459801 1.677378
7 -2.181880 0.057722 0.211036
1 1.099577 2.172479 0.171266
1 0.809894 -2.075908 -0.779522
1 1.830658 -0.493432 1.448991
1 -2.579937 -0.620675 -0.434649
1 -2.490687 0.994569 -0.039055
1 -2.469576 -0.159490 1.162317

HF=-1924.71243230
RMSD=1.327e-08
S2=0.7534

ZnZNSt1

2,1
Zn
N,1,2.092046578
N,1,2.1014889889,2,109.47122063
N,1,2.0698741107,2,109.47122063,3,120.
N,1,2.0638843509,2,109.47122063,3,-120.

H, 2, 1.0244256839, 1, 114.16934879, 3, 56.11134187
H, 2, 1.0243153586, 1, 112.8222358, 3, 176.39093265
H, 2, 1.0247364646, 1, 112.87129375, 3, -64.39651998
H, 3, 1.0243901963, 1, 114.36800519, 2, 17.4943823
H, 3, 1.0236021031, 1, 114.33682581, 2, 139.14615199
H, 3, 1.0246702752, 1, 111.47340786, 2, -101.97330702
C, 4, 1.4796564991, 1, 116.67325199, 2, 62.28172377
C, 4, 1.2796594982, 1, 125.07331685, 2, -116.13359339
H, 13, 1.0923963252, 4, 121.87066204, 12, 0.76224853
H, 13, 1.0885295008, 4, 120.70028833, 12, 180.93768548
H, 12, 1.0936739555, 4, 111.56535168, 13, -4.41811074
H, 12, 1.0948893584, 4, 109.08722872, 13, 115.90157689
H, 12, 1.0937645872, 4, 109.44005502, 13, -125.49229753
C, 5, 1.4780949609, 1, 119.14155561, 2, 24.95557376
C, 5, 1.2803230884, 1, 122.28376136, 2, -156.29573288
H, 20, 1.0924549043, 5, 121.79979793, 19, -0.16485867
H, 20, 1.0892177027, 5, 120.36358217, 19, 179.80396526
H, 19, 1.0937551055, 5, 111.53355688, 20, -0.19500588
H, 19, 1.0945605454, 5, 109.22816531, 20, 120.2261824
H, 19, 1.0948760686, 5, 109.33291293, 20, -120.79393302

HF=-2160.0651334
RMSD=3.796e-09
Dipole=1.010846, -0.1893998, 0.3045577
PG=C01 [X(C4H16N4Zn1)]

ZnZNSt2

1, 1
Zn
O, 1, 2.0222701245
N, 1, 2.0960110004, 2, 109.47122063
N, 1, 2.0803819195, 2, 109.47122063, 3, 120.
O, 1, 1.9180479507, 2, 109.47122063, 3, -120.
H, 2, 0.9709433122, 1, 131.12865202, 3, -3.64011648
H, 2, 1.0192235329, 1, 95.25479326, 3, 119.23132056
H, 3, 1.0232061824, 1, 109.53177164, 2, -57.35520837
H, 3, 1.0220829768, 1, 116.72419391, 2, 63.64557027
H, 3, 1.0230951729, 1, 111.10269384, 2, 186.38114572
H, 4, 1.0233395433, 1, 110.89531971, 2, 11.3646775
H, 4, 1.0234666396, 1, 108.67023837, 2, 127.85337058
H, 4, 1.021562189, 1, 117.17428168, 2, -111.15252971
C, 5, 1.3004413453, 1, 115.69395984, 2, -0.50983559
H, 14, 1.0986548231, 5, 114.56874068, 1, 179.95696067
O, 14, 1.2415259163, 5, 125.74621316, 15, 180.11380172

HF=-2158.1092144
RMSD=4.875e-09
Dipole=1.907443, -2.5226461, -1.0538322
PG=C01 [X(C1H9N2O3Zn1)]

ZnZNSt3

1,1
Zn
O,1,2.0852679916
O,1,2.0109778068,2,109.47122063
N,1,2.0578107511,2,109.47122063,3,120.
O,1,1.9093362292,2,109.47122063,3,-120.
H,2,0.9728844615,1,127.54275879,3,-23.7998906
H,2,0.9747675208,1,117.45730466,3,121.55527263
H,3,1.0217429938,1,95.11256783,2,-116.54027415
H,3,0.9714419022,1,131.17702724,2,5.82100624
H,4,1.0223933644,1,115.9542546,2,-2.86083153
H,4,1.0235535376,1,108.38008344,2,117.06740093
H,4,1.0230743436,1,111.79049427,2,-125.7053997
C,5,1.302615681,1,115.78749587,2,117.54782126
H,13,1.0983776439,5,114.42672255,1,180.15927516
O,13,1.2401807255,5,125.69063459,14,180.21663432

HF=-2177.9681568
RMSD=4.989e-09
Dipole=-0.1867769,-2.3141363,1.8775408
PG=C01 [X(C1H8N104Zn1)]

ZnZNSt4

1,1
Zn
S,1,2.4984047577
N,1,2.0885302134,2,109.47122063
O,1,1.9462713952,2,109.47122063,3,120.
N,1,2.0605506248,2,109.47122063,3,-120.
H,2,1.351493945,1,96.06934422,3,-164.94456095
H,2,1.3546756927,1,88.2239449,3,-71.08183872
H,3,1.0219064793,1,113.71655382,2,-173.66547546
H,3,1.0213192824,1,119.41618834,2,-45.91989102
H,3,1.0259993807,1,101.35131407,2,71.81553998
C,4,1.29847211,1,106.5027002,2,-63.35172768
H,11,1.0997799467,4,115.32467539,1,180.37163733
O,11,1.2415790857,4,123.4649005,12,180.07592545
C,5,1.4690866991,1,122.63723218,2,60.79705265
C,5,1.2788739164,1,117.63054214,2,-119.66829617
H,15,1.0931926081,5,121.64432207,14,0.11169967
H,15,1.0893422951,5,119.6099667,14,180.05190168
H,14,1.0948164427,5,111.68339335,15,0.10004536
H,14,1.0944909568,5,109.19650247,15,121.1377848
H,14,1.0946409999,5,109.13960632,15,-120.77218499

HF=-2558.4743264
RMSD=7.867e-09
Dipole=0.1422999,2.2528627,-0.5063038
PG=C01 [X(C3H11N202S1Zn1)]

ZnZNSt5

O,1
Zn
N,1,2.0852517329
N,1,2.0853534603,2,109.47122063
O,1,1.9559369845,2,109.47122063,3,120.
O,1,1.9560517397,2,109.47122063,3,-120.
H,2,1.0355966802,1,97.90476108,3,-115.14245465
H,2,1.0199336608,1,112.72120504,3,130.45588264
H,2,1.0186513479,1,119.43529174,3,2.31701294
H,3,1.0356487639,1,97.87339203,2,-115.48224333
H,3,1.0186584186,1,119.38861174,2,1.88142499
H,3,1.0199100263,1,112.80130674,2,130.07502773
C,4,1.2912187505,1,119.93758563,2,-5.27307776
H,12,1.1050296534,4,113.75768691,1,179.01057226
O,12,1.2417101414,4,127.14734682,1,-0.99609502
C,5,1.2912071974,1,119.94848738,2,115.17722342
H,15,1.1050259171,5,113.75785918,1,178.75595529
O,15,1.2417118576,5,127.1502969,16,180.02850844

HF=-2271.1200301
RMSD=7.490e-09
Dipole=1.6140733,0.0026958,1.1457796
PG=C01 [X(C2H8N2O4Zn1)]

ZnZNSt6

O,1
Zn
S,1,2.4578566202
S,1,2.452479758,2,109.47122063
O,1,1.9409697641,2,109.47122063,3,120.
O,1,1.9394734595,2,109.47122063,3,-120.
H,2,1.38163488,1,79.86205016,3,-125.74009116
H,2,1.35163013,1,96.26799792,3,-33.30594799
H,3,1.3816,1,79.76133275,2,-117.48390186
H,3,1.3516,1,93.30923331,2,148.57920331
C,4,1.2907116895,1,123.55601327,2,6.09180548
H,10,1.1033676431,4,113.85514644,1,177.31743037
O,10,1.2427668676,4,127.38248639,1,-2.71399135
C,5,1.2891586094,1,123.41582602,2,116.90915221
H,13,1.1031425475,5,113.94759476,1,179.92846939
O,13,1.2442998438,5,127.38196656,14,180.09132496

HF=-2956.7648226
RMSD=8.926e-09
Dipole=0.9962439,-0.3475684,0.3178687
PG=C01 [X(C2H6O4S2Zn1)]

ZnZNSt7

O,1
Zn
O,1,1.8990320015

O,1,1.8894991874,2,109.47122063
N,1,2.1556494488,2,109.47122063,3,120.
N,1,2.1478166414,2,109.47122063,3,-120.
H,2,0.9681505785,1,119.91367715,3,-187.8588022
H,3,0.96956331,1,105.18571038,2,-1.18865874
H,4,1.0187297626,1,123.15206419,2,119.40326087
H,4,1.0209779923,1,103.73336664,2,242.10408529
H,4,1.019982146,1,105.14868295,2,-5.13877245
C,5,1.4569466361,1,125.09840467,2,-51.66180786
C,5,1.2743872923,1,113.40578598,2,-244.60748781
H,12,1.0966482247,5,121.98192453,11,-1.03244758
H,12,1.0909032249,5,118.36094952,11,177.63866126
H,11,1.0984740659,5,112.43955543,12,1.35375125
H,11,1.0957124555,5,109.24073316,12,122.82551499
H,11,1.0949818894,5,108.46902993,12,-119.85343973

HF=-2121.7072932
RMSD=8.407e-09
Dipole=-2.8172712,0.2537533,-1.4950541
PG=C01 [X(C2H10N2O2Zn1)]

ZnZNSt8

O,1
Zn
S,1,2.4532640255
N,1,2.0771167672,2,109.47122063
O,1,1.9573503532,2,109.47122063,3,120.
O,1,1.9435598867,2,109.47122063,3,-120.
H,2,1.4316348828,1,77.13840245,3,-128.17504082
H,2,1.3516301282,1,96.95911806,3,-36.83805
H,3,1.0373385183,1,97.54654413,2,-117.5808632
H,3,1.0188248698,1,118.39594959,2,-1.21840977
H,3,1.0201026442,1,114.05013256,2,127.60097468
C,4,1.2845229511,1,121.96223347,2,9.38528353
H,11,1.1029659632,4,114.55752691,1,175.96518785
O,11,1.249072452,4,127.39697748,1,-4.15863711
C,5,1.2926222785,1,120.08902168,2,116.69524133
H,14,1.1042598869,5,113.61980985,1,180.03422492
O,14,1.2408300651,5,127.11559119,15,180.10715411

HF=-2613.9423245
RMSD=3.089e-09
Dipole=1.6804672,-0.7475259,0.3929117
PG=C01 [X(C2H7N10S1Zn1)]

ZnZNSt9

-1,1
Zn
O,1,1.9476794609
O,1,1.9388420886,2,109.47122063
S,1,2.4150651266,2,109.47122063,3,120.

N, 1, 2.1649569189, 2, 109.47122063, 3, -120.
H, 2, 0.9696914828, 1, 103.66933231, 3, -116.44634523
H, 3, 0.9708385794, 1, 101.51299369, 2, 7.32444724
H, 4, 1.3520271021, 1, 89.8894525, 2, -124.8992094
C, 5, 1.4516200768, 1, 115.84667301, 2, 51.06091492
C, 5, 1.268818854, 1, 122.67778355, 2, -128.38208859
H, 10, 1.0999224704, 5, 122.15918362, 9, 0.12338099
H, 10, 1.090995031, 5, 118.29662417, 9, 180.26177816
H, 9, 1.1019525349, 5, 112.73836302, 10, 1.03010974
H, 9, 1.0953735152, 5, 107.9883618, 10, 123.23161644
H, 9, 1.0953949131, 5, 108.05158913, 10, -120.95295109

HF=-2464.018206
RMSD=4.427e-09
Dipole=-1.516848, 2.9946521, -0.8479096
PG=C01 [X(C2H8N102S1Zn1)]

ZnZNSt10

-1, 1
Zn
O, 1, 1.9575700466
O, 1, 1.9583708557, 2, 109.47122063
O, 1, 1.9784786618, 2, 109.47122063, 3, 120.
N, 1, 2.1697964762, 2, 109.47122063, 3, -120.
H, 2, 0.9707630056, 1, 103.56159834, 3, -137.21919961
H, 3, 0.9707760513, 1, 103.88683657, 2, -221.1634143
H, 4, 0.9697329173, 1, 102.21060079, 2, -62.11264818
H, 5, 1.0176348704, 1, 107.56225512, 2, 118.74546329
H, 5, 1.0176389153, 1, 107.62403392, 2, 0.46922129
H, 5, 1.0172935838, 1, 111.96105841, 2, 239.57953692

HF=-2063.6107066
RMSD=8.325e-09
Dipole=-1.6245299, 1.8498063, -1.1756054
PG=C01 [X(H6N103Zn1)]

CdZNSt1

2, 1
Cd
N, 1, 2.3211365195
N, 1, 2.3267519474, 2, 109.47122063
N, 1, 2.2979714346, 2, 109.47122063, 3, 120.
N, 1, 2.2930477046, 2, 109.47122063, 3, -120.
H, 2, 1.02442568, 1, 114.16934879, 3, 56.11134187
H, 2, 1.02431536, 1, 112.8222358, 3, 176.39093265
H, 2, 1.02473646, 1, 112.87129375, 3, -64.39651998
H, 3, 1.0243902, 1, 114.36800519, 2, 17.4943823
H, 3, 1.0236021, 1, 114.33682581, 2, 139.14615199
H, 3, 1.02467028, 1, 111.47340786, 2, -101.97330702
C, 4, 1.4796565, 1, 116.67325199, 2, 62.28172377
C, 4, 1.2796595, 1, 125.07331685, 2, -116.13359339

H, 13, 1.09239633, 4, 121.87066204, 12, 0.76224853
H, 13, 1.0885295, 4, 120.70028833, 12, 180.93768548
H, 12, 1.09367396, 4, 111.56535168, 13, -4.41811074
H, 12, 1.09488936, 4, 109.08722872, 13, 115.90157689
H, 12, 1.09376459, 4, 109.44005502, 13, -125.49229753
C, 5, 1.47809496, 1, 119.14155561, 2, 24.95557376
C, 5, 1.28032309, 1, 122.28376136, 2, -156.29573288
H, 20, 1.0924549, 5, 121.79979793, 19, -0.16485867
H, 20, 1.0892177, 5, 120.36358217, 19, 179.80396526
H, 19, 1.09375511, 5, 111.53355688, 20, -0.19500588
H, 19, 1.09456055, 5, 109.22816531, 20, 120.2261824
H, 19, 1.09487607, 5, 109.33291293, 20, -120.79393302

HF=-547.6131487
RMSD=4.326e-09
Dipole=0.8783601, -0.1696878, 0.2515144
PG=C01 [X(C4H16Cd1N4)]

CdZNSt2

1, 1
Cd
O, 1, 2.2633479519
N, 1, 2.3320003964, 2, 109.47122063
N, 1, 2.3168565114, 2, 109.47122063, 3, 120.
O, 1, 2.101196316, 2, 109.47122063, 3, -120.
H, 2, 0.97094331, 1, 131.12865202, 3, -3.64011648
H, 2, 1.01922353, 1, 95.25479326, 3, 119.23132056
H, 3, 1.02320618, 1, 109.53177164, 2, -57.35520837
H, 3, 1.02208298, 1, 116.72419391, 2, 63.64557027
H, 3, 1.02309517, 1, 111.10269384, 2, 186.38114572
H, 4, 1.02333954, 1, 110.89531971, 2, 11.3646775
H, 4, 1.02346664, 1, 108.67023837, 2, 127.85337058
H, 4, 1.02156219, 1, 117.17428168, 2, -111.15252971
C, 5, 1.30044135, 1, 115.69395984, 2, -0.50983559
H, 14, 1.09865482, 5, 114.56874068, 1, 179.95696067
O, 14, 1.24152592, 5, 125.74621316, 15, 180.11380172

HF=-545.6475068
RMSD=9.990e-09
Dipole=2.0103025, -2.7043207, -0.9206969
PG=C01 [X(C1H9Cd1N2O3)]

CdZNSt3

1, 1
Cd
O, 1, 2.3167587009
O, 1, 2.2534379936, 2, 109.47122063
N, 1, 2.2951335699, 2, 109.47122063, 3, 120.
O, 1, 2.0929231712, 2, 109.47122063, 3, -120.
H, 2, 0.97288446, 1, 127.54275879, 3, -23.7998906
H, 2, 0.97476752, 1, 117.45730466, 3, 121.55527263

H, 3, 1.02174299, 1, 95.11256783, 2, -116.54027415
H, 3, 0.9714419, 1, 131.17702724, 2, 5.82100624
H, 4, 1.02239336, 1, 115.9542546, 2, -2.86083153
H, 4, 1.02355354, 1, 108.38008344, 2, 117.06740093
H, 4, 1.02307434, 1, 111.79049427, 2, -125.7053997
C, 5, 1.30261568, 1, 115.78749587, 2, 117.54782126
H, 13, 1.09837764, 5, 114.42672255, 1, 180.15927516
O, 13, 1.24018073, 5, 125.69063459, 14, 180.21663432

HF=-565.5076434

RMSD=5.288e-09

Dipole=-0.0348694, -2.5019264, 1.8665125

PG=C01 [X(C1H8Cd1N104)]

CdZNSt4

1, 1

Cd

S, 1, 2.7137040682

N, 1, 2.323805474, 2, 109.47122063

O, 1, 2.1471097522, 2, 109.47122063, 3, 120.

N, 1, 2.3006493442, 2, 109.47122063, 3, -120.

H, 2, 1.35149394, 1, 96.06934422, 3, -164.94456095

H, 2, 1.35467569, 1, 88.2239449, 3, -71.08183872

H, 3, 1.02190648, 1, 113.71655382, 2, -173.66547546

H, 3, 1.02131928, 1, 119.41618834, 2, -45.91989102

H, 3, 1.02599938, 1, 101.35131407, 2, 71.81553998

C, 4, 1.29847211, 1, 106.5027002, 2, -63.35172768

H, 11, 1.09977995, 4, 115.32467539, 1, 180.37163733

O, 11, 1.24157909, 4, 123.4649005, 12, 180.07592545

C, 5, 1.4690867, 1, 122.63723218, 2, 60.79705265

C, 5, 1.27887392, 1, 117.63054214, 2, -119.66829617

H, 15, 1.09319261, 5, 121.64432207, 14, 0.11169967

H, 15, 1.0893423, 5, 119.6099667, 14, 180.05190168

H, 14, 1.09481644, 5, 111.68339335, 15, 0.10004536

H, 14, 1.09449096, 5, 109.19650247, 15, 121.1377848

H, 14, 1.094641, 5, 109.13960632, 15, -120.77218499

HF=-946.0195419

RMSD=7.441e-09

Dipole=0.2855088, 2.4785527, -0.3750302

PG=C01 [X(C3H11Cd1N202S1)]

CdZNSt5

0, 1

Cd

N, 1, 2.3247745296

N, 1, 2.3248495383, 2, 109.47122063

O, 1, 2.1491197976, 2, 109.47122063, 3, 120.

O, 1, 2.1491549423, 2, 109.47122063, 3, -120.

H, 2, 1.03559668, 1, 97.90476108, 3, -115.14245465

H, 2, 1.01993366, 1, 112.72120504, 3, 130.45588264

H, 2, 1.01865135, 1, 119.43529174, 3, 2.31701294
H, 3, 1.03564876, 1, 97.87339203, 2, -115.48224333
H, 3, 1.01865842, 1, 119.38861174, 2, 1.88142499
H, 3, 1.01991003, 1, 112.80130674, 2, 130.07502773
C, 4, 1.29121875, 1, 119.93758563, 2, -5.27307776
H, 12, 1.10502965, 4, 113.75768691, 1, 179.01057226
O, 12, 1.24171014, 4, 127.14734682, 1, -0.99609502
C, 5, 1.2912072, 1, 119.94848738, 2, 115.17722342
H, 15, 1.10502592, 5, 113.75785918, 1, 178.75595529
O, 15, 1.24171186, 5, 127.1502969, 16, 180.02850844

HF=-658.6556038
RMSD=5.496e-09
Dipole=1.9136212, 0.002826, 1.3578438
PG=C01 [X(C2H8Cd1N2O4)]

CdZNSt6

O, 1
Cd
S, 1, 2.6794761316
S, 1, 2.6739190959, 2, 109.47122063
O, 1, 2.1270273932, 2, 109.47122063, 3, 120.
O, 1, 2.1248975875, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135
C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-1344.3078296
RMSD=9.773e-09
Dipole=1.4216928, -0.3653579, 0.6019329
PG=C01 [X(C2H6Cd1O4S2)]

CdZNSt7

O, 1
Cd
O, 1, 2.1073901155
O, 1, 2.1060007468, 2, 109.47122063
N, 1, 2.4135618353, 2, 109.47122063, 3, 120.
N, 1, 2.41019231, 2, 109.47122063, 3, -120.
H, 2, 0.96815058, 1, 119.91367715, 3, -187.8588022
H, 3, 0.96956331, 1, 105.18571038, 2, -1.18865874
H, 4, 1.01872976, 1, 123.15206419, 2, 119.40326087
H, 4, 1.02097799, 1, 103.73336664, 2, 242.10408529
H, 4, 1.01998215, 1, 105.14868295, 2, -5.13877245

C, 5, 1.45694664, 1, 125.09840467, 2, -51.66180786
C, 5, 1.27438729, 1, 113.40578598, 2, -244.60748781
H, 12, 1.09664822, 5, 121.98192453, 11, -1.03244758
H, 12, 1.09090322, 5, 118.36094952, 11, 177.63866126
H, 11, 1.09847407, 5, 112.43955543, 12, 1.35375125
H, 11, 1.09571246, 5, 109.24073316, 12, 122.82551499
H, 11, 1.09498189, 5, 108.46902993, 12, -119.85343973

HF=-509.2378737

RMSD=7.298e-09

Dipole=-3.030946, 0.248793, -1.6495686

PG=C01 [X(C2H10Cd1N2O2)]

CdZNSt8

O, 1

Cd

S, 1, 2.673644838

N, 1, 2.3141951556, 2, 109.47122063

O, 1, 2.141155548, 2, 109.47122063, 3, 120.

O, 1, 2.1379187796, 2, 109.47122063, 3, -120.

H, 2, 1.43163488, 1, 77.13840245, 3, -128.17504082

H, 2, 1.35163013, 1, 96.95911806, 3, -36.83805

H, 3, 1.03733852, 1, 97.54654413, 2, -117.5808632

H, 3, 1.01882487, 1, 118.39594959, 2, -1.21840977

H, 3, 1.02010264, 1, 114.05013256, 2, 127.60097468

C, 4, 1.28452295, 1, 121.96223347, 2, 9.38528353

H, 11, 1.10296596, 4, 114.55752691, 1, 175.96518785

O, 11, 1.24907245, 4, 127.39697748, 1, -4.15863711

C, 5, 1.29262228, 1, 120.08902168, 2, 116.69524133

H, 14, 1.10425989, 5, 113.61980985, 1, 180.03422492

O, 14, 1.24083007, 5, 127.11559119, 15, 180.10715411

HF=-1001.4808955

RMSD=9.510e-09

Dipole=2.1066023, -0.6130611, 0.6708014

PG=C01 [X(C2H7Cd1N104S1)]

CdZNSt9

-1, 1

Cd

O, 1, 2.1709199096

O, 1, 2.1636250947, 2, 109.47122063

S, 1, 2.5924046477, 2, 109.47122063, 3, 120.

N, 1, 2.4532651848, 2, 109.47122063, 3, -120.

H, 2, 0.96969148, 1, 103.66933231, 3, -116.44634523

H, 3, 0.97083858, 1, 101.51299369, 2, 7.32444724

H, 4, 1.3520271, 1, 89.8894525, 2, -124.8992094

C, 5, 1.45162008, 1, 115.84667301, 2, 51.06091492

C, 5, 1.26881885, 1, 122.67778355, 2, -128.38208859

H, 10, 1.09992247, 5, 122.15918362, 9, 0.12338099

H, 10, 1.09099503, 5, 118.29662417, 9, 180.26177816

H, 9, 1.10195253, 5, 112.73836302, 10, 1.03010974
H, 9, 1.09537352, 5, 107.9883618, 10, 123.23161644
H, 9, 1.09539491, 5, 108.05158913, 10, -120.95295109

HF=-851.5578239
RMSD=8.581e-09
Dipole=-1.6430895, 3.1074977, -0.9532266
PG=C01 [X(C2H8Cd1N102S1)]

CdZNSt10

-1, 1
Cd
O, 1, 2.1797760195
O, 1, 2.1803299481, 2, 109.47122063
O, 1, 2.2007321332, 2, 109.47122063, 3, 120.
N, 1, 2.4489978949, 2, 109.47122063, 3, -120.
H, 2, 0.97076301, 1, 103.56159834, 3, -137.21919961
H, 3, 0.97077605, 1, 103.88683657, 2, -221.1634143
H, 4, 0.96973292, 1, 102.21060079, 2, -62.11264818
H, 5, 1.01763487, 1, 107.56225512, 2, 118.74546329
H, 5, 1.01763892, 1, 107.62403392, 2, 0.46922129
H, 5, 1.01729358, 1, 111.96105841, 2, 239.57953692

HF=-451.1452303
RMSD=8.829e-09
Dipole=-1.7115816, 2.0888536, -1.2350778
PG=C01 [X(Cd1H6N103)]

HgZNSt1

2, 1
Hg
N, 1, 2.3644485578
N, 1, 2.371622466, 2, 109.47122063
N, 1, 2.338418321, 2, 109.47122063, 3, 120.
N, 1, 2.3311350979, 2, 109.47122063, 3, -120.
H, 2, 1.02442568, 1, 114.16934879, 3, 56.11134187
H, 2, 1.02431536, 1, 112.8222358, 3, 176.39093265
H, 2, 1.02473646, 1, 112.87129375, 3, -64.39651998
H, 3, 1.0243902, 1, 114.36800519, 2, 17.4943823
H, 3, 1.0236021, 1, 114.33682581, 2, 139.14615199
H, 3, 1.02467028, 1, 111.47340786, 2, -101.97330702
C, 4, 1.4796565, 1, 116.67325199, 2, 62.28172377
C, 4, 1.2796595, 1, 125.07331685, 2, -116.13359339
H, 13, 1.09239633, 4, 121.87066204, 12, 0.76224853
H, 13, 1.0885295, 4, 120.70028833, 12, 180.93768548
H, 12, 1.09367396, 4, 111.56535168, 13, -4.41811074
H, 12, 1.09488936, 4, 109.08722872, 13, 115.90157689
H, 12, 1.09376459, 4, 109.44005502, 13, -125.49229753
C, 5, 1.47809496, 1, 119.14155561, 2, 24.95557376
C, 5, 1.28032309, 1, 122.28376136, 2, -156.29573288
H, 20, 1.0924549, 5, 121.79979793, 19, -0.16485867

H, 20, 1.0892177, 5, 120.36358217, 19, 179.80396526
H, 19, 1.09375511, 5, 111.53355688, 20, -0.19500588
H, 19, 1.09456055, 5, 109.22816531, 20, 120.2261824
H, 19, 1.09487607, 5, 109.33291293, 20, -120.79393302

HF=-534.4261992
RMSD=6.086e-09
Dipole=0.5461541, -0.1486169, 0.0548731
PG=C01 [X(C4H16Hg1N4)]

HgZNSt2

1, 1
Hg
O, 1, 2.3625830493
N, 1, 2.381915796, 2, 109.47122063
N, 1, 2.361172361, 2, 109.47122063, 3, 120.
O, 1, 2.1469480652, 2, 109.47122063, 3, -120.
H, 2, 0.97094331, 1, 131.12865202, 3, -3.64011648
H, 2, 1.01922353, 1, 95.25479326, 3, 119.23132056
H, 3, 1.02320618, 1, 109.53177164, 2, -57.35520837
H, 3, 1.02208298, 1, 116.72419391, 2, 63.64557027
H, 3, 1.02309517, 1, 111.10269384, 2, 186.38114572
H, 4, 1.02333954, 1, 110.89531971, 2, 11.3646775
H, 4, 1.02346664, 1, 108.67023837, 2, 127.85337058
H, 4, 1.02156219, 1, 117.17428168, 2, -111.15252971
C, 5, 1.30044135, 1, 115.69395984, 2, -0.50983559
H, 14, 1.09865482, 5, 114.56874068, 1, 179.95696067
O, 14, 1.24152592, 5, 125.74621316, 15, 180.11380172

HF=-532.4533634
RMSD=7.173e-09
Dipole=1.8619769, -2.463515, -0.9092361
PG=C01 [X(C1H9Hg1N2O3)]

HgZNSt3

1, 1
Hg
O, 1, 2.4187647187
O, 1, 2.3474588973, 2, 109.47122063
N, 1, 2.3285872258, 2, 109.47122063, 3, 120.
O, 1, 2.1366531554, 2, 109.47122063, 3, -120.
H, 2, 0.97288446, 1, 127.54275879, 3, -23.7998906
H, 2, 0.97476752, 1, 117.45730466, 3, 121.55527263
H, 3, 1.02174299, 1, 95.11256783, 2, -116.54027415
H, 3, 0.9714419, 1, 131.17702724, 2, 5.82100624
H, 4, 1.02239336, 1, 115.9542546, 2, -2.86083153
H, 4, 1.02355354, 1, 108.38008344, 2, 117.06740093
H, 4, 1.02307434, 1, 111.79049427, 2, -125.7053997
C, 5, 1.30261568, 1, 115.78749587, 2, 117.54782126
H, 13, 1.09837764, 5, 114.42672255, 1, 180.15927516
O, 13, 1.24018073, 5, 125.69063459, 14, 180.21663432

HF=-552.3113945
RMSD=7.949e-09
Dipole=-0.0791261, -2.2453639, 1.5519263
PG=C01 [X(C1H8Hg1N104)]

HgZNSt4

1,1
Hg
S,1,2.7531156417
N,1,2.3822315923,2,109.47122063
O,1,2.2064135298,2,109.47122063,3,120.
N,1,2.3455259613,2,109.47122063,3,-120.
H,2,1.35149394,1,96.06934422,3,-164.94456095
H,2,1.35467569,1,88.2239449,3,-71.08183872
H,3,1.02190648,1,113.71655382,2,-173.66547546
H,3,1.02131928,1,119.41618834,2,-45.91989102
H,3,1.02599938,1,101.35131407,2,71.81553998
C,4,1.29847211,1,106.5027002,2,-63.35172768
H,11,1.09977995,4,115.32467539,1,180.37163733
O,11,1.24157909,4,123.4649005,12,180.07592545
C,5,1.4690867,1,122.63723218,2,60.79705265
C,5,1.27887392,1,117.63054214,2,-119.66829617
H,15,1.09319261,5,121.64432207,14,0.11169967
H,15,1.0893423,5,119.6099667,14,180.05190168
H,14,1.09481644,5,111.68339335,15,0.10004536
H,14,1.09449096,5,109.19650247,15,121.1377848
H,14,1.094641,5,109.13960632,15,-120.77218499

HF=-932.831659
RMSD=6.102e-09
Dipole=0.2548701, 2.3969621, -0.3515911
PG=C01 [X(C3H11Hg1N202S1)]

HgZNSt5

0,1
Hg
N,1,2.3841454709
N,1,2.3842689589,2,109.47122063
O,1,2.2014945417,2,109.47122063,3,120.
O,1,2.2015433259,2,109.47122063,3,-120.
H,2,1.03559668,1,97.90476108,3,-115.14245465
H,2,1.01993366,1,112.72120504,3,130.45588264
H,2,1.01865135,1,119.43529174,3,2.31701294
H,3,1.03564876,1,97.87339203,2,-115.48224333
H,3,1.01865842,1,119.38861174,2,1.88142499
H,3,1.01991003,1,112.80130674,2,130.07502773
C,4,1.29121875,1,119.93758563,2,-5.27307776
H,12,1.10502965,4,113.75768691,1,179.01057226
O,12,1.24171014,4,127.14734682,1,-0.99609502
C,5,1.2912072,1,119.94848738,2,115.17722342

H, 15, 1.10502592, 5, 113.75785918, 1, 178.75595529
O, 15, 1.24171186, 5, 127.1502969, 16, 180.02850844

HF=-645.4602269
RMSD=4.886e-09
Dipole=1.9055485, 0.0025834, 1.3520147
PG=C01 [X(C2H8Hg1N2O4)]

HgZNSt6

O, 1
Hg
S, 1, 2.7241961078
S, 1, 2.7206220267, 2, 109.47122063
O, 1, 2.1801782927, 2, 109.47122063, 3, 120.
O, 1, 2.1770295353, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135
C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-1331.1197638
RMSD=6.599e-09
Dipole=1.4156794, -0.3624944, 0.5963678
PG=C01 [X(C2H6Hg1O4S2)]

HgZNSt7

O, 1
Hg
O, 1, 2.1569973753
O, 1, 2.1498374707, 2, 109.47122063
N, 1, 2.5174575439, 2, 109.47122063, 3, 120.
N, 1, 2.5248568448, 2, 109.47122063, 3, -120.
H, 2, 0.96815058, 1, 119.91367715, 3, -187.8588022
H, 3, 0.96956331, 1, 105.18571038, 2, -1.18865874
H, 4, 1.01872976, 1, 123.15206419, 2, 119.40326087
H, 4, 1.02097799, 1, 103.73336664, 2, 242.10408529
H, 4, 1.01998215, 1, 105.14868295, 2, -5.13877245
C, 5, 1.45694664, 1, 125.09840467, 2, -51.66180786
C, 5, 1.27438729, 1, 113.40578598, 2, -244.60748781
H, 12, 1.09664822, 5, 121.98192453, 11, -1.03244758
H, 12, 1.09090322, 5, 118.36094952, 11, 177.63866126
H, 11, 1.09847407, 5, 112.43955543, 12, 1.35375125
H, 11, 1.09571246, 5, 109.24073316, 12, 122.82551499
H, 11, 1.09498189, 5, 108.46902993, 12, -119.85343973

HF=-496.0479564
RMSD=7.054e-09
Dipole=-2.8055237, 0.2184043, -1.4878779
PG=C01 [X(C2H10Hg1N2O2)]

HgZNSt8

0, 1
Hg
S, 1, 2.7133575629
N, 1, 2.373507658, 2, 109.47122063
O, 1, 2.1928543515, 2, 109.47122063, 3, 120.
O, 1, 2.1897143554, 2, 109.47122063, 3, -120.
H, 2, 1.43163488, 1, 77.13840245, 3, -128.17504082
H, 2, 1.35163013, 1, 96.95911806, 3, -36.83805
H, 3, 1.03733852, 1, 97.54654413, 2, -117.5808632
H, 3, 1.01882487, 1, 118.39594959, 2, -1.21840977
H, 3, 1.02010264, 1, 114.05013256, 2, 127.60097468
C, 4, 1.28452295, 1, 121.96223347, 2, 9.38528353
H, 11, 1.10296596, 4, 114.55752691, 1, 175.96518785
O, 11, 1.24907245, 4, 127.39697748, 1, -4.15863711
C, 5, 1.29262228, 1, 120.08902168, 2, 116.69524133
H, 14, 1.10425989, 5, 113.61980985, 1, 180.03422492
O, 14, 1.24083007, 5, 127.11559119, 15, 180.10715411

HF=-988.2888925
RMSD=8.092e-09
Dipole=2.1289921, -0.5549116, 0.6552501
PG=C01 [X(C2H7Hg1N104S1)]

HgZNSt9

-1, 1
Hg
O, 1, 2.2331129731
O, 1, 2.2207803456, 2, 109.47122063
S, 1, 2.6099123316, 2, 109.47122063, 3, 120.
N, 1, 2.6004091764, 2, 109.47122063, 3, -120.
H, 2, 0.96969148, 1, 103.66933231, 3, -116.44634523
H, 3, 0.97083858, 1, 101.51299369, 2, 7.32444724
H, 4, 1.3520271, 1, 89.8894525, 2, -124.8992094
C, 5, 1.45162008, 1, 115.84667301, 2, 51.06091492
C, 5, 1.26881885, 1, 122.67778355, 2, -128.38208859
H, 10, 1.09992247, 5, 122.15918362, 9, 0.12338099
H, 10, 1.09099503, 5, 118.29662417, 9, 180.26177816
H, 9, 1.10195253, 5, 112.73836302, 10, 1.03010974
H, 9, 1.09537352, 5, 107.9883618, 10, 123.23161644
H, 9, 1.09539491, 5, 108.05158913, 10, -120.95295109

HF=-838.3731627
RMSD=6.587e-09
Dipole=-1.4425069, 2.7662813, -0.838124
PG=C01 [X(C2H8Hg1N102S1)]

HgZNSt10

-1,1

Hg

O,1,2.2317701856

O,1,2.2327032892,2,109.47122063

O,1,2.2667923896,2,109.47122063,3,120.

N,1,2.5805871131,2,109.47122063,3,-120.

H,2,0.97076301,1,103.56159834,3,-137.21919961

H,3,0.97077605,1,103.88683657,2,-221.1634143

H,4,0.96973292,1,102.21060079,2,-62.11264818

H,5,1.01763487,1,107.56225512,2,118.74546329

H,5,1.01763892,1,107.62403392,2,0.46922129

H,5,1.01729358,1,111.96105841,2,239.57953692

HF=-437.9540124

RMSD=9.900e-09

Dipole=-1.5611815,1.9338618,-1.1263043

PG=C01 [X(H6Hg1N103)]

5. Cd2+-specific sites

CoCDSt1

2,4

Co

O,1,2.0163013766

O,1,2.0214518927,2,109.47122063

S,1,2.4245679785,2,109.47122063,3,120.

O,1,1.9730066602,2,109.47122063,3,-120.

H,2,0.97710956,1,126.72351565,3,-32.42515075

H,2,0.97756217,1,125.23198546,3,137.32199183

H,3,0.97720206,1,125.08548378,2,128.90568232

H,3,0.97691541,1,127.26501921,2,-43.6894312

H,4,1.35409598,1,98.71271852,2,3.90805121

H,4,1.35439907,1,98.51076654,2,100.10143429

C,5,1.23465919,1,146.23736757,2,123.86702845

H,12,1.09868727,5,121.69940132,1,-2.09235282

H,12,1.09751386,5,118.89820982,13,179.94205073

HF=-2049.1268687

S2=3.75537

S2-1=0.

S2A=3.750013

RMSD=9.300e-09

Dipole=0.7595132,0.8853164,0.4200273

PG=C01 [X(C1H8Co103S1)]

CoCDSt2

2,4
Co
S,1,2.420587473
O,1,2.0219333498,2,109.47122063
O,1,1.9756591249,2,109.47122063,3,120.
O,1,1.983872307,2,109.47122063,3,-120.
H,2,1.35379864,1,99.7819091,3,-18.12579641
H,2,1.35393714,1,100.2118578,3,78.80693391
H,3,0.97744477,1,125.63242174,2,115.40313724
H,3,0.97598732,1,126.75833562,2,-68.51929524
C,4,1.23376805,1,147.69191231,2,68.13943977
H,10,1.09887316,4,121.64827332,1,-0.69344272
H,10,1.09752428,4,118.93131886,11,180.32903525
C,5,1.23366055,1,147.88558831,2,157.60744208
H,13,1.09904483,5,121.69558296,1,-0.62863977
H,13,1.09770407,5,118.96648232,14,179.92854414

HF=-2087.2171898
S2=3.755846
S2-1=0.
S2A=3.750015
RMSD=9.026e-09
Dipole=0.3542477,0.3829661,-1.1073728
PG=C01 [X(C2H8Co103S1)]

CoCDSt3

2,4
Co
S,1,2.4213256482
O,1,1.9795595321,2,109.47122063
O,1,1.982137398,2,109.47122063,3,120.
O,1,1.9779377647,2,109.47122063,3,-120.
H,2,1.35382234,1,99.42346635,3,-24.86006571
H,2,1.35394345,1,99.35041753,3,71.37040763
C,3,1.23439672,1,142.62314323,2,115.8445957
H,8,1.09877467,3,121.73254404,1,0.69876845
H,8,1.09753352,3,118.90990393,9,180.08272977
C,4,1.23419868,1,143.32350114,2,80.31278782
H,11,1.09872769,4,121.76269088,1,2.16299582
H,11,1.09740596,4,118.89863073,12,180.01844807
C,5,1.23372739,1,144.93803684,2,112.4054566
H,14,1.09881591,5,121.71095223,1,1.03525778
H,14,1.09752425,5,118.92338792,15,180.0617941

HF=-2125.3101554
S2=3.757198
S2-1=0.
S2A=3.750023
RMSD=6.759e-09
Dipole=0.2643819,0.0889337,-1.1144103
PG=C01 [X(C3H8Co103S1)]

CoCDSt4

2,4

Co

S,1,2.4341811212

O,1,1.9784622955,2,109.47122063

O,1,1.9922223802,2,109.47122063,3,120.

N,1,2.0623883128,2,109.47122063,3,-120.

H,2,1.35370225,1,100.67403997,3,-47.42763211

H,2,1.35408901,1,99.62884198,3,48.89193922

C,3,1.23388199,1,144.85377957,2,127.8430108

H,8,1.09869892,3,121.67597912,1,-2.16876368

H,8,1.09746485,3,118.92495585,9,179.91268855

C,4,1.23209511,1,151.41275636,2,28.9978892

H,11,1.09950782,4,121.58841047,1,-0.87424889

H,11,1.09801294,4,119.2932244,12,179.8790918

H,5,1.02597301,1,112.96295399,2,158.00819994

H,5,1.02537065,1,113.04635429,2,38.41966235

H,5,1.02551705,1,113.357995,2,-81.86571236

HF=-2067.3645927

S2=3.756686

S2-1=0.

S2A=3.75002

RMSD=9.743e-09

Dipole=-0.147763,-0.2033227,-0.83564

PG=C01 [X(C2H9Co1N102S1)]

CoCDSt5

2,4

Co

S,1,2.4381337976

O,1,2.0255191485,2,109.47122063

O,1,1.9713854469,2,109.47122063,3,120.

N,1,2.0567400597,2,109.47122063,3,-120.

H,2,1.3532682,1,101.52794537,3,-71.45930587

H,2,1.35375954,1,101.36172376,3,25.96769013

H,3,0.97657675,1,125.34039764,2,40.55857074

H,3,0.9772854,1,124.99395005,2,-162.43509427

C,4,1.23078918,1,166.98888266,2,-5.875825

H,10,1.09927299,4,121.0481255,1,1.19440852

H,10,1.09851533,4,119.75500726,11,179.97862286

H,5,1.02591479,1,113.7585246,2,183.68402475

H,5,1.02570578,1,113.14704837,2,62.87609203

H,5,1.02595319,1,112.1546187,2,-56.67361772

HF=-2029.2727891

S2=3.75581

S2-1=0.

S2A=3.750015

RMSD=5.972e-09

Dipole=0.2913515,-0.1906211,-0.8947771

PG=C01 [X(C1H9Co1N102S1)]

CoCDSt6

2,4

Co

O,1,2.0230795277

O,1,2.0228991729,2,109.47122063

S,1,2.4268133448,2,109.47122063,3,120.

S,1,2.426904336,2,109.47122063,3,-120.

H,2,0.97715546,1,126.00530669,3,-137.28671058

H,2,0.97721096,1,126.72613851,3,37.77615189

H,3,0.97717428,1,125.96028173,2,223.41524284

H,3,0.97720322,1,126.74413777,2,38.09497653

H,4,1.35436319,1,98.61472212,2,-175.53081491

H,4,1.35444234,1,100.57257274,2,-79.16407195

H,5,1.35447271,1,100.52722432,2,38.8404492

H,5,1.35436768,1,98.61819189,2,-57.52868001

HF=-2333.9954643

S2=3.755949

S2-1=0.

S2A=3.750016

RMSD=8.237e-09

Dipole=1.1681075,-0.0057592,0.8345326

PG=C01 [X(Co1H802S2)]

CoCDSt7

1,4

Co

O,1,2.0594080542

O,1,1.9965378522,2,109.47122063

S,1,2.4414209071,2,109.47122063,3,120.

O,1,1.9002321392,2,109.47122063,3,-120.

H,2,0.97304987,1,129.08906844,3,-92.60346916

H,2,0.97474217,1,118.79945451,3,114.21728494

H,3,1.02084268,1,95.67672252,2,-119.05786808

H,3,0.97258209,1,126.58711976,2,0.93577882

H,4,1.3523873,1,94.04096012,2,120.26596053

H,4,1.35233137,1,96.0652197,2,215.1457816

C,5,1.30489723,1,115.95687296,2,120.60279574

H,12,1.09833869,5,114.23891506,1,179.81220999

O,12,1.23877975,5,125.70918421,13,180.21989236

HF=-2124.2082208

S2=3.755735

S2-1=0.

S2A=3.750015

RMSD=7.627e-09

Dipole=-0.1927124,-1.4683346,1.7646664

PG=C01 [X(C1H7Co104S1)]

CoCDSt8

1, 4
Co
S, 1, 2.4231430964
N, 1, 2.0808942456, 2, 109.47122063
O, 1, 1.8954500469, 2, 109.47122063, 3, 120.
O, 1, 2.0679500442, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.64107442, 3, -132.34729509
H, 2, 1.35163013, 1, 96.11149781, 3, -39.14270577
H, 3, 1.02324409, 1, 114.14255374, 2, -133.93875655
H, 3, 1.02176858, 1, 114.21620804, 2, -11.14508144
H, 3, 1.02380537, 1, 108.33284024, 2, 107.85234365
C, 4, 1.30526952, 1, 122.86903562, 2, 14.16423746
H, 11, 1.09978935, 4, 113.7139494, 1, 178.97461085
O, 11, 1.23588904, 4, 126.296095, 1, -1.21412678
H, 5, 0.9735806, 1, 124.20061642, 2, 18.55214804
H, 5, 0.97497082, 1, 117.71800181, 2, -121.1507242

HF=-2104.3425007
S2=3.756202
S2-1=0.
S2A=3.750018
RMSD=9.092e-09
Dipole=1.6960181, 1.9937161, -1.2558493
PG=C01 [X(C1H8Co1N103S1)]

CoCDSt9

1, 4
Co
S, 1, 2.4594660519
N, 1, 2.0724938961, 2, 109.47122063
O, 1, 2.0318832539, 2, 109.47122063, 3, 120.
O, 1, 1.9233862824, 2, 109.47122063, 3, -120.
H, 2, 1.35555116, 1, 87.18674496, 3, 75.74742417
H, 2, 1.35174477, 1, 97.8295942, 3, 169.76240196
H, 3, 1.02223766, 1, 114.056871, 2, 176.52904891
H, 3, 1.02180832, 1, 118.28414373, 2, 49.7214649
H, 3, 1.02586929, 1, 101.96538083, 2, -68.4277988
C, 4, 1.22912758, 1, 127.78102097, 2, 118.13609683
H, 11, 1.09986557, 4, 121.5658166, 1, -0.65425365
H, 11, 1.09814039, 4, 119.228673, 12, 179.9641778
C, 5, 1.29983846, 1, 106.55781519, 2, 62.50959276
H, 14, 1.0995402, 5, 115.17801117, 1, 179.45159566
O, 14, 1.24073079, 5, 123.44459098, 15, 179.85979299

HF=-2142.4348664
S2=3.757533
S2-1=0.
S2A=3.750025
RMSD=9.704e-09
Dipole=-0.2990566, -1.7365779, -0.8317288

PG=C01 [X(C2H8Co1N103S1)]

CoCDSt10

0, 4

Co

S, 1, 2.4394280074

S, 1, 2.4391906711, 2, 109.47122063

O, 1, 1.9314603917, 2, 109.47122063, 3, 120.

O, 1, 1.9299000316, 2, 109.47122063, 3, -120.

H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116

H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799

H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186

H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331

C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548

H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037

O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135

C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221

H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939

O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-2560.188402

S2=3.757318

S2-1=0.

S2A=3.750025

RMSD=7.993e-09

Dipole=0.8587331, -0.3385929, 0.2344246

PG=C01 [X(C2H6Co104S2)]

NiCDSt1

2, 3

Ni

O, 1, 2.0953697135

O, 1, 1.9959507162, 2, 109.47122063

S, 1, 2.3772099312, 2, 109.47122063, 3, 120.

O, 1, 1.9553646075, 2, 109.47122063, 3, -120.

H, 2, 0.97710956, 1, 126.72351565, 3, -32.42515075

H, 2, 0.97756217, 1, 125.23198546, 3, 137.32199183

H, 3, 0.97720206, 1, 125.08548378, 2, 128.90568232

H, 3, 0.97691541, 1, 127.26501921, 2, -43.6894312

H, 4, 1.35409598, 1, 98.71271852, 2, 3.90805121

H, 4, 1.35439907, 1, 98.51076654, 2, 100.10143429

C, 5, 1.23465919, 1, 146.23736757, 2, 123.86702845

H, 12, 1.09868727, 5, 121.69940132, 1, -2.09235282

H, 12, 1.09751386, 5, 118.89820982, 13, 179.94205073

HF=-2174.6414061

S2=2.004114

S2-1=0.

S2A=2.00001

RMSD=9.557e-09

Dipole=0.6365806, 0.8648129, 0.2956387

PG=C01 [X(C1H8Ni103S1)]

NiCDSt2

2,3

Ni

S,1,2.3693672637

O,1,2.075188284,2,109.47122063

O,1,1.9847057428,2,109.47122063,3,120.

O,1,1.9589544302,2,109.47122063,3,-120.

H,2,1.35379864,1,99.7819091,3,-18.12579641

H,2,1.35393714,1,100.2118578,3,78.80693391

H,3,0.97744477,1,125.63242174,2,115.40313724

H,3,0.97598732,1,126.75833562,2,-68.51929524

C,4,1.23376805,1,147.69191231,2,68.13943977

H,10,1.09887316,4,121.64827332,1,-0.69344272

H,10,1.09752428,4,118.93131886,11,180.32903525

C,5,1.23366055,1,147.88558831,2,157.60744208

H,13,1.09904483,5,121.69558296,1,-0.62863977

H,13,1.09770407,5,118.96648232,14,179.92854414

HF=-2212.732204

S2=2.004385

S2-1=0.

S2A=2.000012

RMSD=9.453e-09

Dipole=0.2536251,0.2769589,-0.9995597

PG=C01 [X(C2H8Ni103S1)]

NiCDSt3

2,3

Ni

S,1,2.5090171228

O,1,1.9523050236,2,109.47122063

O,1,1.9547141558,2,109.47122063,3,120.

O,1,1.9608126782,2,109.47122063,3,-120.

H,2,1.35382234,1,99.42346635,3,-24.86006571

H,2,1.35394345,1,99.35041753,3,71.37040763

C,3,1.23439672,1,142.62314323,2,115.8445957

H,8,1.09877467,3,121.73254404,1,0.69876845

H,8,1.09753352,3,118.90990393,9,180.08272977

C,4,1.23419868,1,143.32350114,2,80.31278782

H,11,1.09872769,4,121.76269088,1,2.16299582

H,11,1.09740596,4,118.89863073,12,180.01844807

C,5,1.23372739,1,144.93803684,2,112.4054566

H,14,1.09881591,5,121.71095223,1,1.03525778

H,14,1.09752425,5,118.92338792,15,180.0617941

HF=-2250.8227561

S2=2.004947

S2-1=0.

S2A=2.000016

RMSD=8.329e-09
Dipole=0.2759412, 0.1194238, -1.3305388
PG=C01 [X(C3H8Ni103S1)]

NiCDSt4

2,3
Ni
S,1,2.3871414967
O,1,2.0715544085,2,109.47122063
O,1,1.9795237921,2,109.47122063,3,120.
N,1,2.0213402333,2,109.47122063,3,-120.
H,2,1.35370225,1,100.67403997,3,-47.42763211
H,2,1.35408901,1,99.62884198,3,48.89193922
C,3,1.23388199,1,144.85377957,2,127.8430108
H,8,1.09869892,3,121.67597912,1,-2.16876368
H,8,1.09746485,3,118.92495585,9,179.91268855
C,4,1.23209511,1,151.41275636,2,28.9978892
H,11,1.09950782,4,121.58841047,1,-0.87424889
H,11,1.09801294,4,119.2932244,12,179.8790918
H,5,1.02597301,1,112.96295399,2,158.00819994
H,5,1.02537065,1,113.04635429,2,38.41966235
H,5,1.02551705,1,113.357995,2,-81.86571236

HF=-2192.8803185
S2=2.00434
S2-1=0.
S2A=2.000012
RMSD=6.827e-09
Dipole=-0.3254334, -0.2311663, -0.7127552
PG=C01 [X(C2H9N1Ni102S1)]

NiCDSt5

2,3
Ni
S,1,2.3838774911
O,1,2.0604030568,2,109.47122063
O,1,2.0181711007,2,109.47122063,3,120.
N,1,2.0138584204,2,109.47122063,3,-120.
H,2,1.3532682,1,101.52794537,3,-71.45930587
H,2,1.35375954,1,101.36172376,3,25.96769013
H,3,0.97657675,1,125.34039764,2,40.55857074
H,3,0.9772854,1,124.99395005,2,-162.43509427
C,4,1.23078918,1,166.98888266,2,-5.875825
H,10,1.09927299,4,121.0481255,1,1.19440852
H,10,1.09851533,4,119.75500726,11,179.97862286
H,5,1.02591479,1,113.7585246,2,183.68402475
H,5,1.02570578,1,113.14704837,2,62.87609203
H,5,1.02595319,1,112.1546187,2,-56.67361772

HF=-2154.7896726
S2=2.004041

S2-1=0.
S2A=2.00001
RMSD=8.549e-09
Dipole=0.2300342, -0.1961467, -0.7811571
PG=C01 [X(C1H9N1Ni102S1)]

NiCDSt6

2, 3
Ni
O, 1, 2.059616
O, 1, 2.064869, 2, 109.47122063
S, 1, 2.378973, 2, 109.47122063, 3, 120.
S, 1, 2.378402, 2, 109.47122063, 3, -120.
H, 2, 0.97715546, 1, 126.00530669, 3, -137.28671058
H, 2, 0.97721096, 1, 126.72613851, 3, 37.77615189
H, 3, 0.97717428, 1, 125.96028173, 2, 223.41524284
H, 3, 0.97720322, 1, 126.74413777, 2, 38.09497653
H, 4, 1.35436319, 1, 98.61472212, 2, -175.53081491
H, 4, 1.35444234, 1, 100.57257274, 2, -79.16407195
H, 5, 1.35447271, 1, 100.52722432, 2, 38.8404492
H, 5, 1.35436768, 1, 98.61819189, 2, -57.52868001

HF=-2459.5120511
S2=2.004459
S2-1=0.
S2A=2.000012
RMSD=8.306e-09
Dipole=1.0348311, -0.001469, 0.7425669
PG=C01 [X(H8Ni102S2)]

NiCDSt7

1, 3
Ni
O, 1, 2.1786067455
O, 1, 1.9683660241, 2, 109.47122063
S, 1, 2.3855056359, 2, 109.47122063, 3, 120.
O, 1, 1.8872979623, 2, 109.47122063, 3, -120.
H, 2, 0.97304987, 1, 129.08906844, 3, -92.60346916
H, 2, 0.97474217, 1, 118.79945451, 3, 114.21728494
H, 3, 1.02084268, 1, 95.67672252, 2, -119.05786808
H, 3, 0.97258209, 1, 126.58711976, 2, 0.93577882
H, 4, 1.3523873, 1, 94.04096012, 2, 120.26596053
H, 4, 1.35233137, 1, 96.0652197, 2, 215.1457816
C, 5, 1.30489723, 1, 115.95687296, 2, 120.60279574
H, 12, 1.09833869, 5, 114.23891506, 1, 179.81220999
O, 12, 1.23877975, 5, 125.70918421, 13, 180.21989236

HF=-2249.7258602
S2=2.004642
S2-1=0.
S2A=2.000013

RMSD=9.850e-09
Dipole=-0.2672723, -1.4582693, 1.587782
PG=C01 [X(C1H7Ni104S1)]

NiCDSt8

1, 3
Ni
S, 1, 2.3730878614
N, 1, 2.0332744692, 2, 109.47122063
O, 1, 1.8853076532, 2, 109.47122063, 3, 120.
O, 1, 2.1921196977, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.64107442, 3, -132.34729509
H, 2, 1.35163013, 1, 96.11149781, 3, -39.14270577
H, 3, 1.02324409, 1, 114.14255374, 2, -133.93875655
H, 3, 1.02176858, 1, 114.21620804, 2, -11.14508144
H, 3, 1.02380537, 1, 108.33284024, 2, 107.85234365
C, 4, 1.30526952, 1, 122.86903562, 2, 14.16423746
H, 11, 1.09978935, 4, 113.7139494, 1, 178.97461085
O, 11, 1.23588904, 4, 126.296095, 1, -1.21412678
H, 5, 0.9735806, 1, 124.20061642, 2, 18.55214804
H, 5, 0.97497082, 1, 117.71800181, 2, -121.1507242

HF=-2229.8623734
S2=2.005112
S2-1=0.
S2A=2.000015
RMSD=2.686e-09
Dipole=1.714135, 1.8343395, -1.133383
PG=C01 [X(C1H8N1Ni103S1)]

NiCDSt9

1, 3
Ni
S, 1, 2.6014555251
N, 1, 2.0263233036, 2, 109.47122063
O, 1, 2.001263077, 2, 109.47122063, 3, 120.
O, 1, 1.9071087249, 2, 109.47122063, 3, -120.
H, 2, 1.35555116, 1, 87.18674496, 3, 75.74742417
H, 2, 1.35174477, 1, 97.8295942, 3, 169.76240196
H, 3, 1.02223766, 1, 114.056871, 2, 176.52904891
H, 3, 1.02180832, 1, 118.28414373, 2, 49.7214649
H, 3, 1.02586929, 1, 101.96538083, 2, -68.4277988
C, 4, 1.22912758, 1, 127.78102097, 2, 118.13609683
H, 11, 1.09986557, 4, 121.5658166, 1, -0.65425365
H, 11, 1.09814039, 4, 119.228673, 12, 179.9641778
C, 5, 1.29983846, 1, 106.55781519, 2, 62.50959276
H, 14, 1.0995402, 5, 115.17801117, 1, 179.45159566
O, 14, 1.24073079, 5, 123.44459098, 15, 179.85979299

HF=-2267.9522044
S2=2.004672

S2-1=0.
S2A=2.000014
RMSD=4.917e-09
Dipole=-0.3078154, -1.7062702, -1.0339239
PG=C01 [X(C2H8N1Ni103S1)]

NiCDSt10

0, 3
Ni
S, 1, 2.5573416994
S, 1, 2.3952064792, 2, 109.47122063
O, 1, 1.9134791979, 2, 109.47122063, 3, 120.
O, 1, 1.9145248764, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135
C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-2685.7044773
S2=2.005206
S2-1=0.
S2A=2.000016
RMSD=4.314e-09
Dipole=0.9234086, -0.1943949, 0.0448965
PG=C01 [X(C2H6Ni104S2)]

CuCDSt1

2, 2
Cu
O, 1, 2.028337331
O, 1, 2.0972199983, 2, 109.47122063
S, 1, 2.3414701318, 2, 109.47122063, 3, 120.
O, 1, 1.9866487012, 2, 109.47122063, 3, -120.
H, 2, 0.97710956, 1, 126.72351565, 3, -32.42515075
H, 2, 0.97756217, 1, 125.23198546, 3, 137.32199183
H, 3, 0.97720206, 1, 125.08548378, 2, 128.90568232
H, 3, 0.97691541, 1, 127.26501921, 2, -43.6894312
H, 4, 1.35409598, 1, 98.71271852, 2, 3.90805121
H, 4, 1.35439907, 1, 98.51076654, 2, 100.10143429
C, 5, 1.23465919, 1, 146.23736757, 2, 123.86702845
H, 12, 1.09868727, 5, 121.69940132, 1, -2.09235282
H, 12, 1.09751386, 5, 118.89820982, 13, 179.94205073

HF=-2306.8002193
S2=0.753504

S2-1=0.
S2A=0.750007
RMSD=6.892e-09
Dipole=0.2733347,0.4564418,0.2489854
PG=C01 [X(C1H8Cu103S1)]

CuCDSt2

2,2
Cu
S,1,2.3572317542
O,1,2.0227074905,2,109.47122063
O,1,1.9860677083,2,109.47122063,3,120.
O,1,2.0381253348,2,109.47122063,3,-120.
H,2,1.35379864,1,99.7819091,3,-18.12579641
H,2,1.35393714,1,100.2118578,3,78.80693391
H,3,0.97744477,1,125.63242174,2,115.40313724
H,3,0.97598732,1,126.75833562,2,-68.51929524
C,4,1.23376805,1,147.69191231,2,68.13943977
H,10,1.09887316,4,121.64827332,1,-0.69344272
H,10,1.09752428,4,118.93131886,11,180.32903525
C,5,1.23366055,1,147.88558831,2,157.60744208
H,13,1.09904483,5,121.69558296,1,-0.62863977
H,13,1.09770407,5,118.96648232,14,179.92854414

HF=-2344.8939548
S2=0.753285
S2-1=0.
S2A=0.750008
RMSD=6.997e-09
Dipole=0.2041608,0.2425672,-0.7805962
PG=C01 [X(C2H8Cu103S1)]

CuCDSt3

2,2
29 0.006019 0.018117 0.005914
16 -0.756943 2.155705 -0.777528
8 0.904176 0.237013 1.700583
8 -1.601477 -1.238778 0.240322
8 1.288882 -0.773104 -1.338742
1 -0.852973 2.804488 0.406826
1 0.434910 2.707918 -1.105718
6 0.831422 -0.064256 2.895438
1 0.015156 -0.687821 3.285543
1 1.603563 0.303454 3.583310
6 -2.376712 -1.978981 -0.371524
1 -2.282230 -2.148364 -1.452998
1 -3.180814 -2.479348 0.182870
6 2.461353 -1.095316 -1.547488
1 3.239363 -0.972096 -0.781386
1 2.730553 -1.514638 -2.525373

HF=-2382.98051311
RMSD=5.697e-08
S2=0.7532

CuCDSt4

2,2
Cu
S,1,2.334815679
O,1,2.0552724304,2,109.47122063
O,1,2.0473250795,2,109.47122063,3,120.
N,1,2.0449511349,2,109.47122063,3,-120.
H,2,1.35370225,1,100.67403997,3,-47.42763211
H,2,1.35408901,1,99.62884198,3,48.89193922
C,3,1.23388199,1,144.85377957,2,127.8430108
H,8,1.09869892,3,121.67597912,1,-2.16876368
H,8,1.09746485,3,118.92495585,9,179.91268855
C,4,1.23209511,1,151.41275636,2,28.9978892
H,11,1.09950782,4,121.58841047,1,-0.87424889
H,11,1.09801294,4,119.2932244,12,179.8790918
H,5,1.02597301,1,112.96295399,2,158.00819994
H,5,1.02537065,1,113.04635429,2,38.41966235
H,5,1.02551705,1,113.357995,2,-81.86571236

HF=-2325.037945
S2=0.753291
S2-1=0.
S2A=0.750007
RMSD=8.522e-09
Dipole=-0.3459557, -0.2062259, -0.2493061
PG=C01 [X(C2H9Cu1N102S1)]

CuCDSt5

2,2
Cu
S,1,2.3516417955
O,1,2.113048824,2,109.47122063
O,1,2.0145301498,2,109.47122063,3,120.
N,1,2.024328946,2,109.47122063,3,-120.
H,2,1.3532682,1,101.52794537,3,-71.45930587
H,2,1.35375954,1,101.36172376,3,25.96769013
H,3,0.97657675,1,125.34039764,2,40.55857074
H,3,0.9772854,1,124.99395005,2,-162.43509427
C,4,1.23078918,1,166.98888266,2,-5.875825
H,10,1.09927299,4,121.0481255,1,1.19440852
H,10,1.09851533,4,119.75500726,11,179.97862286
H,5,1.02591479,1,113.7585246,2,183.68402475
H,5,1.02570578,1,113.14704837,2,62.87609203
H,5,1.02595319,1,112.1546187,2,-56.67361772

HF=-2286.950123
S2=0.753346

S2-1=0.
S2A=0.750008
RMSD=7.910e-09
Dipole=0.0360713, -0.3264369, -0.4836236
PG=C01 [X(C1H9Cu1N102S1)]

CuCDSt6

2, 2
Cu
O, 1, 2.0859266095
O, 1, 2.0860297814, 2, 109.47122063
S, 1, 2.3687626466, 2, 109.47122063, 3, 120.
S, 1, 2.3689517076, 2, 109.47122063, 3, -120.
H, 2, 0.97715546, 1, 126.00530669, 3, -137.28671058
H, 2, 0.97721096, 1, 126.72613851, 3, 37.77615189
H, 3, 0.97717428, 1, 125.96028173, 2, 223.41524284
H, 3, 0.97720322, 1, 126.74413777, 2, 38.09497653
H, 4, 1.35436319, 1, 98.61472212, 2, -175.53081491
H, 4, 1.35444234, 1, 100.57257274, 2, -79.16407195
H, 5, 1.35447271, 1, 100.52722432, 2, 38.8404492
H, 5, 1.35436768, 1, 98.61819189, 2, -57.52868001

HF=-2591.676322
S2=0.753712
S2-1=0.
S2A=0.75001
RMSD=6.625e-09
Dipole=0.6966356, -0.0042208, 0.5026641
PG=C01 [X(Cu1H802S2)]

CuCDSt7

1, 2
Cu
O, 1, 2.1422629059
O, 1, 2.0065767637, 2, 109.47122063
S, 1, 2.4471839651, 2, 109.47122063, 3, 120.
O, 1, 1.8752225855, 2, 109.47122063, 3, -120.
H, 2, 0.97304987, 1, 129.08906844, 3, -92.60346916
H, 2, 0.97474217, 1, 118.79945451, 3, 114.21728494
H, 3, 1.02084268, 1, 95.67672252, 2, -119.05786808
H, 3, 0.97258209, 1, 126.58711976, 2, 0.93577882
H, 4, 1.3523873, 1, 94.04096012, 2, 120.26596053
H, 4, 1.35233137, 1, 96.0652197, 2, 215.1457816
C, 5, 1.30489723, 1, 115.95687296, 2, 120.60279574
H, 12, 1.09833869, 5, 114.23891506, 1, 179.81220999
O, 12, 1.23877975, 5, 125.70918421, 13, 180.21989236

HF=-2381.8918589
S2=0.753016
S2-1=0.
S2A=0.750006

RMSD=7.730e-09
Dipole=-0.2940471, -1.0221327, 1.4171872
PG=C01 [X(C1H7Cu104S1)]

CuCDSt8

1,2
Cu
S,1,2.3734421747
N,1,2.125591476,2,109.47122063
O,1,1.8738374712,2,109.47122063,3,120.
O,1,2.1564204643,2,109.47122063,3,-120.
H,2,1.38163488,1,79.64107442,3,-132.34729509
H,2,1.35163013,1,96.11149781,3,-39.14270577
H,3,1.02324409,1,114.14255374,2,-133.93875655
H,3,1.02176858,1,114.21620804,2,-11.14508144
H,3,1.02380537,1,108.33284024,2,107.85234365
C,4,1.30526952,1,122.86903562,2,14.16423746
H,11,1.09978935,4,113.7139494,1,178.97461085
O,11,1.23588904,4,126.296095,1,-1.21412678
H,5,0.9735806,1,124.20061642,2,18.55214804
H,5,0.97497082,1,117.71800181,2,-121.1507242

HF=-2362.0278005
S2=0.75367
S2-1=0.
S2A=0.75001
RMSD=5.042e-09
Dipole=1.3984655, 1.454031, -1.0021374
PG=C01 [X(C1H8Cu1N103S1)]

CuCDSt9

1,2
Cu
S,1,2.4965568278
N,1,2.0870296455,2,109.47122063
O,1,2.0912137289,2,109.47122063,3,120.
O,1,1.8910989402,2,109.47122063,3,-120.
H,2,1.35555116,1,87.18674496,3,75.74742417
H,2,1.35174477,1,97.8295942,3,169.76240196
H,3,1.02223766,1,114.056871,2,176.52904891
H,3,1.02180832,1,118.28414373,2,49.7214649
H,3,1.02586929,1,101.96538083,2,-68.4277988
C,4,1.22912758,1,127.78102097,2,118.13609683
H,11,1.09986557,4,121.5658166,1,-0.65425365
H,11,1.09814039,4,119.228673,12,179.9641778
C,5,1.29983846,1,106.55781519,2,62.50959276
H,14,1.0995402,5,115.17801117,1,179.45159566
O,14,1.24073079,5,123.44459098,15,179.85979299

HF=-2400.1145905
S2=0.752817

S2-1=0.
S2A=0.750006
RMSD=4.889e-09
Dipole=-0.4081796, -1.3229594, -0.929709
PG=C01 [X(C2H8Cu1N103S1)]

CuCDSt10

0, 2
Cu
S, 1, 2.4955993025
S, 1, 2.4148136711, 2, 109.47122063
O, 1, 1.9583105179, 2, 109.47122063, 3, 120.
O, 1, 1.8970449954, 2, 109.47122063, 3, -120.
H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116
H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799
H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186
H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331
C, 4, 1.29071169, 1, 123.55601327, 2, 6.09180548
H, 10, 1.10336764, 4, 113.85514644, 1, 177.31743037
O, 10, 1.24276687, 4, 127.38248639, 1, -2.71399135
C, 5, 1.28915861, 1, 123.41582602, 2, 116.90915221
H, 13, 1.10314255, 5, 113.94759476, 1, 179.92846939
O, 13, 1.24429984, 5, 127.38196656, 14, 180.09132496

HF=-2817.8676241
S2=0.753088
S2-1=0.
S2A=0.750008
RMSD=8.814e-09
Dipole=0.901348, 0.1378658, -0.0793716
PG=C01 [X(C2H6Cu104S2)]

ZnCDSt1

2, 1
Zn
O, 1, 2.0248748007
O, 1, 2.0320650735, 2, 109.47122063
S, 1, 2.4078220904, 2, 109.47122063, 3, 120.
O, 1, 1.9951315152, 2, 109.47122063, 3, -120.
H, 2, 0.9771095556, 1, 126.72351565, 3, -32.42515075
H, 2, 0.9775621694, 1, 125.23198546, 3, 137.32199183
H, 3, 0.977202058, 1, 125.08548378, 2, 128.90568232
H, 3, 0.9769154149, 1, 127.26501921, 2, -43.6894312
H, 4, 1.3540959795, 1, 98.71271852, 2, 3.90805121
H, 4, 1.3543990659, 1, 98.51076654, 2, 100.10143429
C, 5, 1.2346591895, 1, 146.23736757, 2, 123.86702845
H, 12, 1.0986872672, 5, 121.69940132, 1, -2.09235282
H, 12, 1.0975138561, 5, 118.89820982, 13, 179.94205073

HF=-2445.7032657
RMSD=3.835e-09

Dipole=0.6848931,0.7636877,0.3867849
PG=C01 [X(C1H8O3S1Zn1)]

ZnCDSt2

2,1
Zn
S,1,2.4122281973
O,1,2.0372884118,2,109.47122063
O,1,1.9876994534,2,109.47122063,3,120.
O,1,2.0043726643,2,109.47122063,3,-120.
H,2,1.353798643,1,99.7819091,3,-18.12579641
H,2,1.3539371411,1,100.2118578,3,78.80693391
H,3,0.9774447739,1,125.63242174,2,115.40313724
H,3,0.9759873199,1,126.75833562,2,-68.51929524
C,4,1.2337680548,1,147.69191231,2,68.13943977
H,10,1.0988731592,4,121.64827332,1,-0.69344272
H,10,1.097524276,4,118.93131886,11,180.32903525
C,5,1.2336605452,1,147.88558831,2,157.60744208
H,13,1.0990448318,5,121.69558296,1,-0.62863977
H,13,1.0977040721,5,118.96648232,14,179.92854414

HF=-2483.7924735
RMSD=9.111e-09
Dipole=0.329338,0.3716629,-0.9950634
PG=C01 [X(C2H8O3S1Zn1)]

ZnCDSt3

2,1
Zn
S,1,2.4108255694
O,1,2.0105739574,2,109.47122063
O,1,2.0024719737,2,109.47122063,3,120.
O,1,2.0008303077,2,109.47122063,3,-120.
H,2,1.3538223383,1,99.42346635,3,-24.86006571
H,2,1.3539434454,1,99.35041753,3,71.37040763
C,3,1.2343967233,1,142.62314323,2,115.8445957
H,8,1.0987746744,3,121.73254404,1,0.69876845
H,8,1.0975335236,3,118.90990393,9,180.08272977
C,4,1.2341986774,1,143.32350114,2,80.31278782
H,11,1.0987276915,4,121.76269088,1,2.16299582
H,11,1.0974059638,4,118.89863073,12,180.01844807
C,5,1.2337273857,1,144.93803684,2,112.4054566
H,14,1.0988159062,5,121.71095223,1,1.03525778
H,14,1.0975242516,5,118.92338792,15,180.0617941

HF=-2521.8830342
RMSD=9.212e-09
Dipole=0.255214,0.1113741,-0.9450055
PG=C01 [X(C3H8O3S1Zn1)]

ZnCDSt4

2,1
Zn
S,1,2.4412597989
O,1,2.0083703414,2,109.47122063
O,1,2.0248813513,2,109.47122063,3,120.
N,1,2.0488842983,2,109.47122063,3,-120.
H,2,1.3537022461,1,100.67403997,3,-47.42763211
H,2,1.3540890086,1,99.62884198,3,48.89193922
C,3,1.2338819874,1,144.85377957,2,127.8430108
H,8,1.098698924,3,121.67597912,1,-2.16876368
H,8,1.0974648457,3,118.92495585,9,179.91268855
C,4,1.2320951112,1,151.41275636,2,28.9978892
H,11,1.0995078184,4,121.58841047,1,-0.87424889
H,11,1.0980129429,4,119.2932244,12,179.8790918
H,5,1.0259730071,1,112.96295399,2,158.00819994
H,5,1.0253706547,1,113.04635429,2,38.41966235
H,5,1.0255170513,1,113.357995,2,-81.86571236

HF=-2463.9404647
RMSD=9.146e-09
Dipole=-0.18375, -0.1120297, -0.7437482
PG=C01 [X(C2H9N102S1Zn1)]

ZnCDSt5

2,1
Zn
S,1,2.4416776177
O,1,2.044241751,2,109.47122063
O,1,2.0060836101,2,109.47122063,3,120.
N,1,2.0465793351,2,109.47122063,3,-120.
H,2,1.3532682048,1,101.52794537,3,-71.45930587
H,2,1.3537595425,1,101.36172376,3,25.96769013
H,3,0.9765767453,1,125.34039764,2,40.55857074
H,3,0.9772854035,1,124.99395005,2,-162.43509427
C,4,1.2307891828,1,166.98888266,2,-5.875825
H,10,1.0992729929,4,121.0481255,1,1.19440852
H,10,1.0985153345,4,119.75500726,11,179.97862286
H,5,1.0259147941,1,113.7585246,2,183.68402475
H,5,1.0257057794,1,113.14704837,2,62.87609203
H,5,1.0259531894,1,112.1546187,2,-56.67361772

HF=-2425.8495469
RMSD=4.557e-09
Dipole=0.2868596, -0.092368, -0.8029059
PG=C01 [X(C1H9N102S1Zn1)]

ZnCDSt6

2,1
Zn
O,1,2.0435532408
O,1,2.0432911029,2,109.47122063
S,1,2.4331503936,2,109.47122063,3,120.
S,1,2.4329764402,2,109.47122063,3,-120.
H,2,0.9771554647,1,126.00530669,3,-137.28671058
H,2,0.9772109636,1,126.72613851,3,37.77615189
H,3,0.9771742845,1,125.96028173,2,223.41524284
H,3,0.9772032191,1,126.74413777,2,38.09497653
H,4,1.3543631929,1,98.61472212,2,-175.53081491
H,4,1.354442342,1,100.57257274,2,-79.16407195
H,5,1.3544727095,1,100.52722432,2,38.8404492
H,5,1.3543676792,1,98.61819189,2,-57.52868001

HF=-2730.5748123
RMSD=6.319e-09
Dipole=1.0555906,-0.0057908,0.755076
PG=C01 [X(H802S2Zn1)]

ZnCDSt7

1,1
Zn
O,1,2.0689295133
O,1,2.0009224139,2,109.47122063
S,1,2.4443351969,2,109.47122063,3,120.
O,1,1.9058150348,2,109.47122063,3,-120.
H,2,0.9730498746,1,129.08906844,3,-92.60346916
H,2,0.9747421703,1,118.79945451,3,114.21728494
H,3,1.0208426778,1,95.67672252,2,-119.05786808
H,3,0.9725820872,1,126.58711976,2,0.93577882
H,4,1.3523873031,1,94.04096012,2,120.26596053
H,4,1.3523313741,1,96.0652197,2,215.1457816
C,5,1.3048972336,1,115.95687296,2,120.60279574
H,12,1.0983386896,5,114.23891506,1,179.81220999
O,12,1.238779754,5,125.70918421,13,180.21989236

HF=-2520.7851071
RMSD=8.581e-09
Dipole=-0.2131346,-1.6232767,1.7668001
PG=C01 [X(C1H704S1Zn1)]

ZnCDSt8

1,1
Zn
S,1,2.4303383932
N,1,2.0754776648,2,109.47122063
O,1,1.9044165621,2,109.47122063,3,120.
O,1,2.0785575615,2,109.47122063,3,-120.
H,2,1.38163488,1,79.64107442,3,-132.34729509

H, 2, 1.35163013, 1, 96.11149781, 3, -39.14270577
H, 3, 1.0232440853, 1, 114.14255374, 2, -133.93875655
H, 3, 1.021768581, 1, 114.21620804, 2, -11.14508144
H, 3, 1.0238053735, 1, 108.33284024, 2, 107.85234365
C, 4, 1.3052695188, 1, 122.86903562, 2, 14.16423746
H, 11, 1.0997893512, 4, 113.7139494, 1, 178.97461085
O, 11, 1.2358890403, 4, 126.296095, 1, -1.21412678
H, 5, 0.973580604, 1, 124.20061642, 2, 18.55214804
H, 5, 0.9749708199, 1, 117.71800181, 2, -121.1507242

HF=-2500.9192832

RMSD=8.219e-09

Dipole=1.8257473, 2.1010721, -1.1904445

PG=C01 [X(C1H8N103S1Zn1)]

ZnCDSt9

1, 1

Zn

S, 1, 2.4703107109

N, 1, 2.0657760689, 2, 109.47122063

O, 1, 2.0647839452, 2, 109.47122063, 3, 120.

O, 1, 1.9412657965, 2, 109.47122063, 3, -120.

H, 2, 1.3555511589, 1, 87.18674496, 3, 75.74742417

H, 2, 1.3517447718, 1, 97.8295942, 3, 169.76240196

H, 3, 1.0222376595, 1, 114.056871, 2, 176.52904891

H, 3, 1.0218083175, 1, 118.28414373, 2, 49.7214649

H, 3, 1.0258692858, 1, 101.96538083, 2, -68.4277988

C, 4, 1.2291275766, 1, 127.78102097, 2, 118.13609683

H, 11, 1.0998655664, 4, 121.5658166, 1, -0.65425365

H, 11, 1.0981403908, 4, 119.228673, 12, 179.9641778

C, 5, 1.2998384629, 1, 106.55781519, 2, 62.50959276

H, 14, 1.0995401972, 5, 115.17801117, 1, 179.45159566

O, 14, 1.240730792, 5, 123.44459098, 15, 179.85979299

HF=-2539.0079758

RMSD=7.937e-09

Dipole=-0.2528124, -1.9231678, -0.758627

PG=C01 [X(C2H8N103S1Zn1)]

ZnCDSt10

0, 1

Zn

S, 1, 2.4578566202

S, 1, 2.452479758, 2, 109.47122063

O, 1, 1.9409697641, 2, 109.47122063, 3, 120.

O, 1, 1.9394734595, 2, 109.47122063, 3, -120.

H, 2, 1.38163488, 1, 79.86205016, 3, -125.74009116

H, 2, 1.35163013, 1, 96.26799792, 3, -33.30594799

H, 3, 1.3816, 1, 79.76133275, 2, -117.48390186

H, 3, 1.3516, 1, 93.30923331, 2, 148.57920331

C, 4, 1.2907116895, 1, 123.55601327, 2, 6.09180548

H, 10, 1.1033676431, 4, 113.85514644, 1, 177.31743037
O, 10, 1.2427668676, 4, 127.38248639, 1, -2.71399135
C, 5, 1.2891586094, 1, 123.41582602, 2, 116.90915221
H, 13, 1.1031425475, 5, 113.94759476, 1, 179.92846939
O, 13, 1.2442998438, 5, 127.38196656, 14, 180.09132496

HF=-2956.7648226

RMSD=8.926e-09

Dipole=0.9962439, -0.3475684, 0.3178687

PG=C01 [X(C2H6O4S2Zn1)]

CdCDSt1

2,1

Cd

O, 1, 2.2503997553

O, 1, 2.2593276469, 2, 109.47122063

S, 1, 2.6120156394, 2, 109.47122063, 3, 120.

O, 1, 2.2390628455, 2, 109.47122063, 3, -120.

H, 2, 0.97710956, 1, 126.72351565, 3, -32.42515075

H, 2, 0.97756217, 1, 125.23198546, 3, 137.32199183

H, 3, 0.97720206, 1, 125.08548378, 2, 128.90568232

H, 3, 0.97691541, 1, 127.26501921, 2, -43.6894312

H, 4, 1.35409598, 1, 98.71271852, 2, 3.90805121

H, 4, 1.35439907, 1, 98.51076654, 2, 100.10143429

C, 5, 1.23465919, 1, 146.23736757, 2, 123.86702845

H, 12, 1.09868727, 5, 121.69940132, 1, -2.09235282

H, 12, 1.09751386, 5, 118.89820982, 13, 179.94205073

HF=-833.2615841

RMSD=6.869e-09

Dipole=0.7972036, 0.6374707, 0.5159218

PG=C01 [X(C1H8Cd103S1)]

CdCDSt2

2,1

Cd

S, 1, 2.6145162605

O, 1, 2.2580573744, 2, 109.47122063

O, 1, 2.2326695034, 2, 109.47122063, 3, 120.

O, 1, 2.2467829001, 2, 109.47122063, 3, -120.

H, 2, 1.35379864, 1, 99.7819091, 3, -18.12579641

H, 2, 1.35393714, 1, 100.2118578, 3, 78.80693391

H, 3, 0.97744477, 1, 125.63242174, 2, 115.40313724

H, 3, 0.97598732, 1, 126.75833562, 2, -68.51929524

C, 4, 1.23376805, 1, 147.69191231, 2, 68.13943977

H, 10, 1.09887316, 4, 121.64827332, 1, -0.69344272

H, 10, 1.09752428, 4, 118.93131886, 11, 180.32903525

C, 5, 1.23366055, 1, 147.88558831, 2, 157.60744208

H, 13, 1.09904483, 5, 121.69558296, 1, -0.62863977

H, 13, 1.09770407, 5, 118.96648232, 14, 179.92854414

HF=-871.3505304
RMSD=9.287e-09
Dipole=0.2821798, 0.3816551, -0.8218362
PG=C01 [X(C2H8Cd103S1)]

CdCDSt3

2,1
Cd
S,1,2.6168440217
O,1,2.2544492626,2,109.47122063
O,1,2.2445732254,2,109.47122063,3,120.
O,1,2.246208368,2,109.47122063,3,-120.
H,2,1.35382234,1,99.42346635,3,-24.86006571
H,2,1.35394345,1,99.35041753,3,71.37040763
C,3,1.23439672,1,142.62314323,2,115.8445957
H,8,1.09877467,3,121.73254404,1,0.69876845
H,8,1.09753352,3,118.90990393,9,180.08272977
C,4,1.23419868,1,143.32350114,2,80.31278782
H,11,1.09872769,4,121.76269088,1,2.16299582
H,11,1.09740596,4,118.89863073,12,180.01844807
C,5,1.23372739,1,144.93803684,2,112.4054566
H,14,1.09881591,5,121.71095223,1,1.03525778
H,14,1.09752425,5,118.92338792,15,180.0617941

HF=-909.4398653
RMSD=9.611e-09
Dipole=0.2592291, 0.1044666, -0.8061459
PG=C01 [X(C3H8Cd103S1)]

CdCDSt4

2,1
Cd
S,1,2.645287936
O,1,2.2530058306,2,109.47122063
O,1,2.266739584,2,109.47122063,3,120.
N,1,2.2773371427,2,109.47122063,3,-120.
H,2,1.35370225,1,100.67403997,3,-47.42763211
H,2,1.35408901,1,99.62884198,3,48.89193922
C,3,1.23388199,1,144.85377957,2,127.8430108
H,8,1.09869892,3,121.67597912,1,-2.16876368
H,8,1.09746485,3,118.92495585,9,179.91268855
C,4,1.23209511,1,151.41275636,2,28.9978892
H,11,1.09950782,4,121.58841047,1,-0.87424889
H,11,1.09801294,4,119.2932244,12,179.8790918
H,5,1.02597301,1,112.96295399,2,158.00819994
H,5,1.02537065,1,113.04635429,2,38.41966235
H,5,1.02551705,1,113.357995,2,-81.86571236

HF=-851.4969842
RMSD=7.542e-09
Dipole=-0.1934349, -0.0945706, -0.6034204

PG=C01 [X(C2H9Cd1N102S1)]

CdCDSt5

2,1

Cd

S,1,2.6455520965

O,1,2.2699496177,2,109.47122063

O,1,2.2459029234,2,109.47122063,3,120.

N,1,2.2716939165,2,109.47122063,3,-120.

H,2,1.3532682,1,101.52794537,3,-71.45930587

H,2,1.35375954,1,101.36172376,3,25.96769013

H,3,0.97657675,1,125.34039764,2,40.55857074

H,3,0.9772854,1,124.99395005,2,-162.43509427

C,4,1.23078918,1,166.98888266,2,-5.875825

H,10,1.09927299,4,121.0481255,1,1.19440852

H,10,1.09851533,4,119.75500726,11,179.97862286

H,5,1.02591479,1,113.7585246,2,183.68402475

H,5,1.02570578,1,113.14704837,2,62.87609203

H,5,1.02595319,1,112.1546187,2,-56.67361772

HF=-813.4069375

RMSD=7.684e-09

Dipole=0.2294452,-0.0634398,-0.6208046

PG=C01 [X(C1H9Cd1N102S1)]

CdCDSt6

2,1

Cd

O,1,2.266907438

O,1,2.2666079465,2,109.47122063

S,1,2.6411861935,2,109.47122063,3,120.

S,1,2.6410144797,2,109.47122063,3,-120.

H,2,0.97715546,1,126.00530669,3,-137.28671058

H,2,0.97721096,1,126.72613851,3,37.77615189

H,3,0.97717428,1,125.96028173,2,223.41524284

H,3,0.97720322,1,126.74413777,2,38.09497653

H,4,1.35436319,1,98.61472212,2,-175.53081491

H,4,1.35444234,1,100.57257274,2,-79.16407195

H,5,1.35447271,1,100.52722432,2,38.8404492

H,5,1.35436768,1,98.61819189,2,-57.52868001

HF=-1118.1382042

RMSD=7.152e-09

Dipole=1.153564,-0.0052942,0.8238598

PG=C01 [X(Cd1H802S2)]

CdCDSt7

1,1
Cd
O,1,2.3014627688
O,1,2.2477905106,2,109.47122063
S,1,2.6619550991,2,109.47122063,3,120.
O,1,2.0875852632,2,109.47122063,3,-120.
H,2,0.97304987,1,129.08906844,3,-92.60346916
H,2,0.97474217,1,118.79945451,3,114.21728494
H,3,1.02084268,1,95.67672252,2,-119.05786808
H,3,0.97258209,1,126.58711976,2,0.93577882
H,4,1.3523873,1,94.04096012,2,120.26596053
H,4,1.35233137,1,96.0652197,2,215.1457816
C,5,1.30489723,1,115.95687296,2,120.60279574
H,12,1.09833869,5,114.23891506,1,179.81220999
O,12,1.23877975,5,125.70918421,13,180.21989236

HF=-908.3294203
RMSD=7.761e-09
Dipole=-0.085655,-1.852611,1.7573845
PG=C01 [X(C1H7Cd104S1)]

CdCDSt8

1,1
Cd
S,1,2.6498520409
N,1,2.311537842,2,109.47122063
O,1,2.0898565072,2,109.47122063,3,120.
O,1,2.3165383062,2,109.47122063,3,-120.
H,2,1.38163488,1,79.64107442,3,-132.34729509
H,2,1.35163013,1,96.11149781,3,-39.14270577
H,3,1.02324409,1,114.14255374,2,-133.93875655
H,3,1.02176858,1,114.21620804,2,-11.14508144
H,3,1.02380537,1,108.33284024,2,107.85234365
C,4,1.30526952,1,122.86903562,2,14.16423746
H,11,1.09978935,4,113.7139494,1,178.97461085
O,11,1.23588904,4,126.296095,1,-1.21412678
H,5,0.9735806,1,124.20061642,2,18.55214804
H,5,0.97497082,1,117.71800181,2,-121.1507242

HF=-888.4641957
RMSD=7.089e-09
Dipole=2.044845,2.312774,-0.914225
PG=C01 [X(C1H8Cd1N103S1)]

CdCDSt9

1,1
Cd
S,1,2.6833372005
N,1,2.3041322508,2,109.47122063
O,1,2.326567465,2,109.47122063,3,120.

O,1,2.1387555612,2,109.47122063,3,-120.
H,2,1.35555116,1,87.18674496,3,75.74742417
H,2,1.35174477,1,97.8295942,3,169.76240196
H,3,1.02223766,1,114.056871,2,176.52904891
H,3,1.02180832,1,118.28414373,2,49.7214649
H,3,1.02586929,1,101.96538083,2,-68.4277988
C,4,1.22912758,1,127.78102097,2,118.13609683
H,11,1.09986557,4,121.5658166,1,-0.65425365
H,11,1.09814039,4,119.228673,12,179.9641778
C,5,1.29983846,1,106.55781519,2,62.50959276
H,14,1.0995402,5,115.17801117,1,179.45159566
O,14,1.24073079,5,123.44459098,15,179.85979299

HF=-926.555449
RMSD=9.435e-09
Dipole=-0.0685782,-2.0288146,-0.5829031
PG=C01 [X(C2H8Cd1N103S1)]

CdCDSt10

O,1
Cd
S,1,2.6794761316
S,1,2.6739190959,2,109.47122063
O,1,2.1270273932,2,109.47122063,3,120.
O,1,2.1248975875,2,109.47122063,3,-120.
H,2,1.38163488,1,79.86205016,3,-125.74009116
H,2,1.35163013,1,96.26799792,3,-33.30594799
H,3,1.3816,1,79.76133275,2,-117.48390186
H,3,1.3516,1,93.30923331,2,148.57920331
C,4,1.29071169,1,123.55601327,2,6.09180548
H,10,1.10336764,4,113.85514644,1,177.31743037
O,10,1.24276687,4,127.38248639,1,-2.71399135
C,5,1.28915861,1,123.41582602,2,116.90915221
H,13,1.10314255,5,113.94759476,1,179.92846939
O,13,1.24429984,5,127.38196656,14,180.09132496

HF=-1344.3078296
RMSD=9.773e-09
Dipole=1.4216928,-0.3653579,0.6019329
PG=C01 [X(C2H6Cd104S2)]

HgCDSt1

2,1
Hg
O,1,2.3260860017
O,1,2.3384235249,2,109.47122063
S,1,2.5949167829,2,109.47122063,3,120.
O,1,2.3182781442,2,109.47122063,3,-120.
H,2,0.97710956,1,126.72351565,3,-32.42515075
H,2,0.97756217,1,125.23198546,3,137.32199183
H,3,0.97720206,1,125.08548378,2,128.90568232

H, 3, 0.97691541, 1, 127.26501921, 2, -43.6894312
H, 4, 1.35409598, 1, 98.71271852, 2, 3.90805121
H, 4, 1.35439907, 1, 98.51076654, 2, 100.10143429
C, 5, 1.23465919, 1, 146.23736757, 2, 123.86702845
H, 12, 1.09868727, 5, 121.69940132, 1, -2.09235282
H, 12, 1.09751386, 5, 118.89820982, 13, 179.94205073

HF=-820.066316
RMSD=5.525e-09
Dipole=0.2084679, 0.4251699, 0.0216
PG=C01 [X(C1H8Hg103S1)]

HgCDSt2

2, 1
Hg
S, 1, 2.6015465589
O, 1, 2.3404238774, 2, 109.47122063
O, 1, 2.3110045761, 2, 109.47122063, 3, 120.
O, 1, 2.3298046068, 2, 109.47122063, 3, -120.
H, 2, 1.35379864, 1, 99.7819091, 3, -18.12579641
H, 2, 1.35393714, 1, 100.2118578, 3, 78.80693391
H, 3, 0.97744477, 1, 125.63242174, 2, 115.40313724
H, 3, 0.97598732, 1, 126.75833562, 2, -68.51929524
C, 4, 1.23376805, 1, 147.69191231, 2, 68.13943977
H, 10, 1.09887316, 4, 121.64827332, 1, -0.69344272
H, 10, 1.09752428, 4, 118.93131886, 11, 180.32903525
C, 5, 1.23366055, 1, 147.88558831, 2, 157.60744208
H, 13, 1.09904483, 5, 121.69558296, 1, -0.62863977
H, 13, 1.09770407, 5, 118.96648232, 14, 179.92854414

HF=-858.1553668
RMSD=8.711e-09
Dipole=0.0996899, 0.4190725, -0.4834695
PG=C01 [X(C2H8Hg103S1)]

HgCDSt3

2, 1
Hg
S, 1, 2.604459039
O, 1, 2.3446827952, 2, 109.47122063
O, 1, 2.3300367, 2, 109.47122063, 3, 120.
O, 1, 2.3329101221, 2, 109.47122063, 3, -120.
H, 2, 1.35382234, 1, 99.42346635, 3, -24.86006571
H, 2, 1.35394345, 1, 99.35041753, 3, 71.37040763
C, 3, 1.23439672, 1, 142.62314323, 2, 115.8445957
H, 8, 1.09877467, 3, 121.73254404, 1, 0.69876845
H, 8, 1.09753352, 3, 118.90990393, 9, 180.08272977
C, 4, 1.23419868, 1, 143.32350114, 2, 80.31278782
H, 11, 1.09872769, 4, 121.76269088, 1, 2.16299582
H, 11, 1.09740596, 4, 118.89863073, 12, 180.01844807
C, 5, 1.23372739, 1, 144.93803684, 2, 112.4054566

H, 14, 1.09881591, 5, 121.71095223, 1, 1.03525778
H, 14, 1.09752425, 5, 118.92338792, 15, 180.0617941

HF=-896.2457555
RMSD=8.155e-09
Dipole=0.2795919, 0.1111078, -0.5528969
PG=C01 [X(C3H8Hg103S1)]

HgCDSt4

2, 1
Hg
S, 1, 2.6477043273
O, 1, 2.3391700363, 2, 109.47122063
O, 1, 2.3673835569, 2, 109.47122063, 3, 120.
N, 1, 2.3005677574, 2, 109.47122063, 3, -120.
H, 2, 1.35370225, 1, 100.67403997, 3, -47.42763211
H, 2, 1.35408901, 1, 99.62884198, 3, 48.89193922
C, 3, 1.23388199, 1, 144.85377957, 2, 127.8430108
H, 8, 1.09869892, 3, 121.67597912, 1, -2.16876368
H, 8, 1.09746485, 3, 118.92495585, 9, 179.91268855
C, 4, 1.23209511, 1, 151.41275636, 2, 28.9978892
H, 11, 1.09950782, 4, 121.58841047, 1, -0.87424889
H, 11, 1.09801294, 4, 119.2932244, 12, 179.8790918
H, 5, 1.02597301, 1, 112.96295399, 2, 158.00819994
H, 5, 1.02537065, 1, 113.04635429, 2, 38.41966235
H, 5, 1.02551705, 1, 113.357995, 2, -81.86571236

HF=-838.3063725
RMSD=6.471e-09
Dipole=-0.1573949, -0.0795047, -0.3439319
PG=C01 [X(C2H9Hg1N102S1)]

HgCDSt5

2, 1
Hg
S, 1, 2.6441370758
O, 1, 2.3543359361, 2, 109.47122063
O, 1, 2.3406773454, 2, 109.47122063, 3, 120.
N, 1, 2.2925398875, 2, 109.47122063, 3, -120.
H, 2, 1.3532682, 1, 101.52794537, 3, -71.45930587
H, 2, 1.35375954, 1, 101.36172376, 3, 25.96769013
H, 3, 0.97657675, 1, 125.34039764, 2, 40.55857074
H, 3, 0.9772854, 1, 124.99395005, 2, -162.43509427
C, 4, 1.23078918, 1, 166.98888266, 2, -5.875825
H, 10, 1.09927299, 4, 121.0481255, 1, 1.19440852
H, 10, 1.09851533, 4, 119.75500726, 11, 179.97862286
H, 5, 1.02591479, 1, 113.7585246, 2, 183.68402475
H, 5, 1.02570578, 1, 113.14704837, 2, 62.87609203
H, 5, 1.02595319, 1, 112.1546187, 2, -56.67361772

HF=-800.2152378

RMSD=6.793e-09
Dipole=0.1033565, -0.0176841, -0.2457376
PG=C01 [X(C1H9Hg1N102S1)]

HgCDSt6

2,1
Hg
O,1,2.3559336623
O,1,2.3555386274,2,109.47122063
S,1,2.6430638373,2,109.47122063,3,120.
S,1,2.6427701036,2,109.47122063,3,-120.
H,2,0.97715546,1,126.00530669,3,-137.28671058
H,2,0.97721096,1,126.72613851,3,37.77615189
H,3,0.97717428,1,125.96028173,2,223.41524284
H,3,0.97720322,1,126.74413777,2,38.09497653
H,4,1.35436319,1,98.61472212,2,-175.53081491
H,4,1.35444234,1,100.57257274,2,-79.16407195
H,5,1.35447271,1,100.52722432,2,38.8404492
H,5,1.35436768,1,98.61819189,2,-57.52868001

HF=-1104.9524275
RMSD=6.234e-09
Dipole=0.4295773, -0.0063098, 0.3126112
PG=C01 [X(H8Hg102S2)]

HgCDSt7

1,1
Hg
O,1,2.4053161547
O,1,2.3416686477,2,109.47122063
S,1,2.6728074565,2,109.47122063,3,120.
O,1,2.1315309567,2,109.47122063,3,-120.
H,2,0.97304987,1,129.08906844,3,-92.60346916
H,2,0.97474217,1,118.79945451,3,114.21728494
H,3,1.02084268,1,95.67672252,2,-119.05786808
H,3,0.97258209,1,126.58711976,2,0.93577882
H,4,1.3523873,1,94.04096012,2,120.26596053
H,4,1.35233137,1,96.0652197,2,215.1457816
C,5,1.30489723,1,115.95687296,2,120.60279574
H,12,1.09833869,5,114.23891506,1,179.81220999
O,12,1.23877975,5,125.70918421,13,180.21989236

HF=-895.1372987
RMSD=7.904e-09
Dipole=-0.1762557, -1.6927439, 1.3984414
PG=C01 [X(C1H7Hg104S1)]

HgCDSt8

1,1
Hg
S,1,2.6803397538
N,1,2.3564019326,2,109.47122063
O,1,2.1356672294,2,109.47122063,3,120.
O,1,2.4258215551,2,109.47122063,3,-120.
H,2,1.38163488,1,79.64107442,3,-132.34729509
H,2,1.35163013,1,96.11149781,3,-39.14270577
H,3,1.02324409,1,114.14255374,2,-133.93875655
H,3,1.02176858,1,114.21620804,2,-11.14508144
H,3,1.02380537,1,108.33284024,2,107.85234365
C,4,1.30526952,1,122.86903562,2,14.16423746
H,11,1.09978935,4,113.7139494,1,178.97461085
O,11,1.23588904,4,126.296095,1,-1.21412678
H,5,0.9735806,1,124.20061642,2,18.55214804
H,5,0.97497082,1,117.71800181,2,-121.1507242

HF=-875.2750574
RMSD=7.471e-09
Dipole=1.9729921,1.9656769,-0.6576557
PG=C01 [X(C1H8Hg1N103S1)]

HgCDSt9

1,1
Hg
S,1,2.7081014621
N,1,2.3490497928,2,109.47122063
O,1,2.4406527081,2,109.47122063,3,120.
O,1,2.1967032782,2,109.47122063,3,-120.
H,2,1.35555116,1,87.18674496,3,75.74742417
H,2,1.35174477,1,97.8295942,3,169.76240196
H,3,1.02223766,1,114.056871,2,176.52904891
H,3,1.02180832,1,118.28414373,2,49.7214649
H,3,1.02586929,1,101.96538083,2,-68.4277988
C,4,1.22912758,1,127.78102097,2,118.13609683
H,11,1.09986557,4,121.5658166,1,-0.65425365
H,11,1.09814039,4,119.228673,12,179.9641778
C,5,1.29983846,1,106.55781519,2,62.50959276
H,14,1.0995402,5,115.17801117,1,179.45159566
O,14,1.24073079,5,123.44459098,15,179.85979299

HF=-913.3659753
RMSD=8.897e-09
Dipole=0.0169896,-1.7060071,-0.443465
PG=C01 [X(C2H8Hg1N103S1)]

HgCDSt10

0,1
Hg

S,1,2.7241961078
 S,1,2.7206220267,2,109.47122063
 O,1,2.1801782927,2,109.47122063,3,120.
 O,1,2.1770295353,2,109.47122063,3,-120.
 H,2,1.38163488,1,79.86205016,3,-125.74009116
 H,2,1.35163013,1,96.26799792,3,-33.30594799
 H,3,1.3816,1,79.76133275,2,-117.48390186
 H,3,1.3516,1,93.30923331,2,148.57920331
 C,4,1.29071169,1,123.55601327,2,6.09180548
 H,10,1.10336764,4,113.85514644,1,177.31743037
 O,10,1.24276687,4,127.38248639,1,-2.71399135
 C,5,1.28915861,1,123.41582602,2,116.90915221
 H,13,1.10314255,5,113.94759476,1,179.92846939
 O,13,1.24429984,5,127.38196656,14,180.09132496

HF=-1331.1197638

RMSD=6.599e-09

Dipole=1.4156794,-0.3624944,0.5963678

PG=C01 [X(C2H6Hg104S2)]

6. ENERGIES OF LIGANDS

Bq[Co]C0St1	E(B3LYP) =	-745.57450102
Bq[Co]C0St2	E(B3LYP) =	-1295.89999805
Bq[Co]C0St3	E(B3LYP) =	-726.31046548
Bq[Co]C0St4	E(B3LYP) =	-820.31102386
Bq[Co]C0St5	E(B3LYP) =	-572.38168620
Bq[Co]C0St6	E(B3LYP) =	-781.49399599
Bq[Co]C0St7	E(B3LYP) =	-762.04298288
Bq[Co]C0St8	E(B3LYP) =	-685.90007320
Bq[Co]C0St9	E(B3LYP) =	-969.46010971
Bq[Co]C0St10	E(B3LYP) =	-966.64072976
Bq[Ni]C0St1	E(B3LYP) =	-745.56945403
Bq[Ni]C0St2	E(B3LYP) =	-1295.89581206
Bq[Ni]C0St3	E(B3LYP) =	-726.30654920
Bq[Ni]C0St4	E(B3LYP) =	-820.30606164
Bq[Ni]C0St5	E(B3LYP) =	-572.38044668
Bq[Ni]C0St6	E(B3LYP) =	-781.48988243
Bq[Ni]C0St7	E(B3LYP) =	-762.03981263
Bq[Ni]C0St8	E(B3LYP) =	-685.89722953
Bq[Ni]C0St9	E(B3LYP) =	-969.45424574
Bq[Ni]C0St10	E(B3LYP) =	-966.63576932
Bq[Cu]C0St1	E(B3LYP) =	-745.57436424
Bq[Cu]C0St2	E(B3LYP) =	-1295.89922407
Bq[Cu]C0St3	E(B3LYP) =	-726.30777968
Bq[Cu]C0St4	E(B3LYP) =	-820.31048739
Bq[Cu]C0St5	E(B3LYP) =	-572.38000871
Bq[Cu]C0St6	E(B3LYP) =	-781.48925149
Bq[Cu]C0St7	E(B3LYP) =	-762.03930288
Bq[Cu]C0St8	E(B3LYP) =	-685.89460434
Bq[Cu]C0St9	E(B3LYP) =	-969.46056524
Bq[Cu]C0St10	E(B3LYP) =	-966.64466595
Bq[Zn]C0St1	E(B3LYP) =	-745.57718301
Bq[Zn]C0St2	E(B3LYP) =	-1295.90302587
Bq[Zn]C0St3	E(B3LYP) =	-726.31429096

Bq[Zn]C0St4	E(B3LYP) =	-820.31391393
Bq[Zn]C0St5	E(B3LYP) =	-572.38247218
Bq[Zn]C0St6	E(B3LYP) =	-781.49593058
Bq[Zn]C0St7	E(B3LYP) =	-762.04602099
Bq[Zn]C0St8	E(B3LYP) =	-685.90160732
Bq[Zn]C0St9	E(B3LYP) =	-969.46289191
Bq[Zn]C0St10	E(B3LYP) =	-966.63992747
Bq[Cd]C0St1	E(B3LYP) =	-745.59187710
Bq[Cd]C0St2	E(B3LYP) =	-1295.91494127
Bq[Cd]C0St3	E(B3LYP) =	-726.32913947
Bq[Cd]C0St4	E(B3LYP) =	-820.32842209
Bq[Cd]C0St5	E(B3LYP) =	-572.39220802
Bq[Cd]C0St6	E(B3LYP) =	-781.51256895
Bq[Cd]C0St7	E(B3LYP) =	-762.06199763
Bq[Cd]C0St8	E(B3LYP) =	-685.91453198
Bq[Cd]C0St9	E(B3LYP) =	-969.49056559
Bq[Cd]C0St10	E(B3LYP) =	-966.65836469
Bq[Hg]C0St1	E(B3LYP) =	-745.59493898
Bq[Hg]C0St2	E(B3LYP) =	-1295.91757856
Bq[Hg]C0St3	E(B3LYP) =	-726.32869071
Bq[Hg]C0St4	E(B3LYP) =	-820.32981636
Bq[Hg]C0St5	E(B3LYP) =	-572.39041581
Bq[Hg]C0St6	E(B3LYP) =	-781.51264066
Bq[Hg]C0St7	E(B3LYP) =	-762.06342737
Bq[Hg]C0St8	E(B3LYP) =	-685.91538097
Bq[Hg]C0St9	E(B3LYP) =	-969.49771373
Bq[Hg]C0St10	E(B3LYP) =	-966.66474785
Bq[Co]N1St1	E(B3LYP) =	-571.67419047
Bq[Co]N1St2	E(B3LYP) =	-611.43640355
Bq[Co]N1St3	E(B3LYP) =	-626.96738731
Bq[Co]N1St4	E(B3LYP) =	-970.27539276
Bq[Co]N1St5	E(B3LYP) =	-744.15218132
Bq[Co]N1St6	E(B3LYP) =	-721.94121231
Bq[Co]N1St7	E(B3LYP) =	-702.04715182
Bq[Co]N1St8	E(B3LYP) =	-531.07093414
Bq[Co]N1St9	E(B3LYP) =	-796.90315582
Bq[Co]N1St10	E(B3LYP) =	-966.64072976
Bq[Ni]N1St1	E(B3LYP) =	-571.66715435
Bq[Ni]N1St2	E(B3LYP) =	-611.43045984
Bq[Ni]N1St3	E(B3LYP) =	-626.96171373
Bq[Ni]N1St4	E(B3LYP) =	-970.27136292
Bq[Ni]N1St5	E(B3LYP) =	-744.14725587
Bq[Ni]N1St6	E(B3LYP) =	-721.93670808
Bq[Ni]N1St7	E(B3LYP) =	-702.04199309
Bq[Ni]N1St8	E(B3LYP) =	-531.06866327
Bq[Ni]N1St9	E(B3LYP) =	-796.89732060
Bq[Ni]N1St10	E(B3LYP) =	-966.63576932
Bq[Cu]N1St1	E(B3LYP) =	-571.67767648
Bq[Cu]N1St2	E(B3LYP) =	-611.43669976
Bq[Cu]N1St3	E(B3LYP) =	-626.96625698
Bq[Cu]N1St4	E(B3LYP) =	-970.27445100
Bq[Cu]N1St5	E(B3LYP) =	-744.15102526
Bq[Cu]N1St6	E(B3LYP) =	-721.93596089
Bq[Cu]N1St7	E(B3LYP) =	-702.04671472
Bq[Cu]N1St8	E(B3LYP) =	-531.06768865
Bq[Cu]N1St9	E(B3LYP) =	-796.89971179
Bq[Cu]N1St10	E(B3LYP) =	-966.64466595
Bq[Zn]N1St1	E(B3LYP) =	-571.67777692
Bq[Zn]N1St2	E(B3LYP) =	-611.43933820
Bq[Zn]N1St3	E(B3LYP) =	-626.97012647
Bq[Zn]N1St4	E(B3LYP) =	-970.27703232

Bq[Zn]NIST5	E(B3LYP) =	-744.15444918
Bq[Zn]NIST6	E(B3LYP) =	-721.94294997
Bq[Zn]NIST7	E(B3LYP) =	-702.04924098
Bq[Zn]NIST8	E(B3LYP) =	-531.07155500
Bq[Zn]NIST9	E(B3LYP) =	-796.90483154
Bq[Zn]NIST10	E(B3LYP) =	-966.63992747
Bq[Cd]NIST1	E(B3LYP) =	-571.69583234
Bq[Cd]NIST2	E(B3LYP) =	-611.45566404
Bq[Cd]NIST3	E(B3LYP) =	-626.98692927
Bq[Cd]NIST4	E(B3LYP) =	-970.28854896
Bq[Cd]NIST5	E(B3LYP) =	-744.16885344
Bq[Cd]NIST6	E(B3LYP) =	-721.95920026
Bq[Cd]NIST7	E(B3LYP) =	-702.06698347
Bq[Cd]NIST8	E(B3LYP) =	-531.08682631
Bq[Cd]NIST9	E(B3LYP) =	-796.92911641
Bq[Cd]NIST10	E(B3LYP) =	-966.65836469
Bq[Hg]NIST1	E(B3LYP) =	-571.69953366
Bq[Hg]NIST2	E(B3LYP) =	-611.45973142
Bq[Hg]NIST3	E(B3LYP) =	-626.98987271
Bq[Hg]NIST4	E(B3LYP) =	-970.28993876
Bq[Hg]NIST5	E(B3LYP) =	-744.17099198
Bq[Hg]NIST6	E(B3LYP) =	-721.96113155
Bq[Hg]NIST7	E(B3LYP) =	-702.06987768
Bq[Hg]NIST8	E(B3LYP) =	-531.08447413
Bq[Hg]NIST9	E(B3LYP) =	-796.93406285
Bq[Hg]NIST10	E(B3LYP) =	-966.66474785
Bq[Co]CUST1	E(B3LYP) =	-458.53316496
Bq[Co]CUST2	E(B3LYP) =	-400.37267018
Bq[Co]CUST3	E(B3LYP) =	-743.22751314
Bq[Co]CUST4	E(B3LYP) =	-359.00436353
Bq[Co]CUST5	E(B3LYP) =	-665.12331993
Bq[Co]CUST6	E(B3LYP) =	-742.52836344
Bq[Co]CUST7	E(B3LYP) =	-701.16356680
Bq[Co]CUST8	E(B3LYP) =	-664.71053488
Bq[Co]CUST9	E(B3LYP) =	-1007.19384669
Bq[Co]CUST10	E(B3LYP) =	-720.17761492
Bq[Ni]CUST1	E(B3LYP) =	-458.53073988
Bq[Ni]CUST2	E(B3LYP) =	-400.37041868
Bq[Ni]CUST3	E(B3LYP) =	-743.22605205
Bq[Ni]CUST4	E(B3LYP) =	-359.00215966
Bq[Ni]CUST5	E(B3LYP) =	-665.12059691
Bq[Ni]CUST6	E(B3LYP) =	-742.52645511
Bq[Ni]CUST7	E(B3LYP) =	-701.16033980
Bq[Ni]CUST8	E(B3LYP) =	-664.70796103
Bq[Ni]CUST9	E(B3LYP) =	-1007.18932179
Bq[Ni]CUST10	E(B3LYP) =	-720.17391954
Bq[Cu]CUST1	E(B3LYP) =	-458.52739273
Bq[Cu]CUST2	E(B3LYP) =	-400.36950201
Bq[Cu]CUST3	E(B3LYP) =	-743.22611714
Bq[Cu]CUST4	E(B3LYP) =	-358.99953588
Bq[Cu]CUST5	E(B3LYP) =	-665.12030453
Bq[Cu]CUST6	E(B3LYP) =	-742.52603174
Bq[Cu]CUST7	E(B3LYP) =	-701.15875846
Bq[Cu]CUST8	E(B3LYP) =	-664.70961545
Bq[Cu]CUST9	E(B3LYP) =	-1007.19002856
Bq[Cu]CUST10	E(B3LYP) =	-720.17539767
Bq[Zn]CUST1	E(B3LYP) =	-458.53458582
Bq[Zn]CUST2	E(B3LYP) =	-400.37380104
Bq[Zn]CUST3	E(B3LYP) =	-743.22844801
Bq[Zn]CUST4	E(B3LYP) =	-359.00585298
Bq[Zn]CUST5	E(B3LYP) =	-665.12536889

Bq[Zn]CUST6	E(B3LYP) =	-742.53116289
Bq[Zn]CUST7	E(B3LYP) =	-701.16701001
Bq[Zn]CUST8	E(B3LYP) =	-664.71164590
Bq[Zn]CUST9	E(B3LYP) =	-1007.19814671
Bq[Zn]CUST10	E(B3LYP) =	-720.17778121
Bq[Cd]CUST1	E(B3LYP) =	-458.54487728
Bq[Cd]CUST2	E(B3LYP) =	-400.38182261
Bq[Cd]CUST3	E(B3LYP) =	-743.23382954
Bq[Cd]CUST4	E(B3LYP) =	-359.01754001
Bq[Cd]CUST5	E(B3LYP) =	-665.13659936
Bq[Cd]CUST6	E(B3LYP) =	-742.54355012
Bq[Cd]CUST7	E(B3LYP) =	-701.18256681
Bq[Cd]CUST8	E(B3LYP) =	-664.72734181
Bq[Cd]CUST9	E(B3LYP) =	-1007.21242925
Bq[Cd]CUST10	E(B3LYP) =	-720.20062477
Bq[Hg]CUST1	E(B3LYP) =	-458.54624895
Bq[Hg]CUST2	E(B3LYP) =	-400.38211389
Bq[Hg]CUST3	E(B3LYP) =	-743.23407383
Bq[Hg]CUST4	E(B3LYP) =	-359.01867390
Bq[Hg]CUST5	E(B3LYP) =	-665.13872178
Bq[Hg]CUST6	E(B3LYP) =	-742.54627187
Bq[Hg]CUST7	E(B3LYP) =	-701.18533718
Bq[Hg]CUST8	E(B3LYP) =	-664.73225012
Bq[Hg]CUST9	E(B3LYP) =	-1007.21600958
Bq[Hg]CUST10	E(B3LYP) =	-720.20769503
Bq[Co]ZNSt1	E(B3LYP) =	-381.13256870
Bq[Co]ZNSt2	E(B3LYP) =	-378.89968884
Bq[Co]ZNSt3	E(B3LYP) =	-398.77901422
Bq[Co]ZNSt4	E(B3LYP) =	-779.27170138
Bq[Co]ZNSt5	E(B3LYP) =	-491.59277513
Bq[Co]ZNSt6	E(B3LYP) =	-1177.32232827
Bq[Co]ZNSt7	E(B3LYP) =	-342.07764725
Bq[Co]ZNSt8	E(B3LYP) =	-834.45857336
Bq[Co]ZNSt9	E(B3LYP) =	-684.14177903
Bq[Co]ZNSt10	E(B3LYP) =	-283.66431548
Bq[Ni]ZNSt1	E(B3LYP) =	-381.13247219
Bq[Ni]ZNSt2	E(B3LYP) =	-378.89884271
Bq[Ni]ZNSt3	E(B3LYP) =	-398.77886433
Bq[Ni]ZNSt4	E(B3LYP) =	-779.27091809
Bq[Ni]ZNSt5	E(B3LYP) =	-491.59328404
Bq[Ni]ZNSt6	E(B3LYP) =	-1177.32145280
Bq[Ni]ZNSt7	E(B3LYP) =	-342.07685363
Bq[Ni]ZNSt8	E(B3LYP) =	-834.45754766
Bq[Ni]ZNSt9	E(B3LYP) =	-684.13925491
Bq[Ni]ZNSt10	E(B3LYP) =	-283.65807310
Bq[Cu]ZNSt1	E(B3LYP) =	-381.13251106
Bq[Cu]ZNSt2	E(B3LYP) =	-378.89929475
Bq[Cu]ZNSt3	E(B3LYP) =	-398.77848093
Bq[Cu]ZNSt4	E(B3LYP) =	-779.27156549
Bq[Cu]ZNSt5	E(B3LYP) =	-491.59230005
Bq[Cu]ZNSt6	E(B3LYP) =	-1177.32201196
Bq[Cu]ZNSt7	E(B3LYP) =	-342.07650766
Bq[Cu]ZNSt8	E(B3LYP) =	-834.45782270
Bq[Cu]ZNSt9	E(B3LYP) =	-684.14392667
Bq[Cu]ZNSt10	E(B3LYP) =	-283.67029254
Bq[Zn]ZNSt1	E(B3LYP) =	-381.13281407
Bq[Zn]ZNSt2	E(B3LYP) =	-378.89954992
Bq[Zn]ZNSt3	E(B3LYP) =	-398.77877266
Bq[Zn]ZNSt4	E(B3LYP) =	-779.27190406
Bq[Zn]ZNSt5	E(B3LYP) =	-491.59297841
Bq[Zn]ZNSt6	E(B3LYP) =	-1177.32273235

Bq[Zn]ZNSt7	E(B3LYP) =	-342.07731444
Bq[Zn]ZNSt8	E(B3LYP) =	-834.45894755
Bq[Zn]ZNSt9	E(B3LYP) =	-684.13922673
Bq[Zn]ZNSt10	E(B3LYP) =	-283.65187041
Bq[Cd]ZNSt1	E(B3LYP) =	-381.14084762
Bq[Cd]ZNSt2	E(B3LYP) =	-378.90433720
Bq[Cd]ZNSt3	E(B3LYP) =	-398.78269120
Bq[Cd]ZNSt4	E(B3LYP) =	-779.27594108
Bq[Cd]ZNSt5	E(B3LYP) =	-491.60622785
Bq[Cd]ZNSt6	E(B3LYP) =	-1177.32984033
Bq[Cd]ZNSt7	E(B3LYP) =	-342.08976777
Bq[Cd]ZNSt8	E(B3LYP) =	-834.46837876
Bq[Cd]ZNSt9	E(B3LYP) =	-684.15912594
Bq[Cd]ZNSt10	E(B3LYP) =	-283.67445899
Bq[Hg]ZNSt1	E(B3LYP) =	-381.14186117
Bq[Hg]ZNSt2	E(B3LYP) =	-378.90422335
Bq[Hg]ZNSt3	E(B3LYP) =	-398.78262412
Bq[Hg]ZNSt4	E(B3LYP) =	-779.27644132
Bq[Hg]ZNSt5	E(B3LYP) =	-491.60839502
Bq[Hg]ZNSt6	E(B3LYP) =	-1177.33083677
Bq[Hg]ZNSt7	E(B3LYP) =	-342.09342969
Bq[Hg]ZNSt8	E(B3LYP) =	-834.46978377
Bq[Hg]ZNSt9	E(B3LYP) =	-684.16481029
Bq[Hg]ZNSt10	E(B3LYP) =	-283.68478654
Bq[Co]CDSt1	E(B3LYP) =	-666.89030345
Bq[Co]CDSt2	E(B3LYP) =	-704.97377281
Bq[Co]CDSt3	E(B3LYP) =	-743.05820968
Bq[Co]CDSt4	E(B3LYP) =	-685.09578144
Bq[Co]CDSt5	E(B3LYP) =	-647.01153924
Bq[Co]CDSt6	E(B3LYP) =	-951.77386706
Bq[Co]CDSt7	E(B3LYP) =	-741.63315025
Bq[Co]CDSt8	E(B3LYP) =	-721.74843187
Bq[Co]CDSt9	E(B3LYP) =	-759.82942687
Bq[Co]CDSt10	E(B3LYP) =	-1177.32232827
Bq[Ni]CDSt1	E(B3LYP) =	-666.89018453
Bq[Ni]CDSt2	E(B3LYP) =	-704.97369730
Bq[Ni]CDSt3	E(B3LYP) =	-743.05816946
Bq[Ni]CDSt4	E(B3LYP) =	-685.09559597
Bq[Ni]CDSt5	E(B3LYP) =	-647.01138985
Bq[Ni]CDSt6	E(B3LYP) =	-951.77373292
Bq[Ni]CDSt7	E(B3LYP) =	-741.63331731
Bq[Ni]CDSt8	E(B3LYP) =	-721.74806220
Bq[Ni]CDSt9	E(B3LYP) =	-759.82882692
Bq[Ni]CDSt10	E(B3LYP) =	-1177.32145280
Bq[Cu]CDSt1	E(B3LYP) =	-666.89032916
Bq[Cu]CDSt2	E(B3LYP) =	-704.97372336
Bq[Cu]CDSt3	E(B3LYP) =	-743.05829637
Bq[Cu]CDSt4	E(B3LYP) =	-685.09578670
Bq[Cu]CDSt5	E(B3LYP) =	-647.01153967
Bq[Cu]CDSt6	E(B3LYP) =	-951.77381646
Bq[Cu]CDSt7	E(B3LYP) =	-741.63280665
Bq[Cu]CDSt8	E(B3LYP) =	-721.74820416
Bq[Cu]CDSt9	E(B3LYP) =	-759.82903157
Bq[Cu]CDSt10	E(B3LYP) =	-1177.32201196
Bq[Zn]CDSt1	E(B3LYP) =	-666.89023493
Bq[Zn]CDSt2	E(B3LYP) =	-704.97380980
Bq[Zn]CDSt3	E(B3LYP) =	-743.05839033
Bq[Zn]CDSt4	E(B3LYP) =	-685.09594132
Bq[Zn]CDSt5	E(B3LYP) =	-647.01163881
Bq[Zn]CDSt6	E(B3LYP) =	-951.77397100
Bq[Zn]CDSt7	E(B3LYP) =	-741.63308901

Bq[Zn]CDSt8	E(B3LYP) = -721.74845772
Bq[Zn]CDSt9	E(B3LYP) = -759.82964107
Bq[Zn]CDSt10	E(B3LYP) = -1177.32273235
Bq[Cd]CDSt1	E(B3LYP) = -666.89373258
Bq[Cd]CDSt2	E(B3LYP) = -704.97728611
Bq[Cd]CDSt3	E(B3LYP) = -743.06164937
Bq[Cd]CDSt4	E(B3LYP) = -685.10012882
Bq[Cd]CDSt5	E(B3LYP) = -647.01594858
Bq[Cd]CDSt6	E(B3LYP) = -951.77728014
Bq[Cd]CDSt7	E(B3LYP) = -741.63479562
Bq[Cd]CDSt8	E(B3LYP) = -721.75282222
Bq[Cd]CDSt9	E(B3LYP) = -759.83314953
Bq[Cd]CDSt10	E(B3LYP) = -1177.32984033
Bq[Hg]CDSt1	E(B3LYP) = -666.89439438
Bq[Hg]CDSt2	E(B3LYP) = -704.97798531
Bq[Hg]CDSt3	E(B3LYP) = -743.06235375
Bq[Hg]CDSt4	E(B3LYP) = -685.10085318
Bq[Hg]CDSt5	E(B3LYP) = -647.01665559
Bq[Hg]CDSt6	E(B3LYP) = -951.77782533
Bq[Hg]CDSt7	E(B3LYP) = -741.63441453
Bq[Hg]CDSt8	E(B3LYP) = -721.75336158
Bq[Hg]CDSt9	E(B3LYP) = -759.83367067
Bq[Hg]CDSt10	E(B3LYP) = -1177.33083677