

CpZnCp

6	0.999031	2.452578	0.000000
6	0.191809	2.226009	1.155479
6	0.191809	2.226009	-1.155479
6	-1.115971	1.855688	-0.715092
6	-1.115971	1.855688	0.715092
1	0.509940	2.336782	-2.189929
1	-1.968731	1.635794	-1.353665
1	-1.968731	1.635794	1.353665
1	0.509940	2.336782	2.189929
1	2.040707	2.766658	0.000000
30	0.299659	0.306885	0.000000
6	0.895109	-1.616818	0.000000
6	0.191809	-2.184862	-1.169919
6	0.191809	-2.184862	1.169919
6	-0.870225	-2.932136	0.722589
6	-0.870225	-2.932136	-0.722589
1	0.483094	-2.023688	2.208425
1	-1.603649	-3.440933	1.349689
1	-1.603649	-3.440933	-1.349689
1	0.483094	-2.023688	-2.208425
1	1.994292	-1.580059	0.000000

CpZnZnCp

6	-3.086870	0.632725	-1.032887
6	-3.081546	1.180650	0.284299
6	-3.086136	-0.789450	-0.918761
6	-3.081793	-1.120222	0.468997
6	-3.080890	0.097319	1.212381
1	-3.109079	-1.497140	-1.744711
1	-3.100630	-2.124517	0.886867
1	-3.098698	0.184223	2.296685
1	-3.100971	2.238698	0.536763
1	-3.110430	1.199928	-1.960946
30	-1.181568	-0.000381	-0.003879
30	1.181564	0.000202	-0.001364
6	3.086002	0.629896	-1.035557
6	3.085032	-0.791905	-0.917975
6	3.082136	1.181096	0.280251
6	3.082010	0.099989	1.211046
6	3.082072	-1.119376	0.470525
1	3.102180	2.239755	0.530092
1	3.101066	0.189516	2.295116
1	3.101154	-2.122671	0.890781
1	3.106807	-1.501590	-1.742243
1	3.108619	1.194830	-1.965023

Me5CpZnCpMe5

6	-0.536086	-2.684185	0.000000
6	0.210691	-2.289684	1.163292
6	0.210691	-2.289684	-1.163292
6	1.419529	-1.648471	-0.719676
6	1.419529	-1.648471	0.719676
6	-1.801694	-3.496240	0.000000
6	-0.135472	-2.623362	2.587832
6	-0.135472	-2.623362	-2.587832
6	2.549673	-1.193613	-1.600653
6	2.549673	-1.193613	1.600653
30	-0.300375	-0.451121	0.000000
6	-1.268745	1.333391	0.000000
6	-0.646010	2.006027	-1.180571
6	-0.646010	2.006027	1.180571
6	0.295714	2.900662	0.731576
6	0.295714	2.900662	-0.731576
6	-2.793286	1.173406	0.000000
6	-1.079243	1.755801	-2.598008
6	-1.079243	1.755801	2.598008
6	1.220024	3.757376	1.549662
6	1.220024	3.757376	-1.549662
1	-1.582249	-4.579667	0.000000
1	-2.422637	-3.294218	-0.886237
1	-2.422637	-3.294218	0.886237
1	0.286229	-3.601674	2.882900
1	0.258609	-1.877504	3.295040
1	-1.223260	-2.681615	2.746525
1	0.286229	-3.601674	-2.882900
1	0.258609	-1.877504	-3.295040
1	-1.223260	-2.681615	-2.746525
1	3.262986	-2.015948	-1.792567
1	3.119413	-0.369479	-1.145695
1	2.192993	-0.840064	-2.579994
1	3.262986	-2.015948	1.792567
1	2.192993	-0.840064	2.579994
1	3.119413	-0.369479	1.145695
1	-3.155369	0.629385	0.887227
1	-3.284174	2.165865	0.000000
1	-3.155369	0.629385	-0.887227
1	-2.073419	2.196433	-2.803261
1	-0.378968	2.191781	-3.326343
1	-1.164044	0.679731	-2.829485
1	-0.378968	2.191781	3.326343
1	-2.073419	2.196433	2.803261
1	-1.164044	0.679731	2.829485
1	1.060938	4.832480	1.350555

1	1.083703	3.602150	2.629908
1	2.281656	3.554719	1.317869
1	1.060938	4.832480	-1.350555
1	2.281656	3.554719	-1.317869
1	1.083703	3.602150	-2.629908

Me5CpZnZnZnMe5

30	-1.178693	-0.041574	0.066859
30	1.179273	0.037577	-0.087336
6	-3.102636	-0.685727	0.957259
6	-3.073392	-1.143083	-0.406316
6	-3.074596	0.753076	0.940516
6	-3.028340	0.009768	-1.259319
6	-3.032388	1.178690	-0.429610
6	-3.094054	2.601385	-0.910433
6	-3.213814	1.648580	2.140089
6	-3.291727	-1.548742	2.173944
6	-3.205363	-2.570658	-0.858769
6	-3.081950	-0.005414	-2.761297
6	3.112943	0.367186	-1.112224
6	3.075105	-1.004176	-0.679232
6	3.079850	1.200902	0.060716
6	3.022708	0.344260	1.210771
6	3.226788	2.697024	0.078679
6	3.317377	0.842456	-2.523948
6	3.209531	-2.210704	-1.566053
6	3.018682	-1.014477	0.754269
6	3.060396	-2.237862	1.626319
6	3.072086	0.792804	2.644419
1	-2.693465	-2.748894	-1.817434
1	-4.265472	-2.851581	-1.001961
1	-2.781323	-3.276254	-0.127424
1	-2.857360	-2.551726	2.040385
1	-4.364384	-1.689233	2.404269
1	-2.825424	-1.108748	3.069300
1	-2.785274	1.193735	3.046765
1	-4.275849	1.866610	2.358959
1	-2.710570	2.617024	1.993140
1	-2.572119	2.735071	-1.870915
1	-2.637654	3.299886	-0.191741
1	-4.138666	2.931446	-1.062365
1	-2.618123	-0.911705	-3.180996
1	-2.562111	0.859944	-3.201506
1	-4.124709	0.023397	-3.128683
1	2.807232	3.164021	-0.826031
1	4.290148	2.996456	0.133127
1	2.719961	3.151443	0.944328

1	2.884364	0.147494	-3.260191
1	4.392848	0.938640	-2.763730
1	2.859564	1.828657	-2.698640
1	2.562414	0.083909	3.315586
1	2.595629	1.775452	2.786346
1	4.114191	0.884486	3.003350
1	2.585671	-3.105756	1.142352
1	2.544408	-2.077844	2.585968
1	4.100338	-2.529803	1.864004
1	2.686429	-3.087249	-1.152623
1	4.269382	-2.499017	-1.695916
1	2.799272	-2.031662	-2.572092

CpZn radical

6	-0.882992	1.214613	0.000000
6	-0.883069	0.375628	1.154785
6	-0.883069	0.375628	-1.154785
6	-0.883069	-0.981959	-0.713665
6	-0.883069	-0.981959	0.713665
1	-0.907217	0.711951	-2.189135
1	-0.907366	-1.861868	-1.353011
1	-0.907366	-1.861868	1.353011
1	-0.907217	0.711951	2.189135
1	-0.906477	2.302294	0.000000
30	1.034242	-0.000472	0.000000

Cp radical

6	0.000506	1.189902	0.000000
6	-0.000151	0.354710	1.172788
6	-0.000151	0.354710	-1.172788
6	-0.000151	-0.950063	-0.742408
6	-0.000151	-0.950063	0.742408
1	-0.000015	0.706482	-2.202543
1	-0.000148	-1.844723	-1.365106
1	-0.000148	-1.844723	1.365106
1	-0.000015	0.706482	2.202543
1	0.000918	2.281304	0.000000

Me5CpZn radical

6	-0.476728	1.222957	0.000000
6	-0.477872	0.377976	1.163116
6	-0.477872	0.377976	-1.163116
6	-0.479156	-0.989451	-0.718922
6	-0.479156	-0.989451	0.718922
6	-0.607793	2.720359	0.000000
6	-0.608640	0.843123	2.586418
6	-0.608640	0.843123	-2.586418

6	-0.609986	-2.200911	-1.599103
6	-0.609986	-2.200911	1.599103
30	1.412508	-0.001638	0.000000
1	-1.669274	3.029603	0.000000
1	-0.139840	3.175684	-0.886255
1	-0.139840	3.175684	0.886255
1	-1.669836	0.957792	2.874478
1	-0.157026	0.133183	3.296144
1	-0.124008	1.818295	2.748163
1	-1.669836	0.957792	-2.874478
1	-0.157026	0.133183	-3.296144
1	-0.124008	1.818295	-2.748163
1	-1.671260	-2.454288	-1.777234
1	-0.137580	-3.089148	-1.152188
1	-0.145954	-2.046119	-2.585262
1	-1.671260	-2.454288	1.777234
1	-0.145954	-2.046119	2.585262
1	-0.137580	-3.089148	1.152188

Me5Cp

6	-1.075753	0.513959	-0.000022
6	0.170469	1.224860	-0.000069
6	-0.811106	-0.920027	0.000033
6	0.553898	-1.081844	-0.000011
6	1.179899	0.271546	-0.000055
6	-2.441041	1.116861	-0.000057
6	0.309553	2.721337	-0.000011
6	-1.883232	-1.969056	0.000132
6	1.346514	-2.350543	-0.000130
6	2.658826	0.483222	0.000118
1	-3.023145	0.792040	0.882289
1	-3.023608	0.790777	-0.881622
1	-2.413678	2.215529	-0.000791
1	-0.160539	3.183820	0.886278
1	1.365303	3.029943	-0.000553
1	-0.161500	3.183924	-0.885727
1	-2.540573	-1.888351	0.885099
1	-1.462096	-2.985030	-0.000051
1	-2.540885	-1.888188	-0.884579
1	2.008073	-2.418386	0.882881
1	2.006327	-2.419287	-0.884404
1	0.701613	-3.240908	0.000924
1	3.133265	0.018228	0.883840
1	2.929400	1.548544	-0.001381
1	3.133873	0.015457	-0.881776