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Optimized structure of singlet ground state of Zn-2

Zn	-0.00002	-1.59051	0.40888
Cl	-0.00038	-2.25574	2.52236
Cl	0.00042	-2.71826	-1.47545
N	1.36046	0.07372	0.2435
N	-1.36051	0.07376	0.24356
C	0.75584	1.21727	0.17184
C	-0.75585	1.21729	0.17187
C	-1.19203	2.62529	0.17973
C	-2.41708	3.27639	0.25203
H	-3.35914	2.72988	0.255
C	-2.43443	4.69342	0.32626
H	-3.40239	5.196	0.37593
C	-1.27207	5.45159	0.33658
H	-1.32901	6.54101	0.39473
C	0.00007	4.8158	0.28486
C	1.27224	5.45154	0.33638
H	1.32924	6.54096	0.39451
C	2.43457	4.69333	0.32589
H	3.40256	5.19587	0.3754
C	2.41716	3.2763	0.2517
H	3.3592	2.72975	0.25457
C	1.19208	2.62524	0.17962
C	0.00004	3.40404	0.19949
C	-2.75755	-0.10995	0.17292
C	-3.53399	0.4533	-0.85629
H	-3.05331	1.05636	-1.62888
C	-4.89907	0.19045	-0.91936
H	-5.48903	0.61333	-1.734
C	-5.53029	-0.63527	0.03431
C	-4.72519	-1.23362	1.02608
H	-5.18298	-1.90715	1.75314
C	-3.3567	-0.98645	1.09593
H	-2.73598	-1.45507	1.86324
C	-6.98663	-0.93603	-0.0525

C	-7.34525	-2.37682	0.09827
C	-8.38957	-2.78258	0.95224
H	-8.9576	-2.02675	1.49779
C	-8.69494	-4.13529	1.11445
H	-9.50304	-4.42938	1.78816
C	-7.96595	-5.11096	0.42486
H	-8.20579	-6.16892	0.55243
C	-6.91934	-4.7233	-0.41888
H	-6.33892	-5.47688	-0.9557
C	-6.60493	-3.37092	-0.5725
H	-5.77894	-3.07795	-1.22457
C	-7.92316	0.04869	-0.25646
C	-7.59637	1.49837	-0.11174
C	-6.91815	1.98125	1.02502
H	-6.61418	1.27761	1.80242
C	-6.65012	3.34445	1.17485
H	-6.13933	3.69848	2.07381
C	-7.04782	4.25429	0.18773
H	-6.84297	5.32097	0.3067
C	-7.7299	3.78999	-0.9431
H	-8.05063	4.49244	-1.71594
C	-8.01313	2.42947	-1.08433
H	-8.55856	2.07575	-1.96218
C	-9.33731	-0.24644	-0.62821
C	-10.3994	0.43365	0.00098
H	-10.17842	1.16214	0.78446
C	-11.72557	0.17831	-0.35597
H	-12.53458	0.7057	0.15487
C	-12.01743	-0.74487	-1.36616
H	-13.05388	-0.93917	-1.65109
C	-10.97141	-1.41039	-2.01565
H	-11.18798	-2.12216	-2.81554
C	-9.64629	-1.16639	-1.64969
H	-8.83519	-1.68634	-2.16267
C	2.75751	-0.11001	0.17292
C	3.35663	-0.98651	1.09592

H	2.73589	-1.45516	1.86321
C	12.01739	-0.74484	-1.36613
H	13.05383	-0.93912	-1.65108
C	4.72512	-1.23367	1.02611
H	5.1829	-1.90721	1.75318
C	5.53025	-0.6353	0.03437
C	4.89906	0.19045	-0.91929
H	5.48904	0.61335	-1.7339
C	3.53398	0.45329	-0.85625
H	3.05332	1.05638	-1.62883
C	6.98659	-0.93604	-0.05235
C	7.34528	-2.3768	0.09857
C	6.60514	-3.37098	-0.57227
H	5.77923	-3.0781	-1.22448
C	6.91961	-4.72334	-0.41853
H	6.33933	-5.47698	-0.95541
C	7.96611	-5.11088	0.4254
H	8.20602	-6.16881	0.55304
C	8.69491	-4.13513	1.11507
H	9.50291	-4.42913	1.78893
C	8.38947	-2.78244	0.95274
H	8.95736	-2.02655	1.49836
C	7.9231	0.04867	-0.25642
C	7.59629	1.49838	-0.11194
C	8.01312	2.42933	-1.08464
H	8.5586	2.07548	-1.9624
C	7.72988	3.78987	-0.94362
H	8.05065	4.49222	-1.71653
C	7.04772	4.25434	0.1871
H	6.84288	5.32103	0.3059
C	6.64995	3.34463	1.17433
H	6.13911	3.6988	2.07321
C	6.91798	1.98141	1.0247
H	6.61395	1.27789	1.80218
C	9.33727	-0.24646	-0.62814
C	9.64626	-1.16648	-1.64957

H	8.83516	-1.68651	-2.16245
C	10.97138	-1.41046	-2.01554
H	11.18795	-2.12229	-2.81538
C	11.72552	0.17839	-0.356
H	12.53452	0.70585	0.15479
C	10.39935	0.43371	0.00097
H	10.17836	1.16225	0.7844

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Optimized structure of triplet state of Zn-2

Zn	0.00001	-1.08013	1.53759
Cl	-0.00001	-1.3741	3.73585
Cl	0.00003	-2.69918	0.02028
N	1.35914	0.43811	0.9171
N	-1.35914	0.4381	0.91709
C	0.71593	1.59369	0.62481
C	-0.71593	1.59368	0.6248
C	-1.17891	2.97858	0.44882
C	-2.40581	3.6343	0.45544
H	-3.34599	3.0956	0.57632
C	-2.43145	5.04848	0.31275
H	-3.40197	5.54944	0.30658
C	-1.27554	5.80765	0.19324
H	-1.33922	6.89366	0.09272
C	-0.00002	5.17039	0.22684
C	1.27549	5.80766	0.19328
H	1.33916	6.89368	0.09276
C	2.4314	5.04851	0.31282
H	3.40192	5.54949	0.30667
C	2.40578	3.63433	0.4555
H	3.34596	3.09564	0.57641
C	1.17889	2.97859	0.44885
C	-0.00001	3.76985	0.34235
C	-2.66112	0.1508	0.62171
C	-3.37258	0.70766	-0.48168
H	-2.85596	1.38801	-1.16002

C	-4.67824	0.33494	-0.73523
H	-5.19286	0.74758	-1.60421
C	-5.35015	-0.62212	0.07394
C	-4.61515	-1.2152	1.13648
H	-5.09816	-1.96798	1.7618
C	-3.31316	-0.84257	1.40871
H	-2.76561	-1.28169	2.24645
C	-6.72452	-1.05424	-0.22671
C	-7.0016	-2.50691	-0.0346
C	-8.14253	-2.94379	0.66766
H	-8.84215	-2.20511	1.06342
C	-8.37569	-4.30447	0.87294
H	-9.25995	-4.62352	1.42918
C	-7.47763	-5.2566	0.37591
H	-7.66188	-6.32113	0.53657
C	-6.33706	-4.83738	-0.31759
H	-5.62731	-5.57225	-0.7033
C	-6.09545	-3.47566	-0.51275
H	-5.19865	-3.15509	-1.04765
C	-7.70575	-0.17124	-0.65511
C	-7.5638	1.30021	-0.49218
C	-7.11407	1.85703	0.72403
H	-6.85967	1.19286	1.55209
C	-7.0133	3.24022	0.88391
H	-6.67867	3.65022	1.83965
C	-7.35139	4.09849	-0.16969
H	-7.27219	5.18077	-0.04429
C	-7.80798	3.56164	-1.37953
H	-8.07734	4.22398	-2.20537
C	-7.92699	2.17931	-1.53476
H	-8.29081	1.7666	-2.4782
C	-8.97403	-0.62971	-1.27893
C	-10.20182	-0.02438	-0.93547
H	-10.21521	0.7667	-0.18257
C	-11.3954	-0.43687	-1.53085
H	-12.3369	0.03332	-1.23798

C	-11.38634	-1.44592	-2.50059
H	-12.31894	-1.76323	-2.97236
C	-10.17316	-2.04054	-2.86819
H	-10.15461	-2.81814	-3.635
C	-8.98149	-1.64158	-2.26223
H	-8.0391	-2.10548	-2.55805
C	2.66112	0.15081	0.62171
C	3.31317	-0.84256	1.40871
H	2.76562	-1.28166	2.24646
C	11.3863	-1.44592	-2.50067
H	12.31889	-1.76323	-2.97248
C	4.61515	-1.21519	1.13648
H	5.09816	-1.96796	1.7618
C	5.35015	-0.62212	0.07392
C	4.67823	0.33493	-0.73525
H	5.19284	0.74756	-1.60424
C	3.37257	0.70766	-0.48169
H	2.85594	1.38799	-1.16004
C	6.72451	-1.05425	-0.22674
C	7.00156	-2.50693	-0.03468
C	6.09542	-3.47564	-0.51291
H	5.19865	-3.15504	-1.04784
C	6.33701	-4.83737	-0.31781
H	5.62727	-5.57222	-0.70358
C	7.47755	-5.25665	0.37572
H	7.66178	-6.32118	0.53633
C	8.3756	-4.30454	0.87282
H	9.25983	-4.62363	1.42908
C	8.14246	-2.94386	0.6676
H	8.84208	-2.20521	1.06342
C	7.70576	-0.17125	-0.6551
C	7.56385	1.30019	-0.49207
C	7.92704	2.17935	-1.53461
H	8.29082	1.76668	-2.47809
C	7.80808	3.56167	-1.37929
H	8.07744	4.22405	-2.2051

C	7.35154	4.09846	-0.16941
H	7.27239	5.18074	-0.04394
C	7.01347	3.24014	0.88415
H	6.67888	3.65009	1.83992
C	7.11419	1.85695	0.72419
H	6.85979	1.19274	1.55221
C	8.97402	-0.62972	-1.27895
C	8.98144	-1.64152	-2.26232
H	8.03904	-2.10537	-2.55817
C	10.1731	-2.04047	-2.86831
H	10.15452	-2.81803	-3.63517
C	11.39539	-0.43693	-1.53086
H	12.3369	0.0332	-1.23797
C	10.20183	-0.02445	-0.93546
H	10.21524	0.76658	-0.18251