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Optimized structure of singlet ground state of Pd-2

Pd	0.00006	-1.69387	-0.22248
Cl	1.62731	-3.31532	-0.05852
Cl	-1.62698	-3.31548	-0.0582
N	1.33884	-0.10125	-0.33206
N	-1.33884	-0.10127	-0.33192
C	0.74151	1.06361	-0.35783
C	1.19267	2.45735	-0.48043
C	2.41893	3.10193	-0.57791
H	3.36032	2.55677	-0.52523
C	2.4352	4.51176	-0.74423
H	3.40358	5.01109	-0.81189
C	1.27342	5.26748	-0.81706
H	1.33194	6.35099	-0.94371
C	-0.00007	4.63662	-0.73234
C	-0.00005	3.23489	-0.55892
C	-1.27359	5.26745	-0.81698
H	-1.33214	6.35096	-0.94362
C	-2.43534	4.5117	-0.74409
H	-3.40373	5.011	-0.81168
C	-2.41902	3.10187	-0.5778
H	-3.36039	2.55668	-0.5251
C	-1.19273	2.45732	-0.48036
C	-0.74154	1.06359	-0.35777
C	2.75536	-0.2069	-0.26553
C	3.44031	-0.93627	-1.24916
H	2.88067	-1.39378	-2.06411
C	4.82394	-1.06965	-1.16728
H	5.35039	-1.64099	-1.93407
C	5.55444	-0.50538	-0.10201
C	4.84168	0.19095	0.89524
H	5.37908	0.59551	1.7543
C	3.45895	0.34037	0.81933
H	2.91273	0.84793	1.61683
C	7.02278	-0.73199	0.02182

C	7.46124	-2.14045	-0.20261
C	6.72342	-3.21304	0.33832
H	5.83617	-3.00751	0.9413
C	7.11358	-4.53526	0.11262
H	6.53159	-5.35044	0.54796
C	8.23574	-4.8136	-0.67516
H	8.53519	-5.84783	-0.85919
C	8.96349	-3.75874	-1.2382
H	9.83052	-3.96668	-1.8695
C	8.5818	-2.43648	-1.00408
H	9.14918	-1.61879	-1.45243
C	7.89399	0.28377	0.33265
C	7.49697	1.72077	0.25377
C	7.81027	2.61392	1.29806
H	8.3211	2.23684	2.18693
C	7.47046	3.96605	1.21236
H	7.71083	4.63792	2.03962
C	6.83566	4.46224	0.06769
H	6.58832	5.52387	-0.00691
C	6.53979	3.59167	-0.9881
H	6.06882	3.97262	-1.89799
C	6.86193	2.23506	-0.89394
H	6.63895	1.56241	-1.72451
C	9.30181	0.04057	0.76182
C	9.60799	-0.92533	1.74096
H	8.80143	-1.5194	2.17456
C	10.92368	-1.12218	2.16462
H	11.13758	-1.87151	2.9302
C	11.9634	-0.36204	1.61666
H	12.99273	-0.51926	1.94672
C	11.67354	0.60736	0.65021
H	12.47734	1.20854	0.21875
C	-2.75533	-0.20698	-0.26537
C	-3.45897	0.34045	0.8194
H	-2.91278	0.84815	1.61682
C	-4.84169	0.19099	0.89529

H	-5.37913	0.5957	1.75427
C	-5.55442	-0.5055	-0.10186
C	-4.82388	-1.06994	-1.16701
H	-5.3503	-1.64142	-1.93374
C	-3.44025	-0.93654	-1.24889
H	-2.88059	-1.39419	-2.06374
C	-7.02278	-0.73207	0.02195
C	-7.89398	0.28375	0.33258
C	10.35563	0.8146	0.23581
H	10.13566	1.57929	-0.51271
C	-9.30183	0.04058	0.76174
C	-10.35566	0.81445	0.23551
H	-10.13569	1.57899	-0.51317
C	-11.67357	0.60724	0.6499
H	-12.47738	1.20828	0.21828
C	-11.96343	-0.36195	1.61656
H	-12.99277	-0.51916	1.9466
C	-10.92369	-1.12192	2.16475
H	-11.1376	-1.87108	2.93048
C	-9.60799	-0.9251	1.74109
H	-8.80141	-1.51902	2.17487
C	-6.86181	2.23484	-0.89425
H	-6.63865	1.56203	-1.72465
C	-6.53972	3.59145	-0.98863
H	-6.06862	3.97223	-1.89851
C	-6.83583	4.46221	0.06693
H	-6.58853	5.52384	-0.00785
C	-7.47081	3.96623	1.21159
H	-7.71138	4.63825	2.03866
C	-7.81057	2.6141	1.2975
H	-8.32154	2.23717	2.18635
C	-7.49702	1.72074	0.25345
C	-7.46124	-2.14056	-0.20231
C	-8.58173	-2.4367	-1.00384
H	-9.14906	-1.61907	-1.45235
C	-8.9634	-3.75899	-1.2378

H	-9.83038	-3.96702	-1.86915
C	-8.23572	-4.81378	-0.67453
H	-8.53516	-5.84803	-0.85845
C	-7.11362	-4.53533	0.1133
H	-6.53168	-5.35045	0.54882
C	-6.72347	-3.21308	0.33884
H	-5.83627	-3.00747	0.94187

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Optimized structure of triplet state of Pd-2

Pd	-0.00009	-1.65808	-0.79753
Cl	1.60992	-3.31215	-0.60086
Cl	-1.6101	-3.31219	-0.60107
N	1.35552	-0.09045	-0.77713
N	-1.35565	-0.09035	-0.77743
C	0.71141	1.10715	-0.70569
C	1.18067	2.49743	-0.77351
C	2.4081	3.14611	-0.8712
H	3.34965	2.59806	-0.88302
C	2.43162	4.56449	-0.95922
H	3.40277	5.06009	-1.02157
C	1.27534	5.33209	-0.97315
H	1.33792	6.42025	-1.04816
C	0.00025	4.69641	-0.90893
C	0.00016	3.29564	-0.80131
C	-1.27473	5.33222	-0.97385
H	-1.33717	6.42038	-1.04892
C	-2.4311	4.56473	-0.96057
H	-3.40217	5.06044	-1.02349
C	-2.40777	3.14635	-0.87249
H	-3.34937	2.5984	-0.88482
C	-1.18047	2.49754	-0.77406
C	-0.7114	1.10724	-0.70587
C	2.73006	-0.19604	-0.56367
C	3.51281	-1.00595	-1.41741
H	3.0311	-1.50208	-2.25822

C	4.87477	-1.1464	-1.19304
H	5.46442	-1.77053	-1.86699
C	5.51652	-0.50169	-0.10931
C	4.71905	0.29219	0.75103
H	5.17702	0.75772	1.62506
C	3.35788	0.44321	0.53333
H	2.74894	1.01609	1.23495
C	6.95068	-0.73756	0.17099
C	7.41404	-2.14136	-0.02155
C	6.62963	-3.22164	0.43361
H	5.68708	-3.02329	0.94851
C	7.04686	-4.53993	0.23721
H	6.42868	-5.36146	0.60531
C	8.2444	-4.80625	-0.4357
H	8.56585	-5.83761	-0.59713
C	9.0219	-3.74397	-0.91241
H	9.94929	-3.94371	-1.45399
C	8.61312	-2.42566	-0.70607
H	9.21936	-1.60171	-1.08709
C	7.8001	0.26949	0.59014
C	7.44847	1.7088	0.44477
C	7.6858	2.61965	1.49553
H	8.10121	2.2521	2.4364
C	7.38323	3.97506	1.3509
H	7.5589	4.66055	2.18307
C	6.86482	4.45656	0.14292
H	6.64393	5.51991	0.02514
C	6.64743	3.56891	-0.91804
H	6.26625	3.93864	-1.8731
C	6.93043	2.20974	-0.76771
H	6.76993	1.52337	-1.60127
C	9.13088	-0.00418	1.1966
C	9.29138	-0.99556	2.18696
H	8.42607	-1.58287	2.49895
C	10.53525	-1.22101	2.77787
H	10.63494	-1.98718	3.54998

C	11.64923	-0.46753	2.38866
H	12.6231	-0.64825	2.84908
C	11.50488	0.52472	1.41236
H	12.36786	1.11897	1.10326
C	-2.73013	-0.19591	-0.56389
C	-3.35799	0.44356	0.533
H	-2.74906	1.01663	1.23448
C	-4.71913	0.2925	0.75078
H	-5.17709	0.75821	1.62472
C	-5.51659	-0.50166	-0.10934
C	-4.87482	-1.14662	-1.19292
H	-5.46445	-1.77093	-1.8667
C	-3.51288	-1.00615	-1.41737
H	-3.03118	-1.50243	-2.25809
C	-6.95071	-0.73751	0.17103
C	-7.80011	0.26956	0.59023
C	10.25748	0.76246	0.83154
H	10.15043	1.54246	0.07443
C	-9.13087	-0.0041	1.19671
C	-10.25744	0.76267	0.83179
H	-10.15037	1.54274	0.07477
C	-11.50483	0.52494	1.41263
H	-12.36778	1.11928	1.10363
C	-11.64921	-0.46742	2.38882
H	-12.62307	-0.64813	2.84926
C	-10.53527	-1.22101	2.7779
H	-10.63497	-1.98727	3.54992
C	-9.2914	-0.99558	2.18696
H	-8.42611	-1.58298	2.49885
C	-6.93017	2.20974	-0.76752
H	-6.76956	1.52334	-1.60104
C	-6.64711	3.56891	-0.91784
H	-6.26576	3.9386	-1.87284
C	-6.86465	4.45658	0.14307
H	-6.6437	5.51992	0.02529
C	-7.38326	3.97513	1.35097

H	-7.55904	4.66064	2.1831
C	-7.68589	2.61973	1.49559
H	-8.10146	2.25221	2.43641
C	-7.44843	1.70885	0.44488
C	-7.41415	-2.14127	-0.02158
C	-8.61326	-2.42546	-0.70609
H	-9.21946	-1.60145	-1.08706
C	-9.02212	-3.74373	-0.9125
H	-9.94954	-3.9434	-1.45408
C	-8.24467	-4.80609	-0.43586
H	-8.56619	-5.83742	-0.59735
C	-7.04711	-4.53988	0.23704
H	-6.42897	-5.36146	0.60509
C	-6.6298	-3.22162	0.43351
H	-5.68724	-3.02334	0.94841