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Optimized structure of singlet state of 3

N	1.39973	0.40421	-0.50408
N	-1.39974	0.40419	-0.5041
C	0.76194	-0.71077	-0.51694
C	-0.76194	-0.71078	-0.51696
C	-1.18812	-2.13218	-0.58412
C	-2.41366	-2.77984	-0.66123
H	-3.35426	-2.23119	-0.63323
C	-2.43353	-4.19554	-0.774
H	-3.40232	-4.69726	-0.82475
C	-1.27292	-4.9551	-0.81756
H	-1.33219	-6.04281	-0.90421
C	0.00004	-4.32194	-0.75632
C	1.27301	-4.95508	-0.81752
H	1.3323	-6.04278	-0.90417
C	2.4336	-4.19549	-0.77392
H	3.40241	-4.69719	-0.82464
C	2.41371	-2.77979	-0.66115
H	3.35429	-2.23112	-0.63312
C	1.18815	-2.13216	-0.58409
C	0.00002	-2.91125	-0.6352
C	-2.79116	0.50463	-0.39362
C	-3.49589	0.02153	0.72846
H	-2.95094	-0.50078	1.51768
C	-4.86776	0.23491	0.84623
H	-5.39292	-0.13734	1.72804
C	-5.59065	0.93228	-0.14231
C	-4.86826	1.4467	-1.23925
H	-5.39663	2.01734	-2.00644
C	-3.49593	1.24681	-1.36265
H	-2.94558	1.65611	-2.21152
C	-7.05211	1.18565	-0.00098
C	-7.47925	2.59245	-0.26065
C	-8.58098	2.88005	-1.09003
H	-9.14317	2.05627	-1.53382

C	-8.95222	4.19983	-1.35548
H	-9.80552	4.40006	-2.00773
C	-8.23329	5.26167	-0.79486
H	-8.52573	6.29378	-1.00115
C	-7.13018	4.99167	0.0227
H	-6.55877	5.81326	0.46105
C	-6.75002	3.67175	0.27723
H	-5.88101	3.46786	0.90695
C	-7.93914	0.19553	0.3453
C	-7.57009	-1.25129	0.31536
C	-6.94709	-1.81882	-0.81363
H	-6.70821	-1.18025	-1.66629
C	-6.6502	-3.18329	-0.85865
H	-6.18375	-3.60483	-1.75274
C	-6.96059	-4.00993	0.22786
H	-6.72938	-5.07714	0.19244
C	-7.58483	-3.46122	1.35376
H	-7.83603	-4.09795	2.20533
C	-7.89818	-2.10024	1.39113
H	-8.39949	-1.68174	2.26689
C	-9.34096	0.47918	0.7715
C	-10.41143	-0.28665	0.26709
H	-10.20707	-1.07689	-0.45899
C	-11.72472	-0.04077	0.67473
H	-12.54066	-0.63739	0.25982
C	-11.99507	0.96112	1.61349
H	-13.02099	1.14864	1.93849
C	-10.93956	1.71395	2.14056
H	-11.13768	2.4885	2.88517
C	-9.62798	1.47716	1.72373
H	-8.80915	2.06515	2.14244
C	2.79114	0.50466	-0.3936
C	3.49591	1.24687	-1.3626
H	2.94555	1.6562	-2.21146
C	11.99507	0.96109	1.61347
H	13.02099	1.1486	1.93846

C	4.86824	1.44676	-1.23921
H	5.39661	2.01742	-2.00638
C	5.59063	0.9323	-0.14229
C	4.86774	0.23489	0.84623
H	5.39291	-0.13739	1.72802
C	3.49588	0.02152	0.72846
H	2.95093	-0.50083	1.51766
C	7.0521	1.18566	-0.00096
C	7.47923	2.59247	-0.26058
C	6.75	3.67176	0.27734
H	5.881	3.46785	0.90705
C	7.13016	4.99168	0.02285
H	6.55874	5.81326	0.46122
C	8.23326	5.26171	-0.79471
H	8.5257	6.29383	-1.00096
C	8.9522	4.19989	-1.35536
H	9.8055	4.40015	-2.00761
C	8.58096	2.88011	-1.08995
H	9.14315	2.05634	-1.53377
C	7.93913	0.19554	0.34529
C	7.57008	-1.25128	0.31529
C	7.89818	-2.10027	1.39104
H	8.39949	-1.6818	2.26681
C	7.58483	-3.46125	1.35361
H	7.83603	-4.09801	2.20516
C	6.96059	-4.00992	0.2277
H	6.72938	-5.07713	0.19224
C	6.6502	-3.18325	-0.85878
H	6.18374	-3.60475	-1.75288
C	6.94708	-1.81877	-0.81372
H	6.7082	-1.18017	-1.66635
C	9.34095	0.47918	0.77148
C	9.62798	1.47712	1.72375
H	8.80915	2.06509	2.14249
C	10.93957	1.71389	2.14057
H	11.13769	2.48842	2.88521

C	11.72471	-0.04077	0.67467
H	12.54064	-0.63737	0.25973
C	10.41142	-0.28664	0.26703
H	10.20706	-1.07685	-0.45908