

Heterogeneous & Homogeneous & Bio- & Nano-

# CHEM **CAT** CHEM

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CATALYSIS

## Supporting Information

### **Covalent or Non-Covalent? A Mechanistic Insight into the Enantioselective Brønsted Acid Catalyzed Dearomatization of Indoles with Allenamides**

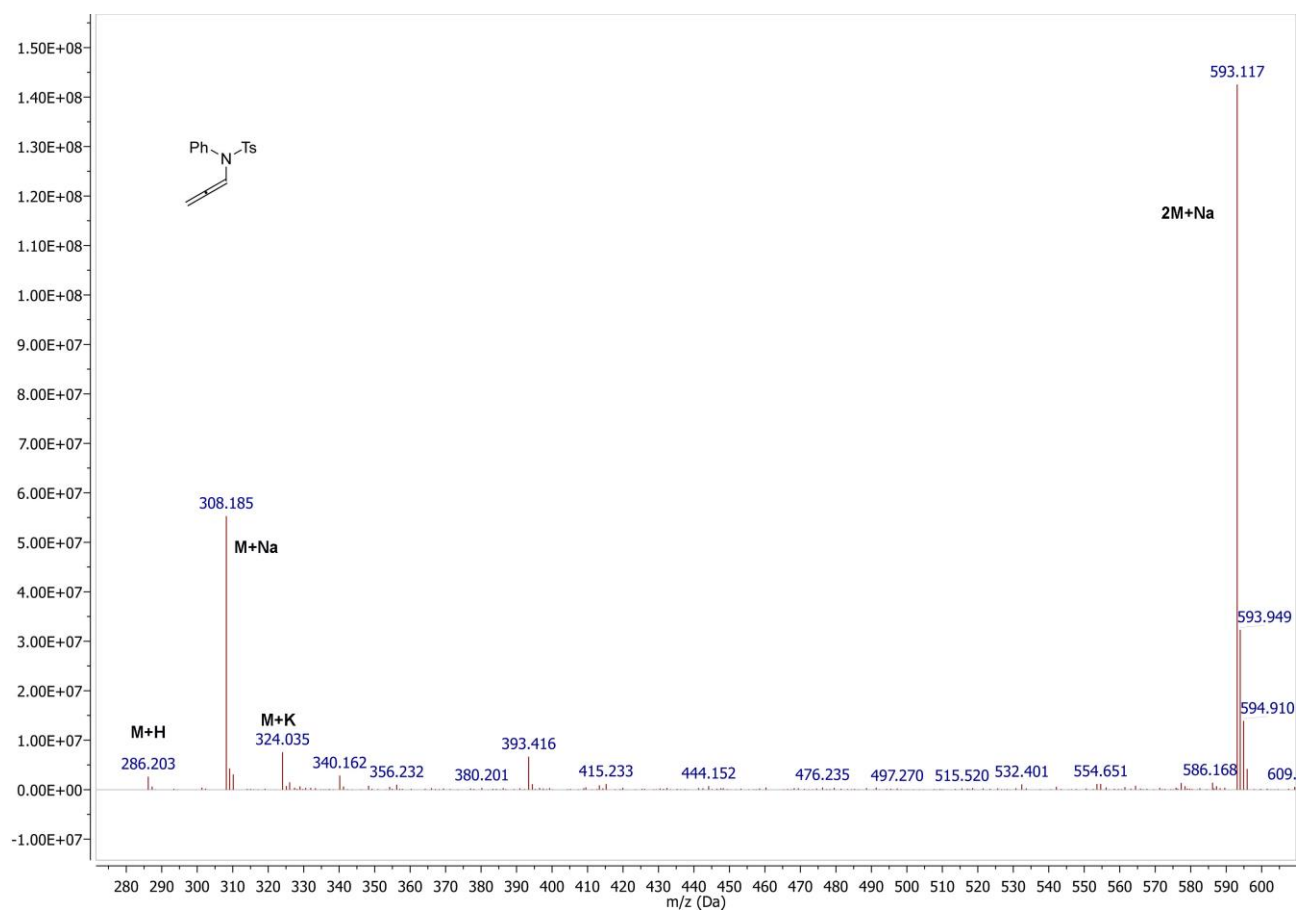
Pietro Giacinto,<sup>[a]</sup> Andrea Bottoni,<sup>[a]</sup> Andrea Garelli,<sup>[a]</sup> Gian Pietro Miscione,<sup>\*[b]</sup> and Marco Bandini<sup>\*[a]</sup>

cctc\_201701933\_sm\_miscellaneous\_information.pdf

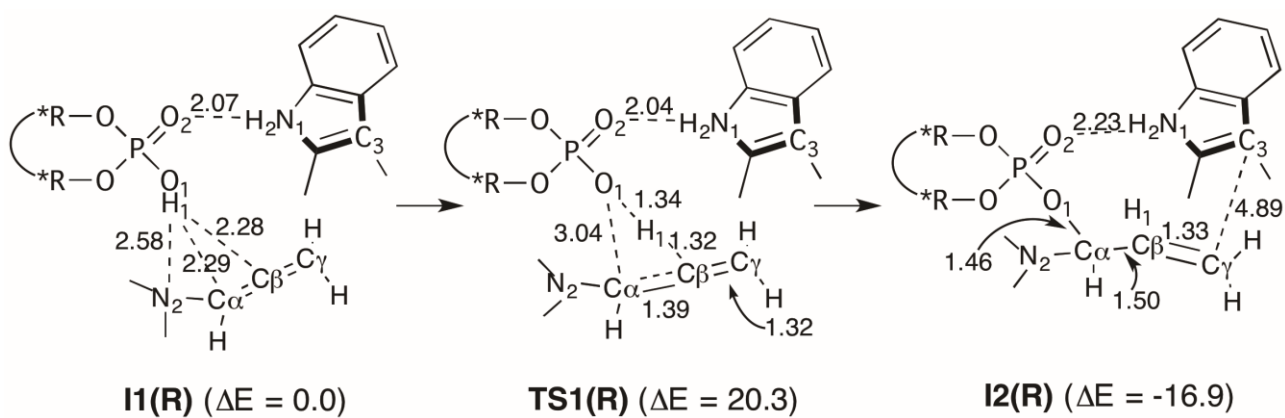
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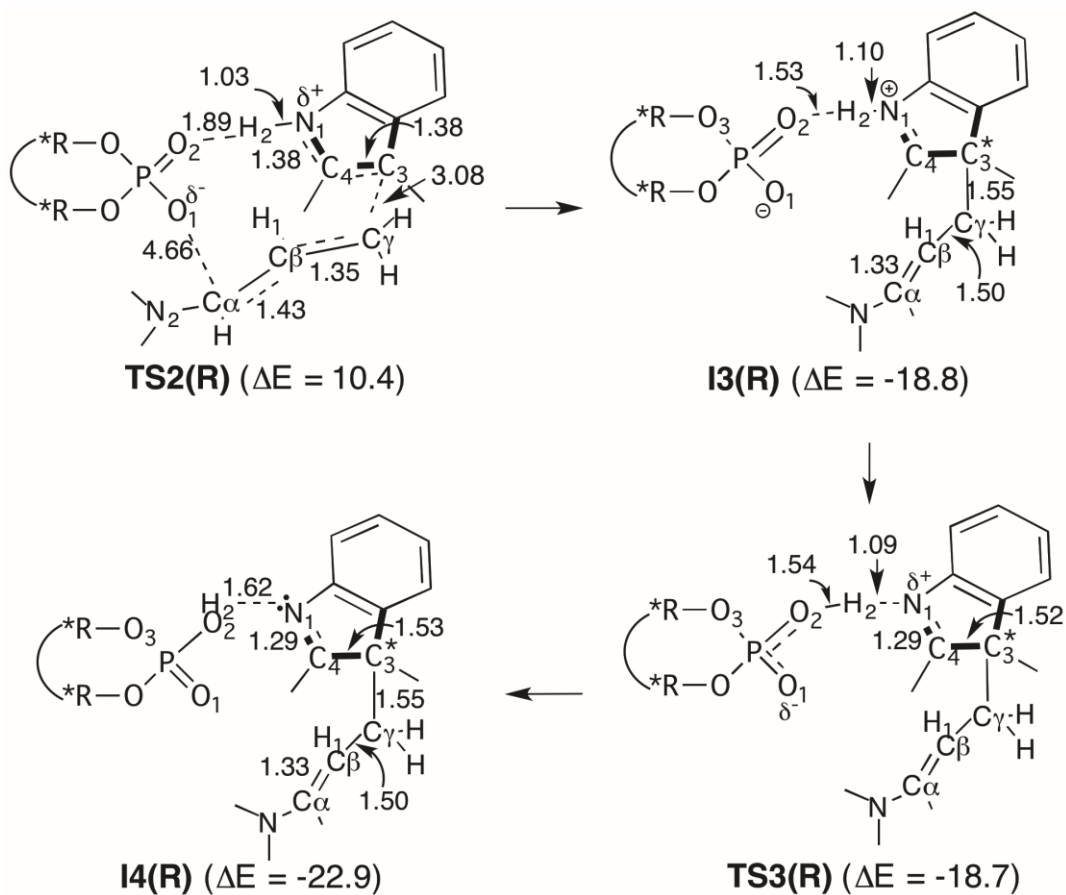
## The MS and MS/MS analyses



**Figure S1:** MS analysis (MSD Ion Trap 1100 Series) of **2a**.



**Figure S2.** A schematic representation of the structures of **I1(R)**, **TS1(R)** and **I2(R)**. Bond lengths are in Angstroms. Energy values are in kcal mol<sup>-1</sup> and refer to initial complex **I1(R)**.



**Figure S3.** A schematic representation of the structures of **TS2(R)**, **I3(R)**, **TS3(R)** and **I4(R)**. Bond lengths are in Angstroms. Energy values are in kcal mol<sup>-1</sup> and refer to initial complex **I1(R)**.

**Computed Cartesian coordinates of all the molecules reported in this study.**

**(S) Pathway**

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**II(S) E(PCM, mixed basis set, opt) = -5013,203937 - E(PCM, 6-31+G\*, single point) = -5023,860211**

C	-4.458870	-2.368373	0.673132
C	-3.161641	-2.410657	1.134452
C	-2.612188	-1.227026	1.723813
C	-3.373691	-0.028200	1.696584
C	-4.661104	-0.033555	1.104504
C	-5.234230	-1.183005	0.618560
H	-0.762843	-2.114709	2.426343
C	-1.345024	-1.201044	2.366699
C	-2.835718	1.156040	2.267116
H	-5.217423	0.898056	1.048354
C	-1.603206	1.170923	2.870927
C	-0.864925	-0.043548	2.920096
H	-3.434383	2.063614	2.227744
H	0.102584	-0.048277	3.416232
C	-2.382933	-3.663837	0.975431
C	-1.136219	-3.679386	0.269250
C	-2.902032	-4.859197	1.425596
C	-0.593595	-2.534355	-0.378182
C	-0.415724	-4.899611	0.171285
C	-2.238746	-6.104755	1.261300
C	0.608631	-2.601528	-1.030908
H	-1.146837	-1.601952	-0.364943
C	0.837472	-4.926052	-0.496934
C	-0.990349	-6.085836	0.688958
C	1.362723	-3.805679	-1.090227
H	0.998808	-1.714677	-1.524247
H	1.373776	-5.871428	-0.546201
H	-0.446112	-7.021998	0.589349
C	-1.027536	2.419667	3.483971
H	-1.720687	3.261353	3.390268
H	-0.084475	2.695252	2.995419
C	2.683756	-3.827996	-1.811578
H	3.154144	-4.814024	-1.741332
H	3.373885	-3.087512	-1.388808
C	-6.587586	-1.178867	0.004186
C	-7.726391	-0.884566	0.784130
C	-6.720452	-1.409908	-1.387325
C	-8.978783	-0.808203	0.159046
C	-7.988300	-1.321335	-1.966643
C	-9.130467	-1.024399	-1.210641
H	-9.849387	-0.589046	0.764114
H	-8.096157	-1.478413	-3.038286
C	-2.894546	-7.380011	1.663752
C	-3.802267	-8.004742	0.764767
C	-2.648013	-7.941339	2.926701
C	-4.492656	-9.132509	1.199542
C	-3.375105	-9.075471	3.325378
C	-4.325118	-9.656037	2.491852
H	-5.221701	-9.601304	0.545399

H	-3.225093	-9.469683	4.324436
O	-4.116873	-4.844359	2.114663
O	-5.042678	-3.537933	0.182482
P	-5.484058	-4.619493	1.294617
O	-6.343077	-3.818986	2.367071
O	-6.108166	-5.814731	0.712433
H	-7.306042	-3.972501	2.257738
C	-5.509616	-1.694182	-2.274527
C	-5.580614	-3.087696	-2.941599
C	-5.342646	-0.604488	-3.359891
H	-4.602056	-1.676225	-1.661142
C	-4.304411	-3.356423	-3.764360
H	-6.452440	-3.121282	-3.611191
H	-5.705603	-3.856191	-2.172018
C	-4.072635	-0.869456	-4.197259
H	-6.221847	-0.614333	-4.017577
H	-5.289381	0.381425	-2.883193
C	-4.124656	-2.270023	-4.844522
H	-4.360073	-4.351539	-4.223980
H	-3.436384	-3.349095	-3.089568
H	-3.962939	-0.098692	-4.968457
H	-3.194008	-0.813047	-3.539961
H	-3.211413	-2.453993	-5.421778
H	-4.975385	-2.312609	-5.538242
C	-10.494086	-1.002322	-1.894705
C	-10.905661	-2.451439	-2.263507
C	-11.604425	-0.367596	-1.032010
H	-10.403172	-0.421650	-2.826152
C	-12.263221	-2.482035	-2.993228
H	-10.966650	-3.028940	-1.331731
H	-10.129737	-2.909783	-2.887995
C	-12.952861	-0.377129	-1.780869
H	-11.713430	-0.958796	-0.113697
H	-11.325261	0.656390	-0.754516
C	-13.355890	-1.825124	-2.126444
H	-12.533349	-3.518215	-3.230043
H	-12.179837	-1.932427	-3.941334
H	-13.724620	0.094280	-1.161898
H	-12.863770	0.205191	-2.708468
H	-14.319384	-1.841097	-2.648381
H	-13.463126	-2.394927	-1.192802
C	-7.637395	-0.625551	2.285001
C	-7.816822	0.884377	2.583744
C	-8.688089	-1.423723	3.089595
H	-6.647241	-0.933806	2.642492
C	-7.657881	1.163911	4.092266
H	-8.821364	1.186800	2.256393
H	-7.091809	1.470556	2.007651
C	-8.535467	-1.159817	4.599900
H	-9.701871	-1.141333	2.779107
H	-8.580399	-2.492868	2.890183
C	-8.683261	0.345295	4.903887
H	-7.783336	2.234451	4.291040
H	-6.642362	0.880516	4.401666
H	-9.292253	-1.736626	5.143271
H	-7.544439	-1.503595	4.927515

H	-8.554400	0.532254	5.976041
H	-9.696397	0.665691	4.625882
C	-3.987070	-7.462245	-0.651112
C	-2.810934	-7.895135	-1.564580
C	-5.304732	-7.892851	-1.335140
H	-3.990474	-6.364845	-0.605681
C	-2.915819	-7.180067	-2.928369
H	-2.860410	-8.984104	-1.701604
H	-1.854492	-7.658539	-1.091103
C	-5.445228	-7.173296	-2.691693
H	-5.290036	-8.977956	-1.508386
H	-6.159848	-7.641843	-0.700675
C	-4.256309	-7.509594	-3.615877
H	-2.077808	-7.469439	-3.572626
H	-2.853032	-6.095263	-2.761556
H	-6.386751	-7.464206	-3.171650
H	-5.484576	-6.089827	-2.510063
H	-4.341947	-6.958839	-4.560353
H	-4.281257	-8.582691	-3.849879
C	-5.236486	-10.790425	2.934545
C	-4.876243	-12.120363	2.229214
C	-5.270083	-11.014596	4.458409
H	-6.256502	-10.519446	2.624390
C	-5.929851	-13.196695	2.566885
H	-3.883946	-12.444299	2.571517
H	-4.825685	-11.965449	1.145015
C	-6.339440	-12.071676	4.803652
H	-4.287981	-11.370903	4.801079
H	-5.492865	-10.067339	4.964607
C	-6.024591	-13.405965	4.092858
H	-5.681223	-14.140552	2.068572
H	-6.907076	-12.861742	2.191680
H	-6.387875	-12.221556	5.888729
H	-7.317968	-11.702386	4.465390
H	-6.795465	-14.150097	4.323905
H	-5.063997	-13.789795	4.462743
C	-1.672489	-7.300532	3.904840
C	-2.434092	-6.605173	5.059130
C	-0.671008	-8.330381	4.475191
H	-1.093986	-6.531654	3.378632
C	-1.446979	-5.930147	6.034103
H	-3.021332	-7.363294	5.597140
H	-3.134026	-5.870775	4.641238
C	0.319340	-7.646722	5.439759
H	-1.219644	-9.107672	5.022720
H	-0.136828	-8.816859	3.650702
C	-0.443447	-6.960202	6.592306
H	-1.995431	-5.450189	6.852512
H	-0.895500	-5.146073	5.497608
H	1.027461	-8.382614	5.836719
H	0.894363	-6.889584	4.889195
H	0.260632	-6.472314	7.275834
H	-0.991058	-7.723073	7.162176
C	-8.212973	-4.614738	5.326904
C	-8.624313	-5.110204	4.193642
C	-9.038343	-5.592717	3.046918



H	-7.155476	-4.437397	5.509064
H	-8.918964	-4.340755	6.106518
N	-9.399003	-4.696008	1.979808
S	-10.975222	-4.018500	2.170299
O	-11.095420	-3.626357	3.563123
O	-11.133439	-3.046543	1.099820
H	-9.142626	-6.663119	2.883802
C	-8.851443	-9.622973	0.943950
C	-8.255342	-9.034711	2.065167
C	-9.896159	-10.508975	1.158493
H	-8.495457	-9.393010	-0.055564
C	-8.655425	-9.363782	3.387191
C	-10.328920	-10.825822	2.462687
H	-10.378642	-10.980703	0.307458
C	-9.712589	-10.270085	3.573216
C	-7.791825	-8.642944	4.282402
C	-6.930034	-7.916744	3.492938
H	-6.757926	-7.640887	1.411478
H	-11.142813	-11.532911	2.594764
H	-10.033802	-10.537600	4.576944
N	-7.226837	-8.136237	2.165341
C	-7.830383	-8.703639	5.776888
H	-7.054838	-8.070387	6.217570
H	-8.794660	-8.358920	6.168747
H	-7.675320	-9.727628	6.140737
C	-5.823741	-6.984235	3.852005
H	-5.011855	-7.060948	3.125630
H	-6.165929	-5.943015	3.865950
H	-5.417354	-7.224474	4.838435
H	-0.813228	2.267928	4.549084
H	2.552698	-3.585628	-2.873704
C	-12.001180	-5.424352	1.849437
C	-12.475654	-5.634086	0.559493
C	-12.088647	-6.414698	2.830892
C	-13.046962	-6.865202	0.248728
H	-12.369772	-4.855053	-0.189899
C	-12.636904	-7.643579	2.492210
H	-11.712220	-6.224274	3.830963
C	-13.110856	-7.889067	1.196186
H	-13.418520	-7.042932	-0.756340
H	-12.684785	-8.434037	3.236253
C	-13.659197	-9.246401	0.845563
H	-12.888880	-10.011316	0.993250
H	-14.507804	-9.505193	1.486701
H	-13.991120	-9.286939	-0.194473
C	-9.145207	-5.153452	0.630816
C	-8.620228	-4.236163	-0.273612
C	-8.383914	-4.636943	-1.585164
C	-8.662885	-5.937807	-1.988719
C	-9.191368	-6.848204	-1.076046
C	-9.440936	-6.458889	0.235777
H	-8.425022	-3.215498	0.043525
H	-7.993261	-3.913398	-2.288321
H	-8.480255	-6.238888	-3.015638
H	-9.440978	-7.856985	-1.390231
H	-9.884332	-7.165055	0.932660

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**TS1(S), E(PCM, mixed basis set, opt) = -5013,171485 - E(PCM, 6-31+G\*, single point) = -5023.828564**

C	-4.355181	-2.412189	0.737646
C	-3.068333	-2.396681	1.229751
C	-2.569919	-1.171458	1.778763
C	-3.359199	0.005468	1.676669
C	-4.614667	-0.053426	1.016943
C	-5.130686	-1.238646	0.556520
H	-0.719439	-1.981378	2.564135
C	-1.321264	-1.085095	2.451878
C	-2.867472	1.224332	2.214757
H	-5.176236	0.864975	0.865902
C	-1.653548	1.296026	2.852553
C	-0.885573	0.105722	2.970243
H	-3.485074	2.115146	2.119377
H	0.068038	0.147098	3.491080
C	-2.236308	-3.621843	1.112289
C	-0.986226	-3.592714	0.410046
C	-2.700971	-4.832887	1.583040
C	-0.502399	-2.440556	-0.271565
C	-0.199582	-4.774215	0.349507
C	-1.962354	-6.042497	1.460606
C	0.703759	-2.461969	-0.921162
H	-1.105627	-1.539570	-0.289857
C	1.055468	-4.752281	-0.315239
C	-0.711853	-5.975481	0.898846
C	1.522594	-3.623967	-0.941443
H	1.045084	-1.570917	-1.442736
H	1.642402	-5.668277	-0.334513
H	-0.117054	-6.883225	0.828062
C	-1.128957	2.584743	3.428524
H	-1.846904	3.399050	3.289600
H	-0.185596	2.872810	2.947453
C	2.846375	-3.596397	-1.658116
H	3.356008	-4.562290	-1.581478
H	3.505069	-2.827181	-1.236087
C	-6.398374	-1.297458	-0.222299
C	-7.644594	-1.186861	0.420455
C	-6.334415	-1.422553	-1.631183
C	-8.812902	-1.156999	-0.353944
C	-7.523762	-1.400975	-2.366139
C	-8.772081	-1.250034	-1.745758
H	-9.767036	-1.062448	0.147854
H	-7.482693	-1.481257	-3.450542
C	-2.568576	-7.334623	1.887715
C	-3.460015	-7.994852	1.000991
C	-2.306663	-7.867682	3.162065
C	-4.133168	-9.123965	1.459328
C	-3.003608	-9.013866	3.580004
C	-3.950287	-9.621627	2.758466
H	-4.860920	-9.611953	0.817574
H	-2.844106	-9.389429	4.584609
O	-3.905055	-4.878215	2.262357
O	-4.908714	-3.611434	0.323338

P	-5.328941	-4.649736	1.507196
O	-6.210636	-3.942852	2.539907
O	-5.860815	-5.877573	0.860504
H	-7.310135	-4.564000	2.792979
C	-4.993939	-1.551736	-2.349558
C	-4.814366	-2.955112	-2.974291
C	-4.807302	-0.469171	-3.437341
H	-4.188483	-1.415025	-1.618662
C	-3.417673	-3.090397	-3.612909
H	-5.577723	-3.091399	-3.754052
H	-4.961786	-3.720354	-2.203420
C	-3.409268	-0.597207	-4.079865
H	-5.574712	-0.595701	-4.212301
H	-4.937927	0.523859	-2.992097
C	-3.215003	-2.002599	-4.688290
H	-3.301527	-4.088863	-4.051643
H	-2.653681	-2.979242	-2.830653
H	-3.276665	0.171409	-4.849552
H	-2.645612	-0.434245	-3.307043
H	-2.217143	-2.088776	-5.133003
H	-3.953796	-2.150158	-5.487898
C	-10.037882	-1.207551	-2.597006
C	-10.438971	-2.637989	-3.038044
C	-11.232404	-0.543970	-1.878920
H	-9.815428	-0.622440	-3.502683
C	-11.690357	-2.614791	-3.939383
H	-10.638853	-3.231633	-2.135306
H	-9.602483	-3.108037	-3.565867
C	-12.466137	-0.495488	-2.803066
H	-11.490879	-1.140526	-0.994895
H	-10.955757	0.463535	-1.546260
C	-12.866150	-1.925674	-3.218484
H	-11.961481	-3.638877	-4.222356
H	-11.462970	-2.060562	-4.860477
H	-13.297907	-0.000537	-2.289404
H	-12.229455	0.090149	-3.701688
H	-13.753569	-1.906922	-3.861187
H	-13.113753	-2.497694	-2.313110
C	-7.735746	-1.107797	1.937062
C	-7.967160	0.338697	2.433014
C	-8.854943	-2.014523	2.483389
H	-6.791364	-1.471308	2.359950
C	-7.975226	0.371295	3.977015
H	-8.931274	0.696802	2.045500
H	-7.182977	0.998403	2.044191
C	-8.841941	-2.018435	4.020685
H	-9.834656	-1.663949	2.135341
H	-8.703914	-3.024361	2.095037
C	-9.050002	-0.581139	4.545785
H	-8.150415	1.393745	4.331558
H	-6.988284	0.053730	4.339668
H	-9.626656	-2.686660	4.392606
H	-7.871675	-2.402015	4.367546
H	-9.022723	-0.566364	5.641226
H	-10.041615	-0.229777	4.229278
C	-3.656256	-7.475993	-0.420816

C	-2.464283	-7.879095	-1.327084
C	-4.956054	-7.952120	-1.106582
H	-3.698700	-6.379602	-0.383878
C	-2.585640	-7.171304	-2.693496
H	-2.481415	-8.969274	-1.461077
H	-1.516809	-7.611855	-0.851757
C	-5.115366	-7.226088	-2.458054
H	-4.904826	-9.035449	-1.284667
H	-5.814586	-7.733061	-0.466400
C	-3.918266	-7.532235	-3.382662
H	-1.740600	-7.442475	-3.336680
H	-2.547683	-6.085146	-2.527823
H	-6.054167	-7.525780	-2.938941
H	-5.172960	-6.145236	-2.266003
H	-4.015108	-6.982133	-4.326498
H	-3.917609	-8.605350	-3.618224
C	-4.847374	-10.763915	3.212709
C	-4.427718	-12.100887	2.552911
C	-4.915253	-10.952568	4.740292
H	-5.866883	-10.523756	2.869207
C	-5.447836	-13.208277	2.891137
H	-3.432771	-12.378233	2.927125
H	-4.354526	-11.971556	1.466468
C	-5.967083	-12.029402	5.078125
H	-3.934104	-11.275476	5.116578
H	-5.177139	-10.002429	5.221145
C	-5.590677	-13.373588	4.418675
H	-5.141695	-14.156626	2.434434
H	-6.423541	-12.929323	2.469732
H	-6.051740	-12.150095	6.164790
H	-6.942050	-11.692641	4.695997
H	-6.347206	-14.133622	4.645600
H	-4.633211	-13.718054	4.832783
C	-1.392366	-7.122561	4.128441
C	-2.244867	-6.184495	5.019051
C	-0.528632	-8.040097	5.022262
H	-0.707113	-6.495762	3.544241
C	-1.347585	-5.333583	5.937594
H	-2.909606	-6.808445	5.632548
H	-2.875031	-5.545370	4.389744
C	0.383475	-7.184380	5.929455
H	-1.175942	-8.657660	5.658238
H	0.070467	-8.711614	4.396282
C	-0.460634	-6.242303	6.813209
H	-1.965106	-4.682870	6.566780
H	-0.707363	-4.691270	5.317606
H	1.007772	-7.833369	6.553863
H	1.050971	-6.581202	5.299144
H	0.191533	-5.636482	7.452423
H	-1.103800	-6.847934	7.466151
C	-8.783262	-5.576990	4.279537
C	-8.435187	-5.282422	3.037424
C	-8.697507	-5.645664	1.722405
H	-8.288301	-5.103136	5.122778
H	-9.550792	-6.315755	4.501439
N	-9.579499	-5.184276	0.830085

S	-11.094915	-4.414397	1.228974
O	-11.095792	-4.239851	2.663255
O	-11.236707	-3.300712	0.312552
H	-7.903770	-6.205841	1.231749
C	-8.681383	-8.917140	1.066324
C	-8.002593	-8.681836	2.267472
C	-9.878860	-9.616527	1.133500
H	-8.283247	-8.563023	0.118059
C	-8.496136	-9.133237	3.521787
C	-10.382188	-10.082619	2.364802
H	-10.434735	-9.812315	0.220477
C	-9.702936	-9.849920	3.552725
C	-7.579606	-8.669971	4.528327
C	-6.605129	-7.959564	3.866674
H	-6.253768	-7.518626	1.833616
H	-11.311665	-10.644990	2.380102
H	-10.101089	-10.214221	4.496437
N	-6.848933	-7.989871	2.514580
C	-7.713525	-8.866880	6.005351
H	-6.897833	-8.374047	6.542614
H	-8.655499	-8.450695	6.383957
H	-7.695509	-9.929718	6.276962
C	-5.493003	-7.103200	4.369192
H	-5.086242	-7.483934	5.309851
H	-4.677246	-7.058320	3.642412
H	-5.849196	-6.077153	4.534944
H	-0.930998	2.480639	4.502593
H	2.710285	-3.364237	-2.721861
C	-12.219680	-5.694309	0.771712
C	-13.074188	-5.495587	-0.305673
C	-12.179742	-6.896753	1.478125
C	-13.927341	-6.532468	-0.672160
H	-13.058924	-4.554499	-0.846403
C	-13.032119	-7.917942	1.087229
H	-11.480186	-7.045465	2.297920
C	-13.918845	-7.749405	0.014156
H	-14.604410	-6.395938	-1.510142
H	-13.002638	-8.864661	1.618930
C	-14.848643	-8.866636	-0.377317
H	-15.649716	-8.973816	0.361749
H	-15.309869	-8.680046	-1.349648
H	-14.316555	-9.821269	-0.423229
C	-9.261440	-5.375714	-0.569422
C	-9.845169	-6.429421	-1.271038
C	-9.453701	-6.656826	-2.586935
C	-8.478290	-5.851463	-3.170720
C	-7.898894	-4.811643	-2.447546
C	-8.291877	-4.554310	-1.137753
H	-10.564456	-7.078778	-0.781029
H	-9.897077	-7.475301	-3.144627
H	-8.162623	-6.039335	-4.192499
H	-7.144190	-4.181143	-2.900697
H	-7.857167	-3.730900	-0.571663

**I1'(S), E(PCM, mixed basis set, opt) = -5013,206344 - E(PCM, 6-31+G\*, single point) = -5023.857095**

C	-4.784598	-2.454116	0.616894
C	-3.495078	-2.483260	1.103602
C	-2.913262	-1.263381	1.573801
C	-3.620810	-0.044488	1.395909
C	-4.888678	-0.066278	0.762131
C	-5.489821	-1.244125	0.393059
H	-1.114571	-2.142232	2.402714
C	-1.655385	-1.216277	2.234544
C	-3.042217	1.172237	1.846069
H	-5.402240	0.873429	0.575071
C	-1.820575	1.204179	2.471458
C	-1.134477	-0.025635	2.667568
H	-3.598223	2.094817	1.690407
H	-0.174958	-0.014029	3.179249
C	-2.750144	-3.765611	1.057321
C	-1.519551	-3.863210	0.329883
C	-3.303251	-4.905845	1.612791
C	-0.957801	-2.784942	-0.412096
C	-0.836570	-5.106494	0.298372
C	-2.650101	-6.169859	1.548583
C	0.222793	-2.937033	-1.090543
H	-1.479824	-1.835624	-0.452504
C	0.392780	-5.223725	-0.403619
C	-1.426322	-6.228360	0.926525
C	0.936617	-4.166344	-1.087908
H	0.626058	-2.099218	-1.654765
H	0.896464	-6.188620	-0.399916
H	-0.914459	-7.185284	0.867221
C	-1.204353	2.489377	2.957855
H	-1.832690	3.349358	2.704614
H	-0.215104	2.643114	2.508411
C	2.237426	-4.280408	-1.837986
H	2.659478	-5.286248	-1.744378
H	2.973857	-3.563033	-1.454475
C	-6.811538	-1.261415	-0.285728
C	-7.973433	-0.895161	0.419904
C	-6.890588	-1.596516	-1.658707
C	-9.196140	-0.829107	-0.262749
C	-8.127275	-1.513738	-2.302699
C	-9.291645	-1.129220	-1.621805
H	-10.084764	-0.547910	0.288688
H	-8.188492	-1.744792	-3.364706
C	-3.284184	-7.426260	2.046371
C	-4.069041	-8.193224	1.144592
C	-3.042327	-7.898446	3.351427
C	-4.596049	-9.407953	1.581992
C	-3.609805	-9.116483	3.751937
C	-4.384916	-9.881449	2.883745
H	-5.206585	-10.001237	0.908034
H	-3.448390	-9.464027	4.763583
O	-4.494095	-4.809370	2.293674
O	-5.398536	-3.632692	0.252773
P	-5.927398	-4.577902	1.493103
O	-6.831828	-3.817448	2.421603
O	-6.388046	-5.875310	0.912889

H	-9.260476	-3.814061	4.421248
C	-5.652680	-2.028285	-2.436685
C	-5.752147	-3.495964	-2.916033
C	-5.363976	-1.107349	-3.645275
H	-4.782799	-1.965255	-1.772889
C	-4.430058	-3.928606	-3.579865
H	-6.563491	-3.575045	-3.655159
H	-5.988303	-4.143898	-2.064384
C	-4.043427	-1.531676	-4.323449
H	-6.186927	-1.184605	-4.369052
H	-5.306673	-0.065499	-3.309142
C	-4.105808	-3.006849	-4.774381
H	-4.498013	-4.973434	-3.909086
H	-3.623005	-3.867369	-2.835768
H	-3.833169	-0.881581	-5.180585
H	-3.222511	-1.413568	-3.603250
H	-3.156227	-3.300559	-5.236227
H	-4.895096	-3.115673	-5.530810
C	-10.618952	-1.101082	-2.374243
C	-11.062486	-2.549805	-2.703095
C	-11.751587	-0.392982	-1.603037
H	-10.462904	-0.567224	-3.324539
C	-12.376199	-2.568104	-3.509390
H	-11.195291	-3.084483	-1.752413
H	-10.270219	-3.061917	-3.260608
C	-13.053646	-0.386148	-2.430237
H	-11.933737	-0.936992	-0.666312
H	-11.450823	0.631256	-1.351458
C	-13.493159	-1.830756	-2.744363
H	-12.672308	-3.603245	-3.717726
H	-12.213279	-2.067722	-4.473739
H	-13.842771	0.139660	-1.881321
H	-12.884203	0.152718	-3.372267
H	-14.419778	-1.830626	-3.329108
H	-13.688677	-2.355238	-1.798432
C	-7.927922	-0.582927	1.910249
C	-8.088255	0.932843	2.174445
C	-9.004640	-1.366341	2.687465
H	-6.958789	-0.907812	2.304742
C	-7.975750	1.227692	3.684227
H	-9.071619	1.256509	1.805319
H	-7.324287	1.490375	1.620291
C	-8.908357	-1.075839	4.197675
H	-10.006295	-1.096131	2.331580
H	-8.827472	-2.428680	2.495704
C	-9.042110	0.437217	4.470235
H	-8.087797	2.302141	3.869603
H	-6.976962	0.927935	4.029435
H	-9.702347	-1.617469	4.728081
H	-7.937918	-1.433826	4.567150
H	-8.947323	0.638277	5.543430
H	-10.039930	0.769221	4.152440
C	-4.258553	-7.733983	-0.299189
C	-3.109018	-8.274980	-1.188055
C	-5.604257	-8.155458	-0.930248
H	-4.230818	-6.637434	-0.321294

C	-3.201426	-7.665785	-2.601472
H	-3.197282	-9.369587	-1.241299
H	-2.139803	-8.038283	-0.740580
C	-5.726937	-7.556128	-2.346246
H	-5.659028	-9.250734	-1.002484
H	-6.419633	-7.785285	-0.302470
C	-4.559066	-8.008089	-3.247756
H	-2.379737	-8.030529	-3.228968
H	-3.103553	-6.573993	-2.519480
H	-6.679565	-7.860396	-2.796274
H	-5.732032	-6.460177	-2.260896
H	-4.640025	-7.537571	-4.235575
H	-4.619767	-9.096269	-3.388725
C	-4.994050	-11.217566	3.289515
C	-4.299461	-12.371691	2.520433
C	-4.917764	-11.510987	4.801375
H	-6.056165	-11.202755	3.002149
C	-4.972959	-13.723453	2.834947
H	-3.243479	-12.401217	2.823385
H	-4.331197	-12.171980	1.443186
C	-5.618062	-12.847415	5.120712
H	-3.862908	-11.579954	5.104339
H	-5.384394	-10.691183	5.360359
C	-4.946504	-14.004104	4.351700
H	-4.471391	-14.531463	2.289912
H	-6.018097	-13.685868	2.497757
H	-5.589132	-13.041135	6.199230
H	-6.671362	-12.772852	4.817762
H	-5.451028	-14.952233	4.570674
H	-3.902528	-14.093928	4.681712
C	-2.130411	-7.133791	4.309996
C	-2.407573	-7.432927	5.802758
C	-0.641082	-7.470793	4.036048
H	-2.266160	-6.054902	4.139327
C	-1.529452	-6.535912	6.698411
H	-2.149327	-8.479930	6.010814
H	-3.469759	-7.303366	6.031674
C	0.278960	-6.603931	4.921560
H	-0.484474	-8.536406	4.252279
H	-0.408242	-7.301460	2.982354
C	-0.036657	-6.811222	6.416821
H	-1.754215	-6.723593	7.754509
H	-1.754483	-5.481542	6.488162
H	1.329599	-6.841874	4.719005
H	0.119203	-5.547963	4.663463
H	0.594317	-6.161021	7.033270
H	0.187867	-7.852208	6.687276
C	-8.882480	-5.827534	5.015607
C	-9.013624	-4.828149	4.136482
C	-8.865024	-5.162125	2.729385
H	-9.027768	-5.656810	6.077807
H	-8.665379	-6.844717	4.702495
N	-9.628255	-4.770964	1.740909
S	-11.178037	-3.896001	1.913981
O	-11.266926	-3.484536	3.296833
O	-11.226193	-2.958197	0.816933



H	-8.121725	-5.910241	2.449010
C	-7.821300	-9.183176	2.211194
C	-7.210661	-8.566935	3.308852
C	-8.576608	-10.320745	2.454929
H	-7.679756	-8.786420	1.209362
C	-7.345278	-9.061860	4.628501
C	-8.724000	-10.833261	3.760811
H	-9.058815	-10.830323	1.625746
C	-8.116894	-10.215789	4.844195
C	-6.609607	-8.172061	5.489120
C	-6.090157	-7.186415	4.680690
H	-6.056238	-6.970652	2.548203
H	-9.317813	-11.729353	3.916467
H	-8.228109	-10.625138	5.845750
N	-6.457855	-7.423885	3.371341
C	-6.493908	-8.303176	6.975429
H	-5.963238	-7.453612	7.414458
H	-7.479148	-8.364888	7.454146
H	-5.944803	-9.211443	7.253842
C	-5.380449	-5.917876	5.016122
H	-4.392306	-5.882559	4.550907
H	-5.942973	-5.062669	4.621453
H	-5.271928	-5.804009	6.097334
H	-1.070411	2.471850	4.046816
H	2.095268	-4.066202	-2.904681
C	-12.266655	-5.243191	1.601131
C	-12.754133	-5.432531	0.311986
C	-12.558985	-6.118555	2.646871
C	-13.574361	-6.529715	0.074755
H	-12.491170	-4.738330	-0.480733
C	-13.374542	-7.208435	2.382185
H	-12.155002	-5.941944	3.639604
C	-13.893827	-7.426233	1.098202
H	-13.968545	-6.694486	-0.923373
H	-13.615380	-7.903283	3.181444
C	-14.794811	-8.603458	0.839836
H	-14.381582	-9.516640	1.277302
H	-15.778308	-8.438471	1.292438
H	-14.939394	-8.766770	-0.230296
C	-9.358146	-5.251564	0.404582
C	-9.535465	-6.607014	0.142768
C	-9.251990	-7.080316	-1.132086
C	-8.829849	-6.190741	-2.119533
C	-8.659825	-4.841100	-1.828188
C	-8.910576	-4.350114	-0.550243
H	-9.878462	-7.273354	0.930978
H	-9.366864	-8.136721	-1.354380
H	-8.621642	-6.554558	-3.120538
H	-8.318301	-4.154108	-2.591494
H	-8.765047	-3.301435	-0.303762

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**TS1'(S), E(PCM, mixed basis set, opt) = -5013,205622 - E(PCM, 6-31+G\*, single point) = -5023.855465**

C	-4.791158	-2.422706	0.720316
C	-3.504123	-2.510603	1.207448

C	-2.875929	-1.322408	1.699066
C	-3.533177	-0.073558	1.536514
C	-4.796921	-0.035104	0.895746
C	-5.442738	-1.181935	0.505478
H	-1.116225	-2.285101	2.517878
C	-1.619393	-1.335776	2.363612
C	-2.908930	1.111906	2.007843
H	-5.271558	0.927054	0.719604
C	-1.690029	1.085564	2.638609
C	-1.053751	-0.173613	2.817656
H	-3.427180	2.058054	1.864885
H	-0.096763	-0.208477	3.332854
C	-2.802019	-3.814457	1.126748
C	-1.578595	-3.931942	0.390126
C	-3.389404	-4.949345	1.654826
C	-0.989185	-2.855408	-0.332845
C	-0.935858	-5.194990	0.326238
C	-2.779078	-6.232136	1.557772
C	0.181378	-3.030052	-1.023093
H	-1.482377	-1.890018	-0.351405
C	0.285375	-5.335363	-0.385707
C	-1.558170	-6.311421	0.931613
C	0.856885	-4.280719	-1.051285
H	0.606578	-2.193725	-1.573117
H	0.758426	-6.315327	-0.406647
H	-1.075439	-7.281554	0.850329
C	-1.026647	2.337900	3.147757
H	-0.033549	2.465400	2.698773
H	-0.891171	2.294422	4.235820
C	2.147637	-4.418174	-1.814510
H	1.997791	-4.200388	-2.879487
H	2.552355	-5.431395	-1.726242
C	-6.758485	-1.135862	-0.180968
C	-7.905089	-0.732658	0.527494
C	-6.845981	-1.455167	-1.557637
C	-9.125196	-0.624187	-0.153488
C	-8.079453	-1.326147	-2.200428
C	-9.230843	-0.911420	-1.514491
H	-10.004790	-0.322090	0.401322
H	-8.149565	-1.543882	-3.264476
C	-3.441218	-7.485674	2.026655
C	-4.232596	-8.221429	1.104586
C	-3.218687	-7.985920	3.324833
C	-4.795379	-9.428036	1.519622
C	-3.820998	-9.194414	3.702123
C	-4.611289	-9.924308	2.817337
H	-5.413511	-9.994920	0.830187
H	-3.676114	-9.561799	4.708976
O	-4.583652	-4.820151	2.335433
O	-5.447776	-3.569160	0.321936
P	-5.986004	-4.576143	1.498510
O	-6.936521	-3.862102	2.439483
O	-6.428433	-5.850340	0.867039
H	-9.059002	-3.672282	4.460847
C	-5.619825	-1.909310	-2.342950
C	-5.758665	-3.365016	-2.847401

C	-5.312628	-0.975391	-3.537171
H	-4.746851	-1.879439	-1.681287
C	-4.452535	-3.819883	-3.528756
H	-6.576926	-3.409574	-3.581189
H	-6.004835	-4.021363	-2.005774
C	-4.009666	-1.422306	-4.235022
H	-6.143470	-1.018233	-4.254746
H	-5.224712	0.058231	-3.183089
C	-4.114974	-2.887325	-4.710965
H	-4.550428	-4.857182	-3.873768
H	-3.637316	-3.790639	-2.791375
H	-3.790835	-0.763184	-5.082989
H	-3.178667	-1.338605	-3.521248
H	-3.177328	-3.197628	-5.186192
H	-4.913863	-2.963037	-5.461561
C	-10.558862	-0.837186	-2.262770
C	-11.038928	-2.268607	-2.614503
C	-11.673060	-0.116968	-1.475975
H	-10.392365	-0.291251	-3.204445
C	-12.351820	-2.239536	-3.421778
H	-11.187190	-2.814302	-1.672363
H	-10.259479	-2.791570	-3.179488
C	-12.975436	-0.062067	-2.301391
H	-11.867566	-0.677001	-0.551161
H	-11.347759	0.894087	-1.203072
C	-13.450256	-1.489387	-2.642618
H	-12.673555	-3.263080	-3.647929
H	-12.176233	-1.725849	-4.376841
H	-13.751048	0.471571	-1.740902
H	-12.793595	0.491003	-3.232875
H	-14.376781	-1.455940	-3.226741
H	-13.657983	-2.027429	-1.706976
C	-7.847691	-0.422749	2.018029
C	-8.002838	1.092435	2.286480
C	-8.921766	-1.206087	2.796970
H	-6.875067	-0.744802	2.407489
C	-7.891568	1.383030	3.797656
H	-8.984849	1.420297	1.917703
H	-7.236039	1.648182	1.733912
C	-8.821318	-0.921413	4.307446
H	-9.923161	-0.931130	2.444766
H	-8.756135	-2.269137	2.598537
C	-8.958567	0.591095	4.582237
H	-8.002874	2.457252	3.984633
H	-6.893385	1.082018	4.143886
H	-9.609570	-1.470979	4.837578
H	-7.847487	-1.274122	4.674305
H	-8.865742	0.791906	5.655615
H	-9.956048	0.922092	4.262642
C	-4.400241	-7.735894	-0.333612
C	-3.255648	-8.280157	-1.226731
C	-5.747730	-8.124191	-0.982392
H	-4.354115	-6.640129	-0.335148
C	-3.329831	-7.637897	-2.627326
H	-3.364719	-9.371525	-1.304319
H	-2.283874	-8.072693	-0.770760

C	-5.854757	-7.487903	-2.383363
H	-5.815126	-9.216870	-1.082053
H	-6.563266	-7.761568	-0.351349
C	-4.689669	-7.938882	-3.288917
H	-2.511957	-8.004027	-3.258851
H	-3.211786	-6.550134	-2.520044
H	-6.810181	-7.764233	-2.844820
H	-5.842920	-6.394119	-2.272094
H	-4.754694	-7.442503	-4.265242
H	-4.769969	-9.021904	-3.457203
C	-5.264380	-11.245806	3.202162
C	-4.594277	-12.412057	2.429596
C	-5.214843	-11.555693	4.711799
H	-6.322326	-11.196610	2.902564
C	-5.307490	-13.748054	2.723625
H	-3.542893	-12.473059	2.743457
H	-4.609299	-12.201854	1.353886
C	-5.958799	-12.873268	5.009156
H	-4.166425	-11.660666	5.026627
H	-5.662217	-10.726975	5.273082
C	-5.310517	-14.041765	4.238068
H	-4.817773	-14.563988	2.179538
H	-6.345850	-13.681795	2.370636
H	-5.948691	-13.077876	6.086036
H	-7.005516	-12.764438	4.694528
H	-5.844503	-14.976929	4.442321
H	-4.274245	-14.164247	4.581556
C	-2.287527	-7.261907	4.296431
C	-2.567594	-7.580533	5.784599
C	-0.805816	-7.625324	4.014594
H	-2.399054	-6.176925	4.146943
C	-1.673510	-6.709286	6.690112
H	-2.325256	-8.634447	5.975702
H	-3.627414	-7.437626	6.018055
C	0.131410	-6.785992	4.908670
H	-0.670310	-8.695943	4.219911
H	-0.570798	-7.449281	2.962558
C	-0.185469	-7.004369	6.402272
H	-1.899319	-6.906190	7.744355
H	-1.882145	-5.649072	6.492653
H	1.177204	-7.040939	4.701785
H	-0.009114	-5.724373	4.662961
H	0.456226	-6.369501	7.023662
H	0.023786	-8.051104	6.661969
C	-8.965888	-5.735387	4.995282
C	-8.937665	-4.702457	4.150265
C	-8.784713	-5.003290	2.727869
H	-9.121590	-5.581998	6.058584
H	-8.863202	-6.761175	4.650906
N	-9.591486	-4.595089	1.763807
S	-11.099098	-3.694421	1.983378
O	-11.149973	-3.290805	3.371414
O	-11.165010	-2.743403	0.895804
H	-8.154990	-5.845719	2.447941
C	-7.993808	-9.088424	2.141835
C	-7.379317	-8.514458	3.259866

C	-8.797992	-10.198472	2.353510
H	-7.822024	-8.680224	1.149506
C	-7.559783	-9.022335	4.568672
C	-8.987840	-10.726273	3.647798
H	-9.285928	-10.674389	1.507879
C	-8.378363	-10.149031	4.751793
C	-6.805885	-8.175973	5.456796
C	-6.230490	-7.201238	4.674591
H	-6.132108	-6.970053	2.546978
H	-9.619904	-11.600016	3.777699
H	-8.524998	-10.568140	5.744661
N	-6.579550	-7.405333	3.354024
C	-6.734969	-8.327260	6.944073
H	-6.076401	-7.578450	7.393017
H	-7.722281	-8.227871	7.412441
H	-6.345668	-9.314550	7.222090
C	-5.480485	-5.966920	5.047182
H	-4.493911	-5.944095	4.578855
H	-6.021355	-5.083393	4.686957
H	-5.364555	-5.891757	6.130921
H	-1.624874	3.224018	2.912550
H	2.900126	-3.713741	-1.438483
C	-12.239811	-5.004119	1.689879
C	-12.758970	-5.176333	0.410675
C	-12.540459	-5.871231	2.739986
C	-13.616124	-6.248621	0.187679
H	-12.489845	-4.489285	-0.386356
C	-13.395519	-6.934344	2.490455
H	-12.113350	-5.708232	3.725144
C	-13.944249	-7.135763	1.216296
H	-14.033104	-6.400646	-0.803175
H	-13.644330	-7.620979	3.294379
C	-14.885610	-8.285091	0.975080
H	-15.855286	-8.090229	1.445469
H	-15.054565	-8.444465	-0.092031
H	-14.492695	-9.210168	1.406225
C	-9.373006	-5.083392	0.421454
C	-9.602290	-6.430852	0.154783
C	-9.361006	-6.905883	-1.128148
C	-8.927307	-6.026630	-2.120255
C	-8.709616	-4.684189	-1.827616
C	-8.917812	-4.194051	-0.541450
H	-9.953175	-7.089957	0.946012
H	-9.520087	-7.955812	-1.353909
H	-8.753423	-6.393064	-3.126833
H	-8.368267	-4.002970	-2.596401
H	-8.742531	-3.150476	-0.292341

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**I2(S), E(PCM, mixed basis set, opt) = -5013,229424 - E(PCM, 6-31+G\*, single point) = -5023.876511**

C	-4.695726	-2.361392	0.857012
C	-3.399825	-2.450273	1.319253
C	-2.807458	-1.292904	1.917341
C	-3.500370	-0.055613	1.860281
C	-4.752537	0.001180	1.201754

C	-5.373651	-1.123149	0.713258
H	-1.020992	-2.273652	2.656604
C	-1.552467	-1.330161	2.582872
C	-2.916091	1.101632	2.440425
H	-5.245893	0.963393	1.084219
C	-1.700187	1.053685	3.075168
C	-1.026146	-0.196986	3.144128
H	-3.463102	2.040151	2.379682
H	-0.071172	-0.248833	3.661311
C	-2.629781	-3.695699	1.089599
C	-1.410245	-3.664044	0.335560
C	-3.132437	-4.910938	1.499586
C	-0.899958	-2.487563	-0.282450
C	-0.688397	-4.872190	0.153186
C	-2.462386	-6.142464	1.258267
C	0.276105	-2.518609	-0.984017
H	-1.456109	-1.559786	-0.211672
C	0.538617	-4.861601	-0.562478
C	-1.236296	-6.082262	0.640520
C	1.034994	-3.712712	-1.124254
H	0.640260	-1.608611	-1.454626
H	1.076176	-5.800863	-0.674258
H	-0.686491	-7.007281	0.485562
C	-1.074377	2.273108	3.698083
H	-1.724427	3.147628	3.595115
H	-0.111612	2.502269	3.223904
C	2.329068	-3.690151	-1.892761
H	2.779543	-4.686631	-1.939029
H	3.050002	-3.008187	-1.424508
C	-6.659296	-1.022646	-0.022411
C	-7.816596	-0.556231	0.629471
C	-6.697817	-1.328092	-1.407510
C	-9.010721	-0.448260	-0.096478
C	-7.897618	-1.159421	-2.100254
C	-9.071789	-0.739081	-1.457800
H	-9.904097	-0.127637	0.425211
H	-7.925515	-1.357472	-3.169777
C	-3.051256	-7.457315	1.634947
C	-3.947687	-8.100631	0.738986
C	-2.723335	-8.056875	2.862328
C	-4.582718	-9.264613	1.161978
C	-3.384702	-9.235044	3.244352
C	-4.350620	-9.819133	2.430260
H	-5.309296	-9.744903	0.513061
H	-3.173669	-9.662045	4.218278
O	-4.336175	-4.903617	2.217014
O	-5.333944	-3.504766	0.372215
P	-5.700431	-4.715185	1.371030
O	-6.717885	-4.095894	2.429876
O	-6.160903	-5.929566	0.685669
H	-8.146865	-3.380848	4.513943
C	-5.449141	-1.773104	-2.164944
C	-5.620038	-3.158511	-2.827877
C	-5.033236	-0.729711	-3.229854
H	-4.612017	-1.855020	-1.463882
C	-4.305492	-3.594705	-3.504926

H	-6.411870	-3.098101	-3.588657
H	-5.924334	-3.892130	-2.073091
C	-3.716827	-1.161563	-3.911301
H	-5.827119	-0.645975	-3.984451
H	-4.916100	0.251146	-2.754182
C	-3.868085	-2.554997	-4.557348
H	-4.434685	-4.579375	-3.971753
H	-3.524461	-3.691955	-2.736560
H	-3.423260	-0.422758	-4.665980
H	-2.920184	-1.204270	-3.154898
H	-2.925031	-2.860147	-5.024947
H	-4.632625	-2.501438	-5.344760
C	-10.370664	-0.646385	-2.253227
C	-10.843536	-2.069548	-2.646057
C	-11.510714	0.065289	-1.495906
H	-10.166783	-0.084634	-3.178073
C	-12.124401	-2.016450	-3.503052
H	-11.024809	-2.637925	-1.722915
H	-10.048480	-2.581732	-3.198130
C	-12.779131	0.145473	-2.370743
H	-11.747535	-0.512003	-0.591148
H	-11.191122	1.068498	-1.189162
C	-13.249045	-1.271717	-2.757218
H	-12.442928	-3.033593	-3.757882
H	-11.906654	-1.487738	-4.441340
H	-13.572070	0.673895	-1.829986
H	-12.556514	0.715691	-3.282777
H	-14.149464	-1.220315	-3.379822
H	-13.500456	-1.825481	-1.842858
C	-7.831796	-0.167621	2.103555
C	-8.207229	1.322068	2.286325
C	-8.805095	-1.064961	2.891860
H	-6.835156	-0.316304	2.532107
C	-8.222362	1.697678	3.782920
H	-9.204956	1.493708	1.860688
H	-7.498458	1.953531	1.735818
C	-8.827344	-0.687099	4.384188
H	-9.817180	-0.978478	2.477224
H	-8.487714	-2.101806	2.759344
C	-9.209817	0.797755	4.555955
H	-8.495236	2.752659	3.900911
H	-7.214246	1.563390	4.198727
H	-9.539923	-1.334135	4.908248
H	-7.829253	-0.850470	4.816729
H	-9.219746	1.069961	5.617583
H	-10.221812	0.951780	4.157791
C	-4.151986	-7.565151	-0.674246
C	-2.989252	-8.023328	-1.593237
C	-5.478609	-7.994050	-1.340872
H	-4.143093	-6.468767	-0.640467
C	-3.097216	-7.318882	-2.961846
H	-3.053134	-9.113198	-1.717796
H	-2.025221	-7.794833	-1.129962
C	-5.628322	-7.269988	-2.693799
H	-5.468026	-9.078766	-1.517507
H	-6.325593	-7.742658	-0.696111

C	-4.453848	-7.621613	-3.631769
H	-2.275371	-7.632921	-3.615609
H	-3.005601	-6.235289	-2.803829
H	-6.579535	-7.545940	-3.164009
H	-5.652279	-6.186979	-2.507310
H	-4.540317	-7.066772	-4.573918
H	-4.500205	-8.693280	-3.869296
C	-5.202810	-11.000964	2.866276
C	-4.820246	-12.291220	2.101327
C	-5.159395	-11.277546	4.380872
H	-6.245410	-10.757601	2.608925
C	-5.806713	-13.425579	2.451141
H	-3.798831	-12.577994	2.386206
H	-4.827718	-12.100604	1.021840
C	-6.168972	-12.387894	4.736422
H	-4.149644	-11.606347	4.666054
H	-5.391604	-10.357162	4.929573
C	-5.825625	-13.684762	3.972454
H	-5.536654	-14.340873	1.912624
H	-6.814272	-13.127576	2.129179
H	-6.166895	-12.571550	5.817256
H	-7.175834	-12.053281	4.448313
H	-6.551380	-14.470390	4.211572
H	-4.834005	-14.034113	4.290628
C	-1.727664	-7.407935	3.816339
C	-2.465022	-6.683036	4.968236
C	-0.721347	-8.428356	4.394677
H	-1.151868	-6.653751	3.266214
C	-1.457776	-5.984789	5.905096
H	-3.038441	-7.428927	5.537472
H	-3.175921	-5.958491	4.550970
C	0.291379	-7.722675	5.319692
H	-1.260242	-9.186767	4.977148
H	-0.205675	-8.940641	3.574237
C	-0.444496	-7.002209	6.468738
H	-1.989415	-5.484043	6.721971
H	-0.916739	-5.214758	5.338127
H	1.004180	-8.451191	5.721891
H	0.858778	-6.984025	4.737081
H	0.275234	-6.497784	7.123204
H	-0.981746	-7.747079	7.071399
C	-8.275024	-5.366680	5.220727
C	-8.147435	-4.440191	4.276602
C	-7.950514	-4.793627	2.830247
H	-8.395310	-5.086469	6.262095
H	-8.274927	-6.429673	4.984802
N	-9.010546	-4.376097	1.922103
S	-10.586616	-3.950107	2.357865
O	-10.574467	-3.473972	3.729799
O	-11.084024	-3.097600	1.290402
H	-7.779544	-5.868139	2.707612
C	-8.991211	-9.686482	1.061652
C	-8.320270	-9.183566	2.180014
C	-9.973329	-10.641339	1.276402
H	-8.724087	-9.358683	0.061879
C	-8.606817	-9.632638	3.494751



C	-10.277707	-11.097084	2.574425
H	-10.505228	-11.059112	0.426775
C	-9.602402	-10.605023	3.680945
C	-7.698983	-8.957553	4.381211
C	-6.907326	-8.153995	3.592643
H	-6.833489	-7.786606	1.512003
H	-11.044057	-11.855576	2.703695
H	-9.828576	-10.973822	4.678673
N	-7.303249	-8.269205	2.275197
C	-7.633067	-9.125413	5.867343
H	-6.802245	-8.554696	6.293712
H	-8.553488	-8.780302	6.354510
H	-7.493880	-10.177596	6.145815
C	-5.760926	-7.265545	3.943108
H	-5.062972	-7.204968	3.106084
H	-6.074279	-6.247486	4.203114
H	-5.214749	-7.670457	4.798892
H	-0.883470	2.110976	4.766093
H	2.166521	-3.338945	-2.919586
C	-11.461305	-5.492790	2.268732
C	-12.304152	-5.731074	1.188519
C	-11.175153	-6.485464	3.201790
C	-12.878148	-6.989980	1.054317
H	-12.485542	-4.943268	0.464976
C	-11.743159	-7.744414	3.039823
H	-10.510249	-6.278322	4.036121
C	-12.602213	-8.011607	1.968275
H	-13.542598	-7.188316	0.217329
H	-11.510770	-8.535021	3.747566
C	-13.226263	-9.371378	1.795023
H	-12.987607	-10.024009	2.637504
H	-14.314723	-9.291751	1.709157
H	-12.854843	-9.853348	0.884623
C	-8.922966	-4.880218	0.570950
C	-8.610299	-3.981829	-0.440179
C	-8.524238	-4.445777	-1.750856
C	-8.747185	-5.786715	-2.041150
C	-9.063249	-6.678910	-1.017424
C	-9.152381	-6.230664	0.294781
H	-8.454883	-2.936750	-0.194283
H	-8.288162	-3.746226	-2.542877
H	-8.683614	-6.138085	-3.066578
H	-9.264315	-7.720302	-1.248190
H	-9.403581	-6.921508	1.096930

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**TS2(S), E(PCM, mixed basis set, opt) = -5013,190441 - E(PCM, 6-31+G\*, single point) = -5023.841447**

C	-4.765289	-2.555912	0.500086
C	-3.429171	-2.589633	0.852768
C	-2.794300	-1.385037	1.289989
C	-3.524605	-0.167413	1.255563
C	-4.861286	-0.177802	0.787244
C	-5.494310	-1.339715	0.417730
H	-0.903022	-2.276731	1.865742
C	-1.466377	-1.351405	1.799174

C	-2.904205	1.035728	1.686000
H	-5.401425	0.763314	0.716012
C	-1.615545	1.055922	2.157705
C	-0.903600	-0.173843	2.215585
H	-3.482709	1.956569	1.642969
H	0.110998	-0.173415	2.607051
C	-2.713003	-3.886311	0.778258
C	-1.550822	-4.066949	-0.033440
C	-3.247284	-4.971409	1.446894
C	-1.005535	-3.041818	-0.857041
C	-0.922774	-5.340850	-0.058118
C	-2.654687	-6.259509	1.401839
C	0.112827	-3.269769	-1.614164
H	-1.493020	-2.073293	-0.891764
C	0.243211	-5.536018	-0.847125
C	-1.493610	-6.405862	0.678426
C	0.773060	-4.529676	-1.614348
H	0.507329	-2.472819	-2.240245
H	0.709514	-6.519595	-0.840244
H	-1.008413	-7.378523	0.651730
C	-0.952838	2.327237	2.618655
H	-1.636592	3.178559	2.540018
H	-0.062272	2.547284	2.016164
C	2.007199	-4.727417	-2.454414
H	2.382089	-5.752458	-2.370263
H	2.806859	-4.043860	-2.141786
C	-6.882930	-1.315731	-0.116392
C	-7.976454	-1.124407	0.746335
C	-7.087227	-1.437260	-1.513411
C	-9.267777	-1.048923	0.202540
C	-8.388255	-1.381781	-2.010224
C	-9.491576	-1.199606	-1.164823
H	-10.104723	-0.913707	0.874555
H	-8.562048	-1.489403	-3.077020
C	-3.264193	-7.444643	2.070126
C	-3.911108	-8.422729	1.275433
C	-3.111458	-7.648682	3.457187
C	-4.332395	-9.606064	1.882269
C	-3.578054	-8.841058	4.029978
C	-4.166413	-9.838349	3.252014
H	-4.816404	-10.371177	1.281063
H	-3.463080	-8.995886	5.095451
O	-4.373546	-4.780904	2.206999
O	-5.401874	-3.728482	0.154435
P	-5.837412	-4.711232	1.414907
O	-6.787747	-4.022559	2.330751
O	-6.122744	-6.072072	0.855029
H	-9.428196	-4.952331	4.713956
C	-5.885322	-1.547225	-2.446362
C	-6.172239	-2.206757	-3.813104
C	-5.305519	-0.130261	-2.695707
H	-5.114805	-2.152473	-1.951020
C	-4.862877	-2.318167	-4.625566
H	-6.885024	-1.592468	-4.379560
H	-6.615098	-3.199624	-3.669063
C	-4.000140	-0.212463	-3.509630

H	-6.057353	0.452346	-3.246223
H	-5.123514	0.368600	-1.739170
C	-4.247259	-0.921462	-4.856494
H	-5.057136	-2.809199	-5.585892
H	-4.149270	-2.938975	-4.067644
H	-3.593711	0.791677	-3.676324
H	-3.259724	-0.782895	-2.931348
H	-3.310587	-1.009631	-5.418656
H	-4.943298	-0.318208	-5.455183
C	-10.889042	-1.268705	-1.769345
C	-11.202559	-2.751536	-2.104176
C	-11.991482	-0.704464	-0.850514
H	-10.893590	-0.694832	-2.708648
C	-12.601888	-2.908904	-2.733101
H	-11.145355	-3.317050	-1.166136
H	-10.430840	-3.148771	-2.774605
C	-13.378588	-0.836736	-1.511997
H	-11.999621	-1.279651	0.082950
H	-11.774639	0.343075	-0.608425
C	-13.682564	-2.320695	-1.802903
H	-12.804855	-3.968454	-2.933762
H	-12.630525	-2.376618	-3.693941
H	-14.146304	-0.414011	-0.854126
H	-13.393869	-0.271594	-2.453693
H	-14.675572	-2.429119	-2.254143
H	-13.678665	-2.873936	-0.852894
C	-7.776176	-1.023955	2.253034
C	-7.838949	0.444708	2.736235
C	-8.799716	-1.865358	3.044400
H	-6.786543	-1.430234	2.491231
C	-7.518197	0.519221	4.244113
H	-8.848505	0.836725	2.546828
H	-7.129298	1.057208	2.168153
C	-8.478848	-1.810673	4.549607
H	-9.816917	-1.487786	2.879650
H	-8.732155	-2.897966	2.691174
C	-8.498672	-0.352867	5.057592
H	-7.558472	1.558800	4.590052
H	-6.495284	0.150549	4.401050
H	-9.210178	-2.412486	5.104189
H	-7.482769	-2.246081	4.707785
H	-8.241663	-0.315493	6.122941
H	-9.513988	0.050655	4.942587
C	-4.088419	-8.241644	-0.229805
C	-3.032673	-9.087709	-0.984906
C	-5.500104	-8.620846	-0.735045
H	-3.939245	-7.183943	-0.475736
C	-3.128855	-8.856543	-2.505797
H	-3.211816	-10.148357	-0.757468
H	-2.028471	-8.836705	-0.627950
C	-5.602778	-8.377624	-2.254975
H	-5.699424	-9.682524	-0.531415
H	-6.232886	-7.998695	-0.212747
C	-4.543423	-9.200943	-3.016305
H	-2.378342	-9.461055	-3.028293
H	-2.915943	-7.799748	-2.716935

H	-6.609802	-8.635180	-2.607002
H	-5.445601	-7.308183	-2.448141
H	-4.614528	-9.013722	-4.094021
H	-4.732555	-10.270072	-2.846889
C	-4.618784	-11.176160	3.821727
C	-3.704959	-12.312889	3.293888
C	-4.640847	-11.233284	5.361622
H	-5.640633	-11.367500	3.460499
C	-4.219026	-13.688530	3.766327
H	-2.688382	-12.142939	3.674228
H	-3.663069	-12.276927	2.199270
C	-5.184874	-12.595751	5.837541
H	-3.618574	-11.104438	5.744726
H	-5.257308	-10.416136	5.753007
C	-4.297215	-13.740494	5.306176
H	-3.564992	-14.484334	3.392332
H	-5.222925	-13.853289	3.350938
H	-5.227701	-12.625441	6.932395
H	-6.206495	-12.721604	5.453299
H	-4.688472	-14.709916	5.635379
H	-3.286152	-13.628289	5.720111
C	-2.379407	-6.612443	4.307304
C	-2.674467	-6.712869	5.820862
C	-0.844325	-6.737212	4.116195
H	-2.685118	-5.611172	3.968874
C	-1.986605	-5.552113	6.570005
H	-2.273293	-7.660908	6.204336
H	-3.754864	-6.708417	6.002825
C	-0.118523	-5.593076	4.853617
H	-0.526542	-7.708440	4.520691
H	-0.595403	-6.714348	3.052093
C	-0.458159	-5.610793	6.357751
H	-2.220770	-5.602190	7.639584
H	-2.372080	-4.598480	6.185170
H	0.964687	-5.678011	4.708921
H	-0.442051	-4.636111	4.420411
H	0.029147	-4.772710	6.868551
H	-0.074698	-6.541739	6.797548
C	-9.106361	-7.058279	5.076552
C	-9.300508	-5.935905	4.281446
C	-9.298326	-6.104434	2.899428
H	-9.164034	-6.965022	6.156652
H	-9.291385	-8.041995	4.666048
N	-9.714098	-5.241510	1.950443
S	-11.135142	-4.263088	2.200889
O	-11.196133	-3.950969	3.613665
O	-11.106662	-3.238478	1.182058
H	-8.896339	-7.031479	2.498708
C	-7.563096	-9.677675	2.109861
C	-7.140654	-8.886795	3.175935
C	-8.169028	-10.893183	2.415539
H	-7.409271	-9.356690	1.084786
C	-7.351831	-9.266108	4.518082
C	-8.361899	-11.299606	3.745930
H	-8.499429	-11.539143	1.608096
C	-7.964205	-10.489051	4.804704

C	-6.952828	-8.138167	5.335745
C	-6.431831	-7.183963	4.445933
H	-6.280042	-7.108166	2.321124
H	-8.831637	-12.257279	3.947910
H	-8.124618	-10.802185	5.833500
N	-6.572713	-7.623097	3.174926
C	-6.824266	-8.153103	6.827011
H	-6.715160	-7.144726	7.234867
H	-7.705602	-8.610511	7.291537
H	-5.951628	-8.737693	7.141782
C	-5.920471	-5.825343	4.745717
H	-4.940570	-5.676964	4.282502
H	-6.586061	-5.072523	4.302783
H	-5.843723	-5.666396	5.822968
H	-0.628544	2.243968	3.663677
H	1.798015	-4.523983	-3.512194
C	-12.401152	-5.425771	1.794134
C	-12.948006	-6.214927	2.803282
C	-12.787139	-5.556532	0.461900
C	-13.916706	-7.149431	2.459858
H	-12.628535	-6.082953	3.832200
C	-13.757678	-6.498816	0.144114
H	-12.340399	-4.927837	-0.302991
C	-14.335613	-7.301905	1.132927
H	-14.361684	-7.767624	3.234314
H	-14.074438	-6.609697	-0.888948
C	-15.414915	-8.291110	0.782281
H	-15.388918	-9.159200	1.445836
H	-16.402518	-7.827607	0.882665
H	-15.315055	-8.638110	-0.249023
C	-9.327200	-5.493146	0.579935
C	-8.695148	-4.476114	-0.126037
C	-8.201522	-4.762932	-1.395244
C	-8.332815	-6.037373	-1.937279
C	-8.988875	-7.039181	-1.223680
C	-9.504580	-6.765888	0.038174
H	-8.554125	-3.495274	0.316162
H	-7.686676	-3.974520	-1.930894
H	-7.918309	-6.255208	-2.916937
H	-9.102276	-8.032001	-1.648452
H	-10.025889	-7.534463	0.604117

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**I3(S), E(PCM, mixed basis set, opt) = -5013,244025 - E(PCM, 6-31+G\*, single point) = -5023.894392**

C	-4.597276	-2.638102	0.577008
C	-3.242029	-2.611666	0.846639
C	-2.643657	-1.373625	1.240890
C	-3.436643	-0.194450	1.249004
C	-4.799844	-0.271702	0.867205
C	-5.397760	-1.465788	0.543184
H	-0.677600	-2.165886	1.696001
C	-1.289991	-1.270478	1.664386
C	-2.850388	1.040226	1.635621
H	-5.389032	0.641560	0.828650
C	-1.537121	1.127913	2.025125

C	-0.761605	-0.063921	2.041372
H	-3.475031	1.931188	1.625616
H	0.274470	-0.010509	2.367448
C	-2.469847	-3.877134	0.730531
C	-1.354092	-4.014198	-0.151420
C	-2.913688	-4.985449	1.426136
C	-0.905491	-2.969749	-1.007674
C	-0.678005	-5.263064	-0.215381
C	-2.290181	-6.257632	1.327758
C	0.167763	-3.154791	-1.838180
H	-1.432562	-2.021564	-1.007169
C	0.440196	-5.412102	-1.079909
C	-1.165025	-6.355996	0.543006
C	0.875130	-4.388087	-1.883136
H	0.487691	-2.343905	-2.488264
H	0.945115	-6.376019	-1.106326
H	-0.651050	-7.310995	0.468842
C	-0.912510	2.433269	2.441959
H	-1.631722	3.255186	2.368197
H	-0.049008	2.675432	1.809651
C	2.048859	-4.544477	-2.813436
H	2.511446	-5.530504	-2.701958
H	2.812415	-3.781931	-2.615201
C	-6.814090	-1.495182	0.081723
C	-7.877526	-1.313883	0.985447
C	-7.074941	-1.618478	-1.305459
C	-9.185382	-1.191703	0.488101
C	-8.388693	-1.504552	-1.756604
C	-9.457037	-1.289741	-0.875141
H	-10.000374	-1.058001	1.190541
H	-8.603053	-1.596278	-2.817071
C	-2.884649	-7.464848	1.977153
C	-3.607555	-8.381359	1.176715
C	-2.707674	-7.719825	3.357055
C	-4.113885	-9.542346	1.770834
C	-3.258062	-8.881729	3.915368
C	-3.960751	-9.804086	3.133344
H	-4.638437	-10.269819	1.158587
H	-3.119470	-9.079506	4.971852
O	-3.994118	-4.839884	2.257187
O	-5.195013	-3.842867	0.266969
P	-5.504234	-4.823662	1.548264
O	-6.402150	-4.180057	2.546300
O	-5.747526	-6.204704	1.018800
H	-8.028435	-5.358008	3.458569
C	-5.934944	-1.851592	-2.291458
C	-6.335668	-2.734081	-3.494205
C	-5.373929	-0.502414	-2.803189
H	-5.125590	-2.377054	-1.772419
C	-5.111799	-2.986498	-4.398915
H	-7.108197	-2.228433	-4.087672
H	-6.747697	-3.683892	-3.131163
C	-4.159147	-0.736307	-3.726197
H	-6.170336	0.016559	-3.354479
H	-5.089833	0.122411	-1.948435
C	-4.542266	-1.646595	-4.911241

H	-5.393438	-3.625425	-5.243592
H	-4.339051	-3.511314	-3.821278
H	-3.773295	0.222090	-4.092180
H	-3.361570	-1.221329	-3.146038
H	-3.670132	-1.825302	-5.550738
H	-5.307239	-1.142058	-5.517244
C	-10.873209	-1.296531	-1.439176
C	-11.234085	-2.762500	-1.796709
C	-11.934765	-0.735962	-0.471985
H	-10.886668	-0.697876	-2.362516
C	-12.648587	-2.871492	-2.399356
H	-11.184996	-3.337983	-0.864638
H	-10.484274	-3.170768	-2.485532
C	-13.343580	-0.821878	-1.096458
H	-11.932012	-1.340388	0.442603
H	-11.689981	0.300002	-0.206658
C	-13.689115	-2.290473	-1.421264
H	-12.880944	-3.920658	-2.623771
H	-12.686159	-2.310848	-3.343813
H	-14.081734	-0.404459	-0.402512
H	-13.374190	-0.227542	-2.020153
H	-14.696295	-2.362085	-1.847791
H	-13.665678	-2.874560	-0.491499
C	-7.646859	-1.290507	2.490932
C	-7.778208	0.138588	3.066501
C	-8.616623	-2.238978	3.236367
H	-6.633283	-1.658136	2.688261
C	-7.453576	0.136687	4.575897
H	-8.806309	0.493190	2.906426
H	-7.101240	0.817834	2.534285
C	-8.273294	-2.263034	4.737503
H	-9.653819	-1.899240	3.109669
H	-8.516661	-3.242177	2.817998
C	-8.373459	-0.843508	5.335703
H	-7.556818	1.147647	4.987147
H	-6.408916	-0.176399	4.709143
H	-8.950282	-2.948718	5.262449
H	-7.248245	-2.644166	4.849545
H	-8.111866	-0.854937	6.400731
H	-9.412627	-0.497296	5.249818
C	-3.791901	-8.161726	-0.320027
C	-2.729638	-8.971439	-1.105751
C	-5.196156	-8.543410	-0.842300
H	-3.655189	-7.094948	-0.531370
C	-2.817782	-8.655804	-2.612069
H	-2.914028	-10.041733	-0.935712
H	-1.727072	-8.743735	-0.730355
C	-5.300508	-8.209197	-2.345414
H	-5.370339	-9.621221	-0.710355
H	-5.940908	-7.974446	-0.277919
C	-4.228632	-8.972913	-3.151405
H	-2.063531	-9.229109	-3.163371
H	-2.604453	-7.588437	-2.760622
H	-6.302226	-8.460089	-2.716691
H	-5.154926	-7.127628	-2.473919
H	-4.294397	-8.714873	-4.214640

H	-4.412324	-10.051943	-3.054543
C	-4.493373	-11.107872	3.706148
C	-3.340215	-12.137510	3.813589
C	-5.175186	-10.947406	5.080925
H	-5.245197	-11.503139	3.006762
C	-3.858919	-13.494626	4.331281
H	-2.588762	-11.737868	4.508491
H	-2.863586	-12.253456	2.833345
C	-5.707638	-12.303661	5.587303
H	-4.448443	-10.558408	5.807431
H	-5.996148	-10.227738	4.995914
C	-4.555386	-13.324376	5.697353
H	-3.030193	-14.206671	4.413251
H	-4.580140	-13.901540	3.609734
H	-6.197053	-12.174744	6.559480
H	-6.458857	-12.679095	4.879263
H	-4.933960	-14.288513	6.054515
H	-3.823198	-12.957853	6.429632
C	-1.870374	-6.764637	4.205776
C	-2.087296	-6.916918	5.728745
C	-0.357951	-6.969353	3.925451
H	-2.130424	-5.733034	3.921933
C	-1.298795	-5.829628	6.487114
H	-1.716860	-7.900993	6.047179
H	-3.152454	-6.866157	5.978662
C	0.474598	-5.907939	4.675194
H	-0.080592	-7.977088	4.263424
H	-0.164675	-6.904745	2.851659
C	0.209684	-5.967956	6.193867
H	-1.482813	-5.913539	7.564116
H	-1.645626	-4.839915	6.161139
H	1.540955	-6.056067	4.471498
H	0.195905	-4.914001	4.299009
H	0.769134	-5.178394	6.707888
H	0.559588	-6.934820	6.580093
C	-8.334852	-6.267702	5.474921
C	-8.786926	-5.737791	4.148179
C	-10.067981	-5.717950	3.780663
H	-7.851854	-5.475400	6.063826
H	-9.181040	-6.643337	6.062312
N	-10.465307	-5.304405	2.490011
S	-12.010302	-4.716541	2.248057
O	-12.640288	-4.686132	3.560812
O	-11.913502	-3.506903	1.444096
H	-10.880081	-6.010191	4.439853
C	-7.404689	-9.394972	2.215434
C	-7.156628	-8.521107	3.258870
C	-8.413796	-10.336023	2.422904
H	-6.843425	-9.335518	1.289933
C	-7.851186	-8.540782	4.464703
C	-9.128770	-10.375095	3.623754
H	-8.647435	-11.047568	1.637614
C	-8.858751	-9.473274	4.656956
C	-7.306985	-7.440619	5.341430
C	-6.181746	-6.909995	4.481877
H	-5.647388	-7.185051	2.475198



H	-9.906835	-11.119755	3.755483
H	-9.422666	-9.509822	5.584647
N	-6.170940	-7.504915	3.329863
C	-6.838439	-7.910002	6.722618
H	-6.483191	-7.064405	7.318573
H	-7.678319	-8.367446	7.253510
H	-6.036526	-8.649396	6.642877
C	-5.315594	-5.775884	4.857432
H	-4.364562	-5.821848	4.324565
H	-5.813860	-4.848894	4.535768
H	-5.161615	-5.755754	5.938292
H	-0.555165	2.382884	3.478318
H	1.736018	-4.429523	-3.859135
C	-12.810506	-5.948862	1.254760
C	-13.599335	-6.910227	1.876822
C	-12.614559	-5.949109	-0.125610
C	-14.208182	-7.886635	1.094359
H	-13.743918	-6.878689	2.951814
C	-13.226987	-6.935004	-0.887345
H	-11.990904	-5.191011	-0.589359
C	-14.032479	-7.912614	-0.291522
H	-14.835538	-8.637053	1.567077
H	-13.080282	-6.945578	-1.964097
C	-14.712005	-8.955451	-1.139898
H	-15.112439	-9.767219	-0.528018
H	-15.543888	-8.514252	-1.699403
H	-14.017203	-9.382070	-1.869069
C	-9.663609	-5.596932	1.332668
C	-9.163380	-4.570888	0.539995
C	-8.422303	-4.882344	-0.600013
C	-8.176603	-6.209007	-0.933439
C	-8.675993	-7.234120	-0.129093
C	-9.421238	-6.934011	1.004201
H	-9.344063	-3.535807	0.797195
H	-8.027940	-4.064287	-1.194249
H	-7.576623	-6.449426	-1.806509
H	-8.483721	-8.272302	-0.387346
H	-9.814910	-7.720832	1.643782

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**TS3(S), E(PCM, mixed basis set, opt) = -5013,241377 - E(PCM, 6-31+G\*, single point) = -5023.890527**

C	-4.596407	-2.637630	0.592125
C	-3.242296	-2.568175	0.859315
C	-2.681471	-1.308108	1.235049
C	-3.513038	-0.156144	1.238655
C	-4.871660	-0.280641	0.856829
C	-5.433048	-1.494074	0.535058
H	-0.689041	-2.034729	1.686520
C	-1.330217	-1.159769	1.652585
C	-2.966412	1.099408	1.616779
H	-5.490547	0.612412	0.810062
C	-1.655727	1.231030	2.002207
C	-0.841078	0.065245	2.021563
H	-3.619481	1.969551	1.603443
H	0.193500	0.154448	2.344285

C	-2.434938	-3.812900	0.763529
C	-1.325651	-3.937112	-0.128240
C	-2.844653	-4.920743	1.477453
C	-0.901238	-2.890979	-0.994340
C	-0.629903	-5.175193	-0.187525
C	-2.219876	-6.190073	1.368239
C	0.167266	-3.065288	-1.833325
H	-1.439859	-1.949441	-0.993058
C	0.482987	-5.312482	-1.060775
C	-1.098873	-6.273061	0.575270
C	0.893458	-4.287639	-1.875802
H	0.469100	-2.253538	-2.490849
H	1.003341	-6.268088	-1.084473
H	-0.580364	-7.224494	0.490839
C	-1.073794	2.557599	2.413172
H	-1.812957	3.358858	2.314280
H	-0.204424	2.813807	1.794886
C	2.061486	-4.431867	-2.815009
H	2.535112	-5.412958	-2.706874
H	2.818504	-3.661471	-2.622341
C	-6.842507	-1.553605	0.054992
C	-7.917572	-1.319612	0.932499
C	-7.083259	-1.734974	-1.332073
C	-9.217517	-1.209588	0.409427
C	-8.387599	-1.623409	-1.807256
C	-9.467688	-1.359246	-0.952452
H	-10.042727	-1.049519	1.094319
H	-8.588052	-1.765223	-2.864544
C	-2.824896	-7.410208	1.982047
C	-3.555468	-8.290910	1.148840
C	-2.657489	-7.709032	3.352471
C	-4.075744	-9.464793	1.702052
C	-3.223601	-8.881396	3.870329
C	-3.929766	-9.771513	3.055471
H	-4.607261	-10.166635	1.066367
H	-3.093031	-9.114185	4.920524
O	-3.909039	-4.776163	2.340403
O	-5.166625	-3.881339	0.341900
P	-5.423274	-4.750370	1.696032
O	-6.321470	-4.093220	2.672311
O	-5.700228	-6.181089	1.233518
H	-8.003494	-5.319823	3.569772
C	-5.931484	-2.063689	-2.278421
C	-6.365232	-2.838862	-3.543120
C	-5.164728	-0.788367	-2.708277
H	-5.230905	-2.714293	-1.741729
C	-5.121622	-3.245087	-4.361842
H	-7.002484	-2.201435	-4.170158
H	-6.944381	-3.726201	-3.258330
C	-3.919707	-1.171663	-3.536096
H	-5.838961	-0.164999	-3.311665
H	-4.869783	-0.213520	-1.824033
C	-4.324376	-1.991320	-4.778838
H	-5.423021	-3.815245	-5.247934
H	-4.482874	-3.891933	-3.745312
H	-3.371573	-0.271094	-3.835467

H	-3.253043	-1.779067	-2.907597
H	-3.435328	-2.279180	-5.351218
H	-4.955038	-1.367464	-5.426730
C	-10.873741	-1.381563	-1.541150
C	-11.232133	-2.861218	-1.843567
C	-11.948395	-0.772767	-0.618593
H	-10.866769	-0.822811	-2.489408
C	-12.641888	-2.998958	-2.450672
H	-11.187436	-3.399940	-0.890035
H	-10.476983	-3.294034	-2.511612
C	-13.349179	-0.889720	-1.255619
H	-11.959625	-1.330145	0.324673
H	-11.705722	0.274801	-0.401801
C	-13.689703	-2.373276	-1.509001
H	-12.870939	-4.057934	-2.626046
H	-12.674673	-2.484554	-3.421399
H	-14.095473	-0.438599	-0.591867
H	-13.370668	-0.342844	-2.208395
H	-14.694299	-2.469662	-1.936563
H	-13.669776	-2.910306	-0.550668
C	-7.719928	-1.252287	2.442583
C	-7.939136	0.177696	2.989352
C	-8.659365	-2.238858	3.179459
H	-6.694346	-1.562265	2.674811
C	-7.661348	0.216389	4.507391
H	-8.978402	0.477621	2.793538
H	-7.281408	0.881711	2.464848
C	-8.371147	-2.214433	4.691639
H	-9.709619	-1.969094	3.001936
H	-8.484929	-3.244535	2.793201
C	-8.559933	-0.790648	5.256894
H	-7.821354	1.229085	4.895663
H	-6.608609	-0.047004	4.678770
H	-9.034677	-2.921340	5.204922
H	-7.334032	-2.544157	4.849552
H	-8.333962	-0.770167	6.329642
H	-9.610573	-0.496169	5.129354
C	-3.735819	-8.014500	-0.339913
C	-2.664982	-8.786709	-1.152127
C	-5.132876	-8.387442	-0.888540
H	-3.602099	-6.939516	-0.513702
C	-2.740337	-8.405872	-2.643662
H	-2.849937	-9.863474	-1.029935
H	-1.666469	-8.575668	-0.757634
C	-5.230152	-7.993295	-2.378440
H	-5.293126	-9.471704	-0.803303
H	-5.897926	-7.860818	-0.309326
C	-4.143787	-8.709171	-3.208641
H	-1.977138	-8.949837	-3.211959
H	-2.532854	-7.331507	-2.743485
H	-6.224836	-8.244862	-2.767597
H	-5.100966	-6.905088	-2.465122
H	-4.204076	-8.402359	-4.259173
H	-4.318669	-9.792829	-3.164119
C	-4.465335	-11.093292	3.583136
C	-3.308664	-12.121154	3.669999

C	-5.159871	-10.973575	4.955194
H	-5.210199	-11.469890	2.866291
C	-3.821561	-13.493531	4.151581
H	-2.561799	-11.735507	4.377698
H	-2.826864	-12.210273	2.689319
C	-5.684636	-12.345582	5.425085
H	-4.442523	-10.595561	5.696711
H	-5.985751	-10.259374	4.878965
C	-4.525346	-13.360084	5.517909
H	-2.988789	-14.202393	4.220238
H	-4.537303	-13.887532	3.417504
H	-6.181402	-12.243185	6.396830
H	-6.428887	-12.709613	4.703791
H	-4.897723	-14.334955	5.851721
H	-3.798965	-13.004555	6.261478
C	-1.803330	-6.794805	4.229750
C	-2.031224	-6.983373	5.746395
C	-0.297010	-7.033941	3.943991
H	-2.039503	-5.750260	3.974217
C	-1.201086	-5.957405	6.544707
H	-1.705522	-7.991726	6.035856
H	-3.094380	-6.892691	5.990504
C	0.572156	-6.035022	4.736409
H	-0.053810	-8.063837	4.239420
H	-0.099513	-6.932649	2.873425
C	0.301219	-6.147444	6.250721
H	-1.393489	-6.072746	7.617365
H	-1.504440	-4.942437	6.255277
H	1.632667	-6.214514	4.527124
H	0.331787	-5.016528	4.402229
H	0.892339	-5.404791	6.798215
H	0.608418	-7.143674	6.596500
C	-8.346427	-6.366118	5.512719
C	-8.772745	-5.751856	4.213678
C	-10.039359	-5.722469	3.803502
H	-7.873206	-5.608671	6.153152
H	-9.208083	-6.765347	6.061161
N	-10.385883	-5.227513	2.521561
S	-11.895468	-4.550943	2.298629
O	-12.470565	-4.411919	3.628377
O	-11.743720	-3.395326	1.426998
H	-10.869365	-6.067949	4.413456
C	-7.402556	-9.388869	2.157626
C	-7.170991	-8.521638	3.212573
C	-8.386145	-10.362188	2.343217
H	-6.839349	-9.303593	1.234590
C	-7.862248	-8.602051	4.421114
C	-9.100102	-10.446357	3.541641
H	-8.598785	-11.065147	1.543855
C	-8.845633	-9.562716	4.595017
C	-7.319351	-7.532056	5.332337
C	-6.206670	-6.971537	4.466846
H	-5.799525	-6.918188	2.238229
H	-9.858986	-11.213262	3.658348
H	-9.399755	-9.638917	5.526719
N	-6.204991	-7.484898	3.278633

C	-6.852160	-8.047716	6.695728
H	-6.497006	-7.223409	7.321387
H	-7.689126	-8.525391	7.214088
H	-6.047837	-8.781086	6.590434
C	-5.328946	-5.862570	4.911253
H	-4.399363	-5.855104	4.339833
H	-5.834703	-4.905263	4.731521
H	-5.117434	-5.957983	5.979388
H	-0.736619	2.529714	3.457203
H	1.739298	-4.320283	-3.858152
C	-12.825162	-5.769393	1.404729
C	-13.710191	-6.585991	2.101757
C	-12.640586	-5.904386	0.029722
C	-14.427803	-7.549772	1.401663
H	-13.842048	-6.450427	3.170277
C	-13.363794	-6.877110	-0.649724
H	-11.943410	-5.258658	-0.496132
C	-14.267277	-7.707206	0.022009
H	-15.128454	-8.186935	1.934318
H	-13.226697	-6.991680	-1.721603
C	-15.074823	-8.729557	-0.734066
H	-14.528384	-9.099318	-1.605576
H	-15.332325	-9.581273	-0.099280
H	-16.011566	-8.289553	-1.093725
C	-9.613345	-5.575035	1.359643
C	-9.088994	-4.584202	0.535386
C	-8.380793	-4.948885	-0.609550
C	-8.195150	-6.290193	-0.923454
C	-8.717867	-7.278223	-0.088273
C	-9.428245	-6.926472	1.053428
H	-9.235532	-3.537776	0.766272
H	-7.969185	-4.159190	-1.228698
H	-7.630218	-6.568686	-1.808290
H	-8.575707	-8.328336	-0.328975
H	-9.835681	-7.686874	1.715681

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**I4(S), E(PCM, mixed basis set, opt) = -5013,245072 - E(PCM, 6-31+G\*, single point) = -5023.895097**

C	-4.599583	-2.639124	0.669001
C	-3.241240	-2.599843	0.909612
C	-2.652473	-1.353548	1.289319
C	-3.462426	-0.186288	1.311361
C	-4.826797	-0.280094	0.937970
C	-5.414897	-1.481315	0.620387
H	-0.668532	-2.122855	1.704551
C	-1.293058	-1.235438	1.687587
C	-2.887684	1.054783	1.694439
H	-5.427673	0.625352	0.896472
C	-1.570112	1.157228	2.065695
C	-0.776768	-0.023329	2.062443
H	-3.523910	1.937280	1.696982
H	0.263294	0.043681	2.372421
C	-2.453773	-3.850856	0.754175
C	-1.377097	-3.958620	-0.180022
C	-2.848791	-4.977926	1.442419

C	-0.973118	-2.890788	-1.028812
C	-0.699313	-5.201772	-0.302708
C	-2.237257	-6.246813	1.284990
C	0.064396	-3.049573	-1.908905
H	-1.502539	-1.945317	-0.981924
C	0.382443	-5.322521	-1.216339
C	-1.149372	-6.317065	0.445982
C	0.776600	-4.276438	-2.012300
H	0.351684	-2.221079	-2.551814
H	0.891375	-6.281854	-1.286704
H	-0.638347	-7.268340	0.324242
C	-0.958190	2.467650	2.484116
H	-1.684046	3.283481	2.408748
H	-0.094751	2.716582	1.854691
C	1.912151	-4.401922	-2.992910
H	2.383971	-5.387476	-2.925490
H	2.678873	-3.639978	-2.805381
C	-6.821308	-1.521327	0.131550
C	-7.904663	-1.329569	1.007439
C	-7.045145	-1.644219	-1.262927
C	-9.198866	-1.196316	0.476137
C	-8.344921	-1.514713	-1.747347
C	-9.434055	-1.287690	-0.894232
H	-10.031108	-1.061517	1.157990
H	-8.532882	-1.602504	-2.812997
C	-2.797199	-7.466785	1.936451
C	-3.523829	-8.392947	1.155044
C	-2.567348	-7.720665	3.309834
C	-3.990645	-9.566207	1.760736
C	-3.070867	-8.894586	3.875754
C	-3.780557	-9.828901	3.112953
H	-4.526979	-10.298540	1.165373
H	-2.895531	-9.096169	4.926486
O	-3.894465	-4.856226	2.343355
O	-5.201945	-3.872162	0.413959
P	-5.404009	-4.767130	1.744529
O	-6.311381	-4.220943	2.767476
O	-5.695556	-6.177605	1.133498
H	-8.049057	-5.423282	3.535090
C	-5.884997	-1.895468	-2.221692
C	-6.271780	-2.771092	-3.434352
C	-5.286131	-0.558252	-2.722600
H	-5.095934	-2.434562	-1.685374
C	-5.027756	-3.054660	-4.301235
H	-7.013018	-2.247809	-4.051637
H	-6.718861	-3.710215	-3.085259
C	-4.051145	-0.818798	-3.611396
H	-6.058657	-0.028282	-3.296851
H	-5.013406	0.066187	-1.863906
C	-4.414903	-1.729781	-4.801956
H	-5.298795	-3.691047	-5.151152
H	-4.283802	-3.593901	-3.699187
H	-3.639770	0.130978	-3.972024
H	-3.277620	-1.313007	-3.006781
H	-3.525953	-1.930532	-5.410835
H	-5.148407	-1.214405	-5.436747

C	-10.832867	-1.280150	-1.499707
C	-11.195356	-2.746292	-1.857419
C	-11.914407	-0.695196	-0.569968
H	-10.810693	-0.688711	-2.427650
C	-12.598699	-2.854461	-2.484920
H	-11.165001	-3.318046	-0.923184
H	-10.434953	-3.159450	-2.531712
C	-13.308266	-0.783451	-1.226123
H	-11.939619	-1.281688	0.355028
H	-11.667835	0.343797	-0.318453
C	-13.653463	-2.255663	-1.533515
H	-12.831624	-3.905427	-2.699558
H	-12.617030	-2.305621	-3.436808
H	-14.059275	-0.350528	-0.555780
H	-13.315799	-0.204552	-2.159888
H	-14.653782	-2.331775	-1.975140
H	-13.646867	-2.825728	-0.594650
C	-7.715843	-1.311931	2.519801
C	-7.936489	0.105383	3.098505
C	-8.659262	-2.319611	3.222253
H	-6.690140	-1.625789	2.749624
C	-7.687127	0.109384	4.621605
H	-8.970500	0.414979	2.890716
H	-7.265457	0.816926	2.601152
C	-8.400409	-2.323247	4.740533
H	-9.708729	-2.055942	3.030543
H	-8.471850	-3.317209	2.820031
C	-8.603855	-0.911274	5.329145
H	-7.851208	1.113952	5.028806
H	-6.638896	-0.161947	4.808155
H	-9.072896	-3.041721	5.224494
H	-7.366684	-2.655186	4.914925
H	-8.404243	-0.912254	6.407026
H	-9.651075	-0.613617	5.181721
C	-3.753316	-8.180171	-0.339254
C	-2.714947	-8.997718	-1.150003
C	-5.171350	-8.573540	-0.814900
H	-3.619076	-7.116114	-0.569645
C	-2.856798	-8.719131	-2.659774
H	-2.884589	-10.064876	-0.949102
H	-1.701975	-8.755228	-0.813777
C	-5.328189	-8.275919	-2.321146
H	-5.336073	-9.648074	-0.653086
H	-5.917482	-8.011344	-0.244737
C	-4.282366	-9.058612	-3.141788
H	-2.118064	-9.302358	-3.221542
H	-2.655180	-7.655018	-2.843809
H	-6.341332	-8.539311	-2.649836
H	-5.190048	-7.198471	-2.486651
H	-4.387540	-8.832247	-4.208765
H	-4.457185	-10.134903	-3.007035
C	-4.281609	-11.122094	3.735240
C	-3.098295	-12.038889	4.127954
C	-5.166588	-10.854733	4.971527
H	-4.895028	-11.648090	2.988689
C	-3.604822	-13.360076	4.744238

H	-2.476139	-11.509060	4.862252
H	-2.479255	-12.236938	3.245226
C	-5.677843	-12.173110	5.585528
H	-4.575574	-10.311246	5.722608
H	-6.010135	-10.224911	4.677306
C	-4.493794	-13.081458	5.974367
H	-2.754714	-13.992172	5.024368
H	-4.193658	-13.903807	3.992942
H	-6.300702	-11.958648	6.462265
H	-6.306031	-12.690298	4.847790
H	-4.860467	-14.023678	6.397453
H	-3.893916	-12.577722	6.744493
C	-1.708600	-6.757410	4.127798
C	-1.884534	-6.891562	5.657002
C	-0.206860	-6.972592	3.801180
H	-1.978869	-5.728366	3.848975
C	-1.054394	-5.813411	6.383574
H	-1.527700	-7.879454	5.978341
H	-2.940733	-6.809273	5.928984
C	0.662710	-5.921851	4.523232
H	0.071145	-7.983118	4.130660
H	-0.045992	-6.913027	2.721032
C	0.441793	-5.978046	6.049304
H	-1.210058	-5.886326	7.465903
H	-1.393615	-4.820066	6.061147
H	1.720385	-6.085255	4.287574
H	0.386797	-4.923835	4.155636
H	1.030203	-5.198686	6.546618
H	0.786236	-6.950963	6.425104
C	-8.461949	-6.433190	5.475536
C	-8.847760	-5.810028	4.169870
C	-10.108320	-5.739689	3.747488
H	-7.966154	-5.692568	6.119220
H	-9.348859	-6.788344	6.014900
N	-10.434169	-5.244252	2.459806
S	-11.941612	-4.575693	2.205880
O	-12.563567	-4.475081	3.517653
O	-11.774505	-3.394458	1.371427
H	-10.954165	-6.052750	4.351798
C	-7.486989	-9.504380	2.140833
C	-7.266451	-8.634795	3.198521
C	-8.545439	-10.408185	2.258442
H	-6.853403	-9.474179	1.260402
C	-8.045302	-8.669437	4.359243
C	-9.344708	-10.434017	3.403606
H	-8.748284	-11.103360	1.449380
C	-9.097919	-9.562198	4.469939
C	-7.488731	-7.636981	5.304817
C	-6.297782	-7.152356	4.483884
H	-5.767752	-6.864865	1.887503
H	-10.160450	-11.146872	3.471088
H	-9.715054	-9.595990	5.364246
N	-6.232886	-7.668394	3.302621
C	-7.111871	-8.199174	6.678696
H	-6.700874	-7.412401	7.319489
H	-8.004804	-8.598745	7.170152



H	-6.376562	-9.003724	6.596360
C	-5.365568	-6.104510	4.977902
H	-4.472871	-6.067862	4.349710
H	-5.852289	-5.122572	4.941844
H	-5.081136	-6.312442	6.014506
H	-0.604199	2.419106	3.521672
H	1.556042	-4.261817	-4.021385
C	-12.830456	-5.776341	1.247285
C	-13.721198	-6.626845	1.892983
C	-12.608812	-5.862494	-0.126860
C	-14.406540	-7.577042	1.142335
H	-13.883293	-6.529335	2.961444
C	-13.299734	-6.820856	-0.856839
H	-11.907750	-5.188890	-0.610838
C	-14.207873	-7.686289	-0.236207
H	-15.111591	-8.241294	1.634314
H	-13.134271	-6.897364	-1.928251
C	-14.973783	-8.695974	-1.050495
H	-15.391345	-9.482629	-0.417330
H	-15.804472	-8.214418	-1.577853
H	-14.332911	-9.162132	-1.804194
C	-9.626376	-5.569908	1.316921
C	-9.104279	-4.562350	0.511997
C	-8.355226	-4.900576	-0.614811
C	-8.124862	-6.235544	-0.928330
C	-8.643433	-7.240897	-0.110577
C	-9.395995	-6.914728	1.011822
H	-9.282145	-3.522220	0.747177
H	-7.949194	-4.095448	-1.218052
H	-7.527818	-6.496995	-1.797487
H	-8.464492	-8.285850	-0.349550
H	-9.798325	-7.689441	1.660381

**(R) Pathway**

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**I1(R), E(PCM, mixed basis set, opt) = -5013.201109 - E(PCM, 6-31+G\*, single point) = -5023.853750**

C	-4.460774	-2.520107	0.877483
C	-3.201402	-2.490557	1.436201
C	-2.838463	-1.354148	2.228421
C	-3.732048	-0.253242	2.308853
C	-4.952286	-0.293858	1.587312
C	-5.337920	-1.403775	0.878633
H	-0.950213	-2.137898	2.950933
C	-1.629479	-1.292019	2.972956
C	-3.377690	0.878102	3.090229
H	-5.592510	0.584294	1.582612
C	-2.200100	0.931143	3.793174
C	-1.328380	-0.189430	3.727627
H	-4.072889	1.714070	3.128764
H	-0.402977	-0.167153	4.298032
C	-2.266797	-3.615419	1.180787
C	-0.987697	-3.413931	0.568601
C	-2.665917	-4.903894	1.453416
C	-0.537867	-2.146429	0.105286
C	-0.137977	-4.535612	0.373035
C	-1.858115	-6.046485	1.218240
C	0.695960	-2.011030	-0.474339
H	-1.188851	-1.283344	0.198599
C	1.141711	-4.350679	-0.214931
C	-0.595655	-5.831048	0.723734
C	1.573772	-3.117291	-0.632860
H	1.015744	-1.034651	-0.830130
H	1.778191	-5.223702	-0.344952
H	0.064937	-6.679861	0.569945
C	-1.820178	2.126230	4.626785
H	-2.584644	2.907430	4.567254
H	-0.867682	2.551990	4.286470
C	2.926226	-2.914871	-1.262943
H	2.830128	-2.456018	-2.254938
H	3.455400	-3.866305	-1.375261
C	-6.544351	-1.407663	0.009499
C	-7.842997	-1.466285	0.549655
C	-6.356058	-1.313887	-1.390811
C	-8.944059	-1.443731	-0.318268
C	-7.479219	-1.311746	-2.219673
C	-8.778756	-1.387021	-1.702723
H	-9.942481	-1.506243	0.095227
H	-7.348277	-1.242205	-3.297586
C	-2.397700	-7.402879	1.508421
C	-2.988839	-8.165057	0.468931
C	-2.364428	-7.898897	2.821736
C	-3.569017	-9.389196	0.791950
C	-2.984748	-9.124446	3.105824
C	-3.616645	-9.863986	2.110640
H	-4.054890	-9.974219	0.015688
H	-3.011200	-9.472438	4.132547
O	-3.923518	-5.086958	2.025698

O	-4.878409	-3.658128	0.188901
P	-5.193837	-4.991101	1.035339
O	-6.341202	-4.592526	2.054993
O	-5.434892	-6.164609	0.182904
H	-7.076939	-5.241424	2.061159
C	-4.967639	-1.156391	-2.007980
C	-4.562220	-2.375062	-2.870426
C	-4.880870	0.138511	-2.851839
H	-4.225066	-1.063710	-1.206767
C	-3.136795	-2.190853	-3.430252
H	-5.269090	-2.469733	-3.708402
H	-4.620066	-3.285991	-2.264661
C	-3.454649	0.322795	-3.410924
H	-5.591452	0.075505	-3.686524
H	-5.167182	0.996295	-2.232673
C	-3.046441	-0.896221	-4.264086
H	-2.859842	-3.058246	-4.040331
H	-2.428138	-2.134616	-2.591954
H	-3.400740	1.240549	-4.007428
H	-2.751485	0.424325	-2.572665
H	-2.030994	-0.764336	-4.654009
H	-3.727435	-0.975294	-5.122570
C	-9.952353	-1.453872	-2.672920
C	-9.979741	-2.857877	-3.333492
C	-11.315111	-1.180155	-2.005415
H	-9.792520	-0.702260	-3.461380
C	-11.131167	-2.973248	-4.352779
H	-10.119160	-3.596964	-2.535085
H	-9.015368	-3.060063	-3.814840
C	-12.461338	-1.281981	-3.031833
H	-11.479900	-1.937728	-1.230081
H	-11.307183	-0.190824	-1.531255
C	-12.480552	-2.688996	-3.661910
H	-11.133410	-3.973978	-4.801434
H	-10.981488	-2.243193	-5.160264
H	-13.418707	-1.074430	-2.540749
H	-12.318525	-0.532415	-3.822182
H	-13.305687	-2.778017	-4.378038
H	-12.635324	-3.429445	-2.864570
C	-8.080759	-1.511897	2.053141
C	-8.562905	-0.123590	2.545463
C	-9.110793	-2.590382	2.455211
H	-7.136866	-1.751027	2.559853
C	-8.782257	-0.123911	4.071867
H	-9.506972	0.113240	2.035145
H	-7.832205	0.643511	2.262388
C	-9.334308	-2.594759	3.978780
H	-10.072552	-2.401672	1.961301
H	-8.759438	-3.570862	2.120025
C	-9.804830	-1.209353	4.466062
H	-9.126801	0.862402	4.403363
H	-7.824883	-0.331732	4.569559
H	-10.077434	-3.360213	4.227834
H	-8.391920	-2.857460	4.480683
H	-9.950928	-1.216709	5.552325
H	-10.771315	-0.977752	3.998007

C	-2.951723	-7.674520	-0.974553
C	-1.643797	-8.158875	-1.652687
C	-4.150033	-8.128159	-1.837822
H	-2.956020	-6.576529	-0.969401
C	-1.512380	-7.562844	-3.068343
H	-1.672322	-9.256092	-1.706991
H	-0.779648	-7.880225	-1.041978
C	-4.040556	-7.515981	-3.249744
H	-4.153599	-9.223077	-1.930692
H	-5.082944	-7.800695	-1.368186
C	-2.728489	-7.952496	-3.933913
H	-0.584952	-7.908731	-3.539259
H	-1.461377	-6.468204	-2.986947
H	-4.902662	-7.820733	-3.855943
H	-4.065658	-6.420990	-3.161388
H	-2.647338	-7.498955	-4.928398
H	-2.739636	-9.043397	-4.062128
C	-4.436578	-11.111858	2.402970
C	-3.774388	-12.390099	1.835935
C	-4.748449	-11.318473	3.897383
H	-5.401925	-10.984664	1.888650
C	-4.728527	-13.592958	2.001920
H	-2.838607	-12.574068	2.380592
H	-3.524971	-12.246373	0.777793
C	-5.722896	-12.500028	4.066117
H	-3.816267	-11.540881	4.437028
H	-5.184801	-10.405981	4.319134
C	-5.110445	-13.791669	3.484589
H	-4.266419	-14.503255	1.603419
H	-5.642550	-13.398007	1.422485
H	-5.971350	-12.637438	5.124465
H	-6.652577	-12.259812	3.531224
H	-5.814196	-14.625959	3.583822
H	-4.207127	-14.045891	4.055333
C	-1.703639	-7.118761	3.950604
C	-2.749015	-6.592785	4.962150
C	-0.649085	-7.978797	4.686981
H	-1.182665	-6.250864	3.527098
C	-2.062812	-5.775385	6.076320
H	-3.275324	-7.450844	5.403024
H	-3.487687	-5.975854	4.435960
C	0.042084	-7.156786	5.794100
H	-1.146044	-8.845258	5.142897
H	0.085396	-8.354869	3.965811
C	-0.999753	-6.626505	6.800892
H	-2.809704	-5.409100	6.789664
H	-1.576016	-4.899747	5.624824
H	0.789528	-7.771470	6.308137
H	0.564848	-6.306354	5.335768
H	-0.506752	-6.035106	7.580719
H	-1.493401	-7.478067	7.288091
C	-8.886188	-5.929231	4.271028
C	-8.898419	-6.226450	3.003536
C	-8.919881	-6.555182	1.731153
H	-7.971427	-5.603774	4.758674
H	-9.791481	-5.996239	4.868489

N	-9.245596	-5.597131	0.713756
S	-10.890953	-5.193409	0.603114
O	-11.375788	-5.040495	1.963497
O	-10.994433	-4.113930	-0.366822
H	-8.706892	-7.575664	1.416483
C	-5.852700	-7.733064	3.500470
C	-6.566561	-8.552090	2.618313
C	-6.178566	-7.818798	4.843950
H	-5.034959	-7.110065	3.145628
C	-7.578264	-9.443051	3.054411
C	-7.188221	-8.693507	5.302389
H	-5.638732	-7.206746	5.560950
C	-7.883528	-9.506787	4.424358
C	-8.053281	-10.141425	1.890914
C	-7.324762	-9.662796	0.823401
H	-5.829967	-8.129039	0.688827
H	-7.410461	-8.734732	6.364463
H	-8.645704	-10.191192	4.788005
N	-6.451648	-8.693064	1.262777
C	-9.092032	-11.219049	1.866037
H	-9.996960	-10.909628	2.401608
H	-9.381684	-11.469718	0.840854
H	-8.733329	-12.139920	2.342585
C	-7.291864	-10.125068	-0.598686
H	-6.721658	-11.058048	-0.689770
H	-8.299188	-10.311426	-0.985476
H	-6.813497	-9.375858	-1.234353
H	-1.697163	1.845968	5.680482
H	3.547200	-2.248613	-0.650819
C	-11.619922	-6.644447	-0.107865
C	-11.781695	-6.717560	-1.487802
C	-11.882339	-7.738491	0.715730
C	-12.226723	-7.911128	-2.047808
H	-11.555061	-5.851923	-2.103489
C	-12.314954	-8.923843	0.134831
H	-11.746436	-7.652514	1.789257
C	-12.494443	-9.026058	-1.249676
H	-12.360832	-7.980009	-3.123753
H	-12.521204	-9.785969	0.764055
C	-12.989800	-10.313305	-1.856465
H	-14.061822	-10.441212	-1.670703
H	-12.833922	-10.329431	-2.937805
H	-12.477322	-11.176447	-1.421546
C	-8.548797	-5.741217	-0.540520
C	-7.938003	-4.616307	-1.081900
C	-8.465981	-6.979448	-1.180879
C	-7.241180	-4.734684	-2.280125
H	-8.016797	-3.654620	-0.587097
C	-7.755661	-7.087064	-2.372412
H	-8.960428	-7.848108	-0.751383
C	-7.143120	-5.962995	-2.924169
H	-6.788552	-3.845424	-2.700791
H	-7.693593	-8.046102	-2.879679
H	-6.596126	-6.045690	-3.858298

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**TS1(R), E(PCM, mixed basis set, opt) = -5013.168780 - E(PCM, 6-31+G\*, single point) = -5023.821232**

C	-4.308082	-2.365904	0.727035
C	-3.031425	-2.321845	1.244016
C	-2.565643	-1.082258	1.788939
C	-3.374912	0.078335	1.662775
C	-4.620840	-0.010664	0.987802
C	-5.107613	-1.210192	0.533334
H	-0.716320	-1.851137	2.616236
C	-1.332393	-0.967041	2.485690
C	-2.916835	1.309943	2.201491
H	-5.201686	0.894541	0.830007
C	-1.717462	1.409518	2.862704
C	-0.929229	0.235444	3.003472
H	-3.549984	2.187835	2.088439
H	0.013049	0.298373	3.542502
C	-2.185641	-3.540153	1.164168
C	-0.919172	-3.515630	0.492380
C	-2.662761	-4.748581	1.631123
C	-0.413079	-2.364541	-0.174489
C	-0.134693	-4.699842	0.450537
C	-1.935116	-5.963307	1.502514
C	0.812481	-2.386789	-0.786210
H	-1.012974	-1.461945	-0.207583
C	1.139513	-4.679392	-0.176651
C	-0.670489	-5.903250	0.972917
C	1.629117	-3.550277	-0.783822
H	1.172110	-1.494871	-1.293921
H	1.724145	-5.597151	-0.181510
H	-0.083361	-6.815881	0.903517
C	-1.230667	2.711750	3.441660
H	-1.964648	3.509366	3.289156
H	-0.286743	3.020184	2.974236
C	2.976283	-3.522658	-1.455548
H	3.479171	-4.491364	-1.369662
H	3.623567	-2.759960	-1.004503
C	-6.379926	-1.324613	-0.230116
C	-7.622469	-1.189107	0.416116
C	-6.328632	-1.557361	-1.625787
C	-8.798486	-1.255886	-0.343734
C	-7.524960	-1.626578	-2.345332
C	-8.770290	-1.466167	-1.722639
H	-9.749502	-1.147758	0.160151
H	-7.492808	-1.790200	-3.420338
C	-2.579916	-7.256972	1.862206
C	-3.362636	-7.919882	0.880940
C	-2.450533	-7.795464	3.153138
C	-4.020782	-9.093635	1.242185
C	-3.171454	-8.953023	3.486720
C	-3.982046	-9.592708	2.553025
H	-4.642141	-9.609467	0.515087
H	-3.135579	-9.320682	4.505954
O	-3.867728	-4.789187	2.301084
O	-4.834226	-3.577512	0.316824
P	-5.292085	-4.575838	1.529472
O	-6.164532	-3.798269	2.509393

O	-5.813010	-5.827919	0.925231
H	-7.231937	-4.432572	3.016554
C	-4.995824	-1.699807	-2.354846
C	-4.811482	-3.119813	-2.935190
C	-4.835037	-0.647911	-3.475888
H	-4.181792	-1.532981	-1.640139
C	-3.428054	-3.264140	-3.599998
H	-5.593187	-3.300406	-3.688151
H	-4.924931	-3.851864	-2.128421
C	-3.445416	-0.784563	-4.134661
H	-5.613864	-0.801351	-4.234575
H	-4.966358	0.355971	-3.056068
C	-3.251172	-2.204874	-4.707839
H	-3.316634	-4.274319	-4.014028
H	-2.649321	-3.129785	-2.835897
H	-3.327281	-0.035726	-4.925892
H	-2.672394	-0.597181	-3.376634
H	-2.259743	-2.296512	-5.165823
H	-4.001079	-2.378255	-5.491884
C	-10.046694	-1.542223	-2.555207
C	-10.402077	-3.019809	-2.857924
C	-11.253412	-0.855871	-1.879870
H	-9.857102	-1.034811	-3.513863
C	-11.669112	-3.121743	-3.731984
H	-10.561284	-3.534379	-1.900274
H	-9.557902	-3.506353	-3.357867
C	-12.503037	-0.933876	-2.779628
H	-11.475394	-1.375666	-0.939660
H	-11.007197	0.187050	-1.646511
C	-12.858001	-2.408518	-3.056488
H	-11.908352	-4.175881	-3.916667
H	-11.477608	-2.647426	-4.704643
H	-13.343571	-0.424241	-2.295484
H	-12.304417	-0.425205	-3.732716
H	-13.754450	-2.477165	-3.683431
H	-13.073974	-2.902263	-2.098306
C	-7.708460	-0.957460	1.917151
C	-7.992134	0.528316	2.241399
C	-8.795994	-1.829126	2.573493
H	-6.751194	-1.239520	2.371520
C	-7.992162	0.748114	3.769703
H	-8.972404	0.797285	1.822582
H	-7.239262	1.167593	1.766182
C	-8.778912	-1.646694	4.100659
H	-9.788143	-1.554709	2.192917
H	-8.608598	-2.874026	2.311540
C	-9.030224	-0.165737	4.457179
H	-8.201372	1.799202	4.000471
H	-6.991961	0.509998	4.157218
H	-9.541647	-2.289224	4.554653
H	-7.797183	-1.959232	4.484195
H	-8.995268	-0.024184	5.543444
H	-10.035695	0.114992	4.115063
C	-3.469181	-7.354621	-0.534885
C	-2.247976	-7.787790	-1.385494
C	-4.754909	-7.757261	-1.290590

H	-3.473183	-6.257499	-0.466617
C	-2.271075	-7.079039	-2.755807
H	-2.291104	-8.877602	-1.520855
H	-1.320656	-7.551245	-0.857078
C	-4.803962	-7.041976	-2.657007
H	-4.768262	-8.843201	-1.457139
H	-5.631786	-7.466895	-0.703535
C	-3.573839	-7.403203	-3.514716
H	-1.400239	-7.375845	-3.351608
H	-2.210336	-5.994035	-2.589438
H	-5.727213	-7.306833	-3.185338
H	-4.819971	-5.958265	-2.480791
H	-3.603023	-6.858399	-4.466219
H	-3.597532	-8.477884	-3.741553
C	-4.895403	-10.757151	2.906871
C	-4.329530	-12.101450	2.388730
C	-5.210408	-10.880781	4.411484
H	-5.853349	-10.575716	2.393403
C	-5.357094	-13.231917	2.610311
H	-3.402590	-12.323544	2.934626
H	-4.080436	-12.015496	1.323925
C	-6.268314	-11.981922	4.625148
H	-4.295704	-11.154062	4.956974
H	-5.573073	-9.922360	4.799956
C	-5.745899	-13.336959	4.100588
H	-4.953507	-14.186914	2.254533
H	-6.257812	-13.007661	2.021788
H	-6.525696	-12.057567	5.687684
H	-7.179003	-11.699538	4.077284
H	-6.502368	-14.117927	4.238937
H	-4.858533	-13.622549	4.681608
C	-1.634375	-7.071452	4.214711
C	-2.569425	-6.230509	5.118804
C	-0.787489	-8.018097	5.095085
H	-0.943793	-6.380650	3.713591
C	-1.748090	-5.410997	6.133232
H	-3.239352	-6.921615	5.650562
H	-3.186448	-5.570283	4.498471
C	0.052939	-7.196156	6.095466
H	-1.450578	-8.686352	5.659820
H	-0.142215	-8.637943	4.462079
C	-0.862208	-6.335928	6.993201
H	-2.415250	-4.820354	6.771091
H	-1.106360	-4.709628	5.582080
H	0.668319	-7.863104	6.709782
H	0.729299	-6.535770	5.535503
H	-0.257959	-5.742396	7.688852
H	-1.505449	-6.998362	7.587899
C	-8.650445	-5.068085	4.722109
C	-8.316232	-5.046739	3.444725
C	-8.601245	-5.594421	2.198362
H	-8.097215	-4.482172	5.449046
H	-9.464111	-5.686359	5.091392
N	-9.442965	-5.177003	1.247526
S	-10.957147	-4.356082	1.552418
O	-10.993225	-4.061773	2.966040



O	-11.081087	-3.331987	0.536436
H	-7.853250	-6.283777	1.800904
C	-5.879307	-7.294345	4.033939
C	-6.799471	-8.000340	3.251641
C	-6.136350	-7.229349	5.392860
H	-4.993250	-6.851423	3.585092
C	-7.959760	-8.611394	3.784328
C	-7.275574	-7.843893	5.955046
H	-5.451452	-6.688370	6.038891
C	-8.186202	-8.532614	5.168245
C	-8.659555	-9.221628	2.682438
C	-7.904734	-8.975374	1.555861
H	-6.119622	-7.812021	1.279308
H	-7.437276	-7.776851	7.027001
H	-9.055094	-9.008784	5.616057
N	-6.795529	-8.239875	1.904819
C	-9.922173	-10.020225	2.782988
H	-10.392594	-10.157100	1.803972
H	-9.744098	-11.015791	3.207780
H	-10.650621	-9.521839	3.434232
C	-8.058463	-9.457396	0.149693
H	-9.097427	-9.719744	-0.067215
H	-7.744059	-8.690853	-0.565629
H	-7.443676	-10.349993	-0.022572
H	-1.047082	2.616038	4.519151
H	2.878001	-3.280735	-2.521368
C	-12.080353	-5.668833	1.186127
C	-12.825083	-5.621857	0.013666
C	-12.133812	-6.755797	2.056697
C	-13.657141	-6.696360	-0.283868
H	-12.738009	-4.767339	-0.650512
C	-12.963066	-7.820833	1.734253
H	-11.527551	-6.770263	2.959003
C	-13.736402	-7.804196	0.565153
H	-14.247452	-6.678546	-1.195338
H	-13.011968	-8.681201	2.395626
C	-14.654967	-8.952816	0.243652
H	-15.636768	-8.795129	0.703376
H	-14.805862	-9.051219	-0.834153
H	-14.258721	-9.896359	0.627230
C	-9.120156	-5.487317	-0.129240
C	-9.700247	-6.596854	-0.739734
C	-9.329626	-6.916717	-2.042504
C	-8.371180	-6.148005	-2.698958
C	-7.792851	-5.049735	-2.065725
C	-8.172090	-4.697046	-0.774347
H	-10.403724	-7.215272	-0.189776
H	-9.770768	-7.780537	-2.529750
H	-8.071867	-6.406399	-3.710207
H	-7.051975	-4.447450	-2.577260
H	-7.738276	-3.828428	-0.279538

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**I2(R), E(PCM, mixed basis set, opt) = -5013.228087 - E(PCM, 6-31+G\*, single point) = -5023.877326**

C	-4.526294	-2.290792	0.753310
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C	-3.272850	-2.353722	1.322981
C	-2.743485	-1.182410	1.949584
C	-3.443707	0.044899	1.820568
C	-4.637269	0.075953	1.059209
C	-5.202268	-1.062691	0.534961
H	-1.012650	-2.134369	2.843590
C	-1.545421	-1.197529	2.713839
C	-2.920403	1.216413	2.429898
H	-5.128298	1.030821	0.885702
C	-1.758975	1.190089	3.161325
C	-1.078544	-0.051448	3.300810
H	-3.469133	2.148422	2.311596
H	-0.167848	-0.084546	3.893605
C	-2.474761	-3.592488	1.175783
C	-1.208538	-3.564746	0.506009
C	-2.996287	-4.802785	1.572476
C	-0.664330	-2.393079	-0.091684
C	-0.471757	-4.772570	0.388134
C	-2.306452	-6.032157	1.401123
C	0.554161	-2.427307	-0.716359
H	-1.227707	-1.467193	-0.065394
C	0.799011	-4.764406	-0.246945
C	-1.043818	-5.977746	0.860549
C	1.325116	-3.620221	-0.791678
H	0.945698	-1.521343	-1.172435
H	1.348408	-5.701383	-0.309460
H	-0.478074	-6.900931	0.764905
C	-1.201493	2.423773	3.820024
H	-1.810681	3.303535	3.590042
H	-0.175687	2.617203	3.482113
C	2.665150	-3.603632	-1.476989
H	3.148937	-4.583991	-1.420604
H	3.331672	-2.864427	-1.015579
C	-6.415114	-0.980386	-0.316710
C	-7.627194	-0.497428	0.214219
C	-6.322173	-1.302620	-1.695102
C	-8.739624	-0.376112	-0.629423
C	-7.444332	-1.124397	-2.506145
C	-8.668155	-0.674214	-1.989472
H	-9.674139	-0.032367	-0.202671
H	-7.368063	-1.335586	-3.570933
C	-2.914772	-7.333505	1.786374
C	-3.691163	-8.052351	0.842470
C	-2.703222	-7.847141	3.078592
C	-4.315847	-9.225782	1.260237
C	-3.363698	-9.022756	3.459482
C	-4.201411	-9.699401	2.574976
H	-4.948441	-9.772436	0.566706
H	-3.253976	-9.381753	4.475666
O	-4.251025	-4.789273	2.197288
O	-5.106967	-3.451904	0.237607
P	-5.537672	-4.648212	1.229004
O	-6.648153	-4.013896	2.175072
O	-5.912697	-5.890403	0.541616
H	-8.216514	-3.260261	4.128530
C	-5.013803	-1.776809	-2.324724

C	-5.140924	-3.177462	-2.967597
C	-4.490661	-0.764579	-3.371421
H	-4.244510	-1.850311	-1.549098
C	-3.772430	-3.642975	-3.504048
H	-5.856786	-3.127686	-3.800728
H	-5.524888	-3.888929	-2.228750
C	-3.120621	-1.225701	-3.914426
H	-5.209078	-0.696141	-4.199480
H	-4.407981	0.227660	-2.912287
C	-3.225201	-2.634820	-4.535875
H	-3.866147	-4.639724	-3.953848
H	-3.069432	-3.722755	-2.661516
H	-2.747881	-0.509962	-4.655859
H	-2.400673	-1.255128	-3.084457
H	-2.244841	-2.960303	-4.901543
H	-3.908759	-2.596941	-5.394978
C	-9.877138	-0.551330	-2.913140
C	-10.338442	-1.960307	-3.366517
C	-11.069821	0.182666	-2.265314
H	-9.570605	0.013296	-3.807079
C	-11.532148	-1.871699	-4.339369
H	-10.616902	-2.535217	-2.472217
H	-9.505644	-2.482222	-3.851086
C	-12.249512	0.292804	-3.252363
H	-11.401726	-0.389670	-1.387887
H	-10.759048	1.178216	-1.926216
C	-12.707738	-1.111852	-3.693973
H	-11.845057	-2.879021	-4.636126
H	-11.216387	-1.336643	-5.245906
H	-13.078505	0.831504	-2.779827
H	-11.935002	0.866340	-4.134887
H	-13.544288	-1.036569	-4.397678
H	-13.053807	-1.668259	-2.812712
C	-7.780594	-0.100282	1.677022
C	-8.110960	1.404799	1.815876
C	-8.862035	-0.948654	2.374930
H	-6.838046	-0.287347	2.202343
C	-8.237915	1.794972	3.303184
H	-9.060977	1.610874	1.304486
H	-7.332495	2.002920	1.325636
C	-8.990887	-0.560010	3.859662
H	-9.831413	-0.816803	1.876363
H	-8.585939	-2.000329	2.276907
C	-9.319989	0.941013	3.997837
H	-8.478928	2.860656	3.391390
H	-7.272792	1.627166	3.800946
H	-9.768733	-1.173650	4.327861
H	-8.038369	-0.764313	4.370439
H	-9.398759	1.218491	5.055236
H	-10.291405	1.137266	3.524051
C	-3.798483	-7.574412	-0.602692
C	-2.574512	-8.046720	-1.428456
C	-5.075564	-8.039345	-1.336908
H	-3.809179	-6.477202	-0.604965
C	-2.604776	-7.396235	-2.828459
H	-2.612813	-9.141507	-1.514218

H	-1.646713	-7.782222	-0.913432
C	-5.146519	-7.366257	-2.722259
H	-5.051407	-9.130134	-1.470938
H	-5.961485	-7.767338	-0.755380
C	-3.912677	-7.741369	-3.571132
H	-1.739188	-7.720868	-3.417528
H	-2.537257	-6.306346	-2.705104
H	-6.065279	-7.665898	-3.240817
H	-5.186823	-6.276699	-2.579658
H	-3.945299	-7.221902	-4.536675
H	-3.934648	-8.821436	-3.770547
C	-5.056149	-10.887243	2.990768
C	-4.591555	-12.197810	2.310294
C	-5.127293	-11.101446	4.514386
H	-6.080202	-10.678166	2.643006
C	-5.586468	-13.335159	2.624693
H	-3.593456	-12.457000	2.688850
H	-4.512966	-12.051647	1.226305
C	-6.132712	-12.223812	4.838952
H	-4.134031	-11.390081	4.888581
H	-5.427945	-10.170444	5.008729
C	-5.718288	-13.540356	4.148627
H	-5.265546	-14.265670	2.142373
H	-6.570586	-13.063716	2.215492
H	-6.204140	-12.366099	5.923445
H	-7.122671	-11.915702	4.474709
H	-6.449654	-14.328996	4.360589
H	-4.748724	-13.865244	4.550030
C	-1.833777	-7.089510	4.074939
C	-2.716187	-6.187552	4.969718
C	-0.966585	-8.005838	4.967732
H	-1.149443	-6.439691	3.515168
C	-1.845924	-5.330973	5.909598
H	-3.367490	-6.841702	5.563563
H	-3.354977	-5.551108	4.345907
C	-0.078759	-7.148614	5.896001
H	-1.613362	-8.639862	5.587693
H	-0.351159	-8.660834	4.340254
C	-0.948511	-6.232421	6.782267
H	-2.480881	-4.699202	6.540810
H	-1.212115	-4.669384	5.302710
H	0.548168	-7.795706	6.519662
H	0.586424	-6.526943	5.281431
H	-0.313152	-5.620554	7.432547
H	-1.584935	-6.856694	7.423917
C	-8.409067	-5.234698	4.864169
C	-8.202765	-4.325848	3.917713
C	-7.894187	-4.706565	2.501089
H	-8.605843	-4.935931	5.889080
H	-8.400225	-6.301256	4.655402
N	-8.882601	-4.295400	1.502551
S	-10.507691	-3.960270	1.818666
O	-10.620677	-3.421011	3.161913
O	-10.980897	-3.193867	0.678091
H	-7.709586	-5.783579	2.417467
C	-6.041787	-7.425838	4.048231

C	-6.976592	-8.202207	3.356659
C	-6.088516	-7.470028	5.433509
H	-5.301948	-6.832033	3.514246
C	-7.899415	-9.050993	4.017133
C	-7.025687	-8.273607	6.114722
H	-5.401975	-6.858657	6.009133
C	-7.922376	-9.071691	5.421700
C	-8.639382	-9.745989	3.000019
C	-8.175072	-9.280622	1.791670
H	-6.644542	-7.854591	1.296810
H	-7.033761	-8.272375	7.200487
H	-8.624742	-9.709551	5.952638
N	-7.188117	-8.339003	2.007442
C	-9.670773	-10.804895	3.234488
H	-10.113572	-11.149974	2.295792
H	-9.237018	-11.677683	3.737898
H	-10.487934	-10.446469	3.872154
C	-8.602035	-9.641434	0.405495
H	-9.470199	-9.050309	0.083941
H	-7.789951	-9.467744	-0.308335
H	-8.879917	-10.697353	0.349881
H	-1.170024	2.303315	4.910192
H	2.559238	-3.333562	-2.535309
C	-11.273422	-5.560867	1.757630
C	-11.870951	-5.983047	0.573875
C	-11.109315	-6.421283	2.838897
C	-12.310269	-7.298583	0.479135
H	-11.970043	-5.290739	-0.255694
C	-11.544506	-7.736323	2.720595
H	-10.650103	-6.063366	3.755250
C	-12.142387	-8.194001	1.541227
H	-12.782490	-7.640526	-0.438023
H	-11.422323	-8.415144	3.559291
C	-12.587682	-9.626432	1.402680
H	-13.559465	-9.689904	0.904805
H	-11.872392	-10.195995	0.797658
H	-12.664475	-10.116223	2.376563
C	-8.669966	-4.803739	0.167711
C	-8.781223	-6.170550	-0.098657
C	-8.556507	-6.633901	-1.389315
C	-8.235279	-5.734641	-2.405661
C	-8.138795	-4.375827	-2.128898
C	-8.351866	-3.899964	-0.837129
H	-9.031699	-6.856504	0.708525
H	-8.637006	-7.693492	-1.610387
H	-8.062132	-6.097600	-3.414381
H	-7.893087	-3.671261	-2.913382
H	-8.289483	-2.843284	-0.602030

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**TS2(R), E(PCM, mixed basis set, opt) = -5013.184586 - E(PCM, 6-31+G\*, single point) = -5023.841507**

C	-4.135153	-2.455102	0.355699
C	-2.832683	-2.459000	0.825764
C	-2.289091	-1.242636	1.352395
C	-3.042435	-0.042431	1.253250

C	-4.328193	-0.081028	0.660253
C	-4.895729	-1.258573	0.241146
H	-0.454416	-2.092557	2.137559
C	-1.029593	-1.181275	2.011876
C	-2.503529	1.170898	1.758890
H	-4.881804	0.847161	0.542833
C	-1.277749	1.217000	2.373996
C	-0.548349	0.003515	2.502724
H	-3.098068	2.077342	1.660973
H	0.412435	0.021436	3.012009
C	-2.048681	-3.721137	0.789490
C	-0.769425	-3.814843	0.153267
C	-2.603524	-4.862805	1.334762
C	-0.171862	-2.742560	-0.566967
C	-0.064257	-5.048217	0.207854
C	-1.947431	-6.122246	1.331868
C	1.059546	-2.885499	-1.150565
H	-0.707303	-1.803834	-0.661300
C	1.216990	-5.153795	-0.398323
C	-0.674936	-6.173346	0.813719
C	1.791075	-4.101533	-1.065911
H	1.491531	-2.052392	-1.700323
H	1.736929	-6.108002	-0.334775
H	-0.144931	-7.123678	0.810386
C	-0.704311	2.497155	2.922403
H	-1.371627	3.343156	2.728298
H	0.270104	2.715912	2.467290
C	3.145200	-4.207981	-1.716386
H	3.569015	-5.208796	-1.584683
H	3.845527	-3.480608	-1.286514
C	-6.246787	-1.270746	-0.387436
C	-7.408555	-1.301229	0.415797
C	-6.356209	-1.197463	-1.794351
C	-8.662513	-1.247691	-0.205192
C	-7.628795	-1.163905	-2.372904
C	-8.790025	-1.181379	-1.594697
H	-9.550680	-1.270051	0.413061
H	-7.726190	-1.121976	-3.454452
C	-2.630002	-7.367608	1.774043
C	-2.818990	-8.406659	0.825117
C	-3.053843	-7.558366	3.104020
C	-3.330621	-9.631826	1.253857
C	-3.600980	-8.793019	3.480487
C	-3.715512	-9.851176	2.581933
H	-3.461431	-10.431028	0.527644
H	-3.930498	-8.917835	4.504679
O	-3.816261	-4.768541	1.957379
O	-4.707981	-3.624167	-0.086790
P	-5.192791	-4.727079	1.057296
O	-6.238482	-4.161099	1.957242
O	-5.419284	-6.016911	0.335173
H	-11.182805	-6.684003	3.311374
C	-5.115919	-1.216379	-2.682451
C	-4.896802	-2.635229	-3.267359
C	-5.179249	-0.185285	-3.833618
H	-4.239769	-0.970095	-2.069790

C	-3.610084	-2.686065	-4.115383
H	-5.765852	-2.887496	-3.894217
H	-4.835110	-3.362950	-2.450760
C	-3.879275	-0.227654	-4.663795
H	-6.023793	-0.422313	-4.493513
H	-5.343121	0.816987	-3.420886
C	-3.659797	-1.639151	-5.247407
H	-3.474348	-3.691544	-4.529868
H	-2.750198	-2.475739	-3.464364
H	-3.924865	0.514278	-5.469439
H	-3.029971	0.030239	-4.016921
H	-2.735254	-1.667562	-5.835054
H	-4.494135	-1.879412	-5.920848
C	-10.149645	-1.203060	-2.281061
C	-10.535348	-2.672533	-2.586504
C	-11.269203	-0.528193	-1.460838
H	-10.061370	-0.667718	-3.238780
C	-11.905751	-2.771622	-3.288550
H	-10.552501	-3.216515	-1.633034
H	-9.756157	-3.127706	-3.207221
C	-12.607498	-0.586150	-2.225094
H	-11.391166	-1.061694	-0.509767
H	-10.991983	0.508629	-1.236982
C	-13.004006	-2.055550	-2.474966
H	-12.167884	-3.826947	-3.448328
H	-11.836478	-2.299522	-4.278475
H	-13.390542	-0.074390	-1.654468
H	-12.501939	-0.069745	-3.189000
H	-13.964124	-2.110972	-3.001515
H	-13.123181	-2.551333	-1.501872
C	-7.303639	-1.319044	1.937247
C	-7.347688	0.126507	2.493252
C	-8.401978	-2.148874	2.638152
H	-6.345573	-1.775849	2.209266
C	-7.099865	0.122360	4.016613
H	-8.335353	0.556623	2.272826
H	-6.592877	0.741254	1.991620
C	-8.132135	-2.190329	4.155210
H	-9.391736	-1.706410	2.462222
H	-8.396921	-3.168036	2.243992
C	-8.137363	-0.762557	4.739803
H	-7.135270	1.145630	4.408482
H	-6.094164	-0.277422	4.204705
H	-8.891535	-2.810375	4.648821
H	-7.150492	-2.657045	4.318936
H	-7.926165	-0.788300	5.815145
H	-9.136493	-0.325736	4.603381
C	-2.558883	-8.212120	-0.665828
C	-1.492845	-9.192394	-1.204862
C	-3.872645	-8.357799	-1.472395
H	-2.197086	-7.193354	-0.836415
C	-1.232008	-8.935561	-2.703772
H	-1.850221	-10.222515	-1.069211
H	-0.564139	-9.083470	-0.630918
C	-3.608934	-8.093660	-2.968932
H	-4.263848	-9.378506	-1.349813

H	-4.605173	-7.648108	-1.071552
C	-2.540116	-9.064281	-3.513111
H	-0.481034	-9.638432	-3.082910
H	-0.833098	-7.919162	-2.825367
H	-4.540487	-8.194677	-3.538226
H	-3.254432	-7.061013	-3.089408
H	-2.347903	-8.866522	-4.574045
H	-2.914704	-10.093634	-3.425343
C	-4.225587	-11.229281	2.991510
C	-3.110540	-12.285963	2.773432
C	-4.697969	-11.295312	4.457710
H	-5.077977	-11.488972	2.342606
C	-3.600958	-13.702485	3.135794
H	-2.258267	-12.014327	3.410679
H	-2.769140	-12.257799	1.732671
C	-5.199453	-12.709108	4.817733
H	-3.848390	-11.048031	5.109931
H	-5.481484	-10.547345	4.628783
C	-4.082398	-13.749369	4.599920
H	-2.798249	-14.430687	2.974377
H	-4.437534	-13.972899	2.476638
H	-5.542233	-12.728832	5.858935
H	-6.053965	-12.968044	4.178476
H	-4.441496	-14.753655	4.851700
H	-3.238693	-13.516169	5.263156
C	-2.938081	-6.478819	4.171030
C	-4.339823	-6.067318	4.681348
C	-2.064981	-6.939320	5.362432
H	-2.464431	-5.590798	3.739615
C	-4.227552	-4.938375	5.723942
H	-4.833767	-6.937567	5.136759
H	-4.951085	-5.736759	3.837352
C	-1.943803	-5.806590	6.403933
H	-2.531196	-7.813613	5.836053
H	-1.074088	-7.239349	5.001289
C	-3.339196	-5.377986	6.906754
H	-5.229470	-4.664354	6.075697
H	-3.786080	-4.055524	5.241452
H	-1.320166	-6.132248	7.244831
H	-1.451523	-4.943697	5.935407
H	-3.243968	-4.566554	7.637732
H	-3.814786	-6.230602	7.410690
C	-10.581525	-8.685500	2.904093
C	-10.671903	-7.367946	2.647189
C	-9.981380	-6.899087	1.482855
H	-11.051959	-9.120972	3.779467
H	-10.037230	-9.353772	2.244690
N	-10.055471	-5.722774	0.915923
S	-11.194718	-4.444950	1.490352
O	-11.139352	-4.467268	2.933763
O	-10.829741	-3.293305	0.705955
H	-9.324220	-7.602856	0.973083
C	-7.706601	-5.883464	4.164317
C	-7.514648	-7.120362	3.535603
C	-8.225211	-5.903661	5.449924
H	-7.435807	-4.962785	3.653065



C	-7.842786	-8.347185	4.158796
C	-8.547840	-7.115113	6.096566
H	-8.380500	-4.962654	5.970073
C	-8.363748	-8.333274	5.463161
C	-7.590826	-9.394303	3.199761
C	-7.109243	-8.773826	2.067101
H	-6.586513	-6.778996	1.613601
H	-8.944865	-7.087861	7.107112
H	-8.623075	-9.262931	5.964600
N	-7.086040	-7.409140	2.256712
C	-7.876281	-10.850639	3.406096
H	-7.287279	-11.480812	2.732881
H	-7.633893	-11.155716	4.429553
H	-8.934489	-11.102144	3.245881
C	-6.632292	-9.329503	0.766974
H	-7.164756	-8.882446	-0.081920
H	-5.569790	-9.100781	0.642468
H	-6.764802	-10.413970	0.731403
H	-0.550356	2.424091	4.006593
H	3.080162	-4.002311	-2.792345
C	-12.708576	-5.114898	0.897565
C	-12.941401	-5.072356	-0.478291
C	-13.624347	-5.662048	1.790599
C	-14.127959	-5.603842	-0.960994
H	-12.212214	-4.626480	-1.150465
C	-14.808846	-6.182566	1.280456
H	-13.423522	-5.658795	2.856918
C	-15.075598	-6.162760	-0.092283
H	-14.328185	-5.575761	-2.028466
H	-15.540913	-6.605614	1.961563
C	-16.373409	-6.701866	-0.630309
H	-16.229257	-7.179532	-1.602659
H	-16.815520	-7.428860	0.054470
H	-17.094141	-5.888099	-0.765591
C	-9.357686	-5.478439	-0.327751
C	-9.744968	-6.201146	-1.458172
C	-9.034393	-6.012484	-2.637896
C	-7.969511	-5.110026	-2.673081
C	-7.616610	-4.386588	-1.538549
C	-8.315575	-4.563705	-0.347936
H	-10.579117	-6.896241	-1.402836
H	-9.309765	-6.572856	-3.525202
H	-7.412031	-4.969208	-3.594198
H	-6.800234	-3.673660	-1.551912
H	-8.006967	-4.038132	0.549312

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**I3(R), E(PCM, mixed basis set, opt) = -5013.231070 - E(PCM, 6-31+G\*, single point) = -5023.884513**

C	-4.182353	-2.642055	0.024464
C	-2.816997	-2.768243	0.220976
C	-2.054930	-1.612335	0.592220
C	-2.689240	-0.343529	0.623494
C	-4.072259	-0.264124	0.340158
C	-4.833223	-1.377126	0.072990
H	-0.182479	-2.632592	1.014332

C	-0.684446	-1.672441	0.975156
C	-1.942321	0.815027	0.967803
H	-4.559357	0.708512	0.355710
C	-0.614187	0.743742	1.302952
C	0.002196	-0.537135	1.314730
H	-2.456182	1.774279	0.972434
H	1.045702	-0.612764	1.611328
C	-2.168363	-4.100524	0.140584
C	-1.018495	-4.363566	-0.671687
C	-2.681844	-5.125861	0.903229
C	-0.502769	-3.429297	-1.611372
C	-0.370904	-5.623404	-0.560735
C	-2.061722	-6.396042	1.015485
C	0.600791	-3.729299	-2.365958
H	-1.002493	-2.473811	-1.734559
C	0.780369	-5.891933	-1.348273
C	-0.899430	-6.604853	0.316104
C	1.276015	-4.974145	-2.240450
H	0.972334	-3.003111	-3.084975
H	1.262507	-6.861541	-1.238885
H	-0.389023	-7.561058	0.403757
C	0.187806	1.964926	1.668333
H	-0.438620	2.862584	1.669810
H	1.007616	2.120856	0.955680
C	2.488049	-5.256181	-3.088469
H	2.908217	-6.241595	-2.862529
H	3.267808	-4.502798	-2.920805
C	-6.294582	-1.210219	-0.170047
C	-7.209984	-1.400129	0.886267
C	-6.745240	-0.768377	-1.436465
C	-8.571704	-1.163159	0.655906
C	-8.108719	-0.530567	-1.618138
C	-9.032887	-0.718152	-0.583605
H	-9.276323	-1.325462	1.461871
H	-8.472297	-0.185256	-2.581174
C	-2.680362	-7.450509	1.859137
C	-3.190845	-8.620587	1.253804
C	-2.736616	-7.299436	3.263580
C	-3.728541	-9.622746	2.068950
C	-3.266019	-8.335566	4.041048
C	-3.758845	-9.507231	3.459876
H	-4.099735	-10.538340	1.614733
H	-3.281522	-8.225984	5.120898
O	-3.829849	-4.904915	1.629019
O	-4.938328	-3.748110	-0.312342
P	-5.231446	-4.962023	0.762818
O	-6.331711	-4.675780	1.712918
O	-5.270038	-6.251387	-0.031747
H	-10.014745	-7.160268	2.740322
C	-5.757269	-0.626874	-2.589846
C	-5.511095	-2.012659	-3.237885
C	-6.194397	0.369195	-3.684648
H	-4.799679	-0.271741	-2.187423
C	-4.425675	-1.922437	-4.329125
H	-6.458504	-2.347164	-3.684339
H	-5.225728	-2.744666	-2.473664

C	-5.091058	0.487821	-4.757331
H	-7.111208	0.006397	-4.168246
H	-6.408591	1.347469	-3.237764
C	-4.819160	-0.887180	-5.403345
H	-4.269596	-2.906324	-4.785711
H	-3.479476	-1.616475	-3.860911
H	-5.387732	1.213810	-5.523169
H	-4.168677	0.853611	-4.286073
H	-4.029063	-0.801178	-6.158121
H	-5.732475	-1.227746	-5.910503
C	-10.506128	-0.448497	-0.859158
C	-11.125260	-1.637073	-1.638232
C	-11.339313	-0.184498	0.411433
H	-10.568507	0.445935	-1.499009
C	-12.595557	-1.335067	-2.002133
H	-11.063557	-2.529921	-1.000619
H	-10.537268	-1.832282	-2.542399
C	-12.796837	0.153146	0.035820
H	-11.344903	-1.090222	1.030124
H	-10.887826	0.629928	0.991035
C	-13.423920	-1.026340	-0.736471
H	-13.032031	-2.178877	-2.553873
H	-12.626784	-0.461083	-2.668300
H	-13.378093	0.363374	0.940621
H	-12.814407	1.053964	-0.593048
H	-14.462359	-0.799266	-1.005952
H	-13.424978	-1.904375	-0.077784
C	-6.706129	-1.772336	2.275519
C	-6.261491	-0.510585	3.057370
C	-7.723018	-2.548363	3.138812
H	-5.835698	-2.427043	2.159207
C	-5.572712	-0.932728	4.373493
H	-7.149451	0.100248	3.272873
H	-5.575127	0.089646	2.451486
C	-7.028830	-3.016106	4.434482
H	-8.569440	-1.897983	3.399987
H	-8.093863	-3.412059	2.582947
C	-6.513845	-1.801267	5.236066
H	-5.254487	-0.047342	4.936737
H	-4.674614	-1.515358	4.124224
H	-7.722578	-3.607470	5.043896
H	-6.187912	-3.664631	4.152598
H	-5.991206	-2.133106	6.141856
H	-7.373530	-1.192398	5.548435
C	-3.093286	-8.866447	-0.247831
C	-2.025506	-9.952772	-0.529171
C	-4.442525	-9.278764	-0.869512
H	-2.788571	-7.938844	-0.743325
C	-1.875638	-10.198627	-2.043032
H	-2.333136	-10.885059	-0.034470
H	-1.066892	-9.648956	-0.092099
C	-4.294693	-9.539537	-2.382647
H	-4.819664	-10.188209	-0.379124
H	-5.142789	-8.458529	-0.702649
C	-3.228618	-10.621132	-2.652372
H	-1.117665	-10.968752	-2.225952

H	-1.537494	-9.270565	-2.524428
H	-5.260149	-9.841317	-2.808358
H	-3.992269	-8.604647	-2.872698
H	-3.124147	-10.790132	-3.730102
H	-3.548459	-11.566744	-2.192473
C	-4.204991	-10.696549	4.294441
C	-2.963214	-11.528501	4.704152
C	-5.007575	-10.305802	5.549396
H	-4.846497	-11.335161	3.667977
C	-3.378319	-12.782081	5.501548
H	-2.317343	-10.891672	5.324078
H	-2.397392	-11.807466	3.807791
C	-5.434103	-11.562579	6.335959
H	-4.384111	-9.678108	6.200032
H	-5.880425	-9.719723	5.253596
C	-4.194708	-12.383984	6.748690
H	-2.490164	-13.353835	5.792888
H	-3.996428	-13.425940	4.860896
H	-6.012401	-11.273540	7.220825
H	-6.080938	-12.183665	5.700499
H	-4.495919	-13.277161	7.307472
H	-3.564568	-11.771164	7.407185
C	-2.158219	-6.071399	3.963833
C	-3.213920	-5.318457	4.807920
C	-0.960331	-6.484301	4.855173
H	-1.781544	-5.370496	3.210883
C	-2.585489	-4.095310	5.506772
H	-3.624652	-6.002334	5.564193
H	-4.027793	-4.983812	4.156325
C	-0.338577	-5.255140	5.548170
H	-1.312002	-7.190606	5.619037
H	-0.213978	-7.000161	4.239607
C	-1.399391	-4.521389	6.394887
H	-3.346879	-3.576451	6.101336
H	-2.229341	-3.394419	4.739344
H	0.505010	-5.564778	6.175482
H	0.046562	-4.567278	4.783548
H	-0.956007	-3.646861	6.884019
H	-1.762880	-5.198995	7.179681
C	-9.821948	-9.221700	1.908077
C	-10.144386	-7.757749	1.841386
C	-10.466729	-7.147311	0.703605
H	-10.318956	-9.704091	2.758228
H	-10.156791	-9.740172	1.002021
N	-10.621560	-5.739826	0.600696
S	-11.945670	-4.992646	1.303821
O	-12.132257	-5.602230	2.609814
O	-11.720643	-3.563855	1.155236
H	-10.581723	-7.694545	-0.233291
C	-6.125033	-6.940005	3.729526
C	-6.785231	-7.803017	2.875109
C	-6.525267	-6.965567	5.064842
H	-5.369083	-6.259518	3.362709
C	-7.768486	-8.694287	3.293699
C	-7.533590	-7.827344	5.504259
H	-6.054658	-6.286013	5.768208

C	-8.159489	-8.714580	4.624077
C	-8.296437	-9.428098	2.083840
C	-7.524977	-8.731299	0.975582
H	-6.043917	-7.232227	0.847460
H	-7.832723	-7.811376	6.547379
H	-8.941105	-9.384117	4.972845
N	-6.677700	-7.884899	1.457821
C	-7.924278	-10.921170	2.099337
H	-8.260998	-11.416887	1.183044
H	-6.840759	-11.046923	2.197606
H	-8.406008	-11.405325	2.953718
C	-7.700762	-8.979050	-0.478347
H	-8.755000	-9.154780	-0.703830
H	-7.336388	-8.129687	-1.060867
H	-7.142216	-9.875658	-0.771831
H	0.635371	1.855699	2.664176
H	2.232507	-5.230197	-4.155628
C	-13.341278	-5.436344	0.304041
C	-13.639243	-4.675800	-0.823279
C	-14.078140	-6.571433	0.629983
C	-14.704028	-5.059945	-1.629957
H	-13.038094	-3.803716	-1.060163
C	-15.139330	-6.939826	-0.189655
H	-13.829995	-7.138557	1.520870
C	-15.469323	-6.190782	-1.324156
H	-14.948230	-4.469137	-2.508831
H	-15.727801	-7.818776	0.058986
C	-16.646832	-6.576909	-2.180868
H	-16.792510	-7.660305	-2.189414
H	-17.566583	-6.123216	-1.795295
H	-16.516836	-6.236065	-3.211050
C	-10.022143	-5.134475	-0.562274
C	-10.545874	-5.363506	-1.835866
C	-9.904821	-4.816909	-2.943715
C	-8.750448	-4.053831	-2.772136
C	-8.232028	-3.835361	-1.497755
C	-8.868161	-4.379373	-0.385267
H	-11.440943	-5.968829	-1.953961
H	-10.306399	-4.987244	-3.938097
H	-8.253333	-3.625049	-3.637369
H	-7.340446	-3.233862	-1.351151
H	-8.456438	-4.235153	0.608919

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**TS3(R), E(PCM, mixed basis set, opt) = -5013.230975 - E(PCM, 6-31+G\*, single point) = -5023.884434**

C	-4.178886	-2.641489	0.012863
C	-2.813819	-2.769014	0.210531
C	-2.050901	-1.613922	0.582661
C	-2.684407	-0.344624	0.614483
C	-4.067883	-0.264629	0.334142
C	-4.829605	-1.376792	0.066534
H	-0.179018	-2.635165	1.005477
C	-0.680290	-1.674782	0.965549
C	-1.936253	0.813791	0.957470
H	-4.554815	0.708049	0.353121

C	-0.607589	0.741858	1.291030
C	0.007702	-0.539659	1.303534
H	-2.449480	1.773419	0.962080
H	1.051430	-0.615941	1.599317
C	-2.166768	-4.102271	0.133491
C	-1.015496	-4.368792	-0.675537
C	-2.683359	-5.125344	0.897080
C	-0.498084	-3.437793	-1.617579
C	-0.368697	-5.628549	-0.559428
C	-2.063949	-6.395746	1.014769
C	0.606797	-3.740394	-2.369320
H	-0.997680	-2.482757	-1.744627
C	0.783804	-5.899890	-1.344278
C	-0.899557	-6.607049	0.319403
C	1.281334	-4.985049	-2.238529
H	0.979560	-3.016718	-3.090240
H	1.265243	-6.869445	-1.231418
H	-0.390190	-7.563456	0.410907
C	0.195941	1.962775	1.653717
H	-0.430488	2.860492	1.658154
H	1.012636	2.118988	0.937539
C	2.494601	-5.270413	-3.083702
H	2.913466	-6.255599	-2.854268
H	3.274839	-4.517333	-2.916860
C	-6.291955	-1.208089	-0.169548
C	-7.203539	-1.401523	0.889746
C	-6.747555	-0.762492	-1.432773
C	-8.566460	-1.164277	0.664720
C	-8.111661	-0.524940	-1.609253
C	-9.032205	-0.716174	-0.572320
H	-9.268757	-1.329188	1.472543
H	-8.478627	-0.176479	-2.570009
C	-2.685598	-7.448261	1.859116
C	-3.190308	-8.622367	1.256082
C	-2.750988	-7.291129	3.262498
C	-3.731954	-9.621219	2.072509
C	-3.283754	-8.324462	4.041488
C	-3.771334	-9.499365	3.462794
H	-4.098170	-10.539889	1.620225
H	-3.306388	-8.209273	5.120573
O	-3.834847	-4.902240	1.617028
O	-4.934556	-3.745925	-0.329221
P	-5.230107	-4.964763	0.739270
O	-6.339067	-4.684154	1.681030
O	-5.257196	-6.253004	-0.056632
H	-10.037647	-7.176679	2.737310
C	-5.763229	-0.616901	-2.589025
C	-5.520596	-2.000817	-3.242723
C	-6.203003	0.383246	-3.679390
H	-4.804159	-0.263823	-2.188671
C	-4.438291	-1.908131	-4.336720
H	-6.469705	-2.332300	-3.687738
H	-5.234154	-2.736242	-2.482508
C	-5.102927	0.504293	-4.755118
H	-7.121743	0.022818	-4.161225
H	-6.414871	1.360430	-3.229047

C	-4.834070	-0.868871	-5.406416
H	-4.284486	-2.890610	-4.797058
H	-3.490378	-1.604668	-3.870304
H	-5.401569	1.232863	-5.517773
H	-4.178821	0.868104	-4.285702
H	-4.046118	-0.780800	-6.163155
H	-5.749145	-1.207049	-5.912022
C	-10.506202	-0.446233	-0.843043
C	-11.128193	-1.633917	-1.621191
C	-11.335226	-0.182451	0.430084
H	-10.569916	0.448658	-1.482158
C	-12.599141	-1.330434	-1.980563
H	-11.066054	-2.527346	-0.984231
H	-10.542752	-1.828935	-2.527027
C	-12.793947	0.155271	0.059197
H	-11.338648	-1.088167	1.048823
H	-10.882043	0.632120	1.008170
C	-13.423499	-1.023445	-0.712183
H	-13.037677	-2.172930	-2.532823
H	-12.631473	-0.455216	-2.645030
H	-13.372478	0.364763	0.965972
H	-12.813166	1.056558	-0.568931
H	-14.462774	-0.796142	-0.978246
H	-13.422364	-1.902255	-0.054478
C	-6.695216	-1.777876	2.276398
C	-6.245080	-0.519281	3.060354
C	-7.709557	-2.555056	3.141949
H	-5.826337	-2.433466	2.155080
C	-5.551638	-0.946929	4.372336
H	-7.130959	0.092471	3.281502
H	-5.560144	0.081804	2.453713
C	-7.009481	-3.028905	4.432479
H	-8.553064	-1.903681	3.410026
H	-8.085400	-3.415725	2.584970
C	-6.490174	-1.817290	5.235963
H	-5.230003	-0.063884	4.937330
H	-4.655339	-1.529744	4.117343
H	-7.699707	-3.623447	5.042932
H	-6.169608	-3.676516	4.144163
H	-5.964672	-2.152118	6.139040
H	-7.348335	-1.208465	5.552876
C	-3.080874	-8.876175	-0.243336
C	-2.009570	-9.962711	-0.509679
C	-4.424813	-9.294003	-0.872601
H	-2.773752	-7.950768	-0.741456
C	-1.847850	-10.219021	-2.020601
H	-2.319805	-10.891850	-0.010580
H	-1.054495	-9.654848	-0.067612
C	-4.264814	-9.564867	-2.382717
H	-4.805070	-10.200372	-0.378879
H	-5.126975	-8.473163	-0.717505
C	-3.195772	-10.647133	-2.637148
H	-1.087736	-10.989592	-2.192442
H	-1.507103	-9.293953	-2.505941
H	-5.226773	-9.870381	-2.813753
H	-3.959622	-8.632934	-2.876794

H	-3.082999	-10.823299	-3.712864
H	-3.518162	-11.589944	-2.173297
C	-4.220527	-10.686649	4.298782
C	-2.980530	-11.522593	4.706120
C	-5.019251	-10.294839	5.555768
H	-4.865113	-11.323172	3.673356
C	-3.398122	-12.776265	5.501847
H	-2.332480	-10.888376	5.326516
H	-2.416146	-11.801542	3.808828
C	-5.450127	-11.552097	6.339136
H	-4.391818	-9.672252	6.207472
H	-5.889578	-9.703634	5.262934
C	-4.213247	-12.378239	6.749851
H	-2.511172	-13.350454	5.792048
H	-4.017749	-13.417740	4.860289
H	-6.027700	-11.263729	7.224661
H	-6.098596	-12.169530	5.701793
H	-4.517139	-13.271592	7.306880
H	-3.581281	-11.768605	7.409518
C	-2.176425	-6.060772	3.961385
C	-3.234014	-5.306577	4.801401
C	-0.980252	-6.471870	4.856181
H	-1.797998	-5.360906	3.208372
C	-2.606764	-4.081785	5.498747
H	-3.647097	-5.988102	5.558489
H	-4.046794	-4.973303	4.147670
C	-0.359758	-5.241376	5.547769
H	-1.333700	-7.177056	5.620346
H	-0.232761	-6.988828	4.242891
C	-1.422309	-4.505480	6.390168
H	-3.369023	-3.561837	6.091155
H	-2.249448	-3.382225	4.730576
H	0.482269	-5.549507	6.177924
H	0.027217	-4.555520	4.782176
H	-0.980043	-3.629495	6.877783
H	-1.787361	-5.180762	7.176251
C	-9.815349	-9.230473	1.893398
C	-10.144787	-7.767807	1.831707
C	-10.450986	-7.152050	0.691832
H	-10.313050	-9.719452	2.739219
H	-10.143508	-9.747680	0.984103
N	-10.619268	-5.746307	0.588106
S	-11.936736	-5.000200	1.304425
O	-12.116411	-5.615442	2.608579
O	-11.709127	-3.571197	1.162476
H	-10.544485	-7.694973	-0.249965
C	-6.137943	-6.918331	3.712925
C	-6.789284	-7.791460	2.861689
C	-6.543202	-6.938003	5.046997
H	-5.387173	-6.233558	3.343704
C	-7.768490	-8.686276	3.281820
C	-7.547224	-7.804028	5.487959
H	-6.080754	-6.249264	5.747031
C	-8.163787	-8.700941	4.610961
C	-8.289486	-9.428864	2.074097
C	-7.518455	-8.734402	0.964382



H	-6.041352	-7.235064	0.834777
H	-7.850106	-7.783839	6.529948
H	-8.941813	-9.373681	4.961342
N	-6.678073	-7.880424	1.445081
C	-7.909760	-10.919913	2.096956
H	-8.242371	-11.421517	1.182381
H	-6.825833	-11.040100	2.197605
H	-8.390620	-11.402800	2.952513
C	-7.687541	-8.991615	-0.488832
H	-8.740898	-9.167424	-0.718416
H	-7.319228	-8.146860	-1.075488
H	-7.129315	-9.891041	-0.773909
H	0.647730	1.853055	2.647597
H	2.240890	-5.247203	-4.151297
C	-13.338819	-5.437113	0.309708
C	-13.642683	-4.671384	-0.811842
C	-14.078466	-6.571477	0.637495
C	-14.715179	-5.050053	-1.613050
H	-13.044433	-3.796525	-1.046955
C	-15.144937	-6.933618	-0.175947
H	-13.828032	-7.139387	1.527317
C	-15.477632	-6.181610	-1.309103
H	-14.966765	-4.452044	-2.484642
H	-15.737601	-7.808898	0.076378
C	-16.633764	-6.596631	-2.181326
H	-16.404958	-7.527131	-2.711819
H	-17.532226	-6.774546	-1.582835
H	-16.863952	-5.831812	-2.926623
C	-10.023005	-5.134198	-0.573132
C	-10.550832	-5.357197	-1.846442
C	-9.912498	-4.805219	-2.953415
C	-8.757648	-4.043075	-2.781330
C	-8.235773	-3.830040	-1.507726
C	-8.868538	-4.379316	-0.395900
H	-11.446479	-5.962082	-1.964003
H	-10.316754	-4.971127	-3.947408
H	-8.262902	-3.610668	-3.645930
H	-7.343622	-3.229520	-1.360750
H	-8.453630	-4.239513	0.597411

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**I4(R), E(PCM, mixed basis set, opt) = -5013.237548 - E(PCM, 6-31+G\*, single point) = -5023.890701**

C	-4.368345	-2.647415	0.358342
C	-3.015037	-2.721192	0.619750
C	-2.341013	-1.551184	1.093416
C	-3.050670	-0.323549	1.154900
C	-4.400765	-0.286760	0.727539
C	-5.075776	-1.418099	0.335781
H	-0.442025	-2.503313	1.541248
C	-0.992252	-1.568021	1.545443
C	-2.392689	0.844665	1.623957
H	-4.916572	0.669350	0.687192
C	-1.086493	0.817273	2.044449
C	-0.394429	-0.424520	2.004921
H	-2.955894	1.775069	1.653228
H	0.633778	-0.461756	2.356539

C	-2.293781	-3.999688	0.405502
C	-1.165619	-4.091140	-0.471122
C	-2.735541	-5.140671	1.033723
C	-0.718189	-3.005760	-1.273557
C	-0.470233	-5.325823	-0.568998
C	-2.070118	-6.389806	0.935263
C	0.372403	-3.142089	-2.091485
H	-1.257871	-2.065055	-1.242368
C	0.665646	-5.423571	-1.416148
C	-0.932360	-6.445541	0.168902
C	1.100153	-4.360968	-2.168891
H	0.691350	-2.300999	-2.702238
H	1.188582	-6.376489	-1.467414
H	-0.372059	-7.374655	0.117660
C	-0.383414	2.048640	2.550405
H	-1.052050	2.915062	2.547179
H	0.487978	2.286355	1.927146
C	2.303946	-4.457818	-3.068082
H	2.733264	-5.464521	-3.044911
H	3.080510	-3.747115	-2.757879
C	-6.447429	-1.308726	-0.236042
C	-7.589686	-1.397476	0.584364
C	-6.574506	-1.028721	-1.617718
C	-8.850916	-1.190111	0.013650
C	-7.852852	-0.833215	-2.146589
C	-8.995632	-0.895475	-1.343458
H	-9.730751	-1.280641	0.637794
H	-7.972111	-0.618620	-3.203834
C	-2.576024	-7.564675	1.695226
C	-3.307867	-8.579318	1.041009
C	-2.309947	-7.656607	3.078360
C	-3.758273	-9.671587	1.790579
C	-2.761429	-8.774279	3.784874
C	-3.489413	-9.788290	3.155222
H	-4.320129	-10.460104	1.300262
H	-2.549057	-8.849814	4.847535
O	-3.840690	-5.050316	1.865468
O	-5.053779	-3.808364	0.013725
P	-5.305921	-4.917111	1.170920
O	-6.316687	-4.604856	2.192386
O	-5.509860	-6.196434	0.290749
H	-9.525151	-6.370297	3.161793
C	-5.343361	-0.996223	-2.521272
C	-5.061244	-2.414648	-3.079583
C	-5.452944	-0.001350	-3.698334
H	-4.473811	-0.696498	-1.922059
C	-3.768207	-2.431159	-3.918468
H	-5.917207	-2.711575	-3.703877
H	-4.981366	-3.131720	-2.255375
C	-4.140301	0.005486	-4.509899
H	-6.269923	-0.305997	-4.365215
H	-5.681521	1.001095	-3.317915
C	-3.848524	-1.403810	-5.066764
H	-3.593140	-3.436718	-4.317662
H	-2.919463	-2.181636	-3.266719
H	-4.209445	0.730472	-5.328864

H	-3.313127	0.314305	-3.856541
H	-2.915988	-1.400967	-5.642102
H	-4.661844	-1.691873	-5.746797
C	-10.365655	-0.696014	-1.972720
C	-10.954416	-2.074447	-2.359016
C	-11.352735	0.051958	-1.050859
H	-10.240413	-0.102526	-2.891798
C	-12.347354	-1.932211	-3.009241
H	-11.019244	-2.673442	-1.441873
H	-10.264509	-2.585450	-3.039275
C	-12.709513	0.239484	-1.759302
H	-11.516912	-0.544297	-0.144327
H	-10.926795	1.018207	-0.755853
C	-13.310739	-1.139341	-2.099335
H	-12.758378	-2.927351	-3.230323
H	-12.248333	-1.400390	-3.966089
H	-13.395039	0.804083	-1.117317
H	-12.564534	0.813166	-2.685319
H	-14.286248	-1.024668	-2.586472
H	-13.463619	-1.687170	-1.159706
C	-7.446529	-1.648424	2.081592
C	-7.297877	-0.301225	2.834438
C	-8.621228	-2.434735	2.707080
H	-6.538376	-2.239724	2.250695
C	-7.018309	-0.550916	4.331758
H	-8.230321	0.267690	2.713292
H	-6.484064	0.284155	2.391824
C	-8.326099	-2.720482	4.192407
H	-9.547818	-1.849993	2.633614
H	-8.778231	-3.378314	2.177291
C	-8.141367	-1.398742	4.966345
H	-6.916456	0.404097	4.860705
H	-6.066506	-1.091594	4.423190
H	-9.149912	-3.300890	4.624854
H	-7.412268	-3.325632	4.252277
H	-7.911813	-1.600801	6.019313
H	-9.081169	-0.830793	4.930429
C	-3.521954	-8.539763	-0.467174
C	-2.396758	-9.333092	-1.179910
C	-4.881645	-9.109864	-0.922792
H	-3.475461	-7.494906	-0.797919
C	-2.528061	-9.194800	-2.710668
H	-2.480156	-10.389555	-0.887784
H	-1.417127	-8.974776	-0.849678
C	-5.039319	-8.944761	-2.447720
H	-4.939401	-10.178989	-0.675096
H	-5.686556	-8.594079	-0.397204
C	-3.909096	-9.691819	-3.187435
H	-1.730176	-9.755422	-3.211074
H	-2.413687	-8.135387	-2.978384
H	-6.017139	-9.322839	-2.769580
H	-4.996003	-7.875166	-2.692783
H	-4.007413	-9.554959	-4.270504
H	-3.994221	-10.766464	-2.975361
C	-3.941659	-11.016116	3.926467
C	-2.717696	-11.850280	4.374853

C	-4.808000	-10.639683	5.147571
H	-4.551854	-11.641064	3.257199
C	-3.162085	-13.108627	5.147610
H	-2.090478	-11.225602	5.025323
H	-2.120742	-12.123589	3.497241
C	-5.245676	-11.898104	5.924515
H	-4.227250	-9.987431	5.813647
H	-5.679442	-10.071296	4.808744
C	-4.014381	-12.714322	6.371779
H	-2.285575	-13.686500	5.461684
H	-3.763201	-13.745071	4.483868
H	-5.849429	-11.608589	6.792321
H	-5.872817	-12.524149	5.274256
H	-4.328143	-13.608838	6.921671
H	-3.404522	-12.100078	7.048021
C	-1.518418	-6.576114	3.804550
C	-2.311050	-5.967964	4.984129
C	-0.163611	-7.131267	4.305540
H	-1.300414	-5.760165	3.105409
C	-1.490141	-4.856196	5.669588
H	-2.532956	-6.758005	5.715427
H	-3.260007	-5.563296	4.611983
C	0.656115	-6.020579	4.994758
H	-0.353221	-7.944299	5.019876
H	0.391470	-7.551252	3.457877
C	-0.138677	-5.408735	6.167102
H	-2.058836	-4.429944	6.503836
H	-1.308524	-4.051316	4.944298
H	1.611637	-6.422369	5.350657
H	0.874414	-5.232206	4.261219
H	0.443131	-4.612540	6.645295
H	-0.323668	-6.187241	6.919791
C	-9.982172	-8.541158	2.839674
C	-9.997468	-7.082763	2.487446
C	-10.482333	-6.651144	1.326616
H	-10.403106	-8.716468	3.837192
H	-10.595767	-9.105349	2.126430
N	-10.399061	-5.284644	0.921857
S	-11.636912	-4.273091	1.441247
O	-11.732101	-4.435932	2.881591
O	-11.385891	-2.971434	0.842223
H	-10.937940	-7.336124	0.608301
C	-5.590660	-7.226789	3.965577
C	-6.605977	-7.851960	3.260687
C	-5.696119	-7.218830	5.357145
H	-4.743894	-6.783637	3.450812
C	-7.672632	-8.488162	3.897302
C	-6.775649	-7.822091	6.006080
H	-4.924103	-6.731177	5.943889
C	-7.775301	-8.475608	5.279461
C	-8.539063	-9.103941	2.828402
C	-7.792210	-8.629992	1.584141
H	-5.947495	-6.945751	0.852229
H	-6.834153	-7.791108	7.089550
H	-8.604829	-8.959146	5.789298
N	-6.735635	-7.944644	1.847246

C	-8.548548	-10.637161	2.911807
H	-9.079151	-11.071534	2.057644
H	-7.525847	-11.027757	2.930298
H	-9.054201	-10.955974	3.828880
C	-8.242848	-8.927068	0.191106
H	-9.315990	-9.130578	0.159810
H	-8.019492	-8.084035	-0.469963
H	-7.722057	-9.813341	-0.191532
H	-0.021280	1.898610	3.575213
H	2.038449	-4.220805	-4.106004
C	-13.120522	-4.930120	0.719426
C	-13.491051	-4.517585	-0.558517
C	-13.847619	-5.897686	1.407428
C	-14.616404	-5.081297	-1.147745
H	-12.901824	-3.767639	-1.076833
C	-14.968576	-6.452954	0.799094
H	-13.543434	-6.193777	2.406117
C	-15.369598	-6.052827	-0.479459
H	-14.916517	-4.759020	-2.141500
H	-15.546181	-7.206266	1.327737
C	-16.606482	-6.634197	-1.113030
H	-16.789726	-7.653231	-0.762732
H	-17.486535	-6.033471	-0.858399
H	-16.522746	-6.651788	-2.202748
C	-9.824913	-5.070673	-0.385593
C	-10.429231	-5.582682	-1.536727
C	-9.799534	-5.421866	-2.768308
C	-8.580730	-4.747927	-2.847667
C	-7.987676	-4.236768	-1.696386
C	-8.604573	-4.406756	-0.460329
H	-11.378504	-6.107929	-1.467121
H	-10.262359	-5.821496	-3.665592
H	-8.093709	-4.620839	-3.810349
H	-7.044863	-3.702935	-1.738347
H	-8.132616	-4.041241	0.444896

## Computed Cartesian coordinates of alternative and less stable conformations of I1(S)

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I1(S)-1, E(PCM, mixed basis set, opt) = -5013.200502 - E(PCM, 6-31+G\*, single point) = -5023.850640

C	-4.855034	-2.500793	0.852254
C	-3.552884	-2.553100	1.299428
C	-2.985738	-1.361464	1.854739
C	-3.730552	-0.152392	1.799437
C	-5.016077	-0.149899	1.201184
C	-5.605118	-1.303223	0.745051
H	-1.143658	-2.257829	2.562734
C	-1.713782	-1.337298	2.487819
C	-3.172726	1.036514	2.340513
H	-5.553860	0.790353	1.112672
C	-1.937104	1.048368	2.938448
C	-1.214195	-0.174014	3.011183
H	-3.757916	1.951858	2.281672
H	-0.243192	-0.179937	3.500522
C	-2.786565	-3.815929	1.143365
C	-1.557305	-3.857633	0.407216
C	-3.313097	-5.001751	1.608981
C	-1.002668	-2.725550	-0.252586
C	-0.872760	-5.096561	0.284357
C	-2.683246	-6.262785	1.437789
C	0.177422	-2.823209	-0.941443
H	-1.528395	-1.777904	-0.219725
C	0.357149	-5.154942	-0.423543
C	-1.457837	-6.271614	0.817982
C	0.895238	-4.047151	-1.028988
H	0.577279	-1.944984	-1.442470
H	0.865388	-6.114616	-0.492164
H	-0.941587	-7.218307	0.683466
C	-1.341624	2.303367	3.519257
H	-2.023606	3.152015	3.407924
H	-0.396922	2.553865	3.020500
C	2.193097	-4.102548	-1.789853
H	2.639938	-5.100339	-1.734189
H	2.913676	-3.380103	-1.387112
C	-6.944001	-1.313784	0.100405
C	-8.096305	-0.968510	0.835928
C	-7.051275	-1.637311	-1.275078
C	-9.336597	-0.930594	0.183988
C	-8.307693	-1.589613	-1.881702
C	-9.462312	-1.238857	-1.169918
H	-10.218790	-0.676833	0.757832
H	-8.396425	-1.821020	-2.941346
C	-3.373776	-7.523426	1.841065
C	-4.184020	-8.192733	0.889706
C	-3.246455	-8.033468	3.151680
C	-4.849331	-9.355218	1.282856
C	-3.947351	-9.194218	3.503911
C	-4.763215	-9.855580	2.585774
H	-5.489834	-9.869776	0.574451
H	-3.877646	-9.566934	4.517695
O	-4.514407	-4.963831	2.308756

O	-5.466311	-3.663126	0.389865
P	-5.895946	-4.770131	1.471044
O	-6.801151	-3.984513	2.511188
O	-6.432444	-5.998043	0.878866
H	-7.456029	-4.572041	2.947213
C	-5.830295	-1.980341	-2.126505
C	-5.930625	-3.393588	-2.746170
C	-5.620831	-0.930189	-3.243831
H	-4.931681	-1.964061	-1.500199
C	-4.662664	-3.722413	-3.559814
H	-6.805435	-3.432851	-3.411376
H	-6.070696	-4.129843	-1.948120
C	-4.353920	-1.258043	-4.062328
H	-6.495863	-0.933284	-3.907172
H	-5.541715	0.067478	-2.796022
C	-4.447811	-2.673575	-4.670283
H	-4.747585	-4.726950	-3.993399
H	-3.794644	-3.723696	-2.884882
H	-4.215080	-0.512326	-4.853199
H	-3.478319	-1.211911	-3.400275
H	-3.540526	-2.902525	-5.240563
H	-5.298915	-2.709428	-5.364016
C	-10.808904	-1.266030	-1.884280
C	-11.232574	-2.739040	-2.120776
C	-11.930791	-0.534736	-1.119192
H	-10.686257	-0.782526	-2.865942
C	-12.567764	-2.821080	-2.887044
H	-11.331857	-3.218174	-1.138141
H	-10.443752	-3.266528	-2.669583
C	-13.255476	-0.596105	-1.907216
H	-12.077831	-1.032374	-0.152369
H	-11.640819	0.506566	-0.931604
C	-13.674540	-2.064723	-2.124878
H	-12.850795	-3.870754	-3.030944
H	-12.444212	-2.368203	-3.880788
H	-14.038508	-0.054795	-1.364613
H	-13.124474	-0.109891	-2.883784
H	-14.620790	-2.115058	-2.675562
H	-13.823816	-2.538884	-1.144901
C	-8.036742	-0.630160	2.321280
C	-8.228716	0.891595	2.542621
C	-9.095115	-1.405548	3.136486
H	-7.051781	-0.912799	2.712218
C	-8.109390	1.241014	4.039734
H	-9.225073	1.174758	2.175372
H	-7.489223	1.451683	1.958132
C	-8.994840	-1.059447	4.633479
H	-10.102946	-1.154345	2.783836
H	-8.951368	-2.480425	2.985303
C	-9.156469	0.458329	4.858505
H	-8.238417	2.319705	4.187090
H	-7.102739	0.971064	4.388377
H	-9.768669	-1.610323	5.179174
H	-8.014574	-1.380810	5.013406
H	-9.061046	0.697243	5.924121
H	-10.161400	0.761570	4.535248

C	-4.324238	-7.666054	-0.536554
C	-3.161250	-8.162259	-1.432892
C	-5.658009	-8.055252	-1.214996
H	-4.288026	-6.568474	-0.505023
C	-3.233158	-7.473880	-2.812549
H	-3.252622	-9.251684	-1.547585
H	-2.197483	-7.954805	-0.960388
C	-5.762615	-7.365362	-2.590012
H	-5.689207	-9.142942	-1.367740
H	-6.493428	-7.752469	-0.576423
C	-4.582337	-7.768090	-3.498816
H	-2.404343	-7.808177	-3.447182
H	-3.130292	-6.388732	-2.668650
H	-6.709199	-7.633389	-3.073305
H	-5.761680	-6.277304	-2.438531
H	-4.642689	-7.237051	-4.456657
H	-4.647454	-8.844762	-3.707634
C	-5.561986	-11.096314	2.952947
C	-4.738002	-12.373815	2.657421
C	-6.039082	-11.113239	4.419715
H	-6.458371	-11.112411	2.315758
C	-5.578119	-13.638135	2.936308
H	-3.846925	-12.368246	3.300183
H	-4.399917	-12.360214	1.614190
C	-6.901813	-12.363004	4.683702
H	-5.166643	-11.144548	5.086569
H	-6.606621	-10.202185	4.635584
C	-6.092757	-13.644332	4.391294
H	-4.982440	-14.536781	2.738814
H	-6.439237	-13.650641	2.254392
H	-7.253013	-12.362154	5.721883
H	-7.785986	-12.328877	4.032209
H	-6.707038	-14.534214	4.571498
H	-5.233230	-13.686073	5.074170
C	-2.351003	-7.328632	4.164679
C	-2.708773	-7.629904	5.637250
C	-0.865256	-7.713400	3.942032
H	-2.438813	-6.242532	4.006230
C	-1.833700	-6.774353	6.576456
H	-2.503869	-8.688654	5.845409
H	-3.775803	-7.455801	5.818235
C	0.046057	-6.886435	4.872477
H	-0.753191	-8.785441	4.153759
H	-0.587597	-7.543579	2.898170
C	-0.339885	-7.096657	6.350842
H	-2.106305	-6.964340	7.620856
H	-2.013335	-5.710141	6.370137
H	1.095232	-7.159589	4.712380
H	-0.065744	-5.823192	4.618729
H	0.285827	-6.471730	6.997919
H	-0.159991	-8.146104	6.620796
C	-8.949294	-4.212599	5.705325
C	-9.213057	-4.821188	4.584157
C	-9.544113	-5.436454	3.469615
H	-9.749288	-3.949734	6.393274
H	-7.932916	-3.939952	5.978729



N	-9.934705	-4.699361	2.306277
S	-11.444298	-3.920998	2.387977
O	-11.588338	-3.424248	3.745683
O	-11.505246	-3.020407	1.247269
H	-9.541351	-6.524416	3.410694
C	-7.708148	-8.472905	2.694149
C	-7.202757	-7.750525	3.776623
C	-8.774735	-9.325692	2.945084
H	-7.285039	-8.341551	1.703020
C	-7.745086	-7.852194	5.078332
C	-9.333397	-9.444364	4.234416
H	-9.196783	-9.904454	2.127512
C	-8.833340	-8.710130	5.300436
C	-7.005159	-6.946422	5.920315
C	-6.077163	-6.334076	5.117394
H	-5.436873	-6.798653	3.152843
H	-10.170100	-10.118822	4.390408
H	-9.274898	-8.798639	6.289618
N	-6.207156	-6.800327	3.814796
C	-7.293288	-6.688896	7.364732
H	-6.587726	-5.973783	7.797010
H	-8.303198	-6.280826	7.496822
H	-7.234944	-7.612403	7.951933
C	-5.123647	-5.223124	5.419897
H	-4.155341	-5.384952	4.938146
H	-5.508162	-4.267533	5.042089
H	-4.961300	-5.133945	6.496982
H	-1.124955	2.174589	4.586994
H	2.036416	-3.855512	-2.847424
C	-12.618214	-5.221156	2.126637
C	-13.035128	-5.510669	0.828497
C	-13.024955	-5.991608	3.211993
C	-13.886086	-6.589284	0.626233
H	-12.699252	-4.892918	0.000585
C	-13.875078	-7.069698	2.986133
H	-12.692488	-5.736985	4.213416
C	-14.313711	-7.383346	1.696966
H	-14.225684	-6.821579	-0.379550
H	-14.207502	-7.673338	3.825797
C	-15.225171	-8.557299	1.451410
H	-16.082331	-8.266051	0.837128
H	-14.695835	-9.353686	0.917689
H	-15.601018	-8.971937	2.389557
C	-9.603626	-5.265041	1.022299
C	-9.827040	-6.618694	0.764284
C	-9.476919	-7.146324	-0.473183
C	-8.940639	-6.317328	-1.456510
C	-8.742896	-4.964934	-1.195161
C	-9.060571	-4.429272	0.049729
H	-10.269969	-7.256104	1.524598
H	-9.637606	-8.201896	-0.672338
H	-8.679055	-6.725801	-2.427581
H	-8.335866	-4.309802	-1.956382
H	-8.907920	-3.375116	0.264157

**I1(S)-2, E(PCM, mixed basis set, opt) = -5013.200659 - E(PCM, 6-31+G\*, single point) = -5023.852609**

C	-4.560373	-2.386919	0.749042
C	-3.250675	-2.418343	1.173919
C	-2.686743	-1.214770	1.705494
C	-3.452380	-0.018282	1.663563
C	-4.745742	-0.036745	1.082617
C	-5.323506	-1.199136	0.633787
H	-0.813169	-2.078723	2.370086
C	-1.400295	-1.168142	2.306871
C	-2.902287	1.181209	2.188508
H	-5.295747	0.896416	0.989563
C	-1.653624	1.214616	2.757911
C	-0.908342	0.004915	2.815352
H	-3.502993	2.086931	2.139964
H	0.074402	0.017279	3.280463
C	-2.476535	-3.676480	1.018380
C	-1.265660	-3.717508	0.252020
C	-2.973822	-4.859464	1.518439
C	-0.746817	-2.590284	-0.443654
C	-0.563061	-4.947606	0.140664
C	-2.328287	-6.113091	1.358009
C	0.418333	-2.682363	-1.158303
H	-1.288818	-1.651463	-0.417194
C	0.650932	-4.999305	-0.594477
C	-1.115252	-6.120306	0.715416
C	1.155107	-3.895547	-1.235975
H	0.790570	-1.808506	-1.687516
H	1.174899	-5.950991	-0.654611
H	-0.584825	-7.061716	0.597714
C	-1.066209	2.480619	3.322738
H	-1.762342	3.318712	3.219944
H	-0.134276	2.742523	2.806365
C	2.436850	-3.944374	-2.024244
H	2.892553	-4.938414	-1.974104
H	3.160084	-3.215070	-1.638818
C	-6.644508	-1.189000	-0.050740
C	-7.816172	-0.814545	0.644599
C	-6.699733	-1.448557	-1.439966
C	-9.009788	-0.660430	-0.067908
C	-7.912141	-1.269060	-2.114173
C	-9.073537	-0.872591	-1.448249
H	-9.912235	-0.385174	0.469743
H	-7.953608	-1.439269	-3.187067
C	-2.989297	-7.360114	1.835490
C	-3.904465	-8.027230	0.980163
C	-2.744648	-7.843269	3.132286
C	-4.557982	-9.158217	1.462353
C	-3.419518	-8.991838	3.573221
C	-4.347828	-9.640362	2.762429
H	-5.287335	-9.664710	0.837361
H	-3.248500	-9.351879	4.580399
O	-4.148285	-4.833332	2.263784
O	-5.171880	-3.574726	0.345265
P	-5.562252	-4.588191	1.533734
O	-6.308309	-3.709859	2.624914
O	-6.276379	-5.782602	1.056904

H	-7.194233	-4.072469	2.842495
C	-5.477616	-1.897309	-2.233105
C	-5.677794	-3.311635	-2.827892
C	-5.116171	-0.902010	-3.361028
H	-4.609352	-1.946257	-1.568228
C	-4.389644	-3.777356	-3.535916
H	-6.499332	-3.280269	-3.558649
H	-5.955508	-4.009792	-2.030523
C	-3.827622	-1.361673	-4.076465
H	-5.940044	-0.857616	-4.085791
H	-4.984903	0.100196	-2.936624
C	-3.999512	-2.784132	-4.650602
H	-4.531808	-4.781498	-3.954748
H	-3.578398	-3.837836	-2.795395
H	-3.569611	-0.658301	-4.876214
H	-3.000387	-1.367010	-3.352934
H	-3.075012	-3.107436	-5.142350
H	-4.796137	-2.769452	-5.407405
C	-10.386668	-0.717163	-2.196473
C	-11.425361	-1.749806	-1.696289
C	-10.954748	0.714606	-2.050672
H	-10.201512	-0.903749	-3.264515
C	-12.760189	-1.602772	-2.454321
H	-11.595603	-1.596996	-0.623539
H	-11.023967	-2.763036	-1.813802
C	-12.287893	0.857566	-2.814449
H	-11.127850	0.919278	-0.985729
H	-10.219569	1.440075	-2.417624
C	-13.315415	-0.171832	-2.301101
H	-13.482763	-2.333245	-2.073301
H	-12.598166	-1.812419	-3.520676
H	-12.677858	1.875091	-2.699661
H	-12.110573	0.685225	-3.884831
H	-14.260751	-0.069609	-2.845941
H	-13.515785	0.021368	-1.238862
C	-7.827296	-0.598986	2.152734
C	-8.068617	0.889361	2.499602
C	-8.904258	-1.472309	2.839687
H	-6.854086	-0.896151	2.562404
C	-8.045968	1.103216	4.027432
H	-9.047271	1.191173	2.100989
H	-7.306992	1.512244	2.015180
C	-8.879966	-1.266674	4.366576
H	-9.901175	-1.209851	2.460200
H	-8.734303	-2.523982	2.586595
C	-9.107737	0.218574	4.714023
H	-8.221296	2.159495	4.261301
H	-7.051600	0.833531	4.409395
H	-9.647840	-1.896975	4.829100
H	-7.901214	-1.583689	4.754955
H	-9.076709	0.364032	5.799763
H	-10.104942	0.517814	4.364151
C	-4.132373	-7.533900	-0.446562
C	-3.006261	-8.062449	-1.372774
C	-5.490801	-7.944985	-1.060175
H	-4.093777	-6.434423	-0.448723

C	-3.127568	-7.433135	-2.774449
H	-3.103422	-9.155255	-1.438933
H	-2.025803	-7.839041	-0.943589
C	-5.646260	-7.319372	-2.461599
H	-5.535823	-9.038975	-1.155023
H	-6.311027	-7.604768	-0.418956
C	-4.500505	-7.759582	-3.396221
H	-2.322420	-7.795393	-3.423900
H	-3.020548	-6.343279	-2.681618
H	-6.611516	-7.611918	-2.890993
H	-5.647195	-6.225704	-2.359669
H	-4.601255	-7.272143	-4.373505
H	-4.569060	-8.844687	-3.554648
C	-5.197250	-10.809289	3.237307
C	-4.786912	-12.126988	2.535464
C	-5.189380	-11.019592	4.763008
H	-6.235332	-10.589477	2.945729
C	-5.775475	-13.252527	2.905479
H	-3.771448	-12.396319	2.856345
H	-4.769187	-11.979859	1.449290
C	-6.195390	-12.127126	5.138958
H	-4.183395	-11.321003	5.089189
H	-5.450873	-10.080248	5.265428
C	-5.826842	-13.450641	4.434777
H	-5.488139	-14.187236	2.410587
H	-6.776576	-12.972625	2.548364
H	-6.216061	-12.267683	6.226041
H	-7.197958	-11.812635	4.815864
H	-6.553262	-14.230819	4.689735
H	-4.840483	-13.781317	4.787498
C	-1.752203	-7.128241	4.041266
C	-2.161697	-7.126492	5.530612
C	-0.351069	-7.770682	3.889626
H	-1.680937	-6.079696	3.721270
C	-1.125564	-6.348891	6.369267
H	-2.205185	-8.157436	5.904631
H	-3.158284	-6.682275	5.637520
C	0.694053	-7.018035	4.737581
H	-0.414687	-8.818350	4.215141
H	-0.060124	-7.765704	2.832701
C	0.270901	-6.988418	6.220815
H	-1.427868	-6.339564	7.422755
H	-1.086432	-5.307799	6.021979
H	1.676801	-7.491230	4.630655
H	0.775765	-5.987137	4.366675
H	1.007229	-6.434759	6.814142
H	0.234543	-8.017260	6.603727
C	-8.656669	-4.559709	5.417209
C	-8.819223	-4.918680	4.174547
C	-8.952045	-5.365991	2.943394
H	-7.796554	-3.968657	5.723255
H	-9.389359	-4.818222	6.177865
N	-9.638364	-4.680247	1.901357
S	-11.280532	-4.319300	2.177429
O	-11.387743	-3.931676	3.573169
O	-11.681780	-3.415637	1.113151

H	-8.493067	-6.311574	2.660192
C	-8.815958	-9.730304	1.194901
C	-8.246986	-9.135939	2.326314
C	-9.775532	-10.711124	1.397411
H	-8.498327	-9.440481	0.197025
C	-8.614021	-9.517444	3.643037
C	-10.153504	-11.105332	2.696753
H	-10.234945	-11.193504	0.539736
C	-9.583146	-10.518060	3.816356
C	-7.798598	-8.755762	4.549711
C	-6.983224	-7.966616	3.773971
H	-6.783175	-7.697169	1.690863
H	-10.895969	-11.888776	2.819168
H	-9.870684	-10.835318	4.815874
N	-7.272026	-8.179643	2.440156
C	-7.833461	-8.840929	6.043042
H	-7.045080	-8.230358	6.492867
H	-8.791010	-8.490354	6.446174
H	-7.692563	-9.873775	6.386089
C	-5.927589	-6.980317	4.150429
H	-5.129289	-6.968973	3.403877
H	-6.335393	-5.966068	4.240812
H	-5.480690	-7.246730	5.112563
H	-0.829232	2.359565	4.387082
H	2.256034	-3.702217	-3.079045
C	-12.052587	-5.891590	1.927226
C	-12.605339	-6.182263	0.683484
C	-11.889227	-6.876927	2.901427
C	-13.012037	-7.485199	0.420718
H	-12.692415	-5.399503	-0.063189
C	-12.283856	-8.177439	2.610756
H	-11.446227	-6.630993	3.861552
C	-12.847194	-8.498419	1.370709
H	-13.445395	-7.724944	-0.546614
H	-12.134949	-8.960044	3.348696
C	-13.288933	-9.905533	1.067256
H	-12.830643	-10.617683	1.757391
H	-14.377270	-9.995800	1.156818
H	-13.018033	-10.190756	0.046368
C	-9.330752	-5.098250	0.554881
C	-8.992905	-4.121409	-0.374195
C	-8.718582	-4.504020	-1.685454
C	-8.751477	-5.845413	-2.051871
C	-9.079969	-6.818184	-1.108411
C	-9.383115	-6.446984	0.197062
H	-8.966966	-3.076919	-0.079727
H	-8.473918	-3.739210	-2.413433
H	-8.527328	-6.132173	-3.074803
H	-9.124483	-7.864717	-1.396519
H	-9.677645	-7.197659	0.928269

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**I1(S)-3, E(PCM, mixed basis set, opt) = -5013.184622 - E(PCM, 6-31+G\*, single point) = -5023.840447**

C	-4.222660	-2.478247	0.678762
C	-2.934138	-2.472629	1.166670
C	-2.418748	-1.258693	1.721327

C	-3.193954	-0.073404	1.621962
C	-4.454673	-0.124323	0.979513
C	-4.999321	-1.302604	0.525119
H	-0.575461	-2.090343	2.504862
C	-1.167661	-1.187866	2.392510
C	-2.687539	1.141434	2.157215
H	-5.018685	0.796622	0.851281
C	-1.471246	1.198740	2.790618
C	-0.717641	-0.001742	2.908521
H	-3.295432	2.038945	2.062568
H	0.237182	0.028894	3.427718
C	-2.111306	-3.700537	1.048534
C	-0.860281	-3.677365	0.349368
C	-2.578858	-4.903464	1.532850
C	-0.372670	-2.530280	-0.337614
C	-0.077978	-4.861311	0.298976
C	-1.836530	-6.111578	1.444489
C	0.832889	-2.561157	-0.986913
H	-0.971132	-1.626483	-0.359463
C	1.176500	-4.849887	-0.367400
C	-0.588687	-6.050030	0.873066
C	1.646301	-3.727605	-1.001843
H	1.178451	-1.674746	-1.513398
H	1.760057	-5.767963	-0.380235
H	0.009761	-6.956731	0.828162
C	-0.927573	2.481187	3.362349
H	-1.635209	3.304746	3.225692
H	0.016872	2.755744	2.875742
C	2.968720	-3.709637	-1.720912
H	3.473985	-4.677426	-1.640674
H	3.631388	-2.941199	-1.303816
C	-6.313059	-1.300398	-0.170440
C	-7.466931	-0.821051	0.493418
C	-6.378881	-1.638074	-1.542071
C	-8.646986	-0.636407	-0.235142
C	-7.576379	-1.429039	-2.231637
C	-8.707684	-0.904806	-1.605888
H	-9.526158	-0.250888	0.274478
H	-7.622397	-1.654180	-3.293003
C	-2.393223	-7.399009	1.940298
C	-3.277255	-8.137540	1.112225
C	-2.055827	-7.868739	3.221814
C	-3.862171	-9.289588	1.629173
C	-2.661048	-9.042650	3.697048
C	-3.586044	-9.742975	2.926126
H	-4.582064	-9.840976	1.032475
H	-2.434154	-9.384506	4.699304
O	-3.808277	-4.928943	2.192209
O	-4.769965	-3.677185	0.231445
P	-5.175138	-4.768449	1.351847
O	-6.093987	-4.031243	2.412435
O	-5.744127	-5.984518	0.754857
H	-7.044655	-4.205667	2.182486
C	-5.179995	-2.168970	-2.318089
C	-5.440373	-3.600560	-2.845885
C	-4.802890	-1.235764	-3.492683

H	-4.306073	-2.214855	-1.661334
C	-4.181595	-4.137882	-3.558965
H	-6.278394	-3.572388	-3.555933
H	-5.717879	-4.252856	-2.011007
C	-3.541040	-1.767327	-4.205001
H	-5.634081	-1.196851	-4.208838
H	-4.634818	-0.220502	-3.114483
C	-3.773571	-3.204452	-4.717557
H	-4.365225	-5.151179	-3.936564
H	-3.360999	-4.199860	-2.829136
H	-3.269922	-1.107269	-5.036711
H	-2.704363	-1.773086	-3.492624
H	-2.869034	-3.581618	-5.208039
H	-4.580139	-3.190902	-5.463707
C	-9.958137	-0.607560	-2.415552
C	-11.140309	-1.499227	-1.979892
C	-10.359491	0.882723	-2.309689
H	-9.741390	-0.826465	-3.471138
C	-12.389601	-1.211067	-2.837696
H	-11.364383	-1.288395	-0.923393
H	-10.849784	-2.552480	-2.055926
C	-11.607659	1.174213	-3.168033
H	-10.582144	1.115650	-1.259418
H	-9.517631	1.511046	-2.621242
C	-12.784915	0.276419	-2.732176
H	-13.223735	-1.851567	-2.524753
H	-12.165145	-1.450078	-3.886068
H	-11.883820	2.231234	-3.083585
H	-11.374661	0.972239	-4.222303
H	-13.666684	0.481812	-3.349551
H	-13.042788	0.505980	-1.689093
C	-7.461740	-0.492666	1.982318
C	-7.761070	1.002655	2.241701
C	-8.473681	-1.366939	2.755435
H	-6.470876	-0.715059	2.393850
C	-7.688785	1.312074	3.751313
H	-8.766984	1.235817	1.866674
H	-7.049000	1.626321	1.688075
C	-8.394302	-1.066977	4.267101
H	-9.492263	-1.166446	2.390854
H	-8.251643	-2.417906	2.553945
C	-8.677803	0.425611	4.537207
H	-7.903681	2.371428	3.930785
H	-6.668534	1.110909	4.106331
H	-9.104545	-1.693611	4.821880
H	-7.385365	-1.315201	4.624412
H	-8.606041	0.637886	5.609731
H	-9.702723	0.659149	4.216035
C	-3.519575	-7.714888	-0.332652
C	-2.331511	-8.158516	-1.225410
C	-4.817261	-8.272502	-0.955626
H	-3.586714	-6.619848	-0.376719
C	-2.490246	-7.572502	-2.643529
H	-2.320915	-9.256298	-1.265713
H	-1.384324	-7.827520	-0.789354
C	-5.014509	-7.658202	-2.356027

H	-4.738812	-9.364564	-1.053180
H	-5.671994	-8.032302	-0.318896
C	-3.827088	-8.014114	-3.275972
H	-1.650653	-7.881120	-3.277177
H	-2.471915	-6.476200	-2.572164
H	-5.953440	-8.014465	-2.795245
H	-5.086829	-6.567164	-2.248529
H	-3.952766	-7.544156	-4.259074
H	-3.808842	-9.102350	-3.425067
C	-4.349077	-10.956549	3.433720
C	-3.926869	-12.244578	2.685365
C	-4.221240	-11.185406	4.950599
H	-5.411958	-10.778270	3.214469
C	-4.831718	-13.420414	3.109642
H	-2.879322	-12.468214	2.930523
H	-3.993728	-12.085883	1.602795
C	-5.135638	-12.349156	5.384114
H	-3.178396	-11.435755	5.195498
H	-4.490464	-10.266781	5.484380
C	-4.749799	-13.642351	4.634525
H	-4.544821	-14.332834	2.574668
H	-5.870301	-13.179549	2.840933
H	-5.070182	-12.501398	6.468113
H	-6.174379	-12.088232	5.137301
H	-5.407509	-14.466105	4.934006
H	-3.720389	-13.917978	4.902308
C	-1.141920	-7.054554	4.132508
C	-1.997817	-6.115696	5.019003
C	-0.226302	-7.921025	5.025377
H	-0.492773	-6.426114	3.510062
C	-1.102786	-5.224980	5.903678
H	-2.641893	-6.739276	5.654599
H	-2.650430	-5.502039	4.386100
C	0.680088	-7.023903	5.895824
H	-0.838000	-8.542919	5.691143
H	0.376520	-8.588872	4.399072
C	-0.176615	-6.093493	6.779210
H	-1.723602	-4.576467	6.532052
H	-0.489311	-4.580491	5.259154
H	1.332088	-7.645557	6.519778
H	1.319851	-6.413357	5.244512
H	0.466386	-5.459674	7.400246
H	-0.792793	-6.707855	7.449875
C	-7.756705	-4.667045	5.324462
C	-8.373104	-5.554385	4.591791
C	-9.032541	-6.425182	3.866299
H	-6.828841	-4.213131	4.981729
H	-8.156304	-4.353049	6.285516
N	-10.053496	-6.025123	2.919068
S	-9.377415	-5.710766	1.399235
O	-8.619280	-4.445095	1.437548
O	-8.689913	-6.916200	0.976202
H	-8.841063	-7.493242	3.918591
C	-8.186915	-9.968950	1.490832
C	-7.540005	-9.362303	2.572919
C	-8.991377	-11.065309	1.757688



H	-8.057348	-9.585282	0.483870
C	-7.698460	-9.828345	3.904565
C	-9.158324	-11.549325	3.071440
H	-9.502660	-11.563076	0.939120
C	-8.525642	-10.938990	4.142674
C	-6.881243	-8.994587	4.745275
C	-6.262689	-8.091032	3.909696
H	-6.421617	-7.699409	1.834121
H	-9.796675	-12.410896	3.243226
H	-8.660831	-11.316259	5.153666
N	-6.665941	-8.309111	2.612401
C	-6.782932	-9.089820	6.236303
H	-5.982039	-8.453891	6.625229
H	-7.716187	-8.778083	6.721808
H	-6.576663	-10.117414	6.560413
C	-5.293734	-6.996092	4.189765
H	-4.385981	-7.130555	3.594990
H	-5.721368	-6.018868	3.939530
H	-5.014989	-6.981244	5.246337
H	-0.725093	2.375729	4.435405
H	2.831171	-3.481873	-2.785350
C	-10.835118	-5.452340	0.439626
C	-11.527720	-6.579063	0.000905
C	-11.318191	-4.164629	0.244165
C	-12.740123	-6.399713	-0.650595
H	-11.117560	-7.569543	0.173600
C	-12.544279	-4.011924	-0.394925
H	-10.745982	-3.307266	0.588896
C	-13.266684	-5.117181	-0.850020
H	-13.292516	-7.265816	-1.004484
H	-12.946983	-3.014127	-0.542435
C	-14.577509	-4.936242	-1.569081
H	-14.988567	-3.937676	-1.401178
H	-14.443603	-5.066651	-2.648548
H	-15.314206	-5.673829	-1.238424
C	-11.064163	-5.084308	3.347380
C	-12.381038	-5.535053	3.401555
C	-13.395534	-4.652972	3.762517
C	-13.094558	-3.324761	4.061164
C	-11.775666	-2.879018	4.003668
C	-10.757170	-3.757998	3.646796
H	-12.591882	-6.568923	3.147260
H	-14.422425	-5.001595	3.804690
H	-13.888876	-2.638100	4.336799
H	-11.535081	-1.843579	4.230173
H	-9.730071	-3.424450	3.579017

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**H(S)-4, E(PCM, mixed basis set, opt) = -5013.197225 - E(PCM, 6-31+G\*, single point) = -5023.845340**

C	-4.450614	-2.380345	0.673742
C	-3.131355	-2.452429	1.068142
C	-2.521533	-1.282707	1.626245
C	-3.242086	-0.059527	1.618863
C	-4.553261	-0.030994	1.083076
C	-5.184693	-1.168156	0.643200
H	-0.672437	-2.223856	2.259710

C	-1.226493	-1.292239	2.212868
C	-2.641161	1.112592	2.149906
H	-5.078033	0.918192	1.023164
C	-1.383754	1.092557	2.699513
C	-0.685132	-0.145868	2.731566
H	-3.210586	2.039276	2.123937
H	0.302098	-0.178581	3.185911
C	-2.379099	-3.715484	0.871619
C	-1.162372	-3.746325	0.115096
C	-2.886195	-4.901828	1.354499
C	-0.640588	-2.611970	-0.567049
C	-0.452781	-4.971738	0.005126
C	-2.232015	-6.151503	1.191769
C	0.534161	-2.694026	-1.266305
H	-1.189173	-1.676778	-0.543761
C	0.772485	-5.013284	-0.712372
C	-1.007742	-6.146900	0.569015
C	1.279256	-3.903047	-1.339960
H	0.908382	-1.815742	-1.786667
H	1.302039	-5.961921	-0.770437
H	-0.466081	-7.084335	0.471677
C	-0.741613	2.327503	3.272892
H	-1.407781	3.192279	3.193588
H	0.191569	2.562759	2.746053
C	2.571899	-3.939918	-2.110567
H	3.034333	-4.930660	-2.057019
H	3.284504	-3.206356	-1.713659
C	-6.559940	-1.110224	0.080199
C	-7.667669	-0.936675	0.933660
C	-6.741011	-1.168376	-1.319939
C	-8.945946	-0.821244	0.372753
C	-8.034083	-1.053356	-1.837208
C	-9.149904	-0.893529	-1.006747
H	-9.798960	-0.707502	1.029734
H	-8.183235	-1.102517	-2.913603
C	-2.869253	-7.415701	1.652545
C	-3.734368	-8.116679	0.769073
C	-2.635567	-7.900597	2.948652
C	-4.378716	-9.256035	1.238826
C	-3.320447	-9.047288	3.384982
C	-4.213531	-9.715837	2.554610
H	-5.073257	-9.785202	0.592931
H	-3.175005	-9.390204	4.403503
O	-4.080192	-4.865820	2.079839
O	-5.084109	-3.528845	0.198455
P	-5.454894	-4.677589	1.265001
O	-6.354105	-3.980313	2.381345
O	-6.020579	-5.875876	0.633714
H	-7.290225	-4.254302	2.300904
C	-5.560918	-1.349737	-2.269036
C	-5.631623	-2.692717	-3.036323
C	-5.460318	-0.178569	-3.276100
H	-4.632959	-1.357030	-1.685181
C	-4.396648	-2.864230	-3.944231
H	-6.542928	-2.706371	-3.652285
H	-5.689486	-3.520185	-2.321375

C	-4.222403	-0.350130	-4.180839
H	-6.363915	-0.162108	-3.899864
H	-5.410507	0.770135	-2.728983
C	-4.287533	-1.691594	-4.940615
H	-4.457443	-3.818263	-4.481155
H	-3.495439	-2.890217	-3.315901
H	-4.155848	0.484978	-4.887257
H	-3.318415	-0.335035	-3.556816
H	-3.402777	-1.811119	-5.576268
H	-5.172514	-1.691167	-5.591069
C	-10.544356	-0.895598	-1.622418
C	-10.898032	-2.343142	-2.053852
C	-11.643280	-0.378872	-0.670939
H	-10.529923	-0.258031	-2.519340
C	-12.281050	-2.399541	-2.733598
H	-10.902721	-2.971636	-1.154155
H	-10.124118	-2.729340	-2.728331
C	-13.021363	-0.408828	-1.363771
H	-11.689188	-1.042000	0.203477
H	-11.400266	0.634910	-0.329344
C	-13.366398	-1.852277	-1.784683
H	-12.510934	-3.432841	-3.017121
H	-12.263780	-1.791915	-3.649248
H	-13.786522	-0.017552	-0.683817
H	-13.000025	0.235177	-2.253423
H	-14.349035	-1.885494	-2.269147
H	-13.404345	-2.485676	-0.888665
C	-7.494629	-0.889140	2.447596
C	-7.476099	0.572987	2.958328
C	-8.611101	-1.646578	3.199895
H	-6.538498	-1.358707	2.709274
C	-7.207030	0.612479	4.477495
H	-8.451053	1.029980	2.737248
H	-6.710489	1.147319	2.427077
C	-8.331236	-1.654111	4.714250
H	-9.562095	-1.127272	3.027236
H	-8.724954	-2.668581	2.814724
C	-8.265418	-0.206194	5.245974
H	-7.203169	1.650209	4.829910
H	-6.211937	0.188993	4.670554
H	-9.121178	-2.209311	5.234359
H	-7.376202	-2.163898	4.901689
H	-8.040124	-0.202517	6.318344
H	-9.249712	0.263618	5.107213
C	-3.907959	-7.660341	-0.676332
C	-2.756990	-8.222353	-1.551333
C	-5.249337	-8.075307	-1.322792
H	-3.858379	-6.563712	-0.707710
C	-2.833044	-7.635838	-2.976353
H	-2.855003	-9.316237	-1.586249
H	-1.789169	-7.986432	-1.099250
C	-5.353317	-7.461842	-2.733950
H	-5.296282	-9.169921	-1.410607
H	-6.086631	-7.729074	-0.708950
C	-4.195259	-7.955453	-3.626426
H	-2.017383	-8.031703	-3.592104

H	-2.708777	-6.545549	-2.914105
H	-6.317115	-7.725043	-3.186676
H	-5.311560	-6.367035	-2.644899
H	-4.258649	-7.496318	-4.619976
H	-4.283717	-9.043510	-3.752112
C	-5.064380	-10.889105	3.012209
C	-4.628450	-12.207657	2.327397
C	-5.097604	-11.092314	4.538330
H	-6.094031	-10.677865	2.689717
C	-5.626688	-13.332646	2.672272
H	-3.622576	-12.474391	2.679348
H	-4.579629	-12.064696	1.241570
C	-6.107347	-12.204581	4.890981
H	-4.098974	-11.384772	4.894512
H	-5.380806	-10.152553	5.028537
C	-5.716459	-13.528368	4.200136
H	-5.327233	-14.268321	2.186266
H	-6.618399	-13.051725	2.289255
H	-6.156906	-12.341556	5.977782
H	-7.101763	-11.895244	4.539434
H	-6.447251	-14.310009	4.437731
H	-4.738352	-13.856031	4.578122
C	-1.693750	-7.186352	3.909638
C	-2.479182	-6.512600	5.060627
C	-0.637505	-8.158464	4.484082
H	-1.158952	-6.397919	3.365938
C	-1.518239	-5.783656	6.023357
H	-3.031245	-7.288143	5.610458
H	-3.210998	-5.813092	4.637842
C	0.322795	-7.421957	5.439570
H	-1.145819	-8.957805	5.038982
H	-0.084345	-8.624432	3.660161
C	-0.467953	-6.761878	6.588406
H	-2.084273	-5.318945	6.838714
H	-1.003102	-4.982318	5.476111
H	1.063193	-8.123039	5.840883
H	0.863064	-6.644542	4.882459
H	0.214099	-6.235577	7.265945
H	-0.979081	-7.544072	7.166048
C	-8.613270	-5.090862	5.423031
C	-8.917371	-5.524454	4.231648
C	-9.264664	-5.950516	3.040885
H	-7.592468	-4.825410	5.686463
H	-9.383998	-4.980081	6.183753
N	-9.677768	-4.999425	2.042340
S	-11.371354	-4.692134	2.024999
O	-11.549682	-3.518045	1.179535
O	-12.088501	-5.924297	1.718830
H	-9.260532	-7.012139	2.796813
C	-8.385172	-9.805945	0.733933
C	-7.956327	-9.191773	1.916137
C	-9.289198	-10.851078	0.844760
H	-8.004831	-9.478498	-0.229694
C	-8.400943	-9.621330	3.194332
C	-9.755422	-11.283159	2.102888
H	-9.640274	-11.349833	-0.053314

C	-9.320896	-10.679592	3.272220
C	-7.691631	-8.841581	4.172497
C	-6.861889	-7.998157	3.469641
H	-6.545428	-7.663406	1.407857
H	-10.463368	-12.104673	2.152058
H	-9.676401	-11.027683	4.238979
N	-7.052667	-8.184173	2.119080
C	-7.839970	-8.946986	5.657592
H	-7.069662	-8.366275	6.174382
H	-8.813295	-8.570385	5.994822
H	-7.755342	-9.987806	5.994536
C	-5.868888	-6.990069	3.938587
H	-4.984818	-6.999488	3.294255
H	-6.284962	-5.975531	3.931517
H	-5.540158	-7.216327	4.956884
H	-0.493042	2.181680	4.331485
H	2.403539	-3.696200	-3.167026
C	-11.714202	-4.260443	3.708303
C	-12.118819	-5.250628	4.601417
C	-11.584563	-2.934258	4.099829
C	-12.373164	-4.894247	5.919597
H	-12.226748	-6.274860	4.259833
C	-11.841587	-2.597038	5.425325
H	-11.303901	-2.182955	3.370660
C	-12.233714	-3.567980	6.349882
H	-12.688838	-5.654158	6.629218
H	-11.738478	-1.563196	5.744592
C	-12.541888	-3.193673	7.775892
H	-11.992964	-2.299090	8.079738
H	-13.611158	-2.984918	7.893356
H	-12.288866	-4.006816	8.461545
C	-9.198100	-5.264626	0.698909
C	-8.664725	-4.197074	-0.013743
C	-8.187680	-4.408647	-1.304506
C	-8.234807	-5.676402	-1.870538
C	-8.779653	-6.740182	-1.151327
C	-9.275031	-6.538351	0.132559
H	-8.641165	-3.202803	0.419772
H	-7.793298	-3.562143	-1.850689
H	-7.857965	-5.833968	-2.876625
H	-8.844020	-7.726939	-1.601024
H	-9.730492	-7.358915	0.678749

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**II(S)-5, E(PCM, mixed basis set, opt) = -5013.199373 - E(PCM, 6-31+G\*, single point) = -5023.849005**

C	-4.404317	-2.381665	0.600329
C	-3.090160	-2.421356	1.011502
C	-2.507444	-1.226201	1.541711
C	-3.255211	-0.019514	1.498343
C	-4.566618	-0.032540	0.964184
C	-5.172635	-1.193185	0.547278
H	-0.646546	-2.113043	2.216098
C	-1.218878	-1.194230	2.141000
C	-2.683973	1.177760	2.006674
H	-5.122571	0.899786	0.912281
C	-1.431019	1.197974	2.565979

C	-0.706295	-0.024015	2.634669
H	-3.273688	2.090677	1.956555
H	0.277221	-0.023630	3.098307
C	-2.328056	-3.684890	0.865783
C	-1.104969	-3.732184	0.120594
C	-2.839784	-4.861307	1.371598
C	-0.574945	-2.612568	-0.580080
C	-0.396578	-4.960350	0.037772
C	-2.186544	-6.112069	1.234531
C	0.603924	-2.710999	-1.270004
H	-1.119551	-1.675181	-0.578774
C	0.832434	-5.019712	-0.672283
C	-0.958897	-6.122443	0.618036
C	1.345897	-3.923297	-1.317762
H	0.983978	-1.843399	-1.803938
H	1.358947	-5.971089	-0.709670
H	-0.423034	-7.064845	0.536333
C	-0.819207	2.460094	3.113042
H	-1.505243	3.306802	3.012900
H	0.109143	2.705407	2.582182
C	2.642226	-3.978440	-2.081183
H	3.097997	-4.971291	-2.012240
H	3.357434	-3.244256	-1.690056
C	-6.572109	-1.196820	0.050459
C	-7.621704	-0.803799	0.909687
C	-6.845202	-1.521269	-1.300764
C	-8.923504	-0.719407	0.399153
C	-8.158148	-1.420073	-1.766278
C	-9.211163	-1.024403	-0.932007
H	-9.726391	-0.431368	1.065100
H	-8.371075	-1.645399	-2.809696
C	-2.814300	-7.376825	1.704175
C	-3.669211	-8.092551	0.825639
C	-2.539586	-7.867039	2.992890
C	-4.238756	-9.280482	1.277879
C	-3.155444	-9.054351	3.413624
C	-4.011023	-9.764507	2.573855
H	-4.912736	-9.836019	0.631293
H	-2.973719	-9.413670	4.419094
O	-4.037595	-4.821301	2.090882
O	-5.013164	-3.557309	0.156545
P	-5.417053	-4.631401	1.287807
O	-6.263483	-3.846248	2.384417
O	-6.032039	-5.839821	0.722784
H	-7.225670	-3.913175	2.213860
C	-5.737159	-1.911196	-2.274989
C	-5.945683	-3.319781	-2.878711
C	-5.605306	-0.868284	-3.409757
H	-4.779853	-1.926380	-1.743267
C	-4.760601	-3.687052	-3.795979
H	-6.874233	-3.327714	-3.468396
H	-6.042139	-4.053854	-2.071477
C	-4.422008	-1.230208	-4.332561
H	-6.533976	-0.852794	-3.995626
H	-5.464952	0.128004	-2.974395
C	-4.604353	-2.644856	-4.922751

H	-4.908751	-4.688172	-4.219564
H	-3.842576	-3.714592	-3.191806
H	-4.331352	-0.491538	-5.136946
H	-3.493157	-1.204193	-3.746475
H	-3.750756	-2.901053	-5.560429
H	-5.507311	-2.657334	-5.548165
C	-10.630127	-0.986118	-1.488274
C	-11.162298	-2.433480	-1.656831
C	-11.611608	-0.187025	-0.606464
H	-10.595688	-0.514798	-2.483006
C	-12.583716	-2.439714	-2.256718
H	-11.171265	-2.903256	-0.664819
H	-10.479981	-3.009030	-2.293783
C	-13.018019	-0.167944	-1.238274
H	-11.680084	-0.675678	0.374367
H	-11.237319	0.833372	-0.459736
C	-13.546415	-1.609405	-1.383554
H	-12.944650	-3.471150	-2.346098
H	-12.552277	-2.006744	-3.266384
H	-13.697498	0.426766	-0.617705
H	-12.967805	0.302274	-2.230154
H	-14.551441	-1.606876	-1.820974
H	-13.610470	-2.066414	-0.386268
C	-7.391905	-0.479021	2.382871
C	-7.575661	1.035096	2.654666
C	-8.348249	-1.271576	3.300212
H	-6.368057	-0.758178	2.656983
C	-7.295301	1.360512	4.136503
H	-8.610689	1.310341	2.407886
H	-6.914464	1.618017	2.003131
C	-8.065186	-0.966434	4.782427
H	-9.388794	-1.012559	3.073212
H	-8.237767	-2.343982	3.112479
C	-8.226981	0.543058	5.056163
H	-7.429345	2.433408	4.316275
H	-6.250194	1.109080	4.365137
H	-8.752418	-1.546951	5.407655
H	-7.037706	-1.270516	5.025424
H	-8.012218	0.765710	6.107556
H	-9.268498	0.829999	4.856495
C	-3.915414	-7.592007	-0.596240
C	-2.779603	-8.052717	-1.545091
C	-5.261750	-8.037102	-1.213953
H	-3.918336	-6.493975	-0.582185
C	-2.936447	-7.374602	-2.922122
H	-2.837714	-9.145035	-1.650607
H	-1.803453	-7.807854	-1.117005
C	-5.454589	-7.349813	-2.581570
H	-5.261703	-9.126841	-1.356908
H	-6.090602	-7.763247	-0.555124
C	-4.306343	-7.713716	-3.546065
H	-2.128278	-7.687824	-3.592925
H	-2.860472	-6.286049	-2.788760
H	-6.417419	-7.645171	-3.016507
H	-5.478791	-6.262591	-2.422677
H	-4.429227	-7.185196	-4.498851

H	-4.345688	-8.791829	-3.753180
C	-4.728510	-11.032211	3.007650
C	-4.135589	-12.281203	2.311000
C	-4.732933	-11.255298	4.531180
H	-5.774059	-10.940153	2.682808
C	-4.984429	-13.524646	2.652040
H	-3.102773	-12.421958	2.658131
H	-4.109810	-12.124662	1.226285
C	-5.600439	-12.481165	4.879488
H	-3.704960	-11.435914	4.878397
H	-5.112884	-10.357180	5.031754
C	-5.047800	-13.740649	4.179126
H	-4.570659	-14.412515	2.160477
H	-6.003402	-13.368128	2.270443
H	-5.629476	-12.630352	5.965311
H	-6.626258	-12.295464	4.532006
H	-5.671694	-14.610710	4.413516
H	-4.035021	-13.941527	4.555190
C	-1.654748	-7.077743	3.951769
C	-2.531279	-6.168117	4.849128
C	-0.755455	-7.967298	4.839830
H	-0.994143	-6.429094	3.362350
C	-1.652149	-5.296039	5.767536
H	-3.181894	-6.810994	5.459011
H	-3.174198	-5.539565	4.222919
C	0.136122	-7.089983	5.744892
H	-1.380473	-8.602923	5.480074
H	-0.142389	-8.621500	4.209161
C	-0.733597	-6.179117	6.636302
H	-2.283371	-4.662718	6.400781
H	-1.032654	-4.635857	5.144860
H	0.779972	-7.724526	6.364285
H	0.784416	-6.465063	5.115994
H	-0.098421	-5.555065	7.275027
H	-1.354641	-6.807027	7.289502
C	-10.419825	-7.597142	4.410665
C	-9.780685	-6.498826	4.117774
C	-9.152341	-5.387206	3.817144
H	-11.345388	-7.562450	4.979928
H	-10.048669	-8.564303	4.076823
N	-9.439204	-4.592224	2.644628
S	-10.838482	-3.633492	2.841408
O	-10.774275	-3.110521	4.196414
O	-10.907360	-2.737138	1.697603
H	-8.409675	-4.961599	4.487254
C	-8.007253	-10.073343	0.727612
C	-7.683708	-9.418021	1.920586
C	-8.729491	-11.255429	0.815202
H	-7.676474	-9.682757	-0.230519
C	-8.037257	-9.953227	3.189238
C	-9.122094	-11.781375	2.060711
H	-8.988963	-11.789222	-0.093793
C	-8.781234	-11.142453	3.244169
C	-7.442113	-9.107451	4.188180
C	-6.774855	-8.116210	3.505033
H	-6.532161	-7.667150	1.462607



H	-9.690044	-12.706051	2.091489
H	-9.067468	-11.566611	4.204081
N	-6.950106	-8.287664	2.151735
C	-7.547944	-9.300542	5.667853
H	-6.857053	-8.645233	6.206629
H	-8.558832	-9.080931	6.035169
H	-7.315381	-10.334538	5.951654
C	-5.904892	-7.002591	3.977765
H	-4.957890	-7.016350	3.426187
H	-6.376338	-6.025894	3.819834
H	-5.680394	-7.105323	5.042367
H	-0.569395	2.344028	4.175012
H	2.480958	-3.747347	-3.141560
C	-12.193786	-4.765025	2.725883
C	-12.572061	-5.232146	1.469371
C	-12.826581	-5.196255	3.888878
C	-13.603845	-6.161558	1.388313
H	-12.075798	-4.865297	0.574959
C	-13.860402	-6.117344	3.783572
H	-12.507799	-4.804573	4.849748
C	-14.257446	-6.616228	2.536886
H	-13.911328	-6.535214	0.416067
H	-14.371695	-6.455506	4.681290
C	-15.375969	-7.621104	2.446980
H	-15.118697	-8.537286	2.987990
H	-16.292913	-7.224102	2.893757
H	-15.589271	-7.887207	1.409419
C	-9.194611	-5.114139	1.318751
C	-8.815532	-4.205891	0.325171
C	-8.567886	-4.667614	-0.963760
C	-8.676274	-6.020350	-1.266221
C	-9.058023	-6.916980	-0.272153
C	-9.324300	-6.471449	1.018968
H	-8.750331	-3.143349	0.545448
H	-8.287507	-3.948197	-1.722420
H	-8.469769	-6.372992	-2.272322
H	-9.171960	-7.972696	-0.495833
H	-9.624571	-7.180625	1.781635

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**I1(R)-1, E(PCM, mixed basis set, opt) = -5013.197492 - E(PCM, 6-31+G\*, single point) = -5023.841185**

C	-4.439547	-2.479423	0.824983
C	-3.160286	-2.487415	1.340699
C	-2.715415	-1.343998	2.078655
C	-3.542515	-0.190743	2.132025
C	-4.790281	-0.202195	1.461155
C	-5.264915	-1.324959	0.830027
H	-0.854807	-2.200951	2.791624
C	-1.484814	-1.317763	2.789930
C	-3.103800	0.954871	2.848018
H	-5.383769	0.707324	1.437494
C	-1.905433	0.971999	3.517571
C	-1.101195	-0.200883	3.484173
H	-3.750241	1.829756	2.864829
H	-0.161528	-0.206654	4.031014
C	-2.284434	-3.661209	1.103407
C	-1.007378	-3.536453	0.466731
C	-2.734730	-4.919142	1.432243
C	-0.509925	-2.306706	-0.046333
C	-0.208394	-4.699438	0.301545
C	-1.978561	-6.101884	1.227940
C	0.721928	-2.244232	-0.642637
H	-1.121347	-1.413513	0.022261
C	1.071102	-4.591328	-0.306444
C	-0.715854	-5.959540	0.707248
C	1.550873	-3.392115	-0.770778
H	1.078599	-1.295158	-1.035146
H	1.667858	-5.495147	-0.411006
H	-0.094983	-6.841887	0.577838
C	-1.436146	2.179086	4.284722
H	-2.165446	2.993036	4.223950
H	-0.479848	2.545394	3.890630
C	2.905237	-3.266895	-1.416096
H	2.821113	-2.825039	-2.416684
H	3.390100	-4.243607	-1.511179
C	-6.539081	-1.308880	0.063451
C	-7.780294	-1.407691	0.719540
C	-6.482645	-1.153813	-1.341319
C	-8.954974	-1.379620	-0.045100
C	-7.676321	-1.155423	-2.066002
C	-8.922036	-1.281460	-1.437621
H	-9.910560	-1.455468	0.458826
H	-7.643372	-1.051883	-3.147960
C	-2.557337	-7.427093	1.575470
C	-3.143397	-8.229749	0.563619
C	-2.547449	-7.862193	2.911197
C	-3.737188	-9.433900	0.934337
C	-3.183462	-9.067443	3.242377
C	-3.808391	-9.846290	2.272836
H	-4.217293	-10.048412	0.177754
H	-3.224769	-9.369000	4.283558
O	-3.992296	-5.026999	2.029253
O	-4.927131	-3.612350	0.174732
P	-5.257257	-4.937921	1.030603
O	-6.416296	-4.534586	2.038533

O	-5.500405	-6.120554	0.192962
H	-7.166756	-5.165924	2.000991
C	-5.152921	-0.949852	-2.064758
C	-4.762975	-2.174931	-2.925982
C	-5.180155	0.323666	-2.944271
H	-4.363397	-0.810926	-1.316600
C	-3.394229	-1.950623	-3.601306
H	-5.530509	-2.321916	-3.699971
H	-4.734102	-3.070492	-2.295621
C	-3.807833	0.547928	-3.612645
H	-5.942807	0.208407	-3.725250
H	-5.457131	1.187155	-2.328623
C	-3.419548	-0.675496	-4.468654
H	-3.131582	-2.822225	-4.211289
H	-2.625446	-1.844555	-2.823432
H	-3.834593	1.452098	-4.231201
H	-3.047893	0.696364	-2.833608
H	-2.442390	-0.516294	-4.938640
H	-4.161479	-0.801650	-5.268811
C	-10.180423	-1.344272	-2.297824
C	-10.171024	-2.645935	-3.142610
C	-11.489143	-1.294569	-1.484109
H	-10.168298	-0.484641	-2.985821
C	-11.388913	-2.692533	-4.087457
H	-10.210341	-3.500331	-2.455233
H	-9.237599	-2.715698	-3.714509
C	-12.715717	-1.332370	-2.419194
H	-11.525462	-2.179995	-0.834131
H	-11.512462	-0.395296	-0.855784
C	-12.695752	-2.616966	-3.272394
H	-11.364844	-3.614090	-4.679634
H	-11.344265	-1.842349	-4.782789
H	-13.635505	-1.286662	-1.824907
H	-12.697162	-0.454180	-3.079046
H	-13.565268	-2.643267	-3.938991
H	-12.744608	-3.487753	-2.606313
C	-7.854881	-1.497531	2.239451
C	-8.068308	-0.083922	2.839714
C	-8.991727	-2.413820	2.735777
H	-6.906589	-1.900230	2.616874
C	-8.085292	-0.136037	4.381396
H	-9.027833	0.303162	2.468554
H	-7.281554	0.593836	2.493229
C	-8.986663	-2.500816	4.274067
H	-9.952596	-1.982719	2.429216
H	-8.911556	-3.409110	2.279261
C	-9.182269	-1.097520	4.883839
H	-8.243674	0.868567	4.789984
H	-7.108430	-0.492290	4.735206
H	-9.784065	-3.176291	4.608542
H	-8.027049	-2.916458	4.611431
H	-9.168702	-1.149965	5.978419
H	-10.165040	-0.711898	4.576636
C	-3.091462	-7.807949	-0.901664
C	-1.816044	-8.390062	-1.564263
C	-4.321604	-8.236387	-1.734470

H	-3.038239	-6.712352	-0.947586
C	-1.668512	-7.874099	-3.009347
H	-1.898303	-9.485991	-1.562595
H	-0.933251	-8.123242	-0.974296
C	-4.191317	-7.702010	-3.176126
H	-4.390240	-9.332369	-1.770592
H	-5.230349	-7.831732	-1.278408
C	-2.911170	-8.243091	-3.846057
H	-0.764646	-8.290757	-3.468344
H	-1.560951	-6.780928	-2.984929
H	-5.074528	-7.986511	-3.761463
H	-4.152976	-6.604362	-3.141581
H	-2.815512	-7.845604	-4.862830
H	-2.981583	-9.337257	-3.916981
C	-4.649022	-11.067909	2.611267
C	-4.018732	-12.378131	2.081126
C	-4.952431	-11.218672	4.113894
H	-5.614647	-10.935782	2.098957
C	-4.997676	-13.553194	2.292894
H	-3.082880	-12.566024	2.624820
H	-3.775377	-12.275097	1.016616
C	-5.948167	-12.374479	4.330196
H	-4.020027	-11.440472	4.653737
H	-5.367536	-10.283448	4.507070
C	-5.368788	-13.696854	3.784431
H	-4.559930	-14.485828	1.918837
H	-5.912496	-13.355256	1.715713
H	-6.188809	-12.473211	5.394992
H	-6.877923	-12.132673	3.796483
H	-6.090145	-14.511321	3.916548
H	-4.465401	-13.952696	4.354477
C	-1.880565	-7.046330	4.011263
C	-2.914773	-6.501340	5.024091
C	-0.811174	-7.885136	4.751063
H	-1.370275	-6.186581	3.559311
C	-2.217082	-5.661989	6.115004
H	-3.437959	-7.348656	5.488368
H	-3.658258	-5.894737	4.492993
C	-0.111866	-7.041355	5.835997
H	-1.298086	-8.747039	5.226253
H	-0.082352	-8.268134	4.027440
C	-1.145717	-6.498555	6.843981
H	-2.956764	-5.283146	6.829421
H	-1.735069	-4.795014	5.642184
H	0.643332	-7.644288	6.352692
H	0.402534	-6.196633	5.358025
H	-0.647450	-5.893492	7.609896
H	-1.633157	-7.343854	7.348278
C	-9.049489	-5.786720	4.201078
C	-9.077093	-6.155139	2.951541
C	-9.123922	-6.551642	1.699935
H	-8.138969	-5.400000	4.650085
H	-9.939094	-5.868767	4.822273
N	-9.540435	-5.650215	0.657184
S	-11.214914	-5.742928	0.336807
O	-11.470233	-4.772987	-0.719448

O	-11.626725	-7.132190	0.163884
H	-8.897281	-7.582068	1.427025
C	-6.018814	-7.609380	3.562705
C	-6.717762	-8.449785	2.689796
C	-6.358505	-7.667355	4.904501
H	-5.198951	-6.992257	3.203450
C	-7.723830	-9.343289	3.134607
C	-7.369645	-8.536651	5.370193
H	-5.830070	-7.036595	5.614147
C	-8.047038	-9.376665	4.502024
C	-8.172628	-10.079384	1.983366
C	-7.440047	-9.612850	0.913036
H	-5.963944	-8.065671	0.757677
H	-7.604366	-8.555193	6.430491
H	-8.806273	-10.061568	4.871682
N	-6.587114	-8.618950	1.339537
C	-9.191802	-11.176116	1.981134
H	-10.112677	-10.862174	2.485104
H	-9.457337	-11.473299	0.962678
H	-8.825148	-12.069750	2.501781
C	-7.378916	-10.104494	-0.497270
H	-6.674201	-10.941423	-0.585114
H	-8.356339	-10.454132	-0.840300
H	-7.037953	-9.312982	-1.169391
H	-1.281534	1.934167	5.342901
H	3.559528	-2.615351	-0.823203
C	-11.883921	-5.145245	1.861615
C	-12.313979	-6.042444	2.832569
C	-11.908152	-3.770316	2.072293
C	-12.754895	-5.541150	4.054463
H	-12.291804	-7.108712	2.631543
C	-12.345500	-3.289751	3.298235
H	-11.580901	-3.100562	1.282552
C	-12.761310	-4.166358	4.308043
H	-13.092703	-6.228822	4.824512
H	-12.354463	-2.218212	3.484120
C	-13.195837	-3.618545	5.641797
H	-14.020553	-2.909318	5.522380
H	-13.523764	-4.413604	6.315328
H	-12.370222	-3.081182	6.122141
C	-8.731370	-5.723573	-0.542956
C	-8.102394	-4.562532	-0.972127
C	-8.578742	-6.924759	-1.237711
C	-7.309742	-4.602450	-2.116468
H	-8.252573	-3.634844	-0.431150
C	-7.777871	-6.954279	-2.375316
H	-9.097835	-7.817148	-0.896191
C	-7.142491	-5.792940	-2.814930
H	-6.840658	-3.686171	-2.451504
H	-7.662650	-7.881501	-2.930501
H	-6.522962	-5.818267	-3.706089

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**I1(R)-2, E(PCM, mixed basis set, opt) = -5013.197144 - E(PCM, 6-31+G\*, single point) = -5023.847127**

C	-4.432562	-2.505843	0.901640
C	-3.151962	-2.480046	1.414547

C	-2.738712	-1.327407	2.157077
C	-3.594288	-0.195546	2.212654
C	-4.836665	-0.234263	1.532159
C	-5.281283	-1.367487	0.897355
H	-0.856140	-2.139063	2.865779
C	-1.508731	-1.272154	2.867786
C	-3.184908	0.958044	2.932529
H	-5.445524	0.664635	1.496076
C	-1.988026	1.003042	3.603218
C	-1.154051	-0.148212	3.565914
H	-3.852265	1.816970	2.950618
H	-0.214289	-0.131628	4.112384
C	-2.236213	-3.618823	1.156510
C	-0.972119	-3.438410	0.505915
C	-2.638353	-4.896907	1.468529
C	-0.521646	-2.183815	0.009164
C	-0.138378	-4.571320	0.307700
C	-1.848777	-6.050487	1.228846
C	0.699235	-2.071003	-0.602690
H	-1.159946	-1.311554	0.101721
C	1.128184	-4.410838	-0.315331
C	-0.599393	-5.855408	0.693883
C	1.562587	-3.188560	-0.763700
H	1.019599	-1.103837	-0.982226
H	1.751821	-5.292914	-0.445684
H	0.047013	-6.713959	0.533920
C	-1.550748	2.219309	4.375100
H	-2.294894	3.018945	4.304962
H	-0.596990	2.603544	3.992227
C	2.902551	-3.008528	-1.425961
H	2.790021	-2.553355	-2.417786
H	3.416657	-3.967482	-1.543976
C	-6.530600	-1.371587	0.088795
C	-7.794846	-1.537244	0.689856
C	-6.419272	-1.181907	-1.307565
C	-8.937342	-1.531515	-0.122398
C	-7.581722	-1.207172	-2.080949
C	-8.845513	-1.392421	-1.509384
H	-9.911381	-1.677300	0.329043
H	-7.509824	-1.085482	-3.159451
C	-2.379600	-7.403305	1.545670
C	-2.928429	-8.204758	0.512114
C	-2.359699	-7.868187	2.870680
C	-3.474288	-9.439974	0.851747
C	-2.949875	-9.104649	3.171081
C	-3.536248	-9.886079	2.179998
H	-3.925321	-10.056106	0.078708
H	-2.985562	-9.431057	4.204865
O	-3.884061	-5.052077	2.079350
O	-4.897495	-3.648931	0.253108
P	-5.155333	-5.003217	1.088575
O	-6.318785	-4.679067	2.118525
O	-5.347983	-6.178328	0.227173
H	-7.060027	-5.318321	2.051029
C	-5.068203	-0.938025	-1.978294
C	-4.630455	-2.149394	-2.837298

C	-5.089121	0.342616	-2.845917
H	-4.305899	-0.793488	-1.203525
C	-3.250496	-1.897922	-3.477961
H	-5.376958	-2.305891	-3.630025
H	-4.600882	-3.048942	-2.211941
C	-3.702718	0.592837	-3.475315
H	-5.828859	0.225832	-3.648098
H	-5.393900	1.196490	-2.229793
C	-3.276221	-0.615519	-4.334391
H	-2.961729	-2.760208	-4.089497
H	-2.500488	-1.787800	-2.682496
H	-3.725717	1.503702	-4.084070
H	-2.964826	0.741872	-2.675314
H	-2.291684	-0.437003	-4.781507
H	-3.998823	-0.745094	-5.151463
C	-10.051824	-1.500092	-2.433215
C	-10.003922	-2.868326	-3.164591
C	-11.409950	-1.361233	-1.716331
H	-9.976217	-0.701989	-3.188101
C	-11.160543	-2.991191	-4.176889
H	-10.089475	-3.659770	-2.409790
H	-9.035621	-2.985857	-3.667063
C	-12.565629	-1.460431	-2.734719
H	-11.514512	-2.183876	-0.997342
H	-11.453623	-0.409955	-1.171300
C	-12.515329	-2.821357	-3.459648
H	-11.114659	-3.965772	-4.676217
H	-11.056745	-2.211975	-4.945027
H	-13.526662	-1.338580	-2.222458
H	-12.472505	-0.651687	-3.472874
H	-13.340252	-2.902745	-4.176642
H	-12.623996	-3.621715	-2.716565
C	-7.908536	-1.684838	2.202620
C	-8.126195	-0.290823	2.844032
C	-9.056778	-2.616340	2.645806
H	-6.967841	-2.103328	2.582960
C	-8.166444	-0.392421	4.381617
H	-9.075718	0.114976	2.467593
H	-7.326417	0.388516	2.533201
C	-9.103486	-2.740752	4.182829
H	-10.007904	-2.180979	2.312441
H	-8.953941	-3.602574	2.174203
C	-9.285844	-1.352131	4.831417
H	-8.315461	0.601123	4.820067
H	-7.200345	-0.775486	4.737020
H	-9.937091	-3.392131	4.469058
H	-8.169439	-3.196095	4.538245
H	-9.295546	-1.440367	5.923651
H	-10.255926	-0.940960	4.517981
C	-2.886022	-7.750824	-0.943742
C	-1.596052	-8.287784	-1.616257
C	-4.104576	-8.189478	-1.787946
H	-2.857757	-6.653813	-0.966690
C	-1.457926	-7.735830	-3.048964
H	-1.651892	-9.385139	-1.640591
H	-0.721066	-8.014193	-1.017547

C	-3.983842	-7.620035	-3.216742
H	-4.147938	-9.285701	-1.849156
H	-5.023009	-7.816499	-1.324535
C	-2.690184	-8.115785	-3.896249
H	-0.543101	-8.120044	-3.514475
H	-1.377220	-6.641063	-2.999365
H	-4.859755	-7.911013	-3.809879
H	-3.970182	-6.522810	-3.157687
H	-2.602493	-7.693822	-4.903854
H	-2.734592	-9.209473	-3.991389
C	-4.324914	-11.150862	2.483990
C	-3.629208	-12.417815	1.930511
C	-4.633740	-11.349634	3.980122
H	-5.291563	-11.052384	1.965795
C	-4.550480	-13.643821	2.109309
H	-2.688710	-12.571695	2.476535
H	-3.384744	-12.279202	0.870499
C	-5.572568	-12.558137	4.162477
H	-3.695924	-11.536050	4.523934
H	-5.100158	-10.446387	4.390372
C	-4.923896	-13.837648	3.594479
H	-4.064201	-14.545093	1.719141
H	-5.470135	-13.478907	1.529519
H	-5.816187	-12.691546	5.222660
H	-6.509236	-12.350773	3.625897
H	-5.603431	-14.690738	3.703408
H	-4.012503	-14.059814	4.166048
C	-1.722690	-7.055557	3.991035
C	-2.771708	-6.564842	5.016581
C	-0.628098	-7.877564	4.712744
H	-1.239736	-6.169979	3.559194
C	-2.095758	-5.726478	6.122304
H	-3.267462	-7.437451	5.463796
H	-3.534862	-5.969838	4.500504
C	0.049416	-7.036678	5.813260
H	-1.090368	-8.761404	5.172153
H	0.109250	-8.227147	3.980969
C	-0.997659	-6.543361	6.833382
H	-2.844291	-5.382212	6.845000
H	-1.640767	-4.837100	5.664148
H	0.821996	-7.628457	6.317020
H	0.539561	-6.168554	5.352173
H	-0.515607	-5.936954	7.608646
H	-1.457683	-7.411768	7.323916
C	-8.968234	-6.091343	4.206621
C	-8.921427	-6.404466	2.942723
C	-8.926873	-6.732502	1.670248
H	-8.094598	-5.701135	4.721009
H	-9.887226	-6.226464	4.773729
N	-9.334258	-5.776397	0.674497
S	-11.009281	-5.805739	0.312114
O	-11.263311	-4.604912	-0.473284
O	-11.381262	-7.113158	-0.221630
H	-8.664844	-7.737545	1.340428
C	-5.834585	-7.775270	3.541342
C	-6.499499	-8.614024	2.640151



C	-6.178548	-7.884198	4.878457
H	-5.038477	-7.116263	3.203705
C	-7.479221	-9.551382	3.051673
C	-7.161056	-8.801511	5.312116
H	-5.676477	-7.256074	5.609251
C	-7.806336	-9.636897	4.415692
C	-7.900475	-10.263443	1.874794
C	-7.177560	-9.741511	0.823376
H	-5.757553	-8.135923	0.726088
H	-7.399405	-8.860616	6.370070
H	-8.544228	-10.356515	4.761680
N	-6.356574	-8.736628	1.286171
C	-8.877011	-11.397686	1.836545
H	-9.805126	-11.139482	2.358589
H	-9.138661	-11.667434	0.809454
H	-8.471521	-12.295011	2.320688
C	-7.093861	-10.180696	-0.602617
H	-6.323827	-10.953221	-0.726006
H	-8.044086	-10.597373	-0.946467
H	-6.826092	-9.342607	-1.251183
H	-1.404519	1.978152	5.435408
H	3.544701	-2.346313	-0.831489
C	-11.754043	-5.641104	1.908718
C	-12.146918	-6.788659	2.594812
C	-11.927800	-4.375920	2.452333
C	-12.709607	-6.654364	3.857412
H	-12.006924	-7.764080	2.140541
C	-12.497920	-4.260791	3.717855
H	-11.630898	-3.488094	1.906275
C	-12.890647	-5.392364	4.437643
H	-13.017155	-7.542418	4.402711
H	-12.633334	-3.274089	4.152577
C	-13.524488	-5.260978	5.797634
H	-14.616229	-5.236452	5.710738
H	-13.263751	-6.107864	6.437858
H	-13.209158	-4.340342	6.294749
C	-8.536223	-5.810492	-0.536350
C	-7.910772	-4.636850	-0.936352
C	-8.391480	-6.988265	-1.272200
C	-7.136142	-4.637245	-2.094119
H	-8.040626	-3.727473	-0.360724
C	-7.605565	-6.979713	-2.420371
H	-8.907442	-7.891535	-0.957038
C	-6.979014	-5.803605	-2.833615
H	-6.673774	-3.707926	-2.402977
H	-7.496684	-7.889461	-3.005166
H	-6.372478	-5.800918	-3.734043

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**I1(R)-3, E(PCM, mixed basis set, opt) = -5013.194831 - E(PCM, 6-31+G\*, single point) = -5023.847446**

C	-4.310508	-2.456818	0.739102
C	-3.059219	-2.378808	1.315935
C	-2.714701	-1.189512	2.034965
C	-3.607652	-0.086039	2.018216
C	-4.820205	-0.188596	1.292646
C	-5.197743	-1.353006	0.669617

H	-0.841555	-1.916155	2.856035
C	-1.521814	-1.072872	2.800757
C	-3.270433	1.099699	2.724326
H	-5.474220	0.677233	1.232181
C	-2.107611	1.204356	3.446058
C	-1.235602	0.081680	3.479567
H	-3.967409	1.934403	2.689702
H	-0.322684	0.144556	4.066705
C	-2.114414	-3.513026	1.174812
C	-0.804323	-3.354187	0.615595
C	-2.527692	-4.778664	1.518467
C	-0.328840	-2.123599	0.084346
C	0.054604	-4.484674	0.550712
C	-1.717321	-5.933467	1.393308
C	0.935524	-2.026849	-0.434619
H	-0.981661	-1.257450	0.080597
C	1.365114	-4.339869	0.022243
C	-0.426585	-5.753196	0.961919
C	1.820381	-3.138987	-0.461786
H	1.275500	-1.077816	-0.841863
H	2.006970	-5.217846	-0.005481
H	0.230356	-6.615274	0.888938
C	-1.744747	2.455376	4.200999
H	-2.515643	3.223665	4.085422
H	-0.793448	2.866214	3.839777
C	3.206282	-2.977659	-1.027275
H	3.166049	-2.647484	-2.072918
H	3.762387	-3.919301	-0.986241
C	-6.457423	-1.435873	-0.115075
C	-7.704749	-1.448651	0.538830
C	-6.394034	-1.441873	-1.528165
C	-8.876224	-1.456813	-0.230348
C	-7.585950	-1.470295	-2.255394
C	-8.835941	-1.488658	-1.625136
H	-9.829551	-1.485327	0.280501
H	-7.546293	-1.487325	-3.342391
C	-2.286276	-7.279843	1.653936
C	-2.572231	-8.132845	0.556430
C	-2.570225	-7.690814	2.966396
C	-3.098545	-9.396546	0.817872
C	-3.123411	-8.960417	3.179991
C	-3.399190	-9.820496	2.120565
H	-3.335357	-10.060657	-0.010114
H	-3.370598	-9.258860	4.192350
O	-3.809180	-4.933469	2.045968
O	-4.712306	-3.631965	0.104056
P	-5.009822	-4.955352	0.973515
O	-6.235153	-4.616793	1.931426
O	-5.135628	-6.169442	0.155574
H	-6.971175	-5.245060	1.787822
C	-5.063170	-1.410285	-2.273836
C	-4.806359	-2.716398	-3.065589
C	-4.986674	-0.197477	-3.232572
H	-4.248361	-1.302992	-1.547724
C	-3.429608	-2.661585	-3.760080
H	-5.594369	-2.836017	-3.823710

H	-4.850841	-3.573163	-2.384783
C	-3.612163	-0.142143	-3.930739
H	-5.773196	-0.292553	-3.992833
H	-5.171887	0.725083	-2.670195
C	-3.346322	-1.447820	-4.708644
H	-3.251050	-3.591846	-4.311809
H	-2.648870	-2.574034	-2.991303
H	-3.569782	0.719534	-4.606543
H	-2.829587	-0.011162	-3.171107
H	-2.363434	-1.407299	-5.191920
H	-4.104950	-1.557091	-5.495460
C	-10.092531	-1.643263	-2.476244
C	-10.171830	-3.119510	-2.950190
C	-11.391376	-1.270260	-1.731177
H	-10.000597	-0.996958	-3.362959
C	-11.423693	-3.381933	-3.810087
H	-10.200927	-3.748729	-2.052494
H	-9.261206	-3.377232	-3.504881
C	-12.628253	-1.511161	-2.620581
H	-11.481540	-1.908625	-0.844970
H	-11.345662	-0.224601	-1.402751
C	-12.696905	-2.996443	-3.030836
H	-11.458010	-4.439626	-4.101136
H	-11.371480	-2.782588	-4.729761
H	-13.535417	-1.224538	-2.076996
H	-12.565230	-0.888435	-3.523779
H	-13.589939	-3.188335	-3.636948
H	-12.759946	-3.614036	-2.123436
C	-7.809298	-1.458994	2.059936
C	-8.225203	-0.061048	2.581337
C	-8.812984	-2.510801	2.584515
H	-6.825554	-1.704017	2.479931
C	-8.263042	-0.042987	4.123443
H	-9.222181	0.173206	2.181830
H	-7.529197	0.698272	2.206569
C	-8.838632	-2.511719	4.125526
H	-9.820511	-2.288287	2.213583
H	-8.538046	-3.502991	2.210843
C	-9.233338	-1.118125	4.656593
H	-8.561514	0.949250	4.480858
H	-7.253377	-0.248749	4.505548
H	-9.548526	-3.269364	4.476099
H	-7.841057	-2.776046	4.502778
H	-9.237168	-1.114442	5.752358
H	-10.250824	-0.883261	4.315908
C	-2.331653	-7.678937	-0.881215
C	-1.007639	-8.258374	-1.436617
C	-3.478833	-8.059962	-1.844610
H	-2.257330	-6.584357	-0.893499
C	-0.718239	-7.687433	-2.841573
H	-1.101991	-9.352414	-1.486921
H	-0.179774	-8.028113	-0.757875
C	-3.214436	-7.474153	-3.247286
H	-3.544423	-9.153013	-1.926321
H	-4.424543	-7.667415	-1.457274
C	-1.877761	-8.001154	-3.810325

H	0.220736	-8.098495	-3.229866
H	-0.599831	-6.597656	-2.759441
H	-4.038263	-7.735940	-3.922263
H	-3.177674	-6.378296	-3.172802
H	-1.678995	-7.561119	-4.794291
H	-1.950874	-9.090034	-3.937555
C	-4.094915	-11.159588	2.311365
C	-3.164883	-12.345688	1.958677
C	-4.667826	-11.366828	3.726378
H	-4.942701	-11.181225	1.609710
C	-3.956340	-13.670002	2.005353
H	-2.342117	-12.375199	2.686049
H	-2.727688	-12.199243	0.963509
C	-5.480708	-12.674708	3.774730
H	-3.839225	-11.431409	4.446942
H	-5.302261	-10.516592	4.001932
C	-4.593460	-13.879321	3.395760
H	-3.302222	-14.513481	1.756949
H	-4.754153	-13.629406	1.249284
H	-5.911576	-12.815998	4.772629
H	-6.312252	-12.591304	3.061441
H	-5.182599	-14.803500	3.405385
H	-3.794416	-13.982761	4.142359
C	-2.290963	-6.795489	4.165923
C	-3.573687	-6.504427	4.981319
C	-1.218214	-7.433440	5.081214
H	-1.898369	-5.833643	3.813575
C	-3.255987	-5.584222	6.178439
H	-3.993911	-7.450529	5.348770
H	-4.317048	-6.033069	4.327905
C	-0.904463	-6.516288	6.280378
H	-1.596381	-8.396462	5.450216
H	-0.311716	-7.630281	4.496632
C	-2.186682	-6.224514	7.087519
H	-4.169585	-5.380402	6.748445
H	-2.878077	-4.625099	5.798927
H	-0.148432	-6.982969	6.922212
H	-0.491801	-5.568481	5.908948
H	-1.960680	-5.565002	7.933038
H	-2.578225	-7.167875	7.492018
C	-10.722820	-9.205434	1.493523
C	-10.139861	-8.093893	1.843977
C	-9.503911	-6.987839	2.143338
H	-11.778569	-9.383885	1.676194
H	-10.141975	-9.969356	0.983353
N	-9.443324	-5.861546	1.238335
S	-10.919077	-5.012278	1.168415
O	-11.341501	-4.834916	2.547788
O	-10.720167	-3.864330	0.297734
H	-8.987105	-6.866563	3.091266
C	-6.192995	-7.940704	2.893395
C	-6.529895	-8.874926	1.907914
C	-6.780710	-8.089109	4.139293
H	-5.439718	-7.182412	2.700145
C	-7.398468	-9.967536	2.154906
C	-7.686998	-9.142068	4.396997

H	-6.530870	-7.390665	4.933188
C	-7.987966	-10.082679	3.425692
C	-7.439931	-10.751006	0.949363
C	-6.619146	-10.110463	0.043579
H	-5.473179	-8.300634	0.186621
H	-8.133349	-9.227198	5.383113
H	-8.665560	-10.903917	3.646572
N	-6.092594	-8.979385	0.618710
C	-8.064167	-12.102981	0.768492
H	-8.953689	-12.225178	1.395641
H	-8.357920	-12.282499	-0.271073
H	-7.368679	-12.906406	1.046958
C	-6.199969	-10.559617	-1.319551
H	-5.429107	-11.338824	-1.253254
H	-7.045483	-10.980138	-1.872733
H	-5.784329	-9.731991	-1.899581
H	-1.625773	2.245753	5.271337
H	3.770288	-2.221397	-0.466835
C	-12.055986	-6.094103	0.346225
C	-11.913372	-6.278534	-1.027773
C	-13.036572	-6.758757	1.075655
C	-12.770203	-7.161240	-1.674457
H	-11.146840	-5.738131	-1.577238
C	-13.888815	-7.629795	0.407656
H	-13.120538	-6.587295	2.144224
C	-13.764528	-7.847139	-0.969362
H	-12.669449	-7.316082	-2.745099
H	-14.664608	-8.152005	0.961503
C	-14.709673	-8.779635	-1.680344
H	-15.673248	-8.289518	-1.857302
H	-14.309473	-9.089022	-2.648766
H	-14.903346	-9.675898	-1.084262
C	-8.667146	-5.965922	0.022092
C	-8.151956	-4.788853	-0.533477
C	-8.399427	-7.194470	-0.586228
C	-7.409457	-4.845022	-1.707713
H	-8.344804	-3.829263	-0.069002
C	-7.639771	-7.234148	-1.753392
H	-8.755496	-8.120793	-0.151163
C	-7.147188	-6.065019	-2.323483
H	-7.039361	-3.912969	-2.115796
H	-7.446158	-8.196401	-2.218108
H	-6.547593	-6.102482	-3.228641

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**I1(R)-4, E(PCM, mixed basis set, opt) = -5013.187015 - E(PCM, 6-31+G\*, single point) = -5023.843983**

C	-4.182679	-2.435637	0.585255
C	-2.912004	-2.402199	1.115527
C	-2.426293	-1.163892	1.642671
C	-3.200598	0.012079	1.463482
C	-4.440175	-0.072784	0.782373
C	-4.965018	-1.273181	0.365138
H	-0.615118	-1.955580	2.534751
C	-1.203406	-1.060418	2.359862
C	-2.717556	1.250892	1.964778
H	-5.005149	0.838690	0.600956

C	-1.526973	1.339617	2.642306
C	-0.776741	0.148178	2.842371
H	-3.322663	2.141427	1.806543
H	0.156242	0.204401	3.397751
C	-2.074164	-3.624490	1.060134
C	-0.799705	-3.605620	0.403066
C	-2.548778	-4.822914	1.549865
C	-0.293100	-2.467331	-0.285115
C	-0.009787	-4.786027	0.396540
C	-1.801702	-6.028335	1.494296
C	0.936231	-2.500214	-0.887858
H	-0.894467	-1.567460	-0.344503
C	1.268476	-4.777210	-0.223304
C	-0.535934	-5.970966	0.964296
C	1.756771	-3.661116	-0.854512
H	1.295932	-1.619401	-1.414334
H	1.856167	-5.692534	-0.201858
H	0.064964	-6.876818	0.947360
C	-1.008774	2.646154	3.182298
H	-1.678331	3.473618	2.927716
H	-0.014816	2.869198	2.774083
C	3.106899	-3.643895	-1.519940
H	3.609044	-4.611169	-1.417391
H	3.751543	-2.874133	-1.077356
C	-6.271218	-1.342281	-0.339870
C	-7.451482	-0.889564	0.296492
C	-6.321970	-1.786237	-1.681939
C	-8.650152	-0.875227	-0.423893
C	-7.539977	-1.743783	-2.365081
C	-8.709092	-1.283910	-1.759160
H	-9.551321	-0.517778	0.066412
H	-7.576198	-2.063575	-3.402682
C	-2.380117	-7.311583	1.972201
C	-3.167817	-8.088567	1.086039
C	-2.139469	-7.750257	3.285572
C	-3.733622	-9.267535	1.564330
C	-2.742470	-8.935934	3.727975
C	-3.554207	-9.693216	2.886758
H	-4.367236	-9.861227	0.912324
H	-2.600862	-9.247024	4.755085
O	-3.794762	-4.850756	2.176133
O	-4.704071	-3.653457	0.159242
P	-5.139625	-4.713525	1.296675
O	-6.073622	-3.954069	2.316793
O	-5.680758	-5.949778	0.708877
H	-7.029667	-4.135484	2.128328
C	-5.086289	-2.252632	-2.440802
C	-5.241304	-3.703890	-2.952053
C	-4.767827	-1.308948	-3.625903
H	-4.215576	-2.230705	-1.778613
C	-3.939695	-4.159360	-3.643818
H	-6.069791	-3.747260	-3.672161
H	-5.483746	-4.361595	-2.110905
C	-3.469189	-1.759450	-4.327282
H	-5.599208	-1.336175	-4.343006
H	-4.671683	-0.280480	-3.258619

C	-3.593376	-3.217807	-4.816352
H	-4.042788	-5.189610	-4.004837
H	-3.123024	-4.145368	-2.906732
H	-3.244352	-1.094618	-5.169148
H	-2.636757	-1.691444	-3.613362
H	-2.660928	-3.536148	-5.296512
H	-4.395005	-3.276814	-5.565493
C	-9.996279	-1.176565	-2.559574
C	-11.160341	-1.921091	-1.872973
C	-10.376172	0.308687	-2.773886
H	-9.830517	-1.632453	-3.546257
C	-12.461116	-1.797749	-2.690788
H	-11.321531	-1.478331	-0.880592
H	-10.891435	-2.973195	-1.724286
C	-11.675822	0.432248	-3.595526
H	-10.519343	0.776210	-1.789790
H	-9.550885	0.827789	-3.274112
C	-12.830835	-0.314230	-2.895688
H	-13.273771	-2.324868	-2.177731
H	-12.320144	-2.273414	-3.671004
H	-11.932848	1.488136	-3.735766
H	-11.516423	-0.008599	-4.589225
H	-13.750988	-0.229408	-3.484984
H	-13.013721	0.148125	-1.915782
C	-7.452991	-0.371092	1.730837
C	-7.798695	1.138396	1.762690
C	-8.423967	-1.149462	2.647699
H	-6.453143	-0.496755	2.158554
C	-7.730991	1.688246	3.201928
H	-8.813453	1.278183	1.365887
H	-7.111351	1.689884	1.109337
C	-8.328580	-0.603984	4.087928
H	-9.454102	-1.043161	2.278097
H	-8.171147	-2.212138	2.622040
C	-8.679133	0.897226	4.126953
H	-7.990935	2.753153	3.210337
H	-6.702212	1.590202	3.574968
H	-8.993848	-1.168308	4.749604
H	-7.302858	-0.745150	4.453897
H	-8.613120	1.278715	5.152031
H	-9.713136	1.033120	3.781228
C	-3.348346	-7.666813	-0.368486
C	-2.130286	-8.104687	-1.221146
C	-4.626588	-8.225084	-1.029020
H	-3.419509	-6.571049	-0.412399
C	-2.251344	-7.534496	-2.650029
H	-2.106521	-9.202762	-1.250267
H	-1.200654	-7.759212	-0.759024
C	-4.781661	-7.627669	-2.440547
H	-4.552914	-9.318724	-1.113714
H	-5.494732	-7.971936	-0.416050
C	-3.565225	-7.992135	-3.318016
H	-1.390704	-7.842314	-3.255221
H	-2.243671	-6.437516	-2.589306
H	-5.706470	-7.989644	-2.904575
H	-4.857682	-6.536128	-2.348407

H	-3.662364	-7.536901	-4.311294
H	-3.537710	-9.082356	-3.450951
C	-4.300316	-10.933539	3.354331
C	-3.797908	-12.206827	2.630956
C	-4.238421	-11.156842	4.875959
H	-5.357723	-10.789515	3.084666
C	-4.676276	-13.416215	3.015750
H	-2.756146	-12.392157	2.927110
H	-3.816417	-12.056103	1.545263
C	-5.128047	-12.350964	5.271121
H	-3.199160	-11.372460	5.166846
H	-4.565470	-10.251821	5.399199
C	-4.667147	-13.631674	4.543858
H	-4.326889	-14.318940	2.501374
H	-5.707878	-13.219212	2.689871
H	-5.102912	-12.497301	6.357241
H	-6.166441	-12.122850	4.990748
H	-5.310809	-14.477484	4.811333
H	-3.644125	-13.874335	4.862881
C	-1.282769	-6.925716	4.240033
C	-2.176363	-6.019095	5.120705
C	-0.376574	-7.796172	5.139837
H	-0.627638	-6.274094	3.648113
C	-1.314845	-5.133841	6.044537
H	-2.830240	-6.664090	5.724231
H	-2.814337	-5.399178	4.479115
C	0.497255	-6.904208	6.045796
H	-0.997502	-8.436629	5.778989
H	0.247767	-8.445936	4.515682
C	-0.393075	-6.002208	6.925528
H	-1.957942	-4.504371	6.669855
H	-0.696513	-4.469876	5.424553
H	1.144282	-7.527322	6.673555
H	1.142170	-6.273125	5.419518
H	0.227212	-5.367232	7.568280
H	-1.012163	-6.636297	7.574613
C	-8.677113	-6.295976	6.420640
C	-8.936649	-6.471566	5.154825
C	-9.206818	-6.694732	3.893925
H	-7.821777	-5.706013	6.739654
H	-9.285108	-6.756910	7.195466
N	-10.143875	-5.919232	3.129742
S	-9.562374	-5.473294	1.611419
O	-8.733152	-4.259728	1.703548
O	-8.981809	-6.668063	1.023961
H	-8.780595	-7.531750	3.347603
C	-5.494214	-7.451873	4.717984
C	-6.307432	-8.256733	3.913792
C	-5.521123	-7.684630	6.083676
H	-4.847613	-6.698717	4.274674
C	-7.124386	-9.282841	4.451115
C	-6.337419	-8.691680	6.642594
H	-4.899819	-7.079220	6.738200
C	-7.134087	-9.491396	5.840156
C	-7.784167	-9.919368	3.342741
C	-7.359073	-9.265498	2.206229



H	-6.052827	-7.607919	1.901184
H	-6.331373	-8.842956	7.718214
H	-7.751026	-10.274478	6.274697
N	-6.484172	-8.258903	2.555791
C	-8.717291	-11.085190	3.439868
H	-9.136054	-11.349774	2.464767
H	-8.207699	-11.974896	3.832039
H	-9.554693	-10.870815	4.114323
C	-7.658605	-9.525615	0.766431
H	-7.827403	-8.584718	0.236163
H	-6.826179	-10.048468	0.279521
H	-8.552415	-10.145134	0.663692
H	-0.912485	2.606478	4.274759
H	3.012633	-3.417667	-2.589440
C	-11.067023	-5.040886	0.793074
C	-11.732175	-6.040063	0.085788
C	-11.602856	-3.766898	0.945546
C	-12.964960	-5.746361	-0.479313
H	-11.281739	-7.021933	-0.016277
C	-12.849652	-3.501725	0.387727
H	-11.055217	-3.003212	1.490720
C	-13.543241	-4.479230	-0.329515
H	-13.492783	-6.511885	-1.041214
H	-13.284328	-2.511987	0.500229
C	-14.882612	-4.184796	-0.952439
H	-15.250715	-3.198721	-0.658657
H	-14.813696	-4.210267	-2.045309
H	-15.625001	-4.931695	-0.654552
C	-10.960129	-4.945321	3.807074
C	-12.324457	-5.210210	3.900613
C	-13.164447	-4.291565	4.521242
C	-12.636377	-3.113369	5.044877
C	-11.269937	-2.856553	4.953387
C	-10.420991	-3.772024	4.334877
H	-12.708512	-6.129468	3.469722
H	-14.228471	-4.492863	4.591686
H	-13.290599	-2.393565	5.526814
H	-10.866254	-1.939527	5.369328
H	-9.354313	-3.584202	4.248380

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**II(R)-5, E(PCM, mixed basis set, opt) = -5013.198880 - E(PCM, 6-31+G\*, single point) = -5023.852098**

C	-4.530372	-2.542886	0.957985
C	-3.284255	-2.506523	1.542122
C	-2.951699	-1.376913	2.355044
C	-3.860317	-0.287631	2.429930
C	-5.052912	-0.323827	1.661572
C	-5.404399	-1.426726	0.923295
H	-1.062905	-2.145782	3.088146
C	-1.754594	-1.309662	3.116994
C	-3.536350	0.834517	3.237706
H	-5.695160	0.553251	1.639863
C	-2.372116	0.890854	3.963850
C	-1.481255	-0.214792	3.893810
H	-4.241805	1.661885	3.276042
H	-0.564426	-0.186778	4.477499

C	-2.324304	-3.597770	1.245593
C	-1.067266	-3.336988	0.611254
C	-2.687771	-4.905628	1.466144
C	-0.669950	-2.041473	0.176972
C	-0.193232	-4.426326	0.347298
C	-1.850965	-6.014017	1.176258
C	0.536827	-1.850345	-0.442636
H	-1.340658	-1.201435	0.321952
C	1.060490	-4.183465	-0.274948
C	-0.605002	-5.745595	0.665049
C	1.440830	-2.924377	-0.667747
H	0.813918	-0.853726	-0.777663
H	1.717312	-5.031831	-0.456121
H	0.078101	-6.568489	0.473820
C	-2.025271	2.076224	4.825189
H	-2.794661	2.851826	4.756402
H	-1.067254	2.514323	4.517899
C	2.763961	-2.661316	-1.336033
H	2.620776	-2.179644	-2.311199
H	3.319103	-3.591671	-1.491466
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C	-7.885314	-1.342855	0.446920
C	-6.282855	-1.393349	-1.407218
C	-8.925889	-1.234979	-0.485047
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H	-7.150175	-1.238553	-3.368626
C	-2.348072	-7.390612	1.446354
C	-2.990522	-8.125671	0.417396
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C	-3.549564	-9.361842	0.735647
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C	-3.528811	-9.870806	2.043209
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C	-4.862752	-1.483522	-1.959462
C	-4.638471	-2.760690	-2.807144
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H	-5.270337	-2.709304	-3.706395
H	-4.929712	-3.644992	-2.231758
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C	-9.563773	-2.600871	3.737839
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H	-3.434526	-12.242714	0.698306
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H	-6.489551	-12.331419	3.521685
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C	-1.554730	-7.153266	3.861875
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H	-1.016670	-6.300693	3.428221
C	-1.890247	-5.771689	5.968253
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C	-12.307675	-8.046401	-1.796458
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H	-11.836010	-7.741945	2.039627
C	-12.578570	-9.150822	-0.984270
H	-12.439006	-8.128808	-2.871720
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C	-13.073953	-10.444422	-1.576230
H	-14.155756	-10.543588	-1.435116
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C	-7.837803	-7.065667	-2.278879
H	-8.926277	-7.912957	-0.618019
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H	-7.163341	-3.756942	-2.658427
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