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SS-9 -1836.63639883 a.u. // (+CPCM) -1836.65869332 a.u.

Rh	-0.41509124	0.89832258	0.16927775
S	1.45435183	-0.31148797	-1.02631581
N	-0.83665197	-1.08015833	0.72996181
O	0.79419487	0.68034898	1.86026738
O	1.95021812	-0.89840632	2.95971129
O	-1.43880856	-3.25627358	0.35505782
O	-2.90762224	-1.56597033	-0.11307672
C	-0.31749594	3.10266908	-0.08336222
C	-0.75247123	2.53771922	-1.33084233
C	-1.98927464	1.83467466	-1.11268642
C	0.88806142	3.95994410	0.16162081
H	1.64985890	3.81870785	-0.60860472
H	1.34254904	3.72865023	1.12834386
H	0.61647822	5.02335200	0.16502016
C	-0.06132231	2.68799386	-2.65227741
H	-0.16742455	1.79242875	-3.26826976
H	1.00497611	2.89111856	-2.53148204
H	-0.49589879	3.52836377	-3.20795762
C	-2.84157694	1.18665710	-2.15983118
H	-3.70555860	1.81807133	-2.40470547
H	-3.20841067	0.22229750	-1.80731603
H	-2.28201409	1.01992763	-3.08316134
C	-1.22752276	3.18069724	2.35221464
H	-2.07161255	2.80104000	2.92984243
H	-1.21396888	4.27276845	2.44544415
H	-0.31009394	2.78378632	2.79900181
C	-2.34705125	2.00399435	0.28215204
C	-1.31609754	2.77964506	0.91256442
C	-3.60946110	1.51183955	0.91566625
H	-3.77159571	0.46160712	0.67146231
H	-4.46526196	2.09347985	0.54986208
H	-3.57673618	1.60816838	2.00231732
C	1.11443624	-0.56194304	2.12851869
C	0.44328421	-1.59378840	1.20882265
C	1.37000730	-1.84321393	0.00009654
H	0.93143061	-2.61360233	-0.63656387
H	2.38486537	-2.13157369	0.28059093
C	2.98832989	0.55069497	-0.38227911
H	3.06375545	1.42413693	-1.03627036
H	2.75572168	0.88480977	0.62918151
C	4.23704029	-0.28400847	-0.43421414
C	4.95861050	-0.43052127	-1.62798653
H	4.60602651	0.06028158	-2.53195446
C	6.12278085	-1.19528279	-1.66289170
H	6.67510638	-1.29709753	-2.59256417
C	6.58012933	-1.82608793	-0.50307649
H	7.48840551	-2.42096835	-0.52978786
C	5.86773075	-1.68784645	0.68845387
H	6.21806276	-2.17528765	1.59335943
C	4.70147752	-0.92092982	0.72692556
H	4.14256829	-0.81920205	1.65436548
C	-1.69105611	-2.04860556	0.32248121
C	-3.97706226	-2.52812977	-0.43447397
C	-3.58502019	-3.38011982	-1.64855923
H	-3.32011197	-2.73536885	-2.49341330

H	-4.43352308	-4.00258173	-1.95233701
H	-2.73755368	-4.02222035	-1.41371402
C	-4.31774227	-3.38504320	0.79241023
H	-3.48631077	-4.03497021	1.05943248
H	-5.19848798	-3.99915909	0.57654516
H	-4.55483112	-2.74227464	1.64656547
H	0.32164057	-2.53751279	1.74506334
H	-4.97539458	-1.01238647	-1.65351968
C	-5.17974772	-1.64496989	-0.78531378
H	-5.45944521	-1.00463740	0.05616880
H	-6.03894404	-2.27757641	-1.02759601

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m1 -1952.36964807 a.u. // (+CPCM) -1952.39066312 a.u.

Rh	0.63622263	1.13221461	-0.41636042
S	-1.75302514	-2.54037584	-0.43928411
N	0.99785797	-0.73050441	-1.06136811
O	-0.78192697	1.05021650	-1.85464380
O	-1.77256522	-0.27872726	-3.35048173
O	2.37538145	-2.46648049	-1.67038597
O	2.79062949	-1.29974951	0.24323631
C	0.20529946	3.23795145	0.15970368
C	0.10945990	2.39340753	1.30987127
C	1.42862984	1.81150151	1.56968212
C	-0.90064084	4.02259705	-0.48358925
H	-1.78576859	4.04980948	0.15427608
H	-1.19109981	3.57405927	-1.43937937
H	-0.58610389	5.05552551	-0.66532242
C	-1.09442571	2.17028774	2.16729818
H	-1.15577379	1.12362599	2.48058172
H	-2.01684492	2.42435223	1.64187525
H	-1.03026761	2.79596200	3.06793178
C	1.75736636	0.97425420	2.76385399
H	1.72313853	1.59402221	3.66953400
H	2.75584249	0.54750329	2.68325487
H	1.03604239	0.16032207	2.88288717
C	2.06846699	3.81194015	-1.56727545
H	2.83809805	3.22443108	-2.07300283
H	2.51783028	4.77054300	-1.27578677
H	1.27250360	4.01791731	-2.28579611
C	2.30670310	2.25314200	0.54768179
C	1.53590782	3.10335428	-0.36183279
C	3.77052544	1.96541813	0.43248375
H	3.97547257	0.91667340	0.64746293
H	4.33975506	2.58472458	1.13695181
H	4.14088936	2.18107320	-0.57208642
C	-0.90139247	-0.07878751	-2.51197626
C	0.11570610	-1.16668807	-2.15830845
C	-0.61265399	-2.50004923	-1.88515365
H	0.12660173	-3.28078523	-1.70750679
H	-1.18773549	-2.76345845	-2.77532411
C	-3.40475531	-2.09105444	-1.18850916
H	-3.19434841	-1.65041482	-2.16333822
H	-3.95534023	-3.02554163	-1.32348465
C	-4.17957992	-1.13292944	-0.32250189
C	-4.13066237	0.24697609	-0.57073994
H	-3.53238109	0.61683852	-1.39858782
C	-4.85193008	1.13370581	0.22937741

H	-4.82003675	2.19847442	0.01384231
C	-5.62519988	0.65913215	1.29171212
H	-6.18876518	1.35159769	1.91060842
C	-5.68077328	-0.71225320	1.54490586
H	-6.28899141	-1.09205182	2.36114055
C	-4.96559780	-1.60060361	0.73967199
H	-5.02380278	-2.66956965	0.93106397
C	2.08362256	-1.56260177	-0.89145561
C	3.86638644	-2.23294314	0.64263967
C	3.30980835	-3.65236516	0.81732441
H	2.45026511	-3.63876149	1.49489198
H	4.08101398	-4.29011262	1.26152184
H	3.00502139	-4.08125669	-0.13563693
C	5.01914217	-2.17872192	-0.36656120
H	4.70546006	-2.55953209	-1.33758268
H	5.85594762	-2.78286169	-0.00049044
H	5.37402775	-1.14968867	-0.48613311
H	0.72124411	-1.34989962	-3.05683471
H	3.49447807	-1.69211186	2.71543013
C	4.32374794	-1.70087570	2.00350016
H	4.73175276	-0.68908398	1.92380740
H	5.11196753	-2.34609103	2.40248697
O	-0.85669537	-1.13288073	2.51048479
H	-1.03532925	-1.33699488	1.57458773
C	-1.72339897	-1.93062999	3.30464038
H	-2.78254446	-1.73129567	3.09313159
H	-1.53851845	-3.00511863	3.16775174
H	-1.52748032	-1.68095533	4.35127894

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 ts12 -1952.36800025 a.u. // (+CPCM) -1952.38993563 a.u.

Rh	-1.49950587	-0.87233338	-0.22915313
S	2.60788050	0.65359798	1.09816738
N	-0.24385228	0.66373154	-0.59573294
O	0.11156096	-1.93876275	-0.82411006
O	2.20049211	-1.80682989	-1.59649309
O	0.05308705	2.73996763	-1.55166875
O	-1.55366079	2.42167389	0.03550285
C	-2.92771041	-2.57402652	-0.35125794
C	-2.98434363	-2.04049327	0.96301097
C	-3.43416215	-0.64689827	0.88139564
C	-2.49081599	-3.94899240	-0.76152161
H	-2.32713106	-4.58880277	0.10730827
H	-1.55213540	-3.90564565	-1.32330858
H	-3.25112683	-4.42400262	-1.39085640
C	-2.70759832	-2.76181123	2.24276131
H	-2.23146534	-2.09501259	2.96224499
H	-2.05091405	-3.61977209	2.08750009
H	-3.64680568	-3.12742942	2.67822283
C	-3.66415107	0.22313397	2.07617749
H	-2.80289389	0.18096904	2.74855138
H	-4.54779374	-0.11629388	2.63149343
H	-3.81841854	1.26245522	1.78983291
C	-3.36580847	-1.64323469	-2.75390597
H	-3.19278299	-0.69097978	-3.25987941
H	-4.36972319	-1.99192506	-3.03097445
H	-2.64255900	-2.36814529	-3.13357099
C	-3.64973719	-0.33382468	-0.48487903

C	-3.26141040	-1.50446159	-1.26778244
C	-4.22992707	0.91939499	-1.05720996
H	-4.08017048	1.76581378	-0.39017842
H	-5.30737936	0.79149618	-1.22275741
H	-3.77386445	1.16991805	-2.01802444
C	1.16205904	-1.26660954	-1.23525122
C	1.01002603	0.25920639	-1.25728302
C	2.26740377	0.94174500	-0.68601516
H	2.17483027	2.02014958	-0.80765433
H	3.13800435	0.60585916	-1.25299462
C	3.81007092	-0.76814454	1.06445173
H	3.93949868	-1.00321118	2.12522405
H	3.32898365	-1.61368213	0.57289014
C	5.13221856	-0.45024927	0.41629578
C	5.39996876	-0.88798017	-0.88869511
H	4.63808450	-1.44826981	-1.42325033
C	6.62673524	-0.60079051	-1.49270454
H	6.82110850	-0.94647286	-2.50418499
C	7.59868435	0.12245193	-0.80232015
H	8.55349241	0.34226895	-1.27154932
C	7.33899713	0.56276465	0.49865649
H	8.09236661	1.12485555	1.04359704
C	6.11507153	0.27995320	1.10057015
H	5.91432248	0.62961301	2.11030449
C	-0.54362245	1.99578833	-0.77803467
C	-1.78424284	3.87095545	0.19466529
C	-0.50612281	4.56083571	0.68982490
H	-0.13641753	4.06885646	1.59497966
H	-0.72881090	5.60375185	0.93738980
H	0.27445573	4.54090957	-0.06940384
C	-2.30240479	4.48715025	-1.11027496
H	-1.54281814	4.44156799	-1.88949749
H	-2.57504670	5.53377795	-0.93805933
H	-3.19737404	3.95967688	-1.45555067
H	0.97508011	0.55804466	-2.31632403
H	-2.51993006	3.43775626	2.19398181
C	-2.85704215	3.94388216	1.28529865
H	-3.79555387	3.48747004	0.95638722
H	-3.06552264	4.98962498	1.52969367
O	-0.16161558	-0.69615544	2.59676511
H	0.40204627	-0.13371750	2.03382136
C	0.66922139	-1.73598607	3.09605194
H	1.07088832	-2.36683240	2.29235358
H	1.50769156	-1.34444863	3.68818766
H	0.05737455	-2.36058081	3.75328181

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m2 -1952.37065640 a.u. // (+CPCM) -1952.39558193 a.u.

Rh	-1.20060088	-0.95990655	-0.01500068
S	2.64156953	1.34874990	-0.55464589
N	-0.54926195	0.85636765	-0.85637610
O	0.23921198	-1.64917050	-1.34558823
O	1.53453946	-1.10449025	-3.07585892
O	-1.02558928	2.97577139	-1.61421083
O	-1.76009961	2.27628554	0.43630126
C	-2.38721133	-2.83592519	-0.13813591
C	-2.32167088	-2.47039998	1.23052052
C	-2.95437454	-1.16173084	1.38582145

C	-1.88509500	-4.09647020	-0.76723583
H	-1.26717662	-4.67409743	-0.07785386
H	-1.29079464	-3.87804492	-1.65814979
H	-2.73129587	-4.72358501	-1.07083294
C	-1.78556106	-3.29956309	2.35538365
H	-1.34567402	-2.67881014	3.13897398
H	-1.03118693	-4.01081842	2.01425911
H	-2.60187029	-3.87170493	2.81313479
C	-3.18534465	-0.47673562	2.69585149
H	-4.07995836	-0.88480830	3.18222506
H	-3.33059757	0.59520922	2.56538994
H	-2.34473804	-0.62432657	3.37811699
C	-3.37201542	-1.75539880	-2.31883824
H	-3.45765488	-0.74395976	-2.72145503
H	-4.33717419	-2.25673640	-2.46279228
H	-2.62571837	-2.29558184	-2.90534714
C	-3.43487814	-0.75196687	0.10858944
C	-3.01243614	-1.73846095	-0.86559120
C	-4.28822995	0.43562630	-0.19304976
H	-4.18592298	1.20876080	0.56545513
H	-5.33802226	0.11817246	-0.22402209
H	-4.04676886	0.87242503	-1.16415017
C	0.73633958	-0.79153793	-2.18702240
C	0.29792466	0.67386002	-2.03610740
C	1.55075185	1.57425057	-2.02792891
H	1.24139895	2.61797329	-2.03247334
H	2.14604334	1.37087414	-2.92008742
C	4.03410027	0.34302236	-1.27289346
H	3.61183590	-0.57017477	-1.69370491
H	4.46396605	0.93699763	-2.08386626
C	5.06458184	0.05078546	-0.21412307
C	5.10767207	-1.20007406	0.41733974
H	4.39645086	-1.96907272	0.12847130
C	6.06111773	-1.47018726	1.40127138
H	6.08436116	-2.44670161	1.87602307
C	6.98431459	-0.48948874	1.76974005
H	7.72741016	-0.69873673	2.53347143
C	6.95104633	0.76086326	1.14660910
H	7.66953579	1.52671449	1.42371162
C	5.99824714	1.02779042	0.16314081
H	5.97893031	2.00043109	-0.32155403
C	-1.11177480	2.08573625	-0.75640465
C	-2.11156279	3.63917546	0.87415915
C	-0.84981258	4.50843269	0.94903994
H	-0.10064095	4.03641665	1.59300580
H	-1.10071309	5.48284263	1.37971390
H	-0.42092178	4.66320023	-0.04076419
C	-3.18213273	4.25904967	-0.03259357
H	-2.79262421	4.43383644	-1.03440329
H	-3.51248607	5.21182224	0.39416505
H	-4.05428037	3.60193203	-0.10189789
H	-0.24862975	0.93642284	-2.95622307
H	-1.94706977	2.91261516	2.91839698
C	-2.67449769	3.42498210	2.28221983
H	-3.59485350	2.83450464	2.25574627
H	-2.91063145	4.39098762	2.73781106
O	0.58634785	-0.51761305	1.35924409

H	1.07897713	0.11362751	0.78959237
C	1.47548374	-1.60140681	1.68289223
H	1.70732554	-2.19446638	0.79383123
H	2.39962596	-1.20803989	2.11606940
H	0.97312859	-2.22651187	2.42098559
72			
ts23	-1952.36695368 a.u. // (+CPCM) -1952.39121737 a.u.		
Rh	-1.69707829	-0.70130982	0.19322133
S	2.67279716	-0.54938134	-0.74248658
N	-0.32764898	0.36122324	-0.96613192
O	-0.78485233	-2.24026120	-0.79875702
O	0.32189474	-2.75809220	-2.66888891
O	0.19926475	2.27456202	-2.12897714
O	-0.67543387	2.39432224	-0.01747047
C	-3.60421355	-1.83993063	0.35376194
C	-3.34342371	-1.26346968	1.62237066
C	-3.33804405	0.19289994	1.47400228
C	-3.68271853	-3.29419840	0.00452805
H	-3.61772499	-3.92567018	0.89264856
H	-2.86070144	-3.56628483	-0.66647697
H	-4.62999461	-3.51580781	-0.49918425
C	-3.16467558	-1.98467867	2.92400179
H	-2.39207985	-1.51164930	3.53581883
H	-2.88309081	-3.02841631	2.77169047
H	-4.09648466	-1.96901430	3.50349896
C	-3.18672758	1.15916563	2.60732159
H	-4.12321965	1.24055934	3.17417207
H	-2.91829338	2.15300982	2.24993977
H	-2.40629308	0.83530191	3.30095347
C	-4.03142015	-0.92469652	-2.06622803
H	-3.67382107	-0.08307037	-2.66351402
H	-5.11950916	-0.98990850	-2.19720145
H	-3.58943987	-1.83735005	-2.47250949
C	-3.60423193	0.49705584	0.11207646
C	-3.68200104	-0.75706342	-0.61848514
C	-3.81490635	1.85168125	-0.48481800
H	-3.31431320	2.62603318	0.09394397
H	-4.88858291	2.07775596	-0.51551519
H	-3.43521801	1.90368039	-1.50747904
C	-0.08468992	-1.92918727	-1.87050640
C	0.21478882	-0.43016778	-2.07417640
C	1.72968680	-0.25221742	-2.29687473
H	1.93240368	0.76103389	-2.64333946
H	2.03641555	-0.98843215	-3.04402651
C	4.38155697	-0.20718422	-1.35497633
H	4.59922555	-0.91233378	-2.16263289
H	4.39983723	0.80625993	-1.76694299
C	5.37961274	-0.35013737	-0.23471841
C	5.95648066	-1.59437149	0.05280600
H	5.68322464	-2.45911817	-0.54614591
C	6.87390695	-1.73006127	1.09456195
H	7.31612889	-2.70053982	1.30088044
C	7.22564291	-0.62180169	1.86720468
H	7.94295252	-0.72580151	2.67616135
C	6.65351621	0.62148970	1.59241381
H	6.92377640	1.48915971	2.18753866
C	5.73582518	0.75427092	0.55039299

H	5.29122194	1.72340159	0.33916765
C	-0.24629854	1.70846773	-1.12985419
C	-0.30255326	3.80630403	0.14544778
C	1.22409804	3.95652480	0.10798140
H	1.68805880	3.29788584	0.84898440
H	1.49913608	4.98879529	0.34818266
H	1.61440752	3.70909391	-0.87886594
C	-0.98711516	4.68832149	-0.90705200
H	-0.62601260	4.44865191	-1.90601028
H	-0.78167827	5.74270734	-0.69241453
H	-2.07244127	4.54681625	-0.88029555
H	-0.25275427	-0.13805073	-3.02696142
H	-0.40204455	3.47013455	2.29147949
C	-0.82315096	4.14904490	1.54469838
H	-1.91468813	4.08093003	1.58729135
H	-0.54264396	5.17329240	1.80829404
O	0.09149067	-0.65461616	1.60343317
H	0.67957959	-0.18614422	0.97789663
C	0.70191935	-1.90547376	1.97673945
H	0.80741135	-2.56270968	1.11144101
H	1.67811103	-1.71755381	2.43299679
H	0.04235250	-2.36700426	2.71384980

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m3 -1952.36773350 a.u. // (+CPCM) -1952.39451859 a.u.

Rh	-1.57233191	-0.63994720	0.13124104
S	2.57461488	-1.15815193	-1.52796569
N	-0.29003813	0.42607585	-1.15747262
O	-1.12865676	-2.11254495	-1.26510573
O	-0.28712976	-2.49953041	-3.29350008
O	0.35874562	2.35865554	-2.21985733
O	-0.20090470	2.38034300	-0.00176626
C	-3.55010885	-1.53571986	0.60938221
C	-2.95527577	-1.15361434	1.83847988
C	-2.74568330	0.29273676	1.81772022
C	-3.96304375	-2.90899845	0.18470416
H	-3.60335484	-3.67207331	0.87685948
H	-3.57610794	-3.14033612	-0.81108361
H	-5.05649252	-2.97407824	0.14653195
C	-2.65932026	-2.04137123	3.00648756
H	-1.76627022	-1.71461457	3.54386055
H	-2.51907707	-3.08047601	2.70349244
H	-3.49584474	-2.00936661	3.71531667
C	-2.24647282	1.09595052	2.97729259
H	-3.06231237	1.27959883	3.68732888
H	-1.85429114	2.06032432	2.65650852
H	-1.45455462	0.57049124	3.51667141
C	-4.34233742	-0.28269354	-1.55513075
H	-4.00641312	0.57919697	-2.13526787
H	-5.42867985	-0.19840585	-1.42719259
H	-4.14465138	-1.18568415	-2.13683618
C	-3.24809120	0.79038200	0.58053104
C	-3.67009000	-0.34229600	-0.21880477
C	-3.39709916	2.22039541	0.17791737
H	-2.72086461	2.86799846	0.73152069
H	-4.42653387	2.54054861	0.38169284
H	-3.21234469	2.36205762	-0.88877773
C	-0.50251787	-1.74219573	-2.34405289

C	0.00440111	-0.29075646	-2.39738873
C	1.50201479	-0.31796151	-2.77645341
H	1.86837701	0.69948011	-2.90563816
H	1.60509222	-0.86434795	-3.71505409
C	3.67360168	0.23348183	-0.97375809
H	4.23985049	0.57729440	-1.84223268
H	3.03492490	1.04704045	-0.62507938
C	4.59449893	-0.24586612	0.11814392
C	5.88212189	-0.70895096	-0.18557826
H	6.22061583	-0.70848986	-1.21836976
C	6.73284501	-1.16146741	0.82459214
H	7.72975457	-1.51152736	0.57347993
C	6.30437226	-1.16088636	2.15377294
H	6.96623451	-1.51042949	2.94052040
C	5.02132486	-0.70492843	2.46740404
H	4.68260884	-0.69791083	3.49922201
C	4.17285777	-0.25207273	1.45634799
H	3.17517978	0.10050147	1.70493200
C	-0.03256577	1.75529661	-1.20996636
C	0.29534372	3.75502115	0.19503557
C	1.80846906	3.81215043	-0.04982007
H	2.32603435	3.09837184	0.59960288
H	2.18080450	4.81332446	0.18886048
H	2.04634587	3.58937959	-1.08967873
C	-0.46516467	4.75423225	-0.68575944
H	-0.25043840	4.58923051	-1.74044193
H	-0.16979107	5.77353546	-0.41615774
H	-1.54370570	4.66386192	-0.52586408
H	-0.49832171	0.18664063	-3.25303230
H	0.47386007	3.27446886	2.30955104
C	0.00577166	4.03107444	1.67336480
H	-1.06937920	4.04209993	1.87330700
H	0.40617567	5.01014703	1.95182624
O	0.46103011	-1.18568378	1.05381653
H	1.03799862	-0.98671881	0.28217448
C	0.70436129	-2.55323526	1.42990685
H	0.40706890	-3.23741335	0.63037103
H	1.76486071	-2.68881568	1.66205338
H	0.11505165	-2.75553806	2.32401484

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ts34 -1952.36487456 a.u. // (+CPCM) -1952.38827750 a.u.

Rh	1.65291152	-0.48869115	0.02571284
S	-2.51702761	-1.10864222	1.75615252
N	0.32289187	0.55117149	1.16564229
O	1.54721964	-1.76767717	1.58967147
O	0.48714876	-2.20332180	3.50769145
O	-0.32656757	2.52729256	2.15144196
O	0.06295916	2.44451381	-0.09424616
C	3.42880420	-1.47332435	-0.88865337
C	2.47557891	-1.25413882	-1.92004534
C	2.23540506	0.18370471	-2.04009418
C	3.95442545	-2.78343625	-0.38314907
H	3.56835367	-3.62104242	-0.96664434
H	3.65711686	-2.93885143	0.65895634
H	5.04819540	-2.80907848	-0.44007335
C	1.82803480	-2.27939628	-2.79489989
H	0.74144859	-2.16649952	-2.77987011



H	2.06595903	-3.29365287	-2.47158070
H	2.17480160	-2.16171257	-3.82904422
C	1.36818278	0.81037648	-3.08595485
H	1.92061429	0.92143900	-4.02832961
H	1.02154183	1.79470458	-2.77508058
H	0.48914599	0.19361403	-3.28819512
C	4.73930503	0.04997397	0.78118501
H	4.52985734	0.97149566	1.32837588
H	5.74901174	0.13265912	0.35758855
H	4.73962350	-0.77604796	1.49541306
C	3.04704212	0.84369391	-1.08107952
C	3.73996990	-0.18411826	-0.30767947
C	3.24160703	2.31613814	-0.91894276
H	2.34193476	2.86366059	-1.19285149
H	4.06676244	2.65592640	-1.55813447
H	3.49149565	2.57697769	0.11195461
C	0.72226681	-1.45976608	2.56860064
C	0.07477350	-0.07028339	2.47828362
C	-1.40863082	-0.16399066	2.88196951
H	-1.82762592	0.83295149	3.02182009
H	-1.44403604	-0.70468034	3.83020030
C	-3.11610399	0.21754721	0.60301158
H	-3.48763500	1.04422919	1.21415273
H	-2.26447671	0.57276293	0.01850184
C	-4.20686146	-0.31838053	-0.28999068
C	-5.54956304	-0.00867673	-0.03855354
H	-5.80183649	0.62017426	0.81146202
C	-6.56172158	-0.49466550	-0.86660071
H	-7.59728653	-0.24031125	-0.65946476
C	-6.24376353	-1.30573736	-1.95657150
H	-7.03024575	-1.68505577	-2.60266060
C	-4.90926442	-1.62874525	-2.21037447
H	-4.65491196	-2.26369267	-3.05448310
C	-3.89715943	-1.13956957	-1.38482980
H	-2.86158363	-1.40938596	-1.57633661
C	0.01435158	1.88937984	1.15692911
C	-0.44182415	3.81962512	-0.28773157
C	-1.91711000	3.91814735	0.12364914
H	-2.51359771	3.17641807	-0.41642210
H	-2.29909779	4.91072713	-0.13630198
H	-2.03875143	3.76520066	1.19484232
C	0.42935558	4.83173873	0.46668722
H	0.34607620	4.69006083	1.54326757
H	0.10926100	5.84832217	0.21492257
H	1.47956390	4.72962159	0.17561440
H	0.54353665	0.53997286	3.26532844
H	-0.88848158	3.27538888	-2.34548392
C	-0.32544108	4.03751603	-1.79941261
H	0.71640953	4.01175936	-2.13232320
H	-0.73235856	5.01813807	-2.06304400
O	-0.62520894	-2.23592581	-0.69422172
H	-1.10163451	-1.82108358	0.05406143
C	-0.47238263	-3.61396918	-0.34797073
H	0.20692211	-3.73801134	0.50261153
H	-1.43825038	-4.07577555	-0.10863858
H	-0.05470972	-4.12705831	-1.21851178

m4 -1952.36658269 a.u. // (+CPCM) -1952.39031751 a.u.

Rh	1.24781054	-0.93745088	-0.00559385
S	-2.48445396	0.12133805	1.89049728
N	0.85370989	0.57558387	1.25947537
O	0.74570271	-2.03716539	1.60169258
O	-0.17062532	-1.95691039	3.63780306
O	1.16411890	2.61529809	2.26504342
O	1.61685203	2.36716156	0.04441244
C	1.48209426	-2.65929577	-1.38635849
C	0.67772906	-1.64179113	-2.00735417
C	1.49126313	-0.44838215	-2.19066858
C	1.00537813	-4.03406868	-1.02989168
H	-0.01914646	-3.99343508	-0.65165891
H	1.62879183	-4.48416317	-0.25564826
H	1.02992116	-4.68739586	-1.91071993
C	-0.72880568	-1.81602191	-2.48118268
H	-1.30173225	-2.44880620	-1.79909430
H	-0.72501804	-2.28940627	-3.47262223
H	-1.24313754	-0.85712291	-2.57579750
C	1.06104993	0.76793235	-2.94740756
H	1.00196953	0.54041922	-4.01928773
H	1.76366800	1.58717137	-2.81195511
H	0.07484285	1.11517738	-2.62918004
C	3.91278050	-2.76067517	-0.43829994
H	4.50502253	-2.06307282	0.15845158
H	4.57485095	-3.19826241	-1.19663424
H	3.57727642	-3.56328583	0.22071543
C	2.76320522	-0.70402412	-1.61666095
C	2.75460708	-2.07647182	-1.09389803
C	3.93293885	0.22883738	-1.59113598
H	3.61348202	1.23703452	-1.32311452
H	4.41636899	0.26687534	-2.57543063
H	4.68340932	-0.09127887	-0.86563860
C	0.28281522	-1.39476434	2.65320914
C	0.32281014	0.13301984	2.56276813
C	-1.06995218	0.69305669	2.91516001
H	-1.05016953	1.78367065	2.92494871
H	-1.30932200	0.33618416	3.91962039
C	-2.41094797	1.27147721	0.44153430
H	-2.32537726	2.29160779	0.82658057
H	-1.50177291	1.04910589	-0.12386210
C	-3.64462657	1.14231891	-0.42215489
C	-4.40613952	2.27836575	-0.72532007
H	-4.11647340	3.24074270	-0.31087923
C	-5.52791519	2.19138348	-1.55080052
H	-6.10347266	3.08526508	-1.77405645
C	-5.91221419	0.95928526	-2.07967330
H	-6.78746574	0.88726792	-2.71881663
C	-5.16836266	-0.18196549	-1.77410593
H	-5.46644908	-1.14801870	-2.17166660
C	-4.04343185	-0.09482182	-0.95356858
H	-3.49156001	-0.99866090	-0.70941195
C	1.21187169	1.90392962	1.26461290
C	1.96950740	3.79895577	-0.08048818
C	0.76915622	4.68588720	0.27761051
H	-0.10753489	4.38626400	-0.30607368
H	1.00040396	5.72632009	0.02692849

H	0.52966508	4.62245128	1.33732836
C	3.20539717	4.11688870	0.76977592
H	2.98971797	4.00627005	1.83137157
H	3.52736292	5.14572521	0.57783797
H	4.03204114	3.44994642	0.50324471
H	0.98887325	0.48972131	3.35935175
H	1.43075768	3.73687203	-2.18935677
C	2.29692172	3.97304799	-1.56581045
H	3.13599642	3.34021033	-1.86912991
H	2.57859047	5.01249266	-1.75752238
O	-2.15306927	-2.92258377	0.29233641
H	-1.96682935	-2.09171319	0.76296691
C	-2.51508341	-3.88072822	1.28617691
H	-1.76132458	-3.94016447	2.07942202
H	-3.48867076	-3.64923238	1.73934430
H	-2.58984819	-4.85263674	0.79017375

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 RS-9 -1836.63174326 a.u. // (+CPCM) -1836.65608420 a.u.

Rh	1.34275800	-0.57330758	0.09224435
S	-0.79749351	-1.84964150	0.23679362
N	0.15361893	0.71463528	1.26735394
O	1.71976302	-1.33956698	1.99144774
O	0.99817280	-1.19335196	4.11216294
O	-1.71436127	2.00204741	1.60713956
O	-0.22339656	2.54761489	-0.04276289
C	3.02705404	-1.60227274	-0.91891880
C	2.08672073	-1.22943748	-1.93382154
C	1.94230899	0.20584097	-1.92567870
C	3.49953901	-2.98148263	-0.57091172
H	2.81583618	-3.74748307	-0.94353336
H	3.57547334	-3.10075821	0.51298703
H	4.48853918	-3.17687165	-1.00460353
C	1.41048841	-2.17580505	-2.87946804
H	0.46655097	-1.77325569	-3.25352876
H	1.20941420	-3.14209031	-2.41142296
H	2.05474368	-2.35766753	-3.74887404
C	1.15368196	1.03391355	-2.89351277
H	1.80561761	1.46064011	-3.66688089
H	0.65543159	1.85426298	-2.37586853
H	0.38865913	0.44122763	-3.40109098
C	4.51182308	-0.34823132	0.81114894
H	4.72212063	0.67226033	1.13525429
H	5.45526302	-0.80672947	0.49335968
H	4.12834783	-0.90522840	1.67288527
C	2.84972709	0.72669882	-0.92380740
C	3.51278085	-0.38290741	-0.30239164
C	3.07864959	2.17763807	-0.64006132
H	2.12690176	2.69127207	-0.49951161
H	3.60982113	2.64661952	-1.47803268
H	3.67781659	2.31970498	0.26085052
C	0.89573565	-0.92359050	2.92589278
C	-0.29844098	-0.13543646	2.36756045
C	-1.34336167	-1.16090116	1.86275173
H	-2.31231301	-0.68523530	1.71081323
H	-1.45897003	-2.00161919	2.55011859
C	-1.91361766	-0.95315678	-0.96263197
H	-1.67408222	0.10786346	-0.89427460

H	-1.57939778	-1.32330286	-1.93575110
C	-3.37962959	-1.21258402	-0.75092999
C	-4.17068797	-0.26689428	-0.08225676
H	-3.71361432	0.64715601	0.28881456
C	-5.53326200	-0.49959485	0.11426622
H	-6.13480921	0.24042704	0.63352404
C	-6.11894151	-1.67545654	-0.35464148
H	-7.17925360	-1.85472267	-0.20325336
C	-5.33727861	-2.62270747	-1.02116865
H	-5.78876878	-3.53899673	-1.39002921
C	-3.97718815	-2.39272488	-1.21676197
H	-3.37213010	-3.13259966	-1.73495880
C	-0.66737722	1.75310313	0.99678525
C	-0.86363819	3.85694808	-0.26160712
C	-2.32214989	3.68862038	-0.70747243
H	-2.38093610	3.00494241	-1.56129859
H	-2.72334185	4.65692611	-1.02559983
H	-2.93480538	3.29895410	0.10347468
C	-0.74157182	4.72413313	0.99808963
H	-1.30779388	4.29441758	1.82346391
H	-1.12250347	5.72969942	0.79111485
H	0.30822535	4.81396135	1.29544976
H	-0.75548025	0.45139836	3.16656052
H	-0.11926940	3.88911861	-2.31444981
C	-0.04862084	4.48282009	-1.39848494
H	1.00543574	4.58033573	-1.12442380
H	-0.43415812	5.48288824	-1.61816126

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methanol -115.723964215 a.u. // (+CPCM) -115.728728805 a.u.

C	0.66191089	-0.01948326	0.00000107
H	1.08177341	0.98959104	-0.00039748
H	1.03810540	-0.54251391	0.89228621
H	1.03804443	-0.54318540	-0.89191321
O	-0.74941723	0.12201963	0.00000151
H	-1.13405077	-0.76314921	0.00000598