

ELECTRONIC SUPPLEMENTARY INFORMATION

**Diastereoselective diazenyl formation: the key for
manganese-catalysed alcohol conversion into (*E*)-alkenes**

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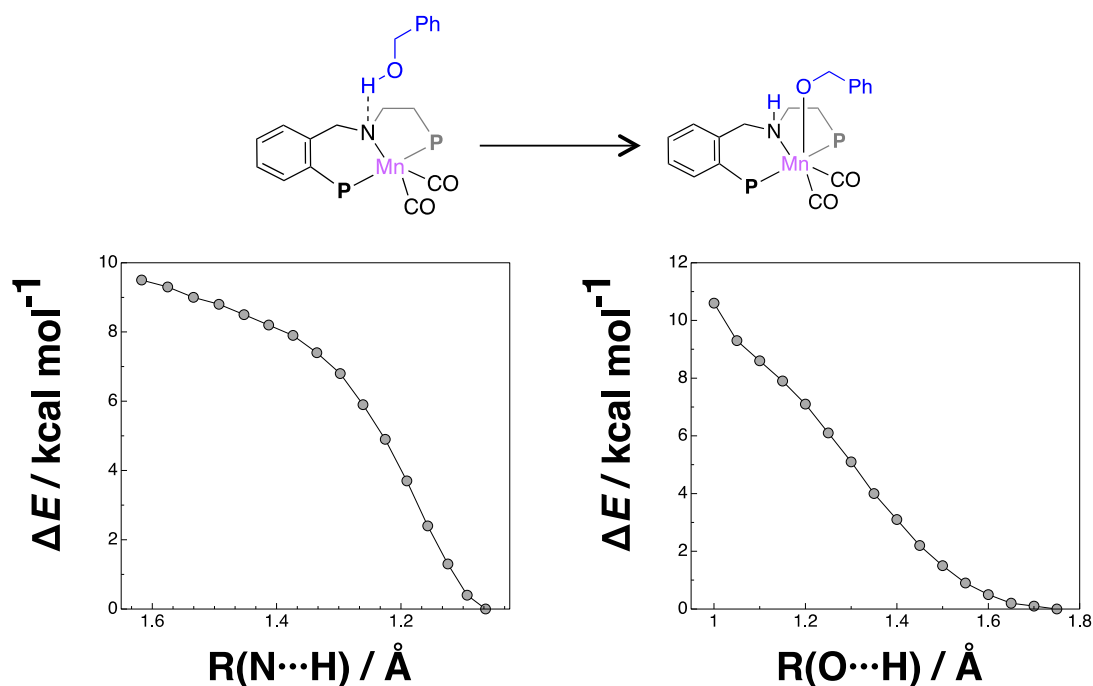


Figure S1. Linear transit calculations corresponding to proton transfer from **A** to **B** (step-wise mechanism), freezing N–H and O–H distances. This suggests that there is no presence of maximum.

Optimised Cartesian coordinates

	A		
Mn	-0.13541254	0.49511465	0.11171320
P	-0.78068374	-1.68945617	-0.20797728
P	0.62174077	2.63652321	0.19202895
O	-2.43892909	1.26320988	-1.57806614
O	-1.52750044	0.93711330	2.66557443
N	1.71276386	0.04423267	0.02317331
C	0.51128775	-2.94725128	0.22135143
C	0.19436631	-4.25876679	0.64974049
C	1.19458488	-5.16956120	1.02701078
C	2.54088184	-4.77127122	0.98919311
C	2.86650338	-3.47620706	0.55755776
C	1.87346389	-2.55068369	0.16104409
C	2.34647685	-1.22012223	-0.40864683
C	2.82136342	1.00015017	0.25700934
C	2.35502871	2.35216783	0.80274196
C	-1.21978458	-2.10223127	-2.01782938
C	-0.06049570	-1.72842078	-2.95754627
C	-1.70137743	-3.53790366	-2.27647337
C	-2.31142065	-2.32079002	0.71986371
C	-3.56298216	-1.49287479	0.37553161
C	-2.10385801	-2.40190511	2.24423374

C	0.87102237	3.62342398	-1.41093268
C	1.60327844	2.77570404	-2.46742459
C	-0.43521807	4.19928428	-1.98799679
C	-0.06127226	3.86976693	1.45395476
C	-1.57983760	4.10535808	1.34862552
C	0.71965713	5.19436352	1.52549394
C	-1.52777122	0.96945876	-0.87978597
C	-1.02030665	0.72959626	1.61519749
H	-0.85662630	-4.58354550	0.69136035
H	0.91934332	-6.18533504	1.35451180
H	3.33846481	-5.46685307	1.29720937
H	3.92506239	-3.16677550	0.52188114
H	3.43884583	-1.17683472	-0.19585553
H	2.28403039	-1.29068945	-1.52218279
H	3.39768226	1.15499505	-0.69077946
H	3.55476210	0.54647000	0.96908695
H	3.06204046	3.16783593	0.53989258
H	2.27605271	2.31279002	1.91032308
H	-2.05595711	-1.39631088	-2.22013948
H	0.29751317	-0.69416720	-2.77072878
H	-0.38993418	-1.79007792	-4.01727355
H	0.79588986	-2.42602451	-2.83772270
H	-0.91578850	-4.28270916	-2.02675535
H	-1.94509247	-3.66478569	-3.35422692
H	-2.61675514	-3.79714030	-1.70619678
H	-2.47075027	-3.35272867	0.33524913
H	-3.46870278	-0.44992518	0.73956941
H	-4.45240329	-1.94075566	0.86959232
H	-3.77162258	-1.45199715	-0.71291367
H	-1.19082635	-2.96451328	2.52414162
H	-2.97246343	-2.92031481	2.70637553
H	-2.03713944	-1.39575150	2.69992893
H	1.53489113	4.46879976	-1.11728694
H	2.60616523	2.44526661	-2.13079772
H	1.74437795	3.36959684	-3.39656344
H	1.01800553	1.86982049	-2.72942111
H	-1.17904158	3.40440382	-2.19981088
H	-0.22009655	4.72176969	-2.94573064
H	-0.91001995	4.93832392	-1.31280792
H	0.11421254	3.30568379	2.39820049
H	-1.84540227	4.73516803	0.47551704
H	-1.93708971	4.63599815	2.25756329
H	-2.14607030	3.15718644	1.27279516
H	1.81184956	5.04291870	1.65223645
H	0.36809282	5.79588281	2.39207320
H	0.56344078	5.81492227	0.61756568
B			
Mn	-0.43303920	0.95451265	0.19946802
P	-1.76139463	-0.92885482	0.69911283

P	0.86511398	2.72615547	-0.54529068
O	-2.87099751	2.60940182	0.18009809
O	0.04668896	1.71384508	3.00760756
O	1.14353336	-0.35662302	-0.00663969
N	-0.37084340	0.36447020	-1.88413127
C	-1.48084425	-2.31226581	-0.51971440
C	-1.42408837	-3.66821810	-0.12426120
C	-1.19535462	-4.70140733	-1.04932979
C	-1.00993423	-4.39098404	-2.40448321
C	-1.05614467	-3.04823992	-2.81240352
C	-1.29142431	-1.99817619	-1.89711115
C	-1.35207979	-0.58748365	-2.45891893
C	-0.12247042	1.47683789	-2.83066434
C	1.05655010	2.32913309	-2.36815965
C	-3.67389035	-0.77178712	0.68579304
C	-4.26079702	-0.32557025	-0.66471554
C	-4.41277869	-2.03487612	1.16662702
C	-1.51408330	-1.75855317	2.38791085
C	-2.11023128	-0.92263194	3.53827507
C	-0.04322986	-2.10198231	2.66768010
C	0.20244417	4.50526535	-0.49824924
C	-0.87835006	4.80111900	-1.55498753
C	-0.28753988	4.88772412	0.91262925
C	2.69135168	2.93496074	-0.05948221
C	2.89854240	3.23107515	1.43604691
C	3.48812265	3.91636382	-0.93833743
C	-1.88406857	1.94971777	0.15925315
C	-0.16003627	1.38709454	1.89083437
C	3.01365043	-1.85038450	0.46354461
C	2.48082541	-2.80641964	-0.42276248
C	3.15881421	-4.01719089	-0.66503134
C	4.37850160	-4.29004536	-0.02252858
C	4.91825971	-3.34040465	0.86774072
C	4.24111813	-2.13340478	1.10476223
C	2.29891656	-0.52460624	0.73393890
H	0.52428725	-0.13652294	-1.64675614
H	-1.55771651	-3.93795484	0.93362566
H	-1.15839777	-5.74716329	-0.70366218
H	-0.82343584	-5.18714344	-3.14308390
H	-0.90457435	-2.79945215	-3.87649853
H	-1.18164187	-0.66542920	-3.55824443
H	-2.36347514	-0.15111511	-2.33541780
H	-1.05020217	2.08430954	-2.90435762
H	0.07889668	1.07268269	-3.85326773
H	1.16861485	3.23370609	-3.00064446
H	1.99588171	1.74187746	-2.45941912
H	-3.84386786	0.05391934	1.41256961
H	-3.81834784	0.61920932	-1.03297136
H	-5.35167181	-0.14700595	-0.54747985

H	-4.14346305	-1.11499148	-1.43760442
H	-4.19342268	-2.90492713	0.51128562
H	-5.51024426	-1.86125231	1.12393453
H	-4.17205514	-2.32019202	2.20940655
H	-2.09167113	-2.70659600	2.32871037
H	-1.58972365	0.04773516	3.65361103
H	-1.98363479	-1.47857250	4.49273617
H	-3.19388679	-0.72138117	3.41927968
H	0.44347791	-2.64098424	1.83125650
H	0.02444215	-2.73790463	3.57715389
H	0.54432394	-1.18322242	2.85996988
H	1.09213805	5.12839211	-0.74189713
H	-0.52523423	4.62741886	-2.59242103
H	-1.17234653	5.87164171	-1.49014140
H	-1.79502804	4.20123663	-1.38556876
H	-1.22419989	4.35469401	1.16921669
H	-0.50160199	5.97813071	0.95230694
H	0.45495699	4.66257043	1.70328042
H	3.07185062	1.90766840	-0.25462069
H	2.61263930	4.27370417	1.69052135
H	3.97347347	3.11865391	1.69627141
H	2.31879704	2.55003003	2.08909600
H	3.40968735	3.69387082	-2.02224111
H	4.56633812	3.86449350	-0.67149913
H	3.17160182	4.96984001	-0.78105542
H	1.52099513	-2.58344594	-0.91356663
H	2.72654181	-4.75411124	-1.36261351
H	4.90932037	-5.23764477	-0.21200299
H	5.87423279	-3.54387894	1.37888332
H	4.67198230	-1.39200288	1.80136418
H	2.11848621	-0.46630679	1.84103609
H	3.06827972	0.28101751	0.55112378
B-C(Ph-Ph)			
Mn	-0.45349014	-0.91458122	-0.26364083
P	-1.43139013	1.11674189	-0.79682556
P	0.49267777	-2.88596317	0.49401156
O	-3.04709404	-2.21744788	-0.82910444
O	0.51854591	-1.48578370	-2.98535253
O	2.08463182	0.10652567	1.99190990
N	-0.54323579	-0.47063444	1.82465770
C	-1.13661435	2.41354185	0.51037907
C	-0.90675524	3.77352632	0.19885867
C	-0.67590829	4.73208290	1.20033305
C	-0.65942660	4.33915170	2.54724497
C	-0.87925934	2.99078231	2.87184380
C	-1.12491257	2.01645952	1.87861525
C	-1.42837989	0.60385517	2.34606788
C	-0.74427949	-1.69134747	2.65839790
C	0.34143100	-2.71967395	2.35395653

C	-3.33952307	1.20805152	-1.00712094
C	-4.13012248	0.77979067	0.24073529
C	-3.85973593	2.57242776	-1.49558822
C	-0.89106395	1.96522554	-2.40750246
C	-1.43301238	1.24072288	-3.65600944
C	0.63088473	2.14604846	-2.48796564
C	-0.31493614	-4.55209157	0.06604116
C	-1.61267985	-4.83703608	0.84469477
C	-0.53841685	-4.69598276	-1.45211788
C	2.35119878	-3.27255920	0.35147428
C	2.86654244	-3.33109040	-1.09628188
C	2.81887233	-4.49461142	1.16318870
C	-2.01442178	-1.71129775	-0.54015582
C	0.09729507	-1.24244738	-1.90678681
C	2.86704520	1.56903616	0.23050863
C	2.60677836	2.76286433	0.93635849
C	3.11006118	3.98515618	0.46381616
C	3.88670024	4.02513194	-0.71132119
C	4.16010356	2.83545100	-1.41317243
C	3.65099158	1.61411720	-0.94286638
C	2.42531924	0.24269537	0.78141627
H	0.45908141	-0.16520836	1.99766106
H	-0.90669715	4.10426512	-0.85039431
H	-0.50629008	5.78484718	0.92175387
H	-0.47263666	5.07601383	3.34504664
H	-0.86385815	2.67686118	3.92922315
H	-1.37089843	0.60671790	3.45967908
H	-2.47113806	0.32757172	2.09213391
H	-1.75962804	-2.09284475	2.45321548
H	-0.71193627	-1.41673610	3.74093302
H	0.14507130	-3.68208382	2.86859152
H	1.31662697	-2.32344428	2.70715729
H	-3.52082633	0.44219029	-1.79367973
H	-3.84025415	-0.22378462	0.60603608
H	-5.21230016	0.73232845	-0.00883057
H	-4.01924110	1.51763822	1.06403709
H	-3.62394698	3.37922424	-0.76882240
H	-4.96677906	2.53411012	-1.59296876
H	-3.45959746	2.87127654	-2.48433241
H	-1.36091630	2.97215298	-2.37522060
H	-1.00269840	0.22629887	-3.76149676
H	-1.14417670	1.81618825	-4.56245259
H	-2.53790608	1.15049727	-3.66494575
H	1.04371908	2.67532597	-1.60713237
H	0.89029694	2.73738554	-3.39318134
H	1.14679112	1.16932598	-2.56481815
H	0.43873066	-5.30678347	0.38266591
H	-1.46696086	-4.82156602	1.94442414
H	-1.98215470	-5.85271958	0.58271826

H	-2.41660551	-4.12064220	0.58402257
H	-1.33367644	-4.01056993	-1.80705280
H	-0.86000706	-5.73386232	-1.68839497
H	0.37404358	-4.48377311	-2.04386488
H	2.78221217	-2.36924857	0.83593073
H	2.52967597	-4.25389536	-1.61456217
H	3.97837622	-3.34508471	-1.10248740
H	2.53098762	-2.46601425	-1.70112407
H	2.48009229	-4.46822900	2.21931590
H	3.93025708	-4.53064153	1.17690737
H	2.47426068	-5.45092213	0.71501815
H	2.01603643	2.70479408	1.86413160
H	2.90303044	4.91514322	1.01827197
H	4.28647627	4.98528354	-1.07704895
H	4.77488293	2.86222187	-2.32774223
H	3.86346054	0.67688558	-1.48603538
H	2.88822364	-0.61274274	0.22273373
H	1.04182525	-0.06575308	-0.17023350
B-C(Ph-ⁱPr)			
Mn	-0.87551783	-0.07538561	0.20255885
P	-0.12910242	-2.19957477	0.78207070
P	-1.48750014	1.99954152	-0.57142885
O	-3.68248639	-0.98349115	0.42020786
O	-0.90183612	0.92234644	2.97553085
O	1.97833140	0.63936942	-1.87946957
N	-0.46249896	-0.45821079	-1.86246930
C	1.07147108	-2.88614885	-0.46944619
C	2.22198524	-3.62611508	-0.10852525
C	3.11980307	-4.11173991	-1.07469490
C	2.88027070	-3.85950653	-2.43407074
C	1.74595483	-3.12166563	-2.80701426
C	0.83176986	-2.62835197	-1.85078228
C	-0.37668787	-1.85801650	-2.35705789
C	-1.31561093	0.34665740	-2.77813499
C	-1.19950431	1.82485624	-2.41333284
C	-1.39144018	-3.64257814	0.93929744
C	-2.19634768	-3.92702717	-0.34031238
C	-0.77960148	-4.95956694	1.45271230
C	0.78043632	-2.40767652	2.44041783
C	-0.17551552	-2.32965854	3.64808907
C	1.93836015	-1.41254501	2.60494630
C	-3.27531736	2.62026472	-0.39963253
C	-4.26016627	1.95239792	-1.37711149
C	-3.78186813	2.49978228	1.05141753
C	-0.45843753	3.54064738	-0.17758245
C	-0.55940698	4.00034426	1.28766450
C	-0.68469552	4.71942424	-1.14172350
C	-2.56009816	-0.62627383	0.28856329
C	-0.89699269	0.49611949	1.87124154

C	2.79475246	1.92589143	-0.01848217
C	3.12773980	3.00872929	-0.86356749
C	3.73591720	4.16127391	-0.33973480
C	4.01818798	4.24635128	1.03711570
C	3.69604816	3.16868808	1.88472768
C	3.09319149	2.01442148	1.35867185
C	2.22091365	0.67401401	-0.63778945
H	0.52215755	-0.06384503	-1.95954809
H	2.43028805	-3.83770983	0.95110020
H	4.00624583	-4.68588019	-0.75947496
H	3.57799151	-4.22676149	-3.20374996
H	1.56131019	-2.91112353	-3.87377551
H	-0.31893224	-1.84730559	-3.47041325
H	-1.32118004	-2.37408752	-2.09761097
H	-2.36379473	-0.01360135	-2.70153864
H	-0.98909431	0.18793599	-3.83486252
H	-1.87241074	2.45598222	-3.02915571
H	-0.15301843	2.15281013	-2.59458370
H	-2.10168323	-3.24378877	1.69780001
H	-2.71641306	-3.03135405	-0.72884072
H	-2.97974475	-4.68327116	-0.11657418
H	-1.55249447	-4.35472241	-1.13828140
H	0.00509470	-5.33603172	0.76199086
H	-1.57008928	-5.73975347	1.50501948
H	-0.33845132	-4.88075410	2.46548564
H	1.20450107	-3.43454810	2.41264332
H	-0.63731462	-1.32812305	3.74244029
H	0.40124314	-2.51592026	4.58028579
H	-0.98748406	-3.08291620	3.61215756
H	2.65141449	-1.44235892	1.75580953
H	2.50746569	-1.64605482	3.53117307
H	1.55276211	-0.37811536	2.69809606
H	-3.21199339	3.70058870	-0.66349443
H	-3.97784846	2.09640374	-2.44027515
H	-5.27030353	2.39886459	-1.24698391
H	-4.35739643	0.86552828	-1.18033094
H	-3.93327855	1.43928811	1.33413144
H	-4.76189224	3.01589664	1.15050049
H	-3.08957468	2.94831085	1.79012635
H	0.57110060	3.15393258	-0.33657657
H	-1.53695560	4.48355129	1.50008240
H	0.22808241	4.75718572	1.49244078
H	-0.42118141	3.16958020	2.00631125
H	-0.53395975	4.44581278	-2.20578825
H	0.03606433	5.53312353	-0.90832956
H	-1.70286213	5.15387641	-1.03962974
H	2.91450961	2.90594443	-1.93949853
H	4.00165248	4.99607476	-1.00929755
H	4.49692283	5.14965312	1.44959351

H	3.91778719	3.22931224	2.96278501
H	2.84095513	1.17276777	2.02203652
H	2.49756611	-0.26701539	-0.09539995
H	0.74309234	0.54079064	0.18811830
A-C(Ph-Ph)			
Mn	-0.43366847	-0.91126120	-0.23902796
P	-1.55622930	1.07011551	-0.71865489
P	0.62928624	-2.87050298	0.45105762
O	-3.00656748	-2.31143674	-0.41481993
O	0.25867028	-1.53172694	-3.04558326
O	2.07520955	0.12220636	1.80162878
N	-0.35269195	-0.45713637	1.78696299
C	-1.16373084	2.40290310	0.51672484
C	-1.03796518	3.76395220	0.15137267
C	-0.74529012	4.75725344	1.09994336
C	-0.56372372	4.39843274	2.44447329
C	-0.67287696	3.05021464	2.81787437
C	-0.97275454	2.03653884	1.87944322
C	-1.14821003	0.62577320	2.41627917
C	-0.45342983	-1.65025437	2.67540374
C	0.60923881	-2.68482793	2.30963922
C	-3.47316532	1.06420304	-0.71242746
C	-4.08976347	0.66538444	0.63930418
C	-4.10097478	2.38638911	-1.19082617
C	-1.22114803	1.88578484	-2.39812479
C	-1.86028587	1.10732696	-3.56499434
C	0.27856691	2.11864427	-2.63472419
C	-0.15353299	-4.55839980	0.07045088
C	-1.34406396	-4.91927030	0.97861621
C	-0.52957278	-4.69018198	-1.41819070
C	2.48142823	-3.17924588	0.15365042
C	2.86862897	-3.26131681	-1.33203451
C	3.05975475	-4.36252212	0.95149250
C	-1.96115939	-1.76046173	-0.33331451
C	-0.03530010	-1.25818032	-1.93393733
C	2.77394131	1.68125983	0.05417679
C	2.65369791	2.78653358	0.91870366
C	3.15816620	4.04357132	0.54199132
C	3.79695399	4.20780606	-0.70153320
C	3.93398429	3.10384814	-1.56488792
C	3.42776797	1.84901562	-1.18522995
C	2.27709585	0.30537362	0.49381101
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H	-0.65627408	5.80877986	0.78273594
H	-0.32732513	5.16327315	3.20177662
H	-0.51865355	2.76469681	3.87202567
H	-0.88762993	0.66369433	3.49996354
H	-2.22269892	0.34374281	2.38075919
H	-1.47858329	-2.07952594	2.61059597

H	-0.30757809	-1.33636030	3.73764847
H	0.44963229	-3.64247668	2.84491814
H	1.60635837	-2.28169913	2.58208893
H	-3.71047045	0.25862360	-1.44243496
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H	-1.40805952	0.10464014	-3.68839323
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H	0.76597162	2.66159811	-1.80136219
H	0.42414863	2.71680354	-3.56051961
H	0.81713395	1.16029708	-2.77126073
H	0.66487052	-5.28012015	0.28756304
H	-1.07512773	-4.93068131	2.05449198
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H	-1.39443800	-4.04612674	-1.67319735
H	-0.81836113	-5.74071716	-1.63982890
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H	2.81987207	-4.31230930	2.03331163
H	4.16799676	-4.36375252	0.86202802
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H	2.17577757	2.62540254	1.89755714
H	3.06137192	4.90123365	1.22835848
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H	4.44628423	3.22094322	-2.53433056
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H	0.79274496	-0.12163267	1.86045814
A-C(Ph-ⁱPr)			
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O	-3.65756778	-0.97189531	0.44530143
O	-1.09534939	0.73550257	3.03557432
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N	-0.47495412	-0.43868659	-1.80543807
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C	0.87914750	-2.58235086	-1.82758374
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C	1.88365763	-1.39726596	2.65208765
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C	-0.45629593	3.54353527	-0.14155240
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C	3.92712774	3.96756218	-0.53855434
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C	3.59428635	3.31770966	1.78192817
C	2.89883169	2.17176278	1.35978998
C	2.01015686	0.64678519	-0.51743760
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H	-0.00483529	-5.33888194	0.68422690
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H	-0.33406630	-4.91857136	2.39926493
H	1.21245315	-3.43567749	2.41245097
H	-0.71030299	-1.42709489	3.77701690
H	0.36687790	-2.59678405	4.59092983
H	-0.99397822	-3.19000264	3.60068076

H	2.59756299	-1.38077855	1.80355822
H	2.45747646	-1.63747815	3.57336477
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Mn	0.20838559	-0.50161855	-0.29510968
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O	-0.11940603	-0.71075224	-3.24761412
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C	-0.57087599	4.20556356	0.52678805
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C	-3.12473437	3.40472262	-0.22408047
C	-2.06482520	2.47033635	-0.30535157
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C	-2.20394426	-2.41413944	0.66823035
C	1.77312264	2.47585088	-1.40918349
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C	2.54586725	3.76198409	-1.07163930
C	1.63935473	2.16218638	1.56401785
C	2.96913443	1.39776528	1.67908159
C	0.77837730	1.95457303	2.82002310
C	-0.33342766	-4.02696085	-1.02248134
C	-1.43046888	-3.91451248	-2.09695701

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C	1.80189841	-3.59874465	1.83000634
C	-0.46249408	-4.65137433	2.29496525
C	-0.00291760	-0.59909246	-2.07229357
C	1.92265734	-0.89065780	-0.45247724
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H	-1.44490871	6.15346902	0.94232799
H	-3.76526307	5.42761801	0.25546454
H	-4.13982711	3.08077860	-0.51071326
H	-3.52616329	1.02068221	-0.86887777
H	-2.03312272	0.92758079	-1.84865354
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H	-2.79861607	-3.33248596	0.48120953
H	-2.26083050	-2.20146599	1.75852119
H	2.50873780	1.66097398	-1.59334613
H	0.43404154	1.73471678	-3.00563259
H	1.60546231	2.97875807	-3.52685869
H	0.17623695	3.46027920	-2.56044706
H	1.86400631	4.61877540	-0.88596216
H	3.18328016	4.04559915	-1.93794394
H	3.21886013	3.65365561	-0.19744335
H	1.86944794	3.24595937	1.47108783
H	2.78903104	0.31534540	1.83525070
H	3.54659071	1.77715179	2.55042631
H	3.61017299	1.49878652	0.77970243
H	-0.14420013	2.57102429	2.80970182
H	1.35821247	2.22931419	3.72829946
H	0.48333139	0.88713460	2.90985908
H	-0.51153478	-4.95685222	-0.43599428
H	-2.45631317	-3.94769046	-1.67435663
H	-1.34702467	-4.76675021	-2.80651952
H	-1.32026511	-2.98380951	-2.69154375
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H	2.09173279	-4.45705290	1.18742495
H	2.15545881	-3.83160344	2.85813443
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H	-1.56187298	-4.51392288	2.35896427
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Mn	-0.20561665	0.52673378	-0.07830388
P	-0.84715856	-1.70686429	-0.07278539

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O	-0.02642290	0.85557480	-3.00679470
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N	1.84166993	-0.00477749	0.12245241
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C	0.25710795	-4.15828892	0.94923571
C	1.28826087	-5.05345855	1.27747361
C	2.62090505	-4.69134067	1.02585448
C	2.89710768	-3.44184504	0.45053762
C	1.87355227	-2.52881415	0.10582738
C	2.28353004	-1.21820251	-0.55142259
C	2.74870943	1.08674570	-0.20304575
C	2.39321920	2.35167903	0.58284192
C	-1.55433540	-2.44308576	-1.68406404
C	-0.46289170	-2.56271192	-2.76394793
C	-2.28773767	-3.78716711	-1.53062049
C	-2.17076053	-2.16643937	1.21728978
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C	-1.72395575	-1.83132962	2.65018552
C	0.40156640	4.05522608	-0.91461123
C	1.42902047	3.96719995	-2.05854888
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C	-1.40335287	3.80831048	2.12078515
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C	-0.11391895	0.71556668	-1.83889518
C	-1.89438787	1.09151933	-0.06778621
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H	1.04620337	-6.02862649	1.73061058
H	3.44535138	-5.37668126	1.28215399
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H	1.98692651	-1.24653688	-1.63808380
H	2.76337763	1.33077482	-1.30340909
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H	2.54451996	2.16574112	1.66857751
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H	0.04707404	-1.60286968	-2.96770483
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H	-1.65902589	4.68697331	1.49135462
H	-1.64217278	4.08415441	3.17095783
H	-2.07133961	2.97565428	1.82693860
H	2.06007474	4.39004481	2.39329467
H	0.72611653	4.96332053	3.43826806
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H	-0.14195471	0.32908588	1.65613354
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O	-0.40439008	0.91799804	-2.94215930
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C	1.28751276	4.58942504	2.35838806
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C	-1.90017126	1.09457090	0.17234963
H	0.52401228	0.14050038	1.49638276

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H	3.50308004	-5.15187896	1.62956813
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H	1.89009606	-1.37023679	-1.71552531
H	2.55771720	1.31665038	-1.61786653
H	3.75575351	0.77746312	-0.41076226
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H	2.76575228	2.17034443	1.34819269
H	-2.22511377	-1.82838995	-2.08757429
H	0.08969185	-1.49892014	-3.02757683
H	-0.72559976	-2.89538534	-3.78594031
H	0.53040560	-3.17555466	-2.54221580
H	-1.21420037	-4.64412581	-1.22704312
H	-2.29466334	-4.31811496	-2.61342459
H	-2.87129603	-4.00357481	-0.95430605
H	-2.28177797	-3.33203951	1.04225658
H	-3.75416651	-0.65195374	0.55941724
H	-4.44385552	-2.15774317	1.23311534
H	-3.89641111	-2.11242915	-0.46583033
H	-1.02243867	-2.06537644	2.87046652
H	-2.78477095	-2.19902866	3.17465086
H	-2.10164576	-0.65608782	2.58442329
H	0.55728427	4.97448490	-0.28550635
H	2.19591393	4.01936728	-1.93945480
H	0.87810711	4.89680473	-2.76809092
H	0.87269674	3.10861787	-2.74451706
H	-1.56594372	3.31349868	-1.82304940
H	-1.42678317	5.09844683	-1.78059887
H	-1.89259958	4.19342595	-0.30431134
H	0.67807622	2.54448185	2.71226563
H	-1.45366910	4.62040268	1.83952282
H	-1.19143675	3.97458521	3.48254939
H	-1.79473177	2.89596618	2.18142678
H	2.35800124	4.36121520	2.18045873
H	1.18565032	4.89205179	3.42354222
H	1.01998783	5.47751883	1.74651958
H	-0.25684337	0.27920431	1.73909936
D-A			
Mn	-0.20531428	0.48767474	0.00197311
P	-0.80543463	-1.76353054	-0.05589053
P	0.63117804	2.62658548	0.21633265
O	-1.20201227	0.93273392	-2.71418082
O	-2.83711093	1.41816197	1.01011988
N	1.73013412	0.04806431	-0.38753528
C	0.62387325	-2.85055500	0.42748147
C	0.46579571	-4.02277434	1.20541970
C	1.56785990	-4.80372695	1.59154028

C	2.85931709	-4.41491630	1.20250326
C	3.02697714	-3.25370037	0.43174266
C	1.93208537	-2.45521588	0.02910562
C	2.21766645	-1.24536423	-0.85183395
C	2.52526572	1.09894933	-1.02119890
C	2.42892110	2.39821366	-0.21512077
C	-1.41509521	-2.52641187	-1.69575508
C	-0.39541190	-2.40108710	-2.84050855
C	-1.88277304	-3.98741873	-1.56990558
C	-2.18416044	-2.31213790	1.13459577
C	-3.58636017	-1.86790796	0.67472582
C	-1.90713472	-1.86612097	2.58140167
C	-0.00017178	4.04272916	-0.87357345
C	0.53334947	3.97359320	-2.31738119
C	-1.53854322	4.12900299	-0.86866750
C	0.74741042	3.38986242	1.95618530
C	-0.61211004	3.68024565	2.61580366
C	1.67375219	4.61739855	2.03804489
C	-0.79360272	0.75849322	-1.61760038
C	-1.78524392	1.01346778	0.64316067
H	0.79634358	0.04236789	1.79316897
H	-0.53758446	-4.34508914	1.52275475
H	1.41269071	-5.71192095	2.19652252
H	3.73701363	-5.01042016	1.50265256
H	4.04191644	-2.94563347	0.12824197
H	3.33106074	-1.19371511	-0.94287365
H	1.87672784	-1.48979706	-1.89440963
H	2.23840058	1.29380056	-2.09177249
H	3.60216749	0.79199263	-1.06393296
H	2.86398597	3.27193839	-0.74332857
H	2.97225128	2.27053744	0.74512552
H	-2.28583218	-1.87845175	-1.94437391
H	-0.04420994	-1.36249398	-2.98792916
H	-0.86876077	-2.72980491	-3.79105710
H	0.48493729	-3.05534121	-2.66755583
H	-1.05160582	-4.64817011	-1.24320506
H	-2.22377809	-4.35471686	-2.56236652
H	-2.72810299	-4.12299309	-0.86638317
H	-2.16223279	-3.42323048	1.10617940
H	-3.69152193	-0.76613819	0.66857525
H	-4.34571362	-2.26783882	1.38185786
H	-3.85046570	-2.24612515	-0.33333547
H	-0.89455821	-2.15555771	2.92997113
H	-2.64620160	-2.33432811	3.26746580
H	-2.01200207	-0.76721195	2.68884402
H	0.40973135	4.96261338	-0.39786691
H	1.64027482	4.00319814	-2.37082743
H	0.15382532	4.84679153	-2.89178301
H	0.18306671	3.05979561	-2.83840043

H	-1.98652015	3.26485454	-1.39893059
H	-1.86356540	5.05133729	-1.39771271
H	-1.97086754	4.15369830	0.15053908
H	1.22851980	2.55493606	2.51546256
H	-1.11320498	4.55359590	2.14709546
H	-0.46418054	3.93124168	3.68876042
H	-1.31025980	2.82247175	2.55957888
H	2.68277782	4.42681834	1.61911170
H	1.80793812	4.91883612	3.09997673
H	1.24288250	5.49398039	1.50840690
H	0.08102189	0.18167793	2.08133767
E (reference)			
Mn	0.15458259	1.29870728	0.07128664
P	-2.14305998	0.98179070	0.45388414
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O	-0.26708449	3.71450371	-1.57914594
O	0.54249049	3.02873531	2.42953222
N	0.09650030	-0.08915692	-1.58142490
N	0.49919656	-0.43273974	1.13274102
N	0.66136367	-1.62752146	0.59814777
C	-2.75135232	-0.62383931	-0.27629280
C	-3.70937426	-1.43950804	0.36913312
C	-4.15708512	-2.64529604	-0.19729880
C	-3.64635115	-3.06317990	-1.43472756
C	-2.68785344	-2.26954365	-2.08408214
C	-2.22682972	-1.05526340	-1.52953321
C	-1.18259200	-0.27587135	-2.31203804
C	1.21756416	0.09802410	-2.53710278
C	2.55121291	0.10521809	-1.79043347
C	-3.41751131	2.23280795	-0.24939011
C	-3.38303213	2.35272577	-1.78330267
C	-4.86785207	1.98608174	0.20690504
C	-2.73131674	0.89263654	2.26139987
C	-2.74066273	2.27193330	2.95023545
C	-1.95759169	-0.12984309	3.11085272
C	3.34686654	2.85996611	-0.90424208
C	3.09574448	3.23768084	-2.37612421
C	3.03323455	4.04984867	0.02390746
C	3.59843193	0.48259722	0.89998651
C	3.68763597	1.23754644	2.23791402
C	4.99903983	0.16949493	0.34317150
C	-0.10848397	2.73638126	-0.92933571
C	0.35936570	2.32936655	1.49357779
C	1.02550217	-2.68761331	1.29807389
C	1.20304864	-4.01126602	0.71943544
C	0.95476887	-4.30358259	-0.65297002
C	1.15159010	-5.59208196	-1.16574540
C	1.59793877	-6.64013367	-0.33408827
C	1.84196363	-6.37215312	1.02640542

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H	0.69737398	-0.41442522	2.15127889
H	-4.12513976	-1.13684268	1.34165062
H	-4.90396669	-3.25618312	0.33509418
H	-3.98150884	-4.00874941	-1.89001361
H	-2.27524236	-2.60048902	-3.05211039
H	-0.98803687	-0.83807947	-3.25494339
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H	1.05924896	1.05053847	-3.08774187
H	1.20998725	-0.72126533	-3.29704969
H	3.39507705	0.33573801	-2.47239804
H	2.73752604	-0.90001161	-1.35589539
H	-3.05674716	3.19760333	0.17360760
H	-2.38289639	2.62170069	-2.17132821
H	-4.08050510	3.15736444	-2.10219486
H	-3.72679227	1.41504596	-2.26994616
H	-5.23345005	0.99336309	-0.13263982
H	-5.53375224	2.75193162	-0.24719351
H	-5.00648400	2.04831337	1.30403107
H	-3.78642266	0.55096031	2.19074255
H	-1.71908702	2.68071712	3.07040808
H	-3.17753652	2.16635186	3.96724324
H	-3.34890275	3.02634606	2.41215520
H	-1.85352173	-1.11570488	2.61548199
H	-2.48689309	-0.28273947	4.07698489
H	-0.94150494	0.24333491	3.35000428
H	4.42385979	2.59827934	-0.79584949
H	3.39212885	2.43708518	-3.08446504
H	3.69798281	4.13607596	-2.63402372
H	2.03226690	3.49500627	-2.55642267
H	1.98627498	4.39039501	-0.10582434
H	3.69753911	4.90619992	-0.22393633
H	3.17502140	3.81191617	1.09636449
H	3.07262797	-0.48043635	1.08171172
H	4.26920010	2.17889791	2.14048116
H	4.21401464	0.61005696	2.98958587
H	2.69239873	1.49765248	2.64893001
H	4.97043569	-0.42337310	-0.59369626
H	5.57296631	-0.42476654	1.08720359
H	5.58680856	1.09237782	0.14814978
H	1.20801736	-2.57436486	2.39297896
H	0.59281305	-3.49705418	-1.30954261
H	0.94996534	-5.78766226	-2.23271540
H	1.75000256	-7.65242644	-0.74191457
H	2.18847538	-7.17931406	1.69349252
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F			
Mn	1.29375498	-1.01981045	0.10534379

P	0.40153582	-1.54766598	-1.98807783
P	1.83343141	-0.42105409	2.26444186
O	3.49480310	-2.98889036	-0.01050217
O	3.19686368	0.94235787	-1.01189896
O	0.02497713	3.40296706	-0.44442696
N	-0.04187950	-2.42450890	1.04652149
N	-0.28835596	0.26151698	0.36958096
N	-1.45486925	-0.09873233	0.86914544
C	-1.07152442	-2.69888491	-1.95739625
C	-2.00454016	-2.72881505	-3.02196211
C	-3.11325491	-3.59107037	-3.01527153
C	-3.31815599	-4.44644977	-1.92217035
C	-2.40520150	-4.42748417	-0.85711206
C	-1.27753367	-3.57443254	-0.85367177
C	-0.32822944	-3.69061237	0.32668280
C	0.31825862	-2.73061876	2.45660111
C	0.61458165	-1.45374159	3.24140552
C	1.58648513	-2.46597513	-3.18545065
C	1.77540582	-3.93609686	-2.76654635
C	1.23433928	-2.39686487	-4.68175837
C	-0.24369318	-0.13011677	-3.08512933
C	0.85733170	0.89985600	-3.39514947
C	-1.51098520	0.56689661	-2.55960179
C	3.53394589	-0.77790593	3.02889617
C	3.74591384	-2.25446992	3.41156769
C	4.66924300	-0.28875574	2.10775234
C	1.41583755	1.32362447	2.88012926
C	2.27113754	2.42198004	2.22516762
C	1.39615298	1.46662849	4.41259069
C	2.60251198	-2.20817757	0.01777128
C	2.39758890	0.18354543	-0.58609622
C	-2.43338736	0.76123461	1.10247326
C	-3.72460931	0.37496371	1.64948878
C	-4.08536933	-0.97621414	1.92660667
C	-5.33874129	-1.29615047	2.46338302
C	-6.28555908	-0.28808851	2.74157060
C	-5.95091050	1.05202214	2.46775633
C	-4.69621573	1.37753087	1.93229702
C	-0.72091890	4.36047157	-0.62721611
C	-0.27357926	5.71030773	-1.04651525
C	1.09940922	5.97449536	-1.26957751
C	-1.22718363	6.73882650	-1.22303541
C	1.50760270	7.25524096	-1.66313875
C	-0.81539042	8.02146370	-1.61792433
C	0.55140478	8.27822410	-1.83705517
H	-0.89978762	-1.80006457	1.05733466
H	-0.21298528	1.27827077	0.16744684
H	-1.87177694	-2.05927550	-3.88483957
H	-3.81729651	-3.58623660	-3.86317942

H	-4.18829332	-5.12181121	-1.89267671
H	-2.56497322	-5.09670706	0.00524243
H	-0.78265110	-4.41964435	1.03703476
H	0.64118450	-4.13352313	0.00901101
H	1.20287766	-3.40334177	2.44913420
H	-0.51309054	-3.29640755	2.94400401
H	0.96477169	-1.68892808	4.26780822
H	-0.31214889	-0.84794618	3.33221377
H	2.54806180	-1.93106965	-3.01696561
H	2.11126000	-4.04327804	-1.71847724
H	2.55499006	-4.40654126	-3.40420016
H	0.83885825	-4.51698495	-2.90409544
H	0.25042841	-2.86776929	-4.89372031
H	1.99316334	-2.96507657	-5.26314682
H	1.22351162	-1.36537761	-5.08596430
H	-0.50565177	-0.63758720	-4.03821849
H	1.09362667	1.51658003	-2.50643209
H	0.50612044	1.58740372	-4.19562200
H	1.80504796	0.43954057	-3.74184455
H	-2.29267610	-0.14147288	-2.22121603
H	-1.94710319	1.19195938	-3.37011627
H	-1.27424670	1.23334211	-1.70964313
H	3.55073162	-0.17503766	3.96512267
H	2.99996968	-2.62170267	4.14610531
H	4.74725216	-2.37501161	3.87998305
H	3.72250848	-2.91355049	2.51972227
H	4.73885205	-0.91518944	1.19613774
H	5.64320592	-0.36025910	2.63943290
H	4.53940908	0.76113361	1.77991004
H	0.37510834	1.43215953	2.50479195
H	3.31892674	2.40140635	2.59352655
H	1.85684277	3.42089483	2.48194527
H	2.28922869	2.34263605	1.12082240
H	0.73654494	0.72567155	4.90853558
H	1.01923266	2.47558531	4.68901744
H	2.41173373	1.37264293	4.85468944
H	-2.26916114	1.84105542	0.88237757
H	-3.36155744	-1.77462997	1.70032156
H	-5.58781228	-2.35197823	2.66512863
H	-7.27100435	-0.54543877	3.16224986
H	-6.67836708	1.85493790	2.67541595
H	-4.44747614	2.43296480	1.72545167
H	-1.83703666	4.25740037	-0.47841677
H	1.82180628	5.15488737	-1.12732467
H	-2.29533813	6.52333364	-1.04757654
H	2.57513646	7.46529906	-1.83798035
H	-1.55753010	8.82402384	-1.75595491
H	0.87651657	9.28487733	-2.14703145

F-G (S_N, S, S)

Mn	-0.62663750	-1.74451510	0.17647392
P	1.52930756	-2.09853778	1.06903777
P	-2.65897180	-1.29686146	-0.86819852
O	-0.93926287	-4.64970418	-0.29145869
O	-2.03865323	-2.14496072	2.73834985
O	-1.91698046	2.14333474	1.04454432
N	0.22238674	-1.27787302	-1.75181212
N	-0.34560566	0.24726357	0.47494949
N	0.22664546	1.03283703	-0.36160440
C	2.85903031	-1.30371244	0.03067223
C	4.00952674	-0.71064907	0.60127617
C	5.00707051	-0.11896928	-0.19220802
C	4.86740899	-0.10639179	-1.58764998
C	3.72753338	-0.68318617	-2.16863803
C	2.71652203	-1.28504854	-1.38760098
C	1.52749385	-1.88576093	-2.11998312
C	-0.74261567	-1.41234462	-2.87282527
C	-2.05689194	-0.70880880	-2.53864184
C	2.19715913	-3.88937230	1.23962726
C	2.38546498	-4.60142353	-0.11232558
C	3.50125335	-4.00205266	2.05201423
C	1.87385265	-1.42945411	2.81575053
C	1.15143586	-2.23898476	3.91046879
C	1.58018841	0.07205994	2.96691530
C	-3.89721215	-2.68754623	-1.24703458
C	-3.50600178	-3.59323482	-2.42903144
C	-4.21693422	-3.53120584	0.00354773
C	-3.75202662	0.12328029	-0.28633988
C	-4.53585984	-0.19631526	1.00033175
C	-4.68786602	0.67426937	-1.37722156
C	-0.80396126	-3.48663583	-0.13252068
C	-1.44602407	-1.96987892	1.73363915
C	0.38267176	2.38797633	0.01702854
C	1.18096151	3.18701684	-0.96224196
C	2.11393258	4.15185836	-0.51707645
C	2.84132540	4.93032436	-1.43250916
C	2.64852224	4.76320353	-2.81650684
C	1.71786796	3.81177848	-3.27404444
C	0.98947569	3.03561758	-2.35648781
C	-1.28865261	3.00599458	0.28347123
C	-1.08138551	4.40520688	0.86438728
C	-0.89636952	5.53365721	0.03857173
C	-1.11350574	4.58097603	2.26385994
C	-0.72862342	6.81190887	0.60114773
C	-0.94040818	5.85569140	2.82845826
C	-0.74457849	6.97666857	1.99845093
H	0.38503931	-0.24539891	-1.57847563
H	-0.77791498	0.77998836	1.27730101
H	4.14193483	-0.70373273	1.69339926

H	5.89025224	0.33410324	0.28635442
H	5.63536352	0.36113928	-2.22422164
H	3.60905446	-0.66341823	-3.26499384
H	1.70450709	-1.73967992	-3.21057215
H	1.46073997	-2.98098442	-1.95888882
H	-0.90754896	-2.49356351	-3.06730116
H	-0.30081526	-0.98110200	-3.80427894
H	-2.80710191	-0.85094463	-3.34355439
H	-1.88258792	0.38398009	-2.43651151
H	1.37588911	-4.40375872	1.78765107
H	1.45603485	-4.65085134	-0.70895008
H	2.70514186	-5.64986772	0.07070614
H	3.18301277	-4.11770119	-0.71534955
H	4.32341649	-3.42376911	1.57860374
H	3.82529354	-5.06501241	2.07903260
H	3.40179121	-3.66901890	3.10326696
H	2.96581732	-1.58093317	2.95528450
H	0.05441804	-2.10010749	3.87103209
H	1.49492152	-1.88812541	4.90778416
H	1.35646402	-3.32723044	3.85846271
H	2.04066145	0.68437742	2.16539576
H	1.98162208	0.43147246	3.93922689
H	0.49034657	0.27213355	2.97010634
H	-4.81689298	-2.12927677	-1.53624327
H	-3.36813207	-3.03345264	-3.37682629
H	-4.31524517	-4.33461310	-2.60784841
H	-2.58209347	-4.16925082	-2.21767916
H	-3.36501949	-4.18392592	0.27761421
H	-5.08713595	-4.19098985	-0.20548786
H	-4.46811695	-2.91541149	0.88798273
H	-3.00901042	0.91175877	0.00285245
H	-5.38766359	-0.88778492	0.82084325
H	-4.95693220	0.74944779	1.40287146
H	-3.89485055	-0.62842921	1.79391543
H	-4.14859226	1.02215136	-2.28188708
H	-5.23615589	1.55276151	-0.97326799
H	-5.45675879	-0.06383822	-1.69801510
H	0.74647670	2.50581716	1.05962486
H	2.26648320	4.29275378	0.56576397
H	3.56441844	5.67536842	-1.06165086
H	3.21690312	5.37565543	-3.53544052
H	1.55343646	3.67806460	-4.35638130
H	0.25516626	2.29810811	-2.71896023
H	-1.64503472	3.09696268	-0.78683597
H	-0.88943736	5.40876891	-1.05729743
H	-1.30714841	3.69361988	2.88813692
H	-0.58718326	7.68586667	-0.05632966
H	-0.97214331	5.98077799	3.92400680
H	-0.61675536	7.97895299	2.43984446

	F-G (S_N, R, S)		
Mn	0.24884673	1.76222658	0.12297014
P	-2.10248532	1.54627160	0.31055735
P	2.54569444	1.92231087	-0.23155489
O	-0.07039677	4.47105939	-1.02132936
O	0.59293998	3.06314553	2.75144932
O	0.23009143	-1.64735516	2.69715459
N	0.23903519	0.75223588	-1.78825730
N	0.72022278	-0.10236644	0.80163204
N	0.92459634	-1.12246960	0.04622655
C	-2.84030491	0.32591922	-0.89040722
C	-4.04912388	-0.34965937	-0.59798529
C	-4.61903760	-1.27015658	-1.49362094
C	-3.97437955	-1.54468783	-2.70924788
C	-2.77881113	-0.87749119	-3.01728983
C	-2.20119456	0.06625187	-2.13715225
C	-0.97489220	0.80957313	-2.63961301
C	1.42482761	1.08883271	-2.62458908
C	2.72178754	0.96280135	-1.82707438
C	-3.09708676	3.14225302	-0.11490773
C	-3.11550290	3.44489213	-1.62478524
C	-4.54016946	3.18722754	0.42100640
C	-2.89383382	1.06988371	1.97330223
C	-2.52438725	2.08491696	3.07236014
C	-2.63325152	-0.36729947	2.44231534
C	3.41575033	3.58288072	-0.52795190
C	3.21584638	4.15906981	-1.94220772
C	3.04486133	4.62358385	0.54783806
C	3.75108721	1.00199751	0.91134473
C	3.85039225	1.61651537	2.31906419
C	5.14592130	0.77249678	0.30110152
C	0.04305268	3.38072450	-0.57914914
C	0.41415887	2.51389817	1.72430652
C	1.56875441	-2.22580669	0.67765206
C	1.96923885	-3.32722169	-0.25439771
C	1.21356961	-3.65347821	-1.40489925
C	1.60549838	-4.70893636	-2.24511861
C	2.75024249	-5.47139270	-1.94657853
C	3.50350503	-5.16484634	-0.79859649
C	3.11707702	-4.10211030	0.03532109
C	0.60030691	-2.73170051	2.04201821
C	-0.50435261	-3.69289261	1.59175525
C	-0.50968752	-5.01850035	2.07229952
C	-1.54611261	-3.28912493	0.72980720
C	-1.53111538	-5.91820931	1.71522474
C	-2.56369935	-4.18499383	0.36008789
C	-2.56302619	-5.50308961	0.85596347
H	0.37925641	-0.23272156	-1.43134931
H	0.84389804	-0.36909345	1.83358496

H	-4.56654932	-0.15766238	0.35303950
H	-5.56403982	-1.77363161	-1.23333517
H	-4.39834032	-2.27397574	-3.41798157
H	-2.27601645	-1.08332013	-3.97736679
H	-0.72981117	0.39005526	-3.64289874
H	-1.21853511	1.88010651	-2.80735127
H	1.29316325	2.12286133	-3.01027248
H	1.46002789	0.41473134	-3.51445498
H	3.59488141	1.28324810	-2.43150413
H	2.88248382	-0.09942547	-1.54559077
H	-2.50476201	3.93738659	0.38930600
H	-2.10412664	3.53774617	-2.06147742
H	-3.62500956	4.41725467	-1.79733082
H	-3.68087759	2.67080957	-2.18556776
H	-5.15678111	2.35662385	0.01488467
H	-5.01942121	4.13429593	0.09004506
H	-4.60285420	3.16316763	1.52601749
H	-3.98155828	1.17724041	1.77306005
H	-1.49953080	1.91236122	3.45110637
H	-3.21901386	1.95828947	3.93053986
H	-2.58743035	3.14351277	2.74517033
H	-3.07667582	-1.12119994	1.76292959
H	-3.11359179	-0.50748665	3.43578314
H	-1.55819635	-0.62822576	2.55366945
H	4.49473558	3.33218161	-0.41495361
H	3.56274697	3.47278454	-2.74158078
H	3.80686674	5.09536157	-2.04235663
H	2.15622798	4.42246806	-2.13360687
H	2.00257457	4.97710288	0.42277138
H	3.71060641	5.50883185	0.45388657
H	3.14506418	4.23564758	1.57998532
H	3.25093120	0.01425605	1.00825972
H	4.41553978	2.57245336	2.30999339
H	4.40015827	0.92231398	2.99032051
H	2.85884736	1.80780635	2.77389003
H	5.11185072	0.25597790	-0.67953887
H	5.74987943	0.13675819	0.98428485
H	5.70671565	1.72314582	0.17152282
H	2.44589955	-1.87784109	1.26802627
H	0.30588858	-3.07312824	-1.63044026
H	1.00361957	-4.94700319	-3.13796137
H	3.05126487	-6.30395364	-2.60320024
H	4.40187813	-5.75488494	-0.55263231
H	3.71820684	-3.86133959	0.92937805
H	1.39594607	-3.35793081	2.54543793
H	0.30245125	-5.34741325	2.74394672
H	-1.55000468	-2.26077412	0.33567213
H	-1.51956705	-6.94826389	2.10909153
H	-3.36202893	-3.85074161	-0.32298095

H	-3.36366450	-6.20495124	0.56934533
	F-G (S_N, S, R)		
Mn	0.60396690	1.66145211	0.09827796
P	-1.62527173	2.29494866	0.56016636
P	2.72390502	0.95473641	-0.50905687
O	1.07612335	4.29895562	-1.16613011
O	1.70249340	2.79010551	2.59770769
O	1.45707221	-1.84260028	2.11115544
N	-0.02996394	0.67456696	-1.71050488
N	0.20782107	-0.16112081	0.90811606
N	-0.45969654	-1.05824786	0.29168419
C	-2.86507028	1.28112959	-0.39321818
C	-4.11859060	0.91734488	0.15109644
C	-5.05030013	0.16059791	-0.57973058
C	-4.73800607	-0.25307970	-1.88277450
C	-3.49484350	0.09377359	-2.43413845
C	-2.54726527	0.85580704	-1.71617541
C	-1.23664936	1.18374558	-2.41441452
C	1.07108527	0.45418857	-2.68276682
C	2.31420665	-0.10837265	-1.99394844
C	-2.19530780	4.07929189	0.13363800
C	-2.21155654	4.36887472	-1.37858872
C	-3.56186903	4.46673511	0.73040050
C	-2.22075704	2.15843687	2.36073277
C	-1.57004017	3.21378354	3.27653434
C	-2.05295617	0.74995567	2.94993825
C	4.03923992	2.18354410	-1.11756594
C	3.81962637	2.70607463	-2.54906924
C	4.23750539	3.35084828	-0.12969978
C	3.70992090	-0.21788519	0.59495209
C	4.24928398	0.43433016	1.88127715
C	4.83198267	-0.96863972	-0.14553655
C	0.88087966	3.24302816	-0.67246192
C	1.23287584	2.32404704	1.62096333
C	-0.77618010	-2.21903403	1.11329881
C	-1.67137647	-3.20191052	0.41202399
C	-2.69898298	-3.85606816	1.12840402
C	-3.52735741	-4.80415894	0.50318955
C	-3.34623002	-5.10971729	-0.85793917
C	-2.32826504	-4.46260990	-1.58296755
C	-1.49560724	-3.52302931	-0.95282266
C	0.62761980	-2.85871794	1.77965091
C	1.23066936	-3.96060003	0.90069943
C	0.77825220	-5.29228256	1.02286244
C	2.25276738	-3.68973034	-0.02975292
C	1.31693876	-6.31851877	0.22771651
C	2.79701950	-4.70988014	-0.83037848
C	2.32819129	-6.03053835	-0.70706026
H	-0.29878906	-0.25067203	-1.26788655

H	0.76090129	-0.69626071	1.78051858
H	-4.38587798	1.22719328	1.17241187
H	-6.01748171	-0.10615397	-0.12403429
H	-5.45247663	-0.85491562	-2.46659211
H	-3.24251187	-0.24064312	-3.45444979
H	-1.28473813	0.73144511	-3.43193608
H	-1.11865498	2.27637690	-2.56489032
H	1.29734261	1.42416464	-3.17488630
H	0.73086336	-0.24272215	-3.48727530
H	3.15756384	-0.20362832	-2.70897059
H	2.09788074	-1.12472180	-1.60017865
H	-1.40084493	4.70704538	0.59635035
H	-1.22802700	4.21722015	-1.85948974
H	-2.48639796	5.43328255	-1.54134201
H	-2.97315613	3.75105055	-1.89993805
H	-4.37011937	3.80301898	0.35521398
H	-3.81863492	5.50093765	0.41393231
H	-3.58525727	4.45343524	1.83717669
H	-3.30768675	2.38406983	2.31003157
H	-0.49762492	3.00478724	3.44919514
H	-2.07574016	3.19607079	4.26631095
H	-1.65263681	4.24770496	2.88484649
H	-2.55032218	-0.02731798	2.33535511
H	-2.50249896	0.71673146	3.96618510
H	-0.98273260	0.47733362	3.04590733
H	4.96889364	1.57064087	-1.12225290
H	3.77754790	1.89375454	-3.30347380
H	4.66868522	3.36545823	-2.83338672
H	2.89689193	3.31530152	-2.62959947
H	3.38171619	4.05326374	-0.15784124
H	5.14805760	3.92443769	-0.40916629
H	4.36179741	3.01390179	0.91731636
H	2.92814677	-0.94640404	0.92207803
H	5.11250487	1.10591084	1.68377256
H	4.60488094	-0.36580560	2.56478078
H	3.47699957	1.01011669	2.42648407
H	4.48493834	-1.48769864	-1.06250233
H	5.25546560	-1.74668901	0.52527229
H	5.67144175	-0.29759354	-0.43165546
H	-1.28200828	-1.85281924	2.03149881
H	-2.85293345	-3.61195748	2.19386236
H	-4.32318798	-5.30263154	1.08102877
H	-3.99473698	-5.85182894	-1.35174112
H	-2.17493006	-4.70082833	-2.64861648
H	-0.68825736	-3.03277633	-1.51875803
H	0.18297488	-3.38703840	2.66923756
H	-0.01002738	-5.52757566	1.75812590
H	2.63944461	-2.66326363	-0.09540803
H	0.94879870	-7.35152747	0.34243249

H	3.60080418	-4.47541144	-1.54862980
H	2.75652487	-6.83393778	-1.32875190
F-G (S_N, R, R)			
Mn	0.46643506	-1.76945065	-0.17793764
P	-1.63435854	-1.95332156	-1.22502407
P	2.44803901	-1.44073463	0.98982458
O	0.59448573	-4.66798851	0.40328593
O	1.96198207	-2.38555986	-2.64974082
O	0.63393729	2.05115472	-2.15296422
N	-0.48654455	-1.29332958	1.70181817
N	0.55626087	0.25064330	-0.35196544
N	-0.03432358	1.07556454	0.43687621
C	-3.07731807	-1.39311511	-0.17990982
C	-4.28468307	-0.95541388	-0.77609587
C	-5.38076516	-0.53146944	-0.00668163
C	-5.28523444	-0.52752069	1.39323084
C	-4.09656002	-0.96042662	2.00006004
C	-2.98953739	-1.40446079	1.24080200
C	-1.79255659	-1.93014927	2.01268333
C	0.41477756	-1.45454520	2.87693604
C	1.78736367	-0.83081998	2.63149388
C	-2.15115433	-3.75308738	-1.66070217
C	-2.60435277	-4.53948109	-0.41612137
C	-3.21488460	-3.89534232	-2.76414259
C	-1.94858964	-1.04671041	-2.86331120
C	-0.94711433	-1.46694320	-3.95479999
C	-2.00839258	0.48391276	-2.74306349
C	3.64186737	-2.85391241	1.40540523
C	3.15685895	-3.77277872	2.54219814
C	4.00090448	-3.67282428	0.14946214
C	3.59804932	-0.01069530	0.49910655
C	4.26458391	-0.19953364	-0.87496185
C	4.62931998	0.36963039	1.57700418
C	0.51714761	-3.51047905	0.17631106
C	1.33849108	-2.10221110	-1.69082161
C	0.34842523	2.43222979	0.37472884
C	-0.32483305	3.28686664	1.39083240
C	-1.68329552	3.07525180	1.73435787
C	-2.32186619	3.89485448	2.68024320
C	-1.62222282	4.94944184	3.29672164
C	-0.27555068	5.17644176	2.95575599
C	0.36443382	4.35590994	2.01240826
C	0.07175513	2.95635539	-1.40563359
C	0.65556940	4.36149038	-1.44320250
C	1.97456308	4.55042210	-1.90878382
C	-0.10254444	5.48863922	-1.06172089
C	2.53289366	5.83774338	-1.97110351
C	0.45244772	6.77913698	-1.12893212
C	1.77383451	6.95776371	-1.57870712

H	-0.62899474	-0.25961123	1.53324509
H	1.08401196	0.76025537	-1.11971587
H	-4.37960612	-0.93825678	-1.87170707
H	-6.30494945	-0.19913768	-0.50653531
H	-6.13026288	-0.18706619	2.01296118
H	-4.01877347	-0.96115084	3.10042671
H	-2.01592836	-1.78732346	3.09494376
H	-1.68200285	-3.02598817	1.86294377
H	0.51175520	-2.54183938	3.08442539
H	-0.05818845	-0.99548337	3.77835635
H	2.47302186	-1.04117882	3.47805986
H	1.69126646	0.27275477	2.54957937
H	-1.19648804	-4.19431493	-2.02428977
H	-1.85239413	-4.54116394	0.39458895
H	-2.77573645	-5.60182955	-0.69371457
H	-3.56079399	-4.14180420	-0.01594856
H	-4.17310220	-3.41298921	-2.47448597
H	-3.43339469	-4.97420634	-2.92077964
H	-2.89606693	-3.48387843	-3.74144157
H	-2.95110558	-1.41861248	-3.16613113
H	0.04803223	-1.01535204	-3.78032284
H	-1.30660853	-1.09892741	-4.93996533
H	-0.81104852	-2.56508644	-4.03617978
H	-2.67181475	0.82524688	-1.92327243
H	-2.41469244	0.89998740	-3.69137249
H	-0.99817309	0.92741811	-2.59472834
H	4.55881672	-2.33169207	1.76004015
H	2.97632721	-3.22712437	3.49107667
H	3.93639485	-4.53680070	2.75336305
H	2.23353817	-4.31955251	2.26407280
H	3.13696085	-4.27270091	-0.19908378
H	4.82486550	-4.38012301	0.38711016
H	4.33352188	-3.04167461	-0.69769986
H	2.87234574	0.82728015	0.40869977
H	5.05937879	-0.97433813	-0.84248353
H	4.74897936	0.74995603	-1.18814977
H	3.54220822	-0.48303696	-1.66517485
H	4.17021416	0.57214130	2.56625181
H	5.16426369	1.29405753	1.26917851
H	5.40262317	-0.41694936	1.71086399
H	1.44709839	2.58606955	0.33086443
H	-2.23432069	2.25408439	1.24848819
H	-3.37949412	3.71264910	2.93443073
H	-2.12542743	5.59495596	4.03505471
H	0.28232436	6.00166904	3.42844359
H	1.41819519	4.54395525	1.74740875
H	-1.05681749	3.00084134	-1.40107413
H	2.53120817	3.66095719	-2.24600182
H	-1.14043038	5.35129334	-0.71493909

H	3.56267001	5.97373268	-2.34256439
H	-0.15171359	7.65193635	-0.83036189
H	2.20780870	7.96979280	-1.63522226
G (S _N , S, S)			
Mn	1.45828937	0.02265909	0.61589490
P	1.12263398	2.32710033	0.35798384
P	1.71434723	-2.27651022	0.64458018
O	4.38789199	0.42401044	0.86248651
O	1.28940606	0.06010563	3.56507229
O	-2.60415430	-1.68792487	1.38010218
N	1.47614035	-0.23388352	-1.52881922
N	-0.55958613	-0.37253476	0.42560424
N	-1.04022292	-0.42074626	-0.72450545
C	0.39657266	2.74161699	-1.31013045
C	-0.58640227	3.74345567	-1.48339643
C	-1.11836695	4.04629804	-2.74869158
C	-0.67203657	3.34131017	-3.87667380
C	0.29400645	2.33469772	-3.71910000
C	0.83861203	2.01638792	-2.45505486
C	1.87498107	0.90553960	-2.39229289
C	2.15444339	-1.47702466	-1.97439101
C	1.64601235	-2.68051985	-1.18156370
C	2.61688064	3.53263892	0.42594631
C	3.66357096	3.30256831	-0.67827925
C	2.21724092	5.02056732	0.43647815
C	-0.05159673	3.17023650	1.58651068
C	0.57503109	3.33402624	2.98574955
C	-1.40146819	2.44765957	1.67345512
C	3.30456801	-3.08947424	1.28917461
C	4.49351530	-3.00625622	0.31404076
C	3.69771443	-2.54933977	2.67850992
C	0.34634159	-3.38500537	1.34117260
C	0.21512887	-3.30704551	2.87290067
C	0.40923559	-4.84558401	0.86060184
C	3.22083468	0.26540959	0.74908598
C	1.33184807	0.07539815	2.38472744
C	-2.49333089	-0.86492083	-0.92918290
C	-2.42562669	-2.09532330	-1.82493884
C	-2.16526497	-1.93424500	-3.20582882
C	-2.05707918	-3.04798715	-4.05709011
C	-2.20713991	-4.34781592	-3.54028891
C	-2.46181522	-4.52138129	-2.16739151
C	-2.56326982	-3.40700751	-1.31464625
C	-3.35389613	-1.05523781	0.35832855
C	-4.07917814	0.21145737	0.84582496
C	-4.74765260	1.08449579	-0.04203581
C	-4.18538421	0.45631372	2.23120976
C	-5.47999286	2.18410765	0.44011971
C	-4.92096297	1.55163783	2.71639138

C	-5.56813378	2.42464068	1.82331917
H	0.42296289	-0.36001887	-1.63494733
H	-1.72924350	-1.16154395	1.35612205
H	-0.95350388	4.30918301	-0.61414778
H	-1.88118333	4.83565414	-2.84706498
H	-1.07834670	3.56629786	-4.87601380
H	0.64026836	1.77099997	-4.60205182
H	2.03084485	0.54027106	-3.43426653
H	2.85771678	1.28338467	-2.04543531
H	3.25110287	-1.34726184	-1.84680091
H	1.97223506	-1.63691327	-3.06540191
H	2.20455748	-3.60225276	-1.44431465
H	0.57659477	-2.86177103	-1.42517200
H	3.08624584	3.27021252	1.40084845
H	4.06839732	2.27378837	-0.68131442
H	4.52383852	3.98657077	-0.51209952
H	3.25089384	3.53903425	-1.68223500
H	1.66916503	5.29760422	-0.48951790
H	3.13428088	5.64809269	0.47231947
H	1.59468134	5.30794204	1.30577475
H	-0.21984521	4.18877964	1.17407416
H	0.73902457	2.35816830	3.48083160
H	-0.12287500	3.91620242	3.62591816
H	1.54058930	3.87891806	2.97607314
H	-1.90281949	2.35159622	0.69003403
H	-2.08791225	3.00559613	2.34528216
H	-1.28444517	1.42506820	2.08243967
H	3.02661257	-4.16269489	1.39510093
H	4.27893406	-3.47193920	-0.66967605
H	5.36221768	-3.54965176	0.74598541
H	4.81597165	-1.95848231	0.14841692
H	4.06327998	-1.50548012	2.61359103
H	4.52114221	-3.16631228	3.09994933
H	2.86007692	-2.56569380	3.40229621
H	-0.56587399	-2.91590089	0.91335279
H	1.03614390	-3.85111216	3.38693952
H	-0.74017555	-3.78115195	3.18361104
H	0.20484619	-2.26471852	3.24723571
H	0.39514076	-4.93900094	-0.24424819
H	-0.47509622	-5.39874872	1.24556696
H	1.30856974	-5.37611875	1.24253897
H	-2.91480761	-0.03610325	-1.53623315
H	-2.05767432	-0.91638917	-3.61711185
H	-1.86490688	-2.89975147	-5.13267975
H	-2.13177791	-5.22266425	-4.20655332
H	-2.58507920	-5.53588756	-1.75367818
H	-2.75069391	-3.54764741	-0.23822466
H	-4.17545584	-1.75894828	0.07856785
H	-4.71476904	0.90336205	-1.12975422

H	-3.68022226	-0.23865935	2.91932163
H	-5.99098168	2.85397413	-0.27134094
H	-4.99106778	1.72305531	3.80354798
H	-6.14468334	3.28431379	2.20237035
G (S_N,R,S)			
Mn	-0.12959550	-1.74588210	-0.19216668
P	-2.19453846	-0.80164992	-0.75929164
P	1.90834707	-2.55723258	0.56040640
O	-1.37869849	-4.41592954	0.16319199
O	0.57419615	-2.52987317	-2.95285003
O	2.97341273	1.23164362	-1.37679168
N	-0.40173557	-1.14498505	1.86399942
N	0.88458767	0.03334268	-0.34973515
N	0.87330748	0.82723787	0.61973318
C	-2.78023192	0.44799338	0.49685015
C	-3.48136181	1.62036550	0.12931645
C	-3.95319891	2.53181937	1.08974695
C	-3.72281229	2.28597639	2.45199925
C	-3.00895615	1.13837567	2.83148860
C	-2.53004140	0.21069574	1.87984902
C	-1.77910957	-1.00432678	2.39883070
C	0.43082443	-1.91665078	2.82176784
C	1.88087850	-1.99404280	2.34594144
C	-3.74625253	-1.92673953	-0.89909222
C	-4.15468729	-2.59174474	0.42741351
C	-4.97700979	-1.22793129	-1.50781512
C	-2.29438429	0.13761434	-2.40246853
C	-2.26323370	-0.79981190	-3.62589492
C	-1.20358633	1.20958767	-2.50667489
C	2.28041707	-4.41883290	0.62028340
C	1.60379136	-5.16156605	1.78724792
C	1.96138660	-5.10622940	-0.72246396
C	3.53843142	-1.81703699	-0.06278502
C	3.87792017	-2.22792823	-1.50729555
C	4.73643509	-2.04481815	0.87652279
C	-0.88746481	-3.34765861	0.03168131
C	0.27074708	-2.18350953	-1.86541724
C	1.88719447	1.94530215	0.66259459
C	1.40694447	3.05010018	1.58529123
C	0.03504658	3.33962370	1.74820193
C	-0.37896595	4.39146665	2.58521060
C	0.56873161	5.16910197	3.27424014
C	1.93862890	4.88048679	3.12939300
C	2.34991091	3.82509679	2.29790388
C	2.51323229	2.39358560	-0.71359273
C	1.69904923	3.31692885	-1.64022145
C	1.17669395	4.56139891	-1.21350949
C	1.59487557	2.98790272	-3.00909883
C	0.53344059	5.42239102	-2.12034180

C	0.95983545	3.85227279	-3.91845622
C	0.41642716	5.07129707	-3.47742331
H	0.02181958	-0.17202562	1.75742206
H	2.17511075	0.59955405	-1.28506746
H	-3.67344623	1.83572705	-0.93220504
H	-4.50135716	3.43179099	0.76711930
H	-4.08753075	2.98815325	3.21888341
H	-2.80966238	0.95216415	3.90019172
H	-1.73485096	-0.91355342	3.50914025
H	-2.33264683	-1.94177755	2.18590830
H	-0.00587316	-2.93305973	2.92917888
H	0.38624644	-1.43936501	3.83161817
H	2.49043249	-2.63580188	3.01468155
H	2.33258088	-0.97894502	2.36211533
H	-3.39718624	-2.72602209	-1.59125508
H	-3.34563097	-3.19788427	0.87448996
H	-5.00721163	-3.28046858	0.24221924
H	-4.50062186	-1.83836449	1.16696058
H	-5.30960750	-0.37504496	-0.87803157
H	-5.82322769	-1.94761681	-1.55264192
H	-4.81421275	-0.85546550	-2.53768622
H	-3.28709439	0.63757203	-2.39014264
H	-1.28018907	-1.29399293	-3.74187030
H	-2.44225274	-0.19907773	-4.54395725
H	-3.03962393	-1.59099252	-3.59581589
H	-1.22241639	1.93058278	-1.66514700
H	-1.32668823	1.78963985	-3.44566295
H	-0.19485520	0.75284080	-2.52174621
H	3.38147914	-4.46091562	0.78298711
H	1.88772063	-4.75742086	2.78054725
H	1.91427879	-6.22917287	1.77266834
H	0.49871180	-5.14413331	1.69850254
H	0.86808747	-5.17545011	-0.88708405
H	2.36474156	-6.14230543	-0.71614323
H	2.39820609	-4.57981990	-1.59268595
H	3.31524054	-0.72802549	-0.08990914
H	4.22959407	-3.28008612	-1.56805142
H	4.69781545	-1.58212858	-1.88728853
H	3.01815138	-2.10959156	-2.19575165
H	4.56124352	-1.66901815	1.90544936
H	5.62393979	-1.50585858	0.47939491
H	5.01861477	-3.11786663	0.94766468
H	2.75527851	1.46399200	1.17520484
H	-0.71164868	2.73342344	1.21262625
H	-1.45468491	4.60422804	2.69573286
H	0.24204147	5.99464819	3.92751198
H	2.69063382	5.47598151	3.67265314
H	3.42568565	3.59927811	2.19661582
H	3.41479684	2.99027358	-0.42991051

H	1.28498290	4.87831081	-0.16640064
H	2.04584476	2.04455584	-3.35122391
H	0.13076484	6.38421703	-1.76149673
H	0.89716136	3.57180116	-4.98325765
H	-0.08167850	5.75124795	-4.18805680
G (S_N, S, R)			
Mn	1.01481166	-1.44576589	-0.38960994
P	-0.94417607	-2.71031467	-0.60763766
P	2.84255045	-0.09261865	0.01835923
O	2.67444692	-3.89225037	-0.12412121
O	1.63624480	-1.44635466	-3.27796087
O	-0.46176914	2.55210503	-1.81510612
N	0.67390299	-1.23028555	1.73257735
N	-0.04894900	0.30491442	-0.51420584
N	-0.57541346	0.76414110	0.51930233
C	-2.12524877	-2.42458345	0.80961881
C	-3.52750635	-2.37485086	0.63015218
C	-4.40465598	-2.15617069	1.70650092
C	-3.88708033	-1.97814044	2.99831184
C	-2.49711412	-2.01612820	3.19182960
C	-1.60082647	-2.23588531	2.12208721
C	-0.11475513	-2.26605012	2.44356508
C	1.90094826	-0.89599517	2.49802008
C	2.63406344	0.27393587	1.84177233
C	-0.84009429	-4.62816231	-0.63204392
C	-0.29078103	-5.23644586	0.67062520
C	-2.16431440	-5.32734801	-0.99381258
C	-2.01556862	-2.40958087	-2.14924615
C	-1.37678766	-2.97747490	-3.43223088
C	-2.37996120	-0.92933803	-2.33133134
C	4.61932368	-0.73144473	-0.17587236
C	5.08823768	-1.63987347	0.97611297
C	4.82994729	-1.42331695	-1.53715299
C	2.91510578	1.64693741	-0.72642078
C	3.14287706	1.65353819	-2.24863684
C	3.89000006	2.59857509	-0.01121149
C	2.00589597	-2.92098560	-0.22016228
C	1.34768099	-1.44542022	-2.13257154
C	-1.30233718	2.11512744	0.44645230
C	-0.52493951	3.08724158	1.31943281
C	-0.65446796	2.99290601	2.72558376
C	0.07321139	3.83924012	3.58022323
C	0.94397548	4.80360756	3.04133342
C	1.08073649	4.90775759	1.64478441
C	0.36189955	4.05323649	0.78963340
C	-1.62871692	2.54253747	-1.01202563
C	-2.37583639	3.86765678	-1.11999886
C	-3.55027666	4.10805493	-0.37211017
C	-1.92801124	4.86252031	-2.01350997

C	-4.25033852	5.31886347	-0.50306420
C	-2.63014234	6.07411311	-2.14728102
C	-3.79145536	6.30976357	-1.39120748
H	0.07168838	-0.35372450	1.66315551
H	-0.11016374	1.61537471	-1.64188418
H	-3.95839542	-2.51263901	-0.37282457
H	-5.49212601	-2.12723014	1.52971517
H	-4.55992789	-1.80372848	3.85335539
H	-2.08598714	-1.86974935	4.20507888
H	-0.01209015	-2.11640657	3.54381638
H	0.32631437	-3.25894151	2.22247340
H	2.54757269	-1.79883899	2.54699642
H	1.63129662	-0.63339461	3.55051134
H	3.59317658	0.49010097	2.35528392
H	2.00700505	1.18936855	1.91074518
H	-0.09339244	-4.81353728	-1.43694636
H	0.70860559	-4.84822292	0.94059534
H	-0.18518010	-6.33546689	0.54261975
H	-0.98984144	-5.07417236	1.51864667
H	-2.96041366	-5.09165445	-0.25529209
H	-2.01658532	-6.42898693	-0.97197673
H	-2.54099309	-5.07235778	-2.00327199
H	-2.95086750	-2.98027745	-1.96218957
H	-0.46507910	-2.42118288	-3.72077886
H	-2.10222226	-2.88271553	-4.26926041
H	-1.10917185	-4.05041347	-3.35190426
H	-2.88858855	-0.50853392	-1.44050300
H	-3.06592334	-0.81575806	-3.19882999
H	-1.47963664	-0.31271581	-2.52415253
H	5.23701549	0.19495981	-0.15217938
H	5.04145650	-1.14143977	1.96599499
H	6.14923952	-1.92738172	0.80893484
H	4.50085269	-2.57921325	1.02334550
H	4.29559936	-2.39299211	-1.57992827
H	5.91186415	-1.63082922	-1.68740258
H	4.48197515	-0.81216011	-2.39220484
H	1.87963975	2.00787193	-0.54486147
H	4.19163742	1.39707101	-2.51014050
H	2.94597649	2.67181835	-2.64671159
H	2.47324695	0.95241164	-2.78374668
H	3.68308621	2.69553149	1.07360074
H	3.80101871	3.61625373	-0.44937589
H	4.94939886	2.28631655	-0.13813030
H	-2.26107770	1.89724438	0.96662008
H	-1.34919135	2.24965631	3.15228138
H	-0.04995112	3.75370357	4.67264553
H	1.50776182	5.47723472	3.70730205
H	1.75246594	5.66787651	1.21281574
H	0.47044883	4.13202669	-0.30192547

H	-2.33331329	1.75361882	-1.38628326
H	-3.93134109	3.33864791	0.32052991
H	-1.02363854	4.66110727	-2.60695479
H	-5.16334589	5.48935069	0.09111902
H	-2.26586682	6.84057854	-2.85157474
H	-4.34061668	7.25993385	-1.49439683
G (S_N,R,R)			
Mn	0.85681147	-1.71952229	0.02470777
P	-1.14484748	-2.27946519	-1.04282550
P	2.71007961	-0.97832852	1.18536106
O	1.38824801	-4.52095738	0.85575476
O	2.54544820	-2.22373322	-2.34798619
O	1.14459331	2.23396241	-1.95240508
N	-0.20606599	-1.24230936	1.84109548
N	0.60007423	0.25292147	-0.38350756
N	-0.06331549	0.97821654	0.39285250
C	-2.65703248	-1.64778476	-0.14592685
C	-3.82917119	-1.25703497	-0.83637006
C	-4.97317839	-0.80291413	-0.15793213
C	-4.96259657	-0.72400968	1.24297665
C	-3.80421530	-1.09670290	1.94226794
C	-2.64749253	-1.56160506	1.27704999
C	-1.46387103	-1.96877295	2.13980165
C	0.66655037	-1.21865046	3.04292701
C	1.92424630	-0.38952541	2.77969079
C	-1.57550905	-4.14212434	-1.23246445
C	-1.86254006	-4.82969445	0.11499279
C	-2.72742809	-4.44576482	-2.20846994
C	-1.41680190	-1.66950499	-2.82240150
C	-0.45943060	-2.33941603	-3.82670058
C	-1.36314727	-0.14104575	-2.95845634
C	4.11406761	-2.14378444	1.70918284
C	3.77444046	-3.02168285	2.92824106
C	4.60105535	-3.01393483	0.53318509
C	3.62553837	0.57004242	0.58231679
C	4.48873928	0.31412550	-0.66653712
C	4.42939093	1.29462891	1.67672331
C	1.16266341	-3.40967045	0.51939925
C	1.83591093	-2.00074696	-1.43094475
C	-0.04456246	2.48429604	0.16165823
C	-1.20093033	3.10402326	0.91545024
C	-2.49505480	2.54107765	0.84035571
C	-3.57745104	3.13803480	1.51138953
C	-3.38303049	4.30394188	2.27399568
C	-2.09721797	4.86808046	2.36251859
C	-1.01802875	4.27101590	1.68883781
C	0.02868559	2.86457587	-1.36401078
C	0.10883315	4.37165351	-1.58066597
C	1.36695429	4.99189221	-1.73160848

C	-1.05358920	5.17075657	-1.62848224
C	1.46178444	6.38316721	-1.91196348
C	-0.96066393	6.56174086	-1.80713193
C	0.29877359	7.17393770	-1.94677057
H	-0.43811811	-0.23369924	1.58903321
H	1.12850557	1.29951000	-1.53441758
H	-3.86232473	-1.30853758	-1.93471388
H	-5.86970023	-0.51259113	-0.72937668
H	-5.84897827	-0.36805487	1.79228098
H	-3.78901613	-1.02496463	3.04274413
H	-1.75264088	-1.78320829	3.20047291
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H	-5.62481907	-4.08910703	3.29290727

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