

Non-covalent interactions between sertraline stereoisomers and the 2-hydroxypropyl- β -cyclodextrin: A quantum chemistry analysis

Joanatan-Michael Bautista-Renedo, Erick Cuevas-Yañez, Horacio Reyes-Pérez
Rubicelia Vargas, Jorge Garza, and Nelly González-Rivas

Supporting Information

1.- Molecular structures with PBE0/6-31G(d,p).

38

cis-(1S,4S)-SRT E(Ha)= -1632.44152388

Cl	-0.0256557380	-5.1479492452	-0.0312626916
Cl	1.8555967542	-2.9189009840	-1.3371198299
N	-0.2481069505	3.0180615937	-2.0923890460
C	0.9939209276	3.7506989819	-2.4576842860
C	-1.7287650681	-1.7271197207	1.1235749721
C	-1.4452030264	-3.0744790404	0.9399555296
C	-0.3477590596	-3.4705600902	0.1787820466
C	0.4740370658	-2.4925605872	-0.3952007185
C	0.1811630336	-1.1456302285	-0.2052618574
C	-0.9204222098	-0.7453131740	0.5501701710
C	-0.1028456134	1.6300095483	0.9777164749
C	0.0674338122	2.8880710754	0.3738147532
C	1.0851800451	3.7470153593	0.8126047364
C	1.9612861771	3.3591252343	1.8152805109
C	1.8137647311	2.1019970817	2.3986311446
C	0.7896243955	1.2586277114	1.9896875894
C	-1.2840505749	0.7218527337	0.6694146212
C	-2.0838344378	1.1614061676	-0.5672954434
C	-2.2253867823	2.6769497932	-0.6505443840
C	-0.8610113467	3.3459118959	-0.7165214617
H	-0.9630013333	3.1889852228	-2.8052721934
H	-0.0627430958	2.0114195908	-2.1108718986
H	1.7620173018	3.5224151003	-1.7201759875
H	0.7820703692	4.8202132349	-2.4610837573
H	1.3136971471	3.4304512910	-3.4498517370
H	-2.5905974146	-1.4434873470	1.7218270359
H	-2.0731512052	-3.8369118353	1.3880212064
H	0.8527423246	-0.4088499469	-0.6368424324
H	1.1698517070	4.7424118790	0.3817474857
H	2.7410050351	4.0349231561	2.1509179804
H	2.4872428744	1.7866305095	3.1894297034
H	0.6665576635	0.2908302152	2.4670895610
H	-1.9587818344	0.8188614537	1.5326873466
H	-1.6058942682	0.7564685293	-1.4726424483
H	-3.0711684892	0.6916522086	-0.5450105487
H	-2.8502712683	2.9756304129	-1.5022368041
H	-2.7268088077	3.0589857918	0.2454381933
H	-0.9505491605	4.4371942773	-0.7214185669

38

cis-(1R,4R)-SRT E(Ha)= -1632.44114287

Cl	1.38400532	2.88731749	-1.86023202
Cl	-0.03373480	5.13270793	-0.08419371
N	-0.79156729	-3.08831058	-1.92216109
C	-1.01849591	-3.38206535	-0.42647439
C	-2.32089595	-2.70827717	-0.02169729
C	-2.16902846	-1.19130266	-0.01276578
C	-1.08071097	-0.72668001	0.96673499
C	1.27588791	-1.22797679	1.69536381
C	2.37962402	-2.05889618	1.83429931
C	2.37585072	-3.33037209	1.26325128
C	1.26634341	-3.74443115	0.54114789
C	0.16110208	-2.89824118	0.37064253
C	0.14700023	-1.62654240	0.97059659
C	-0.76738395	0.73882560	0.73704583
C	0.08299701	1.12925153	-0.29709709
C	0.32014838	2.47344979	-0.56726906
C	-0.30032501	3.45922517	0.21078366
C	-1.14536128	3.07301828	1.24905043
C	-1.37709317	1.72803709	1.50899322
C	0.31689053	-3.82527494	-2.58633676
H	-1.10109108	-4.47298713	-0.38096042
H	-2.56921343	-3.06778550	0.98301799
H	-3.14622537	-3.02614390	-0.67228163
H	-3.11934620	-0.71963661	0.25303963
H	-1.94105416	-0.80717345	-1.01911205
H	-1.50768819	-0.81140845	1.97693180
H	1.27902782	-0.24758901	2.16294624
H	3.23900424	-1.72117383	2.40528834
H	3.22326585	-3.99578894	1.39260636
H	1.24230301	-4.74909931	0.12400132
H	0.60210541	0.38739761	-0.89760010
H	-1.61666257	3.84102302	1.85293512
H	-2.03927219	1.45187820	2.32537178
H	0.36044100	-3.52778042	-3.63473741
H	0.12223920	-4.89545761	-2.51015884
H	1.25046646	-3.57678108	-2.08339575
H	-0.62739880	-2.08183583	-2.01112117
H	-1.66756425	-3.27825095	-2.41718154

38

trans-(1R,4S)-SRT E(Ha)= -1632.43746341

Cl	0.03789968	-5.32525597	-0.02432641
Cl	-1.61249024	-3.33639348	1.84998642
N	0.81979123	4.78657656	0.66636023
C	1.22367196	5.10637842	-0.73439482
C	1.43714895	-1.73238475	-1.05430927
C	1.21992883	-3.10304459	-0.98085703
C	0.28492831	-3.62342395	-0.08981387
C	-0.43843876	-2.74897784	0.73256169
C	-0.21389480	-1.37842623	0.65182796

C	0.72447053	-0.85418311	-0.23835890
C	-0.25278649	1.47183069	-0.51108522
C	-0.44408512	2.71474603	0.11422282
C	-1.65267427	3.40439603	-0.06248834
C	-2.64109142	2.91645063	-0.90372346
C	-2.43100419	1.71076801	-1.57047424
C	-1.25962901	0.99731222	-1.36032557
C	0.99805497	0.63592738	-0.27762670
C	1.72904192	1.08295736	0.99370842
C	1.95799085	2.58821317	0.97295387
C	0.61704428	3.30460875	1.01293813
H	2.22004285	4.71220894	-0.92385295
H	0.49991929	4.65201303	-1.41000507
H	1.22812101	6.19030442	-0.85357334
H	-0.05666531	5.27455831	0.86302324
H	1.51090962	5.17093295	1.31647246
H	2.17232053	-1.34929527	-1.75719667
H	1.77397795	-3.78526346	-1.61658664
H	-0.79852545	-0.72369859	1.29142932
H	-1.85301862	4.32887790	0.48081728
H	-3.56987019	3.46328829	-1.02983405
H	-3.19262981	1.31562980	-2.23534877
H	-1.11999933	0.03714615	-1.84777527
H	1.67678948	0.81505951	-1.12539038
H	1.14492405	0.79868428	1.87777094
H	2.68687777	0.56139898	1.07088636
H	2.57877119	2.90538827	1.81896902
H	2.50145881	2.83864388	0.05384487
H	0.25337847	3.34206765	2.04847774

38

trans-(1S,4R)-SRT E(Ha)= -1632.43746341

Cl	0.25833980	-5.30237000	0.42883204
Cl	-1.32449061	-3.49073945	-1.66999877
N	0.73161835	4.77969114	-0.78974365
C	1.01210057	5.18740614	0.61832670
C	1.44583435	-1.60323652	1.34179657
C	1.28519251	-2.98358130	1.33384854
C	0.43693201	-3.59083048	0.41151097
C	-0.25685083	-2.79415424	-0.50940838
C	-0.08948337	-1.41315052	-0.49369515

C	0.76212688	-0.80194942	0.42772005
C	-0.31541729	1.49534557	0.48922046
C	-0.50095537	2.69419770	-0.21841752
C	-1.74264332	3.34503059	-0.17237233
C	-2.77544549	2.86540712	0.61883582
C	-2.57575987	1.70657190	1.36692683
C	-1.36765396	1.02883896	1.28629633
C	0.97817705	0.69783773	0.39791278
C	1.78604002	1.10077229	-0.84124669
C	1.96203203	2.61239530	-0.89191321
C	0.60437507	3.27506226	-1.06831439
H	1.99841032	4.83186099	0.90950210
H	0.24649944	4.75084859	1.25857808
H	0.98165124	6.27595223	0.67515236
H	-0.14140568	5.22482326	-1.08069928
H	1.45998203	5.15369353	-1.40426739
H	2.11350631	-1.15162037	2.07087575
H	1.81639842	-3.60598118	2.04585899
H	-0.65015876	-0.81968810	-1.20993865
H	-1.93202075	4.23050718	-0.78066279
H	-3.72942667	3.38197143	0.64388198
H	-3.37229272	1.31867830	1.99409052
H	-1.23271257	0.10295313	1.83724641
H	1.58448352	0.95192534	1.28073831
H	1.27896681	0.74566628	-1.74697235
H	2.76400127	0.61238877	-0.81842941
H	2.63153238	2.90522327	-1.70903224
H	2.42880172	2.93381968	0.04705563
H	0.31783687	3.24462918	-2.12798372

147

B-CD E(Ha)= -4270.84685357

O	-4.52024769	3.97281391	1.22337825
O	-1.22942712	4.90429399	-0.08664288
O	0.31407545	6.01768699	1.22962887
O	3.06653242	4.02255867	-0.13176534
O	4.93538479	3.53267680	1.14240400
O	5.05261501	0.11090338	-0.15760895
O	5.83954612	-1.63141945	1.14660325
O	2.33439168	-5.52861962	1.25121310
O	-1.01979492	-4.95518579	-0.10024225

O	-2.90855876	-5.30369698	1.19120651
O	-4.50589867	-2.29506240	-0.15225720
O	-5.99219419	-1.05889012	1.12004180
O	-6.04234050	-1.82671401	-2.42434248
O	-5.82403608	0.91030703	-2.48019524
O	-4.59626936	2.09193450	-0.12170510
O	-4.35062018	-4.07521314	-2.45276530
O	-2.34999966	-5.94905529	-2.33402012
O	-5.19127793	-4.69705793	2.56794990
O	0.46160930	-6.02925790	-2.36818093
O	3.17441312	-5.61434439	-2.27540517
O	0.44180937	-6.88115832	2.68885705
O	6.26305008	-1.00170446	-2.39938284
O	4.88594468	-3.37935798	-2.44477219
O	5.65829627	1.75005252	-2.48596665
O	4.66714912	4.30886993	-2.39025457
O	6.74043654	2.00256609	2.51987655
O	2.62780100	6.43749331	2.62510948
O	-0.45172066	6.41213313	-2.29324230
O	2.16581637	5.59767472	-2.41148579
O	-2.99706089	5.21767459	-2.38065019
O	-5.26301236	3.66829589	-2.31262995
O	-3.41820778	6.02188992	2.66408988
O	-6.96095076	1.09398335	2.51605461
O	5.76287216	-3.97373755	2.57021456
O	3.23320091	-3.88149728	-0.10243439
C	-3.09550380	4.11087986	1.22043854
C	-2.64456384	4.94444456	0.02007489
C	-3.21597872	4.38800765	-1.27093999
C	-4.71952930	4.24408584	-1.14249688
C	-5.07460648	3.39152731	0.07070955
C	-0.50801917	6.08805732	0.09226808
C	1.31014152	4.99008809	1.20819066
C	2.21927682	5.15526697	-0.01051874
C	1.40243027	5.25451683	-1.28572204
C	0.35731746	6.34236560	-1.13723938
C	4.44639135	4.19746818	0.00500392
C	5.14900267	3.65441199	-1.23471494
C	4.94545505	2.15656900	-1.34816686
C	5.41226369	1.48154004	-0.07169293
C	4.75012529	2.11361467	1.15336354
C	6.05026565	-0.85638359	-0.00644380
C	4.61322336	-2.36888665	1.17562481
C	4.52860060	-3.30515625	-0.03055045
C	4.76104140	-2.54565254	-1.32350202
C	6.05835461	-1.76694683	-1.22951651
C	3.09856974	-5.25773162	0.10374405
C	2.42253863	-5.88540055	-1.11037149
C	1.00681342	-5.36489143	-1.25952632
C	0.23636336	-5.60468743	0.02587857
C	0.99088924	-5.03582430	1.22828898
C	-2.18554364	-5.70992615	0.05682442
C	-3.06125327	-5.54841641	-1.18111634
C	-3.52779884	-4.11271030	-1.31724670
C	-4.23612740	-3.68475590	-0.04503294
C	-3.36039548	-3.94578458	1.18131735
C	-5.82625537	-1.85466127	-0.02641408
C	-5.20672493	0.13713958	1.15603853

C	-5.51486514	1.01119331	-0.06031555
C	-5.37177956	0.21911688	-1.34635665
C	-6.20677785	-1.04319193	-1.26034034
C	-5.58262772	0.81771617	2.46145272
C	-4.12978602	-3.77836752	2.48108830
C	0.38547895	-5.48280810	2.54846008
C	4.64082531	-3.12887362	2.49105177
C	5.38187170	1.64401343	2.45305116
C	2.06902530	5.15143282	2.51485013
C	-2.76319609	4.78308516	2.54219605
H	-2.62113877	3.12117490	1.16687089
H	-2.99032972	5.97712570	0.16197545
H	-2.78383779	3.38544848	-1.42695330
H	-5.14906196	5.24466373	-0.98256530
H	-6.15747572	3.38166438	0.23881362
H	-1.18720387	6.92908106	0.27236502
H	0.83138006	4.00190237	1.16526592
H	2.81494145	6.06881790	0.11913255
H	0.88319350	4.29239075	-1.43002305
H	0.87627655	7.30086145	-0.98479340
H	4.68682340	5.25575496	0.15728464
H	6.22600400	3.84763552	-1.11642874
H	3.86591495	1.96060468	-1.45905244
H	6.50103247	1.58790904	0.02525503
H	3.67786558	1.87327806	1.14299013
H	7.02818971	-0.38197160	0.13343103
H	3.75800159	-1.67922591	1.15298978
H	5.29162564	-4.08741144	0.07905456
H	3.93350843	-1.82721734	-1.44696267
H	6.88232963	-2.48541172	-1.10267958
H	4.07673989	-5.71628938	0.28764780
H	2.37452879	-6.97154667	-0.93931322
H	1.05414275	-4.27583031	-1.42632126
H	0.09791768	-6.68343675	0.17831738
H	0.99287819	-3.93899087	1.16204550
H	-1.94117671	-6.76463631	0.22688209
H	-3.94686294	-6.18780282	-1.04629133
H	-2.64021934	-3.47037176	-1.44231305
H	-5.17072724	-4.25078336	0.06606392
H	-2.50016441	-3.26238739	1.15727359
H	-6.50470706	-2.70514689	0.10541079
H	-4.13694136	-0.11420832	1.15318432
H	-6.54335801	1.38556361	0.02911735
H	-4.31287902	-0.07153812	-1.44869296
H	-7.26220853	-0.75072719	-1.15176390
H	-6.06346174	-1.19723182	-3.15862878
H	-5.47303546	1.82074831	-2.46175999
H	-5.26152404	0.17943333	3.29882088
H	-5.05669422	1.77408807	2.53508152
H	-4.80595404	-3.21271130	-2.48925397
H	-2.85563999	-5.59375085	-3.07849866
H	-3.42945180	-3.88401268	3.32381061
H	-4.56502486	-2.77542465	2.51696802
H	-4.79423762	-5.56919999	2.45654879
H	-0.49701001	-5.85036190	-2.40841786
H	2.58276712	-5.82558999	-3.01131061
H	0.90798537	-4.96924528	3.37008741
H	-0.66985270	-5.19635023	2.57739588

H	1.37054463	-7.11957839	2.58270804
H	3.75187650	-3.76244948	2.56177742
H	6.02389623	-1.58820447	-3.13061850
H	4.17334413	-4.04598871	-2.42952365
H	5.71015784	0.77561662	-2.49949068
H	4.96175585	3.76194952	-3.13193704
H	4.80880778	2.05975099	3.29598101
H	5.33158893	0.55255829	2.50594561
H	6.76707341	2.95898841	2.39666692
H	2.89524712	4.43512646	2.54391703
H	1.38730839	4.93023493	3.35040456
H	1.89324938	7.05359852	2.51775946
H	0.16242008	6.32725409	-3.03609960
H	2.95133998	5.01996378	-2.45343862
H	-2.05903534	5.48672669	-2.39914696
H	-4.81218652	4.11245348	-3.04451885
H	-1.68787290	4.97856908	2.58846640
H	-3.02782496	4.09961867	3.36356513
H	-4.35708734	5.83636639	2.54260555
H	-7.40509880	0.24924745	2.37537657
H	6.53071199	-3.40621920	2.43249905
H	4.61736121	-2.40400238	3.31913683

2-HP-B-CD E(Ha)= -5621.40163046

O	-2.7727459824	5.2903013130	-2.2927533349
O	-4.4599789908	2.3690865562	-0.8692675484
O	-5.8966032593	1.1525076940	-2.2228759326
O	-4.6341258013	-2.0096580908	-0.8762865281
O	-4.5527577281	-3.8548844314	-2.2766337213
O	-1.3189941073	-4.8770953886	-0.8975050858
O	0.1841016580	-5.9683105423	-2.2844268657
O	2.9871858932	-4.0712054132	-0.8886027753
O	4.7908551817	-3.5893100650	-2.2626090338
O	5.0505453959	-0.2033821422	-0.8938829626
O	5.8031504636	1.4949397286	-2.2804010751
O	3.3034030501	3.8124717301	-0.9440124935
O	2.4109350539	5.4159895804	-2.3592515046
O	3.3527622755	5.5556911862	1.1280525733
O	0.5208171146	6.0404160011	1.2627571032
O	-0.9278405825	4.9606627808	-0.9282646871
O	4.9734163666	3.3611715015	1.3122998965
O	6.3653141202	0.8453244105	1.2312975966
O	5.6824947766	3.8222383172	-3.7367004060
O	5.7107296705	-1.8083733090	1.3540122091
O	4.6200252735	-4.4670301806	1.2404635215
O	6.5586639188	-2.0611696373	-3.6918756388
O	-0.6119558710	-6.4298307880	1.2120067697
O	2.1446150686	-5.6208156766	1.3388990736
O	-3.0523505080	-5.2025359464	1.3319553478
O	-5.3954330908	-3.5420076035	1.2257502730
O	-3.4297827173	-5.8910098132	-3.7306620252
O	-6.8259445301	-1.0051539724	-3.6451664773
O	-6.0687980522	2.0123506367	1.2848979236
O	-5.9087674207	-0.8565327637	1.3875301132
O	-4.3413655748	4.1323048445	1.3538573437
O	-2.2113229520	6.0575041404	1.1960130425
O	-5.0419186933	4.6604331503	-3.6907700066
O	0.5033854802	6.7400254664	-3.8135025481
O	2.4830262271	-6.3711798521	-3.7179550050
O	-7.0448347385	4.4406737623	2.3423207835
O	-0.9282200089	8.3731772997	2.1721202938
O	5.9376138410	5.9494853162	2.1799081711
O	8.2879126162	-0.9131662952	2.3199877955
O	4.4570695357	-7.0813201013	2.2858959861
O	-2.7684031257	-7.9372702703	2.2307649529
O	-7.9002719081	-2.7613926472	2.2601750921
C	-3.2431083251	3.9400488257	-2.2456671382
C	-4.1453371041	3.7461488340	-1.0286583454
C	-3.4644033816	4.2026213935	0.2560573711
C	-2.9708337151	5.6282190992	0.0900689071
C	-2.0808437873	5.7260124870	-1.1531145537
C	-5.7815955512	1.9477142270	-1.0730263491
C	-5.1280324191	-0.0538697314	-2.2104489486
C	-5.5177337449	-0.9035224995	-1.0023882902
C	-5.4291266922	-0.1098375076	0.2954895706
C	-6.2339839365	1.1709923095	0.1673162225
C	-5.1244316437	-3.3005233451	-1.1220948690
C	-4.8207406756	-4.1690624688	0.1027097888
C	-3.3202291342	-4.3391707916	0.2540075226
C	-2.7324842515	-4.8738014933	-1.0465741875

C	-3.1311349944	-4.0098620983	-2.2415598210
C	-0.6142906820	-6.0660547493	-1.1355888289
C	1.1917967459	-4.9538284372	-2.2454462176
C	2.1053333969	-5.1754537647	-1.0414107558
C	1.3101551105	-5.2983930529	0.2530888459
C	0.2452280358	-6.3682783777	0.0958263821
C	4.3581672740	-4.2635964420	-1.1114267994
C	5.1188796954	-3.7695202627	0.1230382299
C	4.9482855251	-2.2681638686	0.2646821674
C	5.3629141496	-1.5829575087	-1.0320119893
C	4.6304298538	-2.1681051213	-2.2378920683
C	6.0565556420	0.7464695266	-1.1215040627
C	6.1378814666	1.6603164248	0.1050819797
C	4.8569528175	2.4645461901	0.2341250261
C	4.5790815539	3.1986561112	-1.0722224210
C	4.5860157058	2.2463320641	-2.2664265689
C	3.1819172052	5.1841304199	-1.2108691890
C	1.0630200512	4.9402584840	-2.2994385889
C	0.3455206091	5.5672023988	-1.1058057224
C	1.1240073987	5.3618024949	0.1880935295
C	2.5482474311	5.8556880195	0.0113868503
C	0.4440058617	5.3470769628	-3.6263895756
C	4.5620457798	2.9831317828	-3.5951597331
C	5.2097881287	-1.6850885492	-3.5573798298
C	1.9323468569	-5.0856095017	-3.5660212092
C	-2.7729959262	-4.6574649941	-3.5688429169
C	-5.4492829825	-0.7396587813	-3.5279021888
C	-3.9880197946	3.7385990879	-3.5550731691
C	3.6213803468	6.6242943315	2.0295684936
C	7.3342333318	1.3027659822	2.1688239690
C	5.5780666530	-4.9427968284	2.1799386354
C	-0.3943042033	-7.4974543558	2.1281665506
C	-6.1091543723	-4.3782564146	2.1301225085
C	-7.1270274111	2.0273952866	2.2373607492
C	-2.8594703413	6.9217703498	2.1233782027
C	-6.9603768835	3.2628076144	3.1116128878
C	-6.9653895379	-3.4899693139	3.0223302373
C	-1.6319558790	-7.6289825776	3.0051816208
C	4.9027209044	-5.9886653763	3.0564312195
C	7.7116748553	0.1333636489	3.0676563446
C	4.7731092901	6.2027384093	2.9318437686
C	-1.7889505075	7.5946718418	2.9715752470
C	-8.0492383627	3.3182608909	4.1670090839
C	-2.4239641692	8.5118004909	4.0002049138
C	5.0941901777	7.2984757441	3.9311408590
C	8.7226935264	0.5696962312	4.1117069110
C	5.8733735628	-6.5179094729	4.0957528307
C	-1.4475311506	-8.7396067968	4.0225158006
C	-7.7355791274	-4.3284060450	4.0254974191
H	0.9557907613	4.8045984395	-4.4358988261
H	1.2399927687	-4.8390433405	-4.3853855575
H	4.1637573154	5.6231126944	-1.4178094919
H	2.5345793138	6.9408159517	-0.1626487172
H	1.1638981719	4.2815429623	0.3955260064
H	-0.4159118845	5.7625632460	1.2869365241
H	0.2311781745	6.6428179350	-1.2966203291
H	1.0531228837	3.8464425733	-2.1934927149
H	-0.6126668401	5.0656514097	-3.6355391276

H	7.0198708453	0.2531974235	-1.2896798802
H	6.9823516956	2.3491580022	-0.0376523678
H	4.0310836032	1.7594419068	0.4137501645
H	4.1837832482	3.9365090513	1.2941545378
H	5.3534780198	3.9608169162	-1.2327568773
H	3.7244171712	1.5681122397	-2.1920316938
H	4.5014316923	2.2431806954	-4.4077027015
H	3.6745669596	3.6204071286	-3.6413377546
H	6.4550504397	3.2523103964	-3.6403325828
H	4.5735377140	-5.3228610154	-1.2880300272
H	6.1843936842	-3.9990309783	-0.0186738483
H	3.8803526650	-2.0631271814	0.4350088187
H	5.6549418688	-0.8326848521	1.3505052662
H	6.4425146085	-1.7153052913	-1.1849018347
H	3.5643186211	-1.9092375228	-2.1722406383
H	4.5926169157	-2.0788015195	-4.3793162145
H	5.1750680650	-0.5926122930	-3.5912594864
H	6.5760915914	-3.0216968518	-3.6017863074
H	-1.3081105370	-6.8922453957	-1.3242934480
H	0.7323425363	-7.3413685010	-0.0582876150
H	0.8020803421	-4.3392678913	0.4359306581
H	2.8712536677	-4.9672825985	1.3453882714
H	2.6772904409	-6.0985438414	-1.2065202617
H	0.7256523379	-3.9616525149	-2.1670822565
H	2.7629487178	-4.3747521281	-3.5892972620
H	-6.2034372579	-3.2724067104	-1.3079086100
H	-5.2803190443	-5.1548722492	-0.0545589059
H	-2.8841048714	-3.3466312356	0.4444700973
H	-2.0889689699	-5.3670205380	1.3349669835
H	-3.0991457359	-5.8946569194	-1.2194846862
H	-2.6462074140	-3.0274714777	-2.1543115966
H	-3.0164772835	-3.9559289577	-4.3812920266
H	-1.6984909597	-4.8587961325	-3.5963715354
H	-4.3722662670	-5.7027916757	-3.6450605611
H	-6.4378919700	2.8086999488	-1.2392822185
H	-7.2958749045	0.9168406423	0.0415638359
H	-4.3760362310	0.1664767225	0.4571433942
H	-5.4457310015	-1.7169162249	1.3729410172
H	-6.5487518590	-1.2546140389	-1.1442082186
H	-4.0559909894	0.1818326578	-2.1555148478
H	-4.9310141922	-1.7015685619	-3.5724541129
H	-5.0838029896	-0.1089559553	-4.3525515272
H	-7.2697374316	-0.1536652253	-3.5503970472
H	-1.8165235399	6.7711462821	-1.3465543897
H	-3.8335243859	6.2936575442	-0.0547410328
H	-2.5882768493	3.5589057071	0.4278272896
H	-4.7108253623	3.2275945189	1.3674237783
H	-5.0627332262	4.3304932823	-1.1817966030
H	-2.3933340037	3.2461423733	-2.1795648507
H	-4.4307744778	2.7388463335	-3.5708269688
H	-3.2698858294	3.8147366433	-4.3856888167
H	-4.6402447310	5.5346389075	-3.6166826620
H	1.4361495949	6.9770504094	-3.7441554500
H	1.7446725044	-6.9870437876	-3.6366712006
H	-7.1056035883	1.1059363460	2.8322482942
H	-8.0915654419	2.0945595028	1.7140733676
H	-5.4041234105	-4.9796517379	2.7175276155
H	-6.7708678114	-5.0502917153	1.5650202932

H	0.5043545039	-7.2990077146	2.7253820292
H	-0.2562419129	-8.4361107873	1.5725733296
H	5.9642145263	-4.1060072937	2.7750474617
H	6.4127548063	-5.4180627658	1.6449563490
H	6.9266706854	2.1409804620	2.7474626316
H	8.2335862427	1.6395347802	1.6334836070
H	2.7201900296	6.8584195528	2.6096897688
H	3.9256652659	7.5156965368	1.4623040923
H	-3.5618742589	6.3471552577	2.7397818855
H	-3.4137955539	7.6982602750	1.5770362058
H	-5.9779451822	3.1944255859	3.6085451734
H	-1.2236973725	6.8032496038	3.4921271038
H	4.4592947453	5.2964621023	3.4769480402
H	6.7945625550	-0.2119080347	3.5741570429
H	4.0541329471	-5.5035748059	3.5676831826
H	-1.7727989342	-6.6721705416	3.5357350649
H	-6.2907528492	-2.8062170130	3.5647529394
H	6.2544174592	-5.7157286215	4.7344456882
H	6.7198036067	-7.0087826231	3.6050628053
H	5.3727558341	-7.2587836541	4.7229376606
H	-0.5802866649	-8.5567618305	4.6636617064
H	-1.3120641153	-9.6987873916	3.5127722020
H	-2.3385844732	-8.8152491746	4.6495430211
H	-7.0638090224	-4.9171349413	4.6569870952
H	-8.4151678815	-5.0098916242	3.5039780771
H	-8.3370920550	-3.6773348304	4.6635961458
H	-8.0342870506	2.4309241101	4.8065750214
H	-9.0320575095	3.3918806345	3.6907176649
H	-7.9112147296	4.2037866487	4.7912367323
H	-3.1026583306	7.9649838089	4.6612507374
H	-2.9853256485	9.3072888642	3.4999487089
H	-1.6449433709	8.9800603659	4.6057831172
H	4.2284251869	7.5393707201	4.5548899889
H	5.4129807357	8.2048669455	3.4067156766
H	5.9144578001	6.9780436780	4.5771933003
H	8.3323635044	1.3798979924	4.7344447511
H	9.6423366059	0.9111895550	3.6260692788
H	8.9762610180	-0.2764757568	4.7540172810
H	-6.2053845577	4.5495528311	1.8718592883
H	-0.3206180686	7.7718282483	1.7170776199
H	5.8306043115	5.0888470956	1.7485006989
H	7.5741432509	-1.3775614854	1.8586954502
H	3.6479781227	-6.8114057774	1.8271696519
H	-3.0561463682	-7.1250082000	1.7885984450
H	-7.4285410742	-2.0322386425	1.8309492386

B-CD:cis-(1S,4S)-SRT_1_Cl E(Ha)= -5903.32668777

O	-6.9803486124	-3.0799014574	-2.8044246338
O	5.5149237708	-5.3988349652	1.7523591814
O	7.3641370281	-1.6768954125	-2.5754959373
O	4.8544916521	0.8076553240	2.0875346795
O	4.0996007063	1.7146349147	-0.4967261628
O	2.3266213088	2.9989127709	-4.1681518731
O	4.7359486139	2.4229956822	-3.0289871998
O	3.0223319313	-0.9891305167	-7.3400746937
O	-3.2646479514	-1.0790548111	-7.3373834870
O	-0.1050643990	3.3027326778	-5.4680629247
O	-2.6235500635	3.0167169656	-4.4281515909
O	-5.3278650380	1.0859409181	-0.2723372821
O	-4.7461711112	2.3387647178	-2.6903101954
O	-4.9842103678	-6.2433918885	1.9245087918
O	-6.2373264997	-0.5670844898	1.8362113488
O	-4.7800464392	-1.5347241758	3.9657185419
O	0.4257772785	-7.1623595547	4.4888318830
O	-2.7858175639	-2.4309847486	5.7861778310
O	-0.0255475672	-2.3478071290	6.1268985772
O	4.4481371696	-1.8753007642	1.4981851376
O	4.6213291544	-1.0214166285	4.2739904059
O	2.8822699322	-2.3680061619	5.9852658959
O	3.3568388907	-4.8165729637	3.3592295752
O	1.4528041628	-3.6867891360	4.0365613857
O	-1.7539158138	-5.4584725473	4.0877515168
O	-2.8211255570	-3.5742999063	3.2653750164
O	-5.3329257648	-3.8579364554	0.6169808163
O	-4.8531937512	-1.7570865661	-0.2240249281
O	-5.2934491108	-1.0663032282	-3.7992139609
O	-3.3809480803	0.2377835664	-3.8509620215
O	-0.8576062689	-0.0955217106	-6.4741863865
O	0.7443762647	0.6998249839	-5.0031437816
O	4.1330237458	-0.6718946391	-4.8117985049
O	4.1278555256	-0.2918287121	-2.5439303177
O	6.2337057631	-1.8436619039	0.0118482762
C	6.2073922762	-2.4209016763	-2.2732675246
C	2.4421749290	-1.5459866522	-6.1866602656
C	-2.6354855960	-1.5923368961	-6.1910029325
C	-5.5765451477	-3.1777215410	-2.7977423183
C	-3.9161199416	-5.6014266533	1.2746617743
C	0.2494085468	-6.4089404006	3.3140566101
C	4.3114310827	-4.9052325683	1.2246985745
C	3.5504625285	-3.0185113745	4.9248744575
C	3.8013006641	-2.0564373846	3.7819884150
C	4.4242916217	-2.7815423533	2.6013087578
C	3.5925595701	-4.0011087067	2.2118094582
C	2.6983163378	-4.1839726663	4.4296577624
C	-0.4639089138	-5.0966394252	3.5878590282
C	0.2721950506	-4.2346870431	4.6119417000
C	-0.5770525732	-3.0527857197	5.0439971920
C	-1.9483005624	-3.5281109103	5.4829699375
C	-2.5953416897	-4.3732030052	4.3917325952
C	-4.0884148994	-4.0913258585	1.2855140027
C	-4.1253103447	-3.5233060558	2.7034614028
C	-4.5543658138	-2.0674578131	2.6879741143
C	-5.8623012259	-1.9287777784	1.9354593527

C	-5.7534817435	-2.5245632263	0.5368757804
C	-5.2635279748	1.0233508631	-2.6319403211
C	-4.8394672704	0.3248556571	-1.3522371844
C	-5.3647097425	-1.0983985960	-1.3706298113
C	-4.9159120620	-1.8199230481	-2.6426322596
C	-4.7814811576	0.2392577673	-3.8475582992
C	-1.8125177979	-0.5197031283	-5.4935010762
C	-2.6907100961	0.6427934981	-5.0223264087
C	-1.8602855698	1.8623921841	-4.6636910275
C	-0.9214445660	2.1959951057	-5.8052103778
C	-0.0484180706	0.9898089421	-6.1280366820
C	4.2047865183	1.5770333173	-4.0428522266
C	2.6916764036	1.6456412692	-4.0500750102
C	2.1541341695	0.7336897353	-5.1368164370
C	2.7079471946	-0.6855659936	-4.9624205430
C	4.6326557221	0.1373537336	-3.7947849014
C	5.6605691971	-1.2750288137	1.1596355629
C	5.3858157311	0.2117877916	0.9078639512
C	4.4150017976	0.3461569283	-0.2575986016
C	5.0454451211	-0.3303465464	-1.4683001019
C	5.4092303420	-1.7839464699	-1.1488439516
H	-7.2169510925	-2.5372402405	-3.5659213703
H	5.2796012311	-5.9011968290	2.5418447161
H	7.9395695852	-1.7264102901	-1.8033321411
H	4.3591214477	1.9539979593	-1.4202125736
H	1.4510324365	3.0728133139	-4.6066417515
H	3.9750852932	-0.9770266605	-7.1910478513
H	-2.5594381708	-0.7683865023	-7.9175794293
H	-3.2852756290	2.8232270720	-3.7371362636
H	-5.5225868106	0.4889363304	0.4793426029
H	-5.7847199304	-5.9767516532	1.4564234152
H	-4.0105763201	-1.7278676235	4.5330273954
H	-0.4570462491	-7.3371896976	4.8366041764
H	0.9316883481	-2.2440721754	5.9812012026
H	4.6453080383	-0.3255286429	3.5958135892
H	6.4459009330	-3.4559408948	-1.9927074657
H	5.5936020045	-2.4472612622	-3.1782288888
H	2.8108030348	-2.5630159422	-5.9905215033
H	1.3633929939	-1.6008997473	-6.3596775286
H	-3.4248913545	-1.9346710383	-5.5156354356
H	-1.9839875009	-2.4469797282	-6.4261892274
H	-5.3025888269	-3.8075770901	-1.9466081624
H	-5.1955417608	-3.6531007680	-3.7136608633
H	-3.0035978187	-5.8637500512	1.8171833855
H	-3.8096866854	-5.9378480420	0.2322518141
H	1.2464004633	-6.2003617288	2.9153266669
H	-0.3181599329	-6.9645271910	2.5526725601
H	4.5646673282	-4.3316121167	0.3287936193
H	3.6285597493	-5.7157499172	0.9296691345
H	4.5125161785	-3.4234767544	5.2722602807
H	2.8252703668	-1.6645666087	3.4562769187
H	5.4416319809	-3.1128475111	2.8451811351
H	2.6376392141	-3.6599081288	1.7873725329
H	2.5873378308	-4.9528300254	5.2015130710
H	-0.5698700427	-4.5257435945	2.6544420488
H	0.5198670285	-4.8519114683	5.4850330640
H	-0.7081762754	-2.3984375923	4.1658577084
H	-1.8254561754	-4.1682861612	6.3687801969

H	-3.5324755764	-4.8145700945	4.7476907958
H	-3.2691307120	-3.6119247911	0.7310520408
H	-4.8287135090	-4.1163196617	3.3023689313
H	-3.7817559473	-1.4962183183	2.1454828904
H	-6.6353880985	-2.4896460169	2.4807560408
H	-6.7318990378	-2.5556542163	0.0454871018
H	-6.3623015202	1.0507727525	-2.6654412192
H	-3.7381833343	0.2839346428	-1.3312325740
H	-6.4621504986	-1.0817461873	-1.3473769813
H	-3.8236334229	-1.9407761263	-2.6140638289
H	-5.1706241462	0.6782773795	-4.7728609556
H	-1.2906191594	-0.9412782518	-4.6230652989
H	-3.3967046052	0.9021545966	-5.8219807693
H	-1.2549226646	1.6024425893	-3.7790022354
H	-1.5185661384	2.4319383773	-6.6973607803
H	0.5843410324	1.1802075806	-7.0019837525
H	4.5976257661	1.8926136481	-5.0184224929
H	2.3410823402	1.2374692727	-3.0888372550
H	2.4450453277	1.1076119982	-6.1276201442
H	2.2415608079	-1.1354973156	-4.0755632064
H	5.7225996989	0.0273652478	-3.8216428719
H	6.3997772093	-1.3982970041	1.9583593258
H	6.3361127902	0.6901188115	0.6413885467
H	3.4905242529	-0.1828107765	0.0080997716
H	5.9683850504	0.2034298836	-1.7350242832
H	4.4797851475	-2.3488635416	-0.9898178902
Cl	0.5244813448	9.0517088543	0.3889889023
Cl	0.8204542787	10.6643587016	3.1324574437
N	1.6200645456	2.8126330018	-0.0100765003
C	0.9916890696	2.2861208927	1.2769903046
C	1.9516295983	2.5863757305	2.4201575429
C	1.9833265623	4.0802067798	2.7247408896
C	0.6031138583	4.6215735393	3.1253415376
C	-1.8296191893	4.5247039859	2.4926643161
C	-2.9305131824	3.9249461861	1.8967793231
C	-2.7725210403	2.7776510152	1.1202903391
C	-1.4955359462	2.2664174618	0.9354568418
C	-0.3729843992	2.8813223584	1.5064216404
C	-0.5379102504	4.0145179072	2.3205372051
C	0.6091648558	6.1369774443	3.1279149029
C	0.5424469446	6.8460406106	1.9288086788
C	0.6098438704	8.2350066922	1.9084211829
C	0.7404630649	8.9432379527	3.1092626068
C	0.8001041906	8.2403182310	4.3097290929
C	0.7365644299	6.8523887117	4.3182102524
C	0.8081588751	2.6778000836	-1.2443430241
H	1.8224463855	3.8033418663	0.1361966440
H	2.5572259009	2.3400975347	-0.1563594428
H	0.9084769317	1.2069461497	1.1109833776
H	1.5937706344	2.0354932166	3.2973831414
H	2.9483279813	2.1950302253	2.1905407844
H	2.6960858669	4.2877933198	3.5287306543
H	2.3630855495	4.6524183282	1.8645622282
H	0.4273830052	4.3006782944	4.1627005823
H	-1.9670870233	5.4032998979	3.1169147641
H	-3.9205919515	4.3418990138	2.0554733990
H	-3.6337166787	2.2795238748	0.6784816079
H	-1.3630172351	1.3588587144	0.3500090475

H	0.4101134785	6.3224850120	0.9864859419
H	0.8934574847	8.7951855250	5.2369555656
H	0.7836459689	6.3246948881	5.2670129125
H	1.3736309460	3.0706215144	-2.0942615342
H	0.5943252322	1.6209038317	-1.4081469916
H	-0.1272550541	3.2218173050	-1.1213642071
H	5.3725693105	1.5929655893	2.2860950598
H	4.3811719631	3.3026022593	-3.2230196629
H	-0.7125753378	3.9569529977	-5.0929120685
H	-4.9956485212	2.7637117544	-1.8598131648
H	-6.1322683491	-0.2094740127	2.7294595607
H	-2.2660279426	-1.8531386148	6.3605013654
H	3.3668724196	-1.5434266511	6.1267361941

B-CD:cis-(1S,4S)-SRT_2_C1 E(Ha)= -5903.32626406

O	-4.8527314123	-4.9495873213	-3.0223275103
O	6.7918365852	2.3543995536	-2.4165300288
O	2.8309285350	6.7137381168	-1.5681646556
O	4.0710513371	3.2001511458	2.9626792220
O	1.4504330372	4.2251064741	2.7536868439
O	-3.3626596541	4.8957720402	1.6898921446
O	-0.8106114332	5.8035907553	2.2186529800
O	-2.8402360869	6.3247096738	-3.2533141132
O	-6.5020567762	1.2031993985	-4.1538810075
O	-5.8354028385	3.9198487290	0.8403318831
O	-6.5766082730	1.2634746125	0.8559598797
O	-3.5547360579	-3.2700176366	1.6472368116
O	-5.3717856073	-1.1556042156	1.4945333231
O	0.8660240883	-6.5316389783	-3.7498632228
O	-2.0142577243	-5.6374660205	1.2974319057
O	0.7390333371	-5.9310835474	1.3754311035
O	6.2053148062	-3.6795936363	-3.4851192391
O	3.5984403421	-6.0691775293	1.1194043935
O	5.5216245209	-4.0883256791	1.5051508087
O	4.3287898464	2.3262737421	0.3703675892
O	5.9747388397	1.1070913089	2.4598023649
O	6.7441292142	-1.5050925683	1.9046817869
O	6.3508391277	-0.1472942508	-1.4268241500
O	5.2194180915	-1.8686254877	-0.3646390115
O	4.0021369715	-4.7694594479	-2.2348726149
O	2.1481627747	-4.7607141339	-0.8482994253
O	-1.1816031607	-5.4363094096	-2.2248106106
O	-2.2593637702	-3.9266787094	-0.8373127597
O	-5.4267722849	-2.4153729183	-1.9077506617
O	-4.8820659378	-0.3197221491	-1.1021334821
O	-5.1278186255	2.9843710039	-2.5794185112
O	-3.6680549191	3.6336128478	-0.9121876675
O	-0.8061572763	5.8553268638	-1.3997216591
O	0.4857310550	4.6534114025	0.1206985626
O	4.1119715007	4.5015042672	-0.4338402329
C	2.5536570424	5.3888855667	-1.9539476175
C	-2.1921932006	5.0830029134	-3.1373446339
C	-5.1480426006	1.0083834276	-3.8390343525
C	-4.0728930270	-3.7995650824	-3.2533071707
C	0.7555880451	-5.1477022240	-3.5223636112
C	5.0356478314	-2.9322617233	-3.2591262498
C	5.5001205535	1.8014475980	-2.4059412090
C	6.6942419324	-0.5058160751	0.9082115594
C	5.6184480529	0.5152489728	1.2290861176
C	5.4876480960	1.5278111658	0.1042542409
C	5.3240774010	0.8311506773	-1.2486102317
C	6.4135600485	-1.1532343185	-0.4459464939
C	4.3146250570	-3.3927618978	-2.0034879084
C	5.1848917301	-3.2406052034	-0.7547818499
C	4.6199125561	-4.0044456752	0.4301745160
C	4.2553343447	-5.4237761234	0.0454034555
C	3.3432467992	-5.4162492032	-1.1762982897
C	0.1237799845	-4.8478778217	-2.1750636106
C	0.9158060877	-5.4449701778	-1.0133505530
C	0.1449347351	-5.2792524673	0.2831109731
C	-1.2429174229	-5.8687474305	0.1310670806

C	-1.9683037034	-5.2834913914	-1.0764470694
C	-5.2183869987	-2.1089343187	0.4536468063
C	-3.7919662791	-2.6278182521	0.4142583240
C	-3.6271282124	-3.5582213789	-0.7729239337
C	-4.0746415093	-2.8631963179	-2.0590269105
C	-5.6271096645	-1.4848965289	-0.8787904593
C	-4.8064092314	1.5953444316	-2.4785403763
C	-5.5802914851	0.8928957210	-1.3563859592
C	-5.6224072071	1.7132300579	-0.0752637240
C	-5.9440483037	3.1672567212	-0.3536752938
C	-4.9851671018	3.7215570918	-1.3997349012
C	-1.3785826548	5.8993748465	0.9196412234
C	-2.3785506328	4.7820242475	0.6954572493
C	-2.9068253963	4.8179617041	-0.7255183397
C	-1.7368176823	4.8154808253	-1.7134605380
C	-0.2618695756	5.8305083397	-0.1142991578
C	4.5054678403	3.6840468569	0.6355100774
C	3.6840636340	4.0406804008	1.8804197703
C	2.1987526887	3.9014553815	1.5862072418
C	1.8645207571	4.8003828769	0.4056900686
C	2.7328297959	4.4208569887	-0.7977634971
H	-5.7565222712	-4.6466377717	-2.8752552112
H	7.4018699262	1.6101779783	-2.4903857338
H	3.7689643555	6.7484361330	-1.3468430078
H	0.6487220810	4.7346011082	2.4956304553
H	-4.1969633828	4.4864096596	1.3778107761
H	-2.1887050509	7.0005794600	-3.0324609131
H	-6.6473212159	2.1569456265	-4.1509084074
H	-6.2538586991	0.4219330204	1.2262138971
H	-2.9060874537	-3.9895346594	1.5094668050
H	-0.0303020844	-6.8865568069	-3.7128300629
H	1.7073884242	-5.8210195985	1.3260413437
H	5.9256303984	-4.5996693473	-3.5654066399
H	5.8266191659	-3.1895546210	1.7231582958
H	5.3145491738	1.7887101194	2.6649591335
H	3.1914292971	5.0619975060	-2.7870039502
H	1.5126654717	5.3635445666	-2.2862356612
H	-1.3245676788	5.0080907475	-3.8092315705
H	-2.9148912713	4.3146332463	-3.4287695021
H	-4.9727426323	-0.0710686905	-3.8106423765
H	-4.4820796222	1.4483450439	-4.5963044322
H	-3.0503422853	-4.1402182674	-3.4380677880
H	-4.4178956347	-3.2436896929	-4.1370674284
H	1.7692500733	-4.7379703220	-3.5404263948
H	0.1665648780	-4.6497197664	-4.3070388336
H	5.3381180413	-1.8876282777	-3.1390255403
H	4.3403220554	-2.9941450673	-4.1095490659
H	4.7962247855	2.6301445326	-2.2869576988
H	5.2680587376	1.2811928099	-3.3468770248
H	7.6623409612	0.0111390570	0.8346478731
H	4.6610759287	-0.0205548970	1.3146809317
H	6.3814335224	2.1636363115	0.0627739085
H	4.3334310970	0.3583712954	-1.2903646689
H	7.2400877656	-1.8071414491	-0.7448492757
H	3.3904734794	-2.8182443189	-1.8645031007
H	6.1967439282	-3.6019070530	-0.9794218939
H	3.6863705535	-3.5078827995	0.7374561583
H	5.1719525480	-5.9703682104	-0.2201259727

H	3.1427178712	-6.4338226412	-1.5283388408
H	0.0410750724	-3.7606371538	-2.0346424144
H	1.0895653449	-6.5099311967	-1.2140639991
H	0.0436441123	-4.1967421490	0.4737273306
H	-1.1376520073	-6.9505018024	-0.0365559473
H	-2.8929420759	-5.8338609829	-1.2817863053
H	-5.8842926831	-2.9656656542	0.6284555046
H	-3.1092067985	-1.7741381472	0.2782966542
H	-4.2558756835	-4.4456059325	-0.6240427497
H	-3.4136381588	-2.0080013866	-2.2583287451
H	-6.6996448349	-1.2603596292	-0.8825874292
H	-3.7331949702	1.4754654404	-2.2777701434
H	-6.6035936325	0.6951912952	-1.7031040821
H	-4.6149984236	1.6744150806	0.3617807797
H	-6.9627192456	3.2439085588	-0.7587251304
H	-5.2295033311	4.7582445074	-1.6560408412
H	-1.8878216375	6.8666541543	0.8098842548
H	-1.8361259295	3.8278034982	0.7921326822
H	-3.5209656359	5.7113963348	-0.8975072596
H	-1.2347508405	3.8395307353	-1.6558197952
H	0.3926512980	6.7067408597	-0.0569739337
H	5.5632455447	3.9134548928	0.8062526620
H	3.8908555254	5.0882881576	2.1308179525
H	1.9937236051	2.8587536502	1.2964920995
H	2.0891093685	5.8438621432	0.6665980259
H	2.4811291966	3.3999893980	-1.1194869600
Cl	2.2401761434	-1.2538118367	0.3587948484
Cl	1.1387649686	-0.0078155310	-2.3632330943
N	0.9371898151	1.7851711723	3.9797269952
C	-0.2329756320	1.6718505372	4.9427982686
C	-1.3667052303	2.5824028790	4.4999782354
C	-1.8387428140	2.2239737689	3.0950031528
C	-1.9646113152	0.6951759151	2.7967276360
C	-2.0025538413	-1.5274506459	3.9851831679
C	-1.6480263747	-2.3698084224	5.0341078190
C	-0.8391645113	-1.9076613355	6.0693950886
C	-0.3737003567	-0.5991138827	6.0378847841
C	-0.7141090240	0.2479915282	4.9800209589
C	-1.5504721557	-0.2047899489	3.9470159614
C	-1.2080541069	0.4055130545	1.5056024259
C	-0.0091686928	-0.3029457032	1.4824350082
C	0.7323868203	-0.4283815172	0.3042600078
C	0.2573684707	0.1261532281	-0.8832874474
C	-0.9600435664	0.8047668051	-0.8732050970
C	-1.6755424383	0.9512414195	0.3034145321
C	2.1795003269	1.1517174872	4.4823946868
H	0.6679753947	1.3124240405	3.1070596572
H	1.1207093178	2.7817020969	3.6898544024
H	0.1643451791	1.9768520279	5.9158444526
H	-2.1674880956	2.4622938892	5.2363085046
H	-1.0624055569	3.6352045601	4.5284368647
H	-2.7825596554	2.7365243402	2.8927554571
H	-1.1297045902	2.6590736952	2.3825977850
H	-3.0180809058	0.4690789335	2.5900988407
H	-2.6250879769	-1.9157101317	3.1791454521
H	-2.0145883214	-3.3918279537	5.0452812801
H	-0.5764954273	-2.5598154532	6.8962561205
H	0.2478924499	-0.2220650807	6.8468724962

H	0.3528331014	-0.8136267254	2.3710084419
H	-1.3349376579	1.2265815731	-1.7997223473
H	-2.6041031635	1.5106288855	0.2782242317
H	2.9611155924	1.2553888112	3.7313975818
H	2.4857249835	1.6623417781	5.3966997741
H	1.9767313800	0.1029072020	4.6998425515
H	4.2685526265	3.7551027896	3.7226279802
H	-1.5623895983	5.7797328784	2.8264509049
H	-6.3111176815	3.3998737439	1.5050100514
H	-5.1958027309	-1.6235703463	2.3196208682
H	-1.4481193200	-5.9103532053	2.0328325376
H	4.1408165426	-5.8878644223	1.8992141119
H	6.7670716006	-1.0366385454	2.7492703220

B-CD:cis-(1S,4S)-SRT_3_CI E(Ha)= -5903.31722101

O	-1.1226771928	-6.1656883366	-4.2447114886
O	3.9000503359	6.2080151810	-3.2939031851
O	-1.9416755567	7.7611678399	-1.8542204325
O	1.3961687027	5.4782649106	2.3552676499
O	-1.2643246713	4.6378544685	2.1703343698
O	-5.3328718736	2.7464007253	1.7675784401
O	-3.9696900505	5.1393586894	1.7419149020
O	-6.3249537940	3.3302246198	-3.2075650677
O	-6.4412075577	-2.9045973078	-3.2426703609
O	-5.6291746298	-0.0340561339	1.7886882954
O	-4.3647547345	-2.4250475328	1.4870843841
O	-1.2833014454	-5.9524367458	0.7804229652
O	-3.9100982560	-5.0962425616	0.6715915306
O	5.1277836568	-5.1334008137	-2.9031263283
O	1.1498944134	-4.8453249993	1.3851700714
O	3.2532733088	-3.0620515910	1.4689026881
O	7.2051345854	0.9272075354	-3.6012191187
O	5.8984172119	-2.1638854156	1.1458609535
O	6.1936827479	0.5721541350	1.3618964841
O	1.9935244560	5.0458901917	-0.3348932204
O	4.1196709273	5.1809575563	1.7270484953
O	6.1972583806	3.4261681770	1.2699891618
O	5.0091672987	4.0050246186	-2.1004646580
O	5.0435155834	2.0606704723	-0.8533095957
O	5.8935358240	-1.1786383777	-2.3401633458
O	4.2306777492	-2.1748865112	-1.1036013269
O	2.4977340580	-5.2932394687	-1.9452343179
O	0.4245205796	-4.5042145423	-1.2699555887
O	-2.8824615677	-4.6664391754	-2.7680463920
O	-3.5195797159	-3.0834460604	-1.2248630265
O	-6.0716487200	-0.5185549293	-1.7827922322
O	-4.8560619528	1.0916958745	-0.6400873641
O	-4.2484454633	4.4909162430	-1.8071196175
O	-2.3571456369	4.5486288254	-0.4958399486
O	0.5389600733	6.7547719334	-0.9222357138
C	-1.2990293169	6.6268301417	-2.3878708112
C	-5.0421156140	2.7580876338	-3.1771278484
C	-5.3198330242	-2.0678237479	-3.3928072214
C	-0.8884258673	-4.8053951548	-3.9869402017
C	4.1123961139	-4.2403205630	-3.2945646085
C	5.8034609044	0.8205457980	-3.5613087055
C	3.1656520676	5.0229604345	-3.1253035607
C	5.5610996055	4.1211754096	0.2166911409
C	4.1095678886	4.3883125063	0.5633697425
C	3.3936883657	5.0435707778	-0.6064364600
C	3.6169037995	4.2527007961	-1.8960384057
C	5.6510347175	3.3031108567	-1.0666365577
C	5.3319730856	0.1381120542	-2.2878360742
C	5.8044416782	0.8724412922	-1.0320723638
C	5.5895877946	0.0329732113	0.2138273418
C	6.1815775165	-1.3478662889	0.0205264264
C	5.6196115107	-1.9967303008	-1.2390021345
C	3.1021243928	-4.0195283918	-2.1822901729
C	3.7609942570	-3.4967677247	-0.9020573733
C	2.7400010860	-3.4599173984	0.2165713148
C	2.1357235966	-4.8453465685	0.3714329982

C	1.5159895988	-5.3197090174	-0.9428802208
C	-3.1367059235	-5.3239136487	-0.4939331741
C	-1.6759424332	-5.0339016667	-0.2106976620
C	-0.8408488592	-5.1241792515	-1.4827000475
C	-1.4872170258	-4.3802575701	-2.6558025822
C	-3.6402080070	-4.4310483548	-1.6160683880
C	-4.9608774712	-1.3667584690	-2.0946633271
C	-4.7066991946	-2.3607966352	-0.9589086877
C	-4.5263386757	-1.6134300271	0.3475730338
C	-5.7547850179	-0.7494859193	0.5702784445
C	-5.9494098812	0.2138820089	-0.5946516375
C	-4.5210773500	4.5865175605	0.5526343818
C	-4.5637090913	3.0747271721	0.6336525822
C	-5.0856899253	2.4918551337	-0.6691838460
C	-4.3281474097	3.0651231928	-1.8714730465
C	-3.6821228412	5.0158192816	-0.6460992511
C	1.3899705119	6.2356230892	0.0706806028
C	0.5579730220	5.9583355503	1.3231425879
C	-0.5282170361	4.9460859151	0.9947656887
C	-1.3843541748	5.5122376133	-0.1220877847
C	-0.5103772498	5.8782032008	-1.3269507635
H	-2.0802747005	-6.2828239695	-4.2261634954
H	4.8253469226	5.9440644726	-3.3671913941
H	-1.2465636751	8.3576412648	-1.5522656472
H	-2.1983346069	4.8987344559	2.0317209738
H	-5.4590067179	1.7779283766	1.7941410689
H	-6.2016810159	4.2842228704	-3.1375532210
H	-7.1806913722	-2.3365778479	-2.9962641341
H	-4.1694526846	-3.3446646646	1.2127090801
H	-0.4481454186	-5.6347365099	1.1671668002
H	4.6915300363	-5.9675477666	-2.6918511242
H	4.1430892951	-2.6760405108	1.3393386704
H	7.5470772809	0.0263869030	-3.5533677659
H	6.0609016293	1.5386739341	1.3690127914
H	3.2117739140	5.2264236214	2.0708468325
H	-0.6190758324	6.8895875567	-3.2098865814
H	-2.0795670107	5.9735003672	-2.7883178658
H	-4.4168938838	3.1014412484	-4.0141235932
H	-5.1713874658	1.6750817880	-3.2631093172
H	-4.4820873105	-2.7022889668	-3.6973187550
H	-5.4774786469	-1.3098152763	-4.1736351015
H	0.1954117049	-4.6639862146	-3.9475603152
H	-1.2940430604	-4.1612518035	-4.7816027651
H	4.5928307608	-3.2876902454	-3.5372830434
H	3.5804682362	-4.5942022908	-4.1892924775
H	5.4016058338	1.8372212863	-3.5974315354
H	5.4096516612	0.2636880967	-4.4242696233
H	2.1171727961	5.3085464777	-3.0012114149
H	3.2423350819	4.3648974260	-4.0038018212
H	6.0678152961	5.0812472698	0.0388044460
H	3.6220709608	3.4179823616	0.7480810794
H	3.7587404518	6.0682818474	-0.7527876836
H	3.0746309877	3.2999658532	-1.8246111781
H	6.6904963242	3.1796581279	-1.3892843120
H	4.2351657254	0.0791571260	-2.2739911779
H	6.8709237080	1.1100597535	-1.1364494159
H	4.5012457148	-0.0796729272	0.3541764997
H	7.2698298210	-1.2533116279	-0.1027608897

H	6.1084366462	-2.9557143426	-1.4459616323
H	2.3435321667	-3.2950062688	-2.5112139135
H	4.5916098120	-4.1634159145	-0.6351188348
H	1.9456170026	-2.7650166165	-0.0922259130
H	2.9387358966	-5.5515109274	0.6302440723
H	1.2003122665	-6.3656545298	-0.8633602529
H	-3.2420005011	-6.3699316647	-0.8151945798
H	-1.6110092467	-4.0001741207	0.1611466839
H	-0.7137074649	-6.1776653848	-1.7654874847
H	-1.3414545415	-3.3012195042	-2.5089845724
H	-4.6777503495	-4.6609463290	-1.8830374291
H	-4.0533638441	-0.7632039034	-2.2392106160
H	-5.5651444434	-3.0418276181	-0.8879631683
H	-3.6553771091	-0.9499685485	0.2414048534
H	-6.6415964312	-1.3977019800	0.6163572475
H	-6.8865137914	0.7728467238	-0.4916011071
H	-5.5386156997	4.9752483200	0.4100308398
H	-3.5303735889	2.7150748466	0.7496453190
H	-6.1553380029	2.7123951147	-0.7859897136
H	-3.3157577185	2.6381004027	-1.8844211066
H	-3.6886300494	6.1046678983	-0.7685256070
H	2.1368537474	7.0132849228	0.2622075468
H	0.0921988269	6.9074661523	1.6267973841
H	-0.0342695818	4.0302803839	0.6442318126
H	-1.8784468414	6.4264857339	0.2343104554
H	-0.0943784264	4.9552231165	-1.7543542725
Cl	-3.1190716392	-4.7193008117	4.1052408894
Cl	-0.9556758345	-6.6479000709	5.4373399574
N	-1.6894384784	1.4955779289	4.1654664267
C	-0.4067260054	1.5817639162	3.3223206301
C	0.7614373569	1.1932517609	4.2157508262
C	0.6961578832	-0.2830904790	4.5911642010
C	0.6920294472	-1.2107306940	3.3616831145
C	-0.2141494324	-1.4355535702	1.0310977436
C	-0.7669037505	-0.9238693461	-0.1351057437
C	-1.1866653238	0.4040737692	-0.1882122335
C	-1.0647465982	1.2010237239	0.9402662801
C	-0.5267278760	0.6825217131	2.1253279605
C	-0.0698117964	-0.6445947431	2.1753968221
C	0.2560605088	-2.5978899950	3.7957140296
C	-1.0710135827	-3.0177820238	3.7145106922
C	-1.4574501776	-4.2588342597	4.2175953081
C	-0.5149304158	-5.1066883426	4.8084809567
C	0.8146479893	-4.6939104717	4.8799345482
C	1.1941716544	-3.4536716256	4.3828625493
C	-2.9584111300	1.8855190589	3.4873960290
H	-1.7723899354	0.5363090092	4.5118118368
H	-1.5541287611	2.0865991525	4.9892875857
H	-0.3720915602	2.6333021869	3.0187180996
H	1.6762237457	1.3982269164	3.6491719442
H	0.8051617288	1.8265016989	5.1120259104
H	1.5393418998	-0.5446792757	5.2367722843
H	-0.1935142251	-0.4929804848	5.2050436568
H	1.7317150401	-1.3055051878	3.0144445474
H	0.1250067847	-2.4668383228	1.0571072011
H	-0.8547243101	-1.5646770936	-1.0061883368
H	-1.6048460009	0.8162573372	-1.1009189494
H	-1.3689929384	2.2446410580	0.9047973934

H	-1.8247719748	-2.4073468172	3.2242307850
H	1.5454524124	-5.3572627765	5.3302673162
H	2.2376150171	-3.1545722246	4.4374063784
H	-3.7568552429	1.9087042462	4.2290885756
H	-2.8194895103	2.8670119068	3.0382949796
H	-3.1884458993	1.1550846383	2.7130061971
H	0.8268261045	5.3289954747	3.1186567605
H	-4.5464758426	4.8365905906	2.4559503066
H	-5.3813191602	-0.7061099635	2.4394344546
H	-3.4326131880	-5.5486009058	1.3841525850
H	1.5536674728	-4.4751264191	2.1824215257
H	6.1769678054	-1.6415678736	1.9114699268
H	5.9481111241	3.9045692898	2.0733730188

B-CD:cis-(1S,4S)-SRT_4_CI E(Ha)= -5903.2939552168

O	-5.09399117	-4.57021890	0.04078234
O	7.10707918	2.37366344	-1.65171305
O	2.10349649	5.96941304	-3.79919682
O	4.63395939	5.42436672	1.39661562
O	2.23831548	6.75469480	1.25860187
O	-2.90364350	6.43337605	1.91541272
O	-0.46021257	7.48543153	1.24036784
O	-3.99372910	5.84325902	-3.06276251
O	-7.25594031	0.96395651	-1.25535478
O	-5.10695679	4.82502120	2.57331647
O	-5.64848275	2.27433902	3.45043892
O	-4.43097609	-2.50491181	4.68703201
O	-6.11815707	-0.44773074	4.00623088
O	0.51591985	-6.84274683	0.79904283
O	-2.17222980	-4.08264838	5.17573366
O	0.57239010	-4.09114853	5.10366385
O	5.63311627	-3.92522786	-0.63207766
O	3.36787892	-4.06789105	4.68016471
O	5.13209512	-2.06156157	4.06361978
O	3.94216482	3.16526912	-0.15258734
O	4.49112144	3.00330216	2.73950491
O	5.35551389	0.60407063	3.61850773
O	6.21393117	0.30701610	0.10891021
O	4.64078097	-0.91128595	1.29009088
O	3.54947953	-4.37748874	1.08311281
O	1.73686013	-3.86034212	2.42369090
O	-1.57620960	-5.30151465	1.81568313
O	-2.64078167	-3.36980598	2.52191743
O	-5.52827351	-1.96379430	0.76954394
O	-5.04338458	0.16598779	1.52643752
O	-5.62861640	3.10776823	-0.57625013
O	-3.74784728	4.17606855	0.24086139
O	-1.50024220	6.07371440	-1.93259352
O	0.30179694	5.53069635	-0.59311041
O	3.54674581	4.53398141	-1.94483091
C	1.60712186	4.78552622	-3.23542740
C	-3.24016338	4.71316661	-2.71217879
C	-5.85484936	0.89066671	-1.30587866
C	-4.10704926	-3.58742655	-0.13294491
C	0.25966044	-5.52834428	0.37565794
C	4.45821414	-3.17122108	-0.69338793
C	5.93101863	1.62906886	-1.81899369
C	5.68600587	1.01975075	2.31491257
C	4.62407689	1.97584536	1.79838760
C	5.01926484	2.43308539	0.40916630
C	5.31340332	1.22617123	-0.48849843
C	5.83801316	-0.17345529	1.37714323
C	3.80008661	-3.04552580	0.67496652
C	4.68584101	-2.28936329	1.66804211
C	4.19569632	-2.46291603	3.09989739
C	3.92069175	-3.92822810	3.39170714
C	2.96893520	-4.51746680	2.36164905
C	-0.33436143	-4.68441080	1.49226512
C	0.57529347	-4.63363799	2.72017025
C	-0.13308418	-3.98871707	3.89655153
C	-1.45941271	-4.69283237	4.12295859

C	-2.30293232	-4.68423388	2.85248984
C	-5.78553264	-1.47478794	3.09566317
C	-4.39223980	-2.00214934	3.37888545
C	-4.01373807	-3.04311515	2.33903474
C	-4.21307552	-2.49866559	0.92356741
C	-5.88331768	-0.94622754	1.66996242
C	-5.20594657	1.78054082	-0.25873974
C	-5.62567831	1.40902091	1.16434710
C	-5.14166857	2.45145059	2.15606703
C	-5.60140266	3.82589884	1.70571187
C	-5.14603437	4.11246239	0.27971304
C	-1.36397435	7.01342958	0.26217368
C	-2.21490829	5.89083102	0.82298456
C	-3.12864298	5.34957575	-0.26297976
C	-2.33600363	4.99095466	-1.52140412
C	-0.59682981	6.54096419	-0.96637164
C	4.26080117	4.40647465	-0.75233491
C	3.92350038	5.56392331	0.17933546
C	2.43347314	5.63320634	0.44457869
C	1.68011950	5.69981205	-0.87314163
C	2.12342861	4.58316800	-1.81968280
H	-5.94447978	-4.10623576	0.01984903
H	7.75324077	1.79849377	-1.21617883
H	3.06973990	5.90773888	-3.76748386
H	1.27534726	6.91919195	1.35620871
H	-3.57730538	5.79000461	2.22233343
H	-3.35677337	6.54959504	-3.24733430
H	-7.48621165	1.89748483	-1.37516147
H	-5.65357533	1.31867022	3.66947421
H	-3.57210822	-2.92734777	4.89396878
H	-0.33678141	-7.21690299	1.06650963
H	1.52329130	-3.92230708	4.94423091
H	5.38859907	-4.78796309	-0.26335374
H	5.17959901	-1.08386675	4.06617296
H	4.48541601	3.87271122	2.28142730
H	1.87238680	3.90237092	-3.84055851
H	0.51698908	4.87292599	-3.21326124
H	-2.62247067	4.35714703	-3.55287915
H	-3.95402813	3.92687969	-2.44659743
H	-5.58205139	-0.15179119	-1.11747216
H	-5.47009265	1.17709249	-2.29897500
H	-3.13941752	-4.09002792	-0.04328690
H	-4.16761913	-3.12135941	-1.12965479
H	1.22237752	-5.10500029	0.07199619
H	-0.41995304	-5.50420710	-0.48958384
H	4.74536519	-2.17642031	-1.05427596
H	3.73101374	-3.60923833	-1.39863150
H	5.22616435	2.26625176	-2.36300586
H	6.10526577	0.71940227	-2.41518573
H	6.65502531	1.54197452	2.32262648
H	3.67423769	1.41867776	1.72399519
H	5.92076768	3.05533957	0.47206706
H	4.34783600	0.72895082	-0.68758122
H	6.65606578	-0.82386182	1.70093006
H	2.84039232	-2.50522341	0.59343927
H	5.71036967	-2.67300838	1.57990590
H	3.24896375	-1.90911952	3.20492227
H	4.86953528	-4.48137650	3.32530634

H	2.84266180	-5.59485273	2.50406661
H	-0.50820728	-3.65677551	1.13554374
H	0.86315628	-5.65816417	2.98576751
H	-0.33798805	-2.93456531	3.64227218
H	-1.25052065	-5.74381140	4.37307442
H	-3.20261999	-5.29486548	2.97939621
H	-6.49876499	-2.30673568	3.19444076
H	-3.68073239	-1.16350504	3.29298258
H	-4.63888907	-3.93666391	2.46341593
H	-3.46589957	-1.71341251	0.73613135
H	-6.91542000	-0.68158852	1.41783428
H	-4.11040650	1.70759044	-0.33292620
H	-6.72068836	1.34604974	1.20572924
H	-4.03822393	2.43519495	2.15536443
H	-6.70145513	3.83922336	1.71194416
H	-5.58291448	5.04636469	-0.08905388
H	-2.02878812	7.83035211	-0.05514638
H	-1.54528784	5.07285333	1.13888796
H	-3.88223807	6.10486849	-0.52154949
H	-1.71878452	4.10629613	-1.30163267
H	-0.06264510	7.37192853	-1.43875267
H	5.32038843	4.42371449	-1.03090546
H	4.23440888	6.49239337	-0.32131922
H	2.13011794	4.70544602	0.96003297
H	1.86516218	6.66849956	-1.35539727
H	1.74970882	3.62843818	-1.41711107
Cl	-1.34454379	-5.98516617	-3.33871606
Cl	-0.33321685	-7.26917074	-6.08070711
N	1.81063627	-0.47245670	-1.04846068
C	1.73927714	0.29985868	-2.37608668
C	2.81403261	-0.25432424	-3.30031838
C	2.43915023	-1.63371737	-3.82683351
C	1.14472725	-1.58469266	-4.64660991
C	-1.23328916	-0.77317447	-4.49933722
C	-2.22809022	0.07117633	-4.02455197
C	-1.93356673	1.00766653	-3.03576778
C	-0.64544954	1.07116780	-2.52267739
C	0.35569874	0.19539915	-2.96791692
C	0.06974829	-0.73109037	-3.98961791
C	0.70871822	-2.98966381	-5.01437752
C	-0.04750241	-3.76818705	-4.13880499
C	-0.38245956	-5.08310836	-4.45135823
C	0.05253909	-5.64664664	-5.65698183
C	0.80743037	-4.87158339	-6.53508145
C	1.12843307	-3.55809139	-6.21846664
C	1.02459987	0.07875440	0.08881323
H	1.51535681	-1.43684238	-1.22842162
H	2.79438561	-0.52679411	-0.75052257
H	1.96989821	1.33088641	-2.08566393
H	2.91051714	0.44863796	-4.13695062
H	3.79002595	-0.26877869	-2.79855110
H	3.24784222	-2.03259689	-4.44742436
H	2.32502223	-2.35872412	-3.00619874
H	1.39077729	-1.07145683	-5.58950421
H	-1.46335650	-1.48072271	-5.29095421
H	-3.22944257	0.01261838	-4.44140455
H	-2.69706697	1.69319236	-2.68079096
H	-0.40350928	1.83015639	-1.78078655

H	-0.41451977	-3.35224428	-3.20472458
H	1.13425038	-5.30963409	-7.47245435
H	1.71277582	-2.97113621	-6.92299697
H	1.18494297	-0.55919115	0.96022726
H	1.38348908	1.08891706	0.29519092
H	-0.03002366	0.09292753	-0.18363270
H	4.26232024	6.10839504	1.98176514
H	-0.98335508	7.56036998	2.05667007
H	-5.26406767	4.48934145	3.47174197
H	-5.84879218	-0.78388415	4.87804916
H	-1.52839125	-3.95145120	5.89119876
H	3.92525286	-3.51719328	5.25680447
H	5.08237035	1.40916688	4.09133286

B-CD:cis-(1S,4S)-SRT_5_CI E(Ha)= -5903.2932691077

O	-6.83080711	-0.39449937	-4.36790717
O	6.41344030	-2.62212488	-3.86020703
O	6.36141952	3.45903924	-3.46874918
O	6.53622096	0.13218605	1.24660973
O	5.40432987	2.60605059	1.49189585
O	0.80033609	5.06463985	1.54129365
O	3.51560235	4.67677076	1.70555892
O	1.43597286	7.20505052	-3.10637696
O	-4.21336168	5.09283278	-4.21777865
O	-1.79039803	5.99029869	0.98257267
O	-4.02728826	4.40736678	0.87324076
O	-6.07662836	-0.34411519	0.70507621
O	-5.97094962	2.39341830	0.65764486
O	-3.86277231	-5.74473117	-4.21694210
O	-5.89838164	-3.14754195	0.52452511
O	-3.81897415	-4.88785995	0.83250214
O	2.12654717	-7.02692045	-3.41652540
O	-1.24378641	-5.88241684	1.20534891
O	1.39712178	-5.14728894	1.32797276
O	5.12080442	-0.67109761	-1.02068732
O	5.55791191	-2.50902799	1.19965453
O	4.18462213	-4.88055133	1.01397410
O	4.44935820	-3.96083920	-2.48168234
O	2.57865726	-4.25452007	-1.15796809
O	-0.29876808	-6.23413481	-2.27892987
O	-1.79258615	-4.76239993	-1.29616498
O	-4.83366083	-3.54655614	-2.91847589
O	-4.82503282	-1.66411453	-1.57236752
O	-5.69979809	1.64295570	-2.87979326
O	-4.18253037	2.65850763	-1.45368340
O	-2.02467058	5.38989843	-2.58432232
O	-0.36163795	4.81793751	-1.08050804
O	3.17896092	5.42786756	-1.82804529
O	3.77430312	3.44188788	-0.79528239
O	6.11147209	1.03022606	-2.24069383
C	5.13197362	2.77829845	-3.44844706
C	1.41557301	5.81584762	-3.33324405
C	-3.29889825	4.04399671	-4.01770001
C	-5.43863853	-0.27113483	-4.20941154
C	-3.07336914	-4.59384066	-4.05087515
C	1.57924701	-5.74315991	-3.60188381
C	5.12020423	-2.08821783	-3.71838101
C	4.73351070	-4.24660830	-0.12777259
C	4.75838517	-2.74394444	0.06745797
C	5.27523818	-2.07265721	-1.19194362
C	4.47759818	-2.53171880	-2.41422406
C	3.91848061	-4.61501822	-1.36218910
C	0.77559066	-5.29693115	-2.39253801
C	1.61280746	-5.29195814	-1.111103170
C	0.72479204	-5.04447196	0.09243174
C	-0.38401910	-6.08090263	0.10025604
C	-1.17475744	-6.01136943	-1.20287850
C	-3.44254771	-3.85055845	-2.77722972
C	-3.19223568	-4.69807459	-1.52758678
C	-3.84029355	-4.06681537	-0.30759712
C	-5.30061425	-3.78023880	-0.59104218

C	-5.43172188	-2.89932245	-1.82727640
C	-6.12596953	1.64083614	-0.53111387
C	-5.46154573	0.28571676	-0.38961498
C	-5.59840228	-0.48111098	-1.69253190
C	-5.08386590	0.35105433	-2.86912700
C	-5.53429183	2.40117786	-1.71187208
C	-2.67005699	4.11260603	-2.63534375
C	-3.71207333	3.99404582	-1.52117694
C	-3.09638236	4.32967708	-0.17435334
C	-2.42485709	5.68588638	-0.24816847
C	-1.40139404	5.71694677	-1.37643388
C	2.94085913	5.22671097	0.53564628
C	1.51304355	4.74066414	0.36763489
C	0.93690125	5.35601061	-0.89147734
C	1.82895592	5.03892920	-2.09487396
C	3.75739900	4.83408075	-0.69343304
C	6.23829516	0.15819108	-1.14746293
C	6.39167284	0.98285120	0.12588326
C	5.18688692	1.88380935	0.30436342
C	5.01760682	2.76506241	-0.92051916
C	4.99491805	1.92264269	-2.19871326
H	-7.19158237	0.50126562	-4.29239564
H	6.31239777	-3.58452534	-3.81438809
H	7.04553619	2.77490423	-3.41878821
H	4.66738325	3.24049711	1.60833885
H	-0.11491503	5.32947426	1.29985481
H	2.35034169	7.43207240	-2.88213111
H	-3.71255973	5.91363568	-4.10111859
H	-4.61380080	3.62119191	0.83732953
H	-5.88240140	-1.30539214	0.67096660
H	-4.78223963	-5.43947594	-4.21456343
H	-2.88886036	-5.12833930	1.02692962
H	1.37692860	-7.62136879	-3.26499870
H	2.34709379	-4.93674898	1.19396194
H	5.76752061	-1.55262964	1.24651557
H	5.00736560	2.13718494	-4.33466235
H	4.34565115	3.53863371	-3.45844150
H	2.07538839	5.53051394	-4.16623827
H	0.38893200	5.55135796	-3.60255757
H	-3.85849960	3.10962079	-4.11594311
H	-2.49848960	4.05159988	-4.77335999
H	-5.02005712	-1.28015838	-4.26398887
H	-4.99047791	0.33457432	-5.01203380
H	-2.03305318	-4.92564521	-3.98846406
H	-3.16959527	-3.90754698	-4.90641259
H	2.41728362	-5.05722837	-3.75571235
H	0.93197532	-5.70294799	-4.49106359
H	5.22206882	-0.99922469	-3.72297417
H	4.46581760	-2.37994025	-4.55417600
H	5.76420620	-4.59736799	-0.28476086
H	3.72474767	-2.39753044	0.23423915
H	6.33256486	-2.32658250	-1.34429498
H	3.45373639	-2.13911778	-2.34165320
H	3.99609051	-5.68471806	-1.58443851
H	0.37705651	-4.28630253	-2.55968470
H	2.10637519	-6.26757818	-1.00898572
H	0.27324926	-4.04599681	-0.00937173
H	0.06929168	-7.08140162	0.16234847

H	-1.91624730	-6.81595306	-1.25528233
H	-2.86301971	-2.92052968	-2.69581039
H	-3.60239655	-5.70302675	-1.69344699
H	-3.33029716	-3.10868853	-0.11528296
H	-5.81454693	-4.73064560	-0.79761991
H	-6.48169348	-2.76180466	-2.10714232
H	-7.19606290	1.48680125	-0.73332789
H	-4.38631227	0.44269849	-0.20122826
H	-6.65400661	-0.72737458	-1.86743192
H	-3.99361474	0.45697245	-2.77881788
H	-6.07626498	3.33635355	-1.88902704
H	-1.92600077	3.31260050	-2.51673595
H	-4.53831835	4.68461863	-1.73599703
H	-2.32622605	3.56861044	0.03906011
H	-3.19079215	6.44490911	-0.46345764
H	-0.99863820	6.72537793	-1.51886602
H	2.94142072	6.32451692	0.60471827
H	1.54541260	3.64863319	0.23744126
H	0.88334021	6.44661808	-0.77403128
H	1.78122474	3.95969443	-2.29719296
H	4.77576857	5.23338208	-0.63655049
H	7.13872075	-0.43267267	-1.34663077
H	7.29048637	1.60753714	0.01580427
H	4.29013026	1.24847502	0.38786401
H	5.84343392	3.48580471	-0.98450937
H	4.05688074	1.35080165	-2.22791921
Cl	0.78106952	-2.35349630	2.32335031
Cl	0.60890172	-0.41980870	-0.21319752
N	1.42305125	-0.08627486	8.10045314
C	0.37627471	1.04125761	8.19364139
C	0.95569053	2.26192487	7.49377511
C	1.04923542	2.03254065	5.98925482
C	-0.32073559	1.73258593	5.35974477
C	-2.43339623	0.41539007	5.72339445
C	-3.33836624	-0.28603599	6.50902886
C	-3.05254603	-0.54138058	7.84959549
C	-1.84893433	-0.10125877	8.38031520
C	-0.91854177	0.58270180	7.58404232
C	-1.21333996	0.86730195	6.23932554
C	-0.13718863	1.18288467	3.95782439
C	0.15906101	-0.16641775	3.76369416
C	0.40090634	-0.68029560	2.49330090
C	0.32942275	0.17060587	1.38261053
C	0.02927427	1.51739450	1.56945423
C	-0.19272661	2.02272767	2.84547479
C	1.15247285	-1.31358138	8.89720105
H	1.50935758	-0.33953272	7.11079760
H	2.33225707	0.30174392	8.37401662
H	0.26733750	1.21034794	9.27034250
H	0.28422954	3.10198628	7.70663555
H	1.93134805	2.53305802	7.92030086
H	1.48415893	2.91080492	5.50208618
H	1.74591775	1.21209889	5.75537614
H	-0.84426820	2.69564936	5.26593355
H	-2.67347197	0.62644184	4.68499196
H	-4.27782477	-0.62106268	6.07935362
H	-3.76754054	-1.06530089	8.47635414
H	-1.63500062	-0.26743490	9.43467553

H	0.18217845	-0.85529434	4.60453733
H	-0.03163660	2.17180445	0.70626384
H	-0.39199564	3.08526942	2.95448718
H	1.96941085	-2.02084303	8.74424986
H	1.08724594	-1.03970427	9.95126175
H	0.20959273	-1.74407429	8.56075516
H	6.36557461	0.70672911	2.01184231
H	2.82477305	4.75559167	2.38300058
H	-2.44956058	5.76078323	1.65943861
H	-6.15192026	1.76368491	1.37519698
H	-5.55463597	-3.63610996	1.29211508
H	-0.65778992	-5.69531577	1.95634138
H	4.61327063	-4.44158781	1.76788611

B-CD:cis-(1S,4S)-SRT_6_CI E(Ha)= -5903.2918675359

O	1.04138524	-7.33847092	-0.61333890
O	1.94242939	6.94241923	-1.48311342
O	-4.06848499	6.11084054	-1.47946048
O	-1.07491203	6.39614519	3.52990137
O	-3.48215991	5.03426573	3.51339093
O	-6.19060257	0.60334537	3.19146938
O	-5.75405431	3.34183911	3.19424663
O	-6.64758561	0.64052123	-1.94966277
O	-4.18706615	-4.72400912	-1.92239211
O	-6.39971678	-2.21762863	2.86754801
O	-4.64060943	-4.30662752	3.23371980
O	0.55238576	-5.33692348	4.09030093
O	-2.19003895	-5.48400723	3.87732298
O	5.88683867	-3.58682451	-1.18141723
O	3.34653673	-4.87024480	3.95997659
O	4.94417434	-2.60609859	3.79460632
O	5.70201393	2.32119795	-2.01978300
O	6.43377296	-0.24248200	3.20816692
O	5.74460307	2.42816177	3.21478891
O	0.00338166	5.28566199	1.22981478
O	1.69376547	5.82294270	3.54024552
O	4.21624126	4.75625924	3.39379914
O	3.39738461	5.07917184	-0.12576223
O	3.84208161	3.18182660	1.11943135
O	5.56757203	0.27855952	-0.27242998
O	4.67559475	-1.15388045	1.29772381
O	3.83765771	-4.59659063	0.38008737
O	1.89514670	-4.51331951	1.62467922
O	-1.18254362	-6.10680663	0.45202577
O	-2.40744549	-4.35088525	1.32521613
O	-5.06129508	-2.61226262	-0.47705352
O	-4.98785501	-0.80461038	0.96039575
O	-5.51528128	2.57849689	-0.33999344
O	-3.95751637	3.47995576	1.10983877
O	-1.73115508	6.15535054	-0.02713009
C	-3.20774948	5.00050847	-1.43142068
C	-5.26728326	0.67420217	-1.68184108
C	-3.28909416	-3.73093863	-1.50406413
C	0.78253531	-5.97352089	-0.81297497
C	4.61737190	-2.98861077	-1.13440895
C	4.45161070	1.88346073	-1.55350111
C	1.51141155	5.60736386	-1.40383021
C	3.56001598	5.26694435	2.25233787
C	2.05859227	5.11190997	2.38793946
C	1.37844446	5.61675015	1.12788497
C	1.97169018	4.94950040	-0.11384101
C	4.05998291	4.55802974	0.99806093
C	4.55032005	1.27986343	-0.16260709
C	4.93023494	2.29777825	0.91308383
C	5.21470482	1.58676421	2.22735909
C	6.24477508	0.49360718	2.01760012
C	5.81888168	-0.45362287	0.90173741
C	3.94517304	-3.18218743	0.21295308
C	4.73745179	-2.56877064	1.36719170
C	4.14330005	-2.97255984	2.70427400
C	3.99439499	-4.48122296	2.76689449

C	3.20446689	-5.00181200	1.57061436
C	-1.33714164	-5.87217544	2.82236022
C	-0.05159080	-5.06747770	2.85406005
C	0.81879328	-5.44114435	1.66705250
C	0.03023103	-5.36475338	0.35875641
C	-2.04580264	-5.68938001	1.48483843
C	-3.73820887	-3.07686020	-0.20771752
C	-3.74958495	-4.04735879	0.97330479
C	-4.42868285	-3.41014157	2.17508332
C	-5.79898636	-2.89161141	1.78291138
C	-5.69757727	-1.94793060	0.58917085
C	-5.98359218	2.60929272	2.00823134
C	-5.46398203	1.18972173	2.14463464
C	-5.62070718	0.45998936	0.82267186
C	-4.97370237	1.25600741	-0.31055485
C	-5.31795062	3.32397410	0.83701250
C	-0.95074252	6.30225411	1.13271334
C	-1.85511302	6.25643299	2.35982677
C	-2.64184542	4.96085698	2.39247302
C	-3.39806966	4.78431862	1.08810049
C	-2.46077600	4.92728872	-0.11085322
H	0.18269464	-7.75093524	-0.43408569
H	2.89976418	6.92006422	-1.33341863
H	-3.51811546	6.88402933	-1.28343067
H	-4.15840544	4.32823771	3.45023099
H	-6.09644279	-0.37006331	3.14103415
H	-6.96718846	1.54609041	-1.81852447
H	-5.06546979	-4.31420356	-1.89017708
H	-3.77204504	-4.61212832	3.56709217
H	1.47623388	-5.01169980	4.07319287
H	5.76405533	-4.50295060	-0.88879296
H	5.30472993	-1.70830135	3.63906760
H	6.31997344	1.59930294	-1.82565536
H	5.12113698	3.16873646	3.37162165
H	0.71580887	5.87540428	3.58669217
H	-2.47115854	5.02466260	-2.25167047
H	-3.82746452	4.10718842	-1.55118366
H	-4.72259646	1.26508000	-2.43604713
H	-4.90837882	-0.35827597	-1.72409764
H	-2.31926710	-4.21362666	-1.35212507
H	-3.17179225	-2.94231912	-2.26843419
H	1.75277034	-5.47722481	-0.92023740
H	0.19528313	-5.80344083	-1.73147761
H	4.75460606	-1.91942389	-1.32225246
H	3.94996032	-3.39820722	-1.91370368
H	3.78869510	2.75306553	-1.52724198
H	4.01002846	1.12839094	-2.22861526
H	0.41803973	5.61923471	-1.43705354
H	1.88029381	5.01109720	-2.25474793
H	3.78948303	6.33725881	2.13912667
H	1.82670099	4.03848048	2.49054163
H	1.50859941	6.70418044	1.04697351
H	1.69025526	3.88715015	-0.11057973
H	5.12316709	4.76523024	0.83446755
H	3.59341212	0.81449025	0.11124816
H	5.82100746	2.85042705	0.58468294
H	4.27383359	1.11822497	2.56179597
H	7.19155450	0.96612046	1.71470179

H	6.62582948	-1.14857293	0.64571848
H	2.94551258	-2.72665206	0.19289348
H	5.77886901	-2.91231309	1.31363054
H	3.13931832	-2.52113418	2.77717823
H	4.99879594	-4.92852690	2.72307720
H	3.20667120	-6.09649749	1.54616328
H	-1.08319478	-6.93857380	2.91815904
H	-0.31187343	-3.99959053	2.76124849
H	1.19732190	-6.46305535	1.79841081
H	-0.19600790	-4.30846360	0.15012027
H	-2.92322740	-6.34080172	1.41661689
H	-3.08229410	-2.22821315	0.03284854
H	-4.28436451	-4.95979918	0.67765333
H	-3.81293509	-2.55327942	2.49391177
H	-6.42138703	-3.74793670	1.48133525
H	-6.69023996	-1.68129204	0.21186671
H	-7.06322164	2.56036999	1.80127013
H	-4.38764334	1.23399540	2.38201851
H	-6.68798131	0.32913601	0.60157374
H	-3.88754599	1.29753951	-0.14664465
H	-5.78928474	4.29474452	0.65066495
H	-0.46580876	7.27994383	1.03988044
H	-2.56568706	7.09293646	2.28282394
H	-1.92826452	4.12472727	2.48346026
H	-4.19016187	5.54118832	1.01660813
H	-1.76480060	4.07715728	-0.11859243
Cl	-0.42241663	2.30568556	-2.26155358
Cl	-0.18078669	0.87562959	0.58937580
N	2.31906807	-0.08203690	-7.20865397
C	1.85057756	-1.54770749	-7.27867178
C	2.70140214	-2.35061697	-6.30530414
C	2.38329374	-1.96871181	-4.86397826
C	0.90308703	-2.19614611	-4.50864228
C	-1.42928478	-1.98349722	-5.42267597
C	-2.35059077	-1.81531455	-6.44786308
C	-1.91292333	-1.57236696	-7.74911136
C	-0.55145820	-1.48973151	-8.00173340
C	0.38293272	-1.63112630	-6.96546944
C	-0.05182183	-1.89761163	-5.65590389
C	0.56683868	-1.44228169	-3.23563928
C	0.22685222	-0.09101233	-3.28338729
C	-0.00344184	0.63692064	-2.12040369
C	0.10178279	0.01120959	-0.87229613
C	0.43529528	-1.34151330	-0.81890790
C	0.66574842	-2.05895815	-1.98760074
C	1.75309434	0.84586740	-8.22530832
H	2.09207864	0.26691581	-6.27188827
H	3.34282672	-0.07147605	-7.27311407
H	2.04751182	-1.83811156	-8.31619954
H	2.47275499	-3.40886712	-6.47733676
H	3.77115023	-2.22764554	-6.52272579
H	3.01327297	-2.54248031	-4.17664926
H	2.64847069	-0.91776995	-4.66762965
H	0.78570929	-3.26893799	-4.29527297
H	-1.78011520	-2.19568832	-4.41587843
H	-3.41276755	-1.89132843	-6.23501848
H	-2.62672414	-1.46585014	-8.55999391
H	-0.20275821	-1.33989846	-9.02189138

H	0.10251381	0.41487114	-4.23717231
H	0.51184164	-1.82836045	0.14878722
H	0.92383324	-3.11308408	-1.92006223
H	2.16422000	1.84319473	-8.05977335
H	2.02809695	0.48765420	-9.21843167
H	0.66880904	0.85911583	-8.11686792
H	-1.66141716	6.14515058	4.26282892
H	-6.03698237	2.75910199	3.91815883
H	-6.23808892	-2.78737674	3.63884341
H	-1.62047846	-5.38973690	4.65860171
H	3.78634827	-4.37357378	4.66987935
H	6.50562136	0.42780684	3.90917035
H	3.68268234	5.05190392	4.15079569

B-CD:cis-(1S,4S)-SRT_1_MD E(Ha)= -5903.35862005

O	5.3961391826	0.7770469776	0.5411637492
O	4.4577861139	-2.5476445214	-0.6555580530
O	4.4319548253	-4.3467298319	0.8062455386
O	1.2116719070	-5.4188323310	-0.5685313777
O	-0.3723244043	-6.3672343124	0.8287496959
O	-3.0254729520	-4.3742389422	-0.7384174840
O	-4.7254787735	-3.5286202367	0.5744298286
O	-5.6922631822	1.5832618612	-0.1544117036
O	-3.0677920098	3.7296593008	-1.5668225581
O	-2.1764650599	5.4579887148	-0.3309442682
O	1.1210223648	4.8069036565	-1.8031539483
O	2.8521952326	5.0936640187	-0.3007915559
O	2.6911300580	5.4445524023	-3.9007152423
O	4.7568569809	3.5263810416	-3.5523006887
O	4.4468292633	1.9312527609	-1.2260617448
O	-0.3537555155	5.7339334723	-4.0287668641
O	-3.1096903707	5.3214207692	-3.8412630606
O	-0.1133582201	4.6515458344	1.9755575040
O	-4.6304407647	2.9194229608	-3.8660864717
O	-5.9263017822	0.5070357599	-3.6048219271
O	-3.2954317790	3.6811411289	1.5269558804
O	-4.7837437164	-4.8097505601	-2.8098446783
O	-5.7698888803	-2.2421467064	-3.1472983226
O	-2.2492092428	-6.2027819247	-2.7959522036
O	0.4143605293	-7.0323857216	-2.6430954655
O	-2.7646180217	-4.1211238753	2.3537249847
O	2.7076975414	-3.9634400279	3.0750668883
O	5.2888350840	-4.2254823435	-2.7099230181
O	3.0987746253	-5.9351070935	-2.7351975011
O	6.3313885966	-1.6006948614	-2.6377490251
O	6.4467516108	1.1810221088	-2.8983690978
O	3.2839521385	0.1183047013	2.4265666142
O	2.2392573665	3.3603122776	2.0144747996
O	-3.4652236722	-1.3521252753	2.4760722441
O	-4.8431398218	-0.3179146869	-1.1800756777
C	4.5456928352	-0.3640156008	0.4125294952
C	5.2669079838	-1.4016256128	-0.4456040293
C	5.5465418493	-0.7834251310	-1.8122576013
C	6.3137046995	0.5176862488	-1.6607772289
C	5.6352669558	1.4515543365	-0.6653293888
C	4.9930427805	-3.8071052301	-0.3641559374
C	3.0148576760	-4.5160178887	0.7399087818
C	2.6202840290	-5.4603590079	-0.3934690293
C	3.2385654504	-4.9961617023	-1.7025184762
C	4.7266740448	-4.7569039531	-1.5295170094
C	0.4487599663	-6.5569261569	-0.2951095597
C	-0.4132999317	-6.8789139708	-1.5097538115
C	-1.4376509476	-5.7839847433	-1.7317622586
C	-2.2351299941	-5.5259076101	-0.4609666749
C	-1.3052714592	-5.2885159611	0.7331396162
C	-4.3926426414	-4.4028842376	-0.4877704259
C	-4.3718135093	-2.1486039385	0.3382758939
C	-5.2073872890	-1.6500187294	-0.8404257448
C	-4.9331678775	-2.5228362641	-2.0598217435
C	-5.1651598537	-3.9858168957	-1.7317167539
C	-5.8405647151	0.6581799950	-1.2079485969

C	-5.7963867079	1.4108462117	-2.5321493702
C	-4.5142904295	2.2121238821	-2.6615030656
C	-4.3499915498	3.1189657568	-1.4528701527
C	-4.4674342553	2.3123896398	-0.1539167981
C	-2.9536740306	5.1149784449	-1.4669885527
C	-2.3160450683	5.6818259866	-2.7328458755
C	-0.9062145902	5.1579062622	-2.8767885560
C	-0.1015765620	5.4937509219	-1.6366966565
C	-0.7971723633	5.0211400288	-0.3584205847
C	2.3245714919	5.4710804195	-1.5454843743
C	3.0992103816	3.6860078166	-0.1950955995
C	4.1965190019	3.3226698373	-1.1959641599
C	3.7399101946	3.6888017285	-2.6020388379
C	3.3052016570	5.1421625897	-2.6665034495
C	3.4377729270	3.3765439538	1.2424034330
C	-0.1224381850	5.5706513541	0.8959527229
C	-4.5454774020	3.1624924068	1.1118751002
C	-4.5964826373	-1.3946467795	1.6417304339
C	-1.9787709921	-5.2620703915	2.1067470070
C	2.5833847793	-4.9882392082	2.1120975505
C	4.1890508728	-0.7923167666	1.8229097962
H	3.6183193934	-0.0737633550	-0.1041078412
H	6.2152946007	-1.6834690293	0.0349371196
H	4.5698648423	-0.5617979621	-2.2743446712
H	7.3044421841	0.2697243622	-1.2498980592
H	6.3019363370	2.2844140575	-0.4130367168
H	6.0701757977	-3.7345269231	-0.1745611997
H	2.5483602396	-3.5436860774	0.5325532218
H	2.9542003723	-6.4862360558	-0.1783193606
H	2.7696022744	-4.0345550885	-1.9672077141
H	5.2066421478	-5.7153474859	-1.2801395881
H	1.0955668923	-7.4064607874	-0.0460885156
H	-0.9493937742	-7.8166989798	-1.3001906154
H	-0.8993721210	-4.8535353001	-1.9755551581
H	-2.8817519027	-6.3940774982	-0.2619894566
H	-0.7784734480	-4.3389099195	0.5710266278
H	-4.7114034055	-5.3998037133	-0.1594950996
H	-3.3075249391	-2.0857643518	0.0780451901
H	-6.2750432803	-1.6998235630	-0.5811194179
H	-3.8697276371	-2.3915402689	-2.3208040384
H	-6.2356392779	-4.1164724521	-1.5112687722
H	-6.8285106591	0.2081830256	-1.0592719339
H	-6.6373931303	2.1205616623	-2.5287703840
H	-3.6606640561	1.5148510862	-2.6771899171
H	-5.1389818589	3.8857219325	-1.4788134207
H	-3.6096614270	1.6292728958	-0.0740329787
H	-3.9338759052	5.5779059878	-1.2991262853
H	-2.2804636738	6.7770371863	-2.6304644824
H	-0.9518613259	4.0600010284	-2.9569682665
H	0.0655524572	6.5815427750	-1.6056426589
H	-0.7650338312	3.9252090408	-0.3382948310
H	2.1613614732	6.5542925347	-1.4887692961
H	2.1917877394	3.1255214574	-0.4554664166
H	5.1174326975	3.8759576274	-0.9583971112
H	2.8651185661	3.0579300305	-2.8333716200
H	4.1975735019	5.7673834398	-2.5124426549
H	3.2792277608	5.0962929703	-4.5836928818
H	5.1629597497	2.6494191050	-3.4270144621

H	3.9165711153	2.3937771244	1.2947648046
H	4.1317455437	4.1381247339	1.6243173856
H	0.5836092626	5.4746617896	-4.0812023215
H	-2.5790708325	5.5292306266	-4.6234096930
H	0.9094609528	5.8480547789	0.6639319190
H	-0.6584872002	6.4761678138	1.2042386215
H	0.7681468893	4.2067986267	1.9988752477
H	-3.9483332849	3.6139354704	-3.9045730022
H	-5.7077744406	1.0048211068	-4.4045288568
H	-5.2871439174	3.9637549433	0.9794270204
H	-4.9036491097	2.5135498293	1.9157972949
H	-2.9471353580	4.3131138294	0.8670864955
H	-5.4708211714	-1.8403775266	2.1429159257
H	-5.1657218433	-4.3986538468	-3.5979303901
H	-5.6720166646	-1.3042685671	-3.3955480203
H	-2.9980134701	-5.5860669621	-2.8874624691
H	-0.1820712314	-7.0636001600	-3.4033963106
H	-2.5581167485	-6.1880841707	2.2392922681
H	-1.1831645396	-5.2753456956	2.8578275479
H	-3.5641028559	-4.1388829161	1.7995593240
H	3.1704237391	-5.8776731186	2.3863727548
H	1.5296975189	-5.2797024498	2.0827817210
H	3.6499255076	-3.7745300609	3.1508973223
H	4.9182929843	-4.7432861716	-3.4376514560
H	2.1569240708	-6.1740987454	-2.8116934225
H	5.8676547959	-2.4458613768	-2.7864378886
H	6.7238760684	0.5011920606	-3.5277850740
H	5.0961531991	-0.7863138427	2.4356858016
H	3.7839356413	-1.8110249162	1.8142809417
H	2.4150966901	-0.0486755299	2.0418085714
H	2.3616623035	2.7652912007	2.7649707866
H	-3.1236799297	-2.2520360166	2.6078226403
H	-4.8463592671	-0.3562421775	1.4040298171
Cl	0.0255690006	1.2561401006	-1.0139280757
H	-3.6302720748	5.5304028007	4.6998286829
Cl	0.8167361362	-1.8165190618	-1.0467417125
C	0.0239839873	0.3244045904	0.4456992558
C	-2.6988055631	5.7193289203	4.1631412482
H	-2.9185753120	6.2375030478	3.2285669827
H	-0.5946575098	1.9902125275	1.6236117123
C	-0.3385203361	0.9353604998	1.6408523518
C	0.3778813512	-1.0302744454	0.4266873743
H	-1.1582290801	4.6133294139	3.3031320388
H	-2.0395070022	6.3331941393	4.7783417878
N	-2.0370173410	4.4361623704	3.8529486651
H	-2.6255285813	3.9455805349	3.1453203686
H	-2.3938870808	1.8721877090	2.9855701670
C	1.9815228225	3.7513829368	5.6869235172
C	-0.3817256518	0.2074562763	2.8334621664
C	0.3744129522	-1.7482745158	1.6197707245
C	0.6346823185	4.0715514286	5.6171996007
C	2.4067695977	2.5021564781	5.2347537087
H	2.6916531326	4.4583810376	6.1036883037
C	-0.2979136405	3.1676825134	5.0922027456
H	0.2910136430	5.0340233128	5.9912240841
C	-1.7549942988	3.5631268545	5.0654895968
C	1.4871584216	1.5982337870	4.7146717113
H	3.4551599827	2.2244371231	5.2934796176

C	0.1239389320	1.9149130542	4.6278815141
C	-2.2897430040	1.3808084840	3.9601772152
H	1.8406378927	0.6339398387	4.3597803162
C	-0.0084658629	-1.1352683768	2.8074092191
C	-0.8527187104	0.8626421581	4.1180111971
H	0.6798959184	-2.7874584695	1.6220121114
H	-1.9629152737	4.1994968925	5.9316235485
C	-2.6768138601	2.3518135320	5.0669193299
H	-3.7217777032	2.6699526890	4.9636023682
H	-2.9672195953	0.5229946501	3.9228070019
H	-0.0141344925	-1.7232102043	3.7203109337
H	-0.8695079065	0.0774375900	4.8867953051
H	-2.5928877858	1.8732046583	6.0493208434

B-CD:cis-(1S,4S)-SRT_2_MD E(Ha)= -5903.35360389

O	5.2117311967	1.5849302462	1.1989778014
O	4.8118913272	-1.8826646013	0.1466177656
O	5.0148797632	-3.6934396138	1.5737427953
O	2.0140854576	-5.1702424103	0.0868027654
O	0.4611663529	-6.3689682078	1.3031475005
O	-2.2739554976	-4.7809423078	-0.5432009478
O	-4.1498371222	-4.0582704650	0.6015107957
O	-5.7760479394	0.7293881870	-0.8191282761
O	-3.2649664733	3.1077573583	-2.0403699143
O	-2.7876381081	5.0162238246	-0.8404318214
O	0.7283581304	4.8309172374	-1.8695140745
O	2.1901530529	5.4408613333	-0.1860687037
O	2.4325734762	5.6114151768	-3.7932798361
O	4.6838965848	4.0236809647	-3.0931026020
O	4.3165668256	2.5062750060	-0.7271192112
O	-0.5793582830	5.3852442265	-4.3118791993
O	-3.2447209074	4.5371165785	-4.4109607832
O	-0.9585055135	4.6163533419	1.7388567584
O	-4.3151040086	1.8867423993	-4.4685596925
O	-5.3314683002	-0.6534906249	-4.1385200310
O	-3.9405199344	3.2410988856	0.9792036902
O	-3.8194080596	-5.7043357931	-2.6067151419
O	-5.0815801057	-3.3240940609	-3.3103460877
O	-1.0207928813	-6.5038267187	-2.5141662164
O	1.6890527379	-6.9152400092	-2.0623477537
O	-2.0634020902	-6.7654254057	2.5076553033
O	4.1520200528	-5.8851775091	3.0256363784
O	5.9679475065	-3.4163027396	-1.9105365822
O	4.0414756536	-5.3669016155	-2.0456846013
O	6.8156167623	-0.7918075838	-1.6942598599
O	6.5666621587	1.9561336122	-2.1324120621
O	3.0071570766	0.7588105010	2.8922117289
O	1.5349647685	3.6414217385	2.1152399037
O	-3.7895981923	-2.1191573565	2.5795955383
O	-4.5197579956	-1.0929144008	-1.5070422825
C	4.5299676484	0.3407699774	1.0488825445
C	5.4679054907	-0.6413212462	0.3462459954
C	5.8330008791	-0.0577094996	-1.0174387989
C	6.3932623320	1.3479956465	-0.8718864803
C	5.4893868540	2.2286303509	-0.0165100030
C	5.5249285518	-3.0568020816	0.4280067175
C	3.6448320654	-4.0911167879	1.4816532231
C	3.4137534998	-5.0252435838	0.2902495238
C	4.0032062570	-4.4487018900	-0.9857762514
C	5.4368302621	-4.0188462093	-0.7497336066
C	1.4187166834	-6.4237037201	0.2738742381
C	0.7388061421	-6.8742746184	-1.0165063103
C	-0.4116327773	-5.9534577571	-1.3750333415
C	-1.3657833775	-5.8188070672	-0.2017980639
C	-0.6093478228	-5.4512502131	1.0724841529
C	-3.6399305517	-4.9831972563	-0.3316324186
C	-3.9918962653	-2.6901948922	0.2280942159
C	-4.7554237652	-2.4258313259	-1.0679567326
C	-4.2899629651	-3.3843485064	-2.1533441097
C	-4.3740040432	-4.8184311354	-1.6583671211
C	-5.6267720279	-0.2909520183	-1.7829411747

C	-5.4795044353	0.3477276512	-3.1596070754
C	-4.3051041991	1.3097105993	-3.1909033556
C	-4.4585378126	2.3293439944	-2.0746709027
C	-4.6802210292	1.6299315326	-0.7291749865
C	-3.3602789662	4.4987065112	-2.0307114610
C	-2.6599324259	5.0883622652	-3.2520817791
C	-1.1794046036	4.7925818524	-3.1930991673
C	-0.5972901410	5.3186586573	-1.8953608658
C	-1.3672469032	4.7959571336	-0.6813066374
C	1.7768118715	5.6816626340	-1.5053934404
C	2.6219136263	4.0927920220	0.0353217243
C	3.8763673807	3.8483129143	-0.8060753356
C	3.5481726615	4.0847004401	-2.2757798125
C	2.9273464934	5.4553186720	-2.4804210380
C	2.8077276418	3.9042271353	1.5215782405
C	-0.9463527336	5.4831699409	0.6144399999
C	-5.0534415691	2.5743610809	0.4117335280
C	-4.5150325078	-1.8764107947	1.3949095779
C	-1.4752280302	-5.5034841624	2.3164461215
C	3.3343364921	-4.7629351643	2.8081642640
C	4.0588711554	-0.0722499827	2.4291371465
H	3.6452929312	0.4823246362	0.4077067398
H	6.3763145677	-0.7753174494	0.9516307490
H	4.8989513027	0.0016449241	-1.6008847600
H	7.3584854287	1.2676764493	-0.3484674423
H	6.0057658372	3.1581359929	0.2495828429
H	6.5714802169	-2.8254442433	0.6563935490
H	3.0121824803	-3.2021122505	1.3497533055
H	3.8753772946	-5.9981360266	0.5038447960
H	3.4181355037	-3.5541397143	-1.2506328618
H	6.0268640122	-4.9094371123	-0.4858509366
H	2.1626488064	-7.1597897529	0.5983486889
H	0.3329412124	-7.8808918128	-0.8376067980
H	0.0023980619	-4.9532757569	-1.5843728758
H	-1.9004135003	-6.7656005720	-0.0527396190
H	-0.2182781128	-4.4339766283	0.9454364280
H	-3.8249195654	-5.9712575769	0.1029699334
H	-2.9266595218	-2.4670394369	0.0801277442
H	-5.8301362989	-2.5811754895	-0.8918611527
H	-3.2346169011	-3.1544283109	-2.3722143794
H	-5.4342175272	-5.0589792711	-1.4872322018
H	-6.5528955962	-0.8737274758	-1.7317662390
H	-6.3960600280	0.9285670824	-3.3450009174
H	-3.3776032546	0.7427645485	-3.0080379548
H	-5.3214019201	2.9726270371	-2.3036812492
H	-3.7592207282	1.0947656917	-0.4565113599
H	-4.4096998274	4.8170169053	-2.0097679572
H	-2.8085283574	6.1787939258	-3.2315058949
H	-1.0505561497	3.6978790326	-3.1967797339
H	-0.6068972480	6.4192501757	-1.9179892823
H	-1.1735931362	3.7199848793	-0.6015146792
H	1.4524384556	6.7290914510	-1.5352189970
H	1.8466511182	3.3920705397	-0.2997145071
H	4.6753235610	4.5375059839	-0.4949760794
H	2.8026232628	3.3242696079	-2.5650655272
H	3.6976632936	6.2111170352	-2.2652220475
H	3.1449804044	5.3299937914	-4.3822694285
H	5.1825096624	3.2147261593	-2.8767633688

H	3.4706532596	3.0530383068	1.7049271247
H	3.2562321954	4.8126910495	1.9464268602
H	0.3860932797	5.2884178648	-4.2271268654
H	-2.6726830603	4.7981102373	-5.1463977039
H	0.0609963082	5.8916939531	0.4984599647
H	-1.6355564245	6.3155487748	0.7989546291
H	-0.0358535372	4.3038257587	1.8938821101
H	-3.7545867209	2.6826757020	-4.4707697109
H	-5.0541735482	-0.2031478791	-4.9477869906
H	-5.8177089050	3.2893772187	0.0751377403
H	-5.5006753660	1.9659942082	1.2028795325
H	-3.5446673700	3.8579103038	0.3308493152
H	-5.5867747431	-2.0904579731	1.5303866992
H	-4.2153887704	-5.4565053508	-3.4537107328
H	-5.0205275439	-2.4297235670	-3.6916986700
H	-1.8909293119	-6.0840162904	-2.6384943997
H	1.1782482720	-7.0393764627	-2.8742207228
H	-0.8613495692	-5.2041457920	3.1804549943
H	-2.2873524257	-4.7794586685	2.2070375609
H	-1.3383927025	-7.3997119991	2.5632678999
H	2.2992643155	-5.1182466720	2.8001660610
H	3.4384403933	-4.0197684785	3.6140255338
H	5.0626032789	-5.5703987575	2.9716981731
H	5.6629871010	-3.9566349199	-2.6528710691
H	3.1616798074	-5.7783699513	-2.1411757997
H	6.4600119749	-1.6763458748	-1.9065422582
H	7.0132855106	1.2954566029	-2.6797435308
H	4.8806625864	0.0421825075	3.1418821803
H	3.7655067961	-1.1293864332	2.4128827431
H	2.2537679116	0.6268020435	2.3040820474
H	1.6780861279	3.2707618946	2.9959222119
H	-3.9188369005	-3.0523684461	2.7873484597
H	-4.4124928928	-0.8147503375	1.1582042831
Cl	0.0764533256	1.2668942434	-1.0279577546
H	-3.4734020042	6.0462516513	4.2393792878
Cl	1.1890619949	-1.7020948224	-0.9116938889
C	-0.0552807375	0.3275200165	0.4186774204
C	-3.9473985219	5.3272708753	3.5697255570
H	-4.9011374031	5.0060605423	3.9921159343
H	-1.0084398389	1.9129877849	1.4830155021
C	-0.6630102699	0.8848073357	1.5394805034
C	0.4396405090	-0.9811767585	0.4635226100
H	-2.1598435106	4.4582518475	2.9565068298
H	-4.1216155743	5.7884344430	2.5967146119
N	-3.0655003705	4.1562532718	3.3904638321
H	-3.4753290868	3.5768543100	2.6246015985
H	-3.0416303691	1.5133004117	2.5812652552
C	0.7721682864	3.9903396471	5.6656646303
C	-0.8215535948	0.1413756064	2.7125919018
C	0.3081843022	-1.7130658729	1.6405428442
C	-0.5866759821	4.1487255424	5.4396483823
C	1.3827818320	2.7847107465	5.3168516102
H	1.3476245021	4.7884556257	6.1237646233
C	-1.3476550023	3.1257844574	4.8593026296
H	-1.0751905458	5.0757811574	5.7330200322
C	-2.8266912485	3.3476551740	4.6547329648
C	0.6318527700	1.7649334866	4.7435162071
H	2.4426513107	2.6287978956	5.4961107334

C	-0.7389044238	1.9175190265	4.4968957385
C	-2.9826619788	1.0786867004	3.5866704461
H	1.1306724170	0.8397912543	4.4700311165
C	-0.3309619821	-1.1632342798	2.7456092278
C	-1.5192419372	0.7454760440	3.9164526759
H	0.7057632852	-2.7210695270	1.6737231993
H	-3.2027114863	3.9742168816	5.4701134701
C	-3.6009945249	2.0374140106	4.5975181920
H	-4.6546887475	2.2291748963	4.3596858801
H	-3.5459349492	0.1416393537	3.5424286836
H	-0.4475773242	-1.7619293352	3.6439525251
H	-1.5290536769	-0.0249182283	4.6996354476
H	-3.5856736888	1.6004024201	5.6024692746

B-CD:cis-(1S,4S)-SRT_3_MD E(Ha)= -5903.35272501

O	5.3318070255	0.8755310932	0.8919238316
O	4.6120317147	-2.5958447810	0.0079686461
O	4.4434682607	-4.3094407655	1.5593232707
O	1.4301519820	-5.5695086285	-0.0926922707
O	-0.1697575616	-6.6540364778	1.1795772581
O	-2.7651888308	-4.5694126727	-0.3461608373
O	-4.3929044963	-3.6210433760	0.9910067622
O	-5.5530744270	1.3608062100	-0.2195701892
O	-3.0024331299	3.3138996857	-1.9860695009
O	-2.1603628771	5.2664591277	-1.0934323180
O	1.1948423216	4.4176997024	-2.3360521777
O	2.8174834526	4.9328804628	-0.7780268057
O	2.8848505966	4.7487792405	-4.3911388627
O	4.9691120233	2.9559550436	-3.6214041224
O	4.5455873752	1.7223830091	-1.1134173577
O	-0.2365426842	4.8426389637	-4.7339405663
O	-2.9779270752	4.4408458940	-4.5398195181
O	-0.1783552508	5.1147448006	1.3773741634
O	-4.6840364146	2.2401854018	-4.1194729012
O	-5.9875140165	-0.0956169978	-3.5080546022
O	-3.1388026568	3.7058355859	1.0596073633
O	-4.6162367241	-5.2766544713	-2.2195973657
O	-5.7151937497	-2.7887587530	-2.7854455413
O	-1.8931692826	-6.2545388762	-2.5244297352
O	0.7864423246	-7.0624131888	-2.2890322619
O	-2.6140932448	-6.8547108835	2.5298834918
O	2.5474092364	-3.8690302217	3.6246096926
O	5.6858042665	-4.3867327796	-1.8439879553
O	3.5243412020	-6.0942291883	-2.0212986384
O	6.7484778997	-1.8188619755	-1.8262117071
O	6.7681200214	0.8987406569	-2.4288456347
O	3.1558128192	0.3038148244	2.7159148759
O	1.9816087283	3.5619564782	1.6638187289
O	-5.7161263913	-1.5629395206	2.2688831643
O	-4.7106215586	-0.6254738185	-1.0776524684
C	4.5615856050	-0.3245004624	0.8328067890
C	5.3978605422	-1.4261008183	0.1770454239
C	5.8327034560	-0.9573697121	-1.2079258621
C	6.5206315376	0.3933401476	-1.1355625531
C	5.6813610836	1.4009320945	-0.3606374409
C	5.1280857588	-3.8259518553	0.4303213899
C	3.0441648969	-4.5264892973	1.3548035710
C	2.8070565133	-5.5453674434	0.2429157212
C	3.5499311861	-5.1188305917	-1.0136752651
C	5.0081566195	-4.8508920660	-0.6972370198
C	0.6973659038	-6.7461552349	0.0769818477
C	-0.1049759793	-6.9976179387	-1.1946802507
C	-1.1381851543	-5.9034709537	-1.3952153236
C	-1.9871925165	-5.7418270298	-0.1457671736
C	-1.1187904067	-5.5834361860	1.0998062166
C	-4.1155607228	-4.5970906156	0.0174981955
C	-4.1254790662	-2.2772304902	0.5850695212
C	-5.0247457425	-1.9295853337	-0.6016510028
C	-4.7997259200	-2.9227776049	-1.7309762973
C	-4.9700568693	-4.3434104124	-1.2202557962
C	-5.7375464064	0.3151125760	-1.1496182074

C	-5.7888563046	0.9172959575	-2.5495962841
C	-4.5126971971	1.6836986707	-2.8444872279
C	-4.2868859874	2.7309573683	-1.7658578680
C	-4.3485565227	2.0984587245	-0.3714170221
C	-2.8982371540	4.6914157926	-2.1613468482
C	-2.2271413501	5.0146264088	-3.4949867435
C	-0.8063273217	4.4990850371	-3.4999744101
C	-0.0411161153	5.1017564147	-2.3412715973
C	-0.7649570526	4.8958754399	-1.0072363604
C	2.3763896498	5.1232713190	-2.0966366582
C	3.0605734973	3.5564770563	-0.4591670435
C	4.2421314724	3.0903004949	-1.3080920861
C	3.8818171091	3.2299395962	-2.7822202291
C	3.4289415531	4.6467604030	-3.0929802189
C	3.2585740580	3.4643600213	1.0324190204
C	-0.1570965730	5.7447340828	0.1093790277
C	-4.3929655713	3.1100034816	0.7717272151
C	-4.3963180909	-1.4213296664	1.8084556353
C	-1.9106429078	-5.6442896014	2.3926997420
C	2.4909492938	-4.9365121341	2.7015620999
C	4.1211908767	-0.6240584683	2.2523016636
H	3.6678088481	-0.1638354871	0.2102335665
H	6.2832846467	-1.6369575682	0.7947649938
H	4.9140997953	-0.8443732399	-1.8075380923
H	7.4654601838	0.2611098618	-0.5866051058
H	6.2681704525	2.3028375813	-0.1507394999
H	6.1744956232	-3.7201427228	0.7387820039
H	2.5709577266	-3.5836644877	1.0509223366
H	3.1498700858	-6.5446778756	0.5497174530
H	3.0960878156	-4.1747072120	-1.3563203200
H	5.4654725534	-5.7845413815	-0.3367711337
H	1.3614721034	-7.5921414026	0.2898565139
H	-0.6326263625	-7.9554839650	-1.0746773279
H	-0.6010845999	-4.9540654365	-1.5554716132
H	-2.6348738145	-6.6200471498	-0.0276861973
H	-0.5942354782	-4.6199802338	1.0334817245
H	-4.3710515128	-5.5566065894	0.4804657182
H	-3.0721353418	-2.1761922284	0.2876403478
H	-6.0699818850	-1.9711009861	-0.2688552870
H	-3.7607226066	-2.8031807370	-2.0801914581
H	-6.0244190140	-4.4744349951	-0.9335132697
H	-6.6996242162	-0.1357742657	-0.8855188697
H	-6.6287502821	1.6281129308	-2.5674452648
H	-3.6664725037	0.9785054285	-2.8153145204
H	-5.0688473170	3.5002315022	-1.8554224305
H	-3.4730203907	1.4460987768	-0.2422334545
H	-3.8858706266	5.1661262369	-2.1147831557
H	-2.2073087059	6.1102942568	-3.5974486287
H	-0.8322201269	3.4069003989	-3.3576614233
H	0.1106065330	6.1743218033	-2.5385368652
H	-0.6885079149	3.8319069242	-0.7505075429
H	2.2114104600	6.2020262064	-2.2087033489
H	2.1815159087	2.9525544290	-0.7204704921
H	5.1217117747	3.7147479206	-1.0927141063
H	3.0351259328	2.5500857132	-2.9784276314
H	4.3029330194	5.3070532460	-2.9857242895
H	3.5320076693	4.3483798159	-4.9860944483
H	5.4043242562	2.1414277536	-3.3116129264

H	3.7147827823	2.5023927642	1.2868170594
H	3.9210397632	4.2775328125	1.3607457294
H	0.7106361700	4.6224102599	-4.7018975998
H	-2.4195016323	4.4934464076	-5.3282923356
H	0.8765108914	5.9956765733	-0.1393658191
H	-0.7315704426	6.6756318442	0.1729963437
H	0.6586954527	4.5985731669	1.4749595446
H	-3.9536269642	2.8559863397	-4.3089573567
H	-5.7974095498	0.3093149910	-4.3656487945
H	-5.1564890592	3.8738654494	0.5656852235
H	-4.7047365705	2.5699683514	1.6702162191
H	-2.8421139939	4.2465620645	0.3014761350
H	-4.2589783637	-0.3692912116	1.5414138877
H	-5.0797147170	-4.9869454987	-3.0177234775
H	-5.6684881634	-1.8810253233	-3.1367249724
H	-2.7335633175	-5.7615192283	-2.5032208814
H	0.2359089945	-7.0485516394	-3.0831467463
H	-1.2172157535	-5.4812598253	3.2327901755
H	-2.6486377273	-4.8369013753	2.4013415495
H	-1.9577289784	-7.5592691234	2.4702261740
H	3.0454243150	-5.8146268857	3.0661223600
H	1.4421655468	-5.2245440367	2.5966395326
H	3.4804036454	-3.6395889004	3.7094967880
H	5.3715234461	-4.9331500920	-2.5778047409
H	2.5948258431	-6.3043405543	-2.2265998360
H	6.3259650115	-2.6872429088	-1.9666864606
H	7.1512103194	0.1605311837	-2.9228901977
H	4.9863535429	-0.5332501011	2.9169566279
H	3.7500590467	-1.6550304086	2.3063290630
H	2.3182799782	0.0793624683	2.2940003436
H	2.0746025259	3.2641257262	2.5785124565
H	-5.8476628081	-2.5072111862	2.4199528600
H	-3.6591600548	-1.6794468603	2.5854024211
Cl	-0.4003673320	0.8973539721	-0.8092617016
H	-3.2662571955	6.4555060632	2.2386888332
Cl	0.5052252966	-2.0923592300	-0.2485112441
C	-0.3102917204	0.2843944576	0.8051123874
C	-3.0164758674	6.1875942972	3.2660418949
H	-2.5276021582	7.0287094941	3.7594337298
H	-0.9625815358	2.1326028840	1.6351041382
C	-0.6547341449	1.1166723696	1.8634828087
C	0.1080766023	-1.0299560204	1.0510237819
H	-1.2378927416	5.2620553016	2.6954089283
H	-3.9301380103	5.9283534625	3.8037976286
N	-2.1038012695	5.0261910071	3.2421740211
H	-2.5367499236	4.3126411048	2.6152578268
H	-2.6234929940	2.3080671174	3.0905340451
C	2.0035476033	4.6254859366	5.0108297822
C	-0.6091715538	0.6553526225	3.1819345653
C	0.1932652683	-1.4839019901	2.3660955003
C	0.6695779502	4.9856034062	4.8976928896
C	2.3573813305	3.2803035436	4.8899817583
H	2.7598046179	5.3798063853	5.2024013705
C	-0.3223481374	4.0245654303	4.6627515144
H	0.3840583264	6.0293430181	5.0118370300
C	-1.7647417652	4.4691142005	4.6088660674
C	1.3796602670	2.3215406295	4.6493380812
H	3.3948324668	2.9732285756	4.9823488495

C	0.0274613569	2.6747471537	4.5312368678
C	-2.4392376118	2.0953921658	4.1495578846
H	1.6788415324	1.2836707978	4.5326595961
C	-0.1720625123	-0.6481490321	3.4178284575
C	-1.0040824307	1.5721356453	4.3256007783
H	0.5687353510	-2.4812041534	2.5723374161
H	-1.8926241429	5.3121610977	5.2962896197
C	-2.7180760444	3.3417328751	4.9812715778
H	-3.7606237370	3.6611750277	4.8641041154
H	-3.1433583562	1.3004602847	4.4130555898
H	-0.1048032859	-1.0253420245	4.4344038359
H	-0.9826503486	0.9685874300	5.2435433163
H	-2.5778203971	3.1312037625	6.0474245463

B-CD:cis-(1S,4S)-SRT_4_MD E(Ha)= -5903.3524660022

Cl	-0.95099698	1.92929050	-0.42729351
Cl	0.33955233	-0.93489265	-0.86645567
O	-0.78244235	-4.65350078	-2.09927964
O	0.76138496	-4.80027486	1.62432664
O	-2.80862306	3.59507667	3.65339302
O	2.05994736	7.07236421	2.29024631
O	-1.58453510	6.86396364	-2.32997926
O	1.12726153	6.26187424	-2.66551751
O	5.24937420	3.26654777	-3.04095565
O	3.94222182	5.63607154	-2.44385395
O	5.67774100	2.22049952	2.03356374
O	3.64462956	-3.30644256	1.11193511
O	5.66048750	0.60180130	-3.79181490
O	4.60628806	-1.90468543	-4.23789841
O	0.63927083	-5.14094546	-4.48643404
O	3.33641061	-4.43032193	-4.39690632
O	-1.65274246	-3.63712454	1.88121912
O	-2.43701853	-5.23970815	-4.12801144
O	-4.68096127	-3.62898636	-3.41365741
O	-3.08151431	-0.64332164	2.77720487
O	-6.58988965	-1.63590614	-2.35182627
O	-6.82752718	1.09091941	-1.80247484
O	-1.99342847	5.35573775	-0.05822497
O	-4.16755334	5.68108558	-1.96588130
O	-6.14374133	3.77778524	-1.75218187
O	-4.84285554	3.81346482	1.63185819
O	-4.83951406	2.09706249	0.07607206
O	-5.25379968	-1.41228918	1.00098070
O	-4.35386436	-2.25908993	-0.95452706
O	-2.33778817	-5.27916505	-0.51217700
O	2.65832112	-5.03981806	-0.87918862
O	3.26668412	-3.09757442	-1.95920038
O	5.71101223	-0.81283287	-0.45783590
O	4.57906262	1.04488122	-1.26140418
O	4.03677335	4.01792431	0.79426629
O	2.25684512	4.74711775	-0.47628986
O	-0.45834172	6.63045105	1.10566073
N	2.76467697	-4.55529664	3.39375369
C	3.25362203	-2.65187168	4.93256599
C	1.28535625	-1.18523071	4.25669268
C	0.12026304	0.84118192	3.26889439
C	2.76075156	-1.54051975	4.01408676
C	0.41793901	-2.38781172	4.60856967
C	-0.96293026	-2.20426614	4.77234189
C	2.43632634	-3.92045911	4.73231236
C	0.95282756	-3.66052613	4.84403026
C	-1.79050903	-3.25515039	5.15161607
C	0.11166310	-4.71453996	5.22478116
C	-0.41080146	1.54860564	2.19426552
C	0.71087945	-0.40916536	3.08593476
C	-1.25293400	-4.52306745	5.37685661
C	-0.33802303	1.02278582	0.90524579
C	0.74505564	-0.94932672	1.79698672
C	3.68368312	-5.70911658	3.47368650
C	0.24082630	-0.23910251	0.71303421
C	1.42764678	5.81633710	2.25414015

C	4.37796094	1.86306155	1.64184860
C	4.81409313	-2.62573614	0.68781940
C	0.72404422	-5.55515201	0.42397502
C	-2.92365876	-3.78790346	1.24829810
C	-4.13548300	0.19135754	2.32573191
C	-2.94481887	4.66190234	2.73780477
C	-5.49348124	4.29777877	-0.61376276
C	-4.07674655	4.71237698	-0.95731133
C	-3.36016480	5.21266441	0.28591992
C	-3.48001493	4.18187854	1.40601415
C	-5.48480065	3.26169064	0.50940118
C	-4.57082088	-0.16154127	0.91614871
C	-5.49730986	0.85110987	0.23856136
C	-5.85395510	0.32582682	-1.15053350
C	-6.42194885	-1.08018913	-1.06675981
C	-5.52921840	-1.99915091	-0.24238477
C	-2.71559995	-3.92432598	-0.24040546
C	-3.93813247	-3.60240940	-1.09965065
C	-3.57213270	-3.76550126	-2.57032354
C	-2.98237825	-5.14154471	-2.83081102
C	-1.88236677	-5.46959050	-1.82631059
C	2.66451453	-4.99545682	-3.29515713
C	1.19716746	-4.63382236	-3.30603315
C	0.51853979	-5.20058987	-2.07544958
C	1.23813537	-4.78664987	-0.78905812
C	3.31493226	-4.48794582	-2.00990231
C	4.58045155	-1.67310338	-0.48208429
C	4.48175749	-2.35905015	-1.84833228
C	4.48503915	-1.32922100	-2.96626179
C	5.67888114	-0.40564773	-2.80775875
C	5.69196187	0.22141571	-1.41799006
C	4.43374249	4.76242261	-1.44954076
C	4.38874813	3.32500629	-1.93552470
C	4.78341634	2.37992408	-0.81191852
C	3.92114206	2.64281683	0.42157442
C	3.60987567	4.93900772	-0.17881545
C	-1.37603823	6.60399915	0.04066122
C	-0.65145596	6.89032684	-1.26929223
C	0.45829702	5.87893366	-1.49334740
C	1.36952771	5.83759080	-0.28019287
C	0.57437984	5.64334736	1.01053797
H	3.15441638	-2.35614244	5.98308132
H	1.24488238	-0.52225218	5.13233983
H	0.05841976	1.27671007	4.26239438
H	3.37037995	-0.64178375	4.14862630
H	4.31915476	-2.85113663	4.76505702
H	2.71578009	-4.67038786	5.47958875
H	-0.90383467	2.49948228	2.36773454
H	-1.40597526	-1.22925092	4.58749023
H	-2.85508483	-3.07835787	5.27514733
H	0.54127423	-5.69486115	5.42155818
H	-1.89063626	-5.34674167	5.68166597
H	2.90032142	-1.83672520	2.96777878
H	3.18270934	-3.87463691	2.72209076
H	3.92284628	-6.03779230	2.46126083
H	1.88890944	-4.82391989	2.87702302
H	1.16553028	-1.93374349	1.61417915
H	4.60187467	-5.41163172	3.98360943

H	3.20627959	-6.52221607	4.02241932
H	-0.30651219	-5.87195156	0.24311766
H	-0.13179881	-4.40255925	1.75543820
H	-3.69699211	3.25516448	3.80842057
H	1.35970889	7.73416263	2.25099756
H	0.79393213	5.65315726	3.13964400
H	2.21633189	5.05796866	2.25555350
H	-1.06314524	6.86207779	-3.14341143
H	2.02557509	5.88431073	-2.65308387
H	5.25834716	2.35749197	-3.39099945
H	4.38785862	5.37014771	-3.26010814
H	5.67115005	3.18053285	2.13182455
H	3.64640240	2.02252477	2.45072203
H	4.39378356	0.79682964	1.39710097
H	3.32307759	-3.90386582	0.40772050
H	5.15724648	-2.02135082	1.53220967
H	5.61930910	-3.33279324	0.44088339
H	5.45128814	0.16114682	-4.62609600
H	3.99697364	-2.66027608	-4.31446379
H	-0.32323661	-5.00215361	-4.45121300
H	2.78285717	-4.61388001	-5.16851686
H	1.34572188	-6.44955602	0.54845349
H	-1.78546210	-3.20382199	2.73351348
H	-3.44250071	-4.68002966	1.62554283
H	-3.53336383	-2.90220497	1.45209367
H	-3.11727540	-4.91641930	-4.73218208
H	-5.18387616	-2.83955023	-3.14355300
H	-2.27756014	-0.35330698	2.33096524
H	-4.97638455	0.03006285	3.00775455
H	-3.85271237	1.25043971	2.36745571
H	-7.02623162	-0.95088580	-2.87614374
H	-6.50320850	2.00574081	-1.90636402
H	-3.60631873	5.44941404	3.12911631
H	-1.95267515	5.09847512	2.59430554
H	-3.26752171	5.98257046	-2.19105600
H	-5.88766439	4.35378589	-2.48596845
H	-6.03705471	5.17764480	-0.23745227
H	-3.53670422	3.81717865	-1.30734559
H	-3.78930983	6.17780891	0.59422119
H	-2.91267912	3.29424093	1.09753875
H	-6.50920016	3.03857252	0.82980218
H	-3.67184206	-0.27382942	0.29068245
H	-6.41252593	0.97171064	0.83688938
H	-4.91471812	0.28562905	-1.72830315
H	-7.39033939	-1.01579478	-0.54686000
H	-6.05457350	-2.93534962	-0.01896686
H	-1.90153727	-3.24492354	-0.52637042
H	-4.75939151	-4.29046857	-0.84954292
H	-2.79780018	-3.01181590	-2.79511370
H	-3.78564476	-5.88077359	-2.68981376
H	-1.60471421	-6.52842609	-1.89999807
H	2.76258654	-6.09180477	-3.30922602
H	1.11251327	-3.53597969	-3.25819550
H	0.48116027	-6.29767573	-2.16239205
H	1.06986089	-3.71272522	-0.64249489
H	4.34988977	-4.84605468	-1.94630240
H	3.65571885	-1.10587129	-0.30284030
H	5.34329869	-3.03009633	-1.98616579

H	3.56452852	-0.72924989	-2.87583849
H	6.59344318	-1.01082985	-2.90185668
H	6.61915150	0.78122287	-1.25536216
H	5.47926684	5.00907491	-1.20980625
H	3.34928728	3.08958897	-2.21912190
H	5.83627063	2.53339761	-0.54067893
H	2.87409617	2.39915561	0.19272778
H	3.77164494	5.92868632	0.26262324
H	-2.11135207	7.38815904	0.25679774
H	-0.19754045	7.88917319	-1.18824628
H	-0.00027850	4.88241363	-1.60353757
H	1.92787636	6.78062708	-0.21591255
H	0.13185258	4.63736754	1.00132651

255

2-HP-B-CD:cis-(1S,4S)-SRT_1_Ci E(Ha)= -7253.89474094

Cl	-5.2672714305	-2.9789535023	6.3327795704
Cl	-3.2220799798	-0.5740278919	6.8497550889
O	1.1939478474	-5.5598907006	-3.2423391128
O	3.4306786619	-4.0257831486	-0.8080760633
O	5.7099669179	-3.8025961848	-1.2189248026
O	5.4429402992	-0.2378786478	-0.4625837768
O	6.5783409037	1.4336704688	-1.5792743430
O	3.8678219977	3.7970824714	-0.8780538253
O	3.4423176488	5.4926940082	-2.4081703733
O	-0.1680169630	5.1361817601	-1.9329508886
O	-1.6788949654	5.3593096883	-3.6692745948
O	-3.6735532232	2.6568497781	-2.2514935176
O	-5.2920495896	1.4774932442	-3.4164415052
O	-3.7546853103	-1.6710008943	-2.3442522402
O	-3.6189997669	-3.5075340243	-3.7514602810
O	-4.7998106751	-3.2564834882	-0.3159496336
O	-2.4477061682	-4.7311194721	0.0579706171
O	-0.5638150314	-4.6231664220	-2.0732089061
O	-4.5712344162	-0.5363514911	0.1531250584
O	-5.1093219735	2.1968767758	0.1592160626
O	-6.3165281193	-0.8754668573	-4.6579854970
O	-3.9047244074	4.6530871051	-0.2423189435
O	-1.7725584295	6.5657248466	-0.2663300838
O	-3.6985700118	4.6879289401	-5.3803390115
O	3.4204056472	5.4518734316	1.2065309840
O	0.6976738260	6.0835584898	0.6297526821
O	4.6834971634	3.1202082111	1.7347018645
O	6.2262425636	0.7820749861	1.9874699204
O	6.9300649834	3.8595829188	-2.8638022786
O	8.0550640910	-2.2803898868	-1.7477733758
O	3.9245045237	-4.0621276622	1.9672542088
O	4.7015198948	-1.3844025277	2.0296601032
O	2.0863607446	-5.9201820804	0.7886143782
O	-0.4884692094	-6.6683806965	-0.2168806783
O	3.8029045538	-5.9264425032	-3.9894192489
O	-2.2630946827	-5.6884743928	-4.9778004069
O	1.9311467706	6.9661901426	-4.2518985062
O	4.6063831017	-6.7720154641	1.7177222354
O	-3.2786590378	-7.3326780221	-0.4650980904
O	-7.1300469786	-1.5744738029	0.1215602222
O	-6.7104450056	4.4352149094	-0.3899317432
O	-0.5213864860	8.7219370097	1.0031340095
O	5.5344728453	5.5449529931	3.1103783305
O	7.2380366950	-1.6764393202	3.2201454871
N	2.3034565057	-0.5103096586	3.0446411395
C	2.7103761018	0.7279256440	3.7558532111
C	-3.2747199803	-2.7161863940	2.8779464082
C	-4.1517940116	-3.1091037333	3.8803320575
C	-4.1576497534	-2.4644790982	5.1154097292
C	-3.2646740666	-1.4125940935	5.3384893910
C	-2.3860279782	-1.0230330244	4.3307222719
C	-2.3808936430	-1.6644177428	3.0935656634
C	-0.9915659514	0.1588103303	1.9681704951
C	0.3370984319	0.6093619238	1.8810323278
C	0.5975761297	1.9840162059	1.7729588056
C	-0.4320521576	2.9129970273	1.7719970574

C	-1.7518770825	2.4636943892	1.8221196403
C	-2.0240056497	1.1047849742	1.9084484449
C	-1.3589041218	-1.3136748749	2.0266411719
C	-0.1342482224	-2.2236435051	2.1848115803
C	1.0408568408	-1.7503515322	1.3405918692
C	1.4905303532	-0.3557603946	1.7611958628
C	2.1704383140	-4.6394125848	-2.7565141376
C	2.6874611219	-5.0888259127	-1.3923344852
C	1.5607170792	-5.4251992790	-0.4212658566
C	0.6159037184	-6.4226543586	-1.0592219028
C	0.1226414385	-5.8168380222	-2.3805016226
C	4.7261101011	-4.2833608846	-0.3386384042
C	5.6476225506	-2.4054693466	-1.4869235148
C	5.7118531409	-1.6017179734	-0.1861855620
C	4.6562816552	-2.0925408987	0.7892220391
C	4.8605417047	-3.5804308661	1.0178540330
C	6.5155245621	0.6812435228	-0.4101923155
C	6.2831245814	1.5773912837	0.8133325316
C	4.9784188153	2.3260945816	0.6121975809
C	5.1060486722	3.1415560413	-0.6703427741
C	5.4315155038	2.2439343008	-1.8633809193
C	3.8697501430	5.1882281296	-1.1140143787
C	2.1062265959	5.0913552542	-2.7280399552
C	1.1154457002	5.7109059653	-1.7418406805
C	1.5206168920	5.4212767476	-0.3006353110
C	2.9608882937	5.8405729588	-0.0719458787
C	-1.2029888925	5.9200081760	-2.4803730051
C	-2.3237933759	6.0122292981	-1.4387085983
C	-2.8687398948	4.6194324616	-1.1976060326
C	-3.3415759821	4.0110005063	-2.5106697426
C	-2.2366620358	4.0462062295	-3.5650191716
C	-5.0177570567	2.2545200254	-2.2789170772
C	-5.2848636319	1.4295277388	-1.0178085364
C	-4.3601225336	0.2212716928	-1.0222906842
C	-4.6603849034	-0.5766935444	-2.2866801747
C	-4.5062691563	0.2922449705	-3.5361699652
C	-4.2813355678	-2.9417947988	-2.6549428609
C	-2.2173641215	-3.7109303189	-3.5742884644
C	-1.9592482400	-4.5617081131	-2.3302884916
C	-2.6337997033	-3.9533890652	-1.1059284186
C	-4.1170184534	-3.8275520714	-1.4132001745
C	-1.7282087947	-4.3942816246	-4.8396836669
C	-4.9934644175	-0.4145654780	-4.7888236924
C	-2.7665915665	3.7280675571	-4.9540708803
C	1.8620979993	5.5658585773	-4.1504005988
C	5.8057915848	3.0486113602	-3.0975680197
C	6.8214730867	-2.0847818137	-2.3962000142
C	3.2700015779	-4.6409030206	-3.8073086070
C	-6.1311541141	-3.7563088405	-0.1471457826
C	-6.2883137630	2.4519848776	0.9297674410
C	-2.5501120494	7.5513002618	0.4081291590
C	3.5075804505	6.4888109096	2.1843548078
C	7.4852613636	0.6679440398	2.6646838725
C	4.4735172465	-4.7850349581	3.0769188128
C	-0.9708606303	-8.0122316760	-0.2668428726
C	4.2009325164	-6.2857278924	2.9827369151
C	7.4035983340	-0.3816183398	3.7616569507
C	4.2157643134	5.9405702639	3.4141602221

C	-1.7013547746	8.1518981881	1.5205759740
C	-6.6540225146	3.9355061895	0.9322265246
C	-6.9335479324	-2.8229908934	0.7471728044
C	-2.3737620224	-8.0827890133	0.3163495858
C	4.9544641652	-7.0257168522	4.0731069551
C	-2.8585063847	-9.5206354391	0.3486686245
C	-8.2959345337	-3.4227947708	1.0439682239
C	-8.0023375721	4.1421304906	1.5967867007
C	-2.4717817729	9.2426307498	2.2396076795
C	4.2882273943	7.0010029294	4.4969012199
C	8.6802808181	-0.3838197202	4.5821682635
H	1.8228537878	1.2966703312	4.0286279067
H	3.3561151048	1.3311424986	3.1129916837
H	3.2626013799	0.4381666582	4.6512153395
H	-3.2879589545	-3.2427263116	1.9263506298
H	-4.8452178501	-3.9269579689	3.7152070670
H	-1.7163433201	-0.1913105514	4.5254920564
H	1.6244253401	2.3291649192	1.6692490535
H	-0.2040596583	3.9730325396	1.7028751523
H	-2.5696238996	3.1763884008	1.7668670955
H	-3.0532820612	0.7551465395	1.9024516901
H	-1.8200244190	-1.5526129921	1.0577028413
H	0.1382982914	-2.2698891053	3.2508382778
H	-0.4082707642	-3.2481347567	1.9154552609
H	1.8713158310	-2.4623459444	1.4011010819
H	0.7442060686	-1.6999961799	0.2866969461
H	2.2201258083	0.0466630547	1.0499313583
H	3.1801242263	-1.0221642914	2.7665460936
H	1.7728970421	-1.1040364711	3.6851080761
H	1.7306816189	-3.6366273899	-2.6620960489
H	3.3258968395	-5.9701029127	-1.5381021887
H	0.9931874306	-4.5022025456	-0.2328987352
H	1.1556497329	-7.3576829066	-1.2635965762
H	-0.5353561264	-6.5057973079	-2.9211878080
H	4.9147692375	-5.3540895123	-0.2279411110
H	4.7070959015	-2.1562552969	-1.9997550209
H	6.7086381933	-1.7202119421	0.2590993765
H	3.6723443349	-1.9399264727	0.3305349433
H	5.8803752068	-3.7536365517	1.3820132271
H	7.4688447364	0.1442828821	-0.3465628041
H	7.1027868866	2.3018208787	0.9053981759
H	4.1750110776	1.5869525042	0.4632874729
H	5.9153823489	3.8765764908	-0.5602371321
H	4.5630009009	1.6060869915	-2.0777416265
H	4.8880886684	5.5836360836	-1.0349934593
H	2.0203169381	3.9967343473	-2.6776303447
H	1.0828915297	6.7954229506	-1.9101933367
H	1.4514973781	4.3318234702	-0.1533768799
H	3.0414734006	6.9303077620	-0.1832237736
H	-0.8322261591	6.9166618040	-2.7417427914
H	-3.1129543575	6.6679775180	-1.8308856163
H	-2.0400826180	4.0007491899	-0.8222747943
H	-4.2123194116	4.5584080457	-2.8970749391
H	-1.4551915200	3.3277788198	-3.2811429117
H	-5.6967175183	3.1117607078	-2.3192379645
H	-6.3228425799	1.0781349975	-1.0713082940
H	-3.3187228338	0.5710464473	-1.0502220115
H	-5.6927411172	-0.9456014217	-2.2298349415

H	-3.4440058169	0.5522719875	-3.6532241401
H	-5.3310728115	-2.8553107836	-2.9562294207
H	-1.7080104873	-2.7439723757	-3.4556639945
H	-2.3604697595	-5.5710537388	-2.4892748654
H	-2.2241431820	-2.9447950650	-0.9445870731
H	-4.5197153576	-4.8280437716	-1.6245231527
H	-1.9718979415	-3.7541149159	-5.6996204697
H	-0.6410523446	-4.5030362342	-4.7909274607
H	-4.8803027110	0.2701443174	-5.6417331446
H	-4.3664428650	-1.2922559480	-4.9698165050
H	-1.9184768595	3.6421384771	-5.6499122935
H	-3.2861783982	2.7658739700	-4.9231798376
H	2.5808295297	5.0691282477	-4.8186276878
H	0.8535189940	5.2714095496	-4.4539946683
H	5.9681366413	2.3532860618	-3.9339858981
H	4.9773352756	3.7127016134	-3.3584970315
H	6.7719259796	-1.0298109405	-2.6822526356
H	6.7352556011	-2.6909402198	-3.3087964215
H	4.0891091937	-3.9992678791	-3.4701888019
H	2.8676875543	-4.2251510771	-4.7429308499
H	-6.0745098712	-4.7657135647	0.2830598308
H	-6.6356840719	-3.8151291825	-1.1209752642
H	-6.1030202580	2.1022364255	1.9521504333
H	-7.1242409530	1.8725080963	0.5212491189
H	-3.4622386307	7.0920232626	0.8088041098
H	-2.8272184567	8.3440172672	-0.3012369313
H	2.5009662354	6.8458139816	2.4310292280
H	4.0984102112	7.3222618999	1.7794502105
H	7.7391404424	1.6486592661	3.0868242078
H	8.2691799763	0.3703980480	1.9555772998
H	4.0236327164	-4.3769483137	3.9898966098
H	5.5550157523	-4.6109709729	3.1264719662
H	-0.2808443707	-8.6598751689	0.2913425418
H	-1.0152970312	-8.3574706997	-1.3092676415
H	3.1212050883	-6.4500040379	3.1131490588
H	6.5532911938	-0.1204234430	4.4142237626
H	3.6295125501	5.0824319098	3.7867022592
H	-1.4604495472	7.3460990535	2.2347993235
H	-5.8840258313	4.4805340481	1.4998496182
H	-6.3787256931	-2.6969105881	1.6916817135
H	-2.3326192177	-7.6879697896	1.3446784080
H	4.6943449113	-6.6522507875	5.0687088924
H	6.0334325332	-6.9130424476	3.9289125122
H	4.7182119565	-8.0909019087	4.0313702480
H	-2.2028236305	-10.1550054890	0.9519941953
H	-2.9043404304	-9.9263946906	-0.6667928114
H	-3.8649608836	-9.5576567128	0.7703523376
H	-8.2108862211	-4.3823099754	1.5622252887
H	-8.8566063739	-3.5736311104	0.1160279965
H	-8.8660399252	-2.7351887154	1.6719217651
H	-8.0188182138	3.7253522650	2.6087073552
H	-8.7880809434	3.6587448828	1.0080549295
H	-8.2319785591	5.2081263064	1.6554075476
H	-3.3989075405	8.8582770160	2.6744834050
H	-2.7180366839	10.0504293256	1.5436429875
H	-1.8570612946	9.6630646474	3.0382246023
H	3.2919326395	7.3419556736	4.7923884011
H	4.8637121972	7.8623294045	4.1442098367

H	4.7957499087	6.5958517807	5.3747667855
H	8.8541657294	0.5840230561	5.0600934123
H	9.5384202240	-0.6231041175	3.9468256591
H	8.6127012931	-1.1502429610	5.3567457610
H	-1.5888886154	-5.1956627790	-0.0126497480
H	-4.3801923936	-1.4737857119	-0.0495275024
H	-6.8721384065	-0.0975025916	-4.5289900921
H	-4.1559718839	3.7216616529	-0.0655254796
H	-3.2346529338	5.5338981346	-5.3831303694
H	-0.2276887923	6.0246246017	0.3072404570
H	4.0836363629	3.8431529385	1.4417296538
H	7.6677521063	3.2659239592	-2.6816506604
H	8.1276324456	-3.2235632128	-1.5595119664
H	5.1985175645	-0.5346385442	1.8924271071
H	2.5763837510	-5.1794101853	1.1924193081
H	3.0717454201	-6.4847995274	-4.2799845879
H	-3.2200416437	-5.5907418973	-5.0488039346
H	2.8307174952	7.2201336875	-4.0147662332
H	3.8011920056	-6.8582902080	1.1870547700
H	-3.1802572636	-6.4011215802	-0.2068225352
H	-6.3102524208	-1.0628591935	0.2373702917
H	-5.8329371435	4.8011859113	-0.5758511534
H	0.0881739543	7.9993468251	0.7973801087
H	5.4960873776	4.7015734931	2.6388401823
H	6.3074140635	-1.7810845800	2.9769252071

2-HP-B-CD:cis-(1S,4S)-SRT_2_Cl E(Ha)= -7253.88256506
Cl -3.0144868461 15.1637795360 2.5189849790
Cl -1.6131340963 13.1462855486 4.5643988688
O -3.7427851497 -6.7409691115 1.7297194834
O -4.6150247931 -3.3738761605 0.5662461000
O -5.3348206610 -1.8808146890 2.1733305540
O -4.0766386168 0.9454467249 0.2253229967
O -3.4622215383 2.8407936842 1.4012613924
O -0.3712102597 3.0253272240 -0.5413661648
O 1.3797503188 4.2252674018 0.3766341643
O 3.6393517324 1.4537433882 -0.4202801000
O 5.3394317787 0.9543433453 1.0679181635
O 4.9427653104 -2.6363486277 0.4662208958
O 5.1530249194 -4.1490253674 2.2019565422
O 2.5434834966 -6.2893899253 0.7865318714
O 1.2891187063 -7.6174515204 2.2132419123
O 2.4279237342 -8.1765258498 -1.1745153610
O -0.4473845092 -8.1155553712 -1.5040872405
O -1.7885980476 -6.6563814607 0.4898709879
O 4.5807061966 -6.4853071101 -1.1631321138
O 6.3733383946 -4.2258394163 -1.1961933357
O 4.4616841552 -6.1403084123 3.9453323295
O 5.9495431036 -1.6864769381 -2.0471430602
O 5.2626050068 1.0658884539 -2.5410286225
O 6.7723880419 -0.6227379512 2.8744396287
O 0.4510513393 3.8163503142 -3.1175626859
O 2.9123356678 2.3920594696 -3.0192647044
O -2.3271603881 3.5698354974 -2.4977534879
O -4.9218885329 2.5349754298 -1.9283342342
O -1.9496789818 4.6561152574 2.5194349560
O -5.2837900653 0.4445305072 3.6404227457
O -6.7285904472 -2.7871268550 -1.0627465591
O -6.1887848279 0.0017403328 -1.3832175493
O -4.7952311665 -4.8859902196 -1.8079533901
O -3.2010001252 -7.2555513895 -1.8344859647
O -5.8733021872 -5.5062568927 3.1358956988
O -0.8765502587 -8.4801809966 3.6099210317
O 3.8049350981 4.6769810445 1.4896744348
O -7.4679631364 -5.5632432528 -1.3862868910
O -2.5563024787 -9.9604362976 -1.3583538389
O 4.9769212040 -9.2992261815 -1.6913479827
O 8.5497559726 -2.9586880570 -2.4066316791
O 5.3701226405 3.2291052958 -4.3433903311
O -1.1555341390 6.1014972672 -2.7602916705
O -7.4453730244 2.4109822056 -0.7431806854
N -0.4692298313 6.9339881290 2.8758686004
C 0.5028487021 6.6543785027 3.9588815023
C -1.7876822528 12.1812441561 0.1645207132
C -2.3476521990 13.3662150494 0.6251935825
C -2.3112767798 13.6861059672 1.9800539247
C -1.6974122221 12.8010971418 2.8745993735
C -1.1386069504 11.6179094713 2.4027865606
C -1.1782856712 11.2900450547 1.0478237365
C 0.7414873934 9.6194908917 1.0983191391
C 1.1025354480 8.3187942506 1.4892739409
C 2.4314250515 8.0420599646 1.8438536805
C 3.3934637951 9.0413442686 1.8511155799

C	3.0334593859	10.3367313288	1.4858119304
C	1.7272646513	10.6132926250	1.1069517172
C	-0.6409614346	9.9594919830	0.5605973458
C	-1.6704823424	8.8502667466	0.8164877214
C	-1.0864705409	7.4653831102	0.5624990790
C	0.0984629105	7.1952622322	1.4815814846
C	-3.8430389330	-5.3202762857	1.8143718719
C	-4.6075050280	-4.7975322422	0.6005889250
C	-3.9834251160	-5.2570363829	-0.7123610890
C	-3.8479653135	-6.7704132529	-0.6782667762
C	-3.0796292216	-7.1948820802	0.5753330446
C	-5.7295178106	-2.7292386903	1.1220151864
C	-4.3993004044	-0.8697862216	1.8062767116
C	-5.0272186894	0.0049711746	0.7254466665
C	-5.5019944699	-0.8179559935	-0.4647388948
C	-6.4217654500	-1.9297683122	0.0103916394
C	-4.3167681143	2.3039669798	0.4006283101
C	-4.0605199757	3.0214689138	-0.9310144860
C	-2.6062934868	2.8368914043	-1.3280196200
C	-1.7131247442	3.3255910023	-0.1932906596
C	-2.0711400969	2.6825408103	1.1432856061
C	0.5171274450	4.0879711507	-0.7333396207
C	2.2097904820	3.0766314221	0.6279604848
C	3.0073627578	2.7019185371	-0.6241058757
C	2.1307104005	2.5738288736	-1.8713769421
C	1.3206056532	3.8495518113	-2.0092316882
C	5.0345624035	1.4258016360	-0.2120791704
C	5.6671214232	0.5498793481	-1.2931747988
C	5.2528541960	-0.9004390955	-1.1139640378
C	5.5232670703	-1.3503446626	0.3181605287
C	4.9135555131	-0.3881167422	1.3380724810
C	5.7212922803	-3.6740446009	1.0145365484
C	5.8370655894	-4.7937121752	-0.0246806912
C	4.4721588019	-5.4118849280	-0.2622691383
C	3.8693651748	-5.8628018121	1.0631463071
C	3.8492189658	-4.7270168532	2.0836405736
C	2.1651444368	-7.5983586630	1.1190421253
C	0.0608412095	-6.9121146147	2.0259229468
C	-0.6744920127	-7.4743763590	0.8117259147
C	0.2157323779	-7.4953431519	-0.4244826099
C	1.5057383860	-8.2309893906	-0.1118236637
C	-0.7028612466	-7.1162067611	3.3241085545
C	3.5106423805	-5.2145702439	3.4832837863
C	5.3730365666	-0.6835658271	2.7546666696
C	3.0940451266	3.4952775147	1.7880562056
C	-1.3931509967	3.3563599627	2.3236750821
C	-4.1165238850	-0.1142182994	3.0937493946
C	-4.5463728290	-5.0347874370	3.1293149904
C	2.5789371750	-9.3566653833	-1.9587958621
C	7.3541853977	-4.9944690295	-1.8877821464
C	6.2699918530	1.1280412257	-3.5497392875
C	0.5445677668	4.9141425531	-4.0247639570
C	-5.9642888172	3.4104163763	-2.3579605789
C	-8.0768184553	-3.2487728097	-1.0759277299
C	-3.8640258184	-8.3083666502	-2.5327851011
C	-8.1848096586	-4.4879436568	-1.9504272993
C	-7.3374437199	2.7986889174	-2.0996670831
C	-0.7457419450	5.7266262072	-4.0703990092

C	5.7177134953	1.9164874478	-4.7282682658
C	7.9725124517	-4.1164629152	-2.9665916664
C	3.9379411036	-9.3104900789	-2.6443717443
C	-2.9812070125	-9.5451335539	-2.6426224158
C	-9.6363204237	-4.9118698745	-2.0869413169
C	-3.7434380729	-10.6806067132	-3.3021974082
C	4.1279173709	-10.5312625180	-3.5253449262
C	9.0621211016	-4.8737637670	-3.7010042939
C	6.7530643489	2.0133377453	-5.8327737953
C	-0.5530151767	6.9760336665	-4.9076133838
C	-8.4332723582	3.7971275722	-2.4252461385
H	1.1461535832	7.5200853563	4.1073937446
H	1.1071208173	5.7925359271	3.6739310197
H	-0.0502154631	6.4299094953	4.8717882437
H	-1.8267979806	11.9528575990	-0.8972030836
H	-2.8179435333	14.0595924409	-0.0636150693
H	-0.6476478592	10.9607703057	3.1143365895
H	2.7229492734	7.0255621175	2.1012648025
H	4.4172913125	8.8087707310	2.1257446028
H	3.7755370817	11.1291292472	1.4814785304
H	1.4570227216	11.6212518079	0.8056375484
H	-0.5257008468	10.0355324330	-0.5306837354
H	-2.0491557198	8.9446731544	1.8461074478
H	-2.5439382749	9.0154684446	0.1793277788
H	-1.8461501878	6.6863587377	0.7015585654
H	-0.7498464611	7.3846566500	-0.4781242970
H	0.5916665780	6.2509030414	1.2261147460
H	-1.1114807787	6.1093881128	2.7859300553
H	-1.0384753895	7.7406722594	3.1396554136
H	-2.8399305227	-4.8699873074	1.8284532735
H	-5.6380849457	-5.1737614436	0.6372087871
H	-2.9842663481	-4.8096039027	-0.8131393050
H	-4.8567295757	-7.1983407327	-0.6056933902
H	-3.0512916238	-8.2875066176	0.6358371327
H	-6.4110343365	-3.4569237694	1.5750296715
H	-3.4748523134	-1.3254387122	1.4246096052
H	-5.8783777370	0.5366913238	1.1709319050
H	-4.6235312464	-1.2747340896	-0.9433739733
H	-7.3346059770	-1.4735465699	0.4190663770
H	-5.3401060378	2.4973328345	0.7355581878
H	-4.2430027023	4.0932852855	-0.7679981816
H	-2.4187776078	1.7669926342	-1.4916753055
H	-1.8404471794	4.4141072222	-0.1029543171
H	-1.7984528724	1.6189122520	1.1158971056
H	-0.0204231423	5.0365060515	-0.8304063172
H	1.5842840876	2.2212349621	0.9141118154
H	3.7596452981	3.4798103025	-0.8184271215
H	1.4414376726	1.7271632695	-1.7326586292
H	2.0222251975	4.6882411998	-2.1137003291
H	5.4435455166	2.4411573310	-0.2648087809
H	6.7590580980	0.6231718969	-1.1906681987
H	4.1678416011	-0.9688523948	-1.2899103799
H	6.6074931795	-1.3966417725	0.4846158550
H	3.8180188057	-0.4523171822	1.2782202509
H	6.7147721498	-3.3017822940	1.2856442634
H	6.5207432122	-5.5578849142	0.3712835183
H	3.8197478377	-4.6299668759	-0.6813804558
H	4.4599102012	-6.6917793305	1.4754224059

H	3.1268881139	-3.9654123293	1.7583386126
H	3.0371127881	-8.1868072151	1.4239468145
H	0.2600393357	-5.8432703386	1.8632766919
H	-1.0046666165	-8.4943292321	1.0523332969
H	0.4677478855	-6.4573511483	-0.6858280075
H	1.2742619826	-9.2770970238	0.1326165261
H	-0.1668953676	-6.5941082472	4.1320747941
H	-1.7004917880	-6.6798849671	3.2326088830
H	3.4287304200	-4.3438605596	4.1520069929
H	2.5448416415	-5.7271452162	3.4650905753
H	4.8726546669	0.0167391276	3.4412674079
H	5.0709632038	-1.6998261503	3.0224950679
H	2.4612060983	3.6243074228	2.6823574916
H	3.8210981193	2.7061979962	2.0019088045
H	-1.5286652986	2.7548806281	3.2303707996
H	-0.3269113743	3.4832296200	2.1239023146
H	-3.4334574360	0.7144930870	2.8890896088
H	-3.6248932695	-0.8034112489	3.7967700201
H	-4.5888870552	-3.9545833543	3.2937943607
H	-3.9536538393	-5.4814694150	3.9413041546
H	1.7586647831	-9.4230704296	-2.6845772141
H	2.5514436108	-10.2388989483	-1.3044344943
H	6.8903180418	-5.8893504749	-2.3196946107
H	8.1392428733	-5.3011340606	-1.1815110113
H	6.5601490220	0.1136287295	-3.8466362287
H	7.1494829842	1.6543389643	-3.1521207187
H	0.7757969079	4.5143186371	-5.0186777839
H	1.3711563195	5.5704516614	-3.7258756700
H	-5.8227269194	3.6137709069	-3.4261921696
H	-5.8958018520	4.3619901746	-1.8152997747
H	-8.7288864414	-2.4463181627	-1.4495958520
H	-8.3987792878	-3.5212593390	-0.0607071098
H	-4.1404764322	-7.9420185994	-3.5293765588
H	-4.7846760044	-8.5834008333	-2.0035271870
H	-7.7850136204	-4.2343443795	-2.9456748865
H	-7.4492353363	1.9157543643	-2.7462956928
H	-1.5314519549	5.1051129256	-4.5238072773
H	4.8327014313	1.3798273457	-5.1097040291
H	7.1759713877	-3.8448739485	-3.6798572166
H	3.9748005523	-8.4030491513	-3.2699077549
H	-2.1055331531	-9.2928256901	-3.2604149135
H	-10.2475323176	-4.1240809858	-2.5370494906
H	-10.0514418113	-5.1620058640	-1.1053350255
H	-9.6994294516	-5.8041571010	-2.7133332074
H	-4.1148451341	-10.3957714232	-4.2915997304
H	-4.5957850959	-10.9727239989	-2.6805923047
H	-3.0937389700	-11.5515510419	-3.4122624731
H	3.3498387036	-10.5991709045	-4.2911710015
H	4.1043714602	-11.4414210536	-2.9179011688
H	5.1014003192	-10.4816329118	-4.0176548650
H	8.6726987128	-5.7836504804	-4.1666224979
H	9.8621168757	-5.1485214690	-3.0065474528
H	9.4939050181	-4.2387854546	-4.4775782967
H	7.0579340583	1.0231951401	-6.1833540189
H	7.6391037652	2.5474872589	-5.4757079558
H	6.3400815674	2.5715256001	-6.6756103232
H	-0.2014926208	6.7295032069	-5.9139089516
H	0.1828612467	7.6371776024	-4.4383549910

H	-1.4950217153	7.5217711600	-4.9954679553
H	-8.3646750286	4.1464123570	-3.4602441964
H	-8.3652770802	4.6631609862	-1.7589565342
H	-9.4124489058	3.3364644639	-2.2793223320
H	-1.2587435314	-7.5967727783	-1.6733835480
H	3.6894197588	-6.8812145826	-1.2441025116
H	5.3135021696	-5.6877137721	3.9176967961
H	5.8054949658	-2.6254075589	-1.8125320106
H	7.0352376515	0.2653993561	2.6054820084
H	3.5547009623	1.6786688974	-2.8311065294
H	-1.4126398502	3.3530416562	-2.7643024635
H	-2.9109389980	4.5364605817	2.4688333385
H	-5.8947446152	-0.2903632423	3.7770477541
H	-5.5594007706	0.6794869893	-1.6917605907
H	-5.1047054387	-3.9786376581	-1.6425516124
H	-5.8300999965	-6.4546348465	2.9625707835
H	0.0087512494	-8.8619954394	3.6499329098
H	3.2121014953	5.2146371205	0.9494455666
H	-6.5308707843	-5.4538921530	-1.6253050866
H	-1.6790571702	-9.5686714270	-1.2270184877
H	5.0526546095	-8.4007822483	-1.3400497744
H	7.8281271796	-2.3563926493	-2.1745121661
H	4.5329390548	3.1843859574	-3.8603232513
H	-1.7696478050	5.4021159737	-2.4821594367
H	-7.2261135911	1.4650528035	-0.7281885858

255

2-HP-B-CD:cis-(1S,4S)-SRT_3_Ci E(Ha)= -7253.87702866

Cl	-1.39311379	1.44889153	-4.39426726
Cl	-0.06528581	-0.65581520	-2.38046644
O	-5.47723452	1.68415580	-1.38544290
O	-4.58739446	-1.14012482	0.76825685
O	-4.33261464	-3.14504367	-0.35170308
O	-1.28236064	-3.95206943	1.47581131
O	0.00349087	-5.58346338	0.46473277
O	3.01353744	-3.55822488	0.91777527
O	4.57785189	-3.55116678	-0.77955079
O	5.09442751	0.03693940	-0.26829631
O	5.59266335	1.35360714	-2.10620641
O	3.47845994	4.08118122	-0.88237484
O	2.45873276	5.45198713	-2.44716987
O	-0.64852882	5.49381774	-0.51878186
O	-2.61691837	5.95319086	-1.64980394
O	-1.66290268	6.66459824	1.79180477
O	-3.79843504	4.81242094	2.14353248
O	-4.22440202	3.07966035	-0.04331498
O	1.11444698	6.83379339	1.21075749
O	3.89768115	6.16879712	0.79277183
O	0.46937797	6.62973127	-3.87938823
O	5.50926141	3.98015368	1.09103878
O	6.81719613	1.42603965	1.29503376
O	5.27908000	3.32638607	-3.98950150
O	4.97367723	-3.60431368	2.82748464
O	6.09547945	-1.05660147	2.15958051
O	2.32136270	-4.18805589	3.60031559
O	-0.43777208	-4.76469200	3.98870125
O	1.92793275	-6.68619600	-0.99942010
O	-3.02196783	-5.03913768	-1.66616660
O	-5.54735128	-2.43670869	3.01685959
O	-3.18477680	-3.98120720	3.51757573
O	-6.22784268	0.37151335	2.43923373
O	-6.20322231	3.18660217	1.84576715
O	-6.11668311	-0.73050108	-2.54971368
O	-5.11111012	5.20630504	-2.76884671
O	6.13547715	-2.46316831	-2.76446895
O	-8.07295138	-1.69058339	2.06501612
O	-6.24093599	6.08998326	1.84149295
O	-0.51459998	9.12933985	1.10448508
O	6.63747496	6.63215440	1.32529453
O	8.84133563	-0.17818143	2.43499228
O	4.27224937	-6.16943017	3.87318998
O	-2.48790947	-6.65479340	4.03603942
N	-2.05758486	-7.17411829	-3.09515545
C	-1.19151397	-7.80666427	-2.06697635
C	-1.82461258	-2.03951704	-6.29356047
C	-1.86268915	-0.68910632	-5.97172486
C	-1.32911754	-0.23393445	-4.76727987
C	-0.74657771	-1.15527630	-3.89165314
C	-0.70891803	-2.50631262	-4.22536866
C	-1.25165977	-2.96946224	-5.42312197
C	-0.09812545	-5.24250162	-5.25705275
C	-0.21503791	-6.53080615	-4.70408991
C	0.94189870	-7.25955837	-4.39483297
C	2.20548841	-6.71863629	-4.57758256

C	2.32472955	-5.43880582	-5.11364591
C	1.18614990	-4.72254055	-5.45861491
C	-1.29869821	-4.45099332	-5.75063764
C	-2.63245412	-5.05007759	-5.28032148
C	-2.63207377	-6.56805301	-5.41686419
C	-1.55879837	-7.19752230	-4.53859364
C	-4.73239137	0.52713752	-1.00954335
C	-5.37501711	-0.07805329	0.23580011
C	-5.51250206	0.93810214	1.36480369
C	-6.22718858	2.17905016	0.86276769
C	-5.52134800	2.68775308	-0.40199125
C	-5.05112806	-2.44559845	0.65731644
C	-2.92643527	-3.17451553	-0.12553357
C	-2.66485569	-3.92575846	1.17336503
C	-3.38073664	-3.24518245	2.33597051
C	-4.86301963	-3.14234402	2.01512363
C	-0.68025179	-5.20269107	1.64022815
C	0.27383060	-5.13481746	2.83188538
C	1.40703157	-4.16792206	2.53537870
C	2.08269838	-4.57527348	1.22607014
C	1.07052007	-4.70254582	0.08835000
C	4.32547945	-3.91014751	0.55048764
C	4.45328468	-2.14932475	-1.05452049
C	5.36720484	-1.34722125	-0.12840184
C	5.15610833	-1.70014471	1.34287268
C	5.28311309	-3.20260378	1.51180010
C	6.05617437	0.85912896	-0.88026258
C	6.39249015	2.00204954	0.08282072
C	5.17721144	2.89247751	0.26650236
C	4.68261557	3.35967823	-1.09721917
C	4.42804659	2.18286331	-2.03662365
C	3.37404877	5.38548789	-1.38785658
C	2.95220017	6.31100338	-0.24031552
C	1.55040263	5.94496661	0.20883680
C	0.60378515	5.97204827	-0.98381502
C	1.11189481	5.09556837	-2.12598113
C	-1.76648554	6.33451115	-0.59725011
C	-3.09461972	4.61207838	-1.55341678
C	-3.86226135	4.44004829	-0.24521113
C	-3.02644605	4.84791920	0.96150966
C	-2.50983806	6.25958529	0.74016336
C	-3.96290704	4.39333732	-2.77992543
C	0.33509246	5.31201547	-3.41515507
C	4.17706902	2.62794729	-3.46794139
C	4.83101836	-2.00219886	-2.51844280
C	1.63750730	-5.31631536	-1.17928288
C	-2.33835206	-3.82346503	-1.35896046
C	-4.79377444	-0.38683501	-2.22068984
C	-2.02806167	7.85652319	2.48579814
C	4.33786107	7.36650041	1.42604046
C	7.96239224	2.01091726	1.91018691
C	5.92808005	-4.47621739	3.43039717
C	-0.49012291	-5.72979375	5.03879576
C	-6.73024725	-3.04651702	3.53085336
C	-7.39361816	3.97012646	1.89859434
C	-7.92184854	-2.10421592	3.40858603
C	-1.91632015	-6.22762327	5.26208558
C	5.24523136	-5.34291128	4.47752557

C	8.46295248	1.06090270	2.98959785
C	5.61538094	7.05882420	2.19558592
C	-0.89468245	8.87659428	2.44203203
C	-7.11568099	5.28955427	2.60295774
C	-9.19473376	-2.79448116	3.86501201
C	-8.40711484	6.06360258	2.80159466
C	-1.33180299	10.18143743	3.08319415
C	6.10901306	8.29771269	2.92002013
C	9.67487478	1.64767714	3.68966263
C	6.26111100	-6.23046675	5.17388633
C	-1.92803935	-7.38196905	6.24696059
H	-0.20876223	-7.33532684	-2.06783081
H	-1.09319830	-8.87114191	-2.28561922
H	-1.66407786	-7.65991463	-1.09549598
H	-2.24533727	-2.36880659	-7.24010906
H	-2.30379113	0.02936076	-6.65435354
H	-0.22333781	-3.19454347	-3.54136696
H	0.85144637	-8.27569743	-4.01931385
H	3.08651042	-7.29570980	-4.31781987
H	3.30618181	-5.00550898	-5.28202193
H	1.28907041	-3.73597929	-5.90161337
H	-1.28284411	-4.53461892	-6.84807320
H	-2.82285741	-4.75421928	-4.24009713
H	-3.44992896	-4.61875135	-5.86567287
H	-3.61954180	-6.98870516	-5.18609187
H	-2.41543065	-6.85176327	-6.45297928
H	-1.45906948	-8.26597667	-4.76102194
H	-2.95396444	-7.66630159	-3.09539495
H	-2.30506245	-6.21306493	-2.76249523
H	-3.68963685	0.79901257	-0.79551733
H	-6.36847751	-0.45372347	-0.04329207
H	-4.50371675	1.23090848	1.69089733
H	-7.26269121	1.90912379	0.60998927
H	-6.06696764	3.52248663	-0.85513726
H	-6.10390616	-2.47588883	0.36007120
H	-2.52667039	-2.15478660	-0.04312015
H	-3.04803338	-4.95132269	1.06656365
H	-2.97721593	-2.22820674	2.44747690
H	-5.26524987	-4.16137712	1.92465937
H	-1.42697241	-5.98117941	1.82874306
H	0.70239111	-6.13835429	2.95914878
H	0.98577264	-3.15932215	2.40800090
H	2.59815294	-5.53530982	1.37597191
H	0.67827779	-3.69886701	-0.12765671
H	4.46019802	-4.99662620	0.60603713
H	3.41436530	-1.82726132	-0.89898889
H	6.41046230	-1.56061300	-0.39908436
H	4.13349384	-1.40245606	1.62246155
H	6.31124039	-3.49237174	1.25738329
H	6.95848141	0.28308352	-1.11233607
H	7.20724521	2.59231895	-0.35981289
H	4.38256371	2.28934364	0.73272244
H	5.43943837	4.01059339	-1.55563039
H	3.57236608	1.60207329	-1.66393067
H	4.33287961	5.71432932	-1.80280730
H	2.95681227	7.34371070	-0.61698717
H	1.58047845	4.91791307	0.60203849
H	0.50626472	6.99997486	-1.35973426

H	1.06107133	4.04030288	-1.82172515
H	-1.47058297	7.36988672	-0.79596718
H	-2.25119448	3.90622402	-1.56900405
H	-4.76378471	5.06628356	-0.27251413
H	-2.16769313	4.16668671	1.05068581
H	-3.37300426	6.93484631	0.67153359
H	-3.34680957	4.57107133	-3.67466600
H	-4.30533948	3.35491421	-2.80245950
H	0.67685522	4.57682383	-4.16089045
H	-0.72912303	5.14603085	-3.22639896
H	3.92967136	1.74209849	-4.07359177
H	3.32320950	3.31069009	-3.49021451
H	4.08545933	-2.54071409	-3.12639850
H	4.80195115	-0.94491432	-2.79637753
H	0.90597331	-5.17927969	-1.99410809
H	2.55743304	-4.79807342	-1.46651559
H	-1.29175327	-4.07687001	-1.18413716
H	-2.40867447	-3.13036857	-2.20514151
H	-4.26884261	-1.31962583	-1.99956143
H	-4.27963581	0.11370918	-3.05557990
H	-2.27832685	7.59406918	3.52120716
H	-2.91728041	8.29925421	2.02044880
H	3.55010673	7.74677047	2.08821299
H	4.56235590	8.12478541	0.66231543
H	7.69990745	2.99099353	2.32677269
H	8.75487358	2.13947257	1.15899087
H	6.73639815	-3.87812254	3.87175553
H	6.35687840	-5.14398058	2.67007417
H	-0.09785327	-5.26188250	5.94891494
H	0.15640561	-6.58090160	4.79175429
H	-6.55413600	-3.32147852	4.57828763
H	-6.95188553	-3.96226984	2.96739010
H	-8.17425625	3.40089614	2.42335263
H	-7.74665537	4.19778403	0.88247650
H	-7.73577525	-1.22894666	4.04947268
H	-2.51087970	-5.39756842	5.67216564
H	4.77670685	-4.67772569	5.22082081
H	7.65130305	0.92500430	3.72412087
H	5.38360058	6.27478045	2.93637489
H	-0.03977582	8.46751618	3.00305348
H	-6.67588540	5.05986281	3.58739584
H	-9.10835542	-3.16168005	4.89247138
H	-9.42112612	-3.64130822	3.20895493
H	-10.03399339	-2.09745312	3.81517113
H	-9.12560453	5.50346206	3.40719720
H	-8.86510175	6.29270178	1.83386876
H	-8.19121598	7.01031517	3.30138462
H	-1.67134001	10.03018917	4.11269061
H	-2.14945850	10.62727584	2.50786764
H	-0.50060690	10.88996423	3.09096373
H	5.36142129	8.67663243	3.62302259
H	6.34712508	9.08674168	2.19965660
H	7.02122439	8.06123346	3.47206899
H	9.44493148	2.61350319	4.14884462
H	10.49388231	1.78345706	2.97622783
H	10.01748147	0.96198400	4.46768769
H	7.04167369	-5.64162597	5.66443604
H	6.73259931	-6.90554002	4.45231477

H	5.75949402	-6.84204315	5.92697136
H	-1.45466216	-7.10459536	7.19398491
H	-1.39151057	-8.23986511	5.82909596
H	-2.95530843	-7.69180923	6.45091587
H	-4.34618811	4.00835968	2.10904935
H	0.22488425	6.53831564	1.48906508
H	1.41651955	6.78487454	-3.97613095
H	4.74316004	4.58740886	1.09039912
H	6.03695690	2.73565357	-3.90632781
H	6.09100122	-0.10890158	1.91764301
H	3.12061348	-3.69883684	3.32184840
H	1.30749489	-6.99763010	-0.32719969
H	-3.96439964	-4.82806583	-1.57890387
H	-2.22651750	-3.96847866	3.70473756
H	-5.73294482	-0.41638319	2.72780947
H	-6.58679039	0.10268845	-2.67580749
H	-4.80391159	6.11937613	-2.72166024
H	6.17536084	-3.36060521	-2.41328340
H	-7.62246640	-0.83301308	2.00348627
H	-5.33373679	5.78254121	2.01200570
H	0.20889956	8.51531760	0.90856919
H	6.45479841	5.71564964	1.07431106
H	8.03523843	-0.68012129	2.24944156
H	3.45639773	-5.64739912	3.81911124
H	-3.00077645	-5.89996507	3.71036694

2-HP-B-CD:cis-(1S,4S)-SRT_4_Cl E(Ha)= -7253.8770286598

Cl	-1.39311379	1.44889153	-4.39426726
Cl	-0.06528581	-0.65581520	-2.38046644
O	-5.47723452	1.68415580	-1.38544290
O	-4.58739446	-1.14012482	0.76825685
O	-4.33261464	-3.14504367	-0.35170308
O	-1.28236064	-3.95206943	1.47581131
O	0.00349087	-5.58346338	0.46473277
O	3.01353744	-3.55822488	0.91777527
O	4.57785189	-3.55116678	-0.77955079
O	5.09442751	0.03693940	-0.26829631
O	5.59266335	1.35360714	-2.10620641
O	3.47845994	4.08118122	-0.88237484
O	2.45873276	5.45198713	-2.44716987
O	-0.64852882	5.49381774	-0.51878186
O	-2.61691837	5.95319086	-1.64980394
O	-1.66290268	6.66459824	1.79180477
O	-3.79843504	4.81242094	2.14353248
O	-4.22440202	3.07966035	-0.04331498
O	1.11444698	6.83379339	1.21075749
O	3.89768115	6.16879712	0.79277183
O	0.46937797	6.62973127	-3.87938823
O	5.50926141	3.98015368	1.09103878
O	6.81719613	1.42603965	1.29503376
O	5.27908000	3.32638607	-3.98950150
O	4.97367723	-3.60431368	2.82748464
O	6.09547945	-1.05660147	2.15958051
O	2.32136270	-4.18805589	3.60031559
O	-0.43777208	-4.76469200	3.98870125
O	1.92793275	-6.68619600	-0.99942010
O	-3.02196783	-5.03913768	-1.66616660
O	-5.54735128	-2.43670869	3.01685959
O	-3.18477680	-3.98120720	3.51757573
O	-6.22784268	0.37151335	2.43923373
O	-6.20322231	3.18660217	1.84576715
O	-6.11668311	-0.73050108	-2.54971368
O	-5.11111012	5.20630504	-2.76884671
O	6.13547715	-2.46316831	-2.76446895
O	-8.07295138	-1.69058339	2.06501612
O	-6.24093599	6.08998326	1.84149295
O	-0.51459998	9.12933985	1.10448508
O	6.63747496	6.63215440	1.32529453
O	8.84133563	-0.17818143	2.43499228
O	4.27224937	-6.16943017	3.87318998
O	-2.48790947	-6.65479340	4.03603942
N	-2.05758486	-7.17411829	-3.09515545
C	-1.19151397	-7.80666427	-2.06697635
C	-1.82461258	-2.03951704	-6.29356047
C	-1.86268915	-0.68910632	-5.97172486
C	-1.32911754	-0.23393445	-4.76727987
C	-0.74657771	-1.15527630	-3.89165314
C	-0.70891803	-2.50631262	-4.22536866
C	-1.25165977	-2.96946224	-5.42312197
C	-0.09812545	-5.24250162	-5.25705275
C	-0.21503791	-6.53080615	-4.70408991
C	0.94189870	-7.25955837	-4.39483297
C	2.20548841	-6.71863629	-4.57758256

C	2.32472955	-5.43880582	-5.11364591
C	1.18614990	-4.72254055	-5.45861491
C	-1.29869821	-4.45099332	-5.75063764
C	-2.63245412	-5.05007759	-5.28032148
C	-2.63207377	-6.56805301	-5.41686419
C	-1.55879837	-7.19752230	-4.53859364
C	-4.73239137	0.52713752	-1.00954335
C	-5.37501711	-0.07805329	0.23580011
C	-5.51250206	0.93810214	1.36480369
C	-6.22718858	2.17905016	0.86276769
C	-5.52134800	2.68775308	-0.40199125
C	-5.05112806	-2.44559845	0.65731644
C	-2.92643527	-3.17451553	-0.12553357
C	-2.66485569	-3.92575846	1.17336503
C	-3.38073664	-3.24518245	2.33597051
C	-4.86301963	-3.14234402	2.01512363
C	-0.68025179	-5.20269107	1.64022815
C	0.27383060	-5.13481746	2.83188538
C	1.40703157	-4.16792206	2.53537870
C	2.08269838	-4.57527348	1.22607014
C	1.07052007	-4.70254582	0.08835000
C	4.32547945	-3.91014751	0.55048764
C	4.45328468	-2.14932475	-1.05452049
C	5.36720484	-1.34722125	-0.12840184
C	5.15610833	-1.70014471	1.34287268
C	5.28311309	-3.20260378	1.51180010
C	6.05617437	0.85912896	-0.88026258
C	6.39249015	2.00204954	0.08282072
C	5.17721144	2.89247751	0.26650236
C	4.68261557	3.35967823	-1.09721917
C	4.42804659	2.18286331	-2.03662365
C	3.37404877	5.38548789	-1.38785658
C	2.95220017	6.31100338	-0.24031552
C	1.55040263	5.94496661	0.20883680
C	0.60378515	5.97204827	-0.98381502
C	1.11189481	5.09556837	-2.12598113
C	-1.76648554	6.33451115	-0.59725011
C	-3.09461972	4.61207838	-1.55341678
C	-3.86226135	4.44004829	-0.24521113
C	-3.02644605	4.84791920	0.96150966
C	-2.50983806	6.25958529	0.74016336
C	-3.96290704	4.39333732	-2.77992543
C	0.33509246	5.31201547	-3.41515507
C	4.17706902	2.62794729	-3.46794139
C	4.83101836	-2.00219886	-2.51844280
C	1.63750730	-5.31631536	-1.17928288
C	-2.33835206	-3.82346503	-1.35896046
C	-4.79377444	-0.38683501	-2.22068984
C	-2.02806167	7.85652319	2.48579814
C	4.33786107	7.36650041	1.42604046
C	7.96239224	2.01091726	1.91018691
C	5.92808005	-4.47621739	3.43039717
C	-0.49012291	-5.72979375	5.03879576
C	-6.73024725	-3.04651702	3.53085336
C	-7.39361816	3.97012646	1.89859434
C	-7.92184854	-2.10421592	3.40858603
C	-1.91632015	-6.22762327	5.26208558
C	5.24523136	-5.34291128	4.47752557

C	8.46295248	1.06090270	2.98959785
C	5.61538094	7.05882420	2.19558592
C	-0.89468245	8.87659428	2.44203203
C	-7.11568099	5.28955427	2.60295774
C	-9.19473376	-2.79448116	3.86501201
C	-8.40711484	6.06360258	2.80159466
C	-1.33180299	10.18143743	3.08319415
C	6.10901306	8.29771269	2.92002013
C	9.67487478	1.64767714	3.68966263
C	6.26111100	-6.23046675	5.17388633
C	-1.92803935	-7.38196905	6.24696059
H	-0.20876223	-7.33532684	-2.06783081
H	-1.09319830	-8.87114191	-2.28561922
H	-1.66407786	-7.65991463	-1.09549598
H	-2.24533727	-2.36880659	-7.24010906
H	-2.30379113	0.02936076	-6.65435354
H	-0.22333781	-3.19454347	-3.54136696
H	0.85144637	-8.27569743	-4.01931385
H	3.08651042	-7.29570980	-4.31781987
H	3.30618181	-5.00550898	-5.28202193
H	1.28907041	-3.73597929	-5.90161337
H	-1.28284411	-4.53461892	-6.84807320
H	-2.82285741	-4.75421928	-4.24009713
H	-3.44992896	-4.61875135	-5.86567287
H	-3.61954180	-6.98870516	-5.18609187
H	-2.41543065	-6.85176327	-6.45297928
H	-1.45906948	-8.26597667	-4.76102194
H	-2.95396444	-7.66630159	-3.09539495
H	-2.30506245	-6.21306493	-2.76249523
H	-3.68963685	0.79901257	-0.79551733
H	-6.36847751	-0.45372347	-0.04329207
H	-4.50371675	1.23090848	1.69089733
H	-7.26269121	1.90912379	0.60998927
H	-6.06696764	3.52248663	-0.85513726
H	-6.10390616	-2.47588883	0.36007120
H	-2.52667039	-2.15478660	-0.04312015
H	-3.04803338	-4.95132269	1.06656365
H	-2.97721593	-2.22820674	2.44747690
H	-5.26524987	-4.16137712	1.92465937
H	-1.42697241	-5.98117941	1.82874306
H	0.70239111	-6.13835429	2.95914878
H	0.98577264	-3.15932215	2.40800090
H	2.59815294	-5.53530982	1.37597191
H	0.67827779	-3.69886701	-0.12765671
H	4.46019802	-4.99662620	0.60603713
H	3.41436530	-1.82726132	-0.89898889
H	6.41046230	-1.56061300	-0.39908436
H	4.13349384	-1.40245606	1.62246155
H	6.31124039	-3.49237174	1.25738329
H	6.95848141	0.28308352	-1.11233607
H	7.20724521	2.59231895	-0.35981289
H	4.38256371	2.28934364	0.73272244
H	5.43943837	4.01059339	-1.55563039
H	3.57236608	1.60207329	-1.66393067
H	4.33287961	5.71432932	-1.80280730
H	2.95681227	7.34371070	-0.61698717
H	1.58047845	4.91791307	0.60203849
H	0.50626472	6.99997486	-1.35973426

H	1.06107133	4.04030288	-1.82172515
H	-1.47058297	7.36988672	-0.79596718
H	-2.25119448	3.90622402	-1.56900405
H	-4.76378471	5.06628356	-0.27251413
H	-2.16769313	4.16668671	1.05068581
H	-3.37300426	6.93484631	0.67153359
H	-3.34680957	4.57107133	-3.67466600
H	-4.30533948	3.35491421	-2.80245950
H	0.67685522	4.57682383	-4.16089045
H	-0.72912303	5.14603085	-3.22639896
H	3.92967136	1.74209849	-4.07359177
H	3.32320950	3.31069009	-3.49021451
H	4.08545933	-2.54071409	-3.12639850
H	4.80195115	-0.94491432	-2.79637753
H	0.90597331	-5.17927969	-1.99410809
H	2.55743304	-4.79807342	-1.46651559
H	-1.29175327	-4.07687001	-1.18413716
H	-2.40867447	-3.13036857	-2.20514151
H	-4.26884261	-1.31962583	-1.99956143
H	-4.27963581	0.11370918	-3.05557990
H	-2.27832685	7.59406918	3.52120716
H	-2.91728041	8.29925421	2.02044880
H	3.55010673	7.74677047	2.08821299
H	4.56235590	8.12478541	0.66231543
H	7.69990745	2.99099353	2.32677269
H	8.75487358	2.13947257	1.15899087
H	6.73639815	-3.87812254	3.87175553
H	6.35687840	-5.14398058	2.67007417
H	-0.09785327	-5.26188250	5.94891494
H	0.15640561	-6.58090160	4.79175429
H	-6.55413600	-3.32147852	4.57828763
H	-6.95188553	-3.96226984	2.96739010
H	-8.17425625	3.40089614	2.42335263
H	-7.74665537	4.19778403	0.88247650
H	-7.73577525	-1.22894666	4.04947268
H	-2.51087970	-5.39756842	5.67216564
H	4.77670685	-4.67772569	5.22082081
H	7.65130305	0.92500430	3.72412087
H	5.38360058	6.27478045	2.93637489
H	-0.03977582	8.46751618	3.00305348
H	-6.67588540	5.05986281	3.58739584
H	-9.10835542	-3.16168005	4.89247138
H	-9.42112612	-3.64130822	3.20895493
H	-10.03399339	-2.09745312	3.81517113
H	-9.12560453	5.50346206	3.40719720
H	-8.86510175	6.29270178	1.83386876
H	-8.19121598	7.01031517	3.30138462
H	-1.67134001	10.03018917	4.11269061
H	-2.14945850	10.62727584	2.50786764
H	-0.50060690	10.88996423	3.09096373
H	5.36142129	8.67663243	3.62302259
H	6.34712508	9.08674168	2.19965660
H	7.02122439	8.06123346	3.47206899
H	9.44493148	2.61350319	4.14884462
H	10.49388231	1.78345706	2.97622783
H	10.01748147	0.96198400	4.46768769
H	7.04167369	-5.64162597	5.66443604
H	6.73259931	-6.90554002	4.45231477

H	5.75949402	-6.84204315	5.92697136
H	-1.45466216	-7.10459536	7.19398491
H	-1.39151057	-8.23986511	5.82909596
H	-2.95530843	-7.69180923	6.45091587
H	-4.34618811	4.00835968	2.10904935
H	0.22488425	6.53831564	1.48906508
H	1.41651955	6.78487454	-3.97613095
H	4.74316004	4.58740886	1.09039912
H	6.03695690	2.73565357	-3.90632781
H	6.09100122	-0.10890158	1.91764301
H	3.12061348	-3.69883684	3.32184840
H	1.30749489	-6.99763010	-0.32719969
H	-3.96439964	-4.82806583	-1.57890387
H	-2.22651750	-3.96847866	3.70473756
H	-5.73294482	-0.41638319	2.72780947
H	-6.58679039	0.10268845	-2.67580749
H	-4.80391159	6.11937613	-2.72166024
H	6.17536084	-3.36060521	-2.41328340
H	-7.62246640	-0.83301308	2.00348627
H	-5.33373679	5.78254121	2.01200570
H	0.20889956	8.51531760	0.90856919
H	6.45479841	5.71564964	1.07431106
H	8.03523843	-0.68012129	2.24944156
H	3.45639773	-5.64739912	3.81911124
H	-3.00077645	-5.89996507	3.71036694

2-HP-B-CD:cis-(1S,4S)-SRT_5_Cl E(Ha)= -7253.8647645931

Cl	2.28981923	1.21727412	2.52028158
Cl	0.42190036	2.06473956	0.06385863
O	-6.03509629	-1.38208314	-2.21509285
O	-2.20321270	-4.67024922	-3.73352667
O	1.14933478	-4.33893033	-2.31551649
O	3.02248794	-4.32796851	-3.68610051
O	4.45693486	-1.50012898	-1.83861477
O	5.87738802	-0.05687231	-2.96924391
O	4.37645978	2.84702642	-1.32552493
O	4.12666190	4.80279675	-2.53505298
O	0.86601366	5.37954837	-0.97305651
O	-0.80368615	6.32226511	-2.27601734
O	-3.39232423	4.25589301	-0.71854641
O	-5.25528042	3.73469477	-1.99520176
O	-4.95429965	4.34973473	1.57871860
O	-5.64579454	1.58779991	1.52128640
O	-5.05882028	0.24998320	-0.88247088
O	-2.56155649	5.87820062	1.43225701
O	0.14595096	6.84603772	1.17456326
O	-3.19223948	6.53754727	-3.59906478
O	2.65012023	5.69772327	1.21475849
O	5.09862736	4.19824527	0.89202772
O	2.71579360	6.86236428	-3.74489224
O	5.93494556	-1.32100009	0.41597298
O	5.60544706	1.51434549	0.84437067
O	4.28945165	-3.43846545	0.17184885
O	2.53959521	-5.62506327	-0.33037249
O	5.33345115	-3.38351525	-4.85456933
O	-0.28532010	-5.68690236	-5.43974102
O	-2.95597898	-5.71926681	-0.32943561
O	-0.15167426	-5.85225094	-0.31019270
O	-3.90363099	-3.37967126	0.74842928
O	-5.65779292	-1.26593024	1.41123130
O	-5.95076222	-3.64378911	-3.91988628
O	-7.02373945	2.16309865	-3.35994601
O	6.72442446	2.34426831	-4.07046357
O	-5.68525718	-5.51611741	0.74490878
O	-8.05810588	0.20641740	1.60683633
O	-5.04509385	7.16400815	1.43450636
O	2.29746695	8.39197150	2.17282296
O	7.50488404	3.33398074	2.08434389
O	6.45362313	-3.62447061	2.04800772
O	1.31978177	-8.22266267	0.19397244
O	-3.02819398	-3.45507640	-1.94544055
N	-0.70160253	-3.66472001	6.11357089
C	-0.48022423	-4.81020146	5.10543189
C	-1.58499051	-4.71428889	4.06554924
C	-1.40717552	-3.46726891	3.21014921
C	-0.06454389	-3.47619216	2.45871859
C	2.39070952	-3.98098931	2.76698324
C	3.46550827	-4.55442994	3.43898026
C	3.25636586	-5.22894782	4.64103669
C	1.97176103	-5.30859211	5.15892180
C	0.89260398	-4.69497840	4.50653837
C	1.08980357	-4.02363775	3.28470448
C	0.15363633	-2.09859306	1.85255215

C	1.04330882	-1.16491310	2.37937563
C	1.14759005	0.11722430	1.83783082
C	0.33964031	0.48809803	0.75941433
C	-0.55626520	-0.43971503	0.23226291
C	-0.64521816	-1.71366768	0.77089411
C	0.14335751	-3.68286153	7.33552743
C	-4.79407198	-1.94632697	-2.63164405
C	-4.32730384	-2.98505307	-1.61278475
C	-4.26613352	-2.39705382	-0.20838611
C	-5.63702502	-1.82539231	0.11594762
C	-6.00633338	-0.78079028	-0.94457614
C	-2.92083007	-4.73216353	-2.53826277
C	-0.85962690	-4.19284996	-3.62876556
C	-0.07723884	-4.99795980	-2.58932124
C	-0.83652338	-5.08488789	-1.26918442
C	-2.21589403	-5.65466118	-1.53329280
C	2.36480503	-4.96866725	-2.63125393
C	3.22902862	-4.95243155	-1.36507390
C	3.51949891	-3.50836421	-1.00307026
C	4.23813419	-2.85918691	-2.17924505
C	3.40608453	-2.96675736	-3.45768944
C	5.76276115	-0.98251891	-1.92914578
C	5.04134689	1.09980776	-2.85646697
C	5.32954609	1.82028692	-1.54146929
C	5.22885209	0.87500373	-0.35055737
C	6.11263411	-0.33776169	-0.58325617
C	4.77528259	4.18754581	-1.45780584
C	4.45322294	4.90588874	-0.14354055
C	2.94979307	4.94588576	0.06244669
C	2.26748455	5.52709630	-1.16925519
C	2.69894326	4.81714044	-2.45041210
C	0.04296306	6.49910260	-1.17392277
C	-0.76555733	6.73844104	0.10631910
C	-1.74930056	5.60168354	0.31329372
C	-2.59634714	5.41208286	-0.93804261
C	-1.72892467	5.23668898	-2.18200880
C	-4.78524094	4.35786088	-0.82753529
C	-4.96643270	2.34033858	-2.10600023
C	-5.51082931	1.59873081	-0.88670150
C	-5.04294331	2.22867051	0.42012848
C	-5.40477011	3.70097644	0.41200804
C	-5.64459791	1.90293049	-3.39512152
C	-2.54008670	5.30090268	-3.46634830
C	2.23075530	5.54351047	-3.70017486
C	5.37361398	1.95527808	-4.06768480
C	4.20042587	-2.56811225	-4.69111596
C	-0.27065599	-4.34538112	-5.02176758
C	-5.04851191	-2.56608663	-3.99530461
C	-5.92775772	5.10022706	2.30178854
C	-0.07104461	7.91683270	2.08758456
C	5.74123967	4.98198575	1.89226573
C	6.83867166	-1.27467984	1.51792772
C	3.22686548	-6.73162193	0.25301029
C	-3.90433536	-6.78717414	-0.30039655
C	-6.72067132	-1.68858446	2.26434490
C	-4.83643883	-6.62969023	0.89213058
C	2.24161779	-7.58246796	1.04295223
C	6.38663021	-2.30097456	2.54370777

C	6.51908901	4.04022138	2.80042319
C	1.17239921	8.06700972	2.95346879
C	-5.39776061	6.49222653	2.62414609
C	-7.57243739	-0.50807831	2.72210790
C	-5.71383833	-7.86067871	1.03628313
C	-8.75076385	-0.99639551	3.54648819
C	-6.45371341	7.30603113	3.35101328
C	0.97833677	9.17619129	3.97135984
C	7.21736041	4.81769919	3.90052397
C	7.26174352	-2.24311569	3.78127762
C	2.98467817	-8.66126802	1.81153453
H	-2.57543072	-4.73984228	4.53935675
H	-2.23166706	-3.38060679	2.49466443
H	-1.47563409	-2.55225428	3.82093729
H	-0.17919978	-4.18606842	1.62355311
H	2.58229261	-3.50733851	1.80902940
H	4.46487153	-4.48060439	3.01271598
H	4.08439271	-5.70414162	5.15787071
H	1.79322303	-5.87474777	6.07127110
H	1.69363773	-1.42362321	3.20868419
H	-1.18393246	-0.14909333	-0.60383499
H	-1.36601462	-2.41081971	0.35546518
H	-0.10522068	-2.81828964	7.95218203
H	-0.05428381	-4.60319030	7.88596938
H	1.18920922	-3.64564001	7.03322938
H	-0.54540339	-2.79013960	5.60466908
H	-1.68978252	-3.66552298	6.38099220
H	-0.56920136	-5.71778841	5.71179609
H	-1.51946300	-5.60954859	3.43703156
H	-5.15289670	2.40673748	-4.24117379
H	5.10562978	1.39788060	-4.97793803
H	-5.09770758	5.40568874	-0.89049768
H	-6.49588780	3.79248680	0.32802787
H	-3.94853085	2.13955666	0.48310585
H	-5.38581753	0.64783041	1.48064569
H	-6.60798022	1.62874293	-0.93760266
H	-3.88019485	2.18108143	-2.17058751
H	-5.52578597	0.82309691	-3.51967975
H	0.65017451	7.38008339	-1.40730680
H	-1.32139332	7.67905154	-0.01392177
H	-1.17401830	4.67993962	0.48505933
H	-3.19923928	5.14294371	1.51758441
H	-3.23663812	6.29179565	-1.09082058
H	-1.18898515	4.28119066	-2.11836206
H	-1.87110126	5.09606981	-4.31625291
H	-3.31624170	4.53105529	-3.44322010
H	-2.50227933	7.21117306	-3.58078714
H	5.84670021	4.25013421	-1.67672235
H	4.84438287	5.93096791	-0.20387333
H	2.60712553	3.90878869	0.18937948
H	1.68042005	5.81140258	1.23798682
H	2.52758577	6.59028172	-1.25879585
H	2.31148514	3.78877346	-2.44257974
H	2.54272811	4.96247725	-4.58131186
H	1.13878515	5.60296313	-3.69639455
H	3.67796394	6.80061059	-3.73042023
H	6.47319739	-1.78319918	-2.16221837
H	7.16549466	-0.02404631	-0.61818392

H	4.18747923	0.52477347	-0.27936069
H	5.13591665	2.37182888	0.87481909
H	6.34333046	2.24030888	-1.58988996
H	3.98317887	0.80378464	-2.88006310
H	4.77562064	2.87047264	-4.03660570
H	2.18979620	-5.99703961	-2.96713744
H	4.17315294	-5.46927238	-1.57986619
H	2.56049179	-2.98900794	-0.85332016
H	4.64704839	-2.52724918	0.22309046
H	5.19728784	-3.36751971	-2.34890305
H	2.51241226	-2.33478327	-3.35716376
H	3.53682552	-2.60622203	-5.56772755
H	4.55801334	-1.54148458	-4.57307090
H	5.00753427	-4.28395163	-4.96600952
H	-3.91482459	-5.10591782	-2.80817833
H	-2.11900641	-6.66060392	-1.96522397
H	-0.95596721	-4.05658983	-0.90105868
H	0.78963117	-5.57376760	-0.33361865
H	0.10555504	-6.00559178	-2.98737697
H	-0.85907234	-3.13600182	-3.32799397
H	0.77492493	-4.02444789	-5.00675051
H	-0.82375813	-3.69269456	-5.71308813
H	-1.21048920	-5.95687890	-5.46277775
H	-7.01683303	-0.40364699	-0.75685509
H	-6.37440634	-2.63637970	0.04896561
H	-3.53169411	-1.58001968	-0.18665779
H	-3.39407202	-4.07743463	0.28555679
H	-5.04170986	-3.81958137	-1.61124467
H	-4.02831314	-1.16167731	-2.71741556
H	-4.10954259	-2.96134100	-4.39390862
H	-5.40566155	-1.77992930	-4.67593157
H	-6.78461637	-3.28611121	-3.59342851
H	-7.11505441	3.11328748	-3.22137356
H	7.24409078	1.53264135	-4.09582027
H	-3.35867987	-7.73931017	-0.24164627
H	-4.51309103	-6.78643755	-1.21534715
H	4.03114299	-6.35626403	0.89884814
H	3.66404000	-7.35781421	-0.53684961
H	6.83358491	-0.27199659	1.95818743
H	7.85443694	-1.51790587	1.17309244
H	4.99340286	5.55153213	2.45761357
H	6.44379352	5.68138723	1.41627782
H	-0.96039565	7.71123738	2.69690032
H	-6.18855732	4.55460436	3.21824433
H	-6.83595461	5.21324212	1.69639151
H	-6.28399336	-2.20572917	3.12927257
H	-7.36297745	-2.40183572	1.73343198
H	-4.20661640	-6.52591150	1.79391080
H	-6.94438746	0.15033829	3.34264729
H	-4.51446273	6.38390226	3.27382373
H	1.32949758	7.11221559	3.48444115
H	5.79420789	3.34150077	3.25454371
H	5.34759202	-2.04695847	2.81922393
H	1.72457489	-6.92024402	1.75880413
H	6.50312527	5.37777674	4.51099302
H	7.93689946	5.51975326	3.46790933
H	7.76749039	4.12915066	4.54587857
H	7.22135602	-1.25631072	4.25049718

H	8.30056131	-2.46874312	3.52233534
H	6.92802777	-2.98937105	4.50657473
H	3.68815050	-8.23034143	2.52985547
H	3.53684032	-9.30765285	1.12211401
H	2.26752693	-9.28510904	2.34964450
H	-5.11986368	-8.76442602	1.19930730
H	-6.32375638	-7.99803816	0.13796052
H	-6.39208494	-7.72809520	1.88195515
H	-8.42518323	-1.59050179	4.40657661
H	-9.41285013	-1.61123398	2.92864919
H	-9.32800977	-0.14395630	3.91099446
H	-6.78299395	6.81188181	4.27043427
H	-7.32382374	7.45727172	2.70417616
H	-6.05251121	8.28890119	3.60759321
H	0.12163158	8.97940224	4.62267595
H	0.82109471	10.13222626	3.46206665
H	1.87472565	9.26910448	4.58842489
H	-5.16199416	-4.71048754	0.89245578
H	-7.42013385	0.92112148	1.45056547
H	-4.10860779	6.96489762	1.27926674
H	2.58498014	7.58999668	1.71215850
H	7.05904817	2.69521165	1.51025517
H	5.91015147	-3.69245636	1.24953077
H	0.65944719	-7.57411083	-0.09084438
H	-0.22595866	8.85152408	1.52960307

2-HP-B-CD:cis-(1S,4S)-SRT_6_Cl E(Ha)= -7253.8582417411

Cl	-1.29195769	-3.91547386	6.21824194
Cl	-3.57441823	-2.54251706	4.46076172
O	1.50599071	5.78785529	-2.80901483
O	-1.69878648	5.26322530	-1.12990041
O	-3.77109531	5.61264102	-2.12454863
O	-4.24619236	2.16961125	-1.00909495
O	-5.66622338	0.60488368	-1.98367713
O	-3.36867391	-2.26251287	-1.83406969
O	-3.10062050	-3.88320314	-3.45266566
O	0.06901039	-5.07244407	-2.04895264
O	1.82026260	-5.76389937	-3.39174278
O	3.73504038	-3.67085376	-1.12863053
O	5.86499637	-2.79551242	-1.33064307
O	4.65437638	0.58419674	-0.57621218
O	5.47821691	2.42451615	-1.71767666
O	5.08591577	1.83018329	1.85189322
O	3.23382074	3.91618842	1.46755954
O	2.41216092	4.37609926	-1.21964405
O	4.12456719	-0.79744175	1.86775707
O	3.99450070	-3.59932535	1.69508627
O	7.72509664	-0.70020495	-1.76986611
O	3.10501576	-5.96275835	0.55472562
O	0.61463916	-7.16402071	-0.27034447
O	4.43968228	-5.78391732	-4.22338784
O	-4.10497410	-4.17711004	0.03192300
O	-1.79491734	-5.75115202	0.00234715
O	-3.68546244	-1.59224905	0.92738596
O	-4.62639349	0.95822698	1.49933261
O	-6.46719408	-1.75364572	-3.39452829
O	-6.28957797	4.76548615	-2.94621970
O	-2.87251815	6.03344256	1.36897921
O	-4.62052578	3.75256776	1.44719974
O	-0.25818644	6.88404740	0.76020795
O	2.54416811	6.48191457	0.60592644
O	-0.50826333	7.02802245	-4.22198732
O	5.23081092	4.85892427	-3.18639478
O	-1.77114904	-5.67543815	-5.12036013
O	-2.40816952	8.72102425	0.79363193
O	5.19657920	5.89899610	1.58621435
O	6.56673028	-0.36975782	3.08127956
O	5.64232840	-5.81891550	1.93828445
O	-1.94953573	-8.42715208	-0.73312236
O	-6.18190191	-2.72437940	1.37010671
O	-7.03296000	2.23109427	1.95378857
N	-1.24175418	2.27002286	-0.99882455
C	-1.37681574	1.72566407	-2.37209425
C	0.75001034	-1.42105548	3.86324199
C	0.41887827	-2.37708775	4.81373308
C	-0.91184513	-2.73399058	5.02070289
C	-1.90787208	-2.12734405	4.24884177
C	-1.57094205	-1.17271516	3.29198531
C	-0.24155983	-0.80107892	3.09704245
C	0.36089614	-0.27379999	0.66813318
C	0.52641152	0.63640398	-0.39279611
C	1.01858693	0.18622997	-1.62321251
C	1.17914514	-1.16788073	-1.87362439

C	0.86559107	-2.08023522	-0.87115852
C	0.51180380	-1.63430702	0.39775573
C	0.16083614	0.24640165	2.08294207
C	-0.71238216	1.50179553	2.07545405
C	-0.08079008	2.55499005	1.16790183
C	0.09954698	2.07323554	-0.26949186
C	0.17180716	5.32650601	-2.65057073
C	-0.51753084	6.00590827	-1.46616312
C	0.34633796	6.07389874	-0.21246931
C	1.73748306	6.58126648	-0.54423153
C	2.31794381	5.71455270	-1.67155356
C	-2.94321751	5.95345312	-1.05351337
C	-4.03755145	4.22120715	-2.26113167
C	-4.50554482	3.57665928	-0.94880236
C	-3.85428000	4.10775046	0.32893418
C	-3.63800218	5.60609221	0.26531840
C	-5.33626531	1.28164643	-0.80624462
C	-5.00387833	0.29003941	0.30859322
C	-3.92493406	-0.69469517	-0.12671893
C	-4.39684325	-1.38908728	-1.39599855
C	-4.71650676	-0.34825594	-2.47079215
C	-3.77282853	-3.55114718	-2.27863052
C	-1.68017873	-4.03243693	-3.34662651
C	-1.33186885	-5.07818337	-2.28638322
C	-2.00621314	-4.74878780	-0.95835726
C	-3.50010640	-4.58456190	-1.17627151
C	0.87655589	-6.16216971	-2.43873594
C	1.58166272	-6.69313133	-1.18224963
C	2.37493526	-5.55347291	-0.57480746
C	3.31307004	-4.93934215	-1.61446727
C	2.67263980	-4.69385213	-2.98511138
C	4.99231258	-3.54464623	-0.52272138
C	4.82763227	-2.84776818	0.83254517
C	4.26679485	-1.44752599	0.61692599
C	5.21716575	-0.69745074	-0.30753633
C	5.42902984	-1.46661930	-1.61191538
C	5.51315528	1.69691823	-0.51689369
C	4.20757330	2.96969278	-2.05710384
C	3.71937319	3.87810962	-0.92791780
C	3.66999750	3.11349003	0.38922694
C	5.07277175	2.57960080	0.65828712
C	4.40716708	3.73097171	-3.35681958
C	6.51549223	-0.84617121	-2.47342978
C	3.72684219	-4.58469392	-4.07663602
C	-1.21433055	-4.44610833	-4.73261049
C	-5.34210440	-0.97219155	-3.70735073
C	-5.11351984	4.10871413	-3.33384557
C	-0.52594809	5.65124499	-3.96531215
C	6.29136787	1.98546944	2.60681591
C	4.54870156	-3.92910178	2.96974605
C	0.41676047	-8.57803476	-0.30574525
C	-5.40402283	-4.72458509	0.25449458
C	-5.39139720	0.61161326	2.66765208
C	-3.44802393	7.05435119	2.19119268
C	3.58442072	7.45834911	0.68150378
C	-2.62045337	8.33575196	2.14059987
C	-6.31608364	1.75553967	3.08264174
C	-6.00226822	-4.12089451	1.51537853

C	-0.98613367	-8.92469140	0.16944577
C	4.87479856	-5.42066360	3.06065167
C	6.39042549	0.89968892	3.66789025
C	4.52387791	7.11674054	1.82860795
C	-3.33405585	9.45566534	2.87571759
C	5.57016333	8.20375313	1.99348760
C	7.57918975	1.16234276	4.57526410
C	5.65533814	-5.71875278	4.32754409
C	-1.15445990	-10.43112744	0.25929026
C	-7.35633750	-4.73762063	1.81011957
C	-7.29569578	1.28268788	4.14078955
H	-1.22097939	0.64907262	-2.35215416
H	-0.64115221	2.19557574	-3.02485710
H	-2.38580416	1.94356803	-2.71454094
H	1.79476415	-1.16579041	3.70040604
H	1.18808903	-2.85362557	5.41222243
H	-2.36839708	-0.75595733	2.68633305
H	1.24923972	0.90870710	-2.40258226
H	1.53706771	-1.50777580	-2.84058762
H	0.91967460	-3.14150914	-1.07506914
H	0.35790632	-2.35203321	1.19727318
H	1.16517005	0.57753320	2.39081491
H	-1.73755536	1.25770368	1.76177021
H	-0.79331084	1.90301408	3.09011380
H	-0.66283617	3.48493758	1.18698984
H	0.91418108	2.81661709	1.55058545
H	0.78879614	2.73278204	-0.80923627
H	-1.42314216	3.29036636	-1.02721658
H	-2.00849088	1.87208970	-0.44297548
H	0.18068696	4.23748225	-2.49071817
H	-0.79369957	7.02140873	-1.77608067
H	0.47068326	5.05118961	0.17097024
H	1.67962584	7.62440933	-0.88674211
H	3.30398012	6.06772179	-1.99103634
H	-2.77717604	7.03264384	-1.10483546
H	-3.12785909	3.72035095	-2.61358726
H	-5.58446194	3.76166607	-0.86758559
H	-2.85364459	3.66607798	0.42853269
H	-4.60870154	6.11674067	0.25165911
H	-6.22533198	1.85044988	-0.52063666
H	-5.92298312	-0.28187844	0.48443585
H	-2.98980472	-0.15342511	-0.35710231
H	-5.31081783	-1.94969164	-1.16265008
H	-3.78507073	0.15869398	-2.76220636
H	-4.83728713	-3.52933179	-2.53917091
H	-1.22341829	-3.07278951	-3.06441725
H	-1.65583757	-6.06827758	-2.63357430
H	-1.60136364	-3.78705874	-0.60303043
H	-3.91330726	-5.55137954	-1.49824046
H	0.26708653	-6.93957219	-2.91202871
H	2.26301857	-7.50341009	-1.47423640
H	1.65255983	-4.78540148	-0.27381722
H	4.17223659	-5.61079052	-1.74942994
H	2.09420492	-3.76229771	-2.93395009
H	5.46875674	-4.51885649	-0.38065145
H	5.83169059	-2.76905536	1.26816190
H	3.28495165	-1.52940888	0.13512104
H	6.18417259	-0.58055138	0.19942752

H	4.48076496	-1.48786679	-2.16850057
H	6.55295272	1.37119734	-0.40479745
H	3.48049129	2.15823054	-2.21081171
H	4.41795332	4.71653885	-0.81739187
H	2.99314187	2.25195548	0.28137415
H	5.75906060	3.43423122	0.74024790
H	4.81121915	3.03771633	-4.10827501
H	3.43986606	4.09587536	-3.71542451
H	6.63844635	-1.46272827	-3.37590478
H	6.20395594	0.15566030	-2.78336149
H	3.23928101	-4.27964590	-5.01531569
H	4.44855732	-3.81132812	-3.79579321
H	-1.46012000	-3.64081352	-5.44148430
H	-0.12788779	-4.57562054	-4.72230426
H	-5.58336587	-0.17105431	-4.42113140
H	-4.61017242	-1.63614244	-4.17729814
H	-5.36438818	3.05204904	-3.47421264
H	-4.71445496	4.49860604	-4.28145607
H	-1.57711207	5.35264493	-3.89922988
H	-0.05032573	5.07293163	-4.77150606
H	6.29436449	2.98493330	3.06352779
H	7.16549445	1.89771409	1.94631731
H	3.81214117	-3.65206932	3.73338922
H	5.45355315	-3.33540792	3.14591595
H	1.17956399	-9.05912699	0.32163393
H	0.52149067	-8.94832805	-1.33500733
H	-5.31869841	-5.81508865	0.35613770
H	-6.06543191	-4.49969069	-0.59547376
H	-4.68237307	0.37708213	3.46843125
H	-5.97648599	-0.29215094	2.46626077
H	-3.50824347	6.66878265	3.21510260
H	-4.46647020	7.26899080	1.84714078
H	3.13080862	8.44737162	0.83369767
H	4.16422339	7.47533375	-0.25256512
H	-1.65281349	8.14278036	2.62736595
H	-5.70187606	2.56872708	3.49679889
H	-5.31288394	-4.33007586	2.34839325
H	-1.12695321	-8.48346452	1.16960760
H	3.92761653	-5.98030918	3.07891242
H	5.46415377	0.92803709	4.26632766
H	3.92055082	7.04761456	2.74775803
H	-3.56106274	9.17717752	3.90959634
H	-4.27104804	9.70284245	2.36690388
H	-2.71056906	10.35211645	2.88738977
H	5.11307022	9.17395961	2.20778925
H	6.17430452	8.29199873	1.08494627
H	6.23859072	7.94401302	2.81690584
H	7.48907742	2.12208627	5.09202540
H	8.50741999	1.16024600	3.99504884
H	7.64972331	0.36809664	5.32146522
H	5.11957927	-5.37601885	5.21869713
H	6.62910385	-5.22033263	4.29352248
H	5.82770196	-6.79334043	4.41878133
H	-0.44075263	-10.87686489	0.95826660
H	-1.01400177	-10.88786163	-0.72575017
H	-2.16654633	-10.66618192	0.59548474
H	-7.28030365	-5.81851968	1.95774795
H	-8.05207510	-4.54275614	0.98774414

H	-7.77239982	-4.29192819	2.71620160
H	-6.77599356	0.85143473	5.00237441
H	-7.96156987	0.52285871	3.72060465
H	-7.90814703	2.11790127	4.48748556
H	2.78987396	4.70639572	1.10405206
H	4.20128521	0.16367515	1.71366288
H	7.99715612	-1.58425616	-1.49695274
H	3.31533702	-5.13230013	1.02633955
H	3.78865227	-6.46268467	-4.43635823
H	-0.85033655	-6.00328632	-0.01496862
H	-3.51352458	-2.47888993	0.55366440
H	-7.12728057	-1.16682727	-3.00804857
H	-6.08032384	5.70427475	-2.88207147
H	-4.54088044	2.78019498	1.52572419
H	-1.08052863	6.43747176	1.04315422
H	0.41709275	7.28545192	-4.30722557
H	6.09118568	4.53877027	-2.89089292
H	-2.72844930	-5.56141449	-5.11544618
H	-1.51959384	8.41982846	0.56019069
H	4.58763683	5.17061943	1.78925664
H	5.70383560	-0.65632137	2.73542795
H	5.03752310	-6.23305487	1.30967907
H	-2.11569037	-7.50153289	-0.49313939
H	-5.30345115	-2.31335011	1.41888078
H	-6.61639461	3.05914677	1.68715831

2-HP-B-CD:cis-(1S,4S)-SRT_1_MD E(Ha)= -7253.92643884

C	0.6066472852	1.2332603942	3.2628487207
C	0.2848272463	0.6330206038	1.9122278020
C	0.6858839053	-0.6712902394	1.5695498157
C	1.5684313414	-1.5123277968	2.4838559122
C	1.5708026696	-0.9867188888	3.9237572105
C	1.7594762640	0.5199641683	3.9469100553
C	-0.4357218522	1.4084952417	0.9947988907
C	-0.7692736513	0.9119983930	-0.2580428515
C	-0.3709249017	-0.3788459564	-0.6042967133
C	0.3468471219	-1.1526842191	0.2998397697
C	1.2704651599	-2.9981088940	2.4708033917
C	2.2579806935	-3.9224259538	2.1226762858
C	2.0024861443	-5.2877323498	2.1852719254
C	0.7660854862	-5.7588635075	2.6149392582
C	-0.2153984078	-4.8377264248	2.9935523293
C	0.0318278084	-3.4733453987	2.9040712469
Cl	0.4828970329	-7.4608161223	2.6830453209
Cl	-1.7489908521	-5.3672346188	3.6098617385
N	-0.6685440504	1.1929290634	4.0857951076
C	-0.5567177524	1.6607025663	5.4839638766
O	-3.7167169133	6.4895868197	0.3815405025
C	-2.6799309952	5.9384051036	-0.3851276767
C	-1.7538785603	7.0552739807	-0.8312734603
C	-0.7141823997	6.5136003282	-1.8194616142
O	-1.3509393208	5.9149792775	-2.9068790921
C	-2.1512992620	4.7766993134	-2.5799707362
C	-3.2355232015	5.1554286590	-1.5756666619
O	0.0898039111	5.5611624584	-1.1529172037
C	1.3787106485	5.9684855030	-0.7234445605
C	1.5884396155	5.3636175281	0.6551137596
C	3.0169095732	5.6161526043	1.1214911314
C	3.9885070807	5.0900507668	0.0623738432
O	3.7470411315	5.7341062301	-1.1638487014
C	2.4456035777	5.4781118806	-1.7026491806
O	3.2930275276	4.9686894913	2.3469111339
C	3.0549672180	5.7402608049	3.5220037646
C	2.2251344218	4.9622356374	4.5398963416
O	1.0429928686	4.4278250744	3.9654499850
O	0.6803376752	5.9200837483	1.6037702279
C	2.3774405455	6.1978136383	-3.0373565743
O	2.3822944117	7.5988023381	-2.8987700013
O	3.7971172738	3.7125127242	-0.0287403131
C	4.9014993941	2.8126653185	-0.0166412685
C	5.1629889804	2.2555720325	-1.4107103375
O	6.0652409895	1.1565234813	-1.3389563663
C	5.5850106826	0.0727320987	-0.5703549070
C	5.4442350828	0.5350554568	0.8839216016
C	4.4873925022	1.7124064294	0.9581834383
C	5.8059928210	3.2262136587	-2.3827184364
O	6.0316825013	2.5984949921	-3.6281763882
O	4.4599102789	2.2088084359	2.2756412934
O	4.9970045298	-0.5288745206	1.6924199741
C	5.8496483076	-0.8884252817	2.7688223452
C	5.4627084201	-2.2966343680	3.1808667669
O	5.5683912424	-3.1714730800	2.0795455004
O	4.3451071412	-0.3869479176	-1.0208921602

C 4.3783712047 -1.3655327840 -2.0575437296
C 3.1852546125 -1.1232834622 -2.9889479637
O 3.1047528478 -2.1682862617 -3.9583454175
C 2.9134453692 -3.4415602733 -3.4168766933
C 4.1061988782 -3.8041981471 -2.5369844163
C 4.2842551837 -2.7570535484 -1.4491904139
C 3.2676344201 0.1806358035 -3.7614757701
O 4.5216211924 0.3309859434 -4.3664866854
O 5.4574949189 -3.0221572722 -0.7027029170
O 3.9255851485 -5.0566723232 -1.9006581559
C 4.4228944891 -6.1646762587 -2.6559437002
C 3.6747890526 -7.4342675140 -2.2804698996
O 2.3435174528 -7.3890089622 -2.7446808211
O 1.7568661068 -3.4837215523 -2.6145025309
C 0.6844895288 -4.3170200259 -3.0270107536
C 0.0680076018 -4.8032743680 -1.7211158926
C -1.2438415780 -5.5200755660 -1.9754713550
C -2.1317552754 -4.6066376573 -2.8403711372
O -1.5077925985 -4.3083923964 -4.0506263999
C -0.3030722327 -3.5506897257 -3.9053744840
O -1.8678606073 -5.7754837959 -0.7354883538
C -2.8212952989 -6.8374074107 -0.7630380809
C -3.5269098824 -6.9160748220 0.5795700183
O -4.2663561317 -5.7345183608 0.8315172415
O 0.9708255763 -5.6461493932 -1.0353480717
C 0.2195682647 -3.3029645039 -5.3104627027
O 0.7212173509 -4.4675580033 -5.9209253417
O -2.3633989165 -3.4065814357 -2.1245498838
C -3.6089879941 -3.2353673757 -1.4706655294
C -4.5051993482 -2.3131782599 -2.2927175766
O -5.6923391275 -2.0175095217 -1.5491569858
C -5.4589257117 -1.3590939623 -0.3354495501
C -4.6110813220 -2.2466768729 0.5808746890
C -3.3086953397 -2.6087368174 -0.1147992364
C -4.9490980691 -2.9426079021 -3.5996218185
O -5.5486784282 -4.2030727419 -3.4200350159
O -2.5667091186 -3.4719698393 0.7223279932
O -4.3716273390 -1.5422690908 1.8010877384
C -4.2978623616 -2.3755677978 2.9647402134
C -3.5454825454 -1.6207428635 4.0539444927
O -2.3352304060 -1.0869111757 3.5036543292
O -4.7639085928 -0.1529794871 -0.5153464874
C -5.4553665817 1.0831280358 -0.4058743572
C -4.6866424809 1.8914577096 0.6281767222
C -5.2329766594 3.3067487941 0.6989772506
C -5.1395069166 3.9148722239 -0.7072695159
O -5.9190559522 3.1526437027 -1.5881462528
C -5.5108049125 1.7946197769 -1.7598212481
O -4.5020649461 4.1355414838 1.5827890849
C -4.8053388358 4.0389370536 2.9714041057
C -3.5332817508 3.7742904942 3.7676992223
O -2.9200359191 2.5626292227 3.3431981682
O -4.7822640681 1.2600081691 1.8970966928
C -6.5555662923 1.1819389840 -2.6794756737
O -7.8417932827 1.2708752990 -2.1189441301
O -3.7960397415 3.9348899071 -1.0997669442
O -1.1109340292 7.5768937229 0.3184326980
C -0.7806360670 8.9624345858 0.2369047522

C	0.0209293479	9.3628786474	1.4649837445
O	1.2616238544	8.6839143516	1.5103142139
C	-2.7102698225	4.2812644423	-3.8997834432
O	-1.6967889920	3.8449703527	-4.7653490882
C	0.3111704719	10.8511776694	1.4521117017
C	2.9981002019	3.8281232905	5.1853797664
C	6.3381066484	-2.8214718544	4.3012804314
C	4.3442816400	-8.6459105390	-2.9048176330
C	-4.4965336045	-8.0812866110	0.6058028748
C	-4.3574866756	-0.5343592129	4.7398529341
C	-2.5227467900	4.8996793300	3.6522735995
H	3.2052003500	5.8456666498	-3.6693166323
H	6.9001785353	-0.8851769142	2.4411472498
H	-2.4592015856	-1.0421844731	2.5435060607
H	-3.6319740942	-5.0176312269	0.9906284587
H	1.8010189521	-6.9131783984	-2.0937150982
H	5.4072546476	-2.6655985191	1.2647681416
H	0.7718394861	4.9934350899	3.2198116595
H	1.0770708658	7.7496869839	1.6932566189
H	-3.5829295398	1.9959167939	2.8872452787
H	6.0506397181	-3.8471145489	4.5445501324
H	7.3882152932	-2.8296275318	3.9939105870
H	6.2365833988	-2.2115771107	5.2042036928
H	2.3697244334	3.3126205690	5.9179735202
H	3.3344127807	3.1014066549	4.4411684041
H	3.8744823216	4.2134849369	5.7145127092
H	0.8917886602	11.1181021080	0.5637211393
H	-0.6109034593	11.4389457962	1.4596172405
H	0.9004371568	11.1165536566	2.3323018162
H	-1.5994804213	4.6493422736	4.1830580930
H	-2.2755395578	5.0861319318	2.6039279874
H	-2.9230428484	5.8223898243	4.0825853959
H	-4.7380677210	0.2054017183	4.0327525665
H	-5.2089363780	-0.9767763971	5.2657979787
H	-3.7402337036	-0.0178846747	5.4808616103
H	-5.2591495796	-7.9623947479	-0.1704936173
H	-3.9811170111	-9.0329399827	0.4492312387
H	-5.0019181753	-8.1158817330	1.5733127567
H	4.3488071137	-8.5561725805	-3.9958748393
H	5.3749762039	-8.7637790505	-2.5580790425
H	3.7816125967	-9.5450457598	-2.6457329984
H	-3.2486671156	-2.3668791317	4.8014895378
H	-2.7596098750	-7.0561395216	1.3558985088
H	3.7011751538	-7.5310786935	-1.1824382084
H	4.4147289867	-2.2621949401	3.5305411010
H	1.9628500918	5.6933067779	5.3237142864
H	-0.5830768512	9.1157526138	2.3533699689
H	-3.8454684230	3.6771011510	4.8207545273
H	-0.1794380547	9.1642583207	-0.6613991754
H	-1.7097199351	9.5455346135	0.1796049262
H	4.0158695806	6.0159105724	3.9770362483
H	2.5386984074	6.6694546061	3.2569305494
H	5.7419661037	-0.1844541321	3.6052400338
H	4.2743288318	-5.9921315031	-3.7298515286
H	5.5007593395	-6.2718416594	-2.4667632008
H	-3.5713908531	-6.6624156275	-1.5477593899
H	-2.3000045069	-7.7803101225	-0.9789916453
H	-5.3072312861	-2.6337655665	3.3105000327

H	-3.7586138356	-3.2919829337	2.7133125610
H	-5.2523228592	4.9834258372	3.3077887521
H	-5.5317842310	3.2378712472	3.1405490981
H	-0.0139287487	-5.0837925507	-6.0163347895
H	3.2203376209	7.8418339256	-2.4881540949
H	-1.1166714745	4.6024187558	-4.9039957735
H	-3.3711406541	3.4311969415	-3.7088503519
H	-3.3171397122	5.0855580298	-4.3466012442
H	-1.5117078861	3.9974236650	-2.1447357826
H	-4.0078235173	5.7646461298	-2.0679498525
H	-4.0527327279	5.7705875216	0.9422492085
H	-2.0826463172	5.2239458771	0.2028945040
H	-2.3462409885	7.8402874117	-1.3209161694
H	-0.0914795428	7.3157975053	-2.2315534913
H	-8.0267695212	2.2117280114	-2.0143308915
H	-6.4979449910	1.6772414949	-3.6593403230
H	-6.3383394328	0.1189015662	-2.8162363117
H	-4.5173701300	1.7483460706	-2.2262218644
H	-6.4844928835	0.9197373158	-0.0579660787
H	-4.6104029281	0.3043214649	1.7676338552
H	-3.6342009792	1.9482307737	0.3202451332
H	-6.2932447575	3.2847008174	0.9878688848
H	-5.5677251163	4.9223794690	-0.7155415278
H	-6.3422551159	-4.0715708352	-2.8884527549
H	-4.0683861676	-3.0944798794	-4.2307333630
H	-5.6188652216	-2.2415655661	-4.1186925565
H	-3.9560843935	-1.3859886805	-2.5071746805
H	-4.1124169585	-4.1983750370	-1.3189976126
H	-2.0557997863	-4.0874127730	0.1630183475
H	-2.7393133943	-1.6838406943	-0.2855196651
H	-5.1812085612	-3.1615663598	0.7877424373
H	-6.4457159167	-1.1765147870	0.1045668701
H	1.0467719279	-2.5890912662	-5.2612869442
H	-0.5266114270	-2.5840816896	-3.4351344690
H	1.0685447962	-5.1851145491	-3.5783473959
H	1.8187158101	-5.1712178725	-1.0144039129
H	-0.1485611036	-3.9193153146	-1.1034501447
H	-1.0565494608	-6.4606377091	-2.5135843241
H	-3.0834184993	-5.0865691775	-3.0940991525
H	4.7986906957	1.2573838921	-4.2995898049
H	3.0360921767	0.9960633485	-3.0633993923
H	2.4617788712	0.1600092207	-4.5112766436
H	2.2642080953	-1.1086118088	-2.3888951615
H	5.2968895399	-1.2628571268	-2.6475006232
H	5.4291234523	-3.9626148914	-0.4778616734
H	3.4048172012	-2.7787692381	-0.7879448725
H	5.0117119287	-3.8150879759	-3.1592898464
H	2.8088508137	-4.1212724916	-4.2696893529
H	6.5807698553	1.8263104585	-3.4325854968
H	6.7512104018	3.5951929122	-1.9567473711
H	5.1518703493	4.0844852958	-2.5521081303
H	4.2032703516	1.9165023905	-1.8167827225
H	5.7983573336	3.3157476380	0.3753013444
H	3.9683090151	3.0477157068	2.2578621075
H	3.4924280524	1.3591529944	0.6450315409
H	6.4372815410	0.8714736524	1.2114012153
H	6.3461724474	-0.7088074255	-0.6510512784
H	1.4407433378	5.9293389317	-3.5350058849

H	2.3118830157	4.4003136784	-1.8654530176
H	1.4385980686	7.0614011554	-0.6450983203
H	-0.1015111921	6.2643903657	1.1214799102
H	1.4197814720	4.2803522146	0.5926791763
H	3.1795906699	6.6987564708	1.2133478198
H	5.0217667642	5.3327238100	0.3365760146
H	-0.5891491782	-2.8457484959	-5.8987904699
H	2.3689636343	-1.4844176321	4.4829572283
H	1.9012131718	0.8944062106	4.9651376865
H	2.6707047283	0.7944320760	3.4004670916
H	0.8365349903	2.3013835996	3.1754718400
H	-1.0992688437	0.2519557775	4.0445956007
H	-1.3901881680	1.8009807119	3.6364276758
H	0.0170710126	0.9505443525	6.0779959595
H	-1.5646205536	1.7477822155	5.8926646264
H	-0.0705990649	2.6383503135	5.4814499451
H	3.2538881915	-3.5907665852	1.8353979810
H	2.7704464382	-6.0037166650	1.9128662361
H	-0.7561092988	-2.7817892036	3.1866774473
H	-0.7334525216	2.4178047932	1.2728711994
H	-1.3206695103	1.5300380624	-0.9609620646
H	-0.6182509790	-0.7865239904	-1.5804814456
H	0.6677992137	-2.1507577411	0.0168762947
H	2.5898434865	-1.3841379358	2.0962812174
H	0.6321766831	-1.2708412594	4.4204750236

2-HP-B-CD:cis-(1S,4S)-SRT_2_MD E(Ha)= -7253.92393253

C	0.6174126695	1.1969753546	3.2513356556
C	0.3445992839	0.6012523139	1.8887007311
C	0.7418014247	-0.7087851007	1.5642910781
C	1.5669186955	-1.5650689146	2.5172768586
C	1.5321079903	-1.0306775699	3.9538634182
C	1.7386266815	0.4738040676	3.9763003122
C	-0.3207218868	1.3879006730	0.9396481838
C	-0.6034068151	0.8950664809	-0.3270035978
C	-0.2088615612	-0.4016957015	-0.6551130800
C	0.4556737351	-1.1861000438	0.2801600025
C	1.2236890114	-3.0411783687	2.5002269271
C	2.1889323999	-3.9965768424	2.1785831368
C	1.8843773566	-5.3526845339	2.2269516543
C	0.6193613700	-5.7801059889	2.6182795413
C	-0.3453002798	-4.8280205184	2.9663378084
C	-0.0450043229	-3.4737843269	2.8924521876
Cl	0.2725692904	-7.4761014833	2.6649198634
CI	-1.9188215850	-5.3065090687	3.5214954910
N	-0.6883718328	1.1653259812	4.0275439886
C	-0.6204488067	1.6323063194	5.4290187087
O	-3.6502004595	6.6296418664	0.2948497941
C	-2.5985493498	6.0607813268	-0.4396207802
C	-1.6195445328	7.1571718172	-0.8201016050
C	-0.5639370680	6.6127963312	-1.7882248983
O	-1.1809504862	6.0645193888	-2.9131842539
C	-2.0163820964	4.9370947930	-2.6425956418
C	-3.1275102518	5.3159409997	-1.6673065231
O	0.1877819792	5.6194495335	-1.1181697023
C	1.4818626852	5.9788436610	-0.6641393295
C	1.6574257582	5.3411750745	0.7045542317
C	3.0787727435	5.5765278904	1.1996483153
C	4.0619124917	5.0475147141	0.1529751703
O	3.8496235349	5.7035533743	-1.0722570352
C	2.5526853801	5.4798196340	-1.6349106392
O	3.3291918166	4.9174944806	2.4243872316
C	3.0880150011	5.6851958936	3.6010785997
C	2.2439014717	4.9057657705	4.6062193989
O	1.0682009470	4.3765651896	4.0126708191
O	0.7339609783	5.8829608473	1.6461451813
C	2.5189771802	6.2172182890	-2.9609422138
O	2.5543220775	7.6159292333	-2.8044962598
O	3.8562380094	3.6727930169	0.0511434213
C	4.9526735023	2.7630864327	0.0731223749
C	5.2349221626	2.2152551708	-1.3200566716
O	6.1403441180	1.1198966491	-1.2387857905
C	5.6469921125	0.0297781838	-0.4860141749
C	5.4715362876	0.4793488002	0.9677589246
C	4.5150949827	1.6573812265	1.0324983937
C	5.8864108168	3.1918395783	-2.2795530307
O	6.1107047822	2.5752974328	-3.5307737065
O	4.4670260383	2.1455794839	2.3528688428
O	5.0022377070	-0.5914360213	1.7553027433
C	5.8752292516	-1.0090638698	2.7920749975
C	5.4317799192	-2.3963546915	3.2143754625
O	5.4786318143	-3.2883691181	2.1229807889
O	4.4184094537	-0.4285237527	-0.9639877318

C 4.4801782618 -1.3940523377 -2.0120132223
C 3.2835626560 -1.1637040560 -2.9422098423
O 3.2162024152 -2.1972769438 -3.9234347682
C 3.0621686871 -3.4862936557 -3.3928039474
C 4.2964388041 -3.8144282425 -2.5546438469
C 4.4209049499 -2.7982126497 -1.4314933655
C 3.3418442736 0.1513184560 -3.6979971305
O 4.5863363146 0.3267781939 -4.3171211484
O 5.5898657747 -3.0506519532 -0.6714753854
O 4.2442737049 -5.0910460246 -1.9640250386
C 4.6715643406 -6.1467495968 -2.8168677415
C 3.9614518565 -7.4235518009 -2.3982683087
O 2.5706624665 -7.3002238282 -2.5844735492
O 1.9220082778 -3.5647689081 -2.5758416601
C 0.8388889880 -4.3645603836 -3.0099799257
C 0.1089116582 -4.7868675906 -1.7447173827
C -1.2302194136 -5.4277956586 -2.0725490511
C -2.0463509470 -4.4833515771 -2.9570737405
O -1.3399821371 -4.2329452973 -4.1300638912
C -0.0879302053 -3.5624068126 -3.9403044446
O -1.8672858186 -5.6768072122 -0.8320819549
C -2.8772063319 -6.6872314685 -0.8777442641
C -3.5937009334 -6.7365208033 0.4602041594
O -4.2676113335 -5.5184629874 0.7163172381
O 0.9238376992 -5.6625633889 -0.9999801167
C 0.4843354838 -3.3698920223 -5.3354561812
O 0.9189679825 -4.5762067905 -5.9150554277
O -2.2628271500 -3.2695434646 -2.2563598016
C -3.5274039360 -3.0730612793 -1.6475880424
C -4.3923181762 -2.1489231737 -2.5041438723
O -5.6030320271 -1.8459244252 -1.8020552920
C -5.4134380526 -1.1889501261 -0.5793816795
C -4.5993022326 -2.0831903800 0.3594879846
C -3.2719744709 -2.4287997648 -0.2923924479
C -4.7983539834 -2.7832267052 -3.8208242960
O -5.4170665526 -4.0359493569 -3.6485489784
O -2.5476949374 -3.2689764544 0.5860526107
O -4.3946635863 -1.3983492764 1.5950305751
C -4.4341848759 -2.2305652914 2.7595011905
C -3.6631544544 -1.5347666411 3.8767734745
O -2.4105810042 -1.0630733661 3.3683003946
O -4.7107899282 0.0155426346 -0.7331886731
C -5.3942751460 1.2538506075 -0.5988343723
C -4.6207647883 2.0391876377 0.4497501403
C -5.1650201304 3.4545479360 0.5487646836
C -5.0644231135 4.0865334542 -0.8473373647
O -5.8540542690 3.3448576279 -1.7378993473
C -5.4483482715 1.9902506955 -1.9385707266
O -4.4402327008 4.2666356369 1.4532115509
C -4.7137773774 4.1019160721 2.8416402069
C -3.4228671441 3.8062298736 3.6009846121
O -2.7808719822 2.6565650427 3.0603543500
O -4.7148788923 1.3851916832 1.7070644103
C -6.4936729334 1.3955414328 -2.8690026780
O -7.7792592765 1.4669170622 -2.3038273239
O -3.7224838323 4.0924554042 -1.2449277606
O -1.0004594893 7.6177786075 0.3680376169
C -0.6381418692 8.9972309359 0.3520508510

C	0.1259151562	9.3335398080	1.6219679007
O	1.3549617688	8.6347439044	1.6814334670
C	-2.5390896144	4.4844933201	-3.9924760939
O	-1.5056328363	4.0457926423	-4.8327134753
C	0.4362393496	10.8165303667	1.6836491913
C	3.0051979235	3.7664862145	5.2563673205
C	6.2972326158	-2.9515081608	4.3290028732
C	4.4369514853	-8.6045765072	-3.2228471802
C	-4.6246219473	-7.8478117418	0.4752175774
C	-4.4271056382	-0.4068853896	4.5492288456
C	-2.4477542260	4.9672329710	3.5668984044
H	3.3460639053	5.8536567123	-3.5871160098
H	6.9116058539	-1.0591362211	2.4248133606
H	-2.4529890856	-1.1178453675	2.4016669872
H	-3.5976804180	-4.8271928619	0.8440671270
H	2.2149855270	-6.6788925110	-1.9287068381
H	5.3853454315	-2.7888520765	1.2932074440
H	0.8120503701	4.9431310316	3.2627374822
H	1.1504315152	7.6954420218	1.8101303003
H	-3.4581376134	2.0754903838	2.6430855856
H	5.9718765928	-3.9643734501	4.5780158394
H	7.3433073144	-3.0026126045	4.0119827531
H	6.2288321535	-2.3353872740	5.2308645498
H	2.3675082726	3.2513471873	5.9812389843
H	3.3461205964	3.0406741199	4.5134029975
H	3.8776423743	4.1466413539	5.7957245612
H	1.0477036788	11.1144146694	0.8262939042
H	-0.4777245579	11.4168949712	1.6895003251
H	1.0012215202	11.0343685143	2.5924021648
H	-1.5002292337	4.6951055411	4.0407360989
H	-2.2458139997	5.2694489691	2.5358719712
H	-2.8609337391	5.8276403753	4.1015191789
H	-4.7586944531	0.3493729309	3.8346091398
H	-5.3073979743	-0.8037386570	5.0639214065
H	-3.7956944551	0.0778069243	5.3000694068
H	-5.3758401339	-7.6861362676	-0.3044277499
H	-4.1596876918	-8.8249731153	0.3179019941
H	-5.1362901914	-7.8596314631	1.4399599267
H	4.2176971877	-8.4395639311	-4.2825484645
H	5.5124854508	-8.7675418859	-3.1077418563
H	3.9120998309	-9.5092765764	-2.9081883176
H	-3.4364043558	-2.3043463712	4.6257351992
H	-2.8404053387	-6.9248737902	1.2408152815
H	4.1952251407	-7.6051259150	-1.3353753242
H	4.3918672978	-2.3101426439	3.5795692842
H	1.9724262847	5.6338575017	5.3894703906
H	-0.5123009028	9.0577521308	2.4774905857
H	-3.7176546923	3.6125301080	4.6460977084
H	-0.0015029056	9.2203513880	-0.5165208830
H	-1.5520041418	9.6030984620	0.2847846849
H	4.0469715237	5.9512406871	4.0658678563
H	2.5808174759	6.6198885825	3.3374746264
H	5.8372976958	-0.3075759160	3.6371820496
H	4.4062358151	-5.9339688487	-3.8611527067
H	5.7644652842	-6.2590931798	-2.7551570514
H	-3.6069274717	-6.4578091720	-1.6666418863
H	-2.4090315728	-7.6554254409	-1.1033899453
H	-5.4730278779	-2.4045575034	3.0682269399

H	-3.9659817672	-3.1910679762	2.5291507562
H	-5.1551636577	5.0280103598	3.2317498257
H	-5.4345535399	3.2914382997	2.9857242402
H	0.1462168983	-5.1442441506	-6.0117711639
H	3.3956375464	7.8356107254	-2.3875957108
H	-0.9092607355	4.7954772805	-4.9409841075
H	-3.2238348382	3.6448062588	-3.8446997027
H	-3.1135742010	5.3113054134	-4.4411389469
H	-1.4090242546	4.1340717684	-2.2049668900
H	-3.8715271471	5.9507282537	-2.1710412517
H	-4.0076039107	5.9169827726	0.8500970214
H	-2.0530950674	5.3160007947	0.1599521427
H	-2.1678461918	7.9771386069	-1.3036318126
H	0.0965635614	7.4060760591	-2.1560750111
H	-7.9683099060	2.4045361069	-2.1792871728
H	-6.4402659752	1.9132792219	-3.8373345458
H	-6.2727999371	0.3366212824	-3.0318768160
H	-4.4557032031	1.9525017993	-2.4068557988
H	-6.4236918430	1.0894918052	-0.2524210298
H	-4.5555033562	0.4288340224	1.5636709802
H	-3.5690654477	2.1009834660	0.1410368384
H	-6.2268034621	3.4274510605	0.8323498211
H	-5.4799459150	5.0992819343	-0.8407017226
H	-6.2259088174	-3.8886812081	-3.1447744216
H	-3.8997715691	-2.9483047203	-4.4228982438
H	-5.4442871508	-2.0800617912	-4.3662436152
H	-3.8326587206	-1.2250303562	-2.7042113176
H	-4.0476833541	-4.0275707568	-1.5001671452
H	-1.9773116856	-3.8466382900	0.0501414371
H	-2.7075010398	-1.5000364520	-0.4563617726
H	-5.1709764724	-3.0033671452	0.5348714281
H	-6.4151830706	-1.0061372368	-0.1751188795
H	1.3517194562	-2.7071886891	-5.2820657921
H	-0.2649639720	-2.5767106326	-3.4898411266
H	1.2062158620	-5.2617244796	-3.5257011980
H	0.3748422795	-6.0340581897	-0.2974840226
H	-0.0900156356	-3.8744521642	-1.1615905734
H	-1.0639253465	-6.3706637826	-2.6130904878
H	-3.0048062413	-4.9190270356	-3.2610002863
H	4.8603807171	1.2519447724	-4.2280804038
H	3.1083939926	0.9543373802	-2.9862423866
H	2.5282302868	0.1314858206	-4.4394988809
H	2.3650094147	-1.1709682183	-2.3382373060
H	5.3987438814	-1.2602608040	-2.5958300021
H	5.6084030761	-4.0098699283	-0.5383623104
H	3.5322333547	-2.8761962810	-0.7881595352
H	5.1771716438	-3.7246958862	-3.2092723463
H	2.9627091059	-4.1554425641	-4.2546098660
H	6.6503131836	1.7948695841	-3.3418957603
H	6.8326823018	3.5504671902	-1.8470075183
H	5.2382870174	4.0559050924	-2.4419446599
H	4.2827931762	1.8740866311	-1.7421481786
H	5.8469392494	3.2552767703	0.4843033044
H	3.9852320705	2.9898613631	2.3308039265
H	3.5243753522	1.3101011713	0.6997275979
H	6.4550865432	0.8139789385	1.3240801970
H	6.4114142120	-0.7494627586	-0.5564961393
H	1.5819583132	5.9761325004	-3.4717929217

H	2.4003513039	4.4070505828	-1.8149990924
H	1.5705726132	7.0679464615	-0.5608940879
H	-0.0357052446	6.2393011615	1.1538568857
H	1.4841320422	4.2603794003	0.6162694161
H	3.2496368940	6.6568199183	1.3031573795
H	5.0930215326	5.2765392962	0.4461727092
H	-0.2837758035	-2.8742098549	-5.9468033105
H	2.3061405196	-1.5354008558	4.5402616706
H	1.8503308584	0.8512018083	4.9971084048
H	2.6707474812	0.7358360361	3.4592767930
H	0.8586171176	2.2631924617	3.1753116440
H	-1.1229393646	0.2283337191	3.9673255455
H	-1.3872496366	1.7848970070	3.5511801689
H	-0.0674747383	0.9222203741	6.0426102749
H	-1.6397624708	1.7222662030	5.8082723110
H	-0.1324934759	2.6090676674	5.4407848303
H	3.2018157967	-3.6994203813	1.9127194505
H	2.6355009477	-6.0916271147	1.9697006437
H	-0.8165108163	-2.7564510642	3.1550001980
H	-0.6195650872	2.3999087768	1.2063197644
H	-1.1111603600	1.5204921799	-1.0556895676
H	-0.4148645579	-0.8047787914	-1.6426890911
H	0.7815999394	-2.1864122493	0.0092923458
H	2.6046243277	-1.4703812077	2.1653118281
H	0.5753253702	-1.2994076144	4.4248230356

2-HP-B-CD:cis-(1S,4S)-SRT_3_MD E(Ha)= -7253.92257350

C	0.5882002370	1.3362646212	3.1247637723
C	0.2455861617	0.6415334393	1.8252491192
C	0.6155606353	-0.6941862365	1.5856541434
C	1.4637428669	-1.4898830871	2.5687919300
C	1.4765590248	-0.8534982709	3.9625292181
C	1.7203272421	0.6429534936	3.8629276422
C	-0.4504285999	1.3622801478	0.8460077337
C	-0.7847002321	0.7809127234	-0.3697703215
C	-0.4139222494	-0.5407804054	-0.6151266919
C	0.2754847028	-1.2611665438	0.3522902359
C	1.1087639933	-2.9598076304	2.6731021510
C	2.0672623823	-3.9469464378	2.4336380074
C	1.7601396137	-5.2904308704	2.6191081961
C	0.5006832841	-5.6744323299	3.0677632783
C	-0.4541795512	-4.6881280859	3.3335996709
C	-0.1562861444	-3.3481591678	3.1176139209
Cl	0.1557773859	-7.3504651668	3.2987990969
CI	-2.0143142354	-5.1035541012	3.9694106429
N	-0.6813696071	1.4030124459	3.9554724797
C	-0.5383081239	1.9898732967	5.3055363570
O	-3.4820665387	6.5427843310	-0.1773019268
C	-2.4471539738	5.9127509582	-0.8838774587
C	-1.4823161707	6.9724701350	-1.3818569530
C	-0.4403803731	6.3402264811	-2.3082286375
O	-1.0722588265	5.6941698063	-3.3718588140
C	-1.9073562703	4.5988144793	-2.9882313275
C	-3.0000243204	5.0658817548	-2.0311693068
O	0.3146917638	5.4052888487	-1.5642830744
C	1.6192437246	5.7783597179	-1.1553331668
C	1.7898140420	5.2697105752	0.2687153858
C	3.2294488260	5.4701265250	0.7295354155
C	4.1741145201	4.8207046786	-0.2841640546
O	3.9699745813	5.3920139852	-1.5537836632
C	2.6606824957	5.1505559176	-2.0813104157
O	3.4649948468	4.8892202307	1.9958324151
C	3.2541599286	5.7457032937	3.1155824270
C	2.3764006712	5.0730810945	4.1659564555
O	1.1747198970	4.5675029151	3.6062100923
O	0.9183383851	5.9548239152	1.1656170776
C	2.6358683640	5.7401347479	-3.4777656927
O	2.7415287333	7.1434799756	-3.4744614040
O	3.9055470964	3.4541220132	-0.2769416402
C	4.9578672202	2.4938855449	-0.2806192935
C	5.1075035208	1.8353054564	-1.6499997874
O	5.9691100740	0.7102468770	-1.5593532946
C	5.5273928372	-0.3025380711	-0.6830822454
C	5.4436843766	0.2598400646	0.7407879053
C	4.5315031508	1.4724986975	0.7685153737
C	5.6998024579	2.7420556280	-2.7041643283
O	5.4243428314	2.1691853742	-3.9723110512
O	4.5494652322	2.0494204597	2.0534326420
O	4.9851954984	-0.7399670317	1.6188279058
C	5.7790408469	-0.9675114325	2.7724183178
C	5.3272369708	-2.3001562940	3.3416591998
O	5.4011142795	-3.3013822451	2.3511769387
O	4.2807398806	-0.8128051642	-1.0494598486

C 4.3082266755 -1.8925218571 -1.9833375379
C 3.1855968463 -1.6826294716 -3.0014679070
O 3.0277520673 -2.8417780621 -3.8251979452
C 2.7609217175 -4.0246757527 -3.1368197129
C 3.9215872188 -4.3478355415 -2.2028334094
C 4.1282136422 -3.2011701576 -1.2297034192
C 3.4531520719 -0.5227792116 -3.9518402004
O 4.7601860551 -0.5396018571 -4.4546962154
O 5.2745340462 -3.4387281665 -0.4337069780
O 3.6748373351 -5.5213742514 -1.4461251157
C 4.1328771515 -6.7187070147 -2.0808762224
C 3.3518597953 -7.9205433515 -1.5709238882
O 2.0221950147 -7.8935460745 -2.0385972475
O 1.5964735846 -3.9107793503 -2.3497815005
C 0.4887430424 -4.7344698057 -2.6766385088
C -0.1381191023 -5.0789299442 -1.3327225259
C -1.4694409427 -5.7755979693 -1.5276977973
C -2.3310101915 -4.9138705741 -2.4633807404
O -1.7069437566 -4.7391736678 -3.6982976901
C -0.4709354116 -4.0191596351 -3.6257004530
O -2.1057809115 -5.9090092965 -0.2745540846
C -3.0287767374 -6.9940644048 -0.2055684452
C -3.8000899759 -6.9246293685 1.1012274026
O -4.5614178178 -5.7340328868 1.1823378198
O 0.7380073982 -5.8851050265 -0.5729504911
C 0.0536136676 -3.9550019896 -5.0504209695
O 0.4091168284 -5.2256927910 -5.5386208915
O -2.5177213602 -3.6520506885 -1.8517578594
C -3.7738483507 -3.3630655927 -1.2652153254
C -4.5741055126 -2.4514705380 -2.1912442373
O -5.7621154522 -2.0058105475 -1.5282056676
C -5.5328806370 -1.2793095750 -0.3545453633
C -4.7738743485 -2.1422904528 0.6608132592
C -3.4794173408 -2.6524185668 0.0481636621
C -5.0192188875 -3.1523594072 -3.4615733480
O -5.7384314687 -4.3334318075 -3.2027179779
O -2.8311231379 -3.4909431252 0.9806110656
O -4.5197669014 -1.3495029347 1.8218220001
C -4.5087382180 -2.0760592993 3.0570546456
C -3.7462384382 -1.2539031289 4.0905084862
O -2.5108491343 -0.8073443491 3.5199105143
O -4.7603628671 -0.1305380450 -0.5878967223
C -5.3831354985 1.1471156706 -0.6106991312
C -4.5961938456 1.9992362579 0.3692278170
C -5.0946191557 3.4319805482 0.3209792683
C -4.9505768720 3.9312264869 -1.1253717665
O -5.7250117548 3.1253470481 -1.9724061982
C -5.3623997252 1.7427272705 -2.0182939448
O -4.3604721800 4.3015936590 1.1613679488
C -4.6732322456 4.2825898614 2.5514884084
C -3.4076810816 4.0375715597 3.3661032701
O -2.7993573021 2.8117008610 2.9743042574
O -4.7299899785 1.4716749010 1.6814733379
C -6.3944579313 1.0960892639 -2.9283844987
O -7.6946648474 1.2538850843 -2.4171407881
O -3.5985754340 3.8928379228 -1.4858752300
O -0.8419988932 7.5516081325 -0.2585714274
C -0.5014606479 8.9273138229 -0.4184443057

C	0.3456171318	9.3795875504	0.7598815787
O	1.5751664342	8.6814185501	0.8025889277
C	-2.4515828906	4.0308637245	-4.2852113370
O	-1.4285070653	3.5308053097	-5.1034335991
C	0.6571476347	10.8600205415	0.6557305015
C	3.0863830821	3.9425467410	4.8861136834
C	6.1652561644	-2.7295878235	4.5293352709
C	3.9891054450	-9.2086789012	-2.0624605594
C	-4.7597957849	-8.0935933407	1.2134851598
C	-4.5358720380	-0.0888782032	4.6640534946
C	-2.3904854156	5.1531779047	3.2217697562
H	3.4324773806	5.2668028980	-4.0702029147
H	6.8427008523	-1.0298025781	2.4953787657
H	-2.6074563160	-0.8735100926	2.5580874193
H	-3.9425298433	-4.9969619044	1.3055402896
H	1.5000188288	-7.3099722657	-1.4627732843
H	5.2687228171	-2.8864468960	1.4806315635
H	0.9409238551	5.1051902817	2.8281211025
H	1.3801139873	7.7678024376	1.0623073849
H	-3.4830860670	2.2175838231	2.5878856218
H	5.8199679646	-3.7005950937	4.8920847688
H	7.2149946711	-2.8320393672	4.2383316815
H	6.0921914114	-2.0086559691	5.3495164759
H	2.4226004091	3.4920995722	5.6301583145
H	3.4073056111	3.1647115812	4.1886235066
H	3.9670830813	4.3189552361	5.4145934574
H	1.2134429599	11.0683659373	-0.2634151189
H	-0.2556624369	11.4622326359	0.6581011454
H	1.2772952204	11.1642131348	1.5014726684
H	-1.4656679423	4.9094561955	3.7529185802
H	-2.1490793364	5.3169555300	2.1686461920
H	-2.7843773758	6.0864639485	3.6346982336
H	-4.8919105218	0.5931419349	3.8883154439
H	-5.4034817546	-0.4613201956	5.2174155125
H	-3.9154629055	0.4770928311	5.3655365350
H	-5.4885581126	-8.0683432490	0.3971605644
H	-4.2298639657	-9.0497174389	1.1827725057
H	-5.3063307730	-8.0302394144	2.1568684503
H	3.9913563018	-9.2361349644	-3.1567687676
H	5.0180320586	-9.3134802077	-1.7064427210
H	3.4060716126	-10.0608955273	-1.7075468808
H	-3.4881916225	-1.9408355467	4.9059937917
H	-3.0709013641	-6.9677247930	1.9242643083
H	3.3788052523	-7.9013172688	-0.4685296068
H	4.2786572563	-2.1781069461	3.6699544820
H	2.1425619367	5.8595626659	4.9038509128
H	-0.2327139526	9.1923552781	1.6796525260
H	-3.7254392552	3.9732624245	4.4201331920
H	0.0717882883	9.0770115113	-1.3447565180
H	-1.4256233893	9.5182688019	-0.4759577034
H	4.2224150117	6.0036263990	3.5654932518
H	2.7852585721	6.6791401778	2.7859267844
H	5.6522389644	-0.1552908088	3.5004579386
H	3.9806981091	-6.6568982513	-3.1662546483
H	5.2086172377	-6.8358921979	-1.8859179660
H	-3.7428659420	-6.9515791070	-1.0412336449
H	-2.4727444172	-7.9397391222	-0.2704587452
H	-5.5356730332	-2.2581715051	3.3995352079

H	-4.0048309333	-3.0327081292	2.9031919635
H	-5.1065185819	5.2505902361	2.8347614645
H	-5.4129536663	3.5027582218	2.7560062860
H	-0.3891726251	-5.7664376046	-5.5186395378
H	3.5821353588	7.3633637466	-3.0559731975
H	-0.8395631790	4.2728695037	-5.2818568092
H	-3.1258915806	3.2014167546	-4.0551146658
H	-3.0401447784	4.8137313871	-4.7909581182
H	-1.2952655003	3.8359217829	-2.4897804408
H	-3.7497589605	5.6587118698	-2.5755999412
H	-3.8500784928	5.8757175754	0.4260554801
H	-1.8789496194	5.2249787057	-0.2385282026
H	-2.0418058357	7.7380256505	-1.9361134832
H	0.2187055172	7.0948873177	-2.7520126680
H	-7.8630419472	2.2032547404	-2.3919113520
H	-6.2924344431	1.5240233642	-3.9359514555
H	-6.2031153945	0.0214851726	-2.9876812261
H	-4.3540652950	1.6246570881	-2.4385525891
H	-6.4283453078	1.0718060333	-0.2806690098
H	-4.6173150741	0.4998355220	1.6274884029
H	-3.5388231991	1.9924667559	0.0751282286
H	-6.1618444541	3.4632159698	0.5829286655
H	-5.3536281808	4.9449952588	-1.2174691303
H	-6.5334006138	-4.0824841180	-2.7180153918
H	-4.1318997012	-3.4347709193	-4.0362671850
H	-5.6020578548	-2.4442517483	-4.0689494401
H	-3.9479113368	-1.5878539212	-2.4568287658
H	-4.3370918922	-4.2835916127	-1.0650196327
H	-2.3019550457	-4.1518535650	0.4938040579
H	-2.8426278859	-1.7838627847	-0.1743858478
H	-5.4136791354	-2.9930717777	0.9289088766
H	-6.5220464036	-1.0076716338	0.0309006055
H	0.9550564481	-3.3359708450	-5.0754047555
H	-0.6562891109	-3.0023903211	-3.2557077785
H	0.8350472390	-5.6638597173	-3.1471207825
H	1.6054726033	-5.4456102123	-0.6011188794
H	-0.3303388099	-4.1407796159	-0.7941565937
H	-1.3066146487	-6.7618569116	-1.9850480468
H	-3.3002328771	-5.3823299095	-2.6681951168
H	5.1705761129	0.3086525610	-4.2260399528
H	3.2276324480	0.4130629338	-3.4276120672
H	2.7269591255	-0.6167228885	-4.7722918452
H	2.2467208365	-1.4931105966	-2.4617153191
H	5.2592103471	-1.8980316830	-2.5289754582
H	5.2072960525	-4.3542251264	-0.1286614507
H	3.2358649441	-3.1090809965	-0.5932540081
H	4.8353072636	-4.4660896410	-2.8017810531
H	2.6253955113	-4.7972621558	-3.9022476989
H	6.0059950992	2.5611281611	-4.6302568579
H	6.7803155824	2.8185339080	-2.5209070423
H	5.2539130658	3.7415862035	-2.6225739975
H	4.1030571000	1.5267834852	-1.9708469803
H	5.9020712519	2.9641726893	0.0333232911
H	4.0942320481	2.9063380329	1.9876285787
H	3.5176456708	1.1364114931	0.4998043941
H	6.4584509640	0.5764438919	1.0203349811
H	6.2934374514	-1.0826046326	-0.7316055016
H	1.6796474677	5.4910600965	-3.9476071895

H	2.4765539976	4.0698378056	-2.1419534551
H	1.7373556439	6.8695816415	-1.1601619301
H	0.1367686100	6.2705962759	0.6644796528
H	1.5599370804	4.1962151785	0.2870222925
H	3.4537780135	6.5458977158	0.7515306662
H	5.2189041584	5.0245431344	-0.0214472458
H	-0.7098500748	-3.4723953239	-5.6780713770
H	2.2532172384	-1.3319974712	4.5670622726
H	1.8787660464	1.0937171828	4.8470016825
H	2.6387813419	0.8332961631	3.2921990808
H	0.8517553339	2.3857329527	2.9518230689
H	-1.1382352982	0.4764507011	3.9988437231
H	-1.3901379714	1.9934183759	3.4571736405
H	0.0091152597	1.3125997130	5.9598838153
H	-1.5373510955	2.1587012143	5.7106363046
H	-0.0098220568	2.9401399740	5.2083256654
H	3.0799745649	-3.6784883696	2.1388451566
H	2.5054680819	-6.0552848283	2.4294948235
H	-0.9265808717	-2.6080464427	3.3129141714
H	-0.7320654710	2.3938130058	1.0482010569
H	-1.3144659957	1.3576521337	-1.1227487023
H	-0.6575793959	-1.0134126235	-1.5625043729
H	0.5747232772	-2.2846644430	0.1479127299
H	2.4911700418	-1.4288104873	2.1805881914
H	0.5252981513	-1.0650719085	4.4710355408

255

2-HP-B-CD:cis-(1S,4S)-SRT_4_MD E(Ha)= -7253.9086235598

C	0.00933468	0.81781245	-5.54393047
C	-0.94354527	-0.27109226	-5.12761510
C	-0.77706323	-0.94010619	-3.90452217
C	0.47434698	-0.76624699	-3.04859422
C	1.32191461	0.44867553	-3.44852179
C	1.39762327	0.62107059	-4.95695184
C	-2.01981603	-0.58631556	-5.96433260
C	-2.95513544	-1.54005862	-5.59376731
C	-2.80953026	-2.19785919	-4.37430088
C	-1.72768934	-1.90319242	-3.55161917
C	0.23576752	-0.77025012	-1.54725513
C	0.68240516	-1.83006795	-0.75694181
C	0.51838619	-1.82685422	0.62421270
C	-0.06529779	-0.73641334	1.26007170
C	-0.47409986	0.35382026	0.48299002
C	-0.35693869	0.31917275	-0.90374825
Cl	-0.28577098	-0.75494237	2.96924968
Cl	-1.09834092	1.78101016	1.23694154
N	-0.56955901	2.16114809	-5.10737009
C	-1.24755227	2.90813676	-6.18641087
C	0.63753750	-5.11584786	-2.61253202
C	1.72604596	-5.62930969	-1.66989846
C	1.21406452	-6.31825094	-0.40111951
C	-0.09980776	-7.07419784	-0.61087657
C	-1.06985305	-6.30459625	-1.50306163
O	-0.46120607	-6.02416784	-2.72478316
O	-0.77827475	-7.27994201	0.62325332
C	-0.33519374	-8.39307592	1.39855778
C	-0.80749287	-8.23800034	2.83850633
O	-0.22684816	-7.08947156	3.45426777
O	2.20856687	-7.19231451	0.06014445
O	2.49052092	-4.48359445	-1.30280635
C	3.88299100	-4.59485303	-1.21823612
C	4.39251741	-4.20654889	0.18350838
C	4.43091585	-2.70075429	0.41445103
C	4.97492233	-1.92675384	-0.77834243
C	4.27747416	-2.39027145	-2.04882897
O	4.49520338	-3.79313903	-2.20210374
C	4.77462920	-1.73125869	-3.31792665
O	3.92555455	-1.99952794	-4.41178211
O	4.71351155	-0.54452398	-0.52432008
C	5.78499447	0.34112020	-0.38581949
C	5.66371539	1.10938657	0.94218227
C	4.50351921	2.08772022	0.87546012
C	4.57931304	2.96254629	-0.37243574
C	4.70210739	2.08494461	-1.62183623
O	5.84368045	1.24503238	-1.45955101
O	5.48134965	0.17835933	1.98367732
C	6.01260751	0.52992480	3.26926055
C	5.29926646	-0.28854024	4.33825065
O	5.61464171	-1.65936178	4.26385128
O	4.50661479	2.89196755	2.03530454
O	3.37567464	3.72299706	-0.32547100
C	3.39163651	5.09030053	-0.59609533
C	2.68440449	5.84418666	0.53223504
C	1.21496847	5.46260594	0.59142984

C	0.57142776	5.59942062	-0.79130006
C	1.38635653	4.83952529	-1.83913034
O	2.73265628	5.34661287	-1.82388227
C	0.86679867	4.96591544	-3.25829290
O	1.26788264	3.89216462	-4.09669661
O	-0.72486944	5.04505598	-0.66544218
C	-1.81882388	5.71300622	-1.24557203
C	-2.80255099	6.10162585	-0.14384205
C	-3.41853824	4.87856561	0.52270499
C	-3.91736008	3.87660296	-0.51850680
C	-2.92311627	3.65743241	-1.66851801
O	-2.44347132	4.89723398	-2.19631347
C	-3.56699852	2.90447650	-2.82263294
O	-2.72993361	1.87692762	-3.33978947
O	-4.10907891	2.62216564	0.12591776
C	-5.38921830	2.08816181	0.22000632
C	-5.53830534	1.34848757	1.56796277
C	-4.71185818	0.07027806	1.58925420
C	-5.02796649	-0.78026676	0.36137712
C	-4.82221507	0.04845939	-0.90085157
O	-5.67674836	1.19317838	-0.84131291
O	-5.14011946	2.12857403	2.66008823
C	-6.06929187	3.10362371	3.09158845
C	-5.39335168	3.83520483	4.24199903
O	-4.08944016	4.24407159	3.82675623
O	-5.00752032	-0.64309084	2.76152910
O	-4.16862902	-1.91513074	0.35991675
C	-4.71067702	-3.15893478	0.71515200
C	-3.78146813	-3.85634713	1.72274413
C	-2.45880227	-4.23727496	1.06342561
C	-2.71064899	-4.99774176	-0.23837872
C	-3.70263285	-4.25927651	-1.12801897
O	-4.90242312	-3.97927685	-0.40691073
C	-5.18642499	-0.67870837	-2.17770802
O	-4.96998275	0.13806580	-3.31909127
O	-4.48748843	5.27746754	1.33376499
O	-2.12505068	6.87444245	0.82291114
C	-2.41285101	8.26939385	0.78486072
C	-1.28365114	9.04204778	1.44829060
O	-0.08480977	8.88628674	0.71864676
O	0.57139682	6.29156510	1.52634520
O	3.32637198	5.55741685	1.74927287
C	4.21835674	6.57124513	2.21486671
C	5.45272808	5.93780349	2.83817846
O	6.12661749	5.14785410	1.87892043
C	4.97647992	2.80903179	-2.94129002
O	3.89067983	3.55619255	-3.44400314
O	5.22517652	-2.45437431	1.54861322
O	3.56836969	-4.81746599	1.14391861
C	4.21980177	-5.29043386	2.31084462
C	3.14731006	-5.70331380	3.29734863
O	2.42103356	-6.76945864	2.70539789
C	1.17105091	-4.90041626	-4.01425762
O	0.29212190	-4.16529073	-4.82518228
O	-1.44819507	-5.09443588	-0.87895004
O	-3.64912147	-2.96775236	2.80336600
C	-3.07716385	-3.44850151	4.01965764
C	-3.57903668	-2.59252120	5.17993255

O	-3.16563017	-1.25054980	5.05041696
O	-1.67840465	-5.03111363	1.93247305
C	-4.14182365	-5.05075540	-2.34498446
O	-5.05450546	-4.31579900	-3.12373973
C	-5.08143307	-2.71322912	5.40387241
C	-6.15782756	5.06275883	4.68274967
C	-1.61894666	10.52118168	1.51096829
C	6.40439737	7.00710860	3.34369726
C	5.71011966	0.18637919	5.72081569
C	3.74272691	-6.12426868	4.63082357
C	-2.31968752	-8.22640302	2.99039658
H	-4.56202090	-1.56391884	-2.29620157
H	-2.48922226	8.61012247	-0.25775262
H	1.52914109	-6.83685246	3.09936936
H	5.21116572	-2.04587608	3.47500276
H	5.75209532	4.25535445	1.95032567
H	0.33223182	8.06619896	1.02810791
H	-3.66248850	3.43214772	3.51696297
H	-3.77486827	-0.79610461	4.45079853
H	-0.77704388	-6.31932363	3.25128722
H	-0.80104662	11.06314702	1.99068220
H	-1.74379794	10.92617762	0.50142307
H	-2.53740477	10.70093346	2.07712447
H	-6.26607850	5.77060345	3.85469224
H	-7.15521533	4.78864687	5.03861129
H	-5.62804139	5.56299679	5.49665266
H	-5.64295804	-2.35126301	4.53690837
H	-5.37311001	-3.75156069	5.59194985
H	-5.37219632	-2.11265398	6.26940002
H	-2.74909971	-7.35890622	2.48067952
H	-2.76145432	-9.13221864	2.56545455
H	-2.58902930	-8.17496169	4.04856014
H	4.28401970	-5.29828278	5.10299117
H	2.95124841	-6.44619380	5.31348270
H	4.43108250	-6.96379577	4.49276928
H	5.21386962	-0.42700496	6.47605524
H	6.79072049	0.07586231	5.85653683
H	5.43731188	1.23279470	5.88389790
H	6.75969468	7.62295504	2.51099616
H	5.92519025	7.65820223	4.08088758
H	7.27443522	6.53699721	3.80701909
H	2.48472199	-4.83577077	3.44185621
H	4.21735243	-0.12212918	4.20262888
H	5.12767803	5.31233534	3.68461788
H	-1.16404128	8.65505567	2.47329017
H	-5.28732341	3.13441533	5.08271792
H	-3.06101035	-2.97775790	6.06901057
H	-0.39821092	-9.09818415	3.38257532
H	-3.35999007	-4.49905736	4.17204034
H	-1.98661081	-3.38547424	3.95334814
H	-6.29499737	3.81698464	2.28671244
H	-7.00466546	2.63213994	3.42772539
H	-3.37196607	8.45386552	1.28764965
H	4.54902987	7.19512536	1.37350999
H	3.69083096	7.20931751	2.93582224
H	7.08975952	0.31313031	3.29207224
H	5.84487230	1.59558710	3.44508196
H	4.84895146	-6.16244580	2.07022822

H	4.85260771	-4.51277354	2.75123755
H	-0.74915548	-9.32126850	0.97702688
H	0.75524236	-8.45679509	1.36519893
H	3.73052125	4.33555468	-2.88273577
H	-5.65788630	0.81307822	-3.30209698
H	-5.76215852	-4.05014552	-2.52421558
H	-3.27404738	-5.26424742	-2.97643987
H	-4.57587989	-6.00837833	-2.01545575
H	-3.24380025	-3.31539359	-1.44947285
H	-3.09816779	-5.99798196	0.00506591
H	-1.20886087	-5.68996706	1.38281368
H	-1.92454285	-3.30880247	0.81333629
H	-4.28556122	-4.77969099	2.05151056
H	-5.70191787	-3.03162307	1.16510286
H	-0.54708870	-4.63842726	-4.83364674
H	2.09560898	-4.31990618	-3.93765459
H	1.41767079	-5.88178098	-4.45131806
H	0.26036784	-4.16311352	-2.22877895
H	2.36107877	-6.35527544	-2.19934531
H	2.41417937	-6.95583353	0.99043225
H	1.01861677	-5.51952425	0.32653831
H	0.11288298	-8.03925400	-1.09061373
H	-1.95279930	-6.91797758	-1.72152991
H	3.98343238	-2.94591364	-4.58290181
H	5.80764843	-2.05636522	-3.51308182
H	4.78823008	-0.64721119	-3.17583983
H	3.20262466	-2.18378987	-1.95885233
H	6.05735570	-2.10019219	-0.86650701
H	5.33570390	-1.48317876	1.62206846
H	3.39472843	-2.35981419	0.56850874
H	5.42584761	-4.57779926	0.25669801
H	4.18677943	-5.62333593	-1.43730396
H	5.21883315	2.04636186	-3.68638562
H	3.78924171	1.48103493	-1.72004921
H	5.44920460	3.63233978	-0.30241154
H	3.81691726	3.57332031	1.93330614
H	3.57411251	1.50135099	0.82228767
H	6.60162735	1.66664624	1.08298424
H	6.73817487	-0.19984229	-0.40948989
H	2.21625781	3.67846507	-3.97399565
H	1.19046444	5.92839072	-3.67734034
H	-0.22687270	4.94415470	-3.23579788
H	1.39326898	3.77722645	-1.56293828
H	0.51227129	6.66724752	-1.04977623
H	-0.39183765	6.18983724	1.40661210
H	1.13324464	4.40677871	0.89235144
H	2.74434063	6.91751082	0.30534068
H	4.41767172	5.46068244	-0.70900080
H	-3.29334120	1.08760050	-3.45332845
H	-3.81326279	3.63485668	-3.60541609
H	-4.49487890	2.45063997	-2.46724997
H	-2.08397749	3.07343342	-1.27374797
H	-4.87149692	4.25335464	-0.91779551
H	-4.27991363	5.05754076	2.26430402
H	-2.63051442	4.37918239	1.10315334
H	-3.61687687	6.68143283	-0.59786193
H	-1.47882685	6.60600753	-1.78487686
H	-6.23639372	-1.00050038	-2.13387515

H	-3.77244282	0.36992132	-0.95847752
H	-6.07912044	-1.10281061	0.41090586
H	-4.47429120	-1.46493629	2.72993868
H	-3.64694477	0.34515748	1.55018072
H	-6.59935531	1.06652280	1.66581139
H	-6.14378526	2.87768133	0.12547317
H	5.86774817	3.44187110	-2.82667499
H	2.32733530	0.31910139	-3.03785940
H	2.05122021	1.45903695	-5.22577506
H	1.83399649	-0.27706265	-5.40831673
H	0.06719956	0.86757440	-6.63597224
H	0.18342747	2.77315483	-4.70563488
H	-1.28340710	2.00674372	-4.36044966
H	-1.63877392	3.84175121	-5.77894463
H	-2.07209300	2.30993532	-6.57619328
H	-0.53464053	3.12763127	-6.98246531
H	1.18835006	-2.67749626	-1.20617064
H	0.85967940	-2.67095499	1.21578170
H	-0.73612252	1.15922888	-1.47748132
H	-2.10838615	-0.08837369	-6.92788130
H	-3.78777560	-1.77689316	-6.24835616
H	-3.54802005	-2.93711933	-4.07262261
H	-1.59778175	-2.44246629	-2.61691842
H	1.08088615	-1.65497318	-3.27857990
H	0.92392805	1.36228534	-2.98936988

255

2-HP-B-CD:cis-(1S,4S)-SRT_5_MD E(Ha)= -7253.9061410569

C	0.83695785	5.71423904	-3.17463692
C	-0.40490590	4.85358805	-3.30512103
C	-0.35623878	3.45312341	-3.21173370
C	0.95610813	2.71240951	-3.00563157
C	2.05808941	3.62904951	-2.46728964
C	2.12848501	4.91471750	-3.28123280
C	-1.61965138	5.48541955	-3.60100321
C	-2.78496824	4.75179593	-3.78454208
C	-2.74045940	3.36097551	-3.67637387
C	-1.53930616	2.72334763	-3.39569594
C	0.79620897	1.45900155	-2.17240353
C	1.22124319	0.22113756	-2.65577274
C	1.04356413	-0.94089648	-1.91342812
C	0.42972039	-0.88161326	-0.66545629
C	0.02288673	0.35805613	-0.15866937
C	0.20668128	1.51437572	-0.90774761
Cl	0.15513423	-2.34099010	0.21640265
Cl	-0.73160071	0.47554014	1.39704632
N	0.82233185	6.50494206	-1.88512109
C	1.55402898	7.78965360	-1.96525671
O	-2.98255870	5.13310279	-0.48209452
C	-3.29065092	4.08943973	0.42521455
C	-2.85867040	4.45125548	1.83730140
C	-3.37520869	3.41473152	2.85000921
O	-4.77408389	3.17595742	2.67428079
C	-5.13573279	2.72137586	1.40245621
C	-4.78304093	3.79774399	0.37654006
C	-3.24566658	3.89322752	4.28711982
O	-3.89806009	5.12662689	4.48251088
O	-1.44106421	4.48622537	1.83430893
C	-0.77293131	5.36711052	2.69941542
C	0.27997447	6.12581940	1.87435610
C	1.25317833	5.09750652	1.32189844
C	1.90682117	4.36439428	2.47967715
C	0.83869176	3.73642269	3.38019877
O	-0.13104419	4.71325231	3.75716343
C	1.43050955	3.17138740	4.65449970
O	2.27563794	4.14297977	5.22866645
O	2.74000683	3.36542601	1.91768614
C	4.04499816	3.23203779	2.42059420
C	5.00153452	3.19253347	1.23501866
C	4.82633411	1.91553690	0.42482097
C	4.86928223	0.68189253	1.32443537
C	3.92621301	0.84251816	2.52014245
O	4.20176743	2.07918470	3.19365452
O	4.76102327	4.33215399	0.42480330
C	5.92270413	4.93477447	-0.11992375
C	5.57675340	5.60669094	-1.43628055
O	4.46457987	6.48196055	-1.29401296
O	5.83747547	1.85776260	-0.55478430
O	4.47914430	-0.45044729	0.55660767
C	5.49957953	-1.36059563	0.24574314
C	5.15356082	-2.07585993	-1.07399675
C	3.95787139	-2.98777597	-0.87798700
C	4.21716574	-3.95835490	0.26982801
C	4.59321500	-3.17003571	1.51949713

O	5.70492771	-2.31387237	1.25301348
C	4.10401495	-0.22005808	3.58833291
O	5.44721985	-0.35776418	3.99173735
O	2.19145619	5.73720555	0.47928250
O	-0.25063713	6.83027454	0.78033468
C	-1.24488587	7.78174050	1.08200419
C	-1.61747945	8.47670449	-0.22011306
O	-1.74283426	7.51019447	-1.25820625
O	-5.08359430	3.38374825	-0.94172540
C	-6.42988210	3.65105037	-1.33676252
C	-6.77399314	2.83642314	-2.57441961
O	-6.78335504	1.45905604	-2.29134849
O	-4.43457261	1.54840396	1.07017016
C	-5.19645500	0.42032702	0.65924680
C	-4.39147406	-0.25375893	-0.44302722
C	-5.10472193	-1.52269707	-0.88912075
C	-5.37607326	-2.40165312	0.34105709
O	-6.12270416	-1.68981740	1.29695145
C	-5.45905317	-0.53803982	1.81467339
O	-4.33400894	-2.27927410	-1.80693597
C	-4.50054439	-1.93881984	-3.18951737
C	-3.18234609	-2.22974287	-3.89597712
O	-2.14745960	-1.46199999	-3.31208058
O	-4.23574878	0.62897994	-1.54385642
C	-6.38021912	0.04887888	2.86838154
O	-7.57544584	0.54635167	2.31154322
O	-4.14524037	-2.81484798	0.85774523
C	-4.02341200	-4.18505832	1.22435834
C	-3.01619691	-4.27188293	2.36630521
O	-2.72185950	-5.63922337	2.65439014
C	-2.20001131	-6.35560458	1.56724025
C	-3.23626507	-6.41159404	0.43787996
C	-3.56760817	-4.99242098	0.00602125
C	-3.51844703	-3.69503107	3.67779479
O	-2.56594704	-3.85186176	4.69742947
O	-4.56341889	-5.01604953	-0.98478888
O	-2.71205974	-7.14782120	-0.64572937
C	-3.15400662	-8.50277436	-0.69010329
C	-2.20069677	-9.33873586	-1.53105993
O	-0.94262398	-9.44715389	-0.90758289
O	-1.05352626	-5.72579777	1.06088053
C	0.17964415	-6.43055812	1.00672122
C	0.73096301	-6.19423144	-0.39458707
C	2.17529591	-6.64641702	-0.50129299
C	2.98895039	-6.04357407	0.64672248
O	2.44205890	-6.39118509	1.88158033
C	1.12240881	-5.88398614	2.08074708
O	2.74603779	-6.19062237	-1.70923889
C	2.99282616	-7.16800930	-2.71228278
C	3.66068104	-6.47478069	-3.89240650
O	4.87666736	-5.87517636	-3.51020178
O	-0.03105308	-6.85983363	-1.37770597
C	0.67976416	-6.25179273	3.48096384
O	0.35230392	-7.62328858	3.51537397
O	2.99621340	-4.64654119	0.47394849
O	4.84444769	-1.18339599	-2.11683170
C	5.94820072	-0.61160991	-2.78499055
C	5.35286621	0.47022296	-3.67370426

O	4.47285685	1.26269304	-2.86928802
O	3.67044107	-3.65546021	-2.08131337
C	4.99193610	-4.00990433	2.71777632
O	5.05835287	-3.24682772	3.89300360
C	6.39420816	1.37459574	-4.29117987
C	6.78088447	6.32154884	-2.02698569
C	-2.88307861	9.30256318	-0.07419004
C	-8.15090229	3.21275730	-3.09106525
C	-2.83593304	-3.71313577	-3.93518744
C	-2.75304327	-10.74188895	-1.71236513
C	3.95988610	-7.47343657	-4.99520493
H	3.45363132	0.03679186	4.43714041
H	-2.14248673	7.29374425	1.49001554
H	-0.45334360	-8.62719233	-1.08796497
H	-2.20855693	-1.62359915	-2.36237324
H	-5.86937925	1.16800801	-2.12280600
H	-2.23943545	6.74687002	-0.90121538
H	4.69353206	7.15200378	-0.63953728
H	3.94461952	0.60852233	-2.37928496
H	4.66850986	-5.06485481	-3.02155579
H	-2.77003659	10.06735459	0.70086343
H	-3.11861302	9.80163125	-1.01682436
H	-3.73073070	8.66389734	0.19617713
H	6.50681331	6.80608275	-2.96715415
H	7.15498503	7.09283570	-1.34314487
H	7.60103580	5.62491741	-2.22527586
H	7.06972719	0.80072345	-4.93188496
H	5.91657182	2.14408128	-4.90299260
H	6.98937929	1.86724305	-3.51528053
H	4.42413931	-6.96022570	-5.84028758
H	4.66132945	-8.23312082	-4.63619579
H	3.05023374	-7.97150391	-5.34355298
H	-2.05445507	-11.33472386	-2.30669856
H	-2.86489226	-11.23273402	-0.74005905
H	-3.72411223	-10.73317579	-2.21592485
H	-1.86746580	-3.85264127	-4.42141048
H	-2.77487058	-4.14252028	-2.93039110
H	-3.58767653	-4.28006160	-4.49417920
H	-8.20210085	4.26856948	-3.37232986
H	-8.38939495	2.60599473	-3.96714619
H	-8.90999707	3.01368927	-2.32809027
H	-2.10826177	-8.85562404	-2.51832528
H	-3.28409949	-1.86368411	-4.92546798
H	-6.02397139	3.07183523	-3.35043370
H	-0.78969744	9.12839574	-0.52615024
H	5.22896187	4.82748124	-2.12454603
H	4.75959114	-0.01625215	-4.46175916
H	2.95661896	-5.71501715	-4.27267610
H	6.65310346	-0.15640445	-2.07422759
H	6.48267017	-1.36319595	-3.38345033
H	6.32608889	5.67944018	0.58852821
H	6.69041275	4.17609225	-0.30205160
H	-0.89363017	8.51401092	1.82503513
H	-7.12699317	3.36974650	-0.53587394
H	-6.54046133	4.72785655	-1.53278281
H	-5.32271207	-2.52719506	-3.62012604
H	-4.73122099	-0.87502594	-3.28018963
H	-3.16952410	-8.92967156	0.32286122

H	-4.17299845	-8.53140356	-1.10118051
H	3.66888194	-7.94045911	-2.31761077
H	2.04823377	-7.63646133	-3.01657389
H	-8.01040577	-0.19651685	1.87707090
H	5.71175781	0.46740693	4.41139790
H	5.66345103	-2.50557952	3.75209468
H	4.23572630	-4.78444846	2.88049423
H	5.94841306	-4.50881600	2.48925984
H	3.71304584	-2.57018066	1.78946896
H	5.01667037	-4.66012784	-0.01185173
H	3.11346934	-4.42911828	-1.85948908
H	3.10384152	-2.36021044	-0.58017905
H	6.02458497	-2.69007785	-1.34963188
H	6.45495187	-0.83165279	0.15801962
H	0.28047955	-7.89815400	4.43288083
H	1.50151202	-6.00515212	4.16718207
H	-0.18485366	-5.62121292	3.73725208
H	1.14048756	-4.78814907	2.00679868
H	0.02146480	-7.50423469	1.16560677
H	-0.97464585	-6.67954328	-1.19915664
H	0.71273320	-5.11063063	-0.57995747
H	2.23096887	-7.74094074	-0.43544297
H	4.01099547	-6.43975988	0.63685589
H	-2.37814292	-4.79700990	4.73358328
H	-4.47750989	-4.17444593	3.93555295
H	-3.69931198	-2.62369748	3.55827691
H	-2.09462818	-3.75213217	2.07394861
H	-4.99650599	-4.57271471	1.56260822
H	-4.51025502	-4.16183606	-1.44344046
H	-2.64634824	-4.52699515	-0.37301728
H	-4.15144270	-6.88988034	0.81292033
H	-1.95616504	-7.35313895	1.94823819
H	-5.88145302	0.89022693	3.35862160
H	-4.50359502	-0.82199996	2.27654756
H	-6.15911062	0.74493576	0.24264833
H	-4.07066314	1.51040510	-1.17198146
H	-3.40469383	-0.53245475	-0.04696420
H	-6.07402966	-1.25692477	-1.33490802
H	-5.99309518	-3.26061474	0.06124081
H	-4.83362539	4.97260772	4.30838562
H	-2.19269051	4.03780708	4.53950343
H	-3.65072549	3.10964309	4.94332251
H	-2.81553023	2.48095956	2.70848747
H	-3.27116142	5.43325382	2.10995759
H	-3.24352950	4.81114153	-1.35756880
H	-2.74600229	3.17757145	0.14003279
H	-5.33160926	4.71900041	0.62190598
H	-6.21251235	2.52369032	1.44675004
H	2.63947267	3.78309962	6.04192114
H	1.98467146	2.25911764	4.39661225
H	0.60031451	2.90086522	5.32269607
H	0.35040033	2.92211719	2.82716350
H	2.50126298	5.06994094	3.07339974
H	2.99715128	5.18728279	0.40383916
H	0.67069493	4.36600802	0.74194248
H	0.80589111	6.81531540	2.55412291
H	-1.48553843	6.04466106	3.18339393
H	3.78968789	-1.19577603	3.22167219

H	2.88522081	0.83644352	2.16710740
H	5.88647612	0.54453206	1.71302269
H	5.40405593	1.74385914	-1.42193433
H	3.83020309	1.95254679	-0.03965396
H	6.02479199	3.22079188	1.63373879
H	4.27706744	4.06868284	3.08871362
H	-6.57358239	-0.72206446	3.62782389
H	3.01441129	3.10097645	-2.51879442
H	2.97822711	5.52882950	-2.96653917
H	2.28499880	4.66957357	-4.33847838
H	0.80473801	6.47711109	-3.96074193
H	1.26441782	5.98705834	-1.09645316
H	-0.15724614	6.72558205	-1.59084826
H	1.05641896	8.44279988	-2.68398526
H	2.58868535	7.60405643	-2.25498070
H	1.53660593	8.23697048	-0.97135677
H	1.67771548	0.15365306	-3.63945940
H	1.38030654	-1.89757754	-2.30043376
H	-0.15038066	2.45784536	-0.50504167
H	-1.65160947	6.56897474	-3.68375534
H	-3.71321086	5.25802145	-4.03475805
H	-3.63724345	2.76724708	-3.82529944
H	-1.52097630	1.63810360	-3.32691472
H	1.28127565	2.38498205	-4.00471471
H	1.87923622	3.85131732	-1.40724376

2-HP-B-CD:cis-(1S,4S)-SRT_6_MD E(Ha)= -7253.9052157931

C	-3.85053244	-3.78272652	-5.24170550
C	-2.35730941	-3.78487262	-5.48007171
C	-1.59641010	-2.61611537	-5.34740721
C	-2.21362214	-1.27653616	-4.98121663
C	-3.69998025	-1.36845463	-4.59686980
C	-4.45308753	-2.39768868	-5.43078835
C	-1.74288456	-4.97507935	-5.89237817
C	-0.38768102	-5.01816120	-6.18188759
C	0.37415405	-3.85415490	-6.05681771
C	-0.22408686	-2.67087439	-5.63666732
C	-1.44331272	-0.56262396	-3.88885202
C	-0.99612174	0.74502858	-4.06601532
C	-0.36540283	1.43235438	-3.03427386
C	-0.16743331	0.81480984	-1.80207881
C	-0.59793891	-0.50656109	-1.61760735
C	-1.22794655	-1.18529369	-2.65560300
Cl	0.58610086	1.69358846	-0.52184022
Cl	-0.37152286	-1.30392685	-0.10064835
N	-4.18189203	-4.30636393	-3.85791677
C	-5.32638288	-5.23978955	-3.81706561
C	-0.39451932	5.50897201	-3.53208644
O	-1.20289625	4.40934844	-3.87002501
C	0.21097184	5.40451064	-2.13116563
C	-0.67453511	5.90962102	-0.98981791
C	0.06934778	5.91648287	0.34567910
C	1.38365704	6.66042027	0.20139235
C	2.16221711	6.07743871	-0.98367142
O	1.40989327	6.17757647	-2.16155960
O	2.16030073	6.54330191	1.37225110
C	2.79878098	7.75076558	1.78357180
C	4.09931500	7.43396569	2.50695480
O	5.02023532	6.83456638	1.62294131
O	-0.71831829	6.52451267	1.34713220
O	-1.79584558	5.06000694	-0.77158961
C	-3.05071092	5.42059230	-1.26776993
C	-4.04038688	5.49618679	-0.10966545
C	-4.22535830	4.14032790	0.55949144
C	-4.46026806	3.03814013	-0.47310371
C	-3.54154306	3.12432492	-1.68949920
O	-3.49449726	4.46520056	-2.20949191
C	-4.03111172	2.26618137	-2.84172541
O	-5.31319209	2.63267245	-3.28584389
O	-4.20368218	1.76461178	0.10670552
C	-5.24070777	1.20064472	0.85505909
C	-4.72704730	0.80194234	2.25008801
C	-3.84678954	-0.44232184	2.19806401
C	-4.50381144	-1.53515387	1.36605473
C	-4.85840679	-0.97817031	-0.01083857
O	-5.78275295	0.07946479	0.19025844
O	-4.03335233	1.89895399	2.78527851
C	-4.11937511	2.07024343	4.18476266
C	-3.44000671	3.37921378	4.52752673
O	-4.21158732	4.41435489	3.91977012
O	-3.62283663	-0.88565663	3.52443686
O	-3.56953488	-2.61226097	1.31194609
C	-4.05476080	-3.91907689	1.43336778

C	-3.52682992	-4.56149479	2.71445449
C	-2.01783729	-4.71899258	2.68744642
C	-1.54943627	-5.33250874	1.36452339
C	-2.25796658	-4.79810035	0.11234799
O	-3.68143795	-4.67162869	0.29792428
C	-2.05940784	-5.72982634	-1.07602799
O	-2.10685871	-5.06251662	-2.32737871
O	-0.17237065	-5.00744556	1.25989533
C	0.75365653	-5.98483663	0.89967193
C	1.99929772	-5.80202507	1.77801035
C	2.78636704	-4.56795108	1.35802312
C	2.99177969	-4.51779290	-0.15220252
C	1.63698093	-4.65150461	-0.84430923
O	1.07982801	-5.91283837	-0.46794681
C	1.70210661	-4.58193947	-2.35047327
O	0.39641794	-4.32963909	-2.86479057
O	3.60076313	-3.26652911	-0.40292650
C	4.62996748	-3.19348112	-1.35994671
C	5.87754089	-2.64538448	-0.67654914
C	5.65020516	-1.21045013	-0.22426330
C	5.09059204	-0.34866884	-1.35919773
C	3.91354507	-1.03905275	-2.06080861
O	4.26474155	-2.37482698	-2.42770304
O	6.19669558	-3.45241875	0.43853864
C	7.23391796	-4.39718108	0.19312956
C	7.12697006	-5.55549151	1.17262280
O	5.93828047	-6.28420383	0.95305565
O	6.85029289	-0.64967214	0.23630091
O	4.62468829	0.87663790	-0.80610823
C	5.51711206	1.95463127	-0.83668898
C	5.37923159	2.78908933	0.45171206
C	4.01669693	3.45442700	0.50364580
C	3.78672091	4.26201188	-0.76953969
C	3.98405024	3.37406834	-1.99221226
O	5.28666916	2.78678906	-1.95087629
C	3.47573097	-0.37729116	-3.35846399
O	2.24571681	-0.90037371	-3.82329599
O	4.02730442	-4.55893133	2.03225900
O	1.54866808	-5.69976759	3.10325826
C	2.37911883	-6.28133563	4.09029609
C	1.78220863	-5.93056733	5.43656031
O	0.45269997	-6.42492646	5.41268073
O	-1.67331784	-5.52457367	3.77220122
O	-3.89408166	-3.74473244	3.80229336
C	-5.05866043	-4.17627207	4.49667003
C	-5.59667728	-3.03041712	5.33926835
O	-6.00358031	-1.95906758	4.51743189
C	-5.55224273	-1.95363893	-0.95753333
O	-4.65510084	-2.85941777	-1.58149489
O	-5.32967953	4.19061066	1.42060757
O	-3.56728495	6.43011656	0.84352707
C	-4.13376324	7.73222712	0.71112223
C	-3.19790191	8.77461695	1.30420574
O	-2.00448924	8.85387534	0.55780189
O	2.45408579	4.74036195	-0.67771384
O	5.55680661	2.02326375	1.61477848
C	6.88836723	1.96460754	2.08760766
C	6.87404232	1.00943686	3.27073613

O	6.21796253	-0.19678512	2.88172026
O	3.93578394	4.28041332	1.64142681
C	3.91217643	4.08633096	-3.32789782
O	4.05572131	3.16759250	-4.38365920
C	8.26207201	0.66134365	3.75827289
C	8.29966122	-6.50447557	1.00123291
C	2.58646693	-6.52834079	6.57902514
C	-6.79491345	-3.48294270	6.15335696
C	-3.34343290	3.59017530	6.02864486
C	-3.85487988	10.14367050	1.29290611
C	4.72259215	8.70617124	3.05435646
H	3.43952319	0.71235015	-3.24394598
H	2.40322607	-7.37619856	3.97235400
H	-1.41029362	8.15377207	0.87783504
H	-3.69820978	5.22824212	3.91086290
H	-5.20359999	-1.47142359	4.25544649
H	-0.00184225	-6.12633281	6.20635125
H	5.22194539	-5.81563147	1.41217086
H	5.36196014	0.09690924	2.53736409
H	4.84436375	5.87901176	1.62955350
H	2.14126605	-6.26454179	7.54375822
H	2.60693029	-7.61967466	6.50275958
H	3.61545168	-6.15541342	6.57793187
H	9.25499170	-6.00067500	1.17482948
H	8.20744536	-7.33297476	1.70680708
H	8.30321775	-6.92420030	-0.01002366
H	8.84748703	0.19350144	2.96020045
H	8.78936680	1.55844591	4.09526083
H	8.20263998	-0.03818899	4.59528990
H	4.96379700	9.39195373	2.23568051
H	4.05348739	9.21667731	3.75344940
H	5.65291303	8.46467320	3.57301059
H	-4.78279199	10.15195471	1.87228381
H	-3.17016752	10.88144723	1.71660066
H	-4.07998150	10.44721983	0.26536510
H	-4.33968946	3.58932579	6.48085181
H	-2.74245536	2.80588150	6.49869344
H	-2.87061527	4.55109446	6.25399496
H	-7.60410690	-3.80643453	5.49059347
H	-6.53831039	-4.30869195	6.82340242
H	-7.16678018	-2.64919879	6.75270397
H	-2.98344188	8.48635553	2.34713777
H	-2.43435939	3.35681313	4.08201404
H	-4.79351556	-2.70962802	6.02287320
H	1.77599055	-4.83184138	5.51894943
H	7.14304888	-5.13987671	2.19347443
H	6.29733759	1.47589232	4.08326318
H	3.86796946	6.75494987	3.34381841
H	7.56361357	1.58134138	1.30901520
H	7.23618198	2.96029343	2.39963804
H	7.14156377	-4.80837060	-0.82250013
H	8.20770569	-3.89459524	0.27874555
H	3.40149770	-5.89227720	4.02320091
H	-5.84291596	-4.47169562	3.78343263
H	-4.80720401	-5.04498629	5.12113711
H	-5.17189209	2.11222620	4.50775023
H	-3.62607429	1.24698508	4.71497292
H	-4.27736968	7.97848550	-0.35037889

H	-5.11408444	7.74821443	1.20771260
H	3.04667783	8.36518929	0.90709006
H	2.11316161	8.31906149	2.42741317
H	-4.27545608	-3.47320445	-0.92100246
H	1.54203162	-0.46205683	-3.33331880
H	4.90342256	2.73221280	-4.23554204
H	2.94039640	4.57446718	-3.43780478
H	4.68780277	4.86891365	-3.35894841
H	3.22109081	2.58385183	-1.97011532
H	4.49208476	5.10651719	-0.79141708
H	3.12570078	4.81741443	1.55185320
H	3.25121071	2.66491584	0.55224794
H	6.14366615	3.57980110	0.39952992
H	6.54383182	1.59338742	-0.94314750
H	-2.04125339	4.47085183	-3.38399759
H	-0.92710718	6.46606874	-3.64732904
H	0.44153661	5.52414287	-4.23815073
H	0.45551775	4.35191874	-1.94022557
H	-1.01610783	6.93346998	-1.20590623
H	-1.62476612	6.17837630	1.24774843
H	0.28457364	4.87319580	0.61782054
H	1.16517503	7.71542822	-0.01251344
H	3.08232926	6.64834433	-1.15442722
H	-5.26723012	3.56685920	-3.51978444
H	-4.09003903	1.23041255	-2.49566745
H	-3.28991801	2.31335344	-3.65329774
H	-2.53155078	2.81237377	-1.39683627
H	-5.50146131	3.09695419	-0.82003006
H	-4.99222092	4.18322874	2.33558212
H	-3.30464409	3.88448596	1.10000713
H	-5.01617950	5.81193085	-0.50164843
H	-2.99882874	6.37456480	-1.80722125
H	-6.01393944	-1.35817610	-1.74988338
H	-3.94698530	-0.61187630	-0.50558810
H	-5.42308064	-1.86292043	1.87364777
H	-3.32053163	-1.80954270	3.48661732
H	-2.89180295	-0.16994641	1.72453101
H	-5.61285971	0.56408368	2.86042675
H	-6.06233935	1.91156813	0.96464999
H	-1.17800465	-4.83775444	-2.56994300
H	-2.85092617	-6.48775508	-1.05086633
H	-1.09275118	-6.23201668	-0.98645657
H	-1.83713247	-3.81110085	-0.11191657
H	-1.68414333	-6.42225460	1.44323999
H	-0.70911522	-5.60888792	3.86482936
H	-1.56738726	-3.71513466	2.74762098
H	-3.96911625	-5.56253938	2.81302447
H	-5.15211348	-3.92394096	1.44071415
H	0.47998376	-3.95909883	-3.75270715
H	2.09911826	-5.52745662	-2.74576573
H	2.36433184	-3.75756640	-2.63802614
H	0.98684129	-3.83659577	-0.50105075
H	3.65798044	-5.33914952	-0.45601200
H	4.59040061	-3.88576487	1.60595536
H	2.19601330	-3.68402498	1.64359566
H	2.63506388	-6.68993055	1.63942510
H	0.33788302	-6.98787773	1.05445355
H	4.22403893	-0.60605763	-4.12490078

H	3.06703117	-1.06047904	-1.35915881
H	5.89187187	-0.15918028	-2.08958783
H	6.81480642	-0.65143344	1.21140012
H	4.88460455	-1.22160550	0.56538187
H	6.70357648	-2.64510915	-1.39996826
H	4.82281024	-4.18584292	-1.78652439
H	-6.35880162	-2.48917933	-0.43662285
H	-4.16134752	-0.38232541	-4.70822564
H	-5.51895451	-2.40497030	-5.17197039
H	-4.39277291	-2.14861550	-6.49623994
H	-4.31177878	-4.49480904	-5.93403263
H	-4.39794228	-3.53438267	-3.18984834
H	-3.34328006	-4.75202646	-3.40307712
H	-5.54536560	-5.47578958	-2.77490215
H	-5.07594957	-6.15270041	-4.35939487
H	-6.20027088	-4.76967847	-4.27175863
H	-1.14931489	1.25618738	-5.01250198
H	-0.08279976	2.46877128	-3.18399247
H	-1.54731682	-2.20918399	-2.48687794
H	-2.34468116	-5.87443821	-6.00630560
H	0.07128063	-5.94385053	-6.51432742
H	1.43473185	-3.86429501	-6.29186566
H	0.38723536	-1.77850110	-5.52222500
H	-2.14247816	-0.65641048	-5.88586124
H	-3.78153436	-1.61493277	-3.53055682

255

2-HP-B-CD:cis-(1R,4R)-SRT_1_Cl E(Ha)= -7253.9000078227

Cl	2.08693560	2.11721561	3.14332424
Cl	-0.43164706	3.98072412	2.53754371
O	-5.79136556	-0.56998294	-2.28041197
O	-3.17330426	-3.10090896	-1.85729510
O	-2.60190331	-4.53005890	-3.57604018
O	0.64110416	-5.05390771	-1.97131966
O	2.50361778	-5.47002057	-3.29084281
O	4.24622392	-2.87301095	-1.39340252
O	6.04401222	-1.75053635	-2.34328280
O	4.74732507	1.50216120	-1.26742762
O	5.07603682	3.33760140	-2.63991135
O	1.91896586	4.86593582	-1.60422390
O	0.60717907	5.97938851	-3.14921911
O	-2.37554083	4.71425447	-1.46302645
O	-4.35260876	4.39133465	-2.61936673
O	-3.82973059	5.30052278	0.87161236
O	-4.83159103	2.66337906	1.11669946
O	-4.56642612	1.03980545	-1.14633352
O	-1.30238421	6.48566796	0.47735047
O	1.53953873	6.79979295	0.24486097
O	-1.62804955	6.56100193	-4.61733647
O	3.46177669	4.94769842	0.80290034
O	5.45581055	2.88719661	0.92342627
O	4.33142140	5.52913784	-4.20297754
O	5.33989349	-2.70464340	1.05142779
O	5.15350582	0.22862579	1.19170612
O	3.78326656	-4.86110314	0.62955777
O	1.72617159	-6.70046537	0.04766502
O	5.01400006	-5.01094489	-4.30519302
O	-0.89720783	-5.92752368	-5.22569900
O	-3.72143348	-5.22837437	-0.17908542
O	-1.10172098	-6.29908088	-0.16541776
O	-3.89432079	-2.58604358	0.82190225
O	-5.24428907	-0.14296070	1.30241356
O	-6.05914373	-2.93757524	-3.82051923
O	-6.41570810	2.98396228	-3.72329763
O	7.43717719	0.44219845	-3.38544678
O	-6.20020473	-4.13690328	0.89214449
O	-7.41652894	1.64525897	1.46667995
O	-3.62011569	8.03977426	0.25544860
O	3.92977892	7.73723659	1.39504204
O	7.16015002	1.57227447	2.74425480
O	3.29108814	-3.24745088	2.91260342
O	-0.04491154	-8.72075861	-0.97499965
N	1.47621515	-4.83080308	4.05680345
C	-0.02493312	-4.70447688	3.83826503
C	-0.33426257	-4.30393744	2.40461464
C	-0.16542626	-2.80634927	2.18157874
C	-1.11257862	-2.00692662	3.08049889
C	-1.48576514	-1.63624136	5.56183194
C	-1.48435371	-2.05273113	6.88651392
C	-1.03155012	-3.32756281	7.21919192
C	-0.58045116	-4.16500993	6.20970844
C	-0.56225602	-3.74464064	4.87294619
C	-1.02730739	-2.46536093	4.53101804
C	-0.92621014	-0.51080417	2.92724831

C	0.32663867	0.07805920	3.10361720
C	0.49958084	1.45194771	2.97015990
C	-0.60095915	2.26988172	2.68944886
C	-1.85600039	1.69102475	2.51912395
C	-2.01274582	0.31236101	2.62355696
C	2.10936306	-6.05063368	3.49564077
C	-4.65042881	-1.33840772	-2.65943582
C	-4.34101793	-2.34933640	-1.55652150
C	-4.11576934	-1.64977935	-0.22226346
C	-5.36588001	-0.83513547	0.07537764
C	-5.63717393	0.13963855	-1.07713003
C	-3.37237021	-4.37908313	-2.41994315
C	-1.19294700	-4.37154591	-3.40036909
C	-0.69320301	-5.36353659	-2.35264560
C	-1.51007502	-5.29438821	-1.06893426
C	-2.98702633	-5.43124096	-1.36850998
C	1.68274756	-5.94704696	-2.26118409
C	2.50786530	-6.10927634	-0.97913345
C	3.03288731	-4.74627319	-0.56556898
C	3.87977266	-4.20504045	-1.71598452
C	3.11809599	-4.20461120	-3.04486138
C	5.60540326	-2.53347408	-1.27650647
C	5.38581360	-0.48666550	-2.49548471
C	5.50825366	0.31136809	-1.20006551
C	4.99233640	-0.48734360	-0.00729177
C	5.77141458	-1.79295137	0.05706674
C	5.44030918	2.72086687	-1.44195467
C	5.13611861	3.61955937	-0.24032792
C	3.67704708	4.04076710	-0.24952017
C	3.31968962	4.64240179	-1.60297554
C	3.69585231	3.70212342	-2.74594443
C	1.43352509	6.11617146	-2.02738429
C	0.66637672	6.74426746	-0.85966569
C	-0.54775101	5.88999873	-0.55327468
C	-1.39130317	5.68068710	-1.80258323
C	-0.55112398	5.16076257	-2.96822530
C	-3.73381667	5.04297219	-1.53876011
C	-4.27859685	2.96442795	-2.59795659
C	-4.84540718	2.42784646	-1.28359487
C	-4.22500713	3.11547014	-0.07518918
C	-4.39519385	4.61402776	-0.22188354
C	-5.09472957	2.51396481	-3.79950651
C	-1.29823275	5.23598252	-4.29012345
C	3.55254418	4.36280486	-4.10648027
C	6.08007366	0.19814007	-3.66066984
C	4.05743709	-3.98542213	-4.22125245
C	-0.58803441	-4.63555496	-4.76988381
C	-5.01291203	-2.00737303	-3.97370806
C	-4.66064827	6.26744256	1.51363611
C	1.56654691	8.02353742	0.97168993
C	6.09174254	3.61126966	1.97593472
C	5.48173041	-2.34997365	2.42675446
C	1.93842507	-8.10629811	0.23252941
C	-4.95667175	-5.94268763	-0.13653139
C	-6.29918444	-0.34086455	2.24913850
C	-5.78532830	-5.47481530	1.05049969
C	0.62267198	-8.87254279	0.25798577
C	4.11507051	-2.07703035	3.03422151

C	6.33623088	2.65007480	3.12990660
C	2.67776698	7.93382505	2.00841623
C	-3.97848318	7.63053615	1.55879061
C	-6.95580041	0.98282375	2.62609329
C	-7.03053668	-6.33128961	1.19331765
C	-8.12977177	0.74224295	3.55892216
C	-4.90931379	8.66767108	2.16132372
C	2.75416092	9.21458390	2.81864928
C	7.01931336	3.36223749	4.28162960
C	4.21675909	-1.72127545	4.50141299
C	0.88029648	-10.35042524	0.49945464
H	0.28193473	-4.88126984	1.70895926
H	-0.37669672	-2.56169832	1.13573132
H	0.87658280	-2.51312149	2.36171567
H	-2.13391468	-2.23185674	2.73720012
H	-1.84567568	-0.64247600	5.31324876
H	-1.84500472	-1.38337804	7.66168242
H	-1.04461477	-3.66808397	8.24966369
H	-0.26131459	-5.17737455	6.45973804
H	1.19460097	-0.52544795	3.35130049
H	-2.71074630	2.32730680	2.30453030
H	-2.99545158	-0.12322648	2.45722422
H	3.16729774	-6.03652244	3.75858056
H	2.02260887	-6.04478064	2.40767216
H	1.62471609	-6.93374564	3.91526451
H	1.63105723	-4.80303192	5.06677699
H	2.01071435	-4.00773951	3.67090512
H	-0.40880783	-5.71162181	4.03922400
H	-1.36771209	-4.60169039	2.19416840
H	5.94803746	-0.41800615	-4.56223341
H	-3.87603201	6.11710945	-1.69830570
H	-5.46619548	4.84483514	-0.29525575
H	-3.14965086	2.88753633	-0.05665556
H	-4.76705192	1.68734329	1.11284929
H	-5.93117989	2.59703732	-1.28980559
H	-3.23418850	2.63622752	-2.69761845
H	-5.14378206	1.42158601	-3.81569402
H	2.26042403	6.76193987	-2.34152415
H	0.35209080	7.75605661	-1.15077105
H	-0.18386993	4.90586323	-0.22589074
H	-2.03256192	5.87164879	0.69169055
H	-1.86411140	6.62431247	-2.10792249
H	-0.25102686	4.12517952	-2.75575123
H	-0.68577057	4.76041851	-5.07154846
H	-2.23812476	4.68293983	-4.20369176
H	-0.79612926	7.04802489	-4.64558666
H	6.51645865	2.53266818	-1.51837493
H	5.77122407	4.51359821	-0.31045738
H	3.06181788	3.13896427	-0.10433131
H	2.57873509	5.34581715	0.67669645
H	3.85988697	5.58916272	-1.73535953
H	3.06504717	2.80351822	-2.69594735
H	3.81501657	3.62906109	-4.88356004
H	2.51001961	4.65940002	-4.25348236
H	5.24786595	5.26237327	-4.06725142
H	6.22967025	-3.43482893	-1.29061830
H	6.83735725	-1.56681828	0.20643987
H	3.92940848	-0.72056614	-0.17181809

H	4.93847947	1.16952918	1.01901772
H	6.56975815	0.54509027	-1.04132298
H	4.32268916	-0.64059290	-2.72828736
H	5.60884587	1.16928363	-3.83621793
H	1.29102583	-6.91453580	-2.59421836
H	3.36691800	-6.75459290	-1.20047348
H	2.18413414	-4.06442608	-0.41498541
H	4.49322594	-4.18746427	0.60446580
H	4.77565855	-4.83158911	-1.83563579
H	2.35610608	-3.41351918	-3.00893846
H	3.45997340	-3.90335719	-5.14094860
H	4.60291693	-3.04841384	-4.07921721
H	4.52512717	-5.82840714	-4.45453365
H	-4.41340085	-4.49313012	-2.74138202
H	-3.18503682	-6.43452592	-1.77281828
H	-1.34663285	-4.30068346	-0.62386241
H	-0.12994363	-6.23073299	-0.09122200
H	-0.74628464	-6.37358781	-2.78128793
H	-0.96580103	-3.34844539	-3.07078832
H	0.50188994	-4.57258012	-4.70185618
H	-0.93763376	-3.85814064	-5.46517981
H	-1.85833027	-5.97464536	-5.28636485
H	-6.58347782	0.66158627	-0.90087716
H	-6.21686788	-1.52642072	0.12485958
H	-3.25094905	-0.97615605	-0.29942668
H	-3.54153406	-3.39754947	0.41108163
H	-5.20292758	-3.02100216	-1.44914082
H	-3.78062760	-0.68209615	-2.80635250
H	-4.14682428	-2.55803771	-4.35227730
H	-5.26646804	-1.22611556	-4.70460054
H	-6.82300433	-2.44703238	-3.49488094
H	-6.35601076	3.94550714	-3.67541683
H	7.85743385	-0.41724042	-3.26852435
H	-4.74247588	-7.01809540	-0.05732347
H	-5.53537814	-5.76731181	-1.05455299
H	2.49847232	-8.25555636	1.16587114
H	2.54172615	-8.50128993	-0.59287384
H	6.12310172	-1.47277072	2.54009543
H	5.94611933	-3.20624803	2.93169839
H	5.45398518	4.44488586	2.29080406
H	7.05476369	4.00311156	1.61779106
H	0.59319036	8.19458549	1.44867575
H	1.78416730	8.85449078	0.28496376
H	-4.89067195	5.91201844	2.52608714
H	-5.60345159	6.37047454	0.96217429
H	-5.87783520	-0.83031398	3.13630118
H	-7.05773194	-1.00705528	1.82175499
H	-5.16360947	-5.58324666	1.95539012
H	-6.20712794	1.60592395	3.13944196
H	-3.07781521	7.54541920	2.18685445
H	2.43837068	7.09280011	2.68212820
H	5.35038308	2.28098468	3.46615577
H	3.65691755	-1.24859225	2.48031193
H	0.00185387	-8.47403860	1.07681378
H	6.41333317	4.19356729	4.65265431
H	7.99216611	3.74911252	3.96320128
H	7.18915274	2.66000952	5.10105724
H	4.78760888	-0.79727451	4.62615694

H	4.71409634	-2.51705403	5.06584819
H	3.22352363	-1.55921422	4.93106924
H	1.41388030	-10.52400560	1.43920950
H	1.47205909	-10.76894800	-0.32058850
H	-0.06943821	-10.88818360	0.53333291
H	-6.78050886	-7.38346748	1.35663372
H	-7.65075547	-6.25244466	0.29487015
H	-7.62176245	-5.97675231	2.04027983
H	-7.82646915	0.19777044	4.45883170
H	-8.90537568	0.16471559	3.04615254
H	-8.56597072	1.69696651	3.86053382
H	-5.24338060	8.37711586	3.16229848
H	-5.78920416	8.79963170	1.52356110
H	-4.39800664	9.63024503	2.23068795
H	1.81187216	9.42031744	3.33487215
H	2.99078139	10.06077858	2.16595150
H	3.54988125	9.13180499	3.56222164
H	-5.43332196	-3.55946072	1.04718703
H	-6.72151543	2.27448441	1.22196417
H	-2.71094770	7.73173624	0.11942484
H	3.96080701	6.82476310	1.07201399
H	6.68393805	1.06602496	2.07111216
H	3.38804369	-3.64466800	2.02495455
H	-0.68215720	-7.99895015	-0.85820949
H	-4.59007305	2.85379795	-4.71660891

2-HP-B-CD:cis-(1R,4R)-SRT_2_CI E(Ha)= -7253.8951936597

Cl	-5.95566898	-8.50966099	3.62305365
Cl	-4.74029897	-5.57229983	3.29176721
O	-4.88695791	-0.87957395	-3.11613263
O	-1.53601665	-2.36072210	-3.00951103
O	-0.51037491	-3.16928973	-4.91702764
O	2.71428393	-2.51582164	-3.32892679
O	4.55135823	-1.70427505	-4.47623130
O	5.30738333	0.31258503	-1.54479697
O	6.71735321	2.14540556	-1.44149894
O	4.09611427	4.10985038	0.19923148
O	3.92010689	6.36212407	-0.31606162
O	0.28470062	6.34591178	0.08222270
O	-1.08418532	7.41308905	-1.43321844
O	-3.62378257	4.89500127	-0.68850908
O	-5.12576473	4.29614771	-2.34224244
O	-5.55120975	4.39540369	1.27281724
O	-5.57695616	1.58387452	0.76023154
O	-4.29789628	0.80655393	-1.63715157
O	-3.51110831	6.32759652	1.73796764
O	-0.98716166	7.57511826	2.19908688
O	-3.19693310	7.66355876	-3.15635025
O	1.18286108	5.83661369	2.73655890
O	3.76556507	4.57685544	2.82200451
O	2.58318770	8.67232893	-1.28758591
O	5.85792641	-0.32318614	1.02035770
O	4.54493631	2.09900027	2.09399279
O	5.74552641	-2.43989182	-0.56721017
O	4.31215764	-4.34655959	-1.99647952
O	6.70338774	-0.06572114	-4.96267649
O	1.68353917	-3.46344962	-6.65165829
O	-1.10918676	-4.80714154	-1.70773394
O	1.68260330	-4.56630479	-1.68986194
O	-2.36834923	-2.68276995	-0.35626016
O	-4.48107842	-1.00070726	0.51209988
O	-4.31154768	-2.86730523	-5.06519471
O	-6.31241175	2.65544678	-4.16545716
O	7.34799249	4.85592928	-1.16386288
O	-3.89873115	-4.93412015	-0.80136197
O	-7.25017586	-0.68639128	0.70946000
O	-6.13957569	7.15588046	1.28441838
O	1.46104362	8.52065265	3.42690585
O	5.60220737	3.23792705	4.50763863
O	3.92557218	-2.32388038	1.90020866
O	3.06719504	-7.02882346	-2.09600473
N	0.81728256	-4.70640205	0.92595705
C	0.74741445	-3.29723138	1.39119908
C	-2.02730430	-9.17274133	3.33991867
C	-3.39874422	-9.35037723	3.47456783
C	-4.25924206	-8.25505264	3.45878975
C	-3.72429402	-6.96922511	3.31510850
C	-2.34857004	-6.80155843	3.18837981
C	-1.48346202	-7.89640509	3.19166768
C	0.60190955	-6.55100168	3.74140839
C	1.46621807	-5.60640570	3.16704930
C	2.10737413	-4.65694348	3.97347721
C	1.86554994	-4.60884062	5.33921690

C	0.98274794	-5.52352544	5.91143077
C	0.36929104	-6.48539175	5.12024316
C	0.00223689	-7.70620975	2.95349136
C	0.27930834	-7.63250139	1.44038651
C	1.64031810	-7.02981805	1.11241275
C	1.75892966	-5.62438507	1.68996097
C	-3.55729149	-1.11193021	-3.57016743
C	-2.89936955	-2.14137321	-2.65641907
C	-2.92751751	-1.68612217	-1.20492223
C	-4.37903722	-1.43102790	-0.82693578
C	-4.97952412	-0.40292154	-1.79330285
C	-1.23707932	-3.50460815	-3.76998249
C	0.70765585	-2.46580602	-4.67279161
C	1.61201072	-3.29222291	-3.75769840
C	0.86874667	-3.72749547	-2.50354713
C	-0.40506753	-4.45207919	-2.88677492
C	4.00315847	-2.80655383	-3.82629487
C	4.87108291	-3.20773074	-2.63358480
C	4.94363146	-2.05169412	-1.65443615
C	5.48166582	-0.81902241	-2.38211748
C	4.71169098	-0.52940932	-3.67456804
C	6.41404836	0.89454190	-0.90467564
C	5.67171799	3.11933549	-1.35191811
C	5.24184498	3.28146755	0.10404950
C	4.87726356	1.94112781	0.73603741
C	6.07004411	1.00565615	0.58796346
C	4.26801284	5.43076367	0.66551055
C	3.41226951	5.60665100	1.92390119
C	1.93352561	5.55641030	1.57446901
C	1.63762239	6.54538236	0.45570207
C	2.55523642	6.30771610	-0.74106782
C	-0.51539213	7.48128094	-0.15782959
C	-1.59890932	7.52845446	0.92839386
C	-2.45718736	6.28578802	0.80758627
C	-2.99963574	6.16717052	-0.61314848
C	-1.90189736	6.26418052	-1.67092386
C	-4.97663095	4.79868587	-1.03824314
C	-4.53522396	3.01573738	-2.56766485
C	-5.06641160	2.00250172	-1.55588918
C	-4.97530667	2.50490247	-0.11895725
C	-5.64860471	3.86030523	-0.02723388
C	-4.91945810	2.65660211	-3.99480630
C	-2.46743805	6.46684445	-3.06755647
C	2.40377002	7.37800930	-1.80758122
C	6.25753793	4.39886313	-1.92505185
C	5.46262935	0.45314580	-4.56001961
C	1.34789873	-2.24568008	-6.03312788
C	-3.67875887	-1.61044574	-4.99987683
C	-6.75975742	4.89616712	1.84219962
C	-0.81353664	8.89767782	2.70257971
C	3.91310909	4.94869920	4.19118699
C	5.56446964	-0.58618278	2.39439449
C	5.01258124	-5.56785927	-2.24262753
C	-1.98011983	-5.93336509	-1.88658125
C	-5.23758342	-1.83532116	1.39048090
C	-2.99722994	-6.01000853	-0.75554711
C	4.31876798	-6.71115943	-1.52225832
C	4.12601654	-1.05907696	2.53236871

C	4.36199011	3.72116427	4.97077819
C	0.16990629	8.88572490	3.86240124
C	-6.57462442	6.32474571	2.34064576
C	-6.52987218	-1.15063924	1.83372544
C	-3.79718649	-7.29662755	-0.85763975
C	-7.39868821	-2.12045953	2.61424646
C	-7.88310366	6.86822383	2.88668635
C	0.26252973	10.26420072	4.49129664
C	4.51852791	4.05395159	6.44257608
C	3.74033955	-1.19616139	3.99182311
C	5.16626987	-7.96852372	-1.58018108
H	0.40456391	-3.28007243	2.42520895
H	1.74605281	-2.85418114	1.33463243
H	0.03002672	-2.76557337	0.76319679
H	-1.37548713	-10.04231913	3.35416027
H	-3.81824831	-10.34339787	3.59583485
H	-1.95801421	-5.79080883	3.11217358
H	2.81002290	-3.96389720	3.51442921
H	2.36952374	-3.87068895	5.95575895
H	0.78537962	-5.49800827	6.97892801
H	-0.30004846	-7.21033528	5.57576371
H	0.50714837	-8.60883275	3.32662224
H	-0.52379313	-7.05977547	0.95407282
H	0.19905614	-8.63596794	1.01139058
H	1.82766108	-7.04065196	0.03198424
H	2.43457670	-7.63084469	1.56975891
H	2.75102495	-5.19896903	1.50590431
H	1.11090647	-4.70806415	-0.08175441
H	-0.12153084	-5.10816473	0.94287422
H	-2.97504430	-0.17924099	-3.54911499
H	-3.45870814	-3.08281173	-2.73610881
H	-2.35861741	-0.75330505	-1.09473174
H	-4.94592298	-2.36078813	-0.96448357
H	-6.04797595	-0.29423393	-1.58579138
H	-2.15749417	-3.97785540	-4.12886627
H	0.49760333	-1.50073584	-4.19257375
H	1.95039916	-4.17698400	-4.31475123
H	0.60365146	-2.82423111	-1.93675788
H	-0.15392292	-5.35642570	-3.45908140
H	3.95026698	-3.60545368	-4.57508635
H	5.88358872	-3.44276872	-2.98461142
H	3.92192157	-1.81097791	-1.32076759
H	6.54293402	-0.96476016	-2.62804483
H	3.72613426	-0.12602793	-3.40546364
H	7.31130846	0.28005201	-1.04403547
H	4.80597813	2.80072507	-1.94937776
H	6.07844870	3.72327201	0.66215559
H	4.02780318	1.51108203	0.18497260
H	6.93144528	1.43511294	1.12068376
H	5.32323925	5.61615232	0.89240315
H	3.64494574	6.58763738	2.36108009
H	1.69884553	4.54400376	1.21131631
H	1.78724460	7.56646092	0.83072728
H	2.33647630	5.32112554	-1.17354593
H	0.09972494	8.38796492	-0.15172721
H	-2.22780349	8.41680993	0.77399122
H	-1.81845845	5.41038220	0.99757892
H	-3.72967090	6.96708025	-0.79841440

H	-1.28893232	5.35314000	-1.63423993
H	-5.46179335	5.78048364	-1.02337342
H	-3.44210604	3.07934630	-2.46985509
H	-6.11612284	1.79506201	-1.80503942
H	-3.91464056	2.63196784	0.13863612
H	-6.70334277	3.75398458	-0.31320829
H	-4.42246876	3.35827669	-4.68223118
H	-4.56668881	1.64640271	-4.22067795
H	-1.63847349	6.43713312	-3.79139276
H	-3.15895619	5.65160428	-3.29914165
H	3.11062188	7.16197955	-2.62265836
H	1.38981119	7.33451139	-2.21603753
H	6.53556294	4.21923357	-2.97399388
H	5.49702091	5.18440230	-1.90036975
H	4.82742288	0.71641665	-5.41859181
H	5.66402681	1.36396502	-3.98935162
H	2.27738621	-1.68300209	-5.90415464
H	0.66577265	-1.64374241	-6.64981706
H	-2.67996326	-1.73394606	-5.42888601
H	-4.21361791	-0.85252671	-5.58945432
H	-7.06308597	4.23185766	2.66166337
H	-7.55495321	4.89653983	1.08607904
H	-1.78951633	9.28932997	3.02266345
H	-0.41038563	9.55598080	1.91934030
H	2.96009585	5.32941571	4.57680184
H	4.67879279	5.73288072	4.27683004
H	5.73157193	0.30726774	2.99926913
H	6.24729992	-1.37966246	2.72338702
H	6.03973379	-5.46039947	-1.87224566
H	5.04019379	-5.78335826	-3.32033838
H	-1.36820068	-6.84586432	-1.92730097
H	-2.53084080	-5.84068398	-2.83120858
H	-4.60807140	-2.06411957	2.25919424
H	-5.47607299	-2.78130420	0.88847349
H	-2.44921200	-6.01350165	0.20551876
H	4.19894319	-6.40441279	-0.46749852
H	3.48766267	-0.29842453	2.06029164
H	3.57775935	2.95187978	4.85454393
H	-0.20347596	8.16879607	4.61232873
H	-5.82310901	6.31538809	3.14551935
H	-6.26445300	-0.30092373	2.48089772
H	-3.15614714	-8.18013512	-0.78734493
H	-4.34106724	-7.32954203	-1.80672270
H	-4.53034843	-7.32989912	-0.04926004
H	-6.86273865	-2.53962559	3.47239062
H	-7.71919327	-2.94280050	1.96668357
H	-8.29274490	-1.61119580	2.98050315
H	-8.27688669	6.23971069	3.69154591
H	-8.63039401	6.92339208	2.08853157
H	-7.73224381	7.87777702	3.27510529
H	-0.70534755	10.59691618	4.87713557
H	0.61826429	10.99379334	3.75668186
H	0.97879000	10.24236519	5.31548700
H	3.57877978	4.40948798	6.87462689
H	5.28267874	4.82583944	6.57633474
H	4.84106643	3.16465756	6.98880237
H	3.79651610	-0.22639462	4.49410990
H	4.40613901	-1.89771868	4.50589416

H	2.71492123	-1.56561417	4.08231213
H	6.12631019	-7.82690974	-1.07685318
H	5.34906798	-8.25795956	-2.61946410
H	4.63524084	-8.78984160	-1.09382148
H	-5.01497619	0.78585311	0.74472492
H	-4.01972654	5.49967207	1.63357288
H	-2.59093349	8.36945457	-2.90236993
H	0.29653767	6.13819396	2.46073620
H	3.47339722	8.70758678	-0.91915004
H	4.01314416	2.91745779	2.18328533
H	5.94500071	-1.63226765	-0.04879215
H	6.51604809	-0.85896499	-5.47716066
H	0.85644310	-3.92461910	-6.83106284
H	2.62486421	-4.26935273	-1.76311761
H	-1.75813033	-3.20236514	-0.91029442
H	-5.19963716	-2.75047808	-4.70750937
H	-6.61295843	3.53662122	-3.91273683
H	8.02535143	4.17178873	-1.21072156
H	-3.44710894	-4.13850001	-0.46789472
H	-7.00584690	0.24373682	0.59247730
H	-5.17101421	7.16528482	1.33215129
H	1.46404612	7.55766459	3.29615416
H	5.47056878	2.89900469	3.61070974
H	4.47606529	-2.38531151	1.10274569
H	2.50783165	-6.23883886	-2.10463564

2-HP-B-CD:cis-(1R,4R)-SRT_3_C1 E(Ha)= -7253.8909898488

Cl	2.26515414	-4.94786331	-6.06491461
Cl	-0.67691633	-5.46739551	-4.94560754
O	-5.69163501	0.18264117	-1.70187069
O	-3.75041478	-1.89002493	0.61142647
O	-3.23522890	-4.05095667	-0.05546782
O	0.22854262	-3.45032829	0.97268369
O	1.85531323	-4.32471859	-0.42750226
O	4.02136268	-1.43271058	0.17148176
O	5.41920221	-0.70725894	-1.52634000
O	4.80460837	2.79818138	-0.67464572
O	4.89072040	4.39324095	-2.35198842
O	1.88955605	5.98479057	-1.00410686
O	0.57148111	7.28437551	-2.39622096
O	-2.43547361	5.55140762	-1.22120137
O	-4.03112683	4.91628543	-2.76310789
O	-4.34033795	6.71182788	0.38475848
O	-5.80124739	4.31674640	0.91814411
O	-4.99387293	2.10814268	-0.61842005
O	-1.57924183	6.90936248	1.12274422
O	1.18456840	7.55662050	1.18032938
O	-1.77441203	7.79955398	-3.89901058
O	3.75688745	6.43666582	1.06434166
O	5.91295537	4.51347773	1.11379598
O	4.02444986	6.35258063	-4.03774920
O	5.93563566	-0.98214069	2.03961224
O	6.15227666	1.85603773	1.64308971
O	3.91352812	-2.62957929	2.75356740
O	1.64505278	-4.30398614	3.19603100
O	4.05918634	-4.32981519	-2.09705372
O	-1.74414783	-6.09828796	-0.87753429
O	-3.85778514	-2.74648210	3.29415019
O	-1.14681205	-3.64654762	3.43796955
O	-5.69716120	-0.77965550	2.30938759
O	-6.82406376	1.68851671	1.40786913
O	-5.57014363	-2.43160557	-2.51699864
O	-5.73464068	3.17237658	-4.04528374
O	6.50541473	0.99808776	-3.39116337
O	-6.54860091	-3.37468294	2.90632440
O	-8.48247919	3.74475543	0.41190981
O	-2.94319227	9.25658146	0.58255954
O	3.41079336	9.23537962	0.88983024
O	8.37458000	3.63972090	2.20103113
O	6.62395105	-3.23332122	3.59179467
O	-0.36594449	-6.25714179	3.46304001
N	-1.05994392	-7.86676323	1.26610469
C	-2.48148221	-8.09098016	1.61438228
C	2.84442759	-7.67903542	-3.21143027
C	3.05284281	-6.76601880	-4.23779426
C	1.97873077	-6.06729869	-4.78677749
C	0.69136524	-6.29502561	-4.28779380
C	0.49257325	-7.19806497	-3.24570151
C	1.56402754	-7.90242595	-2.69760103
C	0.08833981	-9.59866817	-1.46097066
C	-0.64920267	-9.79479071	-0.27913548
C	-1.74486933	-10.66837851	-0.28283430
C	-2.15026159	-11.30963092	-1.44493653

C	-1.43986611	-11.09425290	-2.62324872
C	-0.32949761	-10.26055221	-2.62099592
C	1.38759775	-8.80885369	-1.49401002
C	1.61442549	-7.98764377	-0.21854490
C	1.23087491	-8.76394463	1.03262059
C	-0.24649395	-9.12703918	1.01437105
C	-4.57989876	-0.60424652	-1.27907738
C	-4.89377334	-1.21729943	0.08271582
C	-5.30990733	-0.16400044	1.10135004
C	-6.46350937	0.64467873	0.53841496
C	-6.05536037	1.22180565	-0.82331433
C	-3.87254576	-3.24092855	0.91610779
C	-1.85503670	-3.76270694	-0.25431418
C	-1.10221649	-3.92071002	1.06177799
C	-1.75072204	-3.20004623	2.23498793
C	-3.23693776	-3.50387025	2.28734737
C	1.26276496	-4.39079111	0.83279292
C	2.28693521	-4.16303603	1.94312653
C	2.93339659	-2.80397775	1.77102483
C	3.53129992	-2.74534121	0.36231239
C	2.50437062	-3.07597036	-0.72271379
C	5.35743098	-1.25998173	-0.24489238
C	4.85780660	0.60365871	-1.66656253
C	5.50706676	1.56621282	-0.67366535
C	5.45999438	1.02316183	0.75020409
C	6.06547737	-0.36782363	0.77809608
C	5.45061007	3.95260195	-1.14739721
C	5.34106094	5.03200572	-0.06469175
C	3.88191499	5.40107574	0.11915391
C	3.28100972	5.81385548	-1.21834600
C	3.50819182	4.75767883	-2.29766643
C	1.31846565	7.24898755	-1.20783567
C	0.42228858	7.56170589	-0.00666686
C	-0.71725451	6.55824030	0.06164794
C	-1.44901780	6.57296728	-1.27480965
C	-0.49575515	6.33656920	-2.44451231
C	-3.70042355	5.84038012	-1.76225628
C	-4.06578185	3.55404506	-2.33663769
C	-5.06504159	3.40903138	-1.19137532
C	-4.79093779	4.39354546	-0.05934623
C	-4.72448883	5.80154837	-0.62027143
C	-4.47580919	2.76699021	-3.57050086
C	-1.16642839	6.53512304	-3.79260324
C	3.18763278	5.28058210	-3.68930154
C	5.12889733	0.99676437	-3.10965441
C	3.14207601	-3.26287570	-2.09043369
C	-1.39334265	-4.77398352	-1.29025681
C	-4.41067205	-1.65405854	-2.36564164
C	-4.97478980	7.98434558	0.27706858
C	1.26471728	8.78774926	1.89708056
C	6.74697382	5.39498744	1.86004266
C	7.09480851	-0.97277081	2.87051611
C	1.90851799	-5.51756805	3.88228955
C	-4.57935571	-3.46459191	4.29410791
C	-8.20472864	1.77262004	1.75635306
C	-6.07480477	-3.16622630	4.22221021
C	0.62938876	-6.08898643	4.47857204
C	6.85253836	-1.91567026	4.04057859

C	7.54277807	4.56696734	2.85962953
C	2.72117754	9.18240843	2.12193337
C	-4.22610783	9.01216667	1.11201930
C	-8.66938969	3.22227626	1.70863451
C	-6.84149049	-4.06149174	5.17865645
C	-10.14156516	3.31851969	2.06816897
C	-4.98294993	10.32858274	1.12830128
C	2.80388469	10.54443681	2.78712239
C	8.42838364	5.46402210	3.70457168
C	8.06016629	-1.94008226	4.95883542
C	0.88121822	-7.41921776	5.15852659
H	-2.97655770	-8.61964224	0.80022623
H	-2.54094359	-8.67336414	2.53462741
H	-2.95636632	-7.12089180	1.76856190
H	3.69404504	-8.22548955	-2.80908402
H	4.04878820	-6.58911897	-4.62900009
H	-0.51369371	-7.34086737	-2.86440079
H	-2.26980256	-10.86996289	0.64842010
H	-3.00007288	-11.98460273	-1.42833154
H	-1.73816434	-11.59317431	-3.54023076
H	0.23685105	-10.12070221	-3.53750427
H	2.18956539	-9.56137190	-1.53906121
H	1.03617153	-7.05897701	-0.29805935
H	2.66289888	-7.67737315	-0.16954281
H	1.47303216	-8.20049412	1.94134657
H	1.79972641	-9.69935977	1.08322792
H	-0.48646359	-9.77939961	1.86115188
H	-0.63413557	-7.32960106	2.05851466
H	-1.05397769	-7.25250725	0.42698459
H	-3.67681199	0.01820349	-1.20464009
H	-5.71325523	-1.93483165	-0.05800505
H	-4.46374238	0.51551088	1.27644659
H	-7.31557746	-0.02959456	0.37697122
H	-6.90669569	1.72947127	-1.28868238
H	-4.91871985	-3.56088713	0.93550169
H	-1.71712957	-2.74216481	-0.63482500
H	-1.09997142	-4.99278080	1.30396261
H	-1.61791077	-2.11682454	2.11886960
H	-3.36520795	-4.57634119	2.49534228
H	0.85308457	-5.40349555	0.92400050
H	3.07513404	-4.92114292	1.84083830
H	2.15897945	-2.02479421	1.84937756
H	4.35031147	-3.47534585	0.29525129
H	1.75719269	-2.27163755	-0.76391736
H	5.86013309	-2.23112673	-0.31174984
H	3.77560919	0.57079633	-1.47734713
H	6.55300303	1.72029372	-0.97207909
H	4.40298281	0.93896812	1.04791976
H	7.12681015	-0.30585478	0.49928442
H	6.50294700	3.74065761	-1.36562682
H	5.90516912	5.91313260	-0.40137100
H	3.35140757	4.50364624	0.47026241
H	3.73799361	6.75410755	-1.55689967
H	2.89415267	3.87516008	-2.06865440
H	2.09025438	8.02026933	-1.30198675
H	-0.00690118	8.55886908	-0.17090549
H	-0.29877998	5.55543152	0.23159864
H	-1.92910840	7.55319674	-1.39578885

H	-0.09644894	5.31409332	-2.37822947
H	-3.69073736	6.81875411	-2.25514188
H	-3.06975603	3.23838059	-1.99607705
H	-6.07188949	3.58816273	-1.59202092
H	-3.81332663	4.15001669	0.38315326
H	-5.71436630	6.06670712	-1.01895972
H	-3.69216396	2.88393955	-4.33455365
H	-4.55675287	1.70652091	-3.31676763
H	-0.41542177	6.37603747	-4.58093283
H	-1.95577350	5.78827643	-3.91773953
H	3.26511186	4.44959594	-4.40750212
H	2.16088912	5.65662717	-3.70460321
H	4.57546005	0.31429246	-3.77295430
H	4.76477961	2.01382964	-3.27970690
H	2.34835198	-3.40367417	-2.83897764
H	3.69824798	-2.35710934	-2.34794145
H	-0.30770874	-4.74027668	-1.40822198
H	-1.85738787	-4.55993671	-2.25894328
H	-3.60183244	-2.33623271	-2.09024628
H	-4.13012976	-1.14831463	-3.30176161
H	-6.01797513	7.89287653	0.61202660
H	-4.96930575	8.32712170	-0.76778591
H	0.73697910	8.67263334	2.85204732
H	0.76911523	9.58207027	1.32576244
H	6.13112402	6.15027708	2.36357143
H	7.44980012	5.89810730	1.18061882
H	7.29622635	0.04885488	3.21376029
H	7.95779581	-1.33666191	2.29450912
H	2.64780864	-5.34088697	4.67447088
H	2.33131601	-6.25942048	3.18959197
H	-4.17265375	-3.18177108	5.27205278
H	-4.42215165	-4.54287026	4.15882426
H	-8.34920064	1.34030032	2.75541170
H	-8.80626108	1.20101991	1.03756999
H	-6.22969768	-2.11564736	4.50952953
H	0.23538340	-5.37504597	5.21448089
H	5.97901226	-1.54194374	4.60118484
H	6.82399159	4.04628130	3.51518200
H	3.18552371	8.43079128	2.77992290
H	-4.15481374	8.62202503	2.14082868
H	-8.08002171	3.79758522	2.44017337
H	-6.47624079	-3.96010867	6.20554904
H	-6.74509027	-5.10917063	4.87511359
H	-7.90243484	-3.80345278	5.16153581
H	-10.34348037	2.90483606	3.06108177
H	-10.74592475	2.77727798	1.33300305
H	-10.45655785	4.36413588	2.05556387
H	-5.98307532	10.21449728	1.55649046
H	-5.07810516	10.72424735	0.11189167
H	-4.42941534	11.05983354	1.72130383
H	2.25141105	10.56503530	3.73174238
H	2.39091617	11.31164573	2.12449245
H	3.84701632	10.79899027	2.98736132
H	7.84087199	6.20441904	4.25516228
H	9.14978739	5.98811475	3.06974226
H	8.98889484	4.85854868	4.42018249
H	8.28747457	-0.94367599	5.34837298
H	8.93638310	-2.31536206	4.42080804

H	7.86957390	-2.61003645	5.80014176
H	1.61515611	-7.31447529	5.96221500
H	1.26572846	-8.15958631	4.44760423
H	-0.04544083	-7.80424346	5.59005323
H	-5.86951662	3.38294922	1.19189836
H	-2.44620938	6.50052022	0.94755953
H	-1.07893233	8.45408527	-3.76509202
H	2.79953153	6.60670129	1.17765321
H	4.92798271	6.02229489	-3.96978644
H	5.81059203	2.76428155	1.51656651
H	4.44515931	-1.84443455	2.50592396
H	3.54841943	-5.13465464	-1.95533755
H	-2.70740122	-6.07796775	-0.79165541
H	-0.19500111	-3.44453602	3.38063173
H	-4.90408673	-1.21206152	2.67381146
H	-6.28017706	-1.81441699	-2.73127370
H	-5.66443018	4.11736929	-4.22543175
H	6.82243191	0.10706498	-3.20359056
H	-6.53607524	-2.50188381	2.48199729
H	-7.59884337	4.14644071	0.40503234
H	-2.36576000	8.52324329	0.85804901
H	3.78917507	8.35480418	0.75032861
H	7.81969337	2.92013928	1.86983789
H	5.72774883	-3.26969260	3.23015200
H	-0.81013213	-5.38202310	3.39713208

255

2-HP-B-CD:cis-(1R,4R)-SRT_4_CI E(Ha)= -7253.8893966519

Cl	-0.21371266	1.29011605	-2.76742427
Cl	-0.25418336	-1.82463696	-3.33554780
O	-5.87153022	0.43420219	-2.34545472
O	-4.21750172	-2.48346911	-0.85030274
O	-4.22500978	-4.47703995	-2.05079994
O	-0.78777580	-5.27090483	-1.07239542
O	0.73345205	-6.17874989	-2.56197024
O	3.20691064	-4.14339115	-0.82901962
O	5.30546297	-3.55679592	-1.61749921
O	4.78272388	-0.01068396	-0.82003371
O	5.74484055	1.65042617	-2.13144844
O	2.86776730	3.85803811	-1.67688878
O	1.96704744	5.43285895	-3.10144041
O	-1.28595808	4.75019166	-1.54535415
O	-3.19824551	4.89441629	-2.85045698
O	-2.51154560	5.88416611	0.55543970
O	-4.52651300	3.84932749	0.91996280
O	-4.53097962	1.92842375	-1.18285827
O	0.15699630	5.56504962	0.69127127
O	2.95950649	5.89628563	0.36834807
O	-0.12111536	6.86444239	-4.29036607
O	3.70971032	3.48757172	1.03971945
O	5.51161736	1.38369881	1.49331900
O	5.74539703	4.03994981	-3.65574167
O	4.17554647	-3.97027594	1.82779492
O	4.62023368	-1.21424201	1.74118390
O	2.55083459	-6.10150252	1.16732002
O	-0.08124474	-7.15408660	0.84109495
O	3.16260180	-6.49927642	-3.79316145
O	-3.04991187	-6.64202845	-3.44742413
O	-4.56633273	-3.80771638	1.48630634
O	-2.17996161	-5.38363256	1.43188755
O	-5.22494542	-1.16438113	1.44186515
O	-5.99463451	1.53876463	1.11050720
O	-6.70602845	-1.95691005	-3.44053049
O	-5.52839268	3.99794022	-4.05860424
O	7.28611877	-1.84636949	-2.59153065
O	-6.92073574	-2.98464102	2.86901023
O	-7.24220711	4.05573703	1.78504778
O	-1.08936704	7.36787567	2.60433368
O	5.72919439	5.45253199	1.13936739
O	7.13807340	-0.74166184	2.77126012
O	5.28354406	-6.52928939	1.77623698
O	-2.80208216	-8.09036626	1.25090915
N	1.37873499	3.95050689	2.77571079
C	0.93612180	2.85066726	3.74825157
C	1.96007102	1.72403976	3.72510338
C	1.83591852	0.90959065	2.44481248
C	0.45645092	0.25631237	2.30467156
C	-1.99905216	0.74219131	2.55175531
C	-3.07680099	1.48831144	3.00609248
C	-2.85167771	2.68410827	3.68784068
C	-1.54925316	3.10648240	3.90977209
C	-0.45759128	2.36547197	3.43797174
C	-0.67875516	1.16246346	2.75205744
C	0.25307889	-0.26587743	0.89649510

C	0.10584759	0.62189975	-0.17218636
C	-0.04477680	0.15558089	-1.47278761
C	-0.06812708	-1.21886592	-1.72663992
C	0.05507360	-2.10878192	-0.66582834
C	0.22189805	-1.63390524	0.63105049
C	1.76569180	5.22637264	3.43057272
C	-4.99247340	-0.69625231	-2.29243676
C	-5.18563311	-1.45314841	-0.97707347
C	-5.03277725	-0.51063594	0.21305396
C	-6.05587150	0.60109679	0.05390669
C	-5.79763899	1.32635863	-1.27060740
C	-4.65607016	-3.82112460	-0.89242045
C	-2.80717481	-4.57685408	-2.19981755
C	-2.20883593	-5.31446924	-1.00327740
C	-2.62031321	-4.65331832	0.30739660
C	-4.13595117	-4.53591573	0.35827953
C	-0.07842978	-6.43209614	-1.45436216
C	0.76537687	-6.87608649	-0.25223313
C	1.71617780	-5.74832228	0.09385488
C	2.54822990	-5.36880698	-1.12832781
C	1.71784484	-5.15597978	-2.39505928
C	4.58220774	-4.15073962	-0.56782541
C	4.99823303	-2.18773594	-1.88213886
C	5.20575260	-1.35625987	-0.61561617
C	4.40394766	-1.93355564	0.54410256
C	4.83995352	-3.37899478	0.73109676
C	5.75502919	1.00048777	-0.88967173
C	5.46003452	2.01026879	0.23061185
C	4.08232137	2.60691488	-0.01959374
C	4.14130495	3.31250468	-1.37228060
C	4.52836617	2.31415949	-2.46767567
C	2.75512650	5.23376114	-1.97384185
C	2.10392196	5.93512817	-0.76402028
C	0.79942639	5.19076802	-0.51361104
C	-0.07119983	5.44436706	-1.74161056
C	0.62242336	4.94670048	-3.01596200
C	-2.49963493	5.43709002	-1.77615026
C	-3.57500025	3.51703090	-2.71403431
C	-4.39315846	3.31628885	-1.44031044
C	-3.70393270	3.91625898	-0.21930409
C	-3.31749612	5.35968655	-0.48590823
C	-4.37971840	3.19414213	-3.96208300
C	-0.07372078	5.45864923	-4.26596604
C	4.78250099	3.02208542	-3.78796651
C	5.94158339	-1.76774273	-2.99686249
C	2.58060576	-5.23010043	-3.64560848
C	-2.57383976	-5.31978928	-3.50375748
C	-5.36486985	-1.54127147	-3.49965622
C	-3.18432599	6.66911950	1.54329523
C	3.96560717	6.92274293	0.36334896
C	6.76319379	1.56762759	2.16752250
C	5.00077545	-4.41389928	2.90726022
C	-0.44689059	-8.52974994	0.94667170
C	-5.11845761	-4.56898981	2.55931995
C	-7.17582691	1.64061217	1.90858929
C	-5.83920342	-3.62120477	3.50812519
C	-1.66615782	-8.67920286	1.84358235
C	4.98809401	-5.93769436	3.02672329

C	6.92111804	0.54780589	3.28671154
C	5.01919379	6.63797754	1.42543524
C	-2.32932538	6.71515456	2.79805113
C	-7.16164825	2.96083145	2.66588482
C	-6.39008248	-4.38555903	4.69823171
C	-8.34969924	3.03820300	3.60777271
C	-3.04952145	7.45367595	3.91022699
C	6.02145003	7.77690759	1.47671273
C	8.11724584	0.90670556	4.15208228
C	6.01485516	-6.39582813	4.04639273
C	-1.96997157	-10.14805439	2.07863898
H	2.97635903	2.12361475	3.82828468
H	2.61054644	0.13767350	2.40684454
H	2.01626990	1.55907693	1.57943175
H	0.43609862	-0.61353491	2.97669746
H	-2.18395300	-0.19651874	2.03598886
H	-4.08525311	1.12650559	2.82715262
H	-3.68531628	3.27245893	4.05773918
H	-1.36790628	4.01390028	4.48272257
H	0.08461869	1.69423398	-0.00125404
H	-0.00491681	-3.17496778	-0.85780159
H	0.32173359	-2.34642725	1.44575290
H	2.16333115	5.88711931	2.66132242
H	2.51642258	5.02441890	4.19575470
H	0.87831330	5.68730930	3.86699948
H	0.64502874	4.20171571	2.09102736
H	2.18315437	3.60836193	2.21454435
H	0.93078837	3.34019628	4.72688177
H	1.77750685	1.09119089	4.60086288
H	5.74132356	-2.39173347	-3.87996773
H	-2.29703807	6.48019723	-2.04296475
H	-4.21990254	5.97312041	-0.60780586
H	-2.77783665	3.34719317	-0.04583477
H	-4.82315195	2.92020597	1.00689027
H	-5.37680489	3.78594939	-1.57780982
H	-2.67820081	2.88595937	-2.66572157
H	-4.71720686	2.15509820	-3.90864838
H	3.74020336	5.64856410	-2.21557904
H	1.89794971	6.98426760	-1.01571650
H	1.02154358	4.11653331	-0.47344400
H	-0.81564377	5.47356455	0.54837485
H	-0.25878594	6.52254797	-1.84215869
H	0.62654109	3.85074092	-3.00156712
H	0.43914104	5.04832150	-5.14720655
H	-1.10734715	5.10092533	-4.27383684
H	0.78861121	7.17250624	-4.36744496
H	6.76007743	0.57679102	-0.78746682
H	6.20651077	2.81578071	0.18502118
H	3.34690486	1.79496678	-0.07277119
H	3.42412936	4.34390002	0.64077534
H	4.89813879	4.10824258	-1.33624664
H	3.71493322	1.58402403	-2.58409358
H	5.07365723	2.27380466	-4.53822898
H	3.85614275	3.49745236	-4.12304786
H	6.57576850	3.61093166	-3.41957398
H	4.96734144	-5.17048381	-0.47235110
H	5.92352402	-3.40058843	0.90434362
H	3.33451569	-1.91320657	0.28986269

H	4.73286879	-0.27173918	1.50725419
H	6.27393911	-1.37354437	-0.36005773
H	3.95402913	-2.08705486	-2.21164219
H	5.74783946	-0.72452336	-3.26226869
H	-0.77999532	-7.21258183	-1.76808787
H	1.34281978	-7.77002075	-0.52643803
H	1.10837050	-4.87501171	0.37017934
H	2.98781940	-5.27306141	1.45047666
H	3.28064833	-6.16406699	-1.32442361
H	1.23381978	-4.17331195	-2.34050805
H	1.96785278	-4.95449239	-4.51688744
H	3.39761350	-4.50768720	-3.55724837
H	2.43248114	-7.12742795	-3.84057898
H	-5.75021212	-3.86003924	-0.91892490
H	-4.57120612	-5.54495410	0.37339226
H	-2.20244699	-3.63537686	0.33373681
H	-1.29590784	-5.75014287	1.23536045
H	-2.55473474	-6.35640481	-1.00715318
H	-2.36667013	-3.57251799	-2.26299858
H	-1.49864801	-5.37377824	-3.69806663
H	-3.04087740	-4.74931070	-4.32017232
H	-3.99805933	-6.59108896	-3.28025374
H	-6.56978232	2.08201602	-1.45401545
H	-7.05851609	0.15604808	0.01444830
H	-4.02594602	-0.06601889	0.17704121
H	-4.74918409	-2.01975955	1.39939758
H	-6.19625783	-1.88394056	-0.97470384
H	-3.94682880	-0.36546738	-2.36745784
H	-4.74920857	-2.44457771	-3.51077884
H	-5.15254934	-0.96518770	-4.41267709
H	-7.24036968	-1.15447779	-3.43002148
H	-5.22402420	4.91006718	-4.12392812
H	7.45106521	-2.76990095	-2.36792949
H	-4.31781684	-5.11493606	3.07335059
H	-5.84669195	-5.28956117	2.16152403
H	0.40679701	-9.09413404	1.34750134
H	-0.70247489	-8.93352025	-0.04340286
H	4.62617605	-3.95134837	3.82800542
H	6.02946079	-4.06778395	2.75074596
H	6.80177833	2.59544932	2.55575863
H	7.59521094	1.42668744	1.46454278
H	3.47505463	7.88710580	0.54846520
H	4.46118456	6.96000397	-0.61459391
H	-4.14787391	6.20638835	1.77942375
H	-3.34851212	7.68497502	1.15658487
H	-7.22481315	0.78552671	2.59526685
H	-8.06235340	1.63009149	1.26013457
H	-5.10526088	-2.87742057	3.86376384
H	-6.23006048	3.00376408	3.25874205
H	-2.16960842	5.66554766	3.09704784
H	4.51492862	6.56173987	2.40355611
H	6.00574982	0.57847611	3.90351400
H	3.98602370	-6.25015093	3.35725232
H	-1.43664838	-8.19708237	2.80831616
H	8.00002779	1.88764796	4.62173958
H	9.03209012	0.91118898	3.55108718
H	8.23664705	0.15433650	4.93438825
H	5.85360248	-5.92209983	5.02006670

H	7.02344393	-6.14793203	3.70089690
H	5.95831283	-7.47904079	4.17351568
H	-1.13396093	-10.66092463	2.56288564
H	-2.18702701	-10.64754510	1.12896845
H	-2.85298715	-10.24060458	2.71452179
H	-5.59577116	-4.89380997	5.25256137
H	-7.11830067	-5.13108402	4.36379966
H	-6.90252837	-3.69562476	5.37222061
H	-8.33438624	2.22818332	4.34238622
H	-9.28458800	2.98217293	3.04154595
H	-8.33630101	3.99358230	4.13672031
H	-3.98678040	6.95760663	4.17719032
H	-3.26824951	8.48151807	3.60573002
H	-2.41283046	7.49769609	4.79719854
H	5.53980141	8.72775893	1.72075326
H	6.53207783	7.87630814	0.51401386
H	6.77612637	7.56267250	2.23597458
H	-6.56291541	-2.30270700	2.28279004
H	-6.38825363	4.15452660	1.34021238
H	-0.64040012	6.99213588	1.83618442
H	5.17432487	4.69341063	1.37106980
H	6.28425931	-1.09286709	2.46668147
H	4.43415039	-6.73686273	1.36171125
H	-2.74349223	-7.13146055	1.39550289
H	-3.72818446	3.29988430	-4.84224002

2-HP-B-CD:cis-(1R,4R)-SRT_5_CI E(Ha)= -7253.8898260358

Cl	0.85338891	-1.34147121	3.37961581
Cl	-0.59273827	1.35221732	2.49414144
O	2.42095179	5.44958732	2.36832974
O	4.03730090	2.43452452	1.02795006
O	5.45148202	1.25637595	2.44406749
O	4.83849918	-1.99997402	0.89368830
O	5.20238782	-3.94369113	2.11079018
O	1.88890751	-5.02580460	0.98839296
O	0.41387545	-6.05031329	2.44714692
O	-2.32714703	-4.24450570	0.83122180
O	-4.42560936	-4.12102446	1.82169883
O	-4.63716143	-0.50117624	1.36435567
O	-5.59791487	1.07310287	2.74929666
O	-3.45413931	3.65296326	1.26064526
O	-2.80310489	5.45801885	2.56766111
O	-3.79152059	5.23540933	-0.89689748
O	-1.01252626	5.98479427	-1.12467344
O	0.51811154	5.07800589	1.10244320
O	-4.74004656	2.72211115	-1.01578144
O	-6.34806701	0.40285726	-0.75346533
O	-5.89090021	3.56115920	3.95855000
O	-4.53008154	-1.40947854	-1.34254101
O	-3.51635223	-4.02377082	-1.71673805
O	-6.55207341	-2.78115069	3.14395859
O	1.24891691	-6.83338503	-1.00357384
O	-1.44667894	-5.91472606	-1.26039153
O	3.38794522	-5.05804698	-1.44782060
O	5.62264100	-3.33107426	-1.44884056
O	4.31255868	-6.31827558	3.36745327
O	6.54238584	-0.77787858	3.90530719
O	5.77897725	2.28936171	-1.00610446
O	6.04590753	-0.56412807	-1.21521016
O	3.65648494	3.97179712	-1.31827839
O	1.75454312	6.06778675	-1.14956032
O	4.82416719	4.75604772	3.62602909
O	-0.97536477	7.15298242	3.80088585
O	-1.94060371	-6.50105028	3.77024535
O	6.23974895	4.79018283	-2.26315581
O	0.22444936	8.45734594	-1.77281468
O	-5.48320856	4.56206259	-3.14879636
O	-7.21905738	-2.22986904	-1.62295994
O	-4.07354327	-6.77592767	-1.73185355
O	3.99382088	-7.75956013	-1.34559111
O	8.23569117	-2.31826772	-1.16434368
N	-3.80050020	0.92865900	-3.07560713
C	2.86477265	4.08653302	2.36930256
C	3.68781133	3.80797364	1.11015266
C	2.90431805	4.17322096	-0.14573888
C	2.51271740	5.63795479	-0.03471026
C	1.68951018	5.83929044	1.24108004
C	5.37286755	2.09216680	1.32734635
C	4.87371116	-0.04665088	2.31840553
C	5.51104137	-0.77434748	1.13722990
C	5.39452220	0.05819603	-0.13344782
C	5.99751259	1.43273529	0.09225628
C	5.54917362	-3.21011229	0.96530411

C	5.21303540	-4.02198770	-0.28979304
C	3.71824434	-4.28450134	-0.31689830
C	3.31371778	-4.98201904	0.97865124
C	3.81156899	-4.24057512	2.22170772
C	1.22976872	-6.22395883	1.32408574
C	-0.62670588	-5.07764778	2.32317009
C	-1.47609779	-5.35890201	1.08458870
C	-0.62949734	-5.57282657	-0.16556480
C	0.39865057	-6.65346106	0.10596558
C	-3.69684679	-4.48157519	0.67440502
C	-4.19771336	-3.67136955	-0.52860712
C	-4.04236610	-2.18345007	-0.24003310
C	-4.81429420	-1.87219246	1.03780671
C	-4.32379640	-2.74917603	2.18931505
C	-5.78268613	0.28264351	1.61996360
C	-6.03455268	1.18178560	0.39179904
C	-4.75464821	1.98167807	0.19160361
C	-4.62146712	2.87405485	1.42385674
C	-4.52434804	2.01931830	2.69270295
C	-3.53419838	5.05086952	1.45544847
C	-1.40677601	5.13705734	2.53405932
C	-0.75195095	5.68505241	1.26673113
C	-1.54376155	5.34248979	0.00955548
C	-3.00515977	5.71204789	0.18117982
C	-0.81653379	5.75693337	3.78971935
C	-4.66916864	2.86427170	3.94783376
C	-5.18826988	-2.57116777	3.42595918
C	-1.43154521	-5.20298821	3.60743825
C	3.66126962	-5.07747955	3.48107895
C	5.16374546	-0.73099986	3.64466962
C	3.68563951	3.92980664	3.63777395
C	-4.08154913	6.16862822	-1.94026649
C	-7.72557833	-0.00261489	-0.81087463
C	-4.31439453	-4.60212801	-2.75275196
C	1.62365795	-8.19402530	-1.22587056
C	6.71740109	-3.89468797	-2.17192436
C	6.89225494	2.49211218	-1.87394384
C	2.28821281	7.19999570	-1.84105765
C	6.52633273	3.56320661	-2.89200698
C	7.80802939	-2.85418067	-2.39912222
C	2.89117009	-8.26147770	-2.06467612
C	-3.99418807	-6.08208060	-2.96001556
C	-7.92739221	-1.04251949	-1.90447975
C	-4.34291258	5.39963999	-3.22290331
C	1.18438044	7.88814601	-2.63101692
C	7.67843225	3.79212202	-3.85314924
C	1.76491144	9.00478806	-3.48035673
C	-4.56293883	6.34719048	-4.38641049
C	-9.39888600	-1.39824900	-2.01513077
C	-4.97114421	-6.69838811	-3.94539549
C	3.19294914	-9.70106492	-2.44348153
C	8.99974241	-3.48172866	-3.09969755
C	-5.09470190	1.15239816	-3.77077639
C	0.72938865	-1.63965866	-0.60192626
C	0.95280125	-1.90171289	0.74232365
C	0.54969324	-0.99070773	1.71359593
C	-0.08788294	0.18709820	1.31954869
C	-0.32565635	0.43608692	-0.03021762

C	0.08201309	-0.47169362	-1.00844821
C	-0.35613744	1.17374104	-2.89593052
C	-1.45134939	1.68180499	-3.60957224
C	-1.44073091	3.01368821	-4.04325905
C	-0.37553951	3.85345542	-3.75327014
C	0.71797794	3.35437077	-3.04562252
C	0.72091675	2.02908714	-2.63239859
C	-0.25898856	-0.27940603	-2.47510817
C	-1.52889268	-1.08794023	-2.78773919
C	-2.19335057	-0.66603423	-4.09097718
C	-2.60198450	0.79870257	-4.01951697
H	2.00055668	3.40821759	2.39478009
H	4.59669568	4.42337347	1.15194817
H	1.98855779	3.56371166	-0.17870548
H	3.42819498	6.23827265	0.04291232
H	1.44854861	6.89881674	1.38510316
H	5.93447660	2.99194226	1.59976989
H	3.78892625	0.03232561	2.15845392
H	6.56754580	-0.95771834	1.37652216
H	4.32372239	0.18703638	-0.35815070
H	7.07571188	1.32363545	0.27565540
H	6.62821884	-3.03178353	1.02059087
H	5.74063709	-4.98197887	-0.21761477
H	3.21091585	-3.31069869	-0.36917096
H	3.72232834	-6.00130357	0.97784842
H	3.24122841	-3.30753553	2.33318125
H	1.95970159	-6.99332714	1.59882614
H	-0.19889552	-4.06946528	2.24586432
H	-2.07654120	-6.25756963	1.28155159
H	-0.09460561	-4.63664440	-0.37940953
H	-0.12239901	-7.59174631	0.34215471
H	-3.90512312	-5.54198425	0.50499815
H	-5.26662580	-3.89660598	-0.63459044
H	-2.97950128	-1.95409174	-0.09194706
H	-5.87820723	-2.09024811	0.87116455
H	-3.28133894	-2.48792729	2.42191711
H	-6.63776773	-0.36490796	1.84441061
H	-6.87352811	1.86035371	0.59815701
H	-3.90775552	1.28227128	0.18555568
H	-5.50320672	3.52434564	1.50882877
H	-3.56005002	1.49463483	2.69304163
H	-4.57114037	5.34845186	1.64599391
H	-1.27561273	4.04827332	2.54931791
H	-0.65660973	6.77577969	1.35964248
H	-1.49395161	4.25164850	-0.12429521
H	-3.11682840	6.79981094	0.27842477
H	-1.27619375	5.28348599	4.66999690
H	0.25823047	5.55362707	3.81458134
H	-4.55823864	2.21230902	4.82567749
H	-3.87226318	3.61276488	3.97297302
H	-4.82280747	-3.24780787	4.21089876
H	-5.09019730	-1.54374314	3.78836372
H	-0.79597145	-4.89972246	4.45259474
H	-2.28793940	-4.52468899	3.56213454
H	4.03634831	-4.49313705	4.33412983
H	2.60024707	-5.28425452	3.65126831
H	4.80980424	-1.76443495	3.60167379
H	4.61060025	-0.20871674	4.44005042

H	4.03905961	2.89791420	3.71265129
H	3.03787024	4.13653821	4.50249369
H	-3.22121414	6.82860540	-2.08861490
H	-4.96134334	6.76691190	-1.66413819
H	-8.33997016	0.88686572	-1.00246981
H	-8.03030687	-0.44242107	0.14684607
H	-4.11891709	-4.04180227	-3.67603860
H	-5.37769589	-4.48837617	-2.50716427
H	0.79259116	-8.71339803	-1.72329076
H	1.82845675	-8.69179820	-0.26769463
H	6.34262107	-4.28653496	-3.12597105
H	7.14786808	-4.72753298	-1.60262450
H	7.14944933	1.54814308	-2.36955234
H	7.75448477	2.83955837	-1.28672653
H	3.10413283	6.86944692	-2.49738741
H	2.68500518	7.92479829	-1.11763614
H	5.64967162	3.20245161	-3.45750846
H	7.39568741	-2.05389726	-3.03407056
H	2.72243233	-7.67297891	-2.98172893
H	-2.97393830	-6.15960957	-3.36495748
H	-7.59228203	-0.60954319	-2.86220617
H	-3.43679964	4.79811976	-3.40283253
H	0.71975780	7.13657526	-3.29433289
H	7.94332542	2.87613260	-4.38921147
H	8.55864664	4.14881265	-3.30917938
H	7.40192638	4.55724927	-4.58183742
H	2.50418715	8.62733175	-4.19242119
H	2.24226577	9.75510066	-2.84237782
H	0.96317585	9.49856156	-4.03363017
H	-3.68124983	6.96858517	-4.56594075
H	-5.42082987	6.99775596	-4.19218480
H	-4.77690409	5.77655314	-5.29356355
H	-10.00751811	-0.52391602	-2.26166738
H	-9.75788792	-1.82475270	-1.07356097
H	-9.53351578	-2.14890233	-2.79638917
H	-4.97555825	-6.16110214	-4.89938629
H	-5.98382118	-6.68238632	-3.53033863
H	-4.70156994	-7.73929972	-4.13592073
H	2.38098667	-10.14573225	-3.02631271
H	3.35210766	-10.30444724	-1.54398472
H	4.10980690	-9.73682363	-3.03561195
H	8.71310303	-3.93920405	-4.05170775
H	9.44814990	-4.25119572	-2.46324809
H	9.75972800	-2.72152685	-3.29296809
H	-0.05808965	5.76677396	-1.15809074
H	-4.21863570	3.54317554	-0.85321744
H	-6.58781933	2.89753513	4.00938049
H	-5.15489654	-0.74009510	-0.97881414
H	-6.64226279	-3.70179966	2.87171313
H	-2.00450537	-5.13352987	-1.43672230
H	2.50198641	-5.44216817	-1.30014353
H	5.24856658	-6.12961570	3.23372256
H	6.84914624	0.13634028	3.91135130
H	5.65581533	-1.45469087	-1.32687448
H	4.20450964	3.17067116	-1.18665506
H	4.50629060	5.66459301	3.57299627
H	-1.92361874	7.32493020	3.80770237
H	-1.17749187	-7.09016566	3.79370646

H	5.36557838	4.71439732	-1.85329874
H	-0.33258072	7.74595933	-1.42465326
H	-5.47237745	4.06523584	-2.32072126
H	-6.27610803	-2.07696355	-1.78445113
H	-3.16724596	-6.84243567	-1.39608049
H	3.98422328	-6.79172408	-1.43208813
H	7.68186267	-1.53957648	-1.00287229
H	-5.09670122	2.15627536	-4.19922498
H	-5.22355284	0.39288868	-4.54319289
H	-5.88633365	1.08551926	-3.02573688
H	1.06391878	-2.36268554	-1.34245246
H	1.42528471	-2.82927055	1.04400777
H	-0.81684557	1.36335184	-0.30771266
H	-2.27083505	3.38263186	-4.64213975
H	-0.38650219	4.88330138	-4.09554531
H	1.57311830	3.98404540	-2.81641029
H	1.58440079	1.64384429	-2.09568490
H	0.56582163	-0.71365540	-3.05876153
H	-2.23633951	-0.97097927	-1.95992060
H	-1.29450515	-2.15601269	-2.80661067
H	-3.06412604	-1.29921469	-4.30129197
H	-1.50504328	-0.77980257	-4.93565895
H	-2.98036550	1.14198257	-4.98707018
H	-3.87423456	0.06930685	-2.50081854
H	-3.70754443	1.70574229	-2.39866013

2-HP-B-CD:cis-(1R,4R)-SRT_6_Cl E(Ha)= -7253.8644732849

Cl	-2.17048388	-5.45835222	3.72568952
Cl	-3.46431868	-2.54885202	3.93514441
O	2.04426628	5.21321203	-2.84209947
O	-1.16647155	5.16938055	-1.08635496
O	-3.12112186	5.87740034	-2.14251984
O	-4.31023542	2.63867732	-1.01057467
O	-6.04722415	1.31685346	-1.79490857
O	-3.97185785	-1.70743246	-1.83961969
O	-3.86595961	-3.40800950	-3.38311767
O	-0.71687394	-4.64190777	-1.98078433
O	0.98134204	-5.41602571	-3.34078243
O	3.34510421	-3.83920282	-1.04897586
O	5.53316955	-3.38376502	-1.67453519
O	4.98934896	0.07411964	-0.59340833
O	5.84763861	1.79294647	-1.88479274
O	5.77455161	1.31554683	1.71717697
O	4.19459595	3.66622255	1.41950699
O	2.97737598	3.94744974	-1.14701081
O	4.79131618	-1.32663488	1.85793082
O	4.14223400	-4.06795477	1.62101543
O	7.65902364	-1.65769548	-2.34604292
O	2.25001006	-5.87121223	0.58983670
O	-0.32908625	-6.77164207	-0.23224278
O	3.51773065	-5.62048545	-4.33369261
O	-4.80773105	-3.51507505	0.13379343
O	-2.56205375	-5.14375789	0.14368852
O	-4.00592659	-1.03814285	0.96163657
O	-4.69037340	1.57723364	1.57711988
O	-7.17352533	-0.99163833	-3.09086426
O	-5.72044562	5.55677416	-3.05959683
O	-2.21396922	6.15568572	1.36378886
O	-4.39329177	4.29519995	1.43752385
O	0.45199603	6.72883321	0.65902269
O	3.24548478	6.18877364	0.44893608
O	0.06885872	6.33376055	-4.37220740
O	5.58696213	4.16151245	-3.46281345
O	-2.61413629	-5.37992809	-4.95574809
O	-1.48711110	8.78627537	0.81594010
O	6.03752423	5.69395231	1.02639216
O	7.40066946	-0.87153158	2.73496890
O	4.83219833	-6.76445044	1.33420683
O	-3.03890189	-7.79927492	-0.47584948
O	-6.61207814	-1.87444789	1.59790941
O	-6.89889336	3.06775371	2.28667916
N	-1.22054714	1.95908190	-0.79443143
C	-1.43673423	1.49647661	-2.19012228
C	0.72453433	-3.07066034	2.37051088
C	-0.00041866	-4.18938645	2.75039185
C	-1.30539989	-4.05330607	3.22532606
C	-1.87200815	-2.77938456	3.30055560
C	-1.15060976	-1.66130585	2.87663277
C	0.15621488	-1.79134495	2.41467609
C	0.46045306	0.74508461	2.31160651
C	-0.00960336	1.68079022	1.37208857
C	-0.43045279	2.94266969	1.81196181
C	-0.43173125	3.27445532	3.15947068

C	0.01782771	2.34555483	4.09353812
C	0.46402742	1.10371586	3.66440003
C	0.99857083	-0.61863901	1.92519995
C	1.22329509	-0.71043997	0.41072984
C	0.03558928	-0.15305906	-0.35328633
C	-0.01188045	1.34510322	-0.10736608
C	0.70008378	4.83361013	-2.58855290
C	0.09949175	5.70840855	-1.49115586
C	0.98613574	5.80600864	-0.25468286
C	2.38817496	6.21511464	-0.66571364
C	2.89688936	5.23056359	-1.72735651
C	-2.26845054	6.07272964	-1.05488906
C	-3.66542125	4.56975807	-2.26297835
C	-4.29893185	4.06748877	-0.96095355
C	-3.57035667	4.47376332	0.31826524
C	-3.04154904	5.89050459	0.25019311
C	-5.51006803	1.96349546	-0.67677850
C	-5.23305935	0.94892932	0.43148429
C	-4.29039428	-0.13609713	-0.07385183
C	-4.90638705	-0.78125140	-1.30635997
C	-5.23965816	0.28236979	-2.35674609
C	-4.48214610	-2.98178195	-2.21009780
C	-2.45333958	-3.61788577	-3.30114026
C	-2.12038747	-4.60820399	-2.18530550
C	-2.75292333	-4.18711412	-0.86462638
C	-4.24328216	-3.98311325	-1.07114367
C	0.01286259	-5.77323526	-2.39527904
C	0.66866822	-6.39411830	-1.15298555
C	1.59883107	-5.36154957	-0.54930079
C	2.61539559	-4.92713585	-1.59978820
C	1.95341674	-4.46735377	-2.89878655
C	4.70359112	-4.01113047	-0.73349807
C	4.93661572	-3.40750493	0.65513345
C	4.60192898	-1.92834497	0.59618707
C	5.45119546	-1.26785233	-0.48061482
C	5.31483688	-1.98192466	-1.82559845
C	5.94247959	1.10478927	-0.66616867
C	4.58225363	2.40611652	-2.11688610
C	4.28377876	3.39559927	-0.99230030
C	4.34773326	2.72963952	0.37735723
C	5.70312911	2.05005504	0.51577921
C	4.68484305	3.08259311	-3.47365557
C	6.34935254	-1.51072729	-2.83432328
C	2.95232044	-4.37029652	-4.04217668
C	-2.03421587	-4.13347348	-4.66781107
C	-6.03055532	-0.29430417	-3.51933565
C	-4.69851849	4.65235144	-3.37885222
C	-0.01712260	5.01150576	-3.92097594
C	6.99919537	1.48883258	2.43451695
C	4.83889882	-4.75375769	2.66569924
C	-0.66336725	-8.16046927	-0.27795352
C	-6.16455250	-3.89853172	0.35286462
C	-5.35653362	1.29163149	2.81660156
C	-2.63536334	7.21122947	2.23368683
C	4.25260081	7.20168834	0.42045378
C	-1.67754206	8.39832073	2.16502898
C	-6.10399868	2.52295612	3.32797914
C	-6.64930313	-3.28893592	1.65896433

C	-2.04053846	-8.39009641	0.32569871
C	4.55428290	-6.25299198	2.62390650
C	7.19372836	0.34442749	3.41742846
C	5.35606274	6.86694331	1.41207464
C	-2.23145328	9.57268536	2.95107318
C	6.36598823	7.99866983	1.47639905
C	8.40830519	0.60475886	4.29128962
C	5.41174821	-6.98129513	3.64334786
C	-2.33063760	-9.87768202	0.42009624
C	-8.07932247	-3.70474131	1.94482480
C	-6.99650022	2.15207528	4.49787465
H	-1.70613581	0.44162195	-2.18531570
H	-0.52190617	1.65374363	-2.76272780
H	-2.25837419	2.06920833	-2.61373293
H	1.75650591	-3.19452682	2.04800710
H	0.43991054	-5.17850794	2.67485725
H	-1.63045217	-0.69017875	2.93037316
H	-0.75834971	3.70239592	1.10780066
H	-0.77823134	4.25563321	3.46741706
H	0.03215516	2.59197536	5.15070991
H	0.82639776	0.38002143	4.38990658
H	1.98308679	-0.72504020	2.40166312
H	2.12502648	-0.14892070	0.13332247
H	1.39550864	-1.74930440	0.11846190
H	0.15135514	-0.37212767	-1.41814713
H	-0.89364191	-0.62614911	-0.00441658
H	0.84535918	1.82353174	-0.60321314
H	-1.13396657	2.98765134	-0.80409658
H	-2.07162507	1.76527732	-0.24950136
H	0.66803710	3.77592218	-2.27774000
H	-0.04774871	6.70947918	-1.91504745
H	1.05750353	4.80967277	0.20810076
H	2.35184782	7.22367929	-1.10221286
H	3.87534472	5.53032451	-2.11658891
H	-1.90847236	7.10224768	-1.11985192
H	-2.86672190	3.87780288	-2.56125968
H	-5.32268076	4.46060345	-0.91431376
H	-2.68939478	3.82662563	0.41681146
H	-3.87742161	6.59960070	0.21875645
H	-6.26684697	2.67709517	-0.33948582
H	-6.19459104	0.48426118	0.67961291
H	-3.34754316	0.33843045	-0.39581747
H	-5.83373933	-1.28537739	-1.00895240
H	-4.30125989	0.70731212	-2.74317562
H	-5.54960984	-2.89417877	-2.44336318
H	-1.94459681	-2.66545738	-3.09190841
H	-2.49182401	-5.60348335	-2.46304930
H	-2.30556442	-3.22563491	-0.56396355
H	-4.69700259	-4.94544593	-1.35012758
H	-0.64566844	-6.49129911	-2.89618015
H	1.25405389	-7.27132274	-1.46135515
H	0.99473676	-4.48535213	-0.27140462
H	3.28880626	-5.76326880	-1.83262354
H	1.47422128	-3.49312154	-2.72461376
H	4.98098043	-5.06992850	-0.73003866
H	5.99913064	-3.53279347	0.89796729
H	3.55118161	-1.83978892	0.29862720
H	6.50460628	-1.28047375	-0.17037835

H	4.30316348	-1.79733069	-2.21613174
H	6.95640282	0.69147151	-0.63637685
H	3.79357680	1.63950739	-2.14794472
H	5.03098088	4.19890823	-1.01577255
H	3.55839093	1.96437908	0.44375693
H	6.47561686	2.83104936	0.50037450
H	4.96276585	2.32296275	-4.21873142
H	3.70796115	3.48984608	-3.75019139
H	6.19653434	-2.06274229	-3.77352631
H	6.19941827	-0.44581646	-3.03533012
H	2.44789279	-3.93279367	-4.91742105
H	3.77197524	-3.70801481	-3.74952082
H	-2.29145468	-3.37530031	-5.42260547
H	-0.94935261	-4.27472535	-4.67864074
H	-6.28239428	0.52281952	-4.21043028
H	-5.40078628	-1.00978352	-4.05689424
H	-5.16388364	3.66894629	-3.50224720
H	-4.19037612	4.91602054	-4.31783979
H	-1.08059198	4.78667711	-3.79577105
H	0.40529934	4.29834584	-4.64552124
H	6.97345291	2.45722999	2.95228060
H	7.84804206	1.48232504	1.73675727
H	4.52491771	-4.32363774	3.62380120
H	5.91723526	-4.59022534	2.55578868
H	0.10626650	-8.72788104	0.26340120
H	-0.69104131	-8.50739617	-1.32043439
H	-6.22269473	-4.99447490	0.39726909
H	-6.80381244	-3.54361123	-0.46938538
H	-4.59516811	0.96934262	3.53502974
H	-6.05802905	0.46275200	2.67405311
H	-2.68489570	6.80812247	3.25152319
H	-3.64279337	7.53721001	1.95103087
H	3.79049937	8.16960655	0.66025436
H	4.70158304	7.26342042	-0.58124526
H	-0.71495633	8.09231010	2.60156901
H	-5.36538153	3.26864274	3.65813303
H	-5.98998628	-3.65115264	2.46232711
H	-2.04540369	-7.95338769	1.33787019
H	3.49242464	-6.41119932	2.86657801
H	6.29505692	0.28689158	4.05374903
H	4.89208389	6.73706506	2.40338464
H	-2.44046039	9.29871102	3.99005857
H	-3.15835052	9.92941976	2.49119491
H	-1.51480938	10.39665424	2.94765172
H	5.90199392	8.93699074	1.79367264
H	6.83106813	8.14946594	0.49691105
H	7.15558038	7.74247828	2.18586316
H	8.30156509	1.52819206	4.86779531
H	9.31024459	0.67696826	3.67512498
H	8.54339063	-0.22799513	4.98470514
H	5.26189999	-6.58446065	4.65238697
H	6.47028679	-6.88260020	3.38311879
H	5.16379149	-8.04485814	3.64788179
H	-1.59897432	-10.39368836	1.04855881
H	-2.32041748	-10.33081922	-0.57652588
H	-3.32508916	-10.02842342	0.84542192
H	-8.17046772	-4.79142600	2.02701539
H	-8.74577591	-3.35480010	1.15004264

H	-8.41046923	-3.25705905	2.88430050
H	-6.42633595	1.67157373	5.29942637
H	-7.77905719	1.46281278	4.16645137
H	-7.47876080	3.04485179	4.90183082
H	3.56360214	4.34635283	1.12386458
H	4.88738766	-0.36360600	1.71597959
H	7.79504432	-2.59958650	-2.19130816
H	2.80116046	-5.14267364	0.94085891
H	2.78426623	-6.20502798	-4.55810663
H	-1.64007147	-5.46368242	0.09628170
H	-4.05558085	-1.95005197	0.60999184
H	-7.75181433	-0.35564512	-2.65437189
H	-5.31515632	6.42950865	-3.00145336
H	-4.44402651	3.32510543	1.56591445
H	-0.40193307	6.37096419	0.97051112
H	1.00673273	6.52821103	-4.48576343
H	6.45368081	3.80631382	-3.23384093
H	-3.56975857	-5.25363719	-4.95206639
H	-0.64529758	8.40356563	0.53417919
H	5.49630761	4.93520169	1.30393051
H	6.53009727	-1.22367387	2.49069450
H	3.98835785	-6.81030440	0.86398807
H	-3.07663680	-6.85826010	-0.23845350
H	-5.68247234	-1.60006193	1.64088652
H	-6.43141950	3.83711781	1.94138426

2-HP-B-CD:cis-(1R,4R)-SRT_1_MD E(Ha)= -7253.92660709

C	0.0973136265	1.2140455078	-3.5414296362
C	0.0850839078	0.7126945546	-2.1168530142
C	0.5137576109	-0.5855586582	-1.8045439193
C	1.0382779355	-1.5508634880	-2.8525540651
C	0.9627127701	-1.0139711496	-4.2962617490
C	1.1648355118	0.4920849940	-4.3482261370
C	-0.2912254578	1.5889732102	-1.0922498224
C	-0.2435404231	1.1971392383	0.2377042052
C	0.1940074723	-0.0870062007	0.5568770917
C	0.5577852197	-0.9636219081	-0.4558551384
C	0.4159768813	-2.9326055241	-2.7931304966
C	1.1637367247	-4.0370027169	-3.2070238150
C	0.6053491047	-5.3074278468	-3.2339894017
C	-0.7219192367	-5.5075125708	-2.8615152519
C	-1.4826170174	-4.4066091361	-2.4599025846
C	-0.9136759732	-3.1334818313	-2.4145314632
Cl	-1.3850244815	-7.0980137857	-2.9046219993
Cl	-3.1507743216	-4.5932230428	-2.0231603138
N	-1.2814989673	1.0897419195	-4.1410760323
C	-1.4137795272	1.6319682466	-5.5096904344
O	-5.4634004823	-2.5970035394	-0.1059662361
C	-4.3410330650	-2.3733441790	0.7213983987
C	-4.3881378864	-3.2847067900	1.9412887031
C	-3.2056696424	-2.9803922821	2.8592356819
O	-3.2577390234	-1.6342621295	3.2387088646
C	-3.1323811805	-0.7316402550	2.1428947490
C	-4.2912705749	-0.9144526404	1.1552949372
O	-2.0238144288	-3.2554219437	2.1464259100
C	-1.1193952301	-4.2205366014	2.6616384848
C	-0.5570557380	-4.9268938805	1.4337251474
C	0.5646317599	-5.8618274376	1.8415267451
C	1.5823267701	-5.0882255922	2.6897215477
O	0.9798911511	-4.5158508055	3.8191736082
C	-0.0331744817	-3.5559009034	3.5039770644
O	2.1238462381	-4.0899058514	1.8638286478
C	3.5231315153	-4.0436973644	1.6341037243
C	3.6461637062	-3.6672446920	0.1623633077
C	5.0690231364	-3.2718140482	-0.1988222377
C	5.5474857203	-2.2196372356	0.8083119605
O	5.5013727160	-2.7275808858	2.1116313544
C	4.1771403261	-3.0248984831	2.5645028860
O	4.6969421724	-1.1100507164	0.6787617586
C	5.2157510968	0.1769992845	0.3817152228
C	4.2756916334	0.7492826828	-0.6730086474
C	4.5999551892	2.2110955268	-0.9194310089
C	4.6238598176	2.9697594533	0.4198972867
O	5.5298781365	2.3858598951	1.3183512905
C	5.2710862563	1.0225633812	1.6486361837
O	3.3037459561	2.9675778170	0.9019672298
C	2.9801914623	3.9136378746	1.9116808504
C	2.7016998437	5.2835000873	1.2976028064
C	1.9859470736	6.1958511109	2.2867175330
C	0.7264106292	5.5042128852	2.8168703834
O	1.1319950483	4.3315788559	3.4663297674
C	1.7058073401	3.3751969633	2.5704861643
O	-0.1055287226	5.1801884180	1.7404008816

C	-1.3381184241	5.8471647057	1.4880727833
C	-1.2862132922	6.0993350873	-0.0260348741
C	-2.6384361132	6.3561343081	-0.6830415021
C	-3.6927331451	5.4064862977	-0.1003636496
O	-3.7026442112	5.4847816362	1.3011681649
C	-2.5133072435	4.9609734785	1.8890411026
O	-3.3866925594	4.1158902587	-0.5329802270
C	-4.4248504558	3.2095769058	-0.8812006854
C	-3.6864215865	2.1495374604	-1.6808341806
C	-4.5861851217	0.9739079114	-2.0055364998
C	-5.1071812639	0.3973932885	-0.6792142185
O	-5.8210472602	1.4049644995	-0.0052553690
C	-5.0831478654	2.5734075156	0.3480907199
O	-2.6639958394	6.0902967026	-2.0649523718
C	-1.6972188316	6.6799947304	-2.9117192452
C	-1.4778815569	5.7379798785	-4.0888817162
O	-1.0233896176	4.4636358274	-3.6359580220
O	-0.4211888379	7.1936930221	-0.2896936149
O	1.6923676489	7.3935205687	1.5879625715
C	1.6076858974	8.5574753844	2.4173762016
C	0.7737108610	9.6271168810	1.7284189258
O	-0.5730196312	9.2190075835	1.6259410376
O	3.9159029156	5.8714668929	0.8779344377
O	3.6361301895	2.7233462518	-1.8157185667
C	3.8936258571	4.0228567807	-2.3109134724
C	2.6682324916	4.4101842828	-3.1198509451
O	1.5096040178	4.2619243414	-2.2963007321
O	4.3982783239	0.0036565499	-1.8655426105
O	5.1581161100	-2.6603035300	-1.4708503968
C	5.2763960090	-3.5369720000	-2.5853652075
C	5.3824930715	-2.7083629297	-3.8577957415
O	4.1869353374	-1.9732744611	-4.0859847954
O	3.1968177430	-4.7280049044	-0.6586128329
O	1.2199882278	-6.3746263892	0.6990133986
C	1.6276107646	-7.7344194522	0.8343704872
C	2.6662313697	-8.0686946026	-0.2235100007
O	3.8692451056	-7.3679155533	0.0067120800
O	-1.5712468949	-5.6548710013	0.7712011290
O	-4.3544942235	-4.6215485189	1.4720749955
C	-5.0292517437	-5.5512585470	2.3230862722
C	-4.4921409171	-6.9563111223	2.0916386548
O	-3.1687186211	-7.0729172587	2.5618038727
O	-4.0044777364	-0.0762597153	0.0370041759
O	-3.8271485893	0.0770124932	-2.7755610847
C	-4.5403352438	-1.0101100020	-3.3305701384
C	-3.9662504298	-1.3128601891	-4.7068557438
O	-2.5416725387	-1.4256900910	-4.6619494562
O	-3.1525391024	2.6861696208	-2.8787310641
C	-6.0809899294	3.4580879614	1.0898990968
O	-6.0690043594	3.2382686923	2.4861177520
C	-2.9852066544	0.6650259480	2.6977783049
O	-4.1706616382	1.1194355443	3.3026755712
C	-0.5532193466	-3.0427364851	4.8350550441
O	-1.2239444790	-4.0424675112	5.5639258101
C	4.3222451479	-3.5367793156	3.9862939688
O	5.0220204914	-4.7545522848	4.0493019618
C	6.4002806543	0.6072421293	2.5766283979
O	7.6528839349	0.6896061562	1.9412542523

C	1.8880333600	2.1104363094	3.3842685838
O	0.6480511759	1.6221620869	3.8390730365
C	-2.7674228537	4.8646862842	3.3819733316
O	-3.6828262751	3.8485607446	3.7022444615
C	-2.7321964263	5.5096905806	-4.9087531397
C	2.7263300169	5.8380440056	-3.6144400122
C	6.6038021370	-1.8021376832	-3.8853758421
C	2.9852865130	-9.5525194776	-0.2018486788
C	-5.3410154661	-7.9725452839	2.8357142005
C	0.8140710102	10.9184329498	2.5262859164
C	-4.5968682854	-2.5429005631	-5.3321671637
H	-4.6899131292	5.7098432652	-0.4397497472
H	-2.9476760696	7.3898440953	-0.4630844145
H	-0.8797465174	5.1833262763	-0.4782661613
H	-1.3819324799	6.8124545032	2.0109817886
H	0.2020253922	6.1156436880	3.5611197767
H	2.6563347270	6.4057996573	3.1313828473
H	2.0408538940	5.1227393461	0.4315689826
H	3.7979558581	3.9959383786	2.6424128101
H	4.9851786515	3.9935044315	0.2980707365
H	5.6042492656	2.2848530725	-1.3653623752
H	3.2460191754	0.6910850210	-0.2899350237
H	6.2269411724	0.0971111019	-0.0390107499
H	6.5897850538	-1.9420976130	0.6174705569
H	5.7375298083	-4.1430698257	-0.1477063643
H	3.0239361217	-2.7770022171	-0.0061683204
H	3.9756115982	-5.0308224903	1.7990761321
H	2.3681326724	-5.7530110582	3.0644643651
H	0.1405903652	-6.6787306299	2.4410291447
H	-0.1500955691	-4.1643886293	0.7534157866
H	-1.6546580579	-4.9540277127	3.2781253679
H	-3.2370859031	-3.5604454252	3.7883158408
H	-5.3220149019	-3.0956382470	2.4890601797
H	-3.4127592048	-2.5847271323	0.1698894855
H	-5.2365370306	-0.6186020008	1.6256323263
H	-5.8362589012	-0.4022037315	-0.8414259089
H	-5.4644424145	1.3159774067	-2.5773954983
H	-2.8781346683	1.7660607591	-1.0433285477
H	-5.1673422422	3.7111658214	-1.5208845866
H	-4.2746739960	2.3094336222	1.0380086433
H	-2.2033906191	-0.9485263104	1.5978307102
H	0.4023736427	-2.7229232784	2.9355190221
H	3.5687524470	-2.1107563685	2.5662459198
H	4.3101851766	0.9293016149	2.1714228935
H	0.9921864573	3.1614069993	1.7682019019
H	-2.3260221949	3.9476638664	1.5132662318
H	0.4007412318	7.0528451405	0.2172397407
H	-2.3393560619	-5.0629414337	0.6924994160
H	-2.6661136490	3.5100530889	-2.6836343990
H	3.6949510982	6.7714556941	0.6056331318
H	4.5003493814	-0.9307907607	-1.5934259283
H	2.3445045323	-5.0370560562	-0.2942765328
H	-5.5343168088	-3.5568888171	-0.1903784506
H	-0.7503486094	6.8336270005	-2.3853509144
H	-2.0421233472	7.6608080624	-3.2741495954
H	-0.7094468770	6.2015363421	-4.7291564135
H	-2.5246830151	4.8484535602	-5.7543371532
H	-3.1084119071	6.4584263164	-5.3010013930

H	-3.5133827187	5.0547170510	-4.2949730421
H	-0.1884461609	4.5629987052	-3.1424423101
H	4.7932152516	4.0339525255	-2.9440518094
H	4.0267308851	4.7450705461	-1.4921619795
H	2.5928488293	3.7202384371	-3.9757257616
H	2.7825818293	6.5338784121	-2.7718300777
H	1.8345777015	6.0794917565	-4.1993252229
H	3.5988473120	5.9912359014	-4.2558542036
H	1.6690123849	3.4669900017	-1.7611547296
H	4.4020756230	-4.1931974089	-2.6357866944
H	6.1749203785	-4.1613952894	-2.4704770168
H	5.4506314874	-3.4307275848	-4.6818274043
H	6.5482539661	-1.0597146913	-3.0834980728
H	6.6571397441	-1.2763087574	-4.8421430202
H	7.5254911283	-2.3772649715	-3.7573736976
H	4.2679346192	-1.1232343803	-3.6311338460
H	0.7466304973	-8.3841874817	0.7395740597
H	2.0870794932	-7.8995278664	1.8194172669
H	2.2402787628	-7.8028000870	-1.2060150641
H	3.7446500896	-9.7746519638	-0.9545459243
H	2.0986482586	-10.1591232882	-0.4069372757
H	3.3882880348	-9.8381603373	0.7750035469
H	3.7649098825	-6.4582617026	-0.3136944531
H	-2.1504477062	0.6476825613	3.4124887683
H	-2.6855521244	1.3105083248	1.8572534187
H	-3.9468997365	1.9793977086	3.6991808335
H	0.2941164132	-2.6244238778	5.3982316606
H	-1.2698626189	-2.2359553900	4.6570768503
H	-0.5894613705	-4.7529653948	5.7153187889
H	-6.1095864574	-5.5043590567	2.1233208717
H	-4.8600708507	-5.2954508560	3.3772791045
H	-4.5404957080	-7.1651311200	1.0100382002
H	-6.3811446684	-7.9578308956	2.4973679364
H	-5.3181581066	-7.7700790963	3.9112322392
H	-4.9348889030	-8.9733725416	2.6751856478
H	-2.5685383031	-6.7153414484	1.8851020719
H	4.8059997945	-2.7532050178	4.5884741490
H	3.3263485150	-3.7136565445	4.4035255884
H	5.9023500714	-4.5904391467	3.6914583038
H	2.6236693500	8.9193588013	2.6268588012
H	1.1244885613	8.3097218179	3.3716276829
H	1.2024257637	9.8054797442	0.7289367852
H	0.4008189883	10.7596684840	3.5273175705
H	0.2023046137	11.6729764276	2.0279912793
H	1.8336815995	11.3019706947	2.6237584240
H	-0.6644317459	8.6623049103	0.8354132410
H	6.3591950861	1.2351688325	3.4788820350
H	6.2575994808	-0.4335326252	2.8807546106
H	7.7729282014	1.6141593631	1.6939518644
H	-5.6057783033	-0.7624337790	-3.4471916029
H	-4.4775537288	-1.8833748887	-2.6652779583
H	-4.1462720507	-0.4398086382	-5.3459091802
H	-4.4234615706	-3.4309196488	-4.7137198641
H	-4.1741689075	-2.7240550844	-6.3230862505
H	-5.6784272295	-2.4169336990	-5.4387332738
H	-2.3063570486	-2.2467018167	-4.2077446501
H	2.3193739968	1.3378162668	2.7449657612
H	2.5811745157	2.3040362006	4.2181049796

H	0.2528397256	2.3298727609	4.3620690926
H	-5.8524254757	4.5157872240	0.9581266496
H	-7.0760298983	3.2630454266	0.6674834500
H	-5.9563419502	2.2887923699	2.6464582340
H	-1.8265412056	4.6132556099	3.8833649765
H	-3.1034937037	5.8436160159	3.7551359357
H	-4.5378086518	3.9890242711	3.2481220991
H	-1.6315871167	0.1107479866	-4.1351250771
H	-1.9598039695	1.6300555177	-3.5491568640
H	-2.4753517369	1.6612681292	-5.7574775607
H	-1.0150774424	2.6473510196	-5.5153238526
H	-0.8902385203	0.9977068179	-6.2238781831
H	2.1952434233	-3.8922273531	-3.5131717529
H	1.1948633375	-6.1628766785	-3.5462701352
H	-1.5126112899	-2.2999737917	-2.0551537432
H	-0.6193226460	2.5942084538	-1.3490209934
H	-0.5323857686	1.8843182871	1.0256704163
H	0.2553863052	-0.3934006024	1.5971813515
H	0.8959638391	-1.9643428268	-0.1997891909
H	2.1073318048	-1.6754421962	-2.6325790101
H	-0.0001199193	-1.2776825677	-4.7522922854
H	1.7340679920	-1.5177375707	-4.8859050693
H	1.1959993941	0.8523121039	-5.3817277889
H	2.1259024255	0.7629248893	-3.8918860070
H	0.2943594001	2.2890941750	-3.5412650212

2-HP-B-CD:cis-(1R,4R)-SRT_2_MD E(Ha)= -7253.92568755

C	0.2939245800	0.9334582727	4.0809949028
C	0.1852978482	0.6962068984	2.5933272529
C	-0.1436129185	-0.5607384703	2.0688913721
C	-0.4492766012	-1.7571125971	2.9551909359
C	-0.1332462829	-1.5118329699	4.4416063794
C	-0.4935141782	-0.0994657848	4.8712071824
C	0.3672327846	1.7848631247	1.7309168326
C	0.2144129902	1.6432285631	0.3598840414
C	-0.1267238954	0.3978717900	-0.1707828386
C	-0.2932173947	-0.6862568520	0.6810485747
C	0.2248631740	-3.0409840171	2.5171947367
C	-0.4794872519	-4.2439786303	2.5086142709
C	0.1693705452	-5.4472269534	2.2551882660
C	1.5392603329	-5.4789079144	2.0127900718
C	2.2460418726	-4.2712914874	1.9892512528
C	1.5924347354	-3.0655300597	2.2258035925
Cl	2.3225533118	-6.9921305637	1.7585405807
Cl	3.9556721325	-4.2494675606	1.6853755133
N	1.7506090519	0.9772761547	4.4812423574
C	1.9985119923	1.4522672415	5.8607344026
C	0.5717220486	5.9007270645	0.4389888349
C	1.8320202154	6.3355366993	1.1835990046
C	3.0829257876	5.7308800951	0.5352854182
O	3.0961597375	5.9602483575	-0.8464175967
C	2.0464514629	5.2757238435	-1.5304579798
C	0.7007509197	5.8410517417	-1.0880882545
O	3.0650468504	4.3683938214	0.8290880113
C	4.2662029810	3.6595791976	1.0975082249
C	3.7528571817	2.4703466386	1.8924586832
C	4.8260911801	1.4260845427	2.0902656052
C	5.3054414998	1.0052621602	0.6913063113
O	5.8640926912	2.1269518744	0.0535312433
C	4.9784451726	3.2216781646	-0.1848037411
O	4.2010256387	0.4714438182	0.0187190058
C	4.4730543113	-0.2091383349	-1.2017083332
C	4.7136659539	-1.6901465994	-0.9444300016
C	4.7953242105	-2.4270845448	-2.2722849254
C	3.5284311824	-2.1709157421	-3.0859705733
O	3.3762899402	-0.7995224772	-3.2910264860
C	3.2247226685	-0.0533576041	-2.0822396480
O	2.4412354550	-2.7089325401	-2.3720869359
C	1.5668364988	-3.6201789577	-3.0125158109
C	1.2169844873	-4.6381547162	-1.9258598842
C	0.1780718478	-5.6167589259	-2.4350541394
C	-1.0143897391	-4.8416316025	-3.0143600549
O	-0.6054242162	-3.9335562783	-4.0045247292
C	0.3006213757	-2.9358241738	-3.5219025907
O	-1.6278273438	-4.1649506468	-1.9543370489
C	-3.0137550970	-4.3508025893	-1.7006460099
C	-3.0952051491	-4.1957004394	-0.1824472263
C	-4.5111237092	-3.9912570163	0.3171948716
C	-5.1787790138	-2.9096989409	-0.5480867246
O	-5.1759408430	-3.3056248694	-1.8958543872
C	-3.8655395803	-3.3391434102	-2.4590949633
O	-4.4364819628	-1.7378190357	-0.3550713189
C	-5.1001262667	-0.5036047133	-0.1311650778

C	-4.1467804488	0.2529428615	0.7885618308
C	-4.6741063450	1.6556864590	1.0241326866
C	-4.8708054259	2.3244520335	-0.3444533630
O	-5.7683000537	1.5890332971	-1.1322320620
C	-5.3687492092	0.2514081946	-1.4301447788
O	-3.5948480395	2.4095653409	-0.9238916041
C	-3.3423059572	3.4282204688	-1.8813856261
C	-3.2075107053	4.7821207790	-1.1910720259
C	-2.5133755493	5.8033058412	-2.0782894606
C	-1.1787876426	5.2463624723	-2.5766755071
O	-1.4303365796	4.0799400250	-3.2909997363
C	-1.9969917698	3.0260553038	-2.5105874026
O	-3.8023874719	2.4717030825	1.7750334368
C	-3.9931205742	2.4782411358	3.1763244139
C	-3.2002339001	3.6652297546	3.7058453125
O	-1.8311935924	3.5127068294	3.3262707634
O	-3.9947242818	-0.4622091431	2.0083599209
O	-4.4722200452	-3.5599690304	1.6637697727
C	-5.6148880129	-3.9387402397	2.4288258865
C	-5.8770268121	-2.9163699151	3.5242883180
O	-6.3362651296	-1.6982125760	2.9795655336
O	-2.4958174064	-5.3223713058	0.4302918346
O	-0.2811417481	-6.4387336370	-1.3844597641
C	-0.5287603693	-7.7892040093	-1.7626360696
C	-1.5880323557	-8.3916102899	-0.8533154503
O	-2.8246915212	-7.7289193394	-1.0280162483
O	2.3693444123	-5.3369190932	-1.5093784447
O	4.9710045531	-3.8068693216	-2.0091794760
C	5.7424471833	-4.4858142004	-3.0051844691
C	5.2904090144	-5.9310056197	-3.1349437087
O	3.9794040693	-5.9901073505	-3.6544621901
O	5.9026351710	-1.8723557964	-0.2042247572
O	4.2652891401	0.3856770355	2.8515625887
C	5.1702662831	-0.6316875718	3.2330465095
C	4.7494176510	-1.1559662365	4.5969416488
O	3.3548856813	-1.4706971642	4.6168851727
O	3.2399347164	2.9057104806	3.1444845493
O	1.8614007155	5.8746433947	2.5167880943
C	0.9016496386	6.4031702418	3.4140850703
C	0.9675536879	5.5929966079	4.7014157288
O	0.6548274529	4.2286957585	4.4501233709
O	-0.4962494721	6.7611298865	0.8055558146
O	-0.3433559012	4.9558319378	-1.4807509908
O	-2.3537089636	6.9706736482	-1.2851383094
C	-2.3075096473	8.1963257684	-2.0197676526
C	-1.7616044166	9.3035277484	-1.1314189306
O	-0.4083722167	9.0684456357	-0.8089804644
O	-4.4815313515	5.2582280980	-0.8120298524
C	-2.0752557337	1.7995254496	-3.3996959978
O	-0.8147085775	1.1740704758	-3.4149217233
C	2.3211481528	5.4082067652	-3.0175481948
O	3.4147548589	4.6330238646	-3.4392400533
C	5.8362211162	4.3067734000	-0.8276155418
O	5.8482558912	4.2232815942	-2.2389066237
C	2.9042514898	1.3714049613	-2.4629371171
O	4.0138618424	1.9877424908	-3.0675260154
C	0.5036535429	-1.9621316482	-4.6642993952
O	-0.6769564110	-1.2219878345	-4.9216435812

C	-4.0452020638	-3.6668105129	-3.9296300459
O	-4.7642657829	-2.6629642914	-4.6025521688
C	-6.5132596707	-0.3319142643	-2.2403891578
O	-7.6926036165	-0.4497478215	-1.4823587803
C	-3.7534813850	4.9991461101	3.2286371385
C	-1.7892180805	-9.8626093561	-1.1701339482
C	6.2097697559	-6.6899741449	-4.0759564460
C	5.5863153239	-2.3394351239	5.0437617982
C	2.3289126528	5.6399051926	5.3674798693
C	-6.9400674888	-3.4288186446	4.4799753638
C	-1.8481390718	10.6423029623	-1.8412438752
H	-5.3162369826	3.3136968007	-0.2250436003
H	-5.6582139483	1.6063126096	1.5143549662
H	-3.1695393009	0.3396784175	0.2953462359
H	-6.0508556016	-0.6770963154	0.3922049275
H	-6.2285458938	-2.7596214139	-0.2729588529
H	-5.0750443064	-4.9286692730	0.2201456534
H	-2.5275269301	-3.2911001270	0.0779669293
H	-3.3126424759	-5.3760355291	-1.9627354010
H	-1.7151352752	-5.5316601469	-3.4973577669
H	0.6280405178	-6.2213944799	-3.2348497156
H	0.7866993911	-4.0875432048	-1.0759748778
H	2.0844988543	-4.1358513555	-3.8345429928
H	3.5967465409	-2.6274058212	-4.0805793062
H	5.6549372380	-2.0345256174	-2.8331767916
H	3.8513528574	-2.0722689051	-0.3781361838
H	5.3359654957	0.2447659587	-1.7034336120
H	6.1189402334	0.2749048921	0.7421563818
H	5.6936498970	1.8594060616	2.6140123978
H	2.9534102342	2.0047797987	1.3025564544
H	4.9301673639	4.2657740992	1.7339153395
H	3.9824998145	6.2103901952	0.9398590860
H	1.9140958202	7.4322254336	1.1382564575
H	0.3531712131	4.8740020097	0.7674755727
H	0.5482636491	6.8490191152	-1.4990984306
H	-0.6843947776	5.9387985186	-3.2690988944
H	-3.1502255358	6.0207909481	-2.9464818178
H	-2.5795624484	4.6121856377	-0.3033502339
H	-4.1438987304	3.4728131719	-2.6330643084
H	-1.3309006531	2.7857497918	-1.6752613975
H	2.0682468378	4.2098451790	-1.2709986205
H	4.2085217079	2.9256883076	-0.9041913203
H	2.3664731826	-0.4443527163	-1.5186530620
H	-0.1651409722	-2.3953892912	-2.6871867487
H	-3.4006575701	-2.3496821087	-2.3715522350
H	-4.4546468774	0.2484428698	-2.0392803423
H	-3.8301080850	-1.3850356535	1.7429996748
H	2.6692815447	3.6773916384	2.9739957940
H	-4.3424780979	6.1498726241	-0.4682097739
H	-1.6208816104	-5.4124232629	0.0089229268
H	3.0587112962	-4.6700727891	-1.3452199146
H	6.0710749753	-2.8236020696	-0.2158620042
H	-1.2326390459	6.6080378588	0.1829634648
H	-3.6302299850	1.5423400893	3.6198472306
H	-5.0571079788	2.5917135964	3.4318742165
H	-3.2137526138	3.6267444155	4.8012265145
H	-4.7531636619	5.1722840647	3.6396218669
H	-3.8276416963	5.0154403706	2.1375131586

H	-3.1047187375	5.8171427572	3.5523290282
H	-1.8351851783	3.2067779852	2.4072694508
H	0.4085603115	-8.3598813076	-1.7075594556
H	-0.9066740589	-7.8367501091	-2.7937358789
H	-1.2392633174	-8.2883802380	0.1869731655
H	-2.5442152510	-10.2835029695	-0.5028620330
H	-0.8621338376	-10.4313958537	-1.0540528940
H	-2.1472880333	-9.9801221042	-2.1977731274
H	-2.8650025844	-6.9862067692	-0.4052090939
H	6.8066877454	-4.4278129984	-2.7363499014
H	5.6055677392	-4.0042921778	-3.9821282690
H	5.3313983486	-6.3938745182	-2.1358899146
H	7.2443853644	-6.6905455488	-3.7204934022
H	6.1823973221	-6.2428527956	-5.0748233143
H	5.8697196601	-7.7238559795	-4.1633524317
H	3.3596685427	-5.9435312805	-2.9059342547
H	6.1943038056	-0.2375261687	3.3126444976
H	5.1821294924	-1.4314249295	2.4776010660
H	4.8496050361	-0.3352834233	5.3172952192
H	5.4834439983	-3.1752676895	4.3421972978
H	5.2673022372	-2.6767618246	6.0324732283
H	6.6464463084	-2.0746755561	5.0962222017
H	3.2199239297	-2.2823098967	4.1103988494
H	1.4505624408	5.0394110282	-3.5688062731
H	2.4655924181	6.4704603220	-3.2637103653
H	4.2278359664	4.8601712686	-2.9471009047
H	5.4513530236	5.3006313830	-0.5911308112
H	6.8516883727	4.2239820253	-0.4162573453
H	5.8191009100	3.2873973778	-2.4857491639
H	-0.1053518273	6.3332958667	2.9872035675
H	1.1060280812	7.4649796471	3.6228917886
H	0.2216059454	6.0309906534	5.3847036377
H	2.3138472669	5.0780359054	6.3052508906
H	2.6094568273	6.6722844420	5.5939217957
H	3.0940331679	5.2102219159	4.7165229350
H	-0.2520945451	4.1659961217	4.0961272878
H	2.0329426952	1.3561791018	-3.1322480520
H	2.5970092372	1.8868744229	-1.5382999667
H	3.7085111852	2.8619191461	-3.3819714513
H	-5.4471319385	-4.9376333444	2.8558588229
H	-6.5091196504	-3.9787730343	1.7927590234
H	-4.9339608852	-2.7650736208	4.0760364798
H	-7.1276813307	-2.6835631055	5.2559113638
H	-6.6389966334	-4.3654897688	4.9580995767
H	-7.8795763418	-3.5958965815	3.9436473224
H	-5.5684894216	-1.1577014358	2.7332474100
H	1.2786089184	-1.2378914564	-4.4017689549
H	0.8243919956	-2.5104914627	-5.5612430873
H	-1.3872449400	-1.8500613690	-5.0985839470
H	-3.3190387133	8.4376716762	-2.3749125519
H	-1.6462889575	8.0933851669	-2.8907789297
H	-2.3770724385	9.3394404619	-0.2172884929
H	-2.8816124672	10.9014479883	-2.0882247427
H	-1.2601431732	10.6247871161	-2.7642888259
H	-1.4370518441	11.4221787702	-1.1972066491
H	-0.3738976071	8.4203937540	-0.0859193872
H	-3.0588868765	-3.7206175345	-4.4000651751
H	-4.5241928839	-4.6532230378	-4.0265549853

H	-5.6784112045	-2.7263532144	-4.3061990926
H	-2.8511491413	1.1318090787	-2.9998957780
H	-2.3894909278	2.1201077650	-4.4044276316
H	-0.8536405395	0.4013186282	-4.0069525000
H	-6.6553606705	0.2998556635	-3.1291817232
H	-6.2396660362	-1.3354189833	-2.5720666802
H	-7.9261910481	0.4414348153	-1.1970172108
H	2.2233898022	0.0650519960	4.3432406845
H	2.2546517660	1.6496874627	3.8559874651
H	1.6286774946	0.7287609007	6.5862420279
H	3.0748051282	1.5750850855	5.9863073433
H	1.5044944613	2.4181371516	5.9773522604
H	-1.5524670257	-4.2510347382	2.6773684980
H	-0.3864464467	-6.3783423200	2.2533463971
H	2.1542850465	-2.1359114956	2.1652496442
H	0.6194854625	2.7550773614	2.1543853425
H	0.3452973756	2.5002457694	-0.2951964319
H	-0.2842401421	0.2995946634	-1.2429608532
H	-0.5555619026	-1.6577841155	0.2685138583
H	-1.5350476387	-1.9138862225	2.8788408700
H	0.9309836541	-1.6966691747	4.6290992645
H	-0.6731373804	-2.2484409302	5.0445719044
H	-0.3528955479	0.0339337092	5.9486581945
H	-1.5539638653	0.0960705341	4.6732925854
H	-0.0789737085	1.9354885389	4.3041679580

255

2-HP-B-CD:cis-(1R,4R)-SRT_3_MD E(Ha)= -7253.92367314

C	-0.4780708368	-1.2427756292	3.9515678326
C	-0.2755805278	-0.7998388259	2.5202882183
C	0.0001024296	0.5335380435	2.1874471892
C	0.1382910167	1.6262352701	3.2353194225
C	-0.3209412993	1.1731487605	4.6274173794
C	0.1238474555	-0.2492703281	4.9343148811
C	-0.3192226838	-1.7726032998	1.5131821134
C	-0.0776272043	-1.4409355168	0.1891597739
C	0.2227900755	-0.1208975767	-0.1475160714
C	0.2477434953	0.8492342377	0.8446122132
C	-0.5667308163	2.9138833896	2.8554773219
C	0.1051949151	4.1345568239	2.8614441837
C	-0.5725539305	5.3199791769	2.5959310284
C	-1.9350091081	5.3111701248	2.3159265723
C	-2.6098584358	4.0845743772	2.2858840778
C	-1.9314358816	2.9018024178	2.5526704108
Cl	-2.7521866917	6.8006945800	2.0212531076
Cl	-4.3052800100	4.0125570822	1.9189261633
N	-1.9491718234	-1.4856837799	4.1969745852
C	-2.2723459756	-2.1312185551	5.4865578395
C	-0.0144523773	-6.0114231257	-0.0923056117
C	-1.3119364092	-6.6239070250	0.4263180107
C	-2.5203351737	-5.9869035666	-0.2722824856
O	-2.3687856518	-6.0218477352	-1.6656786062
C	-1.3071440241	-5.1855980068	-2.1253968604
C	0.0189060347	-5.7267434848	-1.6014080486
O	-2.6234444157	-4.6786375270	0.2015210140
C	-3.8999664483	-4.0935713106	0.4118131835
C	-3.5781585140	-2.9488492399	1.3564972529
C	-4.7706540323	-2.0402520515	1.5501837221
C	-5.1601662685	-1.5083323696	0.1613102243
O	-5.5299914698	-2.5970169388	-0.6458589298
C	-4.5221400150	-3.5789224049	-0.8906367218
O	-4.0672395973	-0.7890842310	-0.3324100748
C	-4.3209822809	0.0146464622	-1.4799209522
C	-4.6996033483	1.4313327830	-1.0670715433
C	-4.7971170701	2.3016339630	-2.3123318867
C	-3.4866771881	2.2490765958	-3.0964263170
O	-3.2005928512	0.9211985122	-3.4291084207
C	-3.0225498489	0.0742521549	-2.2929991206
O	-2.4794084965	2.8108525644	-2.2953230409
C	-1.5970169576	3.7655458801	-2.8588611258
C	-1.3455001628	4.7581812847	-1.7240475524
C	-0.3326974379	5.8025701848	-2.1499140122
C	0.9242671452	5.0972869885	-2.6823041833
O	0.6071478882	4.2056620569	-3.7198987154
C	-0.2786352145	3.1529285666	-3.3273426089
O	1.5047086304	4.4037529642	-1.6101098363
C	2.8197880688	4.7459734502	-1.2003867994
C	2.7848082265	4.5680856456	0.3146415170
C	4.1710211411	4.5335102217	0.9246770532
C	5.0347213226	3.5608234825	0.1105822862
O	5.1064564768	3.9758844570	-1.2301795774
C	3.8496235184	3.8647692494	-1.9016366191
O	4.4108089779	2.3149219117	0.2256397946
C	5.1510863352	1.1273478125	0.4496315433

C	4.1920465865	0.2906268970	1.2957802156
C	4.7491689341	-1.1009634980	1.5137133549
C	5.0762995703	-1.7211555960	0.1400052108
O	5.9695341873	-0.9015894273	-0.5675519902
C	5.5139523446	0.4213032799	-0.8494126405
O	3.8534352088	-1.9039954758	-0.5229475354
C	3.8228962398	-2.8343903504	-1.5990691986
C	3.7786238623	-4.2625588202	-1.0629241932
C	3.3376578323	-5.2466392428	-2.1346260929
C	2.0062794430	-4.7979626617	-2.7363760948
O	2.1827039235	-3.5369773979	-3.2979694412
C	2.5163978635	-2.5211336242	-2.3504966272
O	3.8032143895	-1.8469097028	2.2431359088
C	4.2525522894	-3.1042766919	2.7063368028
C	3.1111902198	-3.6886100248	3.5182425497
O	1.9374310586	-3.7409416685	2.7072761390
O	3.9515909112	0.9486809806	2.5288771232
O	4.0809081810	4.0767046387	2.2589339961
C	5.0687873454	4.6045847375	3.1389960917
C	5.4865229266	3.5446563771	4.1462738251
O	6.1304663410	2.4701798150	3.4900852040
O	2.0256044634	5.6071958787	0.9008939296
O	0.0229472878	6.6104459947	-1.0491113199
C	0.2031782618	7.9868522834	-1.3727889848
C	1.0091793731	8.6702676840	-0.2806195010
O	2.3295365394	8.1721382484	-0.2377584020
O	-2.5516053388	5.3792680792	-1.3360797168
O	-5.1201998800	3.6194791942	-1.9146876739
C	-5.9454968275	4.3342009842	-2.8388118012
C	-5.5054091869	5.7865454668	-2.9390390540
O	-4.2113113166	5.8673597997	-3.4981726392
O	-5.9298785011	1.4258225838	-0.3744253645
O	-4.3907478460	-1.0535131006	2.4765930668
C	-5.3930267316	-0.1083118736	2.7931615362
C	-5.1962496110	0.3420370702	4.2268172862
O	-3.8249366241	0.7364113766	4.3711473431
O	-3.1202088462	-3.4393894614	2.6077302850
O	-1.5393755728	-6.3852874438	1.7973543463
C	-0.5654990457	-6.8086184206	2.7324474313
C	-0.7585153528	-5.9975716452	4.0062739072
O	-0.5964861427	-4.6048558857	3.7470957871
O	1.0695072362	-6.8608510789	0.2551064106
O	1.0345059172	-4.7387334699	-1.7213313225
O	3.2471351365	-6.5149869953	-1.5032052170
C	3.4474439699	-7.6267756939	-2.3832516883
C	2.9061049055	-8.8977272802	-1.7470617450
O	1.4987688242	-8.8556117254	-1.6588410458
O	5.0501124312	-4.6345810533	-0.5679090285
C	2.5284917982	-1.2007672350	-3.0956219013
O	1.2004112735	-0.7608323082	-3.2493950630
C	-1.4040579078	-5.1330720589	-3.6388605166
O	-2.5338131723	-4.4280862847	-4.0871196859
C	-5.2106090812	-4.6505625363	-1.7299529895
O	-5.1042368281	-4.4074277960	-3.1171171155
C	-2.5232735269	-1.2617217129	-2.7874789915
O	-3.5103933903	-1.9267703420	-3.5329775372
C	-0.3863503893	2.2383880734	-4.5294302887
O	0.8487377295	1.5906821172	-4.7877675020

C	4.0901357413	4.2685719017	-3.3454727169
O	4.3696673983	5.6381740618	-3.4967411170
C	6.6509510325	1.0582133606	-1.6305791878
O	6.8961965416	0.3481061666	-2.8174659973
C	3.4070252297	-5.0888894843	4.0077066130
C	1.0861579273	10.1645271295	-0.5374622626
C	-6.4618517408	6.5692330473	-3.8223282523
C	-6.1318981831	1.4792934518	4.5863461147
C	-2.1235056183	-6.1904830156	4.6378626133
C	6.4449203091	4.1293139815	5.1688755396
C	3.2847661443	-10.1080748882	-2.5813744099
H	5.6042635059	-2.6712164536	0.2470394469
H	5.6934641953	-1.0344194762	2.0782941881
H	3.2458110642	0.1922120334	0.7449146273
H	6.0551712105	1.3457852621	1.0376664881
H	6.0637842031	3.5269781882	0.4861157081
H	4.6151300686	5.5366229636	0.8798061075
H	2.3123451001	3.5975238442	0.5227286667
H	3.0346527652	5.7991028797	-1.4236393451
H	1.6307210582	5.8199830767	-3.1053662377
H	-0.7670483010	6.4134655407	-2.9535635507
H	-0.9251974253	4.1984521232	-0.8752249525
H	-2.0877515135	4.2869895762	-3.6935062236
H	-3.5730468309	2.7942129407	-4.0435082234
H	-5.5914701711	1.8905173583	-2.9506305053
H	-3.9007525315	1.8211921481	-0.4183437356
H	-5.1136258290	-0.4357536469	-2.0894274352
H	-6.0526446697	-0.8761498607	0.2029963236
H	-5.6345524895	-2.6064946694	1.9355826927
H	-2.7921342546	-2.3439223770	0.8859370593
H	-4.5658138198	-4.8110660173	0.9168490819
H	-3.4257449160	-6.5613056027	-0.0428298121
H	-1.3102265504	-7.7010727958	0.1987329691
H	0.1038582483	-5.0398352512	0.4081504928
H	0.2968690389	-6.6497943239	-2.1310986278
H	1.6842517535	-5.4616679084	-3.5479774429
H	4.0941295622	-5.2745473247	-2.9310900785
H	3.0328603139	-4.2724536100	-0.2523834224
H	4.7016044503	-2.7055491317	-2.2472976433
H	1.7345523447	-2.4644083803	-1.5865824831
H	-1.4397745231	-4.1698652138	-1.7326758125
H	-3.7160695927	-3.1373635035	-1.4858981063
H	-2.2389392371	0.4879572422	-1.6430901366
H	0.1698390671	2.5896019788	-2.4980508382
H	3.5039455696	2.8234836312	-1.8745260552
H	4.6209977393	0.3839563380	-1.4874582496
H	3.7212063303	1.8645541564	2.2880130251
H	-2.4416002029	-4.1191732050	2.4383470222
H	4.9876618870	-5.5768534920	-0.3639424929
H	1.1990068486	5.6652789251	0.3869335394
H	-3.1857208304	4.6619921755	-1.1656804759
H	-6.1755005454	2.3567889521	-0.2901466424
H	1.8661263344	-6.5276050698	-0.1996885376
H	5.1484344759	-2.9939524889	3.3363154182
H	4.4940017540	-3.7775272454	1.8708251172
H	2.9333717276	-3.0189191029	4.3742637419
H	2.5745262658	-5.4691227689	4.6063516532
H	4.3034599908	-5.1035975845	4.6338762741

H	3.5561023916	-5.7629108387	3.1590184437
H	1.9142691206	-2.9090187991	2.2081729166
H	-0.7811858670	8.4621229237	-1.4864746690
H	0.7568637722	8.0901407165	-2.3167874917
H	0.4932706199	8.4928142119	0.6779695799
H	1.5890096097	10.3571467055	-1.4904412331
H	1.6702437929	10.6426837054	0.2516077445
H	0.0926595748	10.6211060202	-0.5646635299
H	2.3299714198	7.3443271641	0.2687206207
H	-6.9926726335	4.2645047150	-2.5128244789
H	-5.8653668586	3.8889991475	-3.8387237265
H	-5.5132322284	6.2174838761	-1.9253155978
H	-6.1353313459	7.6093696694	-3.8841930864
H	-7.4846353970	6.5465561926	-3.4343162741
H	-6.4630407531	6.1577462855	-4.8368276609
H	-3.5731501283	5.8787126948	-2.7644534431
H	-6.3942355388	-0.5571397996	2.7129696643
H	-5.3472712935	0.7435053431	2.1013057164
H	-5.3818847185	-0.5197110618	4.8866967040
H	-5.9370896278	2.3497795090	3.9526606667
H	-6.0078442572	1.7737150214	5.6342160779
H	-7.1760663020	1.1804517151	4.4575435878
H	-3.7758818802	1.3923500200	5.0745439186
H	-0.5304707741	-4.6003610787	-4.0279718170
H	-1.3907711547	-6.1589786536	-4.0365196610
H	-3.3584762181	-4.8035170319	-3.7219209463
H	-4.7604075056	-5.6312465553	-1.5663207084
H	-6.2618933536	-4.6971207884	-1.4131678078
H	-5.1714294391	-3.4523504970	-3.2635391148
H	0.4463593804	-6.6465206872	2.3469795014
H	-0.6723773960	-7.8826922467	2.9507523379
H	0.0133752092	-6.3392982889	4.7155192973
H	-2.2866429912	-7.2443358659	4.8796210254
H	-2.9147695695	-5.8664351817	3.9574529101
H	-2.2011218203	-5.6143946807	5.5640806596
H	0.2955695978	-4.4474572926	3.3829994944
H	-1.6144318605	-1.0881977790	-3.3802612294
H	-2.2200992909	-1.8365299375	-1.8969875117
H	-3.0802022715	-2.7235519804	-3.9013090056
H	4.6649462046	5.4928489783	3.6441729825
H	5.9631575772	4.9045690559	2.5766134378
H	4.5789370269	3.1895679645	4.6607924575
H	6.7375997564	3.3580048893	5.8843860397
H	5.9939497412	4.9624945478	5.7161263415
H	7.3527616138	4.4884151967	4.6737754535
H	5.4675181137	1.7864913293	3.3034232246
H	-1.1262704588	1.4568677700	-4.3438433250
H	-0.7071789304	2.8219465398	-5.4036991630
H	1.5040439208	2.2831461912	-4.9325275536
H	4.5210215262	-7.7175917891	-2.5990108712
H	2.9133405516	-7.4613123351	-3.3278187596
H	3.3552812697	-8.9917503783	-0.7446976726
H	2.8595185037	-10.0246985200	-3.5865082690
H	2.8763965917	-11.0092219453	-2.1196995697
H	4.3695405916	-10.2179976623	-2.6664605076
H	1.2549774841	-8.3390266042	-0.8726459316
H	4.8928508408	3.6359369239	-3.7520883191
H	3.1809406652	4.0681233485	-3.9210051935

H	5.1894463984	5.8191306474	-3.0229880469
H	3.1246269281	-0.4853935157	-2.5116731640
H	3.0293468992	-1.3521761463	-4.0630893712
H	1.1849364537	0.0116389172	-3.8432654697
H	6.3868916547	2.0820818434	-1.9072903063
H	7.5424293343	1.0981308923	-0.9829586893
H	7.0960440181	-0.5563236806	-2.5486313373
H	-2.5066561366	-0.6174444882	4.1048322498
H	-2.3212498835	-2.1380897381	3.4650723341
H	-2.0368990171	-1.4691407387	6.3190141229
H	-3.3385762237	-2.3595966382	5.4860978824
H	-1.7024437485	-3.0592866790	5.5530584800
H	1.1729825952	4.1758920884	3.0561761796
H	-0.0388537580	6.2634967117	2.6015311512
H	-2.4812735394	1.9658438854	2.5332842590
H	-0.5374016092	-2.8028509437	1.7850413327
H	-0.1090252880	-2.2050977002	-0.5809230550
H	0.4548404055	0.1194251516	-1.1826918015
H	0.4652622671	1.8817839352	0.5813677116
H	1.2146398150	1.8430624959	3.2992546297
H	-1.4137129511	1.2458580367	4.6811354965
H	0.0670730620	1.8690268912	5.3776024925
H	-0.1058727568	-0.5227611972	5.9692529530
H	1.2133415610	-0.3269399676	4.8312281582
H	-0.0213130960	-2.2275257217	4.0870338447

255

2-HP-B-CD:cis-(1R,4R)-SRT_4_MD E(Ha)= -7253.9221000361

C	-0.03776190	-1.18137841	3.60917759
C	-0.00038151	-0.73157160	2.16797742
C	0.37598813	0.57563461	1.82751822
C	0.79794964	1.60187249	2.86272986
C	0.66380126	1.11733683	4.32025638
C	0.94106558	-0.37260429	4.44648067
C	-0.28211650	-1.66274215	1.16156858
C	-0.18968577	-1.31575337	-0.17873383
C	0.19541663	-0.02168629	-0.52633667
C	0.46538988	0.90844964	0.46888343
C	0.11653469	2.94961969	2.72927805
C	0.80170681	4.09770121	3.13149993
C	0.18311710	5.34001289	3.12001800
C	-1.14501025	5.46686487	2.71928517
C	-1.84208031	4.32171121	2.32471551
C	-1.21169395	3.07703891	2.31495056
Cl	-1.88741695	7.02132717	2.72296801
Cl	-3.51023494	4.41762187	1.85999616
N	-1.45254927	-1.10815567	4.12919133
C	-1.62828438	-1.60171139	5.51134851
O	-5.60218936	2.28845099	-0.12268752
C	-4.44301873	2.11226648	-0.90848542
C	-4.49399775	3.00323174	-2.14244924
C	-3.26444092	2.75063597	-3.01567750
O	-3.22443707	1.39576092	-3.36571325
C	-3.08281824	0.52799677	-2.24562903
C	-4.29355580	0.65188946	-1.31252322
O	-2.12598074	3.11096929	-2.27277208
C	-1.28485536	4.14512999	-2.76422638
C	-0.78676343	4.85951482	-1.51265849
C	0.29563310	5.85789248	-1.87187919
C	1.37017712	5.14904032	-2.70661747
O	0.82508537	4.58551165	-3.86217474
C	-0.13854004	3.56830254	-3.59540922
O	1.93649745	4.15324109	-1.88613204
C	3.32412027	4.18074251	-1.59729265
C	3.41303255	3.81360704	-0.11976411
C	4.84209334	3.50068012	0.29408014
C	5.41397008	2.47173654	-0.68752423
O	5.38718012	2.96705866	-1.99472706
C	4.06670252	3.19571908	-2.49839524
O	4.62419165	1.31514944	-0.57805249
C	5.21001382	0.07298404	-0.22484155
C	4.25376191	-0.54530972	0.79055611
C	4.65470149	-1.97977876	1.08399066
C	4.79987267	-2.75114620	-0.24192836
O	5.72890216	-2.12541703	-1.08760240
C	5.40281667	-0.78975708	-1.46629645
O	3.51426065	-2.81326315	-0.80181689
C	3.26928425	-3.80475509	-1.78871277
C	3.01961464	-5.16506142	-1.14185047
C	2.36161147	-6.12861247	-2.12174427
C	1.09014526	-5.50247942	-2.69947803
O	1.45815938	-4.32970749	-3.36791874
C	1.98971583	-3.33453477	-2.48851483
O	0.21181663	-5.18810102	-1.65517536

C	-0.98741531	-5.91948532	-1.41988643
C	-0.97729751	-6.12696151	0.10088880
C	-2.33629833	-6.45397668	0.71396293
C	-3.42755331	-5.59157450	0.06413066
O	-3.37672567	-5.69316450	-1.33364349
C	-2.19613923	-5.11352434	-1.88425199
O	-3.22552133	-4.27753988	0.48432913
C	-4.32723871	-3.42831609	0.76797024
C	-3.67964938	-2.32853127	1.59484491
C	-4.64409432	-1.19451495	1.86549668
C	-5.12580342	-0.65914595	0.50652243
O	-5.76493625	-1.70333088	-0.18637216
C	-4.95688614	-2.83661475	-0.49855984
O	-2.43332994	-6.15389254	2.08557853
C	-1.48265512	-6.69449602	2.98372482
C	-1.33822371	-5.72231685	4.14818436
O	-0.92087302	-4.44095243	3.68444332
O	-0.05498584	-7.15494002	0.42733015
O	2.08878600	-7.31770400	-1.39996423
C	2.06649829	-8.50213443	-2.20504044
C	1.29097977	-9.60085722	-1.49390976
O	-0.07536808	-9.26663852	-1.40080356
O	4.23848015	-5.70484281	-0.67570539
O	3.67326755	-2.53945797	1.92877934
C	3.98301558	-3.80848120	2.46876838
C	2.75658113	-4.23438780	3.25610691
O	1.61758214	-4.17824025	2.39496108
O	4.25893481	0.22578644	1.97220931
O	4.92397314	2.89853830	1.57084281
C	4.94158220	3.77727620	2.68932056
C	5.05982817	2.95255486	3.96478693
O	3.90780186	2.14447996	4.15934406
O	2.87753933	4.84957197	0.67857525
O	0.88971577	6.37702399	-0.69823738
C	1.20749101	7.76494854	-0.77712144
C	2.22407398	8.12583157	0.29514040
O	3.47100947	7.51999099	0.03917803
O	-1.85524094	5.51718031	-0.86240393
O	-4.54775715	4.34265061	-1.68591608
C	-5.22187457	5.23194656	-2.57824351
C	-4.81120176	6.66871657	-2.28972972
O	-3.47611463	6.89981521	-2.67062232
O	-4.01283440	-0.15170943	-0.16894889
O	-3.96387723	-0.25424657	2.65738799
C	-4.75538918	0.80498318	3.15822571
C	-4.24109902	1.17383460	4.54283729
O	-2.82366725	1.35723875	4.53445400
O	-3.17880540	-2.83923961	2.81809990
C	-5.87490972	-3.77614539	-1.27605919
O	-5.79075994	-3.58011445	-2.67325677
C	-2.81715961	-0.86760885	-2.75725555
O	-3.93766129	-1.41082709	-3.41100418
C	-0.60190493	2.99997178	-4.92054505
O	-1.45804525	3.93030607	-5.54772344
C	4.24176368	3.72293428	-3.91169413
O	4.89650151	4.96638482	-3.93491590
C	6.56012198	-0.31093745	-2.32736324
O	7.76581875	-0.27141613	-1.60367927

C	2.13492564	-2.08009826	-3.32495905
O	0.88000066	-1.63667931	-3.78403366
C	-2.38744967	-5.06469930	-3.38923678
O	-3.34291662	-4.11355290	-3.78306295
C	-2.62613777	-5.53339790	4.92696471
C	2.87467206	-5.63921125	3.80357799
C	6.33544226	2.12609230	4.02690248
C	2.43855074	9.62844078	0.33583590
C	-5.68781304	7.63214591	-3.07127751
C	1.40359655	-10.90596051	-2.26184385
C	-4.95043840	2.38697861	5.11426453
H	-4.41541242	-5.95633997	0.36933520
H	-2.57019624	-7.51110174	0.51229127
H	-0.64701518	-5.17548995	0.54306479
H	-0.95556375	-6.89993953	-1.91590766
H	0.61182371	-6.15512775	-3.43990194
H	3.05959005	-6.33749884	-2.94453096
H	2.32770194	-4.99895082	-0.30145653
H	4.11256597	-3.87609181	-2.49100323
H	5.20273644	-3.75471002	-0.08647846
H	5.63440843	-1.98624812	1.58725403
H	3.24636553	-0.56200752	0.34838518
H	6.18797601	0.22803500	0.25053130
H	6.46238716	2.25351136	-0.45681415
H	5.45950950	4.41002264	0.26096772
H	2.83196994	2.89207730	0.02581102
H	3.73283534	5.18945950	-1.74636747
H	2.13892818	5.85452730	-3.04148509
H	-0.14898307	6.66495134	-2.46926367
H	-0.35289542	4.10606949	-0.83895707
H	-1.85858732	4.85476076	-3.37335252
H	-3.29636872	3.30802161	-3.95790728
H	-5.39748083	2.75864240	-2.71962500
H	-3.54718327	2.38394599	-0.32975072
H	-5.19662271	0.29180824	-1.82053190
H	-5.89367949	0.11151491	0.62347411
H	-5.53175553	-1.57117977	2.39984796
H	-2.85635083	-1.91622107	0.99645460
H	-5.07453103	-3.96393830	1.37386763
H	-4.13263966	-2.53916471	-1.15716252
H	-2.19521860	0.82266828	-1.66915104
H	0.33421550	2.75649490	-3.02483769
H	3.50833427	2.25065916	-2.52165231
H	4.47592809	-0.77253458	-2.05409281
H	1.25883200	-3.12639741	-1.70116066
H	-2.08166261	-4.08511643	-1.51920846
H	0.76931843	-6.98490123	-0.06563554
H	-2.59134496	4.88331410	-0.83005918
H	-2.63991663	-3.63228454	2.63643962
H	4.03791671	-6.60399687	-0.38638430
H	4.33532522	1.15979378	1.69239962
H	2.03280470	5.12740436	0.27100797
H	-5.72322379	3.24446993	-0.05611640
H	-0.51223485	-6.82885579	2.49712612
H	-1.81232180	-7.67750803	3.35414770
H	-0.57420111	-6.14573929	4.82123882
H	-3.40992817	-5.12437764	4.28478941
H	-2.47137709	-4.84983031	5.76618502

H	-2.97139505	-6.49040619	5.32795063
H	-0.06877002	-4.51885296	3.21570612
H	4.86318637	-3.75455280	3.12709294
H	4.17930385	-4.54538162	1.67604345
H	2.61926529	-3.51941977	4.08273123
H	1.98022513	-5.90615273	4.37344667
H	3.73557541	-5.72391935	4.47273454
H	2.98904648	-6.35977351	2.98817664
H	1.73720724	-3.38021515	1.85498735
H	4.02480839	4.37452256	2.70849864
H	5.79979482	4.46141018	2.60875152
H	5.05934437	3.67622260	4.79058038
H	7.22186003	2.75889763	3.92375964
H	6.34887679	1.38248580	3.22408624
H	6.39544477	1.60313040	4.98494140
H	4.04882008	1.30571805	3.69857675
H	0.28554341	8.35057283	-0.65602900
H	1.64956886	8.00051209	-1.75557262
H	1.81917019	7.79183509	1.26600035
H	2.82139831	9.98228955	-0.62673654
H	3.18027521	9.87124823	1.09989650
H	1.51139723	10.16224957	0.56327975
H	3.42042609	6.59495970	0.32701144
H	-1.94878090	-0.81016201	-3.42972397
H	-2.51939326	-1.47293535	-1.88731231
H	-3.65010473	-2.27590473	-3.75429103
H	0.29225958	2.79372112	-5.52560682
H	-1.11552800	2.04776872	-4.72300986
H	-1.64369650	3.61982576	-6.43798600
H	-6.30797114	5.10139247	-2.46260480
H	-4.95319338	5.00584262	-3.61865450
H	-4.94781383	6.84832710	-1.21001102
H	-6.74306731	7.53013302	-2.80160630
H	-5.58027577	7.45500783	-4.14627645
H	-5.37160995	8.65758368	-2.86879527
H	-2.88577323	6.55383710	-1.97986212
H	4.77844635	2.96508637	-4.50227091
H	3.25540385	3.86716309	-4.36334871
H	5.76404697	4.83390067	-3.53635896
H	3.10096483	-8.81266823	-2.40698386
H	1.56964709	-8.29859420	-3.16248229
H	1.72880214	-9.73179314	-0.49057434
H	0.98492696	-10.79303130	-3.26693380
H	0.83174133	-11.68061421	-1.74705366
H	2.44261741	-11.23657827	-2.34837519
H	-0.19410996	-8.67705664	-0.63816001
H	6.63330406	-0.96495353	-3.20884551
H	6.35644950	0.70631329	-2.67490549
H	7.93646126	-1.17256231	-1.30676406
H	-5.80873981	0.50053210	3.24776546
H	-4.71820235	1.66461739	2.47388145
H	-4.39525032	0.30913211	5.19968820
H	-6.02660533	2.20872339	5.19905164
H	-4.80549148	3.26298493	4.47186448
H	-4.56204410	2.61898571	6.10868364
H	-2.61450969	2.17658537	4.06560654
H	2.54494820	-1.28526868	-2.69839209
H	2.83327958	-2.26633505	-4.15618828

H	0.49778558	-2.37077292	-4.27881341
H	-5.61315034	-4.82146693	-1.10715152
H	-6.89953588	-3.61483918	-0.91427423
H	-5.68017522	-2.63221371	-2.84305866
H	-1.43972214	-4.77185237	-3.85380616
H	-2.64932740	-6.07052994	-3.75051267
H	-4.20986307	-4.28739022	-3.36487881
H	-1.85163206	-0.15017730	4.06634356
H	-2.06873797	-1.70490366	3.52540590
H	-1.17777468	-2.59269218	5.58173362
H	-1.17383061	-0.91163441	6.22136047
H	-2.69812324	-1.67642212	5.70966314
H	1.83188849	4.00910209	3.46200609
H	0.72392159	6.22933115	3.42619943
H	-1.76321247	2.20854994	1.96190253
H	-0.57546913	-2.67184943	1.44355399
H	-0.40726083	-2.04449226	-0.95256146
H	0.28992619	0.24854827	-1.57452137
H	0.76424952	1.91623223	0.19221808
H	1.87034675	1.76952802	2.69600296
H	-0.33776624	1.34698901	4.70532492
H	1.37046903	1.68470414	4.93252746
H	0.92881270	-0.68999330	5.49430854
H	1.94189393	-0.60247680	4.06002448
H	0.20835073	-2.24590232	3.66170164

2-HP-B-CD:cis-(1R,4R)-SRT_5_MD E(Ha)= -7253.9175047023

C	0.50473260	1.35455705	3.72866884
C	0.27053572	0.95411384	2.29094966
C	-0.18535340	-0.32553585	1.94825454
C	-0.49764778	-1.38797170	2.98853460
C	-0.05029455	-0.99757565	4.40770019
C	-0.29517803	0.47845827	4.68072412
C	0.46138728	1.91611273	1.29150077
C	0.18502360	1.63027410	-0.03681245
C	-0.29173717	0.36618154	-0.38503432
C	-0.45963151	-0.59730572	0.60079463
C	0.06111680	-2.75157133	2.64108835
C	-0.71925095	-3.90342610	2.74754960
C	-0.16707639	-5.16310096	2.53506560
C	1.18144403	-5.29495243	2.21366401
C	1.96664276	-4.14354268	2.09126562
C	1.40708249	-2.88625106	2.28687329
Cl	1.85286647	-6.86430336	1.94826178
Cl	3.65862317	-4.25660423	1.71282119
N	1.98606461	1.34715689	4.01934996
C	2.35563189	1.87268003	5.35141912
C	0.90839493	6.01225642	-0.20338749
C	2.30890674	6.34222413	0.30933701
C	3.36009595	5.53617105	-0.46574453
O	3.16304088	5.67537892	-1.84432118
C	1.97294355	5.03667230	-2.29062423
C	0.78358584	5.80176808	-1.71935585
O	3.21930858	4.20508954	-0.06333504
C	4.36764440	3.41091843	0.18532293
C	3.84461971	2.38558000	1.17445898
C	4.86714192	1.30497191	1.42574495
C	5.20204050	0.68330690	0.06203018
O	5.77137749	1.66112415	-0.75881757
C	4.91109924	2.75356261	-1.08876089
O	3.99914539	0.15228261	-0.44984297
C	4.12496987	-0.66963867	-1.59737684
C	4.38998321	-2.11105237	-1.20055313
C	4.36671053	-3.01757243	-2.42445741
C	3.05506278	-2.86438016	-3.21527234
O	2.87045606	-1.49065511	-3.49785832
C	2.78356497	-0.65266653	-2.34080270
O	2.00064617	-3.40722264	-2.48890652
C	0.99323585	-4.15321453	-3.17064584
C	0.92628886	-5.51619546	-2.47754918
C	-0.38709538	-6.27954766	-2.67346254
C	-1.64042742	-5.39086277	-2.74016830
O	-1.36444482	-4.30357099	-3.58505376
C	-0.34632791	-3.42435914	-3.11469356
O	-2.05014177	-4.99517097	-1.46758873
C	-3.43873608	-4.69941765	-1.26556276
C	-3.52079810	-4.42356608	0.24760906
C	-4.81510390	-3.73876562	0.66643689
C	-5.24932114	-2.63261515	-0.28960220
O	-5.23505917	-3.10210207	-1.60602704
C	-3.94847769	-3.50449460	-2.08740309
O	-4.39433738	-1.52935281	-0.14669088
C	-4.98928318	-0.29214640	0.21909734

C	-3.94466829	0.39832362	1.08292180
C	-4.39422053	1.81059836	1.40797451
C	-4.71598745	2.53692795	0.08612733
O	-5.72140647	1.85011619	-0.61799085
C	-5.37933004	0.52391847	-1.00791760
O	-3.51510616	2.61320881	-0.63064893
C	-3.41393579	3.59122727	-1.66030338
C	-3.13884208	4.96544722	-1.05574824
C	-2.61134188	5.93971298	-2.09874059
C	-1.39310365	5.33270284	-2.79834243
O	-1.80419472	4.15895302	-3.42767242
C	-2.21196532	3.14553542	-2.51160829
O	-3.37757009	2.44753651	2.14598005
C	-3.73654457	3.69316392	2.71278732
C	-2.51320838	4.17873093	3.46899245
O	-1.40254989	4.21587112	2.57411711
O	-3.74849085	-0.36728758	2.26228660
O	-4.66417986	-3.18551568	1.96245971
C	-5.72972174	-3.49826539	2.85557012
C	-5.73934827	-2.51786639	4.01903637
O	-6.07738662	-1.21842327	3.58830931
O	-3.44809654	-5.59363565	1.00786947
O	-0.41238300	-7.22873600	-1.63414651
C	-1.52917620	-8.09190023	-1.54789527
C	-1.56218912	-8.56370120	-0.09746846
O	-1.39015951	-7.42203204	0.73578545
O	1.97780080	-6.31128921	-2.95408819
O	4.60760402	-4.30578701	-1.91046452
C	4.93389391	-5.32189397	-2.84363100
C	5.11919377	-6.59343678	-2.02585349
O	3.98916117	-6.79077658	-1.17895367
O	5.63288961	-2.22688614	-0.54604561
O	4.32003419	0.40667951	2.36244188
C	5.20401468	-0.59767983	2.81401304
C	4.84779579	-0.92970001	4.25528191
O	3.44471834	-1.16832300	4.38879070
O	3.47412231	3.01743782	2.39282988
O	2.48679473	5.98103128	1.66506643
C	1.71365487	6.67952388	2.62489513
C	1.71822079	5.88033381	3.92084692
O	1.19070037	4.57561730	3.71159708
O	0.00502680	7.02626089	0.21194331
O	-0.41321783	5.03949480	-1.83876507
O	-2.30005778	7.13876600	-1.40639822
C	-2.37156158	8.31832003	-2.21349673
C	-1.58199485	9.44365299	-1.56126041
O	-0.20118151	9.16539089	-1.57918285
O	-4.31761593	5.47619954	-0.46540956
C	-2.45340385	1.88179459	-3.30826114
O	-1.21895343	1.30439190	-3.65050558
C	2.02180033	4.95854101	-3.80845687
O	3.11200067	4.20956717	-4.27216356
C	5.70034567	3.70260833	-1.97022420
O	6.54217757	4.50026421	-1.15763147
C	2.33285851	0.71244352	-2.81761469
O	3.25377348	1.33025251	-3.69590199
C	-0.43075910	-2.19644481	-4.00108305
O	-1.57517070	-1.41664793	-3.71821974

C	-4.20757660	-3.72310345	-3.57566448
O	-4.13439386	-2.49351855	-4.28272182
C	-6.60797820	-0.01454061	-1.72256456
O	-7.70762253	-0.15659408	-0.85892539
C	-2.69784913	5.56161748	4.05342510
C	-2.86309522	-9.24159923	0.26787903
C	5.26800871	-7.81874630	-2.90056567
C	5.65877304	-2.09118853	4.79753720
C	3.10048587	5.73064724	4.52864666
C	-6.76448987	-2.94384268	5.05555389
C	-1.80509115	10.74517790	-2.31131281
H	-5.13199868	3.53155869	0.26103175
H	-5.32271602	1.77295063	2.00055499
H	-3.00194947	0.46159986	0.52465691
H	-5.88359462	-0.47123584	0.83216700
H	-6.28538234	-2.33647020	-0.08856012
H	-5.59445577	-4.51132827	0.67037441
H	-2.68716089	-3.73516255	0.47059858
H	-4.04337412	-5.59223177	-1.49329212
H	-2.45166459	-5.93445098	-3.24369526
H	-0.31981823	-6.77921963	-3.65206013
H	1.02291372	-5.31441746	-1.40078440
H	1.28147587	-4.31568038	-4.21931746
H	3.13128348	-3.34293947	-4.19901912
H	5.18604027	-2.71893411	-3.09854889
H	3.57528458	-2.42817012	-0.53097136
H	4.91712508	-0.28751788	-2.25453023
H	5.95977251	-0.10034834	0.14485753
H	5.79819710	1.74246136	1.81969419
H	2.96383983	1.90680629	0.72940599
H	5.15735086	4.01212583	0.65303543
H	4.37204910	5.89975351	-0.25934560
H	2.50747647	7.41350431	0.15524401
H	0.62622407	5.05547268	0.26004221
H	0.68022890	6.77934486	-2.21137954
H	-0.99602290	5.99096458	-3.58053100
H	-3.39348746	6.12918906	-2.84710209
H	-2.35903751	4.82585086	-0.29133246
H	-4.33779915	3.62633038	-2.25591998
H	-1.39780968	2.93708072	-1.81254594
H	1.93582972	4.01226199	-1.89700859
H	4.06791437	2.38226531	-1.67912724
H	2.00790739	-1.03597495	-1.66203233
H	-0.55341168	-3.13162670	-2.07637474
H	-3.23413271	-2.67799218	-1.97612656
H	-4.52950500	0.53343319	-1.70245635
H	-3.79279123	-1.30012302	1.97623878
H	2.98723940	3.83343470	2.16879138
H	-4.11180725	6.38543867	-0.21351277
H	-2.66405180	-6.12989319	0.78016704
H	2.54128222	-6.61652923	-2.21782863
H	5.82359208	-3.17383871	-0.52852191
H	-0.85913903	6.84048624	-0.20045261
H	-4.59124286	3.58205520	3.39724999
H	-3.99890335	4.42530555	1.93468691
H	-2.30719686	3.45647729	4.27538685
H	-3.53084129	5.57738876	4.76190339
H	-2.89427929	6.28951101	3.26059400

H	-1.79554760	5.87267574	4.58745717
H	-1.46674294	3.41281682	2.03331339
H	-1.43495476	-8.93678725	-2.24415993
H	-2.46433684	-7.55942415	-1.76525861
H	-0.71654759	-9.24837579	0.06602442
H	-3.04602144	-10.10706984	-0.37593927
H	-3.69637409	-8.53890102	0.16670136
H	-2.83364748	-9.58622306	1.30416680
H	-0.67915534	-6.92394073	0.30134344
H	5.85709442	-5.07182415	-3.38735216
H	4.11319483	-5.46378386	-3.55678195
H	6.01369508	-6.47290704	-1.39510525
H	6.14061177	-7.72585290	-3.55350975
H	4.37805796	-7.95446316	-3.52294531
H	5.39434180	-8.70918301	-2.28076509
H	3.90161678	-5.98642813	-0.64891375
H	6.24689569	-0.24827985	2.78174604
H	5.13353913	-1.48747412	2.17057906
H	5.02837093	-0.03435130	4.86212255
H	6.73014483	-1.87209978	4.76393592
H	5.48391795	-2.99841138	4.20720405
H	5.38311141	-2.29599207	5.83471700
H	3.24783814	-2.03033494	4.00142527
H	1.05887035	4.55648282	-4.16106346
H	2.13802344	5.97000466	-4.21515154
H	2.97568554	3.26703797	-4.08612934
H	6.27881752	3.08110090	-2.66839388
H	4.99553216	4.30916727	-2.55145229
H	7.01482894	5.10750606	-1.73312634
H	0.68325342	6.80116343	2.27488967
H	2.12936077	7.68389013	2.80216011
H	1.08062497	6.43663411	4.62864027
H	3.04469681	5.18034059	5.47211278
H	3.53222017	6.71371825	4.73634458
H	3.77069447	5.19478070	3.85210379
H	0.30564534	4.63842466	3.30641121
H	1.33787833	0.63688348	-3.27674458
H	2.24318266	1.36188539	-1.94438487
H	3.35873848	0.75163590	-4.46003226
H	-5.60942969	-4.53094208	3.21095395
H	-6.69608478	-3.41331475	2.33851357
H	-4.73587928	-2.52702119	4.47832087
H	-7.76621939	-2.95140158	4.61407133
H	-6.76933809	-2.22974458	5.88189552
H	-6.54855060	-3.94005195	5.45222444
H	-5.27997079	-0.79536851	3.23148419
H	0.44678353	-1.56793083	-3.83082409
H	-0.41461165	-2.51917479	-5.05193565
H	-2.38610055	-1.85577622	-4.04291180
H	-3.42701801	8.59718460	-2.34109963
H	-1.93876144	8.12666852	-3.20395091
H	-1.94457377	9.55633982	-0.52577518
H	-1.46815144	10.64876077	-3.34833640
H	-1.22016755	11.53915537	-1.84260025
H	-2.85902974	11.03788110	-2.30949148
H	0.00021585	8.55493676	-0.85044797
H	-3.46885089	-4.36206306	-4.04704648
H	-5.19892191	-4.18119508	-3.68605629

H	-4.82356825	-1.91819871	-3.93179448
H	-3.04424062	1.20368949	-2.67966326
H	-3.05187417	2.13523146	-4.19855705
H	-1.37792672	0.35910984	-3.83190042
H	-6.83310457	0.65680214	-2.56492214
H	-6.39047639	-1.00830459	-2.12552242
H	-7.88856272	0.71731377	-0.49384235
H	2.40315781	0.40618241	3.90362114
H	2.47453615	1.96107320	3.31782049
H	3.43847016	2.00102997	5.37312448
H	1.87424169	2.84324193	5.47851423
H	2.05473310	1.17513589	6.13232210
H	-1.77800035	-3.82965011	2.98381092
H	-0.78269351	-6.05410309	2.60415834
H	2.02426582	-2.00247380	2.14174146
H	0.82789994	2.90098364	1.57189609
H	0.32382551	2.39490315	-0.79465983
H	-0.55552955	0.15596179	-1.41843993
H	-0.83597385	-1.58124243	0.33057758
H	-1.59310337	-1.46383541	3.00481132
H	1.01216714	-1.23136420	4.54662158
H	-0.58887076	-1.61669358	5.13193534
H	-0.08422839	0.72955283	5.72513452
H	-1.35208520	0.71664089	4.50799216
H	0.22147450	2.40266111	3.85761095

2-HP-B-CD:cis-(1R,4R)-SRT_6_MD E(Ha)= -7253.9181080813

C	-0.27020633	-1.22856821	3.49532835
C	-0.13478491	-0.70884812	2.08325414
C	0.16619253	0.63829724	1.83195269
C	0.50615124	1.61769719	2.94348884
C	0.20495961	1.07374161	4.35016324
C	0.56782550	-0.40051682	4.45678687
C	-0.26711602	-1.60328269	1.01523295
C	-0.11971612	-1.18341791	-0.30071750
C	0.15466257	0.15994937	-0.55258201
C	0.28942956	1.05460946	0.50100384
C	-0.10913032	2.99116705	2.78425066
C	0.64583759	4.13088193	3.06094054
C	0.06815851	5.39407160	3.02062257
C	-1.28027679	5.54207411	2.71243602
C	-2.04645953	4.40780145	2.42089862
C	-1.45530623	3.14659385	2.44319239
Cl	-1.96753383	7.12939906	2.67495296
Cl	-3.72787943	4.54291565	2.04099216
N	-1.73201314	-1.25928344	3.88170195
C	-2.00344898	-1.73384656	5.25566706
C	-0.89934334	-6.46345421	0.24498318
C	-2.36620402	-6.54221711	0.63207546
C	-3.19431653	-5.64832450	-0.31407712
O	-2.87798439	-5.89585806	-1.65122904
C	-1.53874503	-5.51495338	-1.99899907
C	-0.62469230	-6.47987372	-1.25850108
O	-2.95501488	-4.30839417	0.01706356
C	-4.04696675	-3.40668237	0.08676902
C	-3.59577258	-2.37379264	1.10697721
C	-4.64933138	-1.30593103	1.30483541
C	-4.99050059	-0.67606678	-0.05718730
O	-5.34061427	-1.68874060	-0.96972122
C	-4.33046809	-2.66469150	-1.22397845
O	-3.89886423	0.08475287	-0.49578398
C	-4.23729591	1.03598885	-1.50092873
C	-4.57240391	2.38294603	-0.87820184
C	-4.79400116	3.41139868	-1.97886657
C	-3.53720275	3.50595653	-2.84546375
O	-3.32522357	2.22312328	-3.40593747
C	-3.03853542	1.20667109	-2.44139194
O	-2.46253513	3.90787410	-2.05793163
C	-1.52576476	4.84121524	-2.57623225
C	-0.92738481	5.51893425	-1.34695176
C	0.27174084	6.37367053	-1.72441016
C	1.28326165	5.52249805	-2.48654941
O	0.66981711	5.03668626	-3.64369100
C	-0.43237213	4.15494722	-3.41237620
O	1.68560182	4.47702745	-1.63695014
C	3.06642643	4.30975737	-1.35746852
C	3.12284119	3.95508922	0.12352789
C	4.52426171	3.54920813	0.53020740
C	5.04299866	2.48507785	-0.44871750
O	5.00840520	2.95713789	-1.76595661
C	3.68123962	3.22280946	-2.23348885
O	4.23133166	1.35080021	-0.29925324
C	4.82931629	0.10138381	0.00951507

C	3.85053545	-0.57119719	0.96756127
C	4.32773499	-1.97234215	1.30424743
C	4.62000082	-2.75882976	0.00933457
O	5.50413227	-2.04300358	-0.81310247
C	5.04894643	-0.75691290	-1.22824694
O	3.38641223	-3.01685380	-0.60482604
C	3.34513915	-4.07875431	-1.55590700
C	3.41759416	-5.43434725	-0.84933254
C	2.96852763	-6.58228611	-1.74513147
C	1.59190056	-6.26411925	-2.32248769
O	1.68538997	-5.07106769	-3.05497426
C	1.97261322	-3.94049087	-2.23333114
O	3.34281182	-2.58756613	2.10496133
C	3.73125370	-3.79829587	2.72454424
C	2.49121979	-4.31587585	3.43345940
O	1.42110238	-4.39975713	2.49016916
O	3.72814011	0.20282900	2.14943709
O	4.50897786	3.01463783	1.83974049
C	5.67207536	3.32986868	2.60373775
C	5.83937717	2.32901638	3.73749793
O	6.15247298	1.04911456	3.23676499
O	2.69203200	5.05000265	0.90681330
O	0.83213198	6.89685083	-0.53270020
C	1.44675349	8.17708670	-0.71104392
C	2.53084171	8.39949214	0.33253113
O	3.63060141	7.54878401	0.10523948
O	-1.92507884	6.29842399	-0.72665014
O	-5.15675220	4.61515076	-1.35407939
C	-5.90632785	5.51659553	-2.16158390
C	-5.34544911	6.92266325	-2.01352882
O	-4.01035561	6.96123181	-2.46216558
O	-5.73449964	2.27927997	-0.08349841
O	-4.14642653	-0.40246332	2.25546576
C	-5.07749075	0.53084779	2.76665876
C	-4.71552679	0.80970293	4.21757288
O	-3.32652570	1.12485937	4.34464572
O	-3.28566645	-2.97214665	2.35192364
O	-2.63020693	-6.05119673	1.92896137
C	-1.98016606	-6.69886216	3.01195088
C	-1.85761274	-5.71127701	4.16508233
O	-1.20171705	-4.51864110	3.74906466
O	-0.13089940	-7.50760386	0.83566841
O	0.74546172	-6.12205459	-1.23061290
O	2.96496594	-7.72879636	-0.91969970
C	2.99985206	-8.97869596	-1.60325030
C	1.97329395	-9.93107690	-1.00655715
O	0.66645770	-9.43682670	-1.23201785
O	4.72898004	-5.68848448	-0.38620918
C	1.76044516	-2.70897532	-3.09830981
O	0.39847733	-2.38028046	-3.21904564
C	-1.44476866	-5.51273045	-3.52510439
O	-1.55974215	-4.22324482	-4.07200368
C	-4.80463902	-3.50285931	-2.41453312
O	-4.08842986	-3.23074422	-3.60027274
C	-2.69976085	-0.02866554	-3.24859267
O	-3.81974806	-0.52243623	-3.96032232
C	-0.87011322	3.74522046	-4.81098751
O	0.18978790	3.15441981	-5.51760387

C	3.80232434	3.63645847	-3.68815071
O	4.43367924	4.88442194	-3.84455454
C	6.11927746	-0.24554815	-2.17648583
O	6.26454839	-1.10384214	-3.27587829
C	2.69738121	-5.68104853	4.05049823
C	3.03057246	9.83263209	0.27074337
C	-6.15439435	7.91340836	-2.83137415
C	-5.58364028	1.89224878	4.83023660
C	-3.20017445	-5.32074766	4.75565364
C	6.96641476	2.75983543	4.65967667
C	2.08516820	-11.30714245	-1.64004646
H	5.14659686	-3.69005204	0.22560710
H	5.27437440	-1.89917414	1.86347330
H	2.87277017	-0.64571421	0.47063771
H	5.78410915	0.26096151	0.53381007
H	6.09083986	2.24288945	-0.23608709
H	5.17874084	4.43015828	0.48015841
H	2.46196022	3.09251952	0.29076533
H	3.60627343	5.25159339	-1.52318964
H	2.15136439	6.10134259	-2.82052282
H	-0.06816173	7.18996695	-2.37652348
H	-0.59058703	4.72603663	-0.66304036
H	-2.04850953	5.59870176	-3.17917158
H	-3.68125867	4.18640484	-3.69269976
H	-5.60874477	3.05348287	-2.62794957
H	-3.71804880	2.70803257	-0.26746027
H	-5.08852442	0.66716020	-2.08763909
H	-5.88298176	-0.04779122	0.02048062
H	-5.57351131	-1.77524128	1.68127448
H	-2.70162551	-1.88337839	0.69750253
H	-4.94957181	-3.92928309	0.43830893
H	-4.25876694	-5.88563071	-0.19896497
H	-2.72166277	-7.57772196	0.51602576
H	-0.53405757	-5.49352757	0.61445607
H	-0.74437352	-7.49526177	-1.66061181
H	1.23633080	-7.03930982	-3.01105775
H	3.68141499	-6.69536991	-2.57458655
H	2.71788946	-5.37952736	-0.00073122
H	4.16620263	-3.98377913	-2.28061561
H	1.23953321	-3.88628324	-1.41901873
H	-1.33893802	-4.49290421	-1.65467850
H	-3.39311352	-2.17412889	-1.51446675
H	-2.15927862	1.49100723	-1.84804486
H	-0.07759173	3.26989241	-2.86755837
H	3.07411283	2.31051146	-2.16599965
H	4.10163082	-0.85166031	-1.77603443
H	3.73037728	1.13590120	1.86284528
H	-2.80730613	-3.80742369	2.18723359
H	4.72328840	-6.61210568	-0.10109903
H	1.87015217	5.37823594	0.49942265
H	-1.50123847	6.81915365	-0.03318879
H	-6.02172264	3.19357494	0.04855059
H	0.78544493	-7.28281436	0.60756330
H	4.54370673	-3.62841844	3.44692866
H	4.07031733	-4.53777045	1.98415999
H	2.22426814	-3.58856622	4.21687533
H	1.78338145	-6.01870184	4.54715054
H	3.49533400	-5.65201540	4.79796439

H	2.96077827	-6.41442906	3.28239636
H	1.54611228	-3.64384861	1.89407001
H	0.67293298	8.95517098	-0.64797071
H	1.91902886	8.23594740	-1.70027169
H	2.08913374	8.21273322	1.32640939
H	2.22716639	10.55053948	0.45932603
H	3.46293569	10.03942045	-0.71347799
H	3.81434242	9.97894463	1.01688536
H	3.42998817	6.67833249	0.48639486
H	-6.96357263	5.48017455	-1.86181840
H	-5.84333095	5.23059048	-3.22002375
H	-5.40059299	7.19838755	-0.94829629
H	-7.20609498	7.92254601	-2.52948017
H	-6.09861485	7.66053059	-3.89528261
H	-5.74691073	8.91884574	-2.70505371
H	-3.42610276	6.69768007	-1.73306392
H	-6.09903308	0.12323950	2.73194389
H	-5.07088493	1.44829081	2.16142300
H	-4.83273715	-0.12434455	4.78017880
H	-5.30224134	2.06048918	5.87247682
H	-6.64090512	1.61257206	4.80087945
H	-5.47191425	2.83649572	4.28446467
H	-3.18736939	2.02031841	4.01176622
H	-0.47195462	-5.88871286	-3.84588001
H	-2.21451036	-6.19365287	-3.91424387
H	-2.46839049	-3.88650125	-3.91735486
H	-4.66182588	-4.56767660	-2.22714026
H	-5.87823260	-3.31409841	-2.54561567
H	-4.15459610	-2.28177412	-3.81934883
H	-0.98471152	-7.03885618	2.71356250
H	-2.55343166	-7.58133066	3.33497324
H	-1.26446318	-6.21868792	4.94436300
H	-3.06477738	-4.65057217	5.60882694
H	-3.72971287	-6.21023380	5.10802677
H	-3.82180632	-4.81695240	4.01148095
H	-0.35106065	-4.72322012	3.32247388
H	-1.87247251	0.20737661	-3.93025874
H	-2.36141503	-0.82674839	-2.58678096
H	-4.08692149	0.14618665	-4.59997099
H	5.57962323	4.35422154	2.99157499
H	6.57062203	3.27572690	1.97323358
H	4.89518091	2.30420352	4.30773050
H	7.91108743	2.80552026	4.10850936
H	7.08316192	2.02733628	5.46121053
H	6.77235756	3.73993717	5.10493200
H	5.32418028	0.61586642	2.97148956
H	-1.66850016	3.00353194	-4.74517741
H	-1.26266192	4.63551933	-5.32968984
H	0.86917526	3.83235569	-5.60336862
H	4.01065296	-9.40254683	-1.52665803
H	2.76818618	-8.84473624	-2.66754886
H	2.17228516	-10.00951379	0.07325431
H	1.87637166	-11.24739414	-2.71303461
H	1.35062514	-11.98108873	-1.19406593
H	3.08210997	-11.73648014	-1.50216925
H	0.34310963	-8.99740924	-0.43376247
H	4.32483104	2.83803431	-4.23424336
H	2.79687775	3.72861062	-4.10779295

H	5.33672013	4.79019720	-3.52178754
H	2.24713690	-1.85673078	-2.61541328
H	2.24004592	-2.86671444	-4.07557220
H	-0.10606829	-3.09815131	-3.64948703
H	5.83366185	0.73808801	-2.55956185
H	7.06243489	-0.13261492	-1.61514053
H	6.47072996	-1.97191044	-2.91041276
H	-2.18814363	-0.33701477	3.76146479
H	-2.24519934	-1.90752433	3.23360621
H	-1.69607483	-0.98239528	5.98185698
H	-3.07666831	-1.90613988	5.34400222
H	-1.47519076	-2.67607404	5.40371519
H	1.70598764	4.04051290	3.27653107
H	0.66242198	6.27798347	3.22679793
H	-2.04950803	2.27954204	2.16428525
H	-0.48985956	-2.64748445	1.22949298
H	-0.19118780	-1.87524062	-1.13675103
H	0.28217144	0.49804885	-1.57765212
H	0.50850860	2.09842505	0.29238924
H	1.59654855	1.74339610	2.88777093
H	-0.85501006	1.22376882	4.59258527
H	0.76478161	1.66197733	5.08394473
H	0.47084229	-0.76201971	5.48536736
H	1.61403289	-0.55081594	4.16283290
H	0.03551934	-2.27841966	3.53077271

255

2-HP-B-CD:trans-(1R,4S)-SRT_1_Cl E(Ha)= -7253.8912020040

Cl	6.64506052	2.37045265	6.74338580
Cl	4.56535056	-0.02040399	7.16792893
O	-6.96944797	-0.23636639	-0.71935152
O	-4.37621025	-2.81306123	-0.73054747
O	-4.43125708	-4.84107153	-1.81236083
O	-0.77765213	-4.97647613	-1.92084682
O	0.48750145	-5.64481313	-3.71757922
O	3.23358161	-3.71213900	-2.29769978
O	4.99094976	-2.88278066	-3.55493016
O	4.43928954	0.40096342	-2.02802310
O	4.89079369	2.34001815	-3.21299383
O	1.77642461	3.83805744	-1.99292440
O	0.58432643	5.31773513	-3.32421870
O	-2.64706368	4.08689930	-2.10142725
O	-4.56786761	3.85567761	-3.34705939
O	-3.95311374	5.83964770	-0.36803609
O	-6.03682524	4.10916376	0.43356578
O	-5.29400671	1.37808242	-0.83600315
O	-1.44619998	4.89734658	0.30953372
O	1.30673669	5.40875410	0.24905476
O	-1.72882116	6.25630470	-4.68630741
O	3.20795757	3.48767191	0.40887151
O	5.33082991	1.59521155	0.31812039
O	4.27686127	4.77409289	-4.41817443
O	4.94556760	-3.92587570	-0.06229284
O	5.26522591	-1.15710843	0.20378049
O	2.99202314	-5.85011888	-0.43607271
O	0.38243177	-6.92321632	-0.31002148
O	2.57546441	-5.54756205	-5.48742987
O	-3.27550642	-6.85371333	-3.49237705
O	-3.76713449	-4.04675493	1.68089566
O	-1.26732763	-5.05712984	0.89062995
O	-3.72979486	-1.39071582	1.64334025
O	-4.85989755	1.13467654	1.93988383
O	-7.92485485	-2.91648687	-0.93014270
O	-6.87383281	2.54604513	-4.09516773
O	6.55258553	-0.93604775	-4.73319912
O	-5.53982171	-2.54935469	3.43841754
O	-7.14422072	2.55486437	2.50069608
O	-1.79283266	7.68246625	0.12370896
O	3.88917005	5.85313228	1.70337426
O	7.73027427	0.03538321	0.75739913
O	5.69671851	-6.53439513	-0.77685163
O	-2.02176408	-7.73668406	1.05902801
N	-2.03715094	0.80352997	1.72720695
C	-1.56968023	1.35782671	0.43406295
C	3.91195933	3.02081572	3.90041172
C	5.02260997	3.13329257	4.72900756
C	5.24846654	2.20620345	5.74309254
C	4.33784991	1.15903063	5.92598527
C	3.22478160	1.05651622	5.09726937
C	2.99848059	1.97949747	4.07495090
C	1.46136273	0.51555330	2.67254479
C	0.15193179	0.02229700	2.55579393
C	-0.05560371	-1.30394931	2.14895169
C	1.00633422	-2.12192581	1.79112524

C	2.30359898	-1.61136454	1.83068851
C	2.51873008	-0.31298098	2.27503408
C	1.74297203	1.90343079	3.22736200
C	0.54262292	2.41418531	4.03589247
C	-0.73567785	2.33325346	3.21428706
C	-1.05508170	0.88030197	2.87846600
C	-6.16124542	-1.28318915	-1.25270079
C	-5.31695958	-1.93073965	-0.15187984
C	-4.54162630	-0.86156596	0.60099944
C	-5.53252996	0.15235220	1.15687357
C	-6.26884462	0.77340169	-0.03814837
C	-4.59781201	-4.20394337	-0.58683577
C	-3.12608277	-4.69690298	-2.38258275
C	-2.07325425	-5.23155982	-1.41185886
C	-2.18195203	-4.54527221	-0.05386061
C	-3.60401152	-4.73862375	0.45179899
C	-0.08873635	-6.05891742	-2.51839270
C	0.98201584	-6.55186536	-1.53466603
C	1.95841886	-5.42127769	-1.28338099
C	2.51590191	-4.89764741	-2.60263244
C	1.41695953	-4.56186715	-3.60906976
C	4.62647744	-3.68054060	-2.45880145
C	4.56592695	-1.52044797	-3.48620693
C	5.06293461	-0.86579171	-2.19638324
C	4.71399991	-1.70158998	-0.97109160
C	5.24028988	-3.10888619	-1.17665819
C	5.21460164	1.56710350	-2.08670466
C	4.95660487	2.36545988	-0.80193280
C	3.48694694	2.74466221	-0.75604650
C	3.16808491	3.54648993	-2.01287875
C	3.53202231	2.77303620	-3.28021581
C	1.35585157	5.16919087	-2.16272532
C	0.53635938	5.56001979	-0.92441442
C	-0.68980382	4.65940597	-0.86233154
C	-1.48256122	4.89508683	-2.13856399
C	-0.62252630	4.55437748	-3.35708833
C	-3.85654838	4.70416349	-2.50180237
C	-4.82976943	2.56673989	-2.80157962
C	-5.55450195	2.64073558	-1.45313527
C	-5.06660893	3.75369459	-0.51583715
C	-4.69182162	5.02439799	-1.26100981
C	-5.67431635	1.86075358	-3.85138713
C	-1.31325076	4.91162301	-4.66151213
C	3.44415856	3.64583208	-4.52139463
C	5.15003632	-0.85737732	-4.72313454
C	1.97041535	-4.37313643	-5.01244798
C	-3.14581124	-5.46658210	-3.69109436
C	-7.11300293	-2.28185532	-1.88845415
C	-4.06513955	7.24138071	-0.59980245
C	1.75497243	6.64002187	0.82557074
C	6.47476722	2.07207188	1.03393055
C	6.05518186	-4.56732284	0.57283088
C	-0.05957455	-8.27730954	-0.25658358
C	-4.70627513	-4.65777871	2.57128223
C	-5.31995211	1.30045181	3.27967441
C	-4.92232657	-3.77457545	3.79057036
C	-0.83794120	-8.50887815	1.03011747
C	5.89975903	-6.08525105	0.54825507

C	7.18547549	0.91184012	1.71597082
C	2.61530350	6.34868973	2.04591275
C	-3.15288740	7.98624190	0.36421566
C	-6.08655194	2.59813627	3.45267361
C	-5.82223299	-4.47257374	4.79281417
C	-6.60602650	2.74219453	4.87165369
C	-3.32406415	9.48540754	0.20755582
C	2.83518032	7.61747724	2.85046036
C	8.31792752	1.42975704	2.58550119
C	7.14344726	-6.75082428	1.10931299
C	-1.23331700	-9.96846377	1.15430084
H	-1.47698143	2.44008629	0.51826644
H	-0.61199938	0.90285353	0.18031018
H	-2.31434322	1.13120113	-0.32915522
H	-2.32954619	-0.18507720	1.61518519
H	-2.93998042	1.24712171	1.96530563
H	3.77173363	3.75763772	3.11461490
H	5.72636466	3.94830761	4.59437413
H	2.53987127	0.22852746	5.25389656
H	-1.06029641	-1.72482388	2.13056213
H	0.81141664	-3.14917699	1.49685755
H	3.15370895	-2.22046428	1.53630389
H	3.53277777	0.07040120	2.33129406
H	1.89631534	2.57797265	2.37281396
H	0.44642783	1.82390704	4.95654789
H	0.72215436	3.44860844	4.34402408
H	-1.57917632	2.77881267	3.75465840
H	-0.59746456	2.93006088	2.30553868
H	-1.60311560	0.42465654	3.71383473
H	-5.47907583	-0.88678760	-2.01803544
H	-5.97882884	-2.46150104	0.54547316
H	-3.89265207	-0.35782403	-0.12664847
H	-6.26897267	-0.36691956	1.78133632
H	-7.02809792	1.48430091	0.29672100
H	-5.63575626	-4.38906144	-0.28678635
H	-2.92337271	-3.63649276	-2.58618352
H	-2.23201490	-6.30837217	-1.27008605
H	-1.99701357	-3.46944407	-0.19514003
H	-3.78100042	-5.81155724	0.60660985
H	-0.79554805	-6.85405286	-2.78118218
H	1.51346057	-7.40898592	-1.97271074
H	1.40076776	-4.59537413	-0.81528304
H	3.17896292	-5.65010213	-3.05130483
H	0.89555421	-3.65365007	-3.27791399
H	5.02798785	-4.68054900	-2.65293904
H	3.46801422	-1.46500075	-3.50814666
H	6.15310502	-0.74712666	-2.26234926
H	3.61832117	-1.74680887	-0.88419824
H	6.32681415	-3.06417764	-1.32397899
H	6.27877211	1.32449804	-2.18131063
H	5.55517467	3.28500364	-0.84090989
H	2.88721224	1.82296022	-0.76004397
H	3.74772535	4.47960316	-2.00328483
H	2.86223474	1.90685011	-3.37796087
H	2.21894830	5.83080880	-2.29518862
H	0.20845290	6.60285693	-1.02483490
H	-0.34142909	3.61691306	-0.85092598
H	-1.75727483	5.95637308	-2.19067791

H	-0.39027798	3.47964696	-3.34499191
H	-3.63990383	5.60344303	-3.08936352
H	-3.88309976	2.02964556	-2.65656749
H	-6.62826352	2.77388265	-1.63736524
H	-4.15048014	3.37569012	-0.03543094
H	-5.61222736	5.53763173	-1.57139054
H	-5.07347911	1.74315788	-4.76547093
H	-5.94112836	0.86411014	-3.48834062
H	-0.63490677	4.67729154	-5.49422289
H	-2.21118288	4.29631665	-4.77226884
H	3.69038687	3.03272061	-5.40070558
H	2.41986757	4.01261872	-4.63417769
H	4.70617378	-1.32312817	-5.61587340
H	4.88752354	0.20469773	-4.72201150
H	1.15756220	-4.03377487	-5.67234278
H	2.74328747	-3.59922028	-4.99052718
H	-2.19803278	-5.30462187	-4.21295041
H	-3.95365127	-5.06522478	-4.31977619
H	-6.52995807	-3.06344603	-2.38494008
H	-7.70706775	-1.76188216	-2.65297495
H	-5.11001704	7.54520572	-0.44816405
H	-3.77295834	7.49156042	-1.63024829
H	0.87590549	7.23631774	1.10391592
H	2.35138974	7.20877222	0.09797724
H	6.14987359	2.82466268	1.76378364
H	7.18472211	2.53294869	0.33459823
H	6.12272120	-4.19685305	1.60260108
H	6.98134316	-4.29854456	0.05123997
H	0.81601226	-8.94008852	-0.29923520
H	-0.71448327	-8.50622407	-1.11014333
H	-4.31288573	-5.63758970	2.87178418
H	-5.67139165	-4.80398523	2.06632484
H	-4.44386452	1.31330548	3.94086646
H	-5.94581910	0.44968531	3.57497465
H	-3.93786988	-3.58942701	4.25055813
H	-0.18176301	-8.23478296	1.87170524
H	5.03313370	-6.35548857	1.17109642
H	6.45554535	0.38750533	2.35536036
H	2.06279750	5.61911036	2.66599206
H	-3.43568395	7.69009475	1.38733398
H	-5.41546000	3.43776371	3.21004482
H	-5.38463161	-5.41382580	5.13623330
H	-6.79984685	-4.68092947	4.34701502
H	-5.97783378	-3.82492144	5.65823958
H	-5.78526780	2.74568042	5.59533695
H	-7.28656623	1.92170881	5.11839324
H	-7.14707587	3.68609808	4.99218202
H	-4.35220715	9.79535301	0.41426627
H	-3.06128836	9.79504134	-0.80886591
H	-2.65802164	10.00442117	0.90008579
H	1.89202440	8.02233313	3.22754752
H	3.32661574	8.37784283	2.23550913
H	3.48804623	7.40071924	3.69880372
H	7.95056137	2.09311150	3.37406085
H	9.04767804	1.97316101	1.97659248
H	8.83251512	0.58684988	3.05142098
H	7.36375875	-6.40309915	2.12346936
H	8.00621416	-6.53503879	0.47117083

H	7.00655535	-7.83405367	1.13484770
H	-0.35660191	-10.62206271	1.16777109
H	-1.87717750	-10.26114615	0.31876124
H	-1.79358740	-10.11854263	2.07964005
H	-6.23248171	3.36306492	1.02141307
H	-2.38199731	5.01721925	0.04567058
H	-0.93373467	6.79743131	-4.61801478
H	2.37705891	3.98288870	0.25607543
H	5.17844151	4.44251630	-4.33396938
H	5.05444697	-0.20125070	0.21350022
H	3.53679461	-5.06283570	-0.23037626
H	1.89518131	-6.23060680	-5.46968601
H	-4.12019133	-7.00100425	-3.05206244
H	-0.54628517	-5.50485772	0.40393525
H	-3.63374675	-2.36885370	1.51268979
H	-8.48265170	-2.23542258	-0.53787200
H	-6.62959116	3.42446596	-4.40874887
H	6.77207436	-1.87500599	-4.71658058
H	-4.87386603	-2.00376471	2.99552794
H	-7.74739798	3.28621123	2.67611454
H	-1.62047754	6.77779567	0.42957059
H	3.79687081	5.03967551	1.17986133
H	7.02745364	-0.57579162	0.48788075
H	4.73785455	-6.58455980	-0.90240154
H	-1.77299686	-6.81406787	1.23390781

2-HP-B-CD:trans-(1R,4S)-SRT_2_Cl E(Ha)= -7253.8879680249

Cl	-0.23703279	-7.33684230	4.63450559
Cl	-1.43981323	-4.89907668	6.31405428
O	2.40467319	6.41566655	-1.82849602
O	-0.99490917	5.21690689	-1.14297913
O	-2.89611891	5.77670130	-2.32400416
O	-4.52170650	2.65551797	-1.32192594
O	-5.87091703	1.56406659	-2.85197577
O	-4.56895043	-1.59119063	-1.56380637
O	-4.62959165	-3.52472687	-2.83899953
O	-1.07884393	-4.10940081	-2.13987181
O	0.29697412	-4.87597082	-3.83363678
O	3.17535515	-3.20667744	-2.30648419
O	4.81145124	-2.32481854	-3.69783529
O	5.11469278	0.57217508	-1.51771073
O	6.31320902	2.54101247	-1.80105673
O	5.44477283	0.85217793	1.31598290
O	3.70252423	2.98653217	1.42504674
O	3.27353917	4.42660298	-1.06338264
O	6.07358991	-1.55872215	0.16456073
O	5.03255513	-4.12077619	-0.56895480
O	6.45375811	-0.43239788	-4.81389989
O	2.50413208	-5.11164251	-0.32337527
O	-0.16190620	-6.07430790	-0.42847410
O	2.57712027	-4.90597964	-5.43318233
O	-4.76005519	-3.11870198	0.77845463
O	-2.22500218	-4.31023206	0.46378790
O	-6.03195957	-0.63989068	0.65645556
O	-6.33601647	2.21300602	0.69537958
O	-6.79269166	-0.52210764	-4.36429325
O	-5.33973858	5.28284253	-3.62701737
O	-2.21447266	5.94268845	1.25344507
O	-4.19512105	3.92891733	1.17011174
O	0.20425932	4.87254244	1.41635890
O	2.91689650	5.42020192	1.63736294
O	0.30113599	8.14598106	-2.64445737
O	6.52184885	5.35122625	-2.15491104
O	-3.41575773	-5.60869924	-4.33898701
O	-0.00881806	7.43176818	2.48088183
O	5.48111321	4.77121865	2.76943436
O	8.11978382	0.04211557	1.30278344
O	4.75510614	-6.90063758	-0.08439454
O	-2.85370168	-6.99284164	0.21096823
O	-7.57020471	-3.00777822	0.73658505
O	-6.75033285	5.00930100	1.43484845
N	1.08970363	2.12941356	1.68701777
C	0.76111046	1.42968103	0.42151592
C	0.87846407	-4.13389829	2.52585241
C	0.69543833	-5.44069004	2.95989677
C	-0.01678904	-5.70159815	4.12651688
C	-0.54506540	-4.63236966	4.86067356
C	-0.35336944	-3.32634440	4.42050237
C	0.35669054	-3.06138880	3.24848999
C	-0.61223391	-0.76106421	2.69188147
C	-0.50051748	0.63153266	2.84198627
C	-1.64561874	1.43679473	2.80784973
C	-2.89770580	0.88107150	2.58419458

C	-3.00560263	-0.49420651	2.38569934
C	-1.87760057	-1.30517311	2.44271753
C	0.62408255	-1.64018931	2.80342154
C	1.64599394	-0.96441201	3.72789689
C	2.04799561	0.39074260	3.16972138
C	0.84148474	1.31471463	2.94920167
C	1.09414321	5.91767635	-2.11532850
C	0.22077914	5.87348284	-0.85251382
C	0.96090660	5.11693629	0.24358408
C	2.23256045	5.91996547	0.50506583
C	3.07709138	5.79719053	-0.77665746
C	-2.16562629	6.01769304	-1.16755259
C	-3.38099102	4.43844592	-2.47943570
C	-4.20103263	4.03164777	-1.25633960
C	-3.42215118	4.24491886	0.03918285
C	-2.98789846	5.69918420	0.08916917
C	-5.84137909	2.28116977	-1.65413871
C	-6.38378049	1.44309487	-0.48976191
C	-5.53664388	0.19439243	-0.36260916
C	-5.51914944	-0.54724003	-1.69565059
C	-5.11301993	0.35045147	-2.86242590
C	-4.99329953	-2.92843618	-1.62347726
C	-3.22474012	-3.53255474	-3.09738645
C	-2.48215422	-4.22941245	-1.95697854
C	-2.82826859	-3.61231567	-0.60627440
C	-4.34041847	-3.67042262	-0.45411031
C	-0.39728972	-5.22360789	-2.66867073
C	0.56460506	-5.73979183	-1.59081571
C	1.58833960	-4.65859548	-1.29128967
C	2.28832113	-4.28084353	-2.59372321
C	1.28842982	-3.86231802	-3.67062333
C	4.50992548	-3.30174834	-2.73958177
C	5.41233925	-3.14605201	-1.51145754
C	5.23594717	-1.74756527	-0.95131562
C	5.49994638	-0.70099827	-2.02676126
C	4.66530849	-0.96889949	-3.27856262
C	6.09362592	1.42036737	-0.98170369
C	5.16650175	3.34526307	-2.05384468
C	4.51748975	3.81489930	-0.74640234
C	4.27987098	2.62298931	0.17412000
C	5.60718437	1.90840544	0.38808316
C	5.64644460	4.52510082	-2.88259029
C	5.12780949	-0.13722087	-4.46477257
C	1.94330872	-3.71637195	-5.03437622
C	-3.05069628	-4.25291290	-4.42355151
C	-5.41712448	-0.29288793	-4.20662527
C	-4.21460976	4.44948753	-3.74983687
C	0.50743221	6.85309366	-3.15901501
C	6.23077988	0.93775354	2.50997891
C	6.08318100	-4.88576565	0.01575922
C	-0.55792588	-7.44782890	-0.39052216
C	-5.54351515	-3.96799744	1.62338804
C	-7.59560285	2.77578820	1.06861281
C	-2.32163575	7.28060106	1.75265472
C	3.74291527	6.38703730	2.30440137
C	-1.35700974	7.49504099	2.91012982
C	-7.39323750	3.91703434	2.05379305
C	-6.89449329	-3.33222505	1.93634421

C	-1.67585148	-7.65253961	0.62078722
C	5.46586812	-6.04858731	0.78135943
C	7.38395091	-0.06696715	2.50579102
C	4.58212093	5.68811935	3.36342762
C	-1.58074039	8.86291685	3.52840936
C	5.39869279	6.70359529	4.14059626
C	8.30885611	0.18796456	3.68186268
C	6.54848192	-6.86970474	1.45798701
C	-1.99034736	-9.13125518	0.76092397
C	-7.75271302	-4.29054901	2.74298511
C	-8.73390137	4.40047413	2.57805400
H	1.26430793	0.46232422	0.40185843
H	-0.31554588	1.28016869	0.35602674
H	1.11063306	2.03519118	-0.41520099
H	0.56982100	3.02779833	1.72465525
H	2.10637843	2.39467966	1.65957074
H	1.44585728	-3.97445335	1.61264318
H	1.10481026	-6.26261135	2.38306660
H	-0.78325378	-2.51649499	5.00225746
H	-1.55918890	2.51332951	2.95186876
H	-3.77805695	1.51509460	2.55561567
H	-3.97649930	-0.93534760	2.19082445
H	-1.97983428	-2.37556743	2.28297953
H	1.08715334	-1.71035780	1.80564956
H	1.21216057	-0.86070679	4.72992652
H	2.53182752	-1.59886888	3.82884391
H	2.76821369	0.88963280	3.82579234
H	2.57719528	0.22955904	2.22106096
H	0.79751687	2.06811500	3.74330884
H	1.16297650	4.90037041	-2.52580785
H	0.03093794	6.90149409	-0.51730928
H	1.26128130	4.14667566	-0.16690352
H	1.97884537	6.97335536	0.68190585
H	4.04336768	6.30707636	-0.68712590
H	-1.88773986	7.07700315	-1.20803178
H	-2.53508431	3.74593060	-2.59175832
H	-5.11722328	4.63727139	-1.22513622
H	-2.52370889	3.60842885	0.01002546
H	-3.88216901	6.33736675	0.10691023
H	-6.45745377	3.17143720	-1.82234607
H	-7.41962081	1.15250236	-0.71028224
H	-4.50506061	0.49865278	-0.13124643
H	-6.51775767	-0.95524579	-1.90516772
H	-4.04104640	0.57753784	-2.77944362
H	-6.08341199	-3.00334744	-1.54979110
H	-2.85169107	-2.50170586	-3.18533777
H	-2.76965572	-5.28899095	-1.93630437
H	-2.50624482	-2.56111496	-0.59285182
H	-4.65338942	-4.72060837	-0.51305753
H	-1.11172061	-5.99650041	-2.97209157
H	1.09369752	-6.62418593	-1.97393324
H	1.05376696	-3.77068844	-0.91778560
H	2.85273603	-5.14717958	-2.96357560
H	0.81510271	-2.91523706	-3.37484806
H	4.68546969	-4.26372980	-3.23210703
H	6.45515791	-3.29757865	-1.82098270
H	4.18238882	-1.65314312	-0.64746465
H	6.56197149	-0.69808877	-2.30634951

H	3.61021786	-0.75621748	-3.05297076
H	7.05991152	0.91906119	-0.88599245
H	4.41733647	2.77379109	-2.62071804
H	5.18664924	4.53355455	-0.25333598
H	3.60010683	1.92198973	-0.32698623
H	6.35309056	2.61865649	0.76455282
H	6.10863128	4.14183167	-3.80284934
H	4.78439094	5.13736284	-3.16400111
H	4.43444091	-0.30081676	-5.30357198
H	5.09267787	0.92216226	-4.19464024
H	1.17751665	-3.39691687	-5.75678104
H	2.71525545	-2.94326759	-4.98636919
H	-3.63409067	-3.71889519	-5.18814752
H	-1.99710592	-4.22299942	-4.71566274
H	-5.01205087	0.34577693	-5.00638369
H	-4.92149674	-1.26648489	-4.25803622
H	-4.58455796	3.43880360	-3.94380100
H	-3.56969616	4.74825950	-4.58915251
H	-0.46947543	6.47057822	-3.46886935
H	1.16719488	6.85857404	-4.03770320
H	5.56131279	0.74435309	3.35658681
H	6.62673476	1.95500332	2.61721899
H	6.67990778	-4.24463727	0.67710206
H	6.72971218	-5.28941172	-0.77628891
H	0.31731457	-8.06220082	-0.13551166
H	-0.93076380	-7.76283088	-1.37542337
H	-4.97755414	-4.15554329	2.54374486
H	-5.71154863	-4.92949291	1.12444445
H	-8.22015634	1.98507002	1.50606599
H	-8.10470531	3.18070848	0.18273577
H	-3.35509390	7.44457735	2.08424060
H	-2.08577122	8.00413575	0.95978232
H	3.08713942	7.14376361	2.75338881
H	4.41380775	6.87120871	1.58295679
H	-1.55648246	6.71668556	3.66384376
H	-6.79117301	3.53598532	2.89561842
H	-6.72164356	-2.41883945	2.52638130
H	-1.33417181	-7.26335753	1.59339373
H	4.79610710	-5.62769483	1.55086703
H	6.95897376	-1.07826421	2.59131483
H	3.89652948	5.16711990	4.05123370
H	-2.59869282	8.96869480	3.91314094
H	-1.40069714	9.64978343	2.78917068
H	-0.87988525	9.00948611	4.35282974
H	4.75865268	7.43922431	4.63556633
H	6.08744114	7.22871688	3.47176225
H	5.99311993	6.19077043	4.89936166
H	7.76790475	0.16160175	4.63326575
H	8.78634075	1.16731300	3.57867125
H	9.09487467	-0.56953342	3.70954241
H	7.13608330	-6.26606739	2.15594824
H	7.22197265	-7.29723313	0.70859771
H	6.09169496	-7.69542340	2.00754401
H	-1.12026455	-9.69763032	1.10518176
H	-2.32243418	-9.54286985	-0.19770025
H	-2.79978575	-9.26364674	1.48183357
H	-7.25151829	-4.60163874	3.66487007
H	-7.97824557	-5.18274367	2.15047971

H	-8.69908513	-3.81260110	3.00513465
H	-9.27542910	3.60473680	3.09740674
H	-9.35364188	4.76794497	1.75390817
H	-8.57662777	5.22813059	3.27289588
H	3.45712694	3.95029735	1.40930535
H	5.72967510	-0.76857907	0.62521728
H	6.47437347	-1.36978012	-5.03944541
H	3.29483780	-4.53642398	-0.37229897
H	1.89094779	-5.58196637	-5.47821057
H	-1.35059880	-4.62413390	0.16634993
H	-5.46083886	-1.43723254	0.66671443
H	-7.22281803	0.33790310	-4.29370520
H	-5.01371817	6.17990165	-3.49382988
H	-4.76475185	3.16546021	0.93776041
H	-0.73300555	5.15666601	1.26189711
H	1.16930320	8.51516627	-2.44801316
H	7.30988964	4.82864346	-1.96710806
H	-4.34532800	-5.63336828	-4.08401786
H	0.22746032	6.49821105	2.38056086
H	5.00088643	3.95676817	2.57090739
H	7.80275980	-0.65652503	0.71428020
H	3.90171056	-6.48815161	-0.28064387
H	-2.75529219	-6.05312509	0.43915480
H	-7.38677875	-2.07499149	0.55819509
H	-5.80019398	4.81576076	1.41251786

255

2-HP-B-CD:trans-(1R,4S)-SRT_3_Cl E(Ha)= -7253.8840302896

Cl	-0.22931422	0.58251304	-4.88843727
Cl	1.36725879	-1.44442327	-3.02541471
O	-2.08805085	6.24639421	-1.74084365
O	-4.06818812	3.43048487	-0.51672779
O	-5.89527273	2.56699812	-1.65438938
O	-4.75709314	-0.87238999	-1.07660106
O	-4.84781874	-2.54670977	-2.66044758
O	-2.12441140	-4.41207201	-1.06314773
O	-0.79904137	-5.82557801	-2.34721038
O	2.19565517	-4.57280822	-0.67050531
O	4.35173356	-4.82895635	-1.49630402
O	4.72417487	-1.20736862	-1.16981434
O	5.79892323	0.30114757	-2.54252162
O	3.51395485	2.96651471	-1.46908594
O	2.81129465	4.72360126	-2.79664055
O	4.34491639	4.71787363	0.50855323
O	1.76844826	5.67211510	1.11677621
O	-0.23354739	5.18010622	-0.82113197
O	4.57090038	2.11874996	1.03795521
O	6.15850389	-0.13993195	1.05700962
O	6.05275254	2.78678688	-3.90164974
O	4.40865209	-1.99561884	1.57674523
O	3.28450744	-4.54249510	1.98050505
O	6.75830364	-3.74748843	-2.58131083
O	-1.97886164	-6.13930333	1.06215524
O	0.83537270	-5.86665492	1.45774712
O	-4.09601138	-4.44184211	0.95411403
O	-6.08083380	-2.45820859	0.76330792
O	-3.99400026	-4.66947512	-4.19034293
O	-7.31910023	0.53844955	-3.08054841
O	-5.23365066	2.85707380	1.89576132
O	-5.22681727	0.03862760	1.58614424
O	-3.25714952	4.71140412	1.92910471
O	-0.83523960	6.18780810	1.64632814
O	-4.71591568	6.45766787	-2.60995462
O	1.13511821	6.58905710	-3.92170737
O	1.45139113	-6.82372210	-3.53647637
O	-5.66377719	5.26124508	3.39691559
O	1.10121206	8.00531400	2.69961041
O	6.95849617	3.53813156	1.15775727
O	7.11854380	-2.59745728	2.25511058
O	3.12395448	-7.37570794	1.94602409
O	-4.58952110	-7.16097627	1.62144724
O	-7.96819424	-0.44546633	1.66051746
N	3.06582958	0.27189954	2.56339434
C	3.17267214	0.33732006	4.04118165
C	-1.47446964	1.53237805	-1.21425863
C	-1.31131764	1.49505743	-2.59088209
C	-0.42886336	0.58931905	-3.17464022
C	0.26376576	-0.29648798	-2.34820250
C	0.08151367	-0.26713899	-0.96458681
C	-0.77065341	0.66407869	-0.37333155
C	-0.58368183	-0.44608872	1.88254610
C	0.75866588	-0.68280923	2.22442116
C	1.12463188	-1.91991139	2.76132610
C	0.15810292	-2.89667172	2.99554808

C	-1.17984132	-2.64201588	2.70971245
C	-1.54339059	-1.42002422	2.15336323
C	-0.95681724	0.81090684	1.13940604
C	-0.20839080	2.07246674	1.66786925
C	1.05958746	1.76437667	2.47266029
C	1.70166329	0.47141053	1.97417960
C	-2.89917350	5.07357402	-1.81787469
C	-3.58408903	4.76964134	-0.48156868
C	-2.61058872	4.84788166	0.68995206
C	-1.82906978	6.14741377	0.64657190
C	-1.13783745	6.25621377	-0.71457557
C	-5.44908474	3.15777727	-0.46709756
C	-5.29898941	1.30480947	-1.97124426
C	-5.50253917	0.30996741	-0.82652351
C	-5.00375234	0.89547697	0.48692199
C	-5.70183374	2.22726093	0.72334941
C	-5.46137654	-2.01079662	-1.52650743
C	-5.50077563	-3.03811451	-0.38612063
C	-4.08604442	-3.49530836	-0.08206085
C	-3.47007889	-4.05814012	-1.35960172
C	-3.50958168	-3.02511606	-2.48607657
C	-1.70161803	-5.73373126	-1.28003940
C	0.41926276	-5.09230532	-2.20373237
C	1.13547694	-5.49134882	-0.91346289
C	0.19513098	-5.41874155	0.28212061
C	-1.04693581	-6.24404857	0.01078951
C	3.48828535	-5.04333246	-0.40789335
C	4.02261554	-4.27030317	0.80630145
C	3.97652968	-2.78728396	0.46705887
C	4.85730801	-2.56107950	-0.75889565
C	4.44127699	-3.47208525	-1.91787454
C	5.88198552	-0.42360221	-1.35473350
C	5.98903361	0.54980125	-0.16962193
C	4.69295864	1.34998027	-0.15043954
C	4.67992129	2.16937647	-1.43394431
C	4.70241042	1.21801786	-2.63859674
C	3.68525256	4.33851083	-1.78811221
C	1.41217783	4.65743608	-2.49570798
C	1.10755556	5.42963965	-1.21229910
C	2.01571565	4.97295583	-0.06994041
C	3.45676721	5.15490825	-0.50837641
C	0.72191412	5.26436223	-3.70671167
C	4.90100500	1.97820145	-3.93832284
C	5.46475384	-3.43541851	-3.04004896
C	1.23239919	-5.44049476	-3.44036554
C	-3.12688608	-3.62430170	-3.82920899
C	-5.95601890	0.83660706	-3.25789678
C	-3.91075452	5.34969837	-2.91902981
C	5.58021545	5.44149761	0.54196917
C	7.53150743	-0.36807072	1.41113607
C	3.94241391	-5.34645580	2.96645008
C	-2.19171952	-7.31297641	1.84352560
C	-7.48606729	-2.68377888	0.87645306
C	-6.15996151	2.93276408	2.98063718
C	-1.10297038	7.01427549	2.77847772
C	-5.67233925	3.97699515	3.97538963
C	-8.06370217	-1.81630074	1.98416226
C	-3.53528244	-7.20013492	2.55246673

C	3.24503798	-6.68879899	3.17357322
C	7.60188333	-1.31558735	2.59908711
C	6.53380747	4.82818368	1.55660063
C	0.20659091	7.27786823	3.50906916
C	-6.59023382	4.01923842	5.18384144
C	-0.04568412	8.09137225	4.76550910
C	7.77072213	5.69584519	1.70083048
C	9.03925356	-1.46971403	3.06149248
C	4.03838954	-7.54506334	4.14519665
C	-3.75427553	-8.39946736	3.45764810
C	-9.53057976	-2.14255702	2.19801629
H	3.00162103	1.35993967	4.37576241
H	2.43853843	-0.32923433	4.49258569
H	4.17945443	0.02679089	4.32336530
H	3.44939585	-0.64207429	2.22662823
H	3.67711844	1.00792728	2.14523580
H	-2.18569669	2.23584979	-0.79278733
H	-1.87388414	2.16531970	-3.23320975
H	0.60618640	-1.00232543	-0.36224470
H	2.16228896	-2.16251187	2.97594048
H	0.45320005	-3.86272379	3.39163199
H	-1.93645526	-3.39869433	2.89297962
H	-2.58590807	-1.21036213	1.92552267
H	-2.02787264	0.97744354	1.29664240
H	0.04879418	2.70581010	0.81405171
H	-0.88407310	2.66218788	2.29392644
H	1.75781685	2.60664755	2.39150861
H	0.80677320	1.64155675	3.53125706
H	1.89190439	0.57210816	0.89708773
H	-2.27140574	4.21398053	-2.08927408
H	-4.41067445	5.47735372	-0.33378259
H	-1.87906814	4.03810299	0.56058218
H	-2.51041666	7.00183094	0.75610762
H	-0.60816528	7.21090670	-0.80148109
H	-6.01638837	4.08815241	-0.35576356
H	-4.22026523	1.42845669	-2.13831523
H	-6.57193596	0.07955161	-0.73118388
H	-3.92537122	1.08289172	0.38532689
H	-6.78397305	2.05430969	0.79699656
H	-6.47151066	-1.72563805	-1.84227257
H	-6.09215062	-3.90797744	-0.70551987
H	-3.49276238	-2.61622221	0.21406787
H	-4.03154367	-4.94493286	-1.68357191
H	-2.84003881	-2.18988825	-2.23672013
H	-2.55122774	-6.36926264	-1.55229508
H	0.20971125	-4.01482229	-2.17489755
H	1.52922223	-6.51000277	-1.03228053
H	-0.11918516	-4.37315775	0.40984495
H	-0.76754737	-7.29522031	-0.14274527
H	3.50020570	-6.11860424	-0.20525321
H	5.06897774	-4.56884407	0.95212642
H	2.94252499	-2.51367364	0.22786269
H	5.90172130	-2.78041188	-0.49463466
H	3.46871065	-3.12606804	-2.29012811
H	6.76702841	-1.06401835	-1.44645237
H	6.83894361	1.22898053	-0.31724971
H	3.85195778	0.64546268	-0.18932178
H	5.57758784	2.80078973	-1.46622818

H	3.75345240	0.66564194	-2.67263056
H	4.69075307	4.49820015	-2.19372912
H	1.10442996	3.61033013	-2.36706854
H	1.25771064	6.50095595	-1.40354281
H	1.84260351	3.89403252	0.07854000
H	3.63766620	6.21819747	-0.71606189
H	0.91300003	4.62402330	-4.58047986
H	-0.35647194	5.29086092	-3.52785977
H	4.92874068	1.25705445	-4.76668167
H	4.04624726	2.64259222	-4.09462121
H	5.13502926	-4.11663776	-3.83681113
H	5.50556794	-2.42361490	-3.45476922
H	0.71762956	-5.04148810	-4.32710718
H	2.21461341	-4.96416832	-3.37177496
H	-3.11272138	-2.82205712	-4.58204477
H	-2.12208136	-4.05010086	-3.76066999
H	-5.46658204	-0.08328422	-3.59182575
H	-5.80126056	1.60435815	-4.03017808
H	-4.57448549	4.48513190	-3.01964937
H	-3.37345748	5.48409814	-3.86976055
H	5.36295294	6.48378680	0.80934369
H	6.06032666	5.42225797	-0.44655604
H	7.98956132	0.60101230	1.64768198
H	8.06637189	-0.82248762	0.56722142
H	3.95930485	-4.77881850	3.90538639
H	4.97967936	-5.52844449	2.66030183
H	-1.36735885	-7.42934940	2.55927362
H	-2.22266813	-8.19362458	1.18726580
H	-7.65738110	-3.74794051	1.09018977
H	-7.99194181	-2.42686292	-0.06539996
H	-6.25328965	1.94547866	3.45021008
H	-7.14350623	3.24422035	2.60375622
H	-1.83498773	6.51896451	3.42793885
H	-1.51384346	7.97613726	2.44197790
H	-4.65800772	3.68897685	4.30082094
H	-7.50369317	-2.03519374	2.90810810
H	-3.52203434	-6.28256189	3.16517621
H	2.24565301	-6.49804124	3.59466833
H	7.00315389	-0.88018890	3.41738433
H	6.00896311	4.77860554	2.52446640
H	0.64079184	6.30254979	3.78885323
H	-6.63216568	3.05163494	5.69220192
H	-7.60300790	4.30046774	4.87878310
H	-6.23205605	4.77197033	5.88934881
H	-0.72580441	7.57572973	5.44957156
H	-0.47868658	9.06233573	4.50565141
H	0.89989096	8.27401222	5.28052573
H	7.51834256	6.70105451	2.04904928
H	8.29448422	5.77607252	0.74310378
H	8.45405315	5.23938075	2.41992494
H	9.47152853	-0.51058734	3.35974274
H	9.65019438	-1.89792339	2.26101220
H	9.07725430	-2.15162389	3.91330171
H	4.19036185	-7.03668773	5.10259428
H	5.01678683	-7.78896695	3.71948213
H	3.50979157	-8.48251342	4.33005529
H	-2.96879344	-8.48353487	4.21451351
H	-3.77328187	-9.32035702	2.86625966

H	-4.71849169	-8.30589959	3.96165243
H	-9.67292457	-3.18854376	2.48401772
H	-10.10115481	-1.94645047	1.28457950
H	-9.93418790	-1.50624511	2.98848900
H	0.79873354	5.66489158	1.26457060
H	4.30844796	3.04580655	0.80278626
H	6.81177707	2.19594230	-3.84331332
H	5.08909005	-1.35311886	1.25144270
H	6.73452717	-4.66186299	-2.27684481
H	1.56101502	-5.23715428	1.63381749
H	-3.21104307	-4.85944253	0.97621355
H	-4.87843697	-4.28746448	-4.23000851
H	-7.75273066	1.35240241	-2.79991365
H	-5.27932111	-0.88013490	1.25179817
H	-3.81940191	3.90981807	1.87753633
H	-4.12575660	7.21676982	-2.54055742
H	2.08230974	6.55680030	-4.09729070
H	0.57932316	-7.23291925	-3.58221042
H	-4.87969515	5.33723732	2.83559447
H	1.50061416	7.40041059	2.06052639
H	6.23333612	2.92223830	1.33625558
H	6.15308587	-2.58899373	2.30033323
H	2.23603574	-7.18008856	1.60953317
H	-4.65599821	-6.25787971	1.27777580
H	-7.04566306	-0.17472123	1.79793961

255

2-HP-B-CD:trans-(1R,4S)-SRT_4_Cl E(Ha)= -7253.8825483445

Cl	0.57358200	13.66004009	2.80669275
Cl	1.58145683	10.63367024	2.68691850
O	-2.35208435	3.94351193	-1.45407248
O	-4.15707692	0.92510284	-0.44026010
O	-5.66123438	-0.03758220	-1.90712861
O	-4.75328778	-3.41127319	-0.81468110
O	-4.83979552	-5.14740701	-2.34459028
O	-1.73884393	-6.58196317	-1.03105252
O	-0.32406452	-7.69963581	-2.48529864
O	2.61918200	-6.20213915	-0.90520635
O	4.45726543	-5.72420748	-2.23099176
O	4.99210746	-2.57026086	-0.45767089
O	6.09897176	-0.85539177	-1.55510827
O	3.54238171	1.54420687	-0.48588840
O	2.74969954	3.06524824	-2.02910712
O	3.93190468	3.53475595	1.37911871
O	1.18245152	4.30360715	1.56741303
O	-0.49427745	3.09136994	-0.36346189
O	4.77174189	0.82310582	1.97634440
O	6.03420312	-1.70535870	1.98702099
O	6.14140863	1.69319121	-2.84830739
O	5.53612163	-4.47349552	1.55256831
O	4.20189384	-6.99796840	1.14491325
O	6.34910188	-4.21288828	-3.49009849
O	-1.22855046	-8.35846482	0.95183385
O	1.59410196	-7.84664393	1.17295075
O	-3.51212961	-6.88237596	1.17037295
O	-5.69186111	-5.00588710	1.16495566
O	-3.90558547	-7.20529496	-3.92105730
O	-6.79957121	-1.99070633	-3.49572766
O	-5.82460054	0.54760422	1.65480476
O	-5.93036858	-2.32437376	1.53647450
O	-3.75747205	2.26193057	2.06864167
O	-1.57094809	4.07310850	2.10008052
O	-4.91681885	3.69791031	-2.64508087
O	0.95246713	4.29730240	-3.57447426
O	1.98730342	-8.18414048	-3.91244565
O	-6.39717000	2.88459089	3.10729329
O	-0.42594241	6.55697939	1.41406998
O	6.70005909	2.79452918	1.77611374
O	8.16448638	-3.49276896	1.66282703
O	3.69848975	-9.68666136	1.87120738
O	-3.53671130	-9.68264249	1.90895324
O	-8.07300618	-4.09850819	2.38490968
N	-1.26034331	5.90700555	-3.25476461
C	-1.92923771	6.16146898	-4.55443287
C	-1.36943346	12.17577260	-0.34959405
C	-0.90227156	13.03058278	0.64223234
C	0.01144786	12.57764223	1.58931775
C	0.45199151	11.24918205	1.53218396
C	-0.01902615	10.40044761	0.53659132
C	-0.93371570	10.85258888	-0.41666623
C	-0.34604895	9.48648138	-2.46143676
C	-0.19644961	8.16345446	-2.91094771
C	0.82540906	7.85264788	-3.81748228
C	1.67768929	8.83523943	-4.30338119

C	1.52476536	10.14897717	-3.87017937
C	0.52700575	10.46039725	-2.95745084
C	-1.44555693	9.91424558	-1.49289877
C	-2.19547145	8.72885575	-0.87163985
C	-2.44401090	7.63054247	-1.89593739
C	-1.09345885	7.08971927	-2.33666930
C	-2.98268550	2.65009049	-1.60959983
C	-3.76118891	2.27600489	-0.34472304
C	-2.94638525	2.43020320	0.94248862
C	-2.35313784	3.82712145	0.95467903
C	-1.51709203	4.03567497	-0.30417033
C	-5.51797109	0.63435967	-0.69217488
C	-5.03305898	-1.32501682	-1.98349063
C	-5.52452507	-2.22305809	-0.84945745
C	-5.37357206	-1.54828249	0.50952582
C	-6.05436352	-0.19224438	0.47792140
C	-5.36640563	-4.63068899	-1.15534445
C	-5.16250891	-5.60733355	0.00634127
C	-3.68634198	-5.93082748	0.15214320
C	-3.14289195	-6.43266065	-1.18063250
C	-3.44300185	-5.45629022	-2.31641669
C	-1.14911930	-7.81301261	-1.35774506
C	0.77238798	-6.79350385	-2.35019857
C	1.63920850	-7.20048832	-1.16013039
C	0.81431590	-7.35360975	0.11195038
C	-0.34811836	-8.29663539	-0.14508420
C	3.96486467	-6.49414235	-1.16616111
C	4.76843304	-6.22790122	0.11237486
C	4.72993012	-4.74463430	0.42924090
C	5.19719682	-3.94069967	-0.77662151
C	4.41969192	-4.30980329	-2.03764369
C	6.09213862	-1.70711886	-0.43191642
C	6.01742048	-0.87375983	0.85144654
C	4.76745367	-0.00670070	0.83344683
C	4.77322843	0.81861807	-0.44679434
C	4.92438943	-0.06092272	-1.68529751
C	3.58812391	2.87461243	-0.90282056
C	1.39329674	2.69352430	-1.81962882
C	0.82027740	3.52903433	-0.67716448
C	1.67235632	3.42409288	0.58515306
C	3.11770898	3.76179126	0.25898137
C	0.72317916	2.95479701	-3.15510913
C	5.10431853	0.74787689	-2.95828252
C	5.04647496	-3.72815596	-3.29510768
C	1.52368446	-6.88024948	-3.66852407
C	-3.14163558	-6.05065835	-3.68244895
C	-5.40772174	-1.86836815	-3.35239335
C	-3.88014657	2.76555499	-2.82752745
C	4.99487077	4.47778954	1.52455092
C	7.18694409	-1.62022132	2.82538051
C	5.10664359	-7.72685286	1.96904436
C	-1.12877444	-9.50980309	1.78621315
C	-6.44428911	-5.85128637	2.03278586
C	-6.89338550	0.57352259	2.60049677
C	-1.89892062	5.24800346	2.84524381
C	-6.55986916	1.60177428	3.67198494
C	-7.17856286	-4.97233618	3.03542656
C	-2.36222412	-9.56075752	2.67720791

C	4.31383007	-8.77009212	2.74496061
C	7.87424817	-2.97685828	2.94614123
C	6.08859875	3.89539577	2.40705669
C	-0.80369414	6.31148173	2.76783390
C	-7.67665821	1.67958982	4.69608132
C	-1.27688639	7.60582754	3.40004711
C	7.15675211	4.94020371	2.67812084
C	9.16729045	-2.84759805	3.73101326
C	5.22976459	-9.55101501	3.66977309
C	-2.29230767	-10.75527697	3.61070526
C	-7.98246741	-5.82559140	3.99878070
H	-2.98181830	6.38994560	-4.38962597
H	-1.43985529	6.99840643	-5.05190964
H	-1.84263607	5.26462957	-5.16903446
H	-0.33456812	5.45249725	-3.41775811
H	-1.78946987	5.18775117	-2.72540063
H	-2.08503693	12.54940228	-1.07739554
H	-1.24332500	14.05907450	0.69238697
H	0.33392014	9.37315626	0.52712190
H	0.96911814	6.83227303	-4.16592884
H	2.45680791	8.57554986	-5.01317704
H	2.18509945	10.92785177	-4.23858338
H	0.41978831	11.48330667	-2.60754916
H	-2.17090882	10.48293297	-2.09297232
H	-1.62286220	8.30650377	-0.03725092
H	-3.14273834	9.08447101	-0.45557274
H	-3.04187792	6.82421148	-1.45273549
H	-2.99786276	8.03039797	-2.75445392
H	-0.60185138	6.66569905	-1.45111774
H	-2.20970107	1.89090676	-1.78367512
H	-4.64118727	2.92946063	-0.26658461
H	-2.12944902	1.69300309	0.93230898
H	-3.18103111	4.54807601	0.91400623
H	-1.11930349	5.05444474	-0.28654619
H	-6.08761288	1.56476821	-0.79298992
H	-3.94238400	-1.21454382	-1.90422976
H	-6.58360480	-2.45642037	-1.02428497
H	-4.29924348	-1.38565291	0.69122031
H	-7.13372208	-0.33520073	0.32820500
H	-6.43536898	-4.48081420	-1.34123133
H	-5.71319147	-6.53044747	-0.22323158
H	-3.15950099	-4.99803509	0.40728762
H	-3.60644446	-7.39874484	-1.42200565
H	-2.85711777	-4.53867293	-2.16371290
H	-1.91664331	-8.54823246	-1.62216362
H	0.40089635	-5.77100873	-2.19158591
H	2.12408222	-8.15720604	-1.39614984
H	0.39737891	-6.36831181	0.37205029
H	0.04338811	-9.29830685	-0.37171602
H	4.08020097	-7.53793678	-1.47689429
H	5.80804596	-6.53665220	-0.06573041
H	3.68460754	-4.47432194	0.63961663
H	6.26231922	-4.13345305	-0.96454847
H	3.37964892	-3.96868369	-1.93415612
H	7.03603075	-2.26081758	-0.45709812
H	6.89252517	-0.21008510	0.85854758
H	3.88213881	-0.65894398	0.84198959
H	5.61243029	1.52422639	-0.40156298

H	4.03839826	-0.70569264	-1.78097857
H	4.59285831	3.14723333	-1.24202674
H	1.31632149	1.62724987	-1.56953717
H	0.80235550	4.58282013	-0.99478761
H	1.63187761	2.38632363	0.94444830
H	3.17049150	4.81632338	-0.05105321
H	1.11373279	2.25889478	-3.90652592
H	-0.35747172	2.81507588	-3.07318529
H	5.27483535	0.04920666	-3.79031885
H	4.18757972	1.30751211	-3.16543943
H	4.39218903	-3.95316332	-4.15165659
H	5.12153557	-2.64195445	-3.19246735
H	0.86299446	-6.52343183	-4.47361679
H	2.40179868	-6.22951247	-3.62855494
H	-3.31523091	-5.27927081	-4.44875616
H	-2.08963864	-6.34694751	-3.72311872
H	-4.98280685	-2.86921647	-3.46978175
H	-4.97192354	-1.21446049	-4.12409314
H	-4.34984941	1.79552683	-3.01374327
H	-3.25764385	3.01124912	-3.70561769
H	4.59173193	5.40594946	1.95391558
H	5.43802225	4.70392466	0.54418021
H	6.87156593	-1.25314687	3.80974692
H	7.89873843	-0.90010195	2.40338234
H	5.63130292	-7.03777048	2.64301687
H	5.84357215	-8.24456521	1.33852558
H	-0.20653941	-9.46024151	2.37797404
H	-1.10766862	-10.41426502	1.16157596
H	-5.77344445	-6.55895361	2.53427165
H	-7.18488567	-6.41134058	1.44410954
H	-7.02988002	-0.42505212	3.03196535
H	-7.81953738	0.87770877	2.09200183
H	-2.05656739	4.94774686	3.88685200
H	-2.84139586	5.66699704	2.47161790
H	-5.63139042	1.28052044	4.17321095
H	-6.42255146	-4.40189003	3.60171971
H	-2.38435682	-8.63437496	3.27625258
H	3.55764792	-8.23963582	3.34830682
H	7.19585615	-3.66129500	3.47873340
H	5.62773829	3.59153546	3.36098753
H	0.07632894	5.94398510	3.31411806
H	-7.85127522	0.71087020	5.17289804
H	-8.60492526	2.00861852	4.21847009
H	-7.41844741	2.40814439	5.46765017
H	-1.59549625	7.44694847	4.43472796
H	-2.12361768	8.01818476	2.84105260
H	-0.47228177	8.34463402	3.39758655
H	6.74594928	5.81737463	3.18661856
H	7.62093636	5.26137065	1.73998712
H	7.93815114	4.50689655	3.30580361
H	8.99567544	-2.41550218	4.72193650
H	9.87391531	-2.21041736	3.18966432
H	9.62753436	-3.83025225	3.85510705
H	5.73453182	-8.89451141	4.38462967
H	5.98651988	-10.08671852	3.08792137
H	4.64748921	-10.29056745	4.22361867
H	-1.40277344	-10.71661522	4.24614355
H	-2.27235714	-11.68496036	3.03329627

H	-3.17876126	-10.77538305	4.24841118
H	-7.34211785	-6.52217318	4.54746141
H	-8.74002814	-6.39817078	3.45447356
H	-8.49805842	-5.18348163	4.71625266
H	0.31510570	3.96516812	1.86301549
H	4.15372149	1.55554752	1.81379592
H	6.94978569	1.20057687	-2.66308972
H	5.44362637	-3.52158330	1.75106673
H	6.27626878	-5.17412261	-3.52582898
H	2.39698204	-7.29246819	1.22415167
H	-2.57586109	-7.16400628	1.14877564
H	-4.82970216	-6.94093983	-3.84273022
H	-7.16964286	-1.11245068	-3.35015870
H	-5.57651335	-3.23247514	1.44374864
H	-4.28657700	1.44826704	1.93686632
H	-4.52487623	4.50565556	-2.29659856
H	1.89916565	4.45632449	-3.44695890
H	1.20910348	-8.75389058	-3.90928644
H	-5.52554213	2.91140028	2.68963302
H	0.33819758	5.97601534	1.26087473
H	6.14199980	2.01415969	1.94025964
H	7.41377329	-4.05925941	1.42801041
H	2.91916836	-9.25879101	1.48774374
H	-3.72716784	-8.82050290	1.51318266
H	-7.55420454	-3.39901639	1.96466502

2-HP-B-CD:trans-(1R,4S)-SRT_5_Cl E(Ha)= -7253.8574775220

Cl	2.27621471	-0.00996641	-2.18684390
Cl	0.38771850	-1.67367586	-0.20853690
O	-4.52737801	-4.34143434	2.52403206
O	-5.61829665	0.69449969	2.73743422
O	-2.84002611	3.05113019	2.34612063
O	-2.05969920	4.24467584	4.16383827
O	1.22074648	4.45794339	2.56707147
O	3.14306236	4.57558456	3.85844997
O	4.67254738	2.03215037	1.72213452
O	6.31828512	0.61967207	2.54027069
O	4.75945690	-2.29306563	0.95149639
O	4.85165938	-4.33040453	2.04615429
O	1.52542084	-5.27730471	0.84509099
O	0.15290555	-6.48314576	2.26964506
O	0.81005974	-6.79207905	-1.27309215
O	-2.01146513	-6.19963039	-1.23201581
O	-2.80140404	-4.71791198	1.02883655
O	3.03881530	-5.20965637	-1.55661736
O	5.30498860	-3.43263358	-1.42370442
O	3.84029906	-6.59427466	3.29621882
O	5.45221148	-0.71464897	-1.29448120
O	5.85133863	2.06074258	-0.74545717
O	7.46507987	-1.79332604	3.30604721
O	2.33644231	6.07440340	0.66576462
O	4.37041354	4.20550073	-0.07973983
O	-0.35476370	6.04509908	0.85947671
O	-3.11508915	5.36195558	0.86068375
O	-0.18551691	5.29931036	5.87505877
O	-5.62415602	2.90073528	4.50469177
O	-5.38166941	0.60818145	-0.90465982
O	-3.82215333	2.89705598	-0.28596734
O	-5.45260194	-2.27072012	-0.94091340
O	-4.62496488	-5.00724711	-1.05299898
O	-6.23101834	-2.86062849	4.05226931
O	-2.05332903	-7.04054876	3.80305998
O	5.56824169	3.78327621	4.86989419
O	-7.82553467	-0.79811925	-0.95559781
O	-4.25416116	-7.81142102	-0.86030926
O	3.06317569	-7.89892026	-2.57262874
O	7.35200919	-2.17553571	-2.90762566
O	6.72039730	4.59597978	-1.71807956
O	0.93011706	7.98025260	-1.05505189
O	-5.81488475	4.82118030	-0.17680524
O	-4.62408057	-0.87589080	1.34113492
N	-2.07415064	5.29122858	-7.16546816
C	-1.40118362	4.16325530	-6.37040462
C	-2.15080064	2.86066740	-6.60017961
C	-1.64776095	1.81537031	-5.61305435
C	-1.99986959	2.21951247	-4.17779075
C	-1.58289485	4.12272885	-2.57604371
C	-1.18938997	5.41539164	-2.26132834
C	-0.79001449	6.28722924	-3.27582493
C	-0.84355469	5.86014595	-4.59402136
C	-1.29372666	4.57097787	-4.92190859
C	-1.62224058	3.66841461	-3.89891726
C	-1.39109863	1.26094778	-3.17029526

C	-0.00892939	1.07348440	-3.11165817
C	0.56026271	0.17936353	-2.20908802
C	-0.26559668	-0.54121527	-1.33730144
C	-1.64210995	-0.34159700	-1.37731049
C	-2.20122673	0.55013624	-2.28522637
C	-3.45394780	5.67904652	-6.75126284
C	-4.30974594	-2.93099885	2.58924332
C	-5.02109380	-2.24085597	1.42707553
C	-4.69395304	-2.87727760	0.08153121
C	-4.97124650	-4.36520194	0.15232162
C	-4.15261772	-4.94720277	1.31323093
C	-5.61416804	0.10889158	1.46145458
C	-4.40199167	1.34763772	3.10045559
C	-4.09330540	2.44171799	2.08102632
C	-4.03310497	1.87235135	0.66957304
C	-5.35634080	1.17666827	0.39315263
C	-2.84996838	4.29396038	3.01375809
C	-2.32819375	5.35859414	2.03782441
C	-0.88971358	5.04089775	1.68594632
C	-0.06457643	4.91226787	2.96266690
C	-0.68170638	3.92477120	3.95011980
C	2.35913821	5.21296267	2.89098181
C	3.64124241	3.28137197	3.50068310
C	4.41691002	3.34906702	2.18565581
C	3.61863112	4.05812069	1.09808720
C	3.16486383	5.41572442	1.60328224
C	5.99883352	1.59426129	1.58708505
C	6.17225645	1.03728309	0.17010004
C	5.28838778	-0.18576712	0.00035097
C	5.65240135	-1.19813250	1.07877566
C	5.54295562	-0.58142831	2.47338284
C	5.29503806	-3.59271350	0.94195949
C	4.88483959	-4.26922945	-0.36996952
C	3.38241569	-4.48928628	-0.39660608
C	2.94578806	-5.22385227	0.86388358
C	3.43614800	-4.51546896	2.12431136
C	0.90130751	-6.51165908	1.08550719
C	-0.90859821	-5.52731963	2.30538085
C	-1.86664079	-5.78107060	1.14363153
C	-1.13180087	-5.84008302	-0.18872407
C	0.00782777	-6.83865628	-0.11647936
C	-1.57346745	-5.72834197	3.65767739
C	3.20738104	-5.34121587	3.37888414
C	6.11426956	-1.48781237	3.55071745
C	4.52691658	2.86284705	4.66327082
C	-0.03521535	4.01556810	5.32301011
C	-4.62701725	1.90673445	4.49458702
C	-4.87546477	-2.51301422	3.93774670
C	0.67804146	-7.87969885	-2.18150568
C	5.89367220	-4.07607453	-2.54957376
C	6.69319273	2.17860441	-1.88910194
C	2.99939635	6.95896495	-0.23608032
C	-4.20473097	6.28160049	0.90159311
C	-6.45372429	1.01812398	-1.75393661
C	-5.58274175	-5.93355541	-1.56213846
C	-7.35804244	-0.15598138	-2.12188652
C	-5.12941724	6.04689295	-0.28400459
C	2.08171468	7.23889669	-1.41382217

C	6.39810644	3.51276665	-2.55956936
C	6.38034776	-2.99868279	-3.50863083
C	1.80763827	-7.79166701	-3.19869292
C	-4.90523178	-7.23477008	-1.97135854
C	-8.54891822	0.32946492	-2.93015103
C	-5.92947479	-8.22118589	-2.50434827
C	1.69708047	-8.91581087	-4.21260915
C	7.00631491	-3.62808292	-4.73949388
C	7.21711584	3.66196067	-3.82833516
C	2.81213334	8.04870817	-2.46920822
C	-6.17193881	7.14853376	-0.36145920
H	-2.01675069	2.52351159	-7.63492096
H	-2.08893909	0.84128450	-5.84166293
H	-0.56224866	1.69834399	-5.71793903
H	-3.09173410	2.13853560	-4.07004782
H	-1.87048512	3.43559090	-1.78564111
H	-1.15862193	5.73499777	-1.22222367
H	-0.42341858	7.27598023	-3.01383224
H	-0.49730017	6.54597631	-5.36983522
H	0.65732578	1.63363749	-3.76107178
H	-2.27632123	-0.88445497	-0.68423804
H	-3.27666070	0.70378334	-2.26981887
H	-2.07455112	5.02949761	-8.15476965
H	-3.74608415	6.56776693	-7.31152397
H	-3.44056950	5.88988814	-5.68238646
H	-4.14053920	4.86391941	-6.97044599
H	-1.47644938	6.11684829	-7.08657280
H	-0.40586284	4.10005305	-6.83120976
H	-3.22565021	3.00168858	-6.43396055
H	-0.85258609	-5.46507736	4.44675505
H	3.90260372	2.74145638	5.56133347
H	1.65039762	-7.29759562	1.22843266
H	-0.40033573	-7.84925210	0.02419533
H	-0.69927718	-4.84793413	-0.38606741
H	-2.74484788	-5.55524171	-1.22845519
H	-2.38799468	-6.73036479	1.32758438
H	-0.50465158	-4.50813525	2.22518897
H	-2.43600575	-5.06125202	3.74086579
H	6.38628082	-3.55636878	1.02801012
H	5.39431735	-5.24114917	-0.43071696
H	2.89740765	-3.50120299	-0.40785756
H	2.10619915	-5.48263673	-1.46293464
H	3.36346183	-6.23944855	0.85371167
H	2.93249501	-3.54269736	2.21483077
H	3.55618953	-4.76297313	4.24785764
H	2.13686956	-5.52989777	3.49816413
H	4.77996400	-6.41783118	3.17053583
H	6.69682020	2.42135885	1.75814583
H	7.22472313	0.74572064	0.04595404
H	4.24249204	0.12126744	0.14829214
H	5.10181758	-1.62807493	-1.28413386
H	6.68752925	-1.53355895	0.92819062
H	4.48689529	-0.36192434	2.68529120
H	5.97512829	-1.00267305	4.52855621
H	5.56618660	-2.43411475	3.55498068
H	7.93700160	-0.95260023	3.29411852
H	2.07175566	6.17769671	3.32379630
H	4.03634621	6.04254514	1.83859853

H	2.71666113	3.46138342	0.89592422
H	4.68325630	3.31247314	-0.33238399
H	5.35932326	3.88541526	2.36261396
H	2.80634122	2.57672982	3.38248546
H	4.98974485	1.89910005	4.43198086
H	-3.86287146	4.52626834	3.36134559
H	-2.36858965	6.34510510	2.52024632
H	-0.86801324	4.06540242	1.17425855
H	0.60711362	5.86820180	0.79570313
H	0.00677271	5.89363128	3.45106254
H	-0.58925234	2.90653740	3.54872354
H	-0.46661129	3.23721218	5.96985494
H	1.03852749	3.82981938	5.22868538
H	-1.13435843	5.45636130	5.94311244
H	-6.61267004	-0.31573331	1.31680725
H	-6.15741277	1.92177811	0.48175961
H	-3.21382735	1.14278460	0.61062245
H	-3.31572842	3.60529502	0.15840676
H	-4.89418008	3.19284823	2.11992015
H	-3.57191437	0.62663343	3.11814819
H	-3.70423012	2.37378510	4.85061648
H	-4.87327320	1.07487981	5.17022109
H	-6.43808549	2.47973902	4.20443286
H	-4.35606127	-6.01768056	1.42413010
H	-6.03603241	-4.51871901	0.37271299
H	-3.62074236	-2.74517839	-0.11816446
H	-5.20354541	-1.32755485	-0.94305670
H	-6.10255396	-2.30841077	1.60912354
H	-3.23444322	-2.70914861	2.53714481
H	-4.81415653	-1.42594170	4.03609073
H	-4.26609104	-2.96882792	4.73280296
H	-6.27366306	-3.81671514	3.93187954
H	-1.29148616	-7.62167646	3.69347782
H	5.14748162	4.63126397	5.05282081
H	-6.02038251	1.46434200	-2.65929886
H	-7.04975574	1.79012090	-1.25279024
H	-3.80509793	7.30551810	0.88161310
H	-4.78668566	6.15042830	1.82502338
H	3.91821922	6.48705296	-0.59704593
H	3.24469962	7.89922947	0.27925533
H	6.51378786	1.33802762	-2.57022309
H	7.74636369	2.16687022	-1.57396356
H	5.15737322	-4.73063650	-3.03160125
H	-0.30337476	-7.83817552	-2.67141306
H	0.76798344	-8.83000770	-1.63558647
H	-6.10275039	-5.47484105	-2.41387365
H	-6.32481739	-6.16839873	-0.78838349
H	-6.77338920	-0.86462944	-2.72884919
H	-4.17442265	-7.00858504	-2.76433905
H	1.71390322	-6.82345494	-3.72028552
H	5.50149081	-2.40357090	-3.81252386
H	5.32399988	3.52687974	-2.81581218
H	1.79429930	6.26057841	-1.83485135
H	-4.50697667	6.06848883	-1.19589881
H	6.99644094	2.86438068	-4.54359138
H	8.28563523	3.63658116	-3.59314573
H	7.00049918	4.62550146	-4.29546098
H	3.68975262	7.51376803	-2.84224439

H	3.13273895	9.01034533	-2.05719321
H	2.14458438	8.25358892	-3.31048913
H	-5.71206501	8.13199527	-0.49452213
H	-6.77582440	7.16386942	0.55129881
H	-6.84412463	6.95759175	-1.20109429
H	-8.23487844	0.86945846	-3.82956930
H	-9.16932539	0.99543584	-2.32218919
H	-9.16447307	-0.52047030	-3.23243987
H	-6.47965245	-7.81196585	-3.35738246
H	-6.64556460	-8.48271217	-1.71867406
H	-5.42911327	-9.13933595	-2.81970864
H	0.74336156	-8.88306089	-4.74766449
H	1.78722801	-9.88527390	-3.71244380
H	2.50962958	-8.83660168	-4.93817222
H	6.29580589	-4.27156076	-5.26651876
H	7.87830082	-4.22556105	-4.45553854
H	7.34459540	-2.84472381	-5.42156477
H	-7.23181219	-1.54940225	-0.80133348
H	-3.34390542	-7.47524339	-0.87490293
H	3.24526333	-7.06014431	-2.12282668
H	6.90600808	-1.61414928	-2.25661704
H	6.09273827	4.60790007	-0.98256093
H	0.44166829	7.51277205	-0.36508505
H	-5.18075799	4.10121657	-0.33890966
H	6.75294444	-4.67842660	-2.22028673

2-HP-B-CD:trans-(1R,4S)-SRT_6_Cl E(Ha)= -7253.8406217591

Cl	0.45557548	1.51923072	1.20860086
Cl	0.51273018	-1.58228405	0.50029885
O	-5.28730850	-2.47154254	-1.28994600
O	-2.47194097	-4.27631666	0.19258438
O	-1.33272734	-5.78992386	-1.13126179
O	1.84192444	-4.70131771	0.31334810
O	3.76924517	-4.86939609	-0.95200940
O	4.64755098	-1.41815566	-0.08080072
O	5.67994709	-0.10752516	-1.68799448
O	4.04962337	2.99395654	-0.62839212
O	3.72272113	4.70763797	-2.16076710
O	0.35320490	5.27421331	-0.83626317
O	-1.38496420	6.04020006	-2.16896362
O	-3.66884059	3.69873716	-0.52216874
O	-5.35288296	2.68155598	-1.73537005
O	-5.25892385	3.90611959	1.66676970
O	-5.75884466	1.10463595	2.05927846
O	-4.85875037	-0.54695340	-0.07427916
O	-3.05225499	5.52941113	1.58921140
O	-0.53466895	6.83936764	1.25226227
O	-3.87152146	6.06677287	-3.38952644
O	2.05236034	6.07866056	1.36141507
O	4.60569899	4.81194979	1.34032724
O	2.30277567	6.47828386	-3.72302481
O	6.26504718	-0.46789518	1.86248832
O	5.60047302	2.30946068	1.66768872
O	4.87430718	-2.76341277	2.43441067
O	3.29054672	-5.11740348	2.64435067
O	5.91645653	-3.93228527	-2.41849583
O	0.66969657	-6.83896124	-2.59389100
O	-2.29537725	-5.89312391	2.35217446
O	0.59341486	-5.95302618	2.52038504
O	-4.19158145	-3.89753771	2.42696484
O	-5.94274219	-1.62930296	2.16567025
O	-4.76806340	-4.79611620	-2.63987127
O	-6.70200706	0.63662650	-2.98715045
O	6.10237437	1.91940783	-3.46370565
O	-4.83128344	-6.56350004	3.36921297
O	-8.14325062	-0.13123335	3.10534079
O	-5.58707147	6.59124457	2.48214168
O	1.34256021	8.78047084	2.08163220
O	7.23785709	4.58418974	2.34929727
O	7.63636250	-2.52839269	3.21669555
O	2.68526522	-7.84929231	2.62406030
N	-1.68476366	-3.77206810	-6.94664914
C	-1.35415037	-3.15772648	-8.26621472
C	-0.23601336	1.47088823	-2.72435428
C	-0.02321336	1.89327527	-1.41555939
C	0.20577082	0.96695604	-0.40313726
C	0.22840860	-0.39701993	-0.71661145
C	0.01831874	-0.80992689	-2.02906207
C	-0.22396461	0.11428968	-3.04674449
C	0.43373245	-1.38595400	-4.98021895
C	0.04446788	-2.60503042	-5.56044682
C	1.02625229	-3.52143018	-5.96519782
C	2.37663757	-3.21865266	-5.86823995

C	2.76406640	-1.98720081	-5.34352014
C	1.80048614	-1.09787319	-4.89225487
C	-0.55984474	-0.36316773	-4.44883777
C	-2.00490933	-0.87962541	-4.47110627
C	-2.30220036	-1.68556427	-5.72774767
C	-1.42673997	-2.92645575	-5.70273580
C	-3.96700572	-3.00282936	-1.21467934
C	-3.82149947	-3.86403802	0.03790146
C	-4.20551784	-3.07811664	1.28650533
C	-5.59565207	-2.48788886	1.10958970
C	-5.67406324	-1.67864061	-0.19018479
C	-2.14677271	-5.62668681	0.00410134
C	-0.07722199	-5.10605304	-1.07964764
C	0.71984693	-5.54894593	0.14607705
C	-0.10656813	-5.42510042	1.42152767
C	-1.43822297	-6.13610536	1.26427690
C	3.13694374	-5.23656127	0.24762076
C	3.92767309	-4.71872485	1.45165786
C	4.06701256	-3.20790876	1.37546740
C	4.67475081	-2.83554062	0.02612989
C	3.91264601	-3.45914402	-1.14219616
C	5.82857334	-0.75653024	-0.45050141
C	4.72349335	0.95359786	-1.72780328
C	5.07237523	2.00855935	-0.67966564
C	5.19131679	1.37584233	0.70331525
C	6.20192934	0.24153583	0.64981696
C	4.36237976	4.31904455	-0.97222182
C	3.93710504	5.23458903	0.17771504
C	2.42770059	5.18514243	0.34580978
C	1.75266231	5.51918455	-0.98090671
C	2.29694983	4.66197221	-2.12559732
C	-0.55821504	6.32149535	-1.07115961
C	-1.40309856	6.54282981	0.18786996
C	-2.23881829	5.30668415	0.46585168
C	-3.07474579	4.96920183	-0.76230574
C	-2.23505959	4.90104657	-2.03836778
C	-5.05272879	3.55195714	-0.67184080
C	-4.86016066	1.35020663	-1.58419340
C	-5.43544832	0.73319669	-0.31075312
C	-5.13865280	1.60616114	0.90326845
C	-5.63502707	3.01968279	0.64210112
C	-5.30683609	0.62216928	-2.84011115
C	-3.09574679	4.90134644	-3.29168835
C	1.84727308	5.17220381	-3.48504684
C	4.80406229	1.49641634	-3.14495163
C	4.65547647	-3.31510548	-2.45884304
C	0.60635176	-5.45305898	-2.39141008
C	-3.79405536	-3.79780179	-2.49784039
C	-6.27719222	4.27982173	2.59360492
C	-0.91328640	7.91833870	2.10582791
C	5.17745841	5.83061959	2.15849622
C	7.37937701	-0.18136869	2.70492489
C	4.00816038	-6.02478037	3.48001641
C	-2.45081572	-6.95426875	3.29161332
C	-6.82888508	-2.15516128	3.15325912
C	-3.66629049	-6.65054157	4.15696395
C	3.14577745	-7.23712858	3.81339880
C	7.45315448	-1.25235072	3.78463644

C	6.19721984	5.18389664	3.08589938
C	0.30361980	8.33368947	2.92136319
C	-5.80204959	5.50836614	3.35719100
C	-7.40781958	-0.99070047	3.94497703
C	-3.87466976	-7.74978082	5.18211972
C	-8.34152166	-1.50013459	5.02762951
C	-6.84280859	5.93173175	4.37753761
C	-0.05505800	9.46754758	3.86423025
C	6.81415371	6.22532069	4.00128846
C	8.62071611	-0.98246179	4.71602363
C	3.94322601	-8.25250307	4.61138243
H	-2.02688370	-2.32212285	-8.44983319
H	-0.32051456	-2.81504150	-8.23741343
H	-1.48340083	-3.91296042	-9.04207967
H	-1.16167407	-4.64547804	-6.85045121
H	-2.67334778	-4.03775384	-6.93625456
H	-0.41687251	2.21356881	-3.49799795
H	-0.02521987	2.94962085	-1.16368292
H	0.05405999	-1.87299808	-2.24891016
H	0.76018438	-4.50278894	-6.35718098
H	3.12029027	-3.93821480	-6.19510492
H	3.81669541	-1.73228911	-5.27032305
H	2.10569476	-0.15348778	-4.44970688
H	-0.50449853	0.50982595	-5.11473580
H	-2.17987241	-1.50586276	-3.58826766
H	-2.69668439	-0.03681754	-4.39100494
H	-3.36296752	-1.96363537	-5.76184617
H	-2.08287202	-1.07503191	-6.61172935
H	-1.75967202	-3.58100585	-4.88508037
H	-3.22844831	-2.18813117	-1.17402802
H	-4.47896810	-4.73926552	-0.05536363
H	-3.49308815	-2.24624814	1.40169574
H	-6.32156562	-3.31074321	1.03735442
H	-6.71081461	-1.38871897	-0.38980685
H	-3.04851221	-6.21799538	-0.18832220
H	-0.24270781	-4.02267198	-1.01002018
H	1.03745596	-6.59209181	0.00634012
H	-0.32021322	-4.35796047	1.58282889
H	-1.26625978	-7.21564572	1.14794355
H	3.10999725	-6.33163146	0.26577552
H	4.93221608	-5.15881037	1.39919168
H	3.06560306	-2.75824273	1.44149102
H	5.71174678	-3.19680011	-0.00203801
H	2.92419006	-2.98310020	-1.21328970
H	6.63959347	-1.47823213	-0.59565574
H	3.71472711	0.56466227	-1.52551802
H	6.03000324	2.47042692	-0.95606137
H	4.21153127	0.95018037	0.97276790
H	7.18900620	0.66046395	0.40670522
H	5.43561376	4.42365598	-1.16348349
H	4.23777931	6.26041822	-0.07808220
H	2.15401501	4.15522698	0.62196679
H	1.92660017	6.57615891	-1.22219062
H	1.96768801	3.62400422	-1.98374943
H	-0.01976520	7.23889404	-1.33070139
H	-2.06982745	7.39586363	-0.00234348
H	-1.55062101	4.46853932	0.65662445
H	-3.84995634	5.73666920	-0.89008717

H	-1.63849406	3.98061222	-2.00530394
H	-5.51835327	4.50890080	-0.93090323
H	-3.76210475	1.35557694	-1.52143226
H	-6.52291587	0.63880352	-0.43175636
H	-4.04692228	1.64813336	1.04138487
H	-6.72974624	2.99809970	0.54447520
H	-4.80305909	1.08638872	-3.70522604
H	-5.00172612	-0.42670118	-2.77598533
H	-2.43903257	4.77323862	-4.16716130
H	-3.78720669	4.05391257	-3.25189296
H	2.19762803	4.46966628	-4.25800232
H	0.75340422	5.20311139	-3.51522649
H	4.44974884	0.71434997	-3.83906038
H	4.14751435	2.36626671	-3.23890960
H	4.02333728	-3.73237973	-3.25927240
H	4.82002043	-2.25315648	-2.66535576
H	1.63208397	-5.07262884	-2.37948157
H	0.06284023	-4.94703124	-3.21134525
H	-2.81734190	-4.29404750	-2.48372126
H	-3.82542244	-3.08547087	-3.34264628
H	-6.48890388	3.44175074	3.26879556
H	-7.19316140	4.54051674	2.04459841
H	-1.74405549	7.60539813	2.74970145
H	-1.23344617	8.77256900	1.49264457
H	4.38598854	6.34121918	2.72027889
H	5.69635828	6.56174360	1.52251932
H	7.26867421	0.81990641	3.13865272
H	8.30402376	-0.21651414	2.11085022
H	4.31769675	-5.49681890	4.39025163
H	4.90989073	-6.37182747	2.96059579
H	-1.53986177	-7.05173878	3.89492571
H	-2.62918877	-7.89601798	2.75297135
H	-6.28796942	-2.85601755	3.80048285
H	-7.65367299	-2.68636364	2.65731156
H	-3.47995265	-5.69801542	4.68100217
H	2.28849452	-6.89784328	4.41584702
H	6.51414112	-1.21609834	4.36240477
H	5.67069263	4.43139501	3.69707634
H	0.62972147	7.46127366	3.51256363
H	-4.86910198	5.24165022	3.88198194
H	-6.56947403	-0.45009458	4.41575747
H	-3.00078774	-7.86631436	5.82967453
H	-4.07083999	-8.70247886	4.68007093
H	-4.74127401	-7.51317143	5.80308808
H	-7.82638440	-2.17374319	5.71861087
H	-9.18519908	-2.03391057	4.57876280
H	-8.74162414	-0.65628662	5.59373436
H	-7.05241005	5.13198116	5.09381422
H	-7.77506966	6.20689915	3.87420876
H	-6.48565733	6.80725729	4.92393954
H	-0.85785293	9.18141137	4.54992954
H	-0.37476810	10.34573813	3.29441727
H	0.82271404	9.74908675	4.44985102
H	6.05483502	6.72617578	4.60885507
H	7.34636208	6.97855600	3.41177099
H	7.53682470	5.74771957	4.66642327
H	8.53548499	-0.00236075	5.19432136
H	9.56330243	-1.02222461	4.16086803

H	8.65588083	-1.74981613	5.49239673
H	4.35190964	-7.81299700	5.52646841
H	4.77222032	-8.63742883	4.00896110
H	3.30567778	-9.09617668	4.88460999
H	-5.52497277	0.15927602	2.13178880
H	-3.64156389	4.75497501	1.67735923
H	-3.25378921	6.80753580	-3.37596445
H	1.07574061	6.09126130	1.39813311
H	3.26298758	6.45070939	-3.63392194
H	4.99960395	3.07845117	1.60907578
H	5.09002216	-1.82671670	2.26085952
H	5.76292954	-4.84267700	-2.13795641
H	-0.20587924	-7.18041864	-2.37200999
H	1.42126917	-5.43875589	2.61216159
H	-3.33246893	-4.36150762	2.44486133
H	-5.61750069	-4.36655677	-2.47530351
H	-6.96897057	1.56319599	-2.94486606
H	6.68472543	1.17710292	-3.26048121
H	-4.83274689	-5.69846914	2.93557900
H	-7.51368286	0.42109033	2.62037167
H	-4.73905927	6.45233592	2.03727405
H	1.76545846	8.00317381	1.69000093
H	6.90443902	3.75263984	1.98376605
H	6.77996231	-2.82670845	2.87732850
H	1.82514794	-7.44874584	2.43100079

2-HP-B-CD:trans-(1R,4S)-SRT_1_MD E(Ha)= -7253.92292611

C	0.3048797464	1.8942303731	-2.5764649672
C	-0.6398053676	2.4731038598	-3.6148225726
C	-1.1304616821	3.7838089562	-3.5099304375
C	-0.7031825774	4.7238440257	-2.4036922552
C	-0.1677841554	3.9402069349	-1.1953260850
C	0.8932615473	2.9534912703	-1.6566921110
C	-1.0294122162	1.6714818647	-4.6969347990
C	-1.9011124867	2.1496154684	-5.6655210543
C	-2.3943766803	3.4502500322	-5.5666621890
C	-2.0064555104	4.2535875952	-4.4998222402
C	0.3084937605	5.7591662745	-2.8835573084
C	0.6084003172	6.8452007874	-2.0549251442
C	1.5354282921	7.8008092544	-2.4406141539
C	2.1845540688	7.7010772085	-3.6708608307
C	1.9006139522	6.6169589512	-4.5032155802
C	0.9689484250	5.6580596276	-4.1062632729
Cl	3.3298800377	8.9128446428	-4.1223799096
Cl	2.6864080582	6.4274010596	-6.0323601817
N	-0.4359998293	0.8124132847	-1.8339631683
C	0.2757764414	0.1636092333	-0.7132898241
C	-3.2180383640	3.9701956534	1.3837713260
C	-4.6777649536	3.7525703557	1.0154593968
C	-5.2257627939	2.5648486102	1.8127897762
O	-5.1179686563	2.8178806516	3.1798492448
C	-3.7669316654	2.9162314365	3.6391811175
C	-3.0471226052	4.0422324806	2.8976006914
O	-4.4945677053	1.3869757810	1.5454595733
C	-4.8550640943	0.6093996027	0.4197203387
C	-3.5712620888	0.2230582474	-0.3100730260
C	-3.8355815206	-0.8193301733	-1.3931481367
C	-4.6912255716	-1.9765347563	-0.8505879191
O	-5.8546537255	-1.4729915845	-0.2489490819
C	-5.6096258409	-0.6352415099	0.8787368653
O	-3.8891639782	-2.6999800597	0.0441391718
C	-4.3439907133	-4.0105415620	0.3651238764
C	-3.8854454396	-5.0001161441	-0.7019524034
C	-4.0084063432	-6.4329254123	-0.2092257385
C	-3.2355533761	-6.5607009452	1.1011114141
O	-3.8464189504	-5.7281870039	2.0497284224
C	-3.7255473758	-4.3361999029	1.7338268291
O	-1.9284895293	-6.1372907373	0.8438327924
C	-0.7819588638	-6.9243894945	1.1289904799
C	0.0759133634	-6.7327011849	-0.1243121210
C	1.4995418650	-7.2105625622	0.0710177742
C	2.0463559473	-6.5917491364	1.3661530612
O	1.2468681134	-6.9396948437	2.4484582201
C	-0.0757136053	-6.4114239823	2.3848184803
O	2.0563297718	-5.1864558369	1.1974800756
C	3.3048651296	-4.5327110565	1.0996320918
C	3.1472110568	-3.4600475604	0.0356446475
C	4.4632076406	-2.7105282803	-0.1036997825
C	4.8628205335	-2.1345225197	1.2612721701
O	4.9290872943	-3.1607278272	2.2160285165
C	3.7129370993	-3.8866547555	2.4209555554
O	2.2740815412	-6.7852068223	-1.0356458850
C	3.3593766723	-7.6549926054	-1.3560256036

C 4.2660449553 -6.9874540252 -2.3770662688
O 4.8682833949 -5.8278996549 -1.8337830945
O -0.5093605937 -7.3730434802 -1.2382695505
O -3.4795620379 -7.2754151190 -1.2199911264
C -4.0335615008 -8.5959170143 -1.2349131881
C -2.9625300111 -9.6206910865 -1.5750929921
O -1.9727878334 -9.6423043906 -0.5668955930
O -4.6356768840 -4.8159310803 -1.8873440889
O -2.5756851843 -1.2465481089 -1.8773536327
C -2.6279753867 -1.9314951566 -3.1146397033
C -1.2432538415 -2.4592337147 -3.4539876427
O -0.3524276554 -1.3506182807 -3.5284255952
O -2.9151070846 1.3608214114 -0.8451006875
O -4.8635475190 3.4136266743 -0.3374913767
C -4.8959553712 4.4436305823 -1.2977165096
C -5.3048106720 3.7755667108 -2.6038157350
O -4.4148762827 2.6869664301 -2.8774201488
O -2.7411302883 5.1451832645 0.7663954245
O -1.6422138482 3.9531430047 3.1157052547
C -1.0262328490 4.7886198988 4.0513414794
C 0.0506847637 5.5978868321 3.3219420296
C 1.1176216650 4.6590609846 2.7806079789
C 1.6310904035 3.6869123076 3.8365372556
C 0.4916534076 3.0485618815 4.6249280916
O -0.4241577094 4.0465451180 5.0802222821
O -0.5332628069 6.2937732875 2.2328133554
C -0.4822237155 7.7162860334 2.2666373475
C 0.9164577280 8.2830723908 2.0130709293
O 1.4916750569 7.6643935987 0.8794836011
O 2.1605279393 5.4548101275 2.2773393430
O 2.3391189061 2.6450126019 3.1711715869
C 3.7386448356 2.6816153832 3.1543189109
C 4.2362834423 2.5444140624 1.7118036452
C 3.8514724542 1.1784764750 1.1639651179
C 4.4072665145 0.1059245681 2.0916498504
C 3.9633319489 0.3240515172 3.5369691585
O 4.2818065716 1.6576932725 3.9441005237
O 3.7168533101 3.6087935802 0.9402873672
C 4.5996192635 4.0980204011 -0.0717156654
C 4.0994586681 5.4399611933 -0.5659290528
O 4.1841002048 6.3252619484 0.5336777657
O 4.3547941602 1.0454160497 -0.1399453937
O 3.9318333068 -1.1486281217 1.6085916419
O 4.3909023930 -1.6522995605 -1.0399371020
C 4.6584555805 -1.9943521035 -2.3983039915
C 3.5371015943 -1.5086385399 -3.3185987856
O 2.2579282067 -1.8748411710 -2.8118180626
O 2.7867962270 -4.0383136269 -1.2174123263
C 3.9938148948 -4.9111201104 3.5050375609
O 4.9386191547 -5.8693672625 3.0871279042
C 4.7113850979 -0.5678797634 4.5145020445
O 6.0957303598 -0.3260647341 4.4721671632
C 0.9639488510 2.3270010498 5.8731526957
O -0.0974169935 1.6913067646 6.5365140901
C -3.8648027710 3.1696450438 5.1323871255
O -4.5107668434 4.3871962223 5.4194288660
C -6.9641730112 -0.3272277849 1.4848874780
O -7.7729558685 0.4452174149 0.6239861097

C	-4.3883635404	-3.5996818961	2.8828850360
O	-5.7856272194	-3.7548971315	2.9061312790
C	-0.7669541285	-6.8034702164	3.6705976597
O	-0.2078080031	-6.0293578510	4.7053695079
C	5.3749969037	-7.9289515098	-2.8040616868
C	-0.7624602953	-3.5036412260	-2.4597951143
C	-6.7190025523	3.2273165073	-2.5680240286
C	0.8529496184	9.7791947000	1.7810601701
C	4.9340194903	5.9228785257	-1.7433254344
C	-3.5717106859	-11.0071684552	-1.6841541994
C	3.5563618077	-0.0070116695	-3.5268951158
H	3.0540401182	-6.9524661995	1.6004835139
H	1.5190345860	-8.3057819476	0.1533569339
H	0.1149841301	-5.6478272399	-0.3034888997
H	-1.0568166841	-7.9834546022	1.2337832343
H	-3.2569135305	-7.5808951223	1.5013460266
H	-5.0660734609	-6.6689419710	-0.0309853791
H	-2.8219219555	-4.8008012615	-0.8900598196
H	-5.4384083283	-4.0259043511	0.4475375181
H	-5.0497332322	-2.6260832726	-1.6531789584
H	-4.4105535124	-0.3384845455	-2.2008537436
H	-2.8804195319	-0.2090623060	0.4237188334
H	-5.4984125746	1.1776730289	-0.2586985773
H	-6.2900123661	2.4215264606	1.5904339504
H	-5.2659799305	4.6466521961	1.2748589783
H	-2.6684415797	3.0852383405	1.0313239760
H	-3.4289919303	5.0065186939	3.2580624514
H	-1.7583333888	5.4427567758	4.5382250999
H	0.5062162188	6.2991764741	4.0326556884
H	0.6517241574	4.0550737989	1.9877212851
H	2.2996724363	4.2313389816	4.5198377461
H	4.1072585182	3.6183039610	3.5878336105
H	5.3334420495	2.6138220006	1.7389445580
H	2.7518714202	1.1009870780	1.1784700928
H	5.5049010471	0.1283642195	2.0613378270
H	5.8722107168	-1.7127693723	1.2092755811
H	5.2463371218	-3.4213172764	-0.4022598230
H	2.3612739963	-2.7590906353	0.3464077009
H	4.0876611102	-5.2363001630	0.7877251455
H	2.9168310713	-3.2067260564	2.7550905206
H	2.8808219428	0.1496768941	3.6143927611
H	-0.0359173427	2.3389423566	3.9753354279
H	-3.2374898276	1.9728450822	3.4589593049
H	-5.0042197351	-1.1641807655	1.6225293378
H	-2.6631592181	-4.0640599580	1.7009171523
H	-0.0344187164	-5.3157076837	2.3345922069
H	-1.4300938437	-7.0586804528	-1.2935455972
H	2.8059279896	4.9032293342	1.7879596898
H	2.3171584734	-4.8824738400	-1.0472851621
H	-4.4080495231	-5.5616469738	-2.4581482694
H	-3.5573105905	1.9058890227	-1.3509351842
H	-1.9143201927	5.4010709466	1.2130073390
H	4.2924443765	0.1063258643	-0.3922933712
H	2.9571150140	-8.5958316705	-1.7557599373
H	3.9511473916	-7.8787763820	-0.4570558204
H	3.6506447927	-6.7257489303	-3.2536722359
H	6.0279932631	-7.4255351171	-3.5200359619
H	4.9736035010	-8.8319435251	-3.2720320628

H	5.9817441183	-8.2199187795	-1.9409606561
H	4.1687842620	-5.1670632534	-1.7188989255
H	-2.9738612383	-1.2496683302	-3.9067704494
H	-3.3146819728	-2.7883521628	-3.0665763294
H	-1.3197974162	-2.9219971114	-4.4500931840
H	0.2699925688	-3.7968745490	-2.6698866314
H	-1.3759821760	-4.4057680607	-2.5383247214
H	-0.8319589170	-3.1253014533	-1.4364928136
H	0.5796794714	-1.6422003465	-3.4331140541
H	-3.9143854994	4.9248251224	-1.3871433262
H	-5.6270399956	5.2183459346	-1.0197821253
H	-5.2279085728	4.5223008580	-3.4070620260
H	-6.9437166830	2.7080482723	-3.5025412799
H	-7.4404559334	4.0393778307	-2.4392471232
H	-6.8445669947	2.5286702235	-1.7369092386
H	-3.6841137976	3.0215745769	-3.4144243527
H	-0.8792653247	8.0961166213	3.2194366257
H	-1.1549716389	8.0375427943	1.4650279902
H	1.5465601423	8.0783816918	2.8931453366
H	0.4132050710	10.2977261837	2.6381339202
H	0.2491397972	10.0000006329	0.8947846094
H	1.8578844929	10.1750666231	1.6178697410
H	1.6892865535	6.7552314070	1.1880890504
H	4.2978051653	-0.4099448694	5.5213673795
H	4.5608705396	-1.6149932331	4.2407844302
H	6.2124394931	0.6032810912	4.7033620484
H	1.6860188088	1.5569350272	5.5882619375
H	1.4818626881	3.0503774524	6.5235005732
H	-0.7070261431	2.3894799808	6.8015795967
H	4.6579323915	3.3731900021	-0.8893236127
H	5.6036080247	4.2379713714	0.3533981352
H	3.0509798627	5.3237537983	-0.8857444230
H	5.9862400108	6.0070817474	-1.4546046920
H	4.5939617041	6.9096202243	-2.0673239343
H	4.8549614543	5.2447319487	-2.5991537106
H	3.5933820533	7.0772061921	0.3899860147
H	-4.3782420339	2.3154038014	5.5970824593
H	-2.8569973409	3.2263706785	5.5537068915
H	-5.3935124014	4.3218649030	5.0360492899
H	-4.8562107483	-8.6292735838	-1.9618873974
H	-4.4364061586	-8.8441132124	-0.2450803406
H	-2.5162522109	-9.3428253768	-2.5430656572
H	-4.3457683779	-11.0503865998	-2.4559345736
H	-4.0132936231	-11.3030102769	-0.7271798009
H	-2.7920674491	-11.7309167068	-1.9298421374
H	-1.2761835508	-9.0169900226	-0.8271257455
H	-7.4391118718	-1.2803792196	1.7548322892
H	-6.8249271666	0.2509919886	2.4026338423
H	-7.9106438015	-0.0834902157	-0.1705494300
H	4.7795917709	-3.0780138164	-2.4923748079
H	5.6021529397	-1.5278540525	-2.7088044075
H	3.7065355964	-1.9985058412	-4.2911293399
H	4.4838920398	0.2962462446	-4.0210374396
H	3.4856141384	0.5291155016	-2.5753069145
H	2.7265390745	0.2908347656	-4.1748549023
H	2.3418108403	-2.7158726386	-2.3194519756
H	-3.9208536121	-3.9446069592	3.8162530096
H	-4.1846879541	-2.5313398535	2.7856414347

H	-5.9625615229	-4.6914805506	3.0491984837
H	4.3209549661	-4.3836387000	4.4121663392
H	3.0690801754	-5.4468594068	3.7406073427
H	5.7613299682	-5.3960520252	2.9157869219
H	-1.8469222889	-6.6179464993	3.5628354522
H	-0.6147897561	-7.8820441139	3.8281289355
H	-0.4750587999	-6.4097316871	5.5468811960
H	-1.3778901894	1.1340684819	-1.4988444553
H	-0.6270127915	0.0405844949	-2.5106894233
H	0.3857531340	0.8531463159	0.1231531812
H	-0.3358214644	-0.6861800327	-0.4066617719
H	1.2507498071	-0.1913813048	-1.0550587160
H	0.1412189453	6.9497391419	-1.0804418895
H	1.7661692960	8.6268811561	-1.7769649815
H	0.7625617831	4.8350271870	-4.7818361000
H	-0.6483147930	0.6551637688	-4.7689777273
H	-2.1884457541	1.5164462112	-6.4990601280
H	-3.0702530811	3.8400396094	-6.3219190564
H	-2.3652845930	5.2782697975	-4.4337372888
H	-1.5885551357	5.2796672325	-2.0694322590
H	0.2416999221	4.6345754061	-0.4559916078
H	-1.0043279334	3.4235938500	-0.7078295141
H	1.6547311765	3.4877883643	-2.2374922977
H	1.4317226733	2.4971618694	-0.8215907438
H	1.1191375818	1.3665264349	-3.0824104397

255

2-HP-B-CD:trans-(1R,4S)-SRT_2_MD E(Ha)= -7253.91935893

C	2.3655921231	0.9156948779	4.7149394257
C	2.3882332912	-0.4600037505	5.3287534259
C	1.1767210460	-1.1666907515	5.2263783528
C	-0.02111156842	-0.4598844566	4.6228157307
C	-0.1207975393	0.9244359691	5.2802354742
C	1.1783573633	1.7534823194	5.1996245278
C	3.5072078879	-1.0819228010	5.8840072869
C	3.4284447974	-2.3990322484	6.3422884006
C	2.2294693576	-3.0986412595	6.2373563108
C	1.1095922960	-2.4805978870	5.6846152609
C	0.0490982369	-0.4628244400	3.0971595922
C	0.2777671672	-1.6750140463	2.4334215212
C	0.3566671475	-1.7272846043	1.0497028793
C	0.2220891460	-0.5687260972	0.2892511021
C	-0.0289568966	0.6404245500	0.9354402507
C	-0.1267517290	0.6887983754	2.3287712761
Cl	0.3621836332	-0.6667681369	-1.4324073058
CI	-0.1985175217	2.1033012998	0.0284312379
N	3.6574970304	1.6596423854	4.8311457965
C	4.0717954972	2.1342999680	6.1693704194
C	2.7539023958	4.7900639219	2.9935932375
O	3.5165260372	3.5957206936	2.9605144913
C	1.8605470917	4.9504568793	1.7704785093
C	2.6782026464	5.1434686527	0.4944743996
C	1.9569302320	5.8410952409	-0.6595591899
C	1.0702025878	6.9791436687	-0.1771347602
C	0.2348541195	6.4989466883	1.0094235785
O	1.0786654230	6.1034013238	2.0592173685
O	-0.5623874206	5.4283977553	0.5861691870
C	-1.9739363405	5.4617967581	0.7292157630
C	-2.5265603707	5.0968619051	-0.6525697158
C	-4.0316946127	4.8950834311	-0.6101844048
C	-4.4285482875	3.9816589788	0.5555749896
O	-3.8932061229	4.4976564312	1.7604761630
C	-2.4515172405	4.4540322962	1.7693753666
O	-3.9463470438	2.6930408269	0.3314295671
C	-4.8387251096	1.5841648033	0.3933753405
C	-4.3582098606	0.6651345433	-0.7249737845
C	-5.1527858588	-0.6313585888	-0.7783776938
C	-5.3214937315	-1.2543107183	0.6195400429
O	-5.7197297819	-0.2848360610	1.5553387749
C	-4.8261976687	0.8165934168	1.7165736250
O	-4.4775062876	4.3254352177	-1.8175600073
C	-5.6808591925	4.8799214388	-2.3393466260
C	-6.4585892429	3.8077994241	-3.0848754506
O	-6.8501359443	2.7838689431	-2.1946035513
O	-2.2154026063	6.1117433190	-1.5732189955
O	0.1368194947	7.4151142103	-1.1484238365
C	0.6568664219	8.1678647118	-2.2458325981
C	-0.3784111434	8.2233693133	-3.3628556240
O	-0.6487062315	6.9248621244	-3.8813931126
O	2.9422406811	6.3272757781	-1.5407850799
C	3.1036399033	3.8510235690	0.0552489161
O	4.4101436291	3.7127960940	-0.4102932773
C	4.4355462074	3.0957935958	-1.8282895476
C	4.0574078306	1.6208648051	-1.7817270131

C 4.8948252965 0.9074945034 -0.7253857812
C 4.7458339851 1.5599130064 0.6413568609
O 5.1470839170 2.9374434113 0.5221240723
O 3.6114904785 3.9170723264 -2.6238237367
C 3.0485999487 3.4034497797 -3.8307926832
C 2.2014141447 4.4855148088 -4.4795040676
O 1.2037539804 4.8316103565 -3.5489315362
O 4.3097413904 1.0285850250 -3.0366679679
O 4.4362615989 -0.4330104610 -0.7310220300
C 5.3813729741 -1.4698276856 -0.6397805113
C 5.2077648080 -2.4216501497 -1.8267458599
C 3.9300364320 -3.2351601378 -1.7217566789
C 3.8029559271 -3.8450525940 -0.3251628442
C 3.9707487435 -2.7698373279 0.7411172013
O 5.2468564407 -2.1442559309 0.5787313239
O 5.2308613767 -1.6566739217 -3.0085546366
C 6.3073071804 -1.9266149838 -3.8998160497
C 6.5716196600 -0.6901929122 -4.7467626972
O 6.9222340022 0.4012179433 -3.9227131332
O 3.9583549225 -4.2342755471 -2.7011075833
O 2.5037931896 -4.4215151184 -0.2428044757
C 2.3766417486 -5.8065434953 -0.0880796980
C 1.3316246589 -6.3101639588 -1.0896669930
C -0.0219203528 -5.7238343953 -0.7355157360
C -0.3638842151 -5.9161341720 0.7354018693
C 0.7879437108 -5.4986762744 1.6480335910
O 1.9846827849 -6.1482743859 1.2207926536
O 1.7116609692 -5.9328284286 -2.3976846058
C 1.6604514203 -6.8972320906 -3.4547472376
C 0.6015518796 -6.5667836158 -4.5103691855
O -0.6976499934 -6.9302446559 -4.0883167178
O -0.9883565121 -6.3513400303 -1.5296960867
O -1.5172049345 -5.1106387856 0.9445379459
C -2.6510338402 -5.6204400046 1.5937087285
C -3.8472473186 -5.5887291016 0.6448705378
C -4.1761857627 -4.1540253957 0.2378090449
C -4.2421027558 -3.2246832637 1.4532680528
C -3.1225017893 -3.4439552807 2.4688192996
O -2.9159739246 -4.8452618006 2.7375666951
O -3.4929492832 -6.4037993528 -0.4598869697
C -4.5695010718 -6.9002844127 -1.2555244368
C -4.0295822208 -7.3838112970 -2.5930412264
O -3.3966976320 -6.2673341145 -3.2158942611
O -5.4170004860 -4.0977727638 -0.4164396716
O -4.1321767667 -1.8752502273 1.0299607942
O -4.5401304537 -1.5794729923 -1.6132151508
C -4.9278862777 -1.5526371912 -2.9747354915
C -4.2999288122 -2.7514837488 -3.6541464934
O -4.8483349793 -3.9099120641 -3.0455674827
O -4.4754741381 1.3171838948 -1.9775011508
C -5.3530266882 1.5467513842 2.9516011414
O -4.4755329065 2.5152406675 3.4782952301
C -3.4541246339 -2.8058380950 3.8039768897
O -2.3923156312 -2.8646020624 4.7318443949
C 0.5900163742 -5.8465185219 3.1231822318
O -0.2221198243 -4.9138606776 3.7935523739
C 3.9290045010 -3.2678364453 2.1633339665
O 3.8267008808 -2.1216114326 2.9872239773

C	5.6292894997	0.9462358803	1.7428652341
O	4.8997547711	0.3753323148	2.8093311923
C	-1.9701668491	4.6645152974	3.1952895181
O	-1.8483969405	3.4507534392	3.9050948577
C	-7.7042419751	4.3960085836	-3.7217883447
C	3.0044438628	5.6888417500	-4.9600884986
C	7.7087306052	-0.9413918631	-5.7196024958
C	0.6665624152	-5.1098822861	-4.9498399244
C	-3.0956320359	-8.5777816586	-2.4774505818
C	-1.6589208992	8.9503735624	-2.9816879713
C	-4.5696215351	-2.7474543275	-5.1505467644
H	-5.5184462692	3.9774167534	0.6769303204
H	-4.4969098975	5.8765200824	-0.4468042362
H	-2.0653193803	4.1424590033	-0.9495879153
H	-2.3095750474	6.4743072720	0.9983678798
H	-0.3794114411	7.3169458733	1.4026722110
H	1.6914751579	7.8236836344	0.1555481852
H	1.3188279568	5.1081615097	-1.1670669777
H	3.5589391072	5.7630314136	0.7272794639
H	4.9142404422	4.6847652349	-0.4382813878
H	5.4755754654	3.1487008335	-2.1912469578
H	2.9953378769	1.5204978413	-1.5094236109
H	5.9508105068	0.9482177582	-1.0341905651
H	6.3973646931	-1.0579911115	-0.6540830988
H	6.0501835467	-3.1261409525	-1.8101761537
H	3.0736740059	-2.5548009147	-1.8607000298
H	4.5719390276	-4.6210762627	-0.2003263430
H	3.3374208612	-6.3072020254	-0.2521093114
H	1.2826726133	-7.4041124754	-1.0052913341
H	0.0142846156	-4.6425747041	-0.9353478307
H	-0.6003774064	-6.9773808807	0.9041284127
H	-2.4705933750	-6.6431084905	1.9474395461
H	-4.7103019019	-6.0230681386	1.1703728440
H	-3.3686868290	-3.7869580313	-0.4080160546
H	-5.2138755113	-3.3911201011	1.9447806941
H	-6.1317162709	-1.9863918919	0.5838532102
H	-6.1658733010	-0.3914609028	-1.1387909449
H	-3.3050225946	0.4132020371	-0.5306952626
H	-5.8634603367	1.9200160526	0.1778495645
H	-3.8060418580	0.4632993322	1.9268147711
H	-2.1967151170	-3.0111342913	2.0757605068
H	0.9180861165	-4.4127051879	1.5817159842
H	3.1767253253	-2.0202504554	0.6223457087
H	3.6956764443	1.4966072913	0.9583469984
H	1.2235747891	4.0657744428	1.6533338338
H	-2.1239480314	3.4566249797	1.4613360405
H	-1.3080789973	6.4206273959	-1.3645304833
H	-1.8951212897	-6.1068309887	-1.2483633830
H	-4.0572738457	2.1908634079	-1.8906028431
H	3.1568956608	5.5703686069	-2.1170247629
H	4.2907223774	0.0591025026	-2.9189886184
H	3.1125070285	-4.7144805725	-2.6465287273
H	-5.2496059401	-3.8535242542	-1.3542601495
H	-5.4363367294	5.7240757283	-2.9991135835
H	-6.3160983853	5.2487940140	-1.5218858419
H	-5.8055884266	3.3999320319	-3.8730512809
H	-8.2561571331	3.6103901782	-4.2419561284
H	-7.4557780452	5.1845798134	-4.4381511456

H	-8.3621144413	4.8155423445	-2.9536619039
H	-6.1166058370	2.1466662655	-2.1586454729
H	2.4096538422	2.5453576279	-3.6042349046
H	3.8392425512	3.0785269893	-4.5171953954
H	1.7568851120	3.9999712716	-5.3670777077
H	2.3398890744	6.4134444415	-5.4416806031
H	3.7549762794	5.3866757811	-5.6972334284
H	3.5132766241	6.1938495284	-4.1353793079
H	0.6630047093	5.5745802104	-3.8747628321
H	6.0612582378	-2.7962956683	-4.5234528809
H	7.2189075853	-2.1496307856	-3.3276483968
H	5.6540848682	-0.4634048443	-5.3135334136
H	7.4890364601	-1.7802392190	-6.3865459346
H	8.6325548400	-1.1592171469	-5.1742134541
H	7.8788760058	-0.0483258867	-6.3245379770
H	6.0930835750	0.8071219482	-3.6240880487
H	1.4671976125	-7.8961255270	-3.0463751658
H	2.6507063608	-6.8983671091	-3.9261873406
H	0.8337844991	-7.2099055161	-5.3705578427
H	0.4409719521	-4.4484703308	-4.1086548418
H	-0.0656374234	-4.9295399606	-5.7404411107
H	1.6600966305	-4.8479729641	-5.3292889066
H	-0.7972742755	-6.6195310698	-3.1638107717
H	-3.6740015336	-1.7496062118	3.6303407231
H	-4.3620166645	-3.2784068521	4.2071196815
H	-2.2723225772	-3.7858280423	4.9863059903
H	0.2112945768	-6.8758605851	3.2227709047
H	1.5733577233	-5.8170225539	3.6025738358
H	-1.1155534186	-4.9306774079	3.4132362177
H	-5.3092649563	-6.1111921142	-1.4042992279
H	-5.0577456761	-7.7401791374	-0.7398095911
H	-4.9108634485	-7.6790738894	-3.1847053757
H	-2.6804273650	-8.8381653883	-3.4557225365
H	-3.6456562388	-9.4454596291	-2.1013185034
H	-2.2618484238	-8.3670691761	-1.8052235393
H	-2.7434403332	-6.5663853604	-3.8685554586
H	3.0637761690	-3.9250347617	2.2986638114
H	4.8430715954	-3.8409457426	2.3753017048
H	3.7201173201	-2.3776446645	3.9123478513
H	1.5716487601	7.6975650050	-2.6107576232
H	0.8943079383	9.1877679951	-1.9079115313
H	0.1060377995	8.7689590659	-4.1831214479
H	-1.4396778487	9.9754421472	-2.6685487252
H	-2.1728307065	8.4394692973	-2.1631061853
H	-2.3333006496	8.9898719154	-3.8409551072
H	-1.3427248585	6.5131564350	-3.3405766776
H	6.3224813930	0.2071356249	1.3274676852
H	6.2332389857	1.7605364872	2.1560996715
H	4.6592399008	-0.5592235728	2.6373854657
H	-4.5962932814	-0.6266713431	-3.4585724027
H	-6.0239221490	-1.6210591252	-3.0625701511
H	-3.2150712908	-2.7077900634	-3.4707055639
H	-4.1268131388	-3.6310765434	-5.6193501312
H	-4.1430069911	-1.8612906132	-5.6305672103
H	-5.6466926566	-2.7688194162	-5.3422000500
H	-4.2953310479	-4.6907448692	-3.2460793518
H	3.4036544718	5.6712021876	3.0857287863
H	2.1272010852	4.7453713189	3.8890357369

H	4.0652546703	3.5545739943	2.1579750456
H	-6.3390460592	1.9796941348	2.7286693250
H	-5.5061306768	0.7890092513	3.7253832885
H	-4.4892755316	3.3088280989	2.9136988612
H	-0.9716222129	5.1110142956	3.1706868878
H	-2.6435871317	5.3723228032	3.7023213548
H	-2.7128821611	3.0009655237	3.9050432037
H	4.3731049452	1.0736988720	4.3515821243
H	3.5915296455	2.4782384108	4.1762837791
H	5.1173493120	2.4416919370	6.1216979226
H	3.4621214860	2.9902671588	6.4566067205
H	3.9528103462	1.3426152952	6.9079035365
H	0.3663025348	-2.5940537225	3.0075131931
H	0.5388789833	-2.6642323024	0.5336230323
H	-0.3714715206	1.6414275257	2.7913283510
H	4.4637774797	-0.5702086196	5.9475300214
H	4.3037607552	-2.8693991804	6.7802980941
H	2.1627027838	-4.1235382145	6.5894301634
H	0.1804588555	-3.0305466258	5.5756268930
H	-0.9140859257	-1.0365488928	4.8934886196
H	-0.9439833525	1.5092913095	4.8640409649
H	-0.3674466112	0.7504433214	6.3313459930
H	1.0452966606	2.6020488684	4.5202606559
H	1.3949841702	2.1656340715	6.1902864937
H	2.2646012861	0.7736309791	3.6319741098

2-HP-B-CD:trans-(1R,4S)-SRT_3_MD E(Ha)= -7253.92106006

C	0.5852854777	-1.7634235740	2.4505580499
C	-0.3400985504	-2.5324505843	3.3862898080
C	-0.6422003814	-3.8922375929	3.1786804819
C	-0.1249691163	-4.6293649935	1.9569956568
C	1.1622535937	-3.9799477653	1.4463471388
C	0.9447109256	-2.5089759802	1.1725879878
C	-0.8604966542	-1.8795351352	4.5119118703
C	-1.6930180448	-2.5388401527	5.4101030858
C	-1.9997212595	-3.8824185850	5.2028070917
C	-1.4695525246	-4.5439398958	4.1006117307
C	0.0942360936	-6.1147864392	2.1358206389
C	-0.4149762215	-7.0144909976	1.1948509596
C	-0.1302425736	-8.3729469093	1.2827794732
C	0.6673980989	-8.8629607364	2.3150839793
C	1.1751821982	-7.9715937027	3.2679745796
C	0.8880186224	-6.6127328960	3.1706256674
Cl	1.0024304233	-10.5545039075	2.3945106156
Cl	2.1662924321	-8.5241833106	4.5712599542
N	-0.0394515330	-0.4499958864	2.1017713976
C	0.7169449592	0.4052200774	1.1637005139
C	1.3173897297	-2.0059553961	-4.6013568324
C	2.3661135960	-2.9251632968	-3.9791788679
C	1.7726249282	-4.1796760039	-3.3422604053
C	0.6177665592	-4.7764021242	-4.1403528736
C	-0.3473384017	-3.6854313648	-4.6106281309
O	0.3625674159	-2.7464407183	-5.3645252473
O	-0.9127627903	-3.0643049831	-3.4794351724
C	-2.2715581379	-3.3215873375	-3.1641454568
C	-2.3176507933	-3.4227060843	-1.6472980365
C	-3.7510394450	-3.4852856456	-1.1582083715
C	-4.5319855231	-2.2965742085	-1.7496532021
O	-4.4927980331	-2.3655425224	-3.1439984428
C	-3.1768153509	-2.2073422444	-3.6883482781
O	-3.9660940193	-1.0665707182	-1.3591274401
C	-4.4209732258	-0.4485344310	-0.1711025308
C	-3.1862460713	0.0433649137	0.5736967668
C	-3.5586752645	0.9587472174	1.7364708974
C	-4.5148399061	2.0590240428	1.2442972899
O	-5.6451667347	1.4753712064	0.6421833045
C	-5.3604977583	0.7032964491	-0.5222902780
O	-3.7848885249	2.8568776146	0.3564074735
C	-4.1929456336	4.2114185648	0.1996190077
C	-3.6858152883	5.0562542815	1.3629679735
C	-3.6957149313	6.5335971969	1.0038391294
C	-2.8704590482	6.7296380968	-0.2651139538
O	-3.5101154424	6.0530870648	-1.3116953219
C	-3.5588825222	4.6348849292	-1.1376270430
O	-1.6036766312	6.1905201626	-0.0124750309
C	-0.4094881265	6.9247087990	-0.2387851450
C	0.4170424407	6.6658988480	1.0175570047
C	1.8417966690	7.1599998161	0.8707956770
C	2.4394785851	6.5871765851	-0.4217548804
O	1.6430412372	6.9287836964	-1.5166176362
C	0.3093923312	6.4133246633	-1.4826533273
O	2.5134871456	5.1812128816	-0.2917063716
C	3.7912273537	4.5946695745	-0.1102211745

C	3.6309619546	3.5245818490	0.9585455729
C	4.9030013695	2.6993605438	1.0929569664
C	5.3625210805	2.1722148541	-0.2705068200
O	5.4925888783	3.2470476096	-1.1676099144
C	4.2915138579	3.9807231136	-1.4151462251
O	4.4465781067	1.2148898831	-0.7125795503
C	4.9509096460	-0.0157511980	-1.2356810111
C	4.1347695837	-1.1225865770	-0.5780853357
C	4.5668404366	-2.4522563874	-1.1769607296
C	4.3576286956	-2.3932689981	-2.7002438089
O	5.1644682449	-1.3658479689	-3.2341793929
C	4.8658261772	-0.0531559741	-2.7615445687
O	3.0081751171	-2.1579023966	-2.9662015211
O	3.8739024977	-3.5168642846	-0.5712280743
C	4.6113776183	-4.7227130962	-0.6010541848
C	3.8517884924	-5.8283680782	0.1035861003
O	2.6524427570	-6.0653876752	-0.6340872573
O	4.3334099655	-1.1281337432	0.8142365730
O	4.7312307407	1.5927391768	1.9598341740
C	4.8978493971	1.8575428924	3.3503407601
C	3.6757251727	1.4257896126	4.1618653586
O	2.4771771689	1.9792817812	3.6333236588
O	3.3334089000	4.0971502088	2.2219200861
O	2.5733630652	6.7062226300	1.9984968093
C	3.4174244375	7.6252912943	2.6766084585
C	4.8584807248	7.5577459308	2.2030651289
O	4.8529146034	7.9827812675	0.8520227179
O	-0.1834472229	7.2531547227	2.1536015095
O	-3.1530067503	7.2481717641	2.1022946587
C	-3.6487674791	8.5876173558	2.2276838029
C	-2.5348917807	9.5416654088	2.6332912472
O	-1.5509720447	9.5953840649	1.6214658997
O	-4.4732492912	4.8229393863	2.5162474884
O	-2.3532246567	1.4768195885	2.2706324161
C	-2.4553669091	1.9650921131	3.5953706406
C	-1.1090759935	2.4896180338	4.0735598816
O	-0.1848090976	1.4063134354	4.1241764852
O	-2.3876107020	-1.0469830526	0.9876741355
O	-3.7060601348	-3.4630984641	0.2477407769
C	-4.8626398226	-3.8938303330	0.9262257752
C	-4.5132415224	-3.8930790200	2.3994145546
O	-4.0467470867	-2.5776136874	2.7087111247
O	-1.6123110475	-4.5749538914	-1.2057826911
O	-0.0450522797	-5.6933102460	-3.2838729020
C	-0.6582960256	-6.7966524418	-3.9440519005
C	-1.5380935274	-7.5480746766	-2.9565682802
O	-2.6588878005	-6.7817220919	-2.5756540177
O	2.8087700523	-5.1162026298	-3.1940877885
C	1.9120679922	-1.0009461778	-5.5683999277
O	0.9463964966	-0.0972849783	-6.0390738170
C	-3.3361419934	-2.2440663821	-5.1968647736
O	-3.7463948181	-3.5075705956	-5.6631152412
C	-6.6978548019	0.2212851590	-1.0537477502
O	-7.3089758799	-0.7183082636	-0.1959693581
C	-4.3385455663	4.1232311071	-2.3352883890
O	-5.6578549008	4.6071943646	-2.3528312786
C	-0.3307527944	6.8539263657	-2.7862548979
O	0.3312439440	6.3033383397	-3.8937500610

C	4.6597499516	5.0346171105	-2.4432253797
O	5.6669927465	5.9003616389	-1.9673211246
C	5.9056758750	0.8388737044	-3.4204230883
O	7.2110712640	0.4529076708	-3.0596520731
C	4.6868969119	-7.0939035942	0.2012956923
C	5.7643006329	8.4250321361	3.0622146199
C	-3.0881787293	10.9397963559	2.8456639760
C	-0.5786818126	3.6368384872	3.2305474260
C	-5.6936651437	-4.2733745679	3.2733685271
C	3.5221301833	-0.0815627370	4.2342267686
C	-2.0493459053	-8.8382108152	-3.5704532597
H	4.6957757357	-3.3153874241	-3.1805533103
H	5.6487879712	-2.5638417173	-0.9995722503
H	3.0742493091	-0.9595285546	-0.8282303909
H	6.0042033645	-0.1358558840	-0.9479651808
H	6.3645743122	1.7373574944	-0.1893689730
H	5.6997058397	3.3555030428	1.4716929274
H	2.8152457332	2.8580093935	0.6436692138
H	4.5148333282	5.3487169614	0.2243440557
H	3.4268305172	7.0174302813	-0.6005850548
H	1.8650316927	8.2553827604	0.8206233504
H	0.4634349715	5.5746648522	1.1476584275
H	-0.6297384634	7.9985511882	-0.3255361417
H	-2.8058986084	7.7825054815	-0.5612750904
H	-4.7291779681	6.8527103282	0.8150354635
H	-2.6473282943	4.7527723427	1.5441133598
H	-5.2860168645	4.2866415606	0.1288063718
H	-4.9073115320	2.6551184415	2.0718494725
H	-4.0934379503	0.3698204641	2.4981418499
H	-2.5745129526	0.6249216040	-0.1255863524
H	-4.9647322240	-1.1533515736	0.4678660407
H	-5.5909792581	-2.3419716590	-1.4656111719
H	-4.2247118152	-4.4140419429	-1.5163421282
H	-1.8650544138	-2.5211429882	-1.2137866112
H	-2.5933408813	-4.2808134101	-3.5913093129
H	-1.1327493021	-4.0816334682	-5.2648835790
H	1.0263397346	-5.2981254092	-5.0159167832
H	1.3777746222	-3.8644914851	-2.3666151104
H	3.0916860644	-3.2370549917	-4.7449369756
H	0.7981416515	-1.4705483596	-3.7981389579
H	-2.7647586528	-1.2360745946	-3.3884535239
H	-4.8781367826	1.3252919011	-1.2863816225
H	-2.5394447505	4.2292763190	-1.1589543282
H	0.3410187588	5.3164194343	-1.4512120404
H	3.5157584598	3.3185019432	-1.8230945017
H	3.8553006289	0.2511585576	-3.0684904596
H	4.4018535675	-0.1999848114	1.0950846789
H	-2.9492544053	-1.7269673192	1.4210384274
H	2.6443629412	-5.6181243466	-2.3766807335
H	2.9240413978	4.9814692852	2.0966783759
H	-1.1146526080	6.9655035765	2.1613311105
H	-4.2025249834	5.4946741339	3.1559486783
H	-0.8744141336	-4.7188381770	-1.8296702893
H	5.5743544906	-4.5879119817	-0.0850180450
H	4.8148636105	-5.0347530504	-1.6353211392
H	3.5911424807	-5.4732278580	1.1101041942
H	4.9705891249	-7.4482496678	-0.7943743505
H	4.1226474454	-7.8891485384	0.6991830947

H	5.5959674157	-6.9228324615	0.7852135802
H	2.1371627524	-6.7492123243	-0.1898535762
H	3.3688078645	7.3671726793	3.7391971232
H	3.0331495171	8.6457610236	2.5541556039
H	5.1725902909	6.5028124354	2.2736986101
H	5.4367686347	9.4685600426	3.0303142697
H	6.7943262203	8.3859680545	2.6949883761
H	5.7710937767	8.0897504084	4.1040395027
H	5.7101127763	7.8031243163	0.4512281665
H	-4.4640683715	8.5977206094	2.9634787803
H	-4.0474037771	8.9284307310	1.2644188337
H	-2.0959056123	9.1777146002	3.5758469074
H	-3.5152139881	11.3222929915	1.9131743722
H	-2.2804659131	11.6117114962	3.1427516966
H	-3.8614055579	10.9575380276	3.6193485742
H	-0.8749672860	8.9313833635	1.8372029691
H	-2.7884682329	1.1586601613	4.2676779077
H	-3.1826261962	2.7878159695	3.6555156983
H	-1.2782879113	2.8535142360	5.0992155032
H	-1.2375994609	4.5054430587	3.3149769451
H	-0.5137912910	3.3513277606	2.1774855178
H	0.4112083223	3.9482995352	3.5770130643
H	0.7411320962	1.7333256678	4.1214979376
H	-4.0382024897	-1.4505311266	-5.4904562563
H	-2.3698461876	-2.0276813640	-5.6629738347
H	-4.5898087123	-3.7010048707	-5.2369255714
H	-7.3380306089	1.0977816520	-1.2222454090
H	-6.5461221403	-0.2740222235	-2.0170560470
H	-7.4896723878	-0.2588379476	0.6322382878
H	-5.1522443344	-4.9083874652	0.6149122494
H	-5.7193731391	-3.2251079321	0.7428589249
H	-3.6893061025	-4.6060798308	2.5401555840
H	-6.0554918227	-5.2781704644	3.0343600383
H	-6.5152818300	-3.5637913522	3.1390424844
H	-5.4071776745	-4.2662069565	4.3293650307
H	-3.5633032806	-2.6255366763	3.5448176743
H	-3.7882978498	4.3950419321	-3.2478936982
H	-4.3910591193	3.0332442810	-2.2891890579
H	-5.5936939218	5.5677769415	-2.4087948371
H	5.0754762109	2.9267664279	3.4996031386
H	5.7753126525	1.3079280448	3.7154172061
H	3.8420119236	1.8092759127	5.1823128560
H	4.3567289258	-0.5250502966	4.7848942362
H	3.5017198553	-0.5267435307	3.2350504546
H	2.5995438348	-0.3383189974	4.7639213464
H	2.6885204592	2.8383577617	3.2037666772
H	-1.3670510937	6.5038407243	-2.8173541269
H	-0.3434829756	7.9559438354	-2.8176624705
H	1.2409146264	6.6191639726	-3.8492577128
H	0.1252364112	-7.4555509233	-4.3448232056
H	-1.2858294969	-6.4534826869	-4.7792301618
H	-0.9125641281	-7.7858918656	-2.0777411495
H	-2.7069914692	-9.3457479653	-2.8613533631
H	-1.2285658364	-9.5116783967	-3.8328947289
H	-2.6305863673	-8.6260127294	-4.4733421800
H	-2.3551578317	-6.0611781993	-1.9964184351
H	4.9656820752	4.5342850490	-3.3726241299
H	3.7789252629	5.6439246847	-2.6648121148

H	6.4431081276	5.3470915454	-1.8178257175
H	2.6825563166	-0.4225539648	-5.0516330931
H	2.3992624398	-1.5492400646	-6.3915436607
H	0.2601873539	-0.6349322237	-6.4512408746
H	5.7557147222	0.8034736281	-4.5093982909
H	5.7724153647	1.8697733669	-3.0835758556
H	7.3001727793	-0.4676421563	-3.3353909517
H	-0.9924746535	-0.6453975929	1.6976931854
H	-0.1969334767	0.1416453004	2.9437121500
H	0.1170031243	1.3032696561	1.0106645140
H	1.6781659079	0.6730011969	1.6059083906
H	0.8560324946	-0.1045833202	0.2120036164
H	-1.0430537542	-6.6453386262	0.3879892277
H	-0.5334278592	-9.0711715346	0.5564119729
H	1.2921949207	-5.9426626421	3.9233282034
H	-0.6106109539	-0.8384710629	4.7057726733
H	-2.0787168797	-2.0132604153	6.2786574842
H	-2.6305879463	-4.4180703478	5.9065117648
H	-1.6901735105	-5.5968743756	3.9502331556
H	-0.8807036632	-4.5112579090	1.1662164784
H	1.9627872177	-4.1083712089	2.1878254108
H	1.4965748296	-4.4727552326	0.5309618076
H	1.8571333841	-2.0889907575	0.7438002845
H	0.1317388580	-2.4046408307	0.4410646722
H	1.5067939172	-1.5294275731	2.9957887631

2-HP-B-CD:trans-(1R,4S)-SRT_4_MD E(Ha)= -7253.9144206290

C	0.77201456	-1.67064059	2.29032958
C	0.09242588	-2.41853671	3.43131722
C	-0.16022581	-3.80276721	3.36006928
C	0.17433223	-4.60593211	2.11683129
C	1.25056016	-3.90082565	1.29050218
C	0.85269119	-2.47190922	0.99984555
C	-0.25051886	-1.71971939	4.59693102
C	-0.86532776	-2.35862740	5.66908552
C	-1.13226964	-3.72476163	5.59413698
C	-0.77291075	-4.43037288	4.45127681
C	0.60962512	-6.03375348	2.36313508
C	0.09442948	-7.06812256	1.57586187
C	0.58473675	-8.36469973	1.69443673
C	1.59902985	-8.65674926	2.60538070
C	2.11254461	-7.63060787	3.40805519
C	1.61824844	-6.33499585	3.27991248
Cl	2.18942177	-10.27369085	2.72271927
Cl	3.36525351	-7.93618874	4.55719173
N	0.05298437	-0.38468549	2.02779043
C	0.58419742	0.41987413	0.90746159
C	0.35513759	-2.17380167	-4.48105576
C	1.54834387	-3.03022085	-4.06314459
C	1.14183575	-4.29185220	-3.30489729
C	-0.09048989	-4.96649757	-3.89839321
C	-1.18677002	-3.94961724	-4.22110226
O	-0.67237730	-2.97060820	-5.07570733
O	-1.62272540	-3.35442139	-3.02262493
C	-2.90530105	-3.68947177	-2.51493680
C	-2.71592308	-3.73513084	-1.00579568
C	-4.04358970	-3.80387610	-0.27613471
C	-4.95056889	-2.67856477	-0.80919515
O	-5.14555564	-2.85595044	-2.18169796
C	-3.94871059	-2.66024090	-2.94375132
O	-4.35771448	-1.41655524	-0.62122107
C	-4.63471121	-0.67490082	0.54898087
C	-3.30658911	-0.12653860	1.05482752
C	-3.52149235	0.90009076	2.16207946
C	-4.48900330	1.97663574	1.64792061
O	-5.70989557	1.38001925	1.28640416
C	-5.61549493	0.45021095	0.20868495
O	-3.83395839	2.58256028	0.56818128
C	-4.28535583	3.85624107	0.12949610
C	-3.79489908	4.95804950	1.06461797
C	-3.88624222	6.32038347	0.39343554
C	-3.12727651	6.27154140	-0.93111396
O	-3.75666695	5.34151189	-1.76325712
C	-3.67190126	4.00079149	-1.27382879
O	-1.81290718	5.87064274	-0.65674114
C	-0.70425094	6.72422456	-0.89767318
C	0.16444415	6.56855592	0.35120644
C	1.54246201	7.16275308	0.14486950
C	2.14243786	6.59262670	-1.14569220
O	1.31537472	6.90084203	-2.22869745
C	0.02942790	6.28010472	-2.16131278
O	2.24498968	5.19795972	-0.99042832
C	3.53210273	4.61476469	-0.89010020

C	3.45789252	3.57390581	0.21497044
C	4.77094364	2.80437718	0.27577352
C	5.10570585	2.22036217	-1.09998437
O	5.15265821	3.25626949	-2.04830133
C	3.91861305	3.95706830	-2.21320332
O	4.14351104	1.25542800	-1.40860699
C	4.56612820	0.01449544	-1.97433979
C	3.92023775	-1.08029843	-1.13060199
C	4.24291041	-2.42375686	-1.76650288
C	3.72862232	-2.41729975	-3.21606053
O	4.38450174	-1.39926607	-3.93747592
C	4.17330015	-0.07512563	-3.44962323
O	2.34552898	-2.21735348	-3.20936016
O	3.70038811	-3.47910199	-1.01081345
C	4.47253503	-4.65933877	-1.09897769
C	3.88615624	-5.74614274	-0.22122135
O	2.61518968	-6.10044165	-0.76441202
O	4.39469205	-1.03997868	0.19131203
O	4.72966005	1.74440688	1.21282912
C	5.02763324	2.10079867	2.55828713
C	3.92965348	1.63969514	3.51470552
O	2.65547577	2.11253838	3.09937798
O	3.19789330	4.16278919	1.47718982
O	2.37312070	6.80870567	1.23728399
C	3.20032611	7.85191602	1.73195652
C	4.40019083	7.25649926	2.43713392
O	5.18263937	6.63164120	1.43286576
O	-0.44530646	7.16489674	1.47847000
O	-3.32178787	7.26789914	1.28550721
C	-3.81290935	8.59904268	1.09296549
C	-2.80310632	9.61785367	1.60030763
O	-1.62969049	9.59257216	0.81931766
O	-4.54462348	4.94434200	2.26156617
O	-2.25465515	1.42490116	2.50709962
C	-2.18374184	2.01234048	3.79073416
C	-0.80154761	2.61131759	4.00631944
O	0.15125918	1.55406793	3.97878590
O	-2.43695737	-1.16445778	1.45152876
O	-3.76277970	-3.67432600	1.09668920
C	-4.78939217	-4.02226661	1.99502583
C	-4.19688796	-3.91126798	3.38563504
O	-3.70208109	-2.57582355	3.51865075
O	-1.90365343	-4.84728520	-0.65249405
O	-0.55645285	-5.90997592	-2.94635104
C	-1.20241659	-7.04335121	-3.51773849
C	-1.87204271	-7.85757511	-2.42102746
O	-2.95595067	-7.16565681	-1.84406473
O	2.23607796	-5.17105028	-3.30884858
C	0.70330214	-1.12917502	-5.52445019
O	-0.39517638	-0.30510873	-5.81359327
C	-4.34275239	-2.79273623	-4.40315199
O	-4.69991899	-4.10717485	-4.75685885
C	-7.02191321	-0.06897537	-0.02762422
O	-7.48972091	-0.84915019	1.05066642
C	-4.36174283	3.13935695	-2.31528508
O	-5.74833050	3.36039701	-2.37436361
C	-0.68101275	6.66369694	-3.44707259
O	0.02818128	6.22376870	-4.57303824

C	4.14015609	4.97288615	-3.31873659
O	5.06978546	5.96403530	-2.95314151
C	5.04322098	0.80093569	-4.33746271
O	6.39614767	0.42574049	-4.25086768
C	4.80412980	-6.95632961	-0.15968523
C	5.18287366	8.33245400	3.17357201
C	-3.38740130	11.01730548	1.51844970
C	-0.47442052	3.70323554	2.99947018
C	-5.20932107	-4.22626830	4.47140346
C	3.87027552	0.12949273	3.64830798
C	-2.41249736	-9.15999807	-2.98316124
H	3.98021445	-3.35241576	-3.72365373
H	5.33959410	-2.52025495	-1.80910826
H	2.82835129	-0.93510324	-1.16710068
H	5.65870587	-0.07453694	-1.90114029
H	6.10893149	1.77973678	-1.09329659
H	5.57351967	3.50825194	0.53802827
H	2.65352469	2.86547234	-0.03114047
H	4.28039160	5.37212580	-0.62442034
H	3.12246419	7.03203645	-1.36362542
H	1.46456518	8.25428455	0.06052037
H	0.29144832	5.49019649	0.52208448
H	-1.03063823	7.77165549	-0.97987339
H	-3.14615487	7.23225983	-1.45902657
H	-4.94043454	6.56249189	0.19955495
H	-2.73435874	4.75416708	1.27070735
H	-5.38063088	3.88005154	0.05992731
H	-4.74540462	2.71206319	2.41450529
H	-3.98395987	0.40650637	3.03146958
H	-2.81064188	0.38370780	0.22150555
H	-5.08516457	-1.30197905	1.32759770
H	-5.94410860	-2.71565024	-0.34515578
H	-4.53846738	-4.76658035	-0.48399060
H	-2.22678571	-2.80413127	-0.69097608
H	-3.21925961	-4.68235087	-2.86332489
H	-2.02915107	-4.41257449	-4.74840646
H	0.20674337	-5.47606755	-4.82515863
H	0.89429691	-3.96964176	-2.28337378
H	2.12054037	-3.32995772	-4.95386867
H	-0.04637791	-1.67090032	-3.59267548
H	-3.55515814	-1.65206773	-2.76848966
H	-5.26834829	0.95634896	-0.69931640
H	-2.61744430	3.70440208	-1.20775130
H	0.15319708	5.19065896	-2.13266942
H	3.12530927	3.25837785	-2.51391859
H	3.11599599	0.20754794	-3.55245024
H	4.43665513	-0.10514433	0.45307944
H	-2.90250780	-1.79829510	2.04147181
H	2.25536762	-5.64006511	-2.45664589
H	2.85867966	5.07425063	1.35927469
H	-1.38681508	6.91288044	1.46688948
H	-4.29325251	5.74362908	2.74133380
H	-1.24375689	-4.95082267	-1.36447086
H	5.50094464	-4.46179128	-0.75983084
H	4.51648235	-5.02722149	-2.13456305
H	3.74561052	-5.33104925	0.78653186
H	4.97897535	-7.36130004	-1.16128044
H	4.35840157	-7.74590704	0.45379475

H	5.76852983	-6.69854287	0.28793012
H	2.19667427	-6.75641821	-0.19480928
H	2.62260335	8.47877526	2.42385704
H	3.56603991	8.47797113	0.90691457
H	4.03448357	6.50629623	3.15824786
H	5.52372770	9.10587454	2.47830877
H	6.06517268	7.90257326	3.65943590
H	4.57751357	8.80306602	3.95401938
H	6.00234382	6.33363578	1.83890551
H	-4.77468132	8.70225281	1.61441650
H	-3.97642263	8.78956453	0.02420392
H	-2.57549763	9.37944946	2.65233417
H	-3.61605444	11.27066016	0.47821989
H	-2.65565595	11.74031484	1.88464490
H	-4.30114572	11.11173092	2.11221419
H	-1.07050145	8.86196285	1.13330298
H	-2.38022927	1.25445996	4.56523631
H	-2.92603576	2.81615447	3.90280271
H	-0.81296078	3.04992432	5.01653849
H	-1.14857024	4.55481355	3.13027567
H	-0.58373188	3.33413144	1.97641935
H	0.54542290	4.07443045	3.13619273
H	1.06047020	1.89616264	3.82515622
H	-5.15358125	-2.07827805	-4.60591886
H	-3.48815532	-2.51466195	-5.02790148
H	-5.45545779	-4.35254656	-4.21085125
H	-7.67859195	0.78850093	-0.22835591
H	-7.02620928	-0.70720960	-0.91598577
H	-7.51619952	-0.26613260	1.81791641
H	-5.13740241	-5.05179759	1.82316238
H	-5.65933454	-3.35158794	1.90723006
H	-3.35167965	-4.61079304	3.43884913
H	-5.59605626	-5.24472309	4.36673156
H	-6.04944625	-3.52678011	4.42946380
H	-4.74880166	-4.14551954	5.46069798
H	-3.05108836	-2.57223348	4.23317251
H	-3.87326881	3.32185918	-3.28338349
H	-4.21204369	2.08712401	-2.06080402
H	-5.87527899	4.27287826	-2.65639125
H	5.14011196	3.18711926	2.63175172
H	5.97618051	1.63289656	2.85474380
H	4.18386602	2.06931167	4.49827516
H	4.78899533	-0.25038186	4.10477532
H	3.75582971	-0.34785243	2.67035350
H	3.03444159	-0.16072676	4.29262766
H	2.77002617	2.94619063	2.58981142
H	-1.66290708	6.17997111	-3.47113147
H	-0.83586036	7.75577532	-3.45760099
H	0.89092613	6.65146945	-4.53484558
H	-0.45550633	-7.65160599	-4.04793173
H	-1.97376868	-6.73214117	-4.23679217
H	-1.10245131	-8.08222823	-1.66079564
H	-2.90664205	-9.72472365	-2.18948562
H	-1.61611282	-9.77640210	-3.40962019
H	-3.15472446	-8.95617006	-3.76140522
H	-2.61325853	-6.42366010	-1.31789000
H	4.44561422	4.44033583	-4.23092524
H	3.19276404	5.47890225	-3.52638986

H	5.90841012	5.51606791	-2.79468036
H	1.50359790	-0.49093365	-5.14067210
H	1.08284437	-1.64109676	-6.42410611
H	-1.10065996	-0.89592924	-6.10067670
H	4.66498464	0.73460497	-5.36842257
H	4.97853393	1.84132567	-4.00996871
H	6.42823088	-0.50471266	-4.50339429
H	-0.95676430	-0.62385815	1.84398188
H	0.04971268	0.25105109	2.85470497
H	0.00290146	1.34143768	0.86961210
H	1.63491234	0.65281009	1.09036715
H	0.46927962	-0.11765174	-0.03259541
H	-0.69961218	-6.85486147	0.86449106
H	0.17875221	-9.16813303	1.08813390
H	2.03430563	-5.55645726	3.91245557
H	-0.03370982	-0.65721334	4.68321218
H	-1.11371322	-1.79645353	6.56460045
H	-1.59534353	-4.24249604	6.42946840
H	-0.95769371	-5.49996579	4.40098005
H	-0.73601396	-4.64302103	1.49972940
H	2.20361519	-3.91291158	1.83617579
H	1.42142780	-4.43943656	0.35619192
H	1.58973652	-2.02807058	0.32742421
H	-0.12547729	-2.45988494	0.50096929
H	1.78590031	-1.39578092	2.60382546

2-HP-B-CD:trans-(1R,4S)-SRT_5_MD E(Ha)= -7253.9064352402

C	-0.40836972	0.89708724	3.68927846
C	-0.82843860	2.06784203	4.54581660
C	-1.11393500	3.32382699	3.99261789
C	-1.16584349	3.55756001	2.49664216
C	-0.42588886	2.45934206	1.71239863
C	-0.77512609	1.06381822	2.21767387
C	-0.96541091	1.88205764	5.93006867
C	-1.32083265	2.92940717	6.76709662
C	-1.55887605	4.19023068	6.22063642
C	-1.46905127	4.37327548	4.84868408
C	-2.60772166	3.70847175	2.02912525
C	-2.92406484	4.59874817	0.99912104
C	-4.22485396	4.70940471	0.52084685
C	-5.23708058	3.92694864	1.07099343
C	-4.94115364	3.04444025	2.11230325
C	-3.63605577	2.94738780	2.58582497
Cl	-6.84575651	4.06256705	0.44052035
Cl	-6.16753778	2.06396100	2.83873112
N	1.08521933	0.61794594	3.75857102
C	1.83288660	0.94494339	4.98929985
O	3.06737273	1.33647100	2.04743746
C	3.59666228	0.38678467	1.13696665
C	3.97370389	-0.91981210	1.82942786
C	4.60562637	-1.87800276	0.80082155
O	5.70733242	-1.27590795	0.16944505
C	5.39067906	-0.08032146	-0.54453020
C	4.82982936	0.93939655	0.44049002
O	3.58250448	-2.20454808	-0.09373006
C	3.86390555	-3.19772978	-1.06600012
C	3.73926575	-4.58995536	-0.45132612
C	3.66354130	-5.66221866	-1.52576208
C	2.52430192	-5.31688787	-2.48328403
O	2.81264070	-4.09253951	-3.08972147
C	2.82414633	-2.98619435	-2.18251390
O	1.34517477	-5.21370026	-1.73585430
C	0.28452411	-6.15575076	-1.83103086
C	-0.09286182	-6.40922611	-0.36395877
C	-1.48248724	-6.99022840	-0.17430698
C	-2.46938257	-6.20374199	-1.04836699
O	-2.07666467	-6.23584308	-2.39067763
C	-0.86471367	-5.51439549	-2.60493250
O	-2.43376669	-4.89827363	-0.55914535
C	-3.58885649	-4.14476083	-0.24192460
C	-3.03240403	-3.20983593	0.82071607
C	-4.00176439	-2.11081215	1.20469091
C	-4.41079353	-1.40033118	-0.10096084
O	-4.99046423	-2.33334421	-0.98008174
C	-4.09930318	-3.34905165	-1.43659720
O	-3.24784066	-0.81165317	-0.63384413
C	-3.39794016	-0.09377568	-1.85366230
C	-3.91680918	1.32044009	-1.61514550
C	-3.82324985	2.12464208	-2.90682661
C	-2.40540610	2.08190137	-3.48132549
O	-2.02419248	0.75730133	-3.67897024
C	-2.00110965	-0.03268530	-2.49178887
O	-1.53768087	2.74710929	-2.60002602

C	-0.70091163	3.77304683	-3.10579512
C	-0.85407364	4.92280040	-2.11436840
C	0.08000765	6.07858265	-2.41723106
C	1.51027442	5.55330730	-2.64521288
O	1.49585596	4.51828071	-3.60406529
C	0.76338342	3.35846434	-3.20188454
O	-4.26238428	3.43691344	-2.61000152
C	-4.69445330	4.19434029	-3.73089150
C	-5.50582803	5.39547540	-3.26453796
O	-4.80472083	6.19432448	-2.33530274
O	-5.25326191	1.24867324	-1.18506104
O	-3.38567577	-1.19899432	2.08659638
C	-3.83852774	-1.15410827	3.42483380
C	-3.19639262	-2.21440644	4.32820858
O	-1.80951707	-2.32141618	4.02204316
O	-2.61869836	-3.97554711	1.94857887
O	-1.84292264	-6.83154844	1.18435858
C	-2.74768430	-7.81622157	1.67011608
C	-3.48596195	-7.27417211	2.88498203
O	-4.34079520	-6.20806951	2.52272889
O	0.85521323	-7.23846448	0.27451974
O	3.44468114	-6.89472232	-0.85748048
C	3.89811391	-8.04284120	-1.58043796
C	3.18185954	-9.28911862	-1.08111412
O	1.81158918	-9.24368107	-1.40827693
O	4.83025360	-4.83291399	0.41204720
O	2.80835422	-1.45731555	2.41858252
C	3.03365272	-2.52188157	3.31994759
C	1.69144803	-3.10340824	3.73083402
O	0.94810746	-2.05331241	4.33600809
O	4.43590063	2.11564012	-0.23109857
C	5.33842533	3.19086552	-0.23658856
C	4.84539263	4.26669966	0.73153856
C	3.48477430	4.77714773	0.29699208
C	3.41607237	5.09282631	-1.20517789
C	4.12830406	4.04948877	-2.07502288
O	5.40971621	3.72203964	-1.52540342
O	4.72421397	3.72163290	2.03975085
C	5.88753805	3.87688296	2.82945618
C	5.67050804	3.22136920	4.17610503
O	5.47549916	1.83212842	3.93472734
O	3.15527499	5.90250384	1.06278805
O	2.00738353	5.12789077	-1.42262769
O	0.02207241	6.96488119	-1.33258105
C	0.37481273	8.29901047	-1.62011458
C	0.96136090	8.92559084	-0.37237320
O	2.18181888	8.23802364	-0.11928034
O	-2.18033758	5.38563195	-2.11122847
C	1.07346340	2.25865073	-4.20270203
O	2.34309552	1.67417504	-3.99441884
C	4.45071184	4.45862102	-3.50392372
O	4.67157643	3.31019074	-4.30836598
C	6.68831936	0.37019247	-1.18625525
O	7.66578576	0.71004297	-0.22895412
C	3.04245144	-1.75158523	-3.05377272
O	2.57885386	-0.61237655	-2.37586651
C	-0.68069903	-5.41298159	-4.10389187
O	-1.63629501	-4.54634389	-4.67296308

C	-4.83212814	-4.15668653	-2.51458019
O	-4.23214652	-4.04875759	-3.78783220
C	-1.42021486	-1.37282562	-2.88952176
O	-2.25074273	-1.99588131	-3.83641779
C	-5.97180786	6.21316683	-4.46198001
C	-4.34098718	-8.35710112	3.51770313
C	3.77596260	-10.53029542	-1.72357280
C	0.94949940	-3.72438457	2.55799110
C	6.85622797	3.46659585	5.09409740
C	-3.35720913	-1.85867791	5.79024767
C	1.19334831	10.41595033	-0.55376095
H	-2.36674808	2.54955289	-4.47325410
H	-4.49699734	1.66406895	-3.64500753
H	-3.28027317	1.79911667	-0.85416885
H	-4.09015827	-0.62075482	-2.52229341
H	-5.18137484	-0.64709600	0.07909624
H	-4.91467382	-2.53445029	1.64675146
H	-2.15256970	-2.71599151	0.38667644
H	-4.37011588	-4.79002160	0.18699735
H	-3.47848576	-6.62813612	-0.99894478
H	-1.48925311	-8.04926794	-0.46515603
H	-0.09775111	-5.41808298	0.11222545
H	0.62368364	-7.09336636	-2.29408937
H	2.42198044	-6.05179736	-3.29114432
H	4.61105533	-5.69480140	-2.08108825
H	2.79230134	-4.60683266	0.10799026
H	4.88171676	-3.07212752	-1.46304193
H	5.02096875	-2.77348193	1.27063959
H	4.72882493	-0.70467286	2.60302140
H	2.83088837	0.17031153	0.38171385
H	5.59484032	1.16392364	1.19691615
H	6.34975001	2.85025416	0.01622871
H	5.55757551	5.10311623	0.73777604
H	2.77141065	3.95373723	0.46216264
H	3.84260524	6.09454636	-1.37362768
H	2.14763656	6.33768841	-3.07607768
H	-0.25432805	6.55942295	-3.34997900
H	-0.57857656	4.53403479	-1.12076933
H	-1.05296993	4.10199814	-4.09570564
H	1.10013998	3.02315504	-2.21153759
H	3.50787351	3.14662366	-2.10257153
H	4.62806239	-0.27030846	-1.31234899
H	1.84109830	-2.88475455	-1.70674586
H	-0.97317719	-4.49439047	-2.21803153
H	-3.22391915	-2.89311576	-1.90971512
H	-1.31526742	0.41889496	-1.76017262
H	-5.56985541	2.15470230	-1.07910820
H	3.69906846	2.06936790	2.17040044
H	-2.75741602	4.61278292	-1.97221960
H	-2.12363601	-4.73692361	1.58644760
H	1.73948308	-6.90382615	0.03664970
H	4.76604050	-5.76366329	0.66071889
H	2.47765815	6.40943834	0.58367181
H	-5.31333309	3.57012855	-4.39081128
H	-3.82583349	4.54268364	-4.31320543
H	-6.37807190	5.01890570	-2.71631482
H	-6.54034268	7.07770356	-4.11258417
H	-6.61000650	5.62750189	-5.13164442

H	-5.11661527	6.58249982	-5.03988435
H	-3.89234207	6.32083629	-2.63169883
H	-2.18971161	-8.72823058	1.92615468
H	-3.49501346	-8.07039306	0.90484824
H	-2.73155958	-6.93445391	3.61342374
H	-4.86988451	-7.94964597	4.38200941
H	-3.73542752	-9.20674523	3.84563769
H	-5.09035525	-8.71472901	2.80426464
H	-3.81787509	-5.39628676	2.46129502
H	4.98627228	-8.13472288	-1.45631075
H	3.67803604	-7.92825823	-2.64980676
H	3.31959542	-9.34499794	0.01134694
H	3.24933632	-11.41527194	-1.36055618
H	4.84005307	-10.63634081	-1.49336445
H	3.65322747	-10.49007198	-2.81060210
H	1.35374322	-8.71116855	-0.73608336
H	3.57335012	-2.15911546	4.20943958
H	3.63056462	-3.32254693	2.86176899
H	1.89872901	-3.88208058	4.48155582
H	1.50132257	-4.58500378	2.16705089
H	0.82821848	-2.99348726	1.75349912
H	-0.03171776	-4.08967935	2.87420091
H	0.00906031	-2.30418873	4.42077337
H	3.62471107	4.98693363	-3.97264858
H	5.33535689	5.10966765	-3.49441002
H	5.41332557	2.83376332	-3.91733471
H	7.04028115	-0.42615820	-1.85845187
H	6.50469928	1.26461148	-1.78906445
H	7.78451757	-0.07152173	0.32348499
H	6.09764817	4.94590882	2.97410941
H	6.76067501	3.41144558	2.34733781
H	4.75948657	3.65442822	4.61935295
H	6.70157237	2.98033894	6.06368199
H	6.99636469	4.53412596	5.28664787
H	7.77518437	3.06663086	4.65405172
H	5.60905527	1.36951074	4.76772392
H	4.10999011	-1.67541672	-3.32313836
H	2.48653245	-1.93025626	-3.98535405
H	2.56436692	0.14782967	-2.98794782
H	-4.93459511	-1.22287353	3.47917732
H	-3.55340125	-0.16042030	3.78919279
H	-3.66764292	-3.18864512	4.13567652
H	-4.41567999	-1.78210312	6.05604008
H	-2.88153793	-0.89625185	6.00914099
H	-2.90061579	-2.62380905	6.42278745
H	-1.79905533	-2.74035999	3.14418507
H	0.30416218	-4.98680374	-4.32065216
H	-0.73519852	-6.41518123	-4.55326305
H	-2.52842654	-4.79475455	-4.36088156
H	-0.50911414	8.86749555	-1.94542114
H	1.12981940	8.35746567	-2.41779183
H	0.25495251	8.75315988	0.45451366
H	1.87352665	10.60295934	-1.39072321
H	1.63635490	10.85330471	0.34727119
H	0.25293612	10.94219718	-0.74225398
H	2.63398200	8.67438575	0.61040608
H	-4.84891940	-5.22402346	-2.27473283
H	-5.87355995	-3.80731876	-2.53363777

H	-3.95366468	-3.12786143	-3.91134027
H	0.33358144	1.46062074	-4.09059599
H	0.98524480	2.66373928	-5.22076289
H	3.06076709	2.29244754	-4.23017124
H	-0.41475390	-1.18856949	-3.29397974
H	-1.30060925	-1.97261622	-1.97273298
H	-1.81371196	-2.80488935	-4.17318407
H	1.18375103	-0.41067750	3.63242043
H	1.61389503	1.04918063	2.97390401
H	1.65071188	1.97985800	5.27560798
H	1.53105737	0.27175840	5.79137337
H	2.89085221	0.80871843	4.75856027
H	-2.15418423	5.22501224	0.55493721
H	-4.46403812	5.39122005	-0.29249112
H	-3.43916773	2.28273614	3.42002648
H	-0.79085093	0.89418820	6.35138651
H	-1.42065820	2.76483515	7.83560990
H	-1.83557957	5.02128726	6.86248474
H	-1.69873004	5.34422696	4.41671171
H	-0.66438380	4.51010635	2.28417675
H	-0.67232326	2.54105598	0.64856321
H	0.65589609	2.63172243	1.79044187
H	-1.84322358	0.85981858	2.09264477
H	-0.26267697	0.29658043	1.62477445
H	-0.87075826	-0.01683326	4.07634979

255

2-HP-B-CD:trans-(1R,4S)-SRT_6_MD E(Ha)= -7253.9071997225

C	1.56676722	-1.05789377	3.26958466
C	0.79148730	-0.60565924	2.04833730
C	-0.31951517	0.24278064	2.14114381
C	-0.76938125	0.84804758	3.45406113
C	-0.24362468	0.04402279	4.65360132
C	1.24541725	-0.25302485	4.52311152
C	1.22496939	-1.03492148	0.78580206
C	0.54893975	-0.66751485	-0.36899496
C	-0.57955587	0.14802773	-0.27400306
C	-0.99677857	0.60285300	0.96834543
C	-0.38696281	2.31782523	3.54621267
C	-1.30930978	3.24791107	4.03032943
C	-0.96530436	4.58715167	4.16184771
C	0.30943924	5.02409971	3.81546924
C	1.23580887	4.10497937	3.31613565
C	0.88162753	2.76669548	3.17502896
Cl	0.70353758	6.69845817	3.98401310
Cl	2.82656244	4.59500065	2.84934167
N	1.32576858	-2.53473972	3.48835704
C	2.20536002	-3.17489270	4.49528609
O	1.42348967	5.85433777	-0.44655420
C	1.80916354	4.78018010	-1.25272082
C	3.27515988	4.93962476	-1.61359996
C	3.69363273	3.89832844	-2.65578464
O	2.87420004	3.94831527	-3.78208856
C	1.48710055	3.69965885	-3.52460404
C	0.96247783	4.72432516	-2.52464247
O	3.64752233	2.62347375	-2.05314151
C	4.86171318	1.91052189	-1.91172240
C	4.83643573	1.27630870	-0.52506153
C	6.08801878	0.42583416	-0.34152862
C	6.16239967	-0.60270954	-1.47562276
O	6.18205853	0.05862482	-2.70995981
C	5.01041292	0.82957973	-2.97884996
O	4.09481496	4.77261816	-0.47334783
C	5.00354474	5.83961981	-0.22041250
C	6.02932075	5.40037596	0.81393238
O	6.77406863	4.29255556	0.35254699
O	-0.35253860	4.37849744	-2.11232752
C	-1.41161615	5.24223293	-2.39353590
C	-2.24949385	5.39969977	-1.11937948
C	-2.86480121	4.05615325	-0.76932330
C	-3.64402607	3.50817843	-1.95451474
C	-2.76396161	3.44527618	-3.20050564
O	-2.21921518	4.75021443	-3.43566537
O	-1.44636990	5.85005288	-0.04651141
C	-1.81408666	7.08100167	0.57232350
C	-3.08579247	6.99895514	1.42024022
O	-3.01266931	5.91298379	2.31906390
O	-3.69907477	4.23641718	0.34238079
O	-4.11186526	2.21770865	-1.58249239
C	-5.49448401	2.00109206	-1.54968285
C	-5.85679493	1.30833789	-0.22763165
C	-5.25506795	-0.08737471	-0.20057946
C	-5.62591146	-0.85964767	-1.46387614
C	-5.28212501	-0.05271021	-2.70925983

O	-5.92441910	1.21773174	-2.62690515
O	-5.39668641	2.12990217	0.81782539
C	-6.02225962	1.99391157	2.08922155
C	-5.91657394	3.31008456	2.84466971
O	-4.54348459	3.54872077	3.09200539
O	-5.70679497	-0.77654445	0.95330621
O	-4.86279466	-2.05505679	-1.38808207
C	-5.42534929	-3.26923802	-1.80775822
C	-5.54903157	-4.18141770	-0.58972837
C	-4.17182054	-4.40287804	0.00845682
C	-3.15829702	-4.86470417	-1.02698964
C	-3.24513976	-4.05049077	-2.32482184
O	-4.60502406	-3.89483775	-2.74875409
O	-6.33998319	-3.60358458	0.43584301
C	-7.74472391	-3.83051120	0.29700369
C	-8.51530421	-2.80092968	1.11116684
O	-8.36579565	-1.51208553	0.56285119
O	-4.24303538	-5.36054899	1.04818681
O	-1.85151012	-4.67791422	-0.49599860
C	-1.25933588	-5.80908179	0.06893590
C	-0.25372467	-5.35025172	1.14434318
C	0.93014677	-4.64740902	0.49015723
C	1.54617262	-5.53281980	-0.58881434
C	0.44761779	-5.90918070	-1.57960575
O	-0.59699088	-6.59292814	-0.89110841
O	-0.80613268	-4.45970006	2.08661560
C	-1.60627113	-5.08521897	3.06721699
C	-2.14711853	-4.04161796	4.02330106
O	-1.03466557	-3.48735475	4.74099310
O	1.87870388	-4.24169715	1.45258377
O	2.54655762	-4.77643558	-1.24306143
C	3.83417750	-5.32545749	-1.39731067
C	4.74192151	-4.96101392	-0.21693601
C	4.83993637	-3.44872846	-0.11922602
C	5.24986443	-2.85864009	-1.46832662
C	4.42153805	-3.39379875	-2.63572179
O	4.37958973	-4.82588170	-2.57359681
O	4.19487172	-5.57567548	0.93933671
C	5.07971524	-5.74844193	2.04093792
C	4.51272254	-6.81567775	2.95552831
O	3.25453389	-6.33323801	3.41489440
O	5.76317995	-3.09831534	0.88006829
O	5.06190990	-1.45437366	-1.35323007
O	6.10802017	-0.27318830	0.88520311
C	6.58065523	0.45811616	2.01488558
C	5.58511737	0.37690652	3.17180482
O	4.27458833	0.70722153	2.76548712
O	4.78219028	2.27603220	0.48228195
C	5.18851653	1.36248630	-4.38842017
O	5.35477905	0.31607554	-5.30841143
C	5.02445104	-3.06529667	-3.98998242
O	6.35552132	-3.51180906	-4.09766068
C	0.87566599	-6.79945903	-2.72978614
O	-0.06999793	-6.80901792	-3.76350688
C	-2.53647383	-4.72278812	-3.48901617
O	-2.90473527	-6.07556167	-3.64085421
C	-5.75675611	-0.66036405	-4.01665924
O	-5.42391462	0.16372031	-5.10173704

C	-3.52546506	3.07019429	-4.45842944
O	-4.66644348	3.87279721	-4.65444247
C	0.80861937	3.76785241	-4.87993506
O	1.22213620	2.72877079	-5.72693670
C	7.00093852	6.52871458	1.10684951
C	-6.57916472	4.46602610	2.11044159
C	-9.99657836	-3.13330247	1.12119284
C	-2.95016128	-2.95204675	3.33441036
C	4.37696576	-8.17041867	2.28002637
C	-3.26578404	8.27517860	2.21848916
C	5.54162067	-1.00124317	3.80860193
H	4.70936904	4.10993127	-3.01064101
H	3.41793594	5.94070089	-2.04057052
H	1.68606040	3.81482487	-0.73346418
H	0.96529978	5.72393875	-2.98516410
H	-1.04155611	6.21571585	-2.73692601
H	-3.05275476	6.11865543	-1.32973342
H	-2.04371614	3.36070815	-0.53708666
H	-4.49433568	4.16747494	-2.17278253
H	-6.03681286	2.94890172	-1.63133753
H	-6.95376513	1.22382344	-0.18719387
H	-4.15992517	0.00988671	-0.17018183
H	-6.70228673	-1.08574846	-1.43784330
H	-6.39122010	-3.10394294	-2.29993664
H	-5.97192594	-5.14636399	-0.90366229
H	-3.81253840	-3.43923477	0.39847180
H	-3.32898791	-5.92135491	-1.26912749
H	-2.02048536	-6.46738986	0.49904970
H	0.11393065	-6.25732280	1.65260894
H	0.55274041	-3.73734050	0.00648177
H	1.97187679	-6.43877153	-0.13379619
H	3.78072798	-6.41662848	-1.50706181
H	5.73904183	-5.38305577	-0.41145788
H	3.83322100	-3.07257341	0.11515115
H	6.30581023	-3.09103069	-1.65993622
H	7.10216057	-1.16304103	-1.41674882
H	6.97659867	1.06905580	-0.42285361
H	3.95402051	0.62755058	-0.44336806
H	5.71797978	2.60143003	-1.96222665
H	4.12595439	0.17872850	-2.95422220
H	3.40267146	-2.99065642	-2.57686800
H	0.06515253	-4.97235673	-2.00579042
H	-2.80140272	-3.06260341	-2.14786791
H	-4.19305652	0.08418621	-2.75636521
H	-1.94733828	2.72677570	-3.04118010
H	1.36777174	2.68946314	-3.11049572
H	0.48981170	5.72024896	-0.20843746
H	2.65869365	-4.83586745	1.44314302
H	4.23449899	3.02206062	0.15543614
H	-4.12291060	3.39144414	0.58927723
H	-5.53409699	-1.72229706	0.80536932
H	-5.01292553	-5.11510345	1.57668336
H	5.83617569	-2.12535400	0.88670278
H	4.44505090	6.71667381	0.13207743
H	5.53575396	6.10247692	-1.14633134
H	5.49008083	5.14076570	1.74021976
H	6.48225527	7.41543775	1.48301592
H	7.55047939	6.80004518	0.20004030

H	7.72733418	6.20517069	1.85549540
H	6.18789700	3.52201905	0.39480426
H	-5.53435667	1.19387725	2.65692457
H	-7.08039175	1.72717366	1.96008260
H	-6.44528210	3.15021255	3.80029747
H	-6.51085022	5.38305506	2.70521155
H	-7.64046742	4.26233750	1.93839687
H	-6.09179422	4.64268566	1.14828845
H	-4.36763108	4.50116403	3.06315192
H	-7.97788848	-4.85264337	0.62820250
H	-8.04566239	-3.72886239	-0.75407192
H	-8.13008138	-2.83215824	2.14437545
H	-10.39540259	-3.12280461	0.10181046
H	-10.53459888	-2.37774252	1.69756930
H	-10.18865610	-4.11463176	1.56373875
H	-7.49293359	-1.16712018	0.81811951
H	-1.01147420	-5.81978469	3.63243975
H	-2.46440432	-5.59534591	2.61129298
H	-2.78578401	-4.58265320	4.73712243
H	-3.81033623	-3.38761572	2.81978060
H	-2.33322767	-2.43466550	2.59496616
H	-3.32746591	-2.22289810	4.05944666
H	-1.38516364	-2.95114206	5.46003742
H	4.38198140	-3.50413337	-4.76663689
H	5.03140063	-1.98267281	-4.13888462
H	6.32992122	-4.47398633	-4.05494261
H	1.80066124	-6.40016712	-3.15735905
H	1.08252676	-7.80965920	-2.33846102
H	-0.93515253	-7.05563582	-3.40960826
H	5.20388288	-4.80222105	2.57603657
H	6.06768559	-6.06317330	1.68044251
H	5.21646216	-6.90008170	3.80001465
H	3.96321561	-8.91284542	2.97091600
H	5.35233461	-8.54215226	1.95083113
H	3.72058187	-8.09971573	1.40912654
H	2.84978403	-7.03087382	3.93950470
H	-2.74632906	-4.14059186	-4.39643799
H	-1.45730765	-4.71638294	-3.33413038
H	-3.81449426	-6.10193104	-3.95390296
H	-1.91897534	7.87412628	-0.18335808
H	-0.96610030	7.32768790	1.21837462
H	-3.95042215	6.86368595	0.74976711
H	-4.18537990	8.22370717	2.80645964
H	-3.32431029	9.15056965	1.56524140
H	-2.42676948	8.40882942	2.90862660
H	-2.97220386	5.12544690	1.74346485
H	-5.26018403	-1.62321624	-4.17150568
H	-6.84334984	-0.83965321	-3.95692313
H	-5.85429282	1.01397386	-4.94683528
H	6.73855074	1.50489235	1.73667614
H	7.54712010	0.04426599	2.33225369
H	5.94935936	1.09350704	3.92903900
H	6.51789773	-1.27147098	4.22189161
H	5.25376398	-1.76049999	3.07386351
H	4.81874818	-1.00091031	4.63022157
H	4.32907758	1.40872750	2.09345429
H	-2.83342926	3.12834249	-5.31087406
H	-3.87135601	2.03631925	-4.38679558

H	-4.35483800	4.76864015	-4.82223727
H	4.28968177	1.91582612	-4.67508116
H	6.04119839	2.06122051	-4.40540615
H	6.15799985	-0.15208387	-5.05193178
H	-0.27258399	3.67641543	-4.74795654
H	1.00534003	4.76104442	-5.31644365
H	2.16466267	2.85239146	-5.88156853
H	0.34459652	-2.73107458	3.75721703
H	1.47408792	-3.06468584	2.59834563
H	2.25169099	-4.24446835	4.28409266
H	3.20855739	-2.75434192	4.41153322
H	1.81598813	-3.00870139	5.49908983
H	-2.32464781	2.94110635	4.26803775
H	-1.69590041	5.31280730	4.49666762
H	1.61316553	2.08622854	2.75058471
H	2.11135754	-1.66062445	0.71505107
H	0.90466247	-1.00787190	-1.33715559
H	-1.12384893	0.44243904	-1.16747546
H	-1.85836050	1.26279979	1.04424991
H	-1.86581577	0.81092915	3.48013755
H	-0.44035879	0.59512542	5.57852616
H	-0.80785459	-0.89611467	4.71381360
H	1.81225055	0.68082121	4.46215342
H	1.62300527	-0.76490036	5.41488263
H	2.63625914	-0.96450356	3.05007679

2-HP-B-CD:trans-(1S,4R)-SRT_1_Cl E(Ha)= -7253.8924536654

Cl	-7.13295785	-0.85072937	6.77893037
Cl	-4.04714176	-0.81817303	7.60840038
O	-4.11533683	-2.57997958	-3.81401688
O	-1.21644097	-4.32451150	-2.41644820
O	0.25942505	-5.46997785	-3.76755686
O	2.80804276	-4.85172661	-1.23586483
O	5.04669143	-4.68189199	-1.79137576
O	5.05574089	-1.51252190	0.01625485
O	6.80065939	0.01746145	0.08500616
O	4.56742500	2.77259330	-0.79591661
O	4.79778995	4.69045160	-2.03387850
O	1.14971333	4.87850754	-2.21860354
O	-0.21885688	5.49237292	-3.95551311
O	-2.76937772	3.41256943	-2.38010792
O	-4.55642819	2.59060109	-3.61027556
O	-4.31396776	3.36791726	-0.05553357
O	-4.59165520	0.54100456	-0.00588333
O	-3.83364494	-0.78273140	-2.38126636
O	-2.54803068	5.52297149	-0.52706404
O	-0.03912260	6.82681666	-0.56817721
O	-2.42423993	5.34021329	-5.58499163
O	1.54911557	5.04392435	0.59637959
O	4.06407609	4.41717385	1.53006343
O	3.73618891	6.70029841	-3.79021996
O	4.22786326	-0.64696748	2.59449436
O	3.41704705	1.87918464	1.68956477
O	4.56357156	-3.37110368	2.11863466
O	3.51504880	-5.87329341	1.29100056
O	7.46168898	-3.43009501	-2.07984180
O	2.71597536	-6.26560394	-4.68938894
O	-1.59481011	-6.55566943	-0.83172301
O	1.08794976	-6.67172318	0.10233022
O	-2.93088071	-4.18003599	-0.15350683
O	-4.95467002	-2.19830853	-0.29302618
O	-3.23014473	-4.87836790	-5.23542736
O	-6.07609601	0.61395784	-4.86994190
O	8.00205870	2.53303118	-0.52777943
O	-4.48994325	-6.37986996	-0.78101174
O	-7.11238074	-0.48626830	0.80678423
O	-5.34326916	5.92969280	-0.59398619
O	2.32169697	7.75844522	0.80031143
O	5.36763416	2.95400065	3.58468576
O	6.26720823	-2.06287543	3.91582798
O	3.22686708	-8.46565292	0.21828550
N	0.70781743	2.39839341	1.25258470
C	0.14371937	1.89478663	-0.02442279
C	-5.32747024	0.61197026	3.52849439
C	-6.28683562	0.15204620	4.42390775
C	-5.91781151	-0.28738115	5.69159833
C	-4.56485137	-0.27126173	6.05374252
C	-3.61175420	0.19029772	5.15207223
C	-3.97867390	0.64316135	3.88340092
C	-1.82468015	0.21563726	2.62350835
C	-0.48755439	0.62300310	2.50084503
C	0.52267723	-0.33679759	2.33434484
C	0.20830709	-1.68096597	2.18757454

C	-1.12832727	-2.08011999	2.21045871
C	-2.12285605	-1.14209046	2.45024960
C	-2.93822754	1.20414828	2.93466183
C	-2.36386368	2.51282984	3.48885471
C	-1.28776691	3.05262553	2.56174875
C	-0.10775834	2.08777453	2.49416803
C	-2.75739013	-3.02175252	-3.74459394
C	-2.57950041	-3.96366181	-2.55435637
C	-3.02288458	-3.30010282	-1.25437439
C	-4.46980502	-2.86753844	-1.44038278
C	-4.58060236	-1.94465529	-2.65833006
C	-0.83078466	-5.59334872	-2.90376724
C	1.42411696	-4.87260535	-3.19525343
C	1.84963249	-5.62780588	-1.93716385
C	0.69109482	-5.85392728	-0.96949216
C	-0.48290640	-6.47637219	-1.69813183
C	4.09604399	-5.35231057	-1.00293146
C	4.40767021	-5.13944979	0.48413577
C	4.30490949	-3.65280189	0.76414918
C	5.28411770	-2.91029608	-0.13939839
C	5.09537439	-3.26660887	-1.61403579
C	5.92507134	-0.78687812	0.83827032
C	6.16226898	0.96833038	-0.75805362
C	5.26451816	1.88935636	0.07176478
C	4.27490792	1.06389676	0.88858372
C	5.08554840	0.10752922	1.75815444
C	4.91558543	4.14300904	-0.75731921
C	3.95914352	4.88321047	0.19715988
C	2.55003120	4.60232645	-0.30815163
C	2.43146923	5.19361117	-1.70480909
C	3.49990821	4.58513911	-2.62104961
C	0.39062168	5.93148343	-2.78699691
C	-0.66290596	6.38729282	-1.76245344
C	-1.54390495	5.19483195	-1.45200172
C	-2.14617390	4.63697633	-2.73651257
C	-1.09630865	4.37030136	-3.81441369
C	-4.16953167	3.30958813	-2.47456345
C	-4.06976899	1.24782853	-3.67433631
C	-4.48598630	0.47404010	-2.42414790
C	-4.10380693	1.20994246	-1.14527206
C	-4.67009730	2.61668376	-1.20388751
C	-4.67283772	0.65524591	-4.93764108
C	-1.72914987	4.18826499	-5.18568679
C	3.56752479	5.31268438	-3.95260895
C	7.27084953	1.74963146	-1.44249361
C	6.26667706	-2.80519112	-2.46727421
C	2.48137606	-4.94151808	-4.28579714
C	-2.47096861	-3.70556604	-5.07009809
C	-5.39709377	3.90428788	0.71233312
C	0.37386122	8.19523720	-0.57426104
C	5.13842075	4.98100678	2.28888131
C	4.43103616	-0.49810346	4.00605980
C	4.05522841	-7.01579939	1.95617088
C	-2.45879357	-7.65762505	-1.10333120
C	-6.24436038	-2.65383791	0.12459634
C	-3.76006243	-7.50120874	-0.33042786
C	3.26370221	-8.27455463	1.61802039
C	5.08904532	-1.73139942	4.62450846

C	5.14306549	4.35019558	3.67280027
C	1.12256267	8.50766592	0.71304891
C	-5.36679960	5.43010093	0.72968224
C	-6.76807131	-1.78085749	1.25186817
C	-4.63301831	-8.72907602	-0.51481444
C	-8.02075576	-2.39776874	1.84762362
C	-6.59119798	5.97306353	1.44490717
C	1.49070905	9.97851787	0.76569686
C	6.24705414	4.94321720	4.52633009
C	5.43861701	-1.46477031	6.07779849
C	3.90323119	-9.49004557	2.26524512
H	-0.89344818	2.21443533	-0.12465000
H	0.18983830	0.80696708	-0.03109650
H	0.72396151	2.30851310	-0.84984789
H	1.67832897	2.02927799	1.37720001
H	0.83595568	3.43008809	1.17804233
H	-5.64285036	0.91811453	2.53549339
H	-7.33307471	0.12800239	4.13822117
H	-2.56870792	0.17883310	5.45414328
H	1.56988311	-0.03530076	2.31450230
H	1.00164030	-2.41132369	2.05555053
H	-1.40186455	-3.11826854	2.04891641
H	-3.15821207	-1.46471604	2.51025675
H	-3.45295009	1.43108878	1.98994567
H	-1.95003933	2.34380602	4.49132577
H	-3.16633942	3.24791285	3.60308174
H	-0.93516862	4.03692957	2.88948052
H	-1.73061253	3.19075073	1.56711262
H	0.58292805	2.29595845	3.32089119
H	-2.08745659	-2.15854687	-3.62335470
H	-3.19642253	-4.85839187	-2.71125487
H	-2.39926272	-2.41301469	-1.07024188
H	-5.07271897	-3.76606029	-1.62914606
H	-5.62610113	-1.68586652	-2.86024808
H	-1.63814358	-6.02777412	-3.50351515
H	1.21686948	-3.82704382	-2.92861994
H	2.27714648	-6.59382020	-2.23897117
H	0.37245345	-4.86813908	-0.59765070
H	-0.20192891	-7.47886951	-2.05140781
H	4.16524143	-6.41458949	-1.25923964
H	5.43806128	-5.47141557	0.66636062
H	3.28707422	-3.32973789	0.50459913
H	6.31490685	-3.16025912	0.14635646
H	4.16137551	-2.80813608	-1.96950765
H	6.56058815	-1.44260739	1.43871942
H	5.54637906	0.46027617	-1.51418658
H	5.90509958	2.45526025	0.76093259
H	3.64112829	0.47336162	0.21601584
H	5.78475658	0.68704756	2.37251368
H	5.96682648	4.25769605	-0.46860854
H	4.16869312	5.96136338	0.16922836
H	2.46331800	3.51308127	-0.40221493
H	2.57763895	6.28004870	-1.65453665
H	3.25230925	3.52854870	-2.79230973
H	1.05549808	6.75193715	-3.08088286
H	-1.26214523	7.20249237	-2.19075645
H	-0.89117213	4.41478019	-1.03404439
H	-2.88140258	5.34644506	-3.14017641

H	-0.51887195	3.47734000	-3.53919471
H	-4.63199032	4.29828617	-2.55857702
H	-2.97238417	1.24510842	-3.74471455
H	-5.57623867	0.34055538	-2.44820420
H	-3.00583286	1.27111709	-1.10108463
H	-5.76258371	2.55139184	-1.27691707
H	-4.32017908	1.23685145	-5.80224668
H	-4.32588132	-0.37563239	-5.05293843
H	-0.94541630	3.90853908	-5.90485706
H	-2.45870305	3.37499104	-5.13640952
H	4.37036930	4.86681080	-4.55565040
H	2.62291037	5.16429567	-4.48453478
H	7.91479487	1.04314059	-1.98381824
H	6.82969064	2.43570110	-2.17137455
H	6.02920089	-2.99248239	-3.52546911
H	6.40699474	-1.72861479	-2.33389675
H	3.42664049	-4.55244027	-3.89608275
H	2.16420294	-4.30584236	-5.12663183
H	-1.41763141	-3.99871694	-5.10305132
H	-2.65078579	-2.98410481	-5.88081094
H	-5.32514080	3.50406800	1.73121880
H	-6.35025455	3.57172829	0.28559538
H	-0.51739742	8.83031792	-0.66274032
H	1.03601579	8.39531238	-1.42814559
H	4.98904756	6.06658766	2.35538091
H	6.10106162	4.78215807	1.79901866
H	3.44660005	-0.32835977	4.45832750
H	5.05457101	0.38328414	4.19832889
H	4.04260466	-6.82599046	3.03688086
H	5.09629229	-7.16731813	1.64533968
H	-1.94922979	-8.58835894	-0.81652507
H	-2.69699487	-7.70433843	-2.17594389
H	-6.15892259	-3.69781565	0.45472409
H	-6.95338147	-2.60643395	-0.71476128
H	-3.50548499	-7.39231655	0.73653480
H	2.24047914	-8.15482960	2.00645292
H	4.37557716	-2.56687870	4.57109821
H	4.16682333	4.55095602	4.14155730
H	0.45833827	8.26521417	1.55719317
H	-4.46129131	5.75327087	1.26595305
H	-5.98618924	-1.73128947	2.02874167
H	-4.13677140	-9.63421670	-0.15347050
H	-4.88279685	-8.86287361	-1.57223473
H	-5.56666981	-8.59934999	0.03667437
H	-7.81675146	-3.38272142	2.27603492
H	-8.79789979	-2.49707161	1.08331900
H	-8.41017097	-1.75120233	2.63721059
H	-6.67442506	5.57572930	2.46139724
H	-7.49764439	5.70799370	0.89193014
H	-6.53809628	7.06240197	1.50080773
H	0.60332963	10.61606432	0.72387458
H	2.14881787	10.23691349	-0.06975440
H	2.02625357	10.18851247	1.69374047
H	6.12487915	6.02356307	4.64311218
H	7.22427900	4.74619412	4.07519558
H	6.23340436	4.48226417	5.51598104
H	4.55941512	-1.16038426	6.65480979
H	6.19196475	-0.67351770	6.14400953

H	5.85515406	-2.36628288	6.53201355
H	3.98462016	-9.37350523	3.35045496
H	4.90500732	-9.65237047	1.85480765
H	3.30621128	-10.37998353	2.05487983
H	-4.42087387	-0.41607138	-0.12350783
H	-3.04180637	4.69558648	-0.34940855
H	-1.77329958	6.04809315	-5.64973140
H	0.91200107	5.62771369	0.11314001
H	4.60535383	6.83849374	-3.39748605
H	3.70778898	2.82022248	1.59746949
H	4.28996775	-2.44367259	2.25242415
H	7.31134104	-4.37840059	-2.17270363
H	1.86919478	-6.61093406	-4.99546022
H	1.80729582	-6.20421619	0.57156020
H	-2.22010190	-4.82319184	-0.34173724
H	-4.15862613	-4.62040621	-5.20434760
H	-6.37793034	1.52683057	-4.79931480
H	8.43560187	1.92207476	0.07944301
H	-4.05847614	-5.58449634	-0.42484192
H	-6.32166511	-0.05251712	0.45065180
H	-4.42222437	6.14313105	-0.79565144
H	2.10172104	6.86495238	1.09731591
H	4.54814252	2.52166951	3.31352851
H	6.03404420	-2.78051373	3.30977587
H	2.40494221	-8.05156441	-0.08634647

2-HP-B-CD:trans-(1S,4R)-SRT_2_C1 E(Ha)= -7253.8887175250

Cl	-0.90260499	13.26917338	-3.57750892
Cl	1.01730021	10.72749177	-3.33580054
O	-5.61781008	-2.52421175	2.31888767
O	-4.44665730	0.48182951	0.59235745
O	-3.94909353	2.31357076	1.91735424
O	-0.80040367	2.80347207	0.12986827
O	0.68028621	4.07908776	1.37170238
O	3.45291172	1.83879952	0.59086118
O	4.99546240	1.29573647	2.21408200
O	5.07013246	-2.12263653	0.89984377
O	5.47311711	-3.87346436	2.36208867
O	2.92998392	-5.96372096	0.75767046
O	1.80717010	-7.51672854	2.06069654
O	-1.36677036	-6.71566139	0.42780189
O	-3.32886680	-7.11912175	1.59252690
O	-2.64911653	-7.25197107	-1.98100009
O	-4.50377207	-5.10784743	-1.82534355
O	-4.59692714	-3.80143527	0.69192180
O	0.10196011	-7.84849472	-1.69092245
O	2.96581373	-7.65055866	-1.36190886
O	-0.26803558	-8.74398636	3.33485540
O	4.84116353	-5.66698741	-1.31719225
O	6.50407375	-3.33614172	-1.06107021
O	5.00003057	-6.18659215	3.77474075
O	5.46374689	2.11585734	-1.29085656
O	6.19460118	-0.64702541	-1.26052593
O	2.86054862	2.98755296	-1.96704373
O	0.19479026	3.89827302	-2.23358004
O	2.50998733	4.65804449	3.21463813
O	-2.10496741	4.02399655	3.19756549
O	-5.25108114	2.15280044	-1.49159722
O	-2.67598474	3.37768221	-1.84662511
O	-6.34507882	-0.52683011	-1.21127903
O	-6.67334725	-3.36652909	-1.05803656
O	-5.99655712	-0.27953163	3.85938433
O	-5.64521744	-6.28494803	3.00492084
O	6.48924737	-0.40306016	3.81517845
O	-7.85067849	1.71838277	-0.53263926
O	-7.04351039	-6.19463007	-1.60379942
O	-1.79146874	-9.92059784	-1.91969997
O	5.57092251	-8.30826682	-2.25231608
O	8.73622211	-1.85501738	-1.97135085
O	4.81994624	4.88608240	-1.53708283
O	-1.60930390	5.98762836	-1.81502116
N	-0.03807613	6.02176809	3.36417711
C	-0.25268721	6.47156560	4.75966509
C	-1.81563204	11.77288515	0.01043521
C	-1.78424073	12.56747399	-1.12956365
C	-0.91982456	12.26373705	-2.17759980
C	-0.07934470	11.14860801	-2.06885498
C	-0.11764985	10.36001087	-0.92430875
C	-0.98492416	10.65893521	0.12734818
C	0.30701427	9.51095236	1.98229378
C	0.70835542	8.25073783	2.45739863
C	1.97726983	8.10587167	3.03451611
C	2.83131605	9.19074978	3.17865977

C	2.42713931	10.44489147	2.72989775
C	1.18235270	10.59234623	2.13560562
C	-1.05409310	9.75628177	1.34297545
C	-1.78696481	8.45351653	0.99665739
C	-1.66579178	7.44578384	2.13056414
C	-0.20367499	7.05527639	2.27802384
C	-4.77221324	-1.39794080	2.09683877
C	-5.36687328	-0.53264987	0.98836829
C	-5.67315179	-1.33414048	-0.27208983
C	-6.52012188	-2.54386001	0.07424678
C	-5.82321166	-3.33476881	1.19042820
C	-4.74464418	1.81695154	0.85032385
C	-2.55269528	2.15185670	1.69727300
C	-2.17503417	2.94603952	0.45351560
C	-2.98518754	2.52655545	-0.76586091
C	-4.46345099	2.62211567	-0.42841283
C	-0.03518929	3.96662612	0.15803849
C	0.91987492	3.98835416	-1.03231506
C	1.94673945	2.87568286	-0.90766907
C	2.65150262	2.99124310	0.44858878
C	1.63034643	3.04017707	1.58907076
C	4.79793886	1.95579070	0.99975841
C	4.72935269	-0.11670859	2.17875094
C	5.52291690	-0.78990617	1.05761221
C	5.35276788	-0.09065776	-0.29158198
C	5.68068947	1.37816507	-0.10886830
C	5.93598285	-3.17932521	1.23863225
C	6.05498458	-4.10843450	0.02710808
C	4.71509996	-4.76756587	-0.24628866
C	4.23563212	-5.47071345	1.01824267
C	4.20485857	-4.52034972	2.21370624
C	2.66756386	-7.32620509	0.97184971
C	2.06190667	-7.90385559	-0.31268976
C	0.70534245	-7.27084886	-0.55718496
C	-0.17575746	-7.44762855	0.67238391
C	0.50790061	-6.93259904	1.93652971
C	-2.59290676	-7.39473006	0.42717878
C	-3.61905266	-5.73522471	1.78516511
C	-4.41570421	-5.20926134	0.59347965
C	-3.69828286	-5.47228506	-0.72442363
C	-3.37874881	-6.95567037	-0.81195100
C	-4.39245745	-5.65028736	3.08954537
C	-0.22745106	-7.34725798	3.20141095
C	3.98041761	-5.25269924	3.52672793
C	5.12849294	-0.63184456	3.55139931
C	2.22376930	3.28478811	2.97070649
C	-1.86670921	2.64224965	2.95555495
C	-4.71904407	-0.67942374	3.43511231
C	-3.21683810	-8.21972566	-2.86268299
C	3.18854076	-8.71423573	-2.28335137
C	7.49782302	-3.92944998	-1.89483435
C	6.45277590	3.11399247	-1.54023780
C	0.23346728	5.04630338	-3.08032147
C	-6.33297366	2.98925973	-1.90151605
C	-7.94682527	-4.00381275	-1.13872129
C	-7.65897635	2.24031886	-1.83203959
C	-1.11670742	5.75940483	-3.12976503
C	5.84638235	4.28110337	-2.30282031

C	8.10941983	-2.83870443	-2.76316493
C	4.44074684	-8.39480205	-3.08863395
C	-2.22449295	-9.34541741	-3.13535250
C	-7.87973689	-5.17713501	-2.10478183
C	-8.81108281	3.16893262	-2.17197709
C	-9.26324165	-5.76775767	-2.31234461
C	-2.86896130	-10.42458495	-3.98668512
C	4.70368023	-9.48367536	-4.11251118
C	9.15751127	-3.42770097	-3.68929027
C	6.90554799	5.32548036	-2.60427483
C	-0.99568866	7.08379127	-3.85877718
H	-1.29136611	6.77331545	4.88895228
H	0.40723506	7.30879586	4.98146716
H	-0.03499400	5.63676980	5.42646963
H	0.89936060	5.58319526	3.26341908
H	-0.71902439	5.26374635	3.16716298
H	-2.49772680	12.02905076	0.81688127
H	-2.42954515	13.43492030	-1.21743548
H	0.55415364	9.50946814	-0.85828026
H	2.31174238	7.13481327	3.39196568
H	3.80600650	9.05739304	3.63763937
H	3.08291589	11.30341457	2.83617092
H	0.87459177	11.56738157	1.76848773
H	-1.66036304	10.28032381	2.09679573
H	-1.38789063	8.01733109	0.07190115
H	-2.83909766	8.67685023	0.79639872
H	-2.26701661	6.55295532	1.92320609
H	-2.04006639	7.89061996	3.06154340
H	0.10046880	6.51095072	1.37653523
H	-3.76717516	-1.73053893	1.80164094
H	-6.28944968	-0.07556886	1.37034494
H	-4.72120563	-1.69264990	-0.69039804
H	-7.49944199	-2.19930105	0.43673491
H	-6.44203284	-4.17007074	1.53559736
H	-5.78744448	1.94785929	1.15540041
H	-2.30635227	1.09068870	1.55241366
H	-2.39703841	4.00296908	0.65895301
H	-2.74900934	1.48364502	-1.01831930
H	-4.70061729	3.67426246	-0.21659155
H	-0.67369578	4.85375137	0.09942948
H	1.45598424	4.94728121	-0.98954721
H	1.42910638	1.90511519	-0.94141816
H	3.27821342	3.89755351	0.43253167
H	1.12827294	2.06133646	1.60154614
H	5.05212527	3.00971530	1.17221681
H	3.65786032	-0.28723750	2.00665002
H	6.58701742	-0.77616345	1.33067760
H	4.29826081	-0.18307949	-0.59487178
H	6.73162639	1.45817243	0.20026586
H	6.92202396	-2.78919661	1.51306983
H	6.79543579	-4.88475738	0.26659326
H	3.99153648	-3.97580115	-0.49582918
H	4.91646402	-6.29996653	1.25333318
H	3.41572537	-3.77136272	2.05565240
H	3.59052566	-7.85840565	1.22574731
H	1.93924091	-8.98734819	-0.17361097
H	0.86058032	-6.19361751	-0.71833000
H	-0.40307625	-8.51280601	0.81749691

H	0.58912518	-5.83753370	1.88163222
H	-2.44318478	-8.47920319	0.40309347
H	-2.68490458	-5.16141284	1.87273302
H	-5.39194974	-5.71074489	0.56375238
H	-2.75639458	-4.90452692	-0.74123225
H	-4.32637692	-7.51044465	-0.80982327
H	-3.77079669	-6.07962012	3.88948765
H	-4.58171520	-4.60041353	3.33145565
H	0.25675007	-6.86650648	4.06569785
H	-1.26299989	-7.00041063	3.14703966
H	3.89919963	-4.51036864	4.33590514
H	3.04088078	-5.80967439	3.47308692
H	4.47970414	-0.16360301	4.30816461
H	4.97189071	-1.71357476	3.58599912
H	1.49618682	3.00557868	3.73878464
H	3.11279585	2.65722461	3.10890312
H	-0.78742806	2.52616156	2.85002310
H	-2.20706873	2.04327283	3.80940180
H	-4.11880406	0.22939880	3.33660170
H	-4.23176908	-1.34178083	4.16688516
H	-3.50643048	-7.71768795	-3.79427008
H	-4.11886213	-8.64963029	-2.41028347
H	2.31193480	-8.83203694	-2.93222911
H	3.35540334	-9.64968530	-1.73038675
H	7.04563787	-4.72243614	-2.50234467
H	8.28855845	-4.36378005	-1.26669925
H	7.28476842	2.66453804	-2.09836063
H	6.84114740	3.50298785	-0.58823631
H	0.52301619	4.71226348	-4.08280140
H	1.00337595	5.74269911	-2.72451450
H	-6.13363612	3.33766348	-2.92248356
H	-6.39371125	3.86602737	-1.24388040
H	-8.69467975	-3.26776539	-1.46696864
H	-8.24363991	-4.39194463	-0.15369305
H	-7.62934018	1.41864482	-2.56367702
H	-1.82680796	5.11462354	-3.66749922
H	5.43536278	3.89811003	-3.24989281
H	7.30162065	-2.39259616	-3.36736553
H	4.27094055	-7.43863866	-3.61236047
H	-1.36390202	-8.92349354	-3.67810480
H	-7.49851154	-4.79884337	-3.06756491
H	-8.68499880	3.62383041	-3.15947498
H	-8.88567268	3.96678384	-1.42592796
H	-9.75097922	2.61296866	-2.16360573
H	-9.95940553	-5.03206991	-2.72556742
H	-9.66426454	-6.13788351	-1.36322326
H	-9.19888775	-6.61339853	-3.00037191
H	-3.25435002	-10.01879492	-4.92728428
H	-3.69689724	-10.88879749	-3.44143413
H	-2.13883967	-11.20375765	-4.21637455
H	3.86380476	-9.59566991	-4.80435470
H	4.87634255	-10.44069106	-3.61009205
H	5.60039283	-9.23953586	-4.68616938
H	8.73198790	-4.19837287	-4.33842215
H	9.97123679	-3.86968086	-3.10568883
H	9.58195062	-2.63821858	-4.31327546
H	7.72374871	4.90821629	-3.19828725
H	7.31937445	5.72749341	-1.67368493

H	6.45944530	6.15351730	-3.15924965
H	-0.58864003	6.94833899	-4.86555897
H	-0.33602502	7.76539426	-3.31185531
H	-1.97584366	7.55780222	-3.94487660
H	-4.96416961	-4.28200127	-1.59289006
H	-0.75841992	-7.40165979	-1.82041972
H	0.64919153	-9.04228207	3.32861976
H	4.00060725	-6.16289585	-1.37930456
H	5.82735334	-5.69108714	3.78049171
H	6.05564793	-1.61625731	-1.24471278
H	3.61765913	2.39557178	-1.78969840
H	3.20067657	4.94984682	2.60918300
H	-3.06311814	4.13992163	3.23063949
H	-1.73578711	3.23658733	-2.06073255
H	-5.75213907	0.21547747	-1.42811844
H	-6.53170954	-1.08133265	3.89890029
H	-5.47556199	-7.20534736	2.77186791
H	6.62840095	0.54804523	3.74460034
H	-7.53936613	0.79979023	-0.57111341
H	-6.12272192	-5.93746018	-1.78541162
H	-0.98871302	-9.44114153	-1.66549807
H	5.53236190	-7.46406768	-1.78123367
H	8.04816397	-1.28466825	-1.60235732
H	4.00716886	4.39752911	-1.74857098
H	-2.21640759	5.25072171	-1.64044601

2-HP-B-CD:trans-(1S,4R)-SRT_3_Cl E(Ha)= -7253.8882245840

Cl	0.39890023	7.13851250	5.32174277
Cl	0.46657021	4.32402384	6.83276912
O	-3.69279847	3.96624011	-3.63882595
O	-4.93505443	1.11963564	-1.70939241
O	-6.16302344	-0.54523685	-2.73632470
O	-4.21478900	-2.90171637	-0.74236576
O	-4.10904390	-5.15015815	-1.28478946
O	-0.44953680	-5.17470950	-1.11868875
O	0.98867584	-6.35352628	-2.46929796
O	3.64004155	-4.27279273	-1.13009879
O	5.82497538	-3.89424033	-1.80040199
O	5.13243261	-0.32473277	-1.55814328
O	5.78942026	1.31885148	-3.03769662
O	2.60442672	3.08741504	-2.60227348
O	1.48098593	4.20357829	-4.27917109
O	2.59841608	5.37211514	-1.01363433
O	-0.18422580	5.48175396	-0.70432704
O	-1.68989858	3.90117555	-2.46865291
O	3.62876585	3.10259542	0.06947015
O	5.74576785	1.36710139	0.59956203
O	5.31001461	3.51311693	-4.79450680
O	5.19129787	-1.17039743	1.20735430
O	4.30702762	-3.85479670	1.49745052
O	7.87418420	-2.32250064	-2.92667776
O	0.29008559	-6.71949339	1.09121544
O	3.04672298	-6.15336855	1.05491986
O	-1.05414035	-4.35013243	1.48207239
O	-3.75747333	-3.51512208	1.96721813
O	-2.78937672	-7.44765407	-2.28777208
O	-6.75053712	-3.11190072	-3.48456180
O	-6.59077601	1.03442725	0.51030582
O	-5.72739703	-1.60266546	1.24808763
O	-4.78635656	3.15594654	0.26334323
O	-2.83154283	5.16980479	-0.33031169
O	-6.08376383	2.90759954	-4.65114904
O	-0.63775378	5.07909362	-5.79478675
O	3.32890415	-6.77835046	-3.87062738
O	-7.50775576	3.78318640	0.24809801
O	-1.50677769	7.53032232	0.81236568
O	5.34901914	5.25567179	-0.06054998
O	7.69346613	-0.20687585	2.12715058
O	3.32512659	-5.44924791	3.80730762
O	-2.09358795	-6.83070533	2.64874836
O	-6.48613445	-4.10225483	2.30747112
N	0.84824639	-2.20727828	1.30794932
C	0.60680998	-1.89352822	-0.12621074
C	0.86289301	4.51154962	2.34658393
C	0.70973396	5.69123337	3.06769183
C	0.59044206	5.65917102	4.45425752
C	0.61641553	4.42484521	5.11452936
C	0.75077902	3.24899035	4.38286109
C	0.88167848	3.27468039	2.99361387
C	-0.30899612	1.19624737	2.20213289
C	-0.34640799	-0.20991770	2.24783849
C	-1.58050301	-0.86957370	2.33937843
C	-2.77270122	-0.15839352	2.32539415

C	-2.74246034	1.22961502	2.21497598
C	-1.52393097	1.89001778	2.16434562
C	0.99703728	1.98472921	2.20320894
C	2.16986534	1.12002640	2.66914442
C	2.17285672	-0.20213591	1.91672040
C	0.93374843	-1.01557458	2.25749247
C	-4.03903540	2.60287916	-3.38930527
C	-4.79078282	2.48676052	-2.06498187
C	-4.02439909	3.14656182	-0.92556386
C	-3.65872440	4.57109044	-1.30497995
C	-2.91286870	4.57038112	-2.64515052
C	-6.19060316	0.49881105	-1.80125993
C	-5.19111306	-1.56012879	-2.48317075
C	-5.35951072	-2.12171070	-1.07212271
C	-5.46199245	-1.03067561	-0.01326338
C	-6.53782022	-0.03860535	-0.40484689
C	-4.39489284	-4.20987072	-0.27897189
C	-3.45538115	-4.41561053	0.91969589
C	-2.01975021	-4.23019533	0.43245236
C	-1.78953023	-5.26582435	-0.66020814
C	-2.78619710	-5.07074196	-1.80396384
C	0.20090041	-6.42039200	-1.32512446
C	1.98864784	-5.33559383	-2.46659883
C	2.91397486	-5.49093123	-1.26184674
C	2.16620475	-5.73412906	0.04612299
C	1.06040164	-6.75545499	-0.10017815
C	4.99596475	-4.32544741	-0.76276493
C	5.19742712	-3.43133448	0.46790405
C	4.91913191	-1.98798587	0.09578234
C	5.69741718	-1.55813558	-1.14252282
C	5.55466417	-2.57384644	-2.27536253
C	5.94748015	0.81013958	-1.74566457
C	5.53374070	1.85943396	-0.70804949
C	4.06712160	2.20661920	-0.92538978
C	3.96018894	2.76923347	-2.33822489
C	4.46289827	1.74655728	-3.36204459
C	2.34349396	4.34702681	-3.19279240
C	0.17584657	3.69117461	-3.99167495
C	-0.49368390	4.53108355	-2.90487428
C	0.40834434	4.67639645	-1.68484788
C	1.73309669	5.26680763	-2.12513030
C	-0.57388430	3.76188956	-5.31245864
C	4.54000255	2.33617748	-4.75964067
C	6.54932552	-2.31371957	-3.39401424
C	2.74237219	-5.50771852	-3.77681952
C	-2.67985843	-6.16244964	-2.85439595
C	-5.44006179	-2.61504395	-3.55021041
C	-4.89022210	2.17060041	-4.57150237
C	3.51492542	6.46693701	-1.08129422
C	6.91276609	1.90221720	1.23905422
C	4.82029344	-3.77038238	2.83853904
C	-0.30995107	-7.95952660	1.46704833
C	-4.23746814	-4.10079265	3.18589036
C	-7.91553428	1.47619013	0.81581979
C	-3.46783803	6.10819269	0.54129151
C	-7.89159538	2.92003874	1.29434034
C	-5.70563282	-3.76393767	3.43870893
C	-1.04319422	-7.77519855	2.78614896

C	3.70282457	-4.09853882	3.82103594
C	7.24871071	1.08469551	2.47627821
C	4.50817650	6.38364998	0.06879887
C	-2.42766508	6.69849503	1.48240147
C	-9.27209866	3.33970448	1.76783246
C	-3.10116625	7.54803384	2.54521095
C	5.38902746	7.61936206	0.09321524
C	8.36098505	1.75698173	3.26086820
C	4.14897019	-3.78008129	5.23800291
C	-1.65591899	-9.08386715	3.24567803
C	-6.21703261	-4.52757255	4.64753477
H	1.48231560	-1.40789268	-0.55345164
H	-0.25846755	-1.23336720	-0.18880719
H	0.40781034	-2.83158826	-0.64730195
H	0.10914804	-2.88738117	1.59316823
H	1.73766878	-2.71505371	1.38458177
H	0.93895335	4.57779391	1.26491345
H	0.64684079	6.64384263	2.55037624
H	0.73424820	2.30744429	4.92313135
H	-1.63117364	-1.95336260	2.43233502
H	-3.72216789	-0.67728465	2.39896320
H	-3.66299825	1.80292118	2.17433973
H	-1.50705634	2.97452789	2.11052085
H	1.21768406	2.27227409	1.16486503
H	2.11029243	0.93818876	3.74948176
H	3.10556647	1.65229574	2.47670853
H	3.08097922	-0.77699767	2.12781949
H	2.18436525	0.02884961	0.84397707
H	1.06669493	-1.48776401	3.24038301
H	-3.12957512	1.98717596	-3.33618576
H	-5.77543132	2.96195974	-2.17015038
H	-3.09095792	2.58681218	-0.76490753
H	-4.57641604	5.16156959	-1.43384561
H	-2.74230586	5.59845728	-2.98260296
H	-6.94941306	1.20490188	-2.15636580
H	-4.17847924	-1.14496061	-2.58243007
H	-6.26424233	-2.74433000	-1.05574166
H	-4.50246483	-0.49576958	0.01735636
H	-7.50848790	-0.55054622	-0.44777326
H	-5.42764147	-4.39459843	0.03050491
H	-3.58075762	-5.44716100	1.26792903
H	-1.93215401	-3.21785809	0.02015716
H	-1.97216402	-6.25793296	-0.22888185
H	-2.61428188	-4.09105507	-2.27322074
H	-0.54529403	-7.19984541	-1.51496742
H	1.51605709	-4.34436699	-2.43515535
H	3.59307237	-6.33205471	-1.45471062
H	1.68208168	-4.77982944	0.31222749
H	1.50203311	-7.75205288	-0.23264549
H	5.29725722	-5.35638619	-0.54469011
H	6.23700926	-3.53947293	0.80388649
H	3.84998157	-1.92423647	-0.16672755
H	6.76138184	-1.44284724	-0.89553461
H	4.52995144	-2.51890757	-2.66815301
H	7.00610134	0.54401688	-1.64722792
H	6.13301322	2.76694491	-0.85825668
H	3.47030313	1.28457900	-0.86934151
H	4.58305030	3.67111502	-2.40262405

H	3.78196197	0.88350682	-3.36466768
H	3.26968900	4.76405826	-3.60423933
H	0.24828746	2.64953681	-3.64847024
H	-0.71478052	5.52317783	-3.32109577
H	0.59886694	3.66627352	-1.28578847
H	1.55853671	6.26166760	-2.55833594
H	-0.08990640	3.08334324	-6.03085049
H	-1.60352401	3.42663649	-5.15934385
H	4.93176593	1.56883100	-5.44275281
H	3.53177759	2.60313611	-5.08972750
H	6.38697963	-3.05424783	-4.19034853
H	6.35993239	-1.31925367	-3.81010918
H	2.05319298	-5.30759335	-4.61021868
H	3.55282696	-4.77407064	-3.81901384
H	-3.44987647	-5.98775414	-3.61857036
H	-1.70161936	-6.10642952	-3.34113731
H	-4.76797741	-3.46165198	-3.38389993
H	-5.21267238	-2.18184682	-4.53593769
H	-5.17005566	1.12018452	-4.44757996
H	-4.28924956	2.26046506	-5.48877363
H	2.94561569	7.40499543	-1.02983630
H	4.07127431	6.44219322	-2.02924706
H	6.71982726	2.95311750	1.49111891
H	7.76914697	1.85217325	0.55298790
H	5.19462101	-2.75705305	3.00940038
H	5.63995828	-4.49050819	2.96559021
H	0.47676448	-8.71770058	1.57295513
H	-1.02198309	-8.29208860	0.69775266
H	-3.61697773	-3.71412931	4.00330342
H	-4.10931578	-5.18879868	3.14678037
H	-8.34316444	0.81177002	1.57913407
H	-8.54388062	1.43265653	-0.08433201
H	-4.25154403	5.59402299	1.10978865
H	-3.91997321	6.91650053	-0.05086483
H	-7.18341849	2.98858374	2.13692841
H	-5.78477942	-2.68416623	3.63352212
H	-0.31438984	-7.42569970	3.53303626
H	2.84490429	-3.44173460	3.56584385
H	6.34297990	1.03239084	3.10497938
H	3.93040493	6.32802712	1.00592796
H	-1.90845756	5.85668900	1.97130250
H	-9.62213401	2.71780445	2.59681292
H	-9.99220952	3.26947214	0.94632000
H	-9.24326850	4.38006221	2.09834146
H	-3.80446631	6.96035155	3.14167366
H	-3.63916806	8.38089819	2.08172213
H	-2.34327766	7.96578296	3.21173827
H	4.80047087	8.53097334	0.22903412
H	5.95656890	7.70180001	-0.83925233
H	6.10350551	7.54051295	0.91528181
H	8.06856048	2.75484276	3.59915161
H	9.26146770	1.84308541	2.64471031
H	8.60966535	1.14907917	4.13326179
H	4.38958827	-2.72014105	5.35753356
H	5.03071962	-4.37361514	5.49726024
H	3.35283750	-4.04379274	5.93733690
H	-0.89230665	-9.85378285	3.38622940
H	-2.38564914	-9.44236750	2.51306488

H	-2.17534048	-8.93313394	4.19417856
H	-5.61079474	-4.32751185	5.53681563
H	-6.19904879	-5.60340291	4.44735180
H	-7.24903013	-4.24090768	4.86057861
H	-1.10065031	5.15786748	-0.57570795
H	3.06212169	3.78138576	-0.35254149
H	6.20608089	3.27315616	-4.53240067
H	5.22553988	-0.23075230	0.91101398
H	8.05893011	-3.21642729	-2.61785551
H	3.66808076	-5.40819291	1.19270516
H	-0.53165660	-5.16816313	1.31252634
H	-3.66898399	-7.50728157	-1.89675521
H	-7.33477434	-2.35557573	-3.61378492
H	-4.96014331	-2.17445396	1.44889098
H	-5.21072343	2.27802967	0.35177732
H	-5.83419724	3.83033182	-4.77643153
H	0.27322081	5.36980780	-5.91825851
H	2.60917515	-7.41948323	-3.86019639
H	-6.53881377	3.77913462	0.20630234
H	-0.96111176	7.00054817	0.21577448
H	4.82948551	4.47212705	0.18562261
H	6.92513347	-0.72868339	1.85525234
H	2.96484482	-5.70652217	2.94512119
H	-1.72361060	-5.94093012	2.69721484
H	-6.65460078	-3.27830424	1.82980794

255

2-HP-B-CD:trans-(1S,4R)-SRT_4_Cl E(Ha)= -7253.8754928698

Cl	-0.52903700	-1.13049237	13.50827596
Cl	-0.80786207	-0.23701145	10.45462961
O	1.67832174	6.84155807	0.40133221
O	3.85330039	4.16768847	-0.82804720
O	5.59113333	3.44869216	0.52724004
O	4.83210501	-0.05374590	-0.22658232
O	4.82250154	-1.56242082	1.51985294
O	2.24363804	-3.53038414	-0.16711335
O	0.94850221	-4.87963148	1.18689729
O	-2.09880538	-3.72348394	-0.45929468
O	-4.02196438	-3.67172472	0.81958047
O	-4.81477218	-0.34655563	-0.50271391
O	-5.82350663	1.19926418	0.89257111
O	-3.96314626	3.97564156	-0.60121573
O	-3.40071027	5.79245349	0.72118982
O	-4.47305979	5.58503815	-2.72414679
O	-1.81114807	6.63503585	-3.00574309
O	-0.09445229	6.00048463	-0.83111192
O	-5.58168404	3.10390753	-2.77371015
O	-6.40391127	0.36055432	-2.57438792
O	-6.15272554	3.53865926	2.30346666
O	-5.05425603	-1.98893984	-2.82928608
O	-3.56663946	-4.40602171	-2.71446649
O	-6.14926176	-2.49945267	2.13683331
O	2.00434856	-5.34333527	-2.27640221
O	-0.81943835	-5.15359371	-2.53268386
O	4.43734529	-3.86519514	-1.87780608
O	6.35257805	-1.73009476	-1.77659125
O	3.74774366	-3.44482085	3.18505279
O	6.88426644	1.54907503	2.19175086
O	5.34283593	3.75552901	-3.07182457
O	5.72217913	0.92537292	-2.73756016
O	3.32092772	5.62809269	-3.19741568
O	0.86900155	7.13338692	-3.11125438
O	4.08375807	6.83039815	1.71749198
O	-1.79725418	7.59002790	2.02785063
O	-0.92232953	-5.73642061	2.67560429
O	5.90032989	6.26994040	-4.26754845
O	-0.85931831	9.09843537	-4.19011386
O	-7.09668245	5.37634383	-3.74960556
O	-7.80037893	-1.79828246	-3.72194708
O	-2.84086677	-7.07124024	-2.26932937
O	4.29083041	-6.60743318	-1.31669562
O	8.37907286	0.28711323	-2.25315971
N	-1.47723020	-6.77146672	5.12069549
C	-0.62184286	-7.97043167	5.31871737
C	-0.53798393	-4.60316942	11.53897766
C	-0.49933416	-3.64668185	12.54650360
C	-0.58316246	-2.29174824	12.23724304
C	-0.70548259	-1.90207771	10.89720157
C	-0.74364944	-2.86682288	9.89605644
C	-0.66178699	-4.22586087	10.20206401
C	0.21482834	-5.04196632	7.96231658
C	-0.12467237	-5.28076115	6.61992935
C	0.81383642	-5.01395834	5.61247467
C	2.08990097	-4.55571035	5.91107518

C	2.43812253	-4.35517333	7.24546030
C	1.50899413	-4.59075782	8.24860470
C	-0.76447148	-5.26795232	9.10634127
C	-2.20806029	-5.36581398	8.60053873
C	-2.29878704	-6.32503834	7.42334496
C	-1.51350265	-5.75780449	6.25050917
C	2.41281329	5.61797664	0.45946028
C	3.28803558	5.47216527	-0.78416841
C	2.48521665	5.65324550	-2.06672795
C	1.72931239	6.96820962	-2.00955045
C	0.87592587	7.00758512	-0.73735989
C	5.23983317	4.02389009	-0.70628038
C	5.02452721	2.15957726	0.75424932
C	5.49071844	1.20376211	-0.34118368
C	5.16708959	1.74298835	-1.72812224
C	5.73213340	3.14839185	-1.86349952
C	5.52489225	-1.10402107	0.38797248
C	5.68764901	-2.23091989	-0.64252500
C	4.31443562	-2.75536081	-1.02103309
C	3.55461424	-3.14990673	0.24097342
C	3.49569709	-2.00920928	1.25265729
C	1.83364107	-4.83569254	0.07336324
C	-0.24976561	-4.11985724	1.03010837
C	-1.01523776	-4.59115170	-0.20452398
C	-0.13123292	-4.58434932	-1.44927633
C	1.13243093	-5.38154513	-1.17539189
C	-3.41305641	-4.20532936	-0.32848230
C	-4.18727369	-3.82568133	-1.59104179
C	-4.27215804	-2.31564059	-1.71408277
C	-4.87855957	-1.75927712	-0.42718536
C	-4.13584163	-2.23982630	0.82015502
C	-5.98372803	0.39530950	-0.24163283
C	-6.30696547	1.23832307	-1.47778095
C	-5.23273090	2.29079796	-1.68414069
C	-5.06621448	3.10460843	-0.40605249
C	-4.80761643	2.20446556	0.80091118
C	-4.13828734	5.35279456	-0.38581212
C	-1.98332601	5.63279652	0.62160081
C	-1.46014786	6.33662236	-0.62890832
C	-2.22029672	5.90460893	-1.87770445
C	-3.70993095	6.09424997	-1.65619927
C	-1.42886573	6.24053281	1.89997406
C	-4.88439016	2.96462761	2.11451838
C	-4.87769627	-1.90223229	2.10160657
C	-1.00459767	-4.34672022	2.33208463
C	2.94947391	-2.43897621	2.60246609
C	5.49119878	1.73868236	2.13678845
C	3.23332017	5.71261812	1.73569114
C	-4.97712662	6.53644857	-3.65802116
C	-7.48956260	0.58567972	-3.47105127
C	-4.27891269	-5.46529083	-3.35210646
C	2.40400507	-6.60060095	-2.82174360
C	7.75451491	-1.99520771	-1.78822272
C	6.35054723	3.90787524	-4.06910529
C	1.30317783	8.02275777	-4.13649145
C	5.95926998	5.05966269	-4.98570518
C	8.45725337	-1.03459831	-2.73536480
C	3.90683363	-6.81640926	-2.66381293

C	-3.38501954	-6.68816376	-3.52030908
C	-7.57379180	-0.59765881	-4.42489267
C	-6.01831822	5.84428753	-4.52659279
C	0.09288762	8.41610373	-4.97276492
C	6.98220487	5.22254101	-6.09545258
C	0.50852168	9.33629595	-6.10579663
C	-6.57386969	6.80898275	-5.55782600
C	-8.71698209	-0.40709043	-5.40447653
C	-4.17575550	-7.85027879	-4.09227794
C	4.28817002	-8.22502712	-3.08037544
C	9.92477567	-1.40262643	-2.86562638
H	-0.97302003	-8.54360802	6.17573616
H	0.40380140	-7.64451687	5.48599908
H	-0.68037706	-8.58498707	4.41938706
H	-1.20493596	-6.30138565	4.21336436
H	-2.44019989	-7.08084034	4.97067112
H	-0.46973820	-5.65513146	11.80354915
H	-0.40193979	-3.94147687	13.58581533
H	-0.82381754	-2.53737323	8.86442117
H	0.55217412	-5.16657733	4.56800697
H	2.79253190	-4.34437946	5.10787286
H	3.43158545	-4.00094926	7.50326401
H	1.77824833	-4.40679299	9.28463395
H	-0.51186395	-6.23751152	9.56148519
H	-2.56303454	-4.37095708	8.30234879
H	-2.86036266	-5.69822067	9.41296500
H	-3.34398840	-6.48595909	7.13133945
H	-1.88773608	-7.29655806	7.72532181
H	-2.08325236	-4.92271875	5.81990499
H	1.72254430	4.76376766	0.51232488
H	4.08250165	6.22931873	-0.73914325
H	1.74331790	4.84241653	-2.12590430
H	2.44735844	7.79908188	-1.96446694
H	0.40374950	7.98994087	-0.62957893
H	5.73723923	4.99915104	-0.73521375
H	3.92674000	2.22080195	0.73732486
H	6.57677269	1.06515785	-0.26061045
H	4.07453221	1.79618319	-1.84381882
H	6.82811586	3.09595171	-1.80195696
H	6.49511915	-0.76231101	0.76395230
H	6.26311461	-3.05081801	-0.18884684
H	3.76162629	-1.94661475	-1.52064828
H	4.05910872	-4.00094265	0.71831875
H	2.89008033	-1.18715212	0.84697397
H	2.67477498	-5.48527912	0.33373619
H	-0.01803316	-3.05305834	0.91675954
H	-1.37654974	-5.61666448	-0.03343864
H	0.15149340	-3.54481139	-1.67095751
H	0.84578091	-6.42024533	-0.95903411
H	-3.41454241	-5.29525687	-0.21231484
H	-5.20871884	-4.21437806	-1.48374650
H	-3.25397419	-1.91070339	-1.82195121
H	-5.92377591	-2.09126658	-0.36089558
H	-3.13546960	-1.78517385	0.83248498
H	-6.81664797	-0.27888359	-0.01422943
H	-7.27120161	1.73787877	-1.30800397
H	-4.28245740	1.77072169	-1.88371273
H	-5.98162361	3.68225338	-0.21917973

H	-3.82065993	1.73315599	0.69153442
H	-5.18557662	5.57337445	-0.15298850
H	-1.72680264	4.56532631	0.56418956
H	-1.56979438	7.42064422	-0.48964126
H	-2.03826049	4.82992494	-2.03357066
H	-3.92343283	7.16343541	-1.51671470
H	-1.77387593	5.63918530	2.75546947
H	-0.33603950	6.20690296	1.87169033
H	-4.61905309	2.27927686	2.93482522
H	-4.15907287	3.78304416	2.10027371
H	-4.25716731	-2.21250228	2.95883942
H	-5.02354180	-0.81994112	2.16149146
H	-0.55941961	-3.74074397	3.13199116
H	-2.05942548	-4.08342975	2.21271891
H	2.87704503	-1.55419532	3.25166143
H	1.94915342	-2.85974928	2.47423271
H	5.02929729	0.78264302	2.39945663
H	5.15278677	2.49449283	2.86121628
H	3.86944785	4.82731621	1.82347675
H	2.54606010	5.73480855	2.59550383
H	-4.15325321	6.93751509	-4.26059527
H	-5.46126547	7.36071866	-3.11480721
H	-7.33455420	1.52664551	-4.01242826
H	-8.42682497	0.64781821	-2.89935475
H	-4.64674157	-5.11017414	-4.32251377
H	-5.14441102	-5.75035997	-2.74074044
H	2.11705743	-6.61834378	-3.87944888
H	1.86856849	-7.41106249	-2.31120236
H	7.91883122	-3.03910535	-2.09114994
H	8.17792141	-1.84779634	-0.78429800
H	6.46295661	2.96899794	-4.62620922
H	7.30823262	4.15616338	-3.59140677
H	2.07533421	7.53718105	-4.74598690
H	1.72368049	8.93063547	-3.68124676
H	4.97788857	4.82353898	-5.43022758
H	7.97340368	-1.11859754	-3.72230108
H	4.42835920	-6.09530413	-3.31064591
H	-2.57054652	-6.42968241	-4.21445159
H	-6.62391071	-0.64965179	-4.98328912
H	-5.52182303	5.00647561	-5.04529163
H	-0.34107391	7.49423077	-5.39581602
H	7.07269762	4.31295007	-6.69653829
H	7.96264393	5.46403117	-5.67268641
H	6.68687709	6.04651523	-6.74856530
H	1.24513808	8.86067613	-6.75987055
H	0.93853047	10.25929254	-5.70412113
H	-0.36712740	9.60532666	-6.70051256
H	-5.78437053	7.20427280	-6.20351707
H	-7.07410624	7.64608017	-5.06067787
H	-7.31239930	6.29769214	-6.17915566
H	-8.59724512	0.51062503	-5.98749977
H	-9.67003541	-0.36106578	-4.86808835
H	-8.75815844	-1.25569151	-6.09080768
H	-4.64256556	-7.58678342	-5.04620865
H	-4.96142706	-8.15346848	-3.39271439
H	-3.51764342	-8.70707216	-4.25272650
H	3.96933762	-8.44062642	-4.10499789
H	3.82376539	-8.95575923	-2.41025010

H	5.37111638	-8.35286766	-3.02046124
H	10.05459384	-2.41638214	-3.25575937
H	10.42116792	-1.33338352	-1.89223268
H	10.41760023	-0.70151012	-3.54242761
H	-0.83887112	6.55043004	-3.06625271
H	-4.94670934	3.84753733	-2.79937411
H	-6.78829948	2.81504812	2.25299097
H	-5.26667569	-1.03579426	-2.77254877
H	-6.01470915	-3.43563486	1.94821290
H	-1.63762546	-4.63657553	-2.67199515
H	3.53555540	-4.12091614	-2.14725564
H	4.64559010	-3.09016157	3.21057228
H	7.28936897	2.38784829	1.94150313
H	5.57518182	-0.00245655	-2.48161374
H	3.83168800	4.79610133	-3.15658286
H	3.51515992	7.59966514	1.59335998
H	-2.76108862	7.61041546	1.99662637
H	-0.06285222	-6.01343605	2.30763916
H	5.05204142	6.30082405	-3.80212370
H	-1.33071589	8.44638427	-3.65290409
H	-6.80171114	4.58793030	-3.27272951
H	-6.96190060	-2.06717883	-3.32036795
H	-1.98792575	-6.61390248	-2.21076524
H	4.60001439	-5.68908612	-1.27494328
H	7.51052594	0.64202806	-2.50914918

255

2-HP-B-CD:trans-(1S,4R)-SRT_5_Cl E(Ha)= -7253.8730853111

Cl	-0.45037828	2.09502887	-0.41816454
Cl	-0.94320558	1.73667670	2.71822305
O	3.86006312	-3.70721018	-3.58576220
O	6.14383633	0.91229150	-2.47231633
O	3.88161797	3.42712722	-1.06563790
O	3.47065967	5.36098248	-2.26923396
O	0.00286077	5.51758508	-1.10872953
O	-1.63352469	6.27979996	-2.55873520
O	-3.94437463	3.76093064	-1.26138174
O	-5.48549498	2.79022595	-2.69046482
O	-4.80455309	-0.49967853	-1.24885414
O	-5.42689045	-2.42357980	-2.38624069
O	-2.13837463	-3.94399306	-1.83568184
O	-1.09715775	-5.10769297	-3.53659390
O	-1.71462850	-6.03396153	-0.06673893
O	1.13424672	-5.77428317	-0.11224491
O	2.12738662	-4.12940738	-2.09577214
O	-3.12137500	-3.72948421	0.79855505
O	-5.16570471	-1.82585554	1.20466332
O	-4.90171189	-4.78318063	-3.86411997
O	-5.96726893	0.86286303	0.93570043
O	-5.71786388	3.73117125	0.79621082
O	-6.71606246	0.82858261	-4.12920978
O	-1.09122057	6.86571459	0.96506200
O	-3.63113683	5.50179820	0.97343194
O	1.46599943	5.95461889	1.29305250
O	4.10153978	4.79157461	1.24175507
O	1.96347355	7.24579230	-3.63317125
O	6.68225345	3.49595664	-3.36463034
O	5.90014225	-0.45915998	0.86933340
O	4.92352624	2.20498438	1.26377159
O	5.50929565	-2.99919002	0.12655164
O	3.90094332	-5.26897977	-0.27677972
O	5.81707665	-2.27941118	-4.86877221
O	1.03645084	-5.75997618	-5.18224296
O	-3.93969488	6.16020878	-4.06491481
O	5.90870454	-2.45602370	2.99870663
O	2.86122257	-7.01693284	1.64707002
O	-4.49712792	-6.12968424	0.87046829
O	-7.88668713	-1.16821628	1.21887586
O	-6.28463018	6.35026824	1.71618321
O	0.71837652	8.57115276	2.29027950
O	6.36219896	4.16956361	2.80876773
O	4.86092891	-0.81549781	-1.60894222
N	2.65341973	-5.60250724	5.38837396
C	2.07210394	-6.79935507	4.70754636
C	0.80802743	-1.62618906	0.28738168
C	0.47488991	-0.43391574	-0.34047764
C	-0.06585278	0.61978485	0.39071232
C	-0.27260214	0.46315948	1.76550357
C	0.06953448	-0.73559112	2.38734113
C	0.60864468	-1.79596182	1.65971592
C	0.25289492	-3.53700945	3.49998528
C	0.82786315	-4.05782004	4.67151738
C	0.00578289	-4.40846650	5.75176102
C	-1.37583038	-4.32567723	5.66148605

C	-1.95071658	-3.87808631	4.47376719
C	-1.14433708	-3.47714346	3.41752587
C	1.10302669	-3.06208759	2.33389357
C	2.56178498	-2.85195255	2.75672577
C	3.09497332	-4.06729797	3.49526398
C	2.32441827	-4.22902572	4.79321292
C	4.01317928	-2.32299602	-3.26062410
C	4.93543120	-2.15943457	-2.05630733
C	4.53292114	-3.05079689	-0.88315136
C	4.36675488	-4.48126485	-1.35773808
C	3.39805943	-4.52363352	-2.55123468
C	6.04053815	-0.06362648	-1.47884449
C	5.09810536	1.89140518	-2.48494406
C	5.02124652	2.58750544	-1.12769357
C	4.89495390	1.57753788	0.00600750
C	6.03509173	0.57747058	-0.08644056
C	4.07239738	4.82141927	-1.12859995
C	3.49425804	5.44219762	0.14684424
C	1.98375217	5.28708307	0.16850386
C	1.38893652	5.82631358	-1.12673451
C	2.05116389	5.19601780	-2.34989042
C	-0.92406159	6.53876784	-1.37881096
C	-2.39081650	5.06803947	-2.56183328
C	-3.37311935	5.05645889	-1.39197096
C	-2.69105945	5.37082927	-0.06578505
C	-1.87672810	6.64559936	-0.18373278
C	-5.30287498	3.57656583	-1.54233815
C	-5.95007794	2.90869807	-0.32265630
C	-5.34887612	1.52760312	-0.14338334
C	-5.50336317	0.72624704	-1.42913409
C	-4.93213614	1.47401288	-2.63150894
C	-5.54329254	-1.68610608	-1.19339676
C	-5.02955297	-2.52199888	-0.01581018
C	-3.57970920	-2.90729036	-0.26255614
C	-3.50770211	-3.64450182	-1.59240080
C	-4.09419954	-2.80166324	-2.72239597
C	-1.81906563	-5.21588042	-2.34104536
C	0.11198230	-4.35331949	-3.44604495
C	1.00964752	-4.96589230	-2.37393332
C	0.28144131	-5.15034429	-1.04897224
C	-0.98690464	-5.94843829	-1.27294909
C	0.73955552	-4.43115952	-4.82834217
C	-4.19498359	-3.57606996	-4.02526828
C	-5.32368606	0.82800774	-3.95118984
C	-3.09900784	5.04524952	-3.90667204
C	1.64137318	5.87742463	-3.64450444
C	5.45618041	2.85167846	-3.60667193
C	4.59756393	-1.68300748	-4.51076453
C	-2.50043230	-7.21974815	0.04477209
C	-6.04145762	-2.40174328	2.17150329
C	-6.83604194	4.00023630	1.63451312
C	-1.55521202	7.86086366	1.87142739
C	4.47407222	5.61656752	2.34275347
C	6.54093374	-0.25343463	2.13118284
C	4.11689588	-6.66306235	-0.41796405
C	5.79816079	-1.05511264	3.18762793
C	5.19987884	4.74674557	3.35916160
C	-0.46238780	8.10823450	2.90207032

C	-6.50520979	5.20555302	2.50502003
C	-7.25096830	-1.50510067	2.43399282
C	-3.50396851	-7.07743770	1.18056433
C	4.05647691	-7.33212110	0.94729043
C	6.34762809	-0.75212533	4.56898036
C	4.23664338	-8.83682148	0.81331433
C	-4.19713757	-8.40407986	1.43739997
C	-8.24814339	-2.21381072	3.33286613
C	-7.65367993	5.50686661	3.45069815
C	-0.90602927	9.15680760	3.90531904
C	5.61992191	5.57130235	4.56129816
H	0.98719955	-6.71046717	4.74009359
H	2.39482742	-7.68557596	5.25600399
H	3.67361778	-5.68228828	5.39249329
H	1.24150173	-2.42697392	-0.30540762
H	0.63364689	-0.30681534	-1.40620620
H	-0.10044784	-0.82853107	3.45524458
H	0.44179981	-4.74417761	6.69325408
H	-1.99608382	-4.60607317	6.50702036
H	-3.03040623	-3.82413395	4.37205837
H	-1.61531429	-3.11431398	2.50782456
H	1.08869129	-3.86709395	1.58401598
H	2.63255706	-1.95716978	3.38898052
H	3.18122474	-2.66235851	1.87645351
H	4.16271340	-3.92390880	3.70075230
H	2.97619330	-4.94895607	2.85243239
H	2.72101810	-3.53179060	5.54398019
H	2.36189192	-5.61156323	6.36719598
H	2.41829605	-6.84583411	3.67123903
H	0.05960239	-3.95623983	-5.55021532
H	-2.34120078	4.98767240	-4.70295275
H	-2.73073181	-5.76800265	-2.59446761
H	-0.73086313	-6.95405696	-1.63676633
H	-0.01808776	-4.15999744	-0.67820303
H	1.98969683	-5.30405913	-0.16057860
H	1.35260656	-5.94429723	-2.73810566
H	-0.11095862	-3.30980266	-3.18448252
H	1.68424067	-3.88031868	-4.83062839
H	-6.61131467	-1.48809867	-1.06031749
H	-5.63201222	-3.43946206	0.01137919
H	-2.96735885	-1.99642307	-0.31453185
H	-2.41597409	-4.30131567	0.44144381
H	-4.08522455	-4.57492456	-1.50965167
H	-3.46851556	-1.90889886	-2.86694791
H	-4.66112068	-2.92736683	-4.78083458
H	-3.19093872	-3.83772802	-4.37177475
H	-5.78925831	-4.54701974	-3.56977070
H	-5.78955615	4.53437085	-1.75597834
H	-7.02913391	2.81944402	-0.51035217
H	-4.27549734	1.65362200	0.05947037
H	-5.47089619	0.03303199	1.07367814
H	-6.56716018	0.53269137	-1.62389378
H	-3.83814849	1.52602434	-2.53826292
H	-4.80509887	1.35161774	-4.76894493
H	-5.00013531	-0.21651613	-3.95149403
H	-6.99230636	1.75139655	-4.07891840
H	-0.40767609	7.49044319	-1.54335782
H	-2.54974191	7.49755336	-0.35340660

H	-1.99425842	4.55068621	0.16127611
H	-4.17139611	4.68801080	0.97052129
H	-4.15559532	5.80222848	-1.58666062
H	-1.71950818	4.20217444	-2.47477665
H	-3.73066255	4.15425304	-3.96717179
H	5.13923074	5.05360942	-1.21627032
H	3.74876033	6.51131880	0.15469902
H	1.75479648	4.21190433	0.22585948
H	0.49349461	5.97280178	1.19961686
H	1.53706765	6.91358353	-1.17182695
H	1.79753125	4.12722944	-2.38726826
H	2.11832555	5.35143025	-4.48557430
H	0.55664500	5.80369879	-3.76316169
H	2.91740209	7.30127020	-3.50389555
H	6.92011409	-0.70708446	-1.59879155
H	6.99356023	1.09680261	0.05288340
H	3.95045458	1.02631414	-0.12094148
H	4.34540929	2.99344923	1.21490301
H	5.93848793	3.17555165	-0.98821878
H	4.13270791	1.40962078	-2.69543557
H	4.69056935	3.63015500	-3.67008373
H	5.46537878	2.29704764	-4.55689623
H	7.35274413	2.80482594	-3.32048300
H	3.34443951	-5.52952749	-2.98366456
H	5.34513754	-4.85545005	-1.69350924
H	3.56040949	-2.68957127	-0.51402487
H	5.70188542	-2.04778846	0.27899844
H	5.95849806	-2.40965173	-2.36943070
H	3.03488027	-1.88026642	-3.02672469
H	4.80271011	-0.62807189	-4.30887386
H	3.85644028	-1.74252975	-5.32184774
H	5.62628824	-3.20665598	-5.05041414
H	0.19513911	-6.23019550	-5.20864663
H	-3.37740408	6.93846902	-3.97415164
H	6.49984299	0.80798997	2.39052101
H	7.58918877	-0.58003312	2.07266965
H	3.58100870	6.07597890	2.78248697
H	5.15421764	6.40697104	1.99330241
H	-2.48500430	7.52632038	2.34822038
H	-1.74609350	8.79564374	1.32450965
H	-7.06480250	3.11564308	2.24302896
H	-7.71114632	4.24647579	1.01630753
H	-5.47189529	-2.55318954	3.09779495
H	-1.83038632	-8.07383368	0.22264324
H	-3.05945346	-7.40216861	-0.88372743
H	5.10307289	-6.85367632	-0.86276160
H	3.35618043	-7.10767547	-1.07985870
H	4.74345733	-0.73858510	3.13300829
H	4.86615454	-6.91317696	1.55725637
H	-2.94470528	-6.77683317	2.08356335
H	-6.89829943	-0.59058952	2.93542522
H	-5.60558469	4.95979456	3.09473880
H	-0.27878267	7.15663520	3.43034090
H	4.49579335	3.96148098	3.68626268
H	-7.87285518	4.65544026	4.10184258
H	-8.55501794	5.75658742	2.88200869
H	-7.40066907	6.36835043	4.07247096
H	-1.81802869	8.85265485	4.42726511

H	-1.09141401	10.10907178	3.39849056
H	-0.11634749	9.31746030	4.64262862
H	4.75729422	6.03097364	5.05204782
H	6.31255349	6.36104390	4.25421438
H	6.13618639	4.93431829	5.28320100
H	6.22973521	0.30561676	4.81887152
H	7.40908696	-1.01233704	4.62461173
H	5.81776836	-1.34614246	5.31845783
H	5.20244274	-9.08778934	0.36366634
H	3.44634151	-9.27173202	0.19180424
H	4.18761417	-9.30778667	1.79797886
H	-3.48641383	-9.18451831	1.72460075
H	-4.73492909	-8.73061091	0.54169060
H	-4.92869489	-8.28328158	2.23919570
H	-7.78639102	-2.53522073	4.27213046
H	-8.65275403	-3.09414061	2.82344281
H	-9.08106678	-1.54694312	3.56584485
H	5.63723997	-2.69774884	2.10016782
H	2.10677378	-7.00320941	1.03684725
H	-4.10915437	-5.24208876	0.96342758
H	-7.50354729	-0.32274544	0.93890889
H	-5.40073082	6.28261493	1.32675076
H	1.13001161	7.82383256	1.83262465
H	6.08376361	3.52614801	2.14154538
H	-6.38560564	-3.38313932	1.82232216

2-HP-B-CD:trans-(1S,4R)-SRT_6_Cl E(Ha)= -7253.8638721465

Cl	0.42170859	0.09574282	-6.06531708
Cl	2.78222775	0.62680297	-3.99955728
O	-6.12613316	-0.40037912	-0.97902008
O	-3.57352359	-3.02941707	-0.88505881
O	-3.33543267	-4.76468727	-2.39245111
O	0.11883104	-5.17473529	-1.27431440
O	1.91480791	-5.48186375	-2.69055046
O	3.66063370	-3.18113326	-0.46933030
O	5.75541397	-2.21403072	-0.74572883
O	4.42257608	1.13591351	-0.07095290
O	5.17794461	2.94752019	-1.30063959
O	1.96082119	4.64919147	-0.93018039
O	0.90921937	5.61299935	-2.73571831
O	-2.16499548	4.74293691	-0.97570564
O	-4.13945274	4.35658468	-2.13040806
O	-3.61549849	5.62401328	1.24389436
O	-4.81159112	3.08837833	1.75855546
O	-4.56927312	1.19930755	-0.33675289
O	-1.15707227	6.88148567	0.60162510
O	1.70593999	6.95572858	0.54913517
O	-1.24248553	6.08301488	-4.37272377
O	2.88747603	4.61068399	1.73406426
O	4.74391518	2.50452216	2.28579738
O	4.77971012	5.25107043	-2.96339107
O	3.94798283	-2.97383975	2.33902579
O	3.93546779	-0.17739595	2.38515612
O	3.32852872	-5.46990860	1.21947799
O	1.11845044	-7.11092026	0.45751596
O	4.42916567	-4.97520307	-3.68479687
O	-1.84192744	-6.58048693	-3.98768337
O	-3.90243959	-4.85277709	1.20351188
O	-1.34500411	-5.95684250	1.05125421
O	-3.63617887	-2.20489445	1.83979865
O	-4.80074173	0.31348085	2.34948534
O	-6.85619123	-2.92830656	-2.08543416
O	-6.26609000	2.96976171	-3.13466100
O	7.55879187	-0.09434145	-1.24797185
O	-6.00347112	-3.47958490	2.65462987
O	-7.14402735	1.83024283	2.69434038
O	-3.60053561	8.25608417	0.28433160
O	4.46393610	6.90379748	1.44021063
O	6.29398140	0.44879652	3.70562591
O	5.80679132	-5.04516627	2.58509621
O	-1.34210898	-8.67119205	0.42906900
N	0.05812091	-1.45722879	3.94678956
C	-1.39324899	-1.09974975	4.02266271
C	-1.20092136	-0.90006299	-2.55629299
C	-1.01051287	-0.66217681	-3.91242702
C	0.20886982	-0.17886129	-4.37726584
C	1.23745068	0.06844538	-3.45931428
C	1.03294593	-0.14974937	-2.09912395
C	-0.18612972	-0.64641901	-1.63165764
C	-0.18237354	0.19611359	0.76711405
C	0.42926632	0.03828089	2.01924819
C	0.72529350	1.16267237	2.80256815
C	0.30789469	2.42800488	2.41995275

C	-0.39977847	2.57047067	1.22730863
C	-0.60417015	1.47703287	0.39868108
C	-0.39103132	-0.98184563	-0.16766759
C	0.48349701	-2.16706510	0.24114449
C	0.27929212	-2.49118222	1.71233357
C	0.73911925	-1.32597233	2.57455621
C	-5.15523645	-1.29838208	-1.50401298
C	-4.62668170	-2.20747387	-0.39257991
C	-4.09795670	-1.38221880	0.77502300
C	-5.22067717	-0.46320125	1.24295582
C	-5.66055457	0.41716912	0.06667447
C	-3.89523943	-4.38264310	-1.17610208
C	-1.90859991	-4.69368106	-2.46504746
C	-1.26097659	-5.50860579	-1.34485993
C	-1.85608490	-5.15358384	0.01467783
C	-3.36828890	-5.27019401	-0.03857102
C	1.10798842	-6.07716897	-1.71978254
C	1.94711739	-6.48267717	-0.49740400
C	2.54141105	-5.21381142	0.08055509
C	3.35035580	-4.47463032	-0.98226270
C	2.58004992	-4.27935241	-2.29111667
C	4.92826153	-2.96647198	0.09712790
C	5.28230851	-0.90414472	-1.06554461
C	5.05259794	-0.10110604	0.21626103
C	4.13717015	-0.86195818	1.16350351
C	4.74911155	-2.22763238	1.42899025
C	5.22510267	2.30115840	-0.06544530
C	4.72125206	3.21448485	1.06021926
C	3.31424035	3.69397649	0.74527549
C	3.31299264	4.33443468	-0.63847451
C	3.87411859	3.38616956	-1.69346053
C	1.68077255	5.86021956	-1.59584869
C	0.92587695	6.76943512	-0.61358829
C	-0.36291802	6.07210218	-0.22982596
C	-1.15399458	5.62676068	-1.45583468
C	-0.30108305	4.89400717	-2.49029471
C	-3.51526490	5.09876068	-1.11506257
C	-4.16063931	2.94084060	-1.94887391
C	-4.78396881	2.58274936	-0.60018283
C	-4.15613977	3.37066381	0.54346744
C	-4.21713381	4.85353231	0.22651353
C	-4.97930912	2.41167967	-3.11697171
C	-0.99507373	4.80744086	-3.84018711
C	4.04114210	4.05574253	-3.04591923
C	6.35057083	-0.27787677	-1.94543491
C	3.51125130	-3.94069361	-3.44492593
C	-1.53025043	-5.21831016	-3.83947869
C	-5.85126381	-2.08748866	-2.60007326
C	-4.43023502	6.62486733	1.85411033
C	2.57604786	8.08292918	0.48933409
C	5.91599148	2.75604911	3.06318259
C	4.55758421	-3.25360791	3.60368641
C	1.06758644	-8.53267728	0.32372980
C	-5.15185436	-5.45822141	1.54073845
C	-5.58608776	0.18525917	3.53711462
C	-5.68648284	-4.84606733	2.82665014
C	-0.14726857	-9.08680097	1.05275117
C	5.01024987	-4.71067723	3.70585164

C	6.02819587	1.74514970	4.19445939
C	3.59648614	8.00378668	1.61492119
C	-3.83155398	8.01534834	1.65843579
C	-6.39321889	1.45036005	3.82939966
C	-6.95157606	-5.55965520	3.26574226
C	-7.33920868	1.21276554	4.99303050
C	-4.77448845	9.07721332	2.19554050
C	4.44436292	9.26245526	1.64965843
C	7.16301413	2.12599618	5.12829002
C	5.81324820	-4.92837804	4.97593925
C	-0.11788987	-10.60493268	1.04234264
H	-1.97010030	-1.65117529	3.27673407
H	-1.49139967	-0.03227621	3.83196956
H	-1.74553115	-1.34041663	5.02663866
H	0.56789758	-0.87217801	4.61132027
H	0.18741475	-2.42348523	4.25739514
H	-2.14645142	-1.31155988	-2.21411242
H	-1.80381131	-0.85665563	-4.62677067
H	1.84250694	0.07520094	-1.40979868
H	1.30173103	1.05079970	3.72071283
H	0.55031770	3.29418062	3.02641015
H	-0.78263999	3.53760626	0.92570580
H	-1.10361124	1.61506151	-0.55600842
H	-1.43331601	-1.31144594	-0.06588796
H	1.53943999	-1.95823114	0.04292083
H	0.22854779	-3.03731213	-0.36815139
H	0.82985190	-3.39477457	1.99702218
H	-0.78746725	-2.69129589	1.87602766
H	1.81192585	-1.40830409	2.79580789
H	-4.31573825	-0.73297253	-1.93465217
H	-5.45536623	-2.82925592	-0.02991302
H	-3.26965767	-0.74882006	0.43234964
H	-6.08575950	-1.07514199	1.52619797
H	-6.51017376	1.03516500	0.36970989
H	-4.97944383	-4.48393036	-1.29829237
H	-1.58097694	-3.64971845	-2.37072094
H	-1.39087967	-6.58179116	-1.53783389
H	-1.62077520	-4.09686101	0.21126029
H	-3.65044182	-6.31412180	-0.23669300
H	0.64139525	-6.94535545	-2.19838065
H	2.74873448	-7.16351748	-0.81524055
H	1.69793662	-4.57004127	0.35719572
H	4.27104304	-5.03249987	-1.20028482
H	1.84538500	-3.47489714	-2.15443223
H	5.45090283	-3.91128985	0.26779367
H	4.33698202	-0.96743267	-1.62310061
H	6.01976876	0.06732768	0.70894391
H	3.16739588	-0.99538703	0.66446537
H	5.75127394	-2.09569295	1.85323084
H	6.27525898	2.02894679	0.08797076
H	5.37954612	4.09200843	1.12306939
H	2.63689773	2.82750966	0.72780186
H	3.92197397	5.24748723	-0.60621786
H	3.20404247	2.52307347	-1.79639167
H	2.60766907	6.32433621	-1.95048464
H	0.70830116	7.73316318	-1.09512502
H	-0.05878823	5.16628850	0.30961485
H	-1.60665571	6.50232854	-1.94033396

H	-0.06771557	3.88807430	-2.11621474
H	-3.61719149	6.15188366	-1.39594422
H	-3.13841499	2.53654011	-1.99066623
H	-5.86002509	2.79671899	-0.65461095
H	-3.10030420	3.07871907	0.61956906
H	-5.26704007	5.14994583	0.10455803
H	-4.43179031	2.60931350	-4.05101787
H	-5.09934953	1.32968453	-3.01169102
H	-0.38200453	4.19130471	-4.51510577
H	-1.96596508	4.31914603	-3.71343199
H	4.50359393	3.33517210	-3.73572059
H	3.05479089	4.31427671	-3.44183372
H	6.48134535	-0.90728288	-2.83722580
H	6.01343652	0.71067354	-2.27010634
H	2.90626210	-3.71099999	-4.33433650
H	4.08872654	-3.04845866	-3.18655766
H	-0.44861355	-5.11793988	-3.97206219
H	-2.02444917	-4.59595755	-4.59972478
H	-5.12227433	-2.73050758	-3.10276232
H	-6.24961379	-1.37926297	-3.34019743
H	-4.52572693	6.38858695	2.92102558
H	-5.43282825	6.60655553	1.40987599
H	1.97848996	9.00198836	0.57206007
H	3.11845930	8.10270752	-0.46690883
H	5.86309181	3.77859207	3.46160614
H	6.81537135	2.66908820	2.43711426
H	3.81627016	-3.03535659	4.38297380
H	5.40798370	-2.58036211	3.76216432
H	1.99603765	-8.95855493	0.72876209
H	0.98501838	-8.81308300	-0.73564433
H	-4.99755453	-6.53845256	1.66672434
H	-5.88794383	-5.29806280	0.74016004
H	-4.89966268	-0.01987927	4.36906420
H	-6.26199508	-0.67335614	3.44359269
H	-4.91125482	-4.96714750	3.60132337
H	-0.10814201	-8.73000318	2.09527663
H	4.11432750	-5.34914836	3.72731823
H	5.07678938	1.76341822	4.75439139
H	3.04259627	7.91183552	2.56355164
H	-2.88077559	8.06456033	2.21098100
H	-5.68908421	2.25422051	4.09336171
H	-6.76949325	-6.62142898	3.45350518
H	-7.72710920	-5.46554816	2.49924119
H	-7.32926296	-5.10287889	4.18296263
H	-6.80474240	0.87030327	5.88516803
H	-8.08427317	0.45827690	4.72206581
H	-7.86803595	2.13605549	5.23898428
H	-5.01708473	8.90530724	3.24903710
H	-5.70494680	9.08032815	1.61893162
H	-4.31713987	10.06441167	2.10080864
H	3.83353395	10.15525988	1.81115705
H	4.99297337	9.37714143	0.70928223
H	5.17562574	9.18869766	2.45743963
H	7.00007282	3.10788424	5.58130627
H	8.11255138	2.14284348	4.58413348
H	7.24711332	1.38233209	5.92377588
H	5.25071967	-4.62872913	5.86635674
H	6.73939262	-4.34691475	4.93751930

H	6.07989618	-5.98281065	5.07415958
H	0.77811541	-10.99557137	1.53319754
H	-0.14660633	-10.97785937	0.01358145
H	-0.99767762	-10.99018393	1.56198724
H	-4.60716024	2.15644759	1.96557654
H	-1.89384865	6.31885078	0.91213364
H	-0.38426282	6.51477972	-4.45537449
H	2.24530156	5.21320498	1.31319452
H	5.65352024	5.02287965	-2.62639317
H	3.95619802	0.78358988	2.19227088
H	3.46011814	-4.59702690	1.63707392
H	3.90970500	-5.75261220	-3.91947755
H	-2.79889602	-6.66219436	-3.90796574
H	-0.40237152	-6.13937740	0.85877771
H	-3.56043494	-3.12333509	1.50290931
H	-7.51689803	-2.35791456	-1.67552007
H	-6.14536240	3.92435638	-3.20236259
H	7.87270723	-0.97036709	-0.99635462
H	-5.17470020	-2.97890926	2.59495273
H	-6.62644081	2.50838697	2.23573889
H	-2.67073783	8.04191482	0.12053576
H	3.99160015	6.10018686	1.71376782
H	5.47745154	0.11309582	3.30153574
H	5.25936120	-5.56831582	1.98574816
H	-1.53769333	-7.77086280	0.73461350

2-HP-B-CD:trans-(1S,4R)-SRT_1_MD E(Ha)= -7253.92994592

C	0.6161671099	0.4057929131	3.9952712526
C	0.4873167441	0.5645987061	2.4945994482
C	0.8277820286	1.7675271348	1.8577778456
C	1.2062701567	3.0167661362	2.6298877842
C	1.6588292469	2.6847436341	4.0614209031
C	0.6746006322	1.7361198080	4.7280500807
C	0.0958440792	-0.5433324630	1.7358454293
C	0.0766738112	-0.4847089226	0.3498832826
C	0.4443072914	0.6944114727	-0.2944306645
C	0.7909406662	1.8105324512	0.4591473921
C	0.0947528318	4.0550306312	2.6671528250
C	0.4352161116	5.4066750246	2.7957784987
C	-0.5487673704	6.3777770506	2.9076705614
C	-1.8969230344	6.0226798283	2.9202311140
C	-2.2445886738	4.6746949206	2.8135957661
C	-1.2547218462	3.7043890463	2.6634136190
Cl	-3.0957470758	7.2569880156	3.0774187171
Cl	-3.8986055821	4.1668758553	2.9088711047
N	1.8523447852	-0.4384018262	4.2311325350
C	2.3604419669	-0.5156671749	5.6141690585
C	5.4982095760	-0.9947240737	-0.7006760503
C	5.1899965007	-0.0470284705	0.4604996472
C	4.0548973938	-0.5870457772	1.3276047741
C	4.2411025012	-2.0394557401	1.7216438084
C	4.5969411556	-2.8675276695	0.4756816097
O	5.7167034594	-2.2977092811	-0.1568224579
O	3.4706888796	-2.8968108203	-0.3585445215
C	3.4785566464	-3.8935509623	-1.3776616222
C	2.9994085084	-5.2280871427	-0.8138703191
C	2.6673723936	-6.2094247975	-1.9263139431
C	1.6526476669	-5.5675220865	-2.8674657121
O	2.2193649145	-4.4193975268	-3.4238897044
C	2.5040342547	-3.4021960118	-2.4646976295
O	0.5307351757	-5.2575409229	-2.0910003821
C	-0.7809509834	-5.5970972900	-2.5046708741
C	-1.4508363045	-5.9718815473	-1.1893789119
C	-2.9432074263	-6.2120092118	-1.3561928803
C	-3.5463547083	-5.0106941874	-2.1026552459
O	-2.8793288395	-4.8125302966	-3.3154531236
C	-1.5104424341	-4.4245248725	-3.1504354315
O	-3.3994749614	-3.8350956779	-1.3539721579
C	-4.3523931851	-3.3930604190	-0.3852951382
C	-3.4700873697	-2.8050918105	0.7129687391
C	-4.1716240550	-1.7642727201	1.5681802074
C	-4.8264698500	-0.7463193165	0.6310816213
O	-5.8116844293	-1.4171568238	-0.1218675103
C	-5.3213545608	-2.3905545132	-1.0389691854
O	-3.6235652914	-6.3117230529	-0.1242044472
C	-3.5824328719	-7.5789175276	0.5253792952
C	-3.0526417132	-7.4121168126	1.9505645054
O	-1.8754775703	-6.6253637997	1.9460229699
O	-0.7976720005	-7.1082275348	-0.6237824256
O	2.1397127872	-7.3762815195	-1.3154411457
C	2.3862507099	-8.5863780074	-2.0418417371
C	1.1935498128	-9.5227072364	-1.9403668591
O	0.0711764609	-8.9440657109	-2.5770065104

O 3.9779679811 -5.7718211774 0.0493957990
O 3.0510439615 -2.4684261071 2.3452027417
C 3.1776156261 -3.6123038966 3.1676662210
C 1.7858584360 -4.1032613420 3.5388331994
O 1.1087417184 -3.0411923480 4.2014136319
O 3.9688687022 0.2124274567 2.5079447321
O 4.6937510299 1.2366268784 0.0988115382
C 5.4556416254 2.0789959042 -0.7219547031
C 5.2675183852 3.5207463923 -0.2347374086
C 3.8291990918 3.9513800657 -0.4876583073
C 3.3898450300 3.6448863453 -1.9147758680
C 3.6482612585 2.1791557020 -2.2504945302
O 5.0536198718 1.9577366426 -2.0660169148
O 5.6249916451 3.5380064684 1.1239530000
C 6.0289904436 4.7879199169 1.6639355951
C 5.1639959574 5.1607920480 2.8668170449
O 3.7923525747 5.2095603860 2.5206639595
O 3.6589114876 5.3351449260 -0.2232557505
O 2.0103160834 3.9716460536 -1.9587339971
C 1.5318854032 4.8535441317 -2.9421851670
C 0.6251454838 5.8757542860 -2.2506481300
C -0.5928065815 5.1637675420 -1.6992073483
C -1.2757727178 4.3065482713 -2.7630055122
C -0.2715629709 3.4072493918 -3.4855376640
O 0.8452215838 4.1767732143 -3.9467966683
O 1.3889037857 6.4919642438 -1.2357050606
C 1.1551669688 7.8817301041 -1.0170194754
C 2.2456583643 8.4053096953 -0.0954695925
O 3.5193339332 8.2979337368 -0.6916326360
O -1.5177840683 6.0854562551 -1.1526481397
O -2.2064364287 3.5545939234 -2.0018876493
C -3.4476396675 3.2209631350 -2.5514055307
C -4.4870660478 3.2909025099 -1.4357357683
C -4.2657670432 2.1937928804 -0.3958652130
C -4.1858712494 0.8288114121 -1.0760170654
C -3.0881030534 0.9124976033 -2.1489218425
O -3.4486466337 1.9225227080 -3.0921482906
O -4.4732325577 4.5330394953 -0.7646831418
C -5.4084926518 5.5062814141 -1.2232352848
C -4.7084012365 6.7805581197 -1.6709243092
O -3.8230139313 6.4913796115 -2.7385496227
O -5.3261161411 2.2056335261 0.5309675042
O -3.8131796452 -0.1990102356 -0.1695273244
O -3.2300228186 -1.1324278247 2.4058735345
C -3.3594047640 -1.3146590931 3.7975334455
C -2.8322161578 -2.6594583419 4.3147806756
O -1.5799992771 -2.9634740339 3.7121809429
O -2.9480085905 -3.8187176447 1.5560270719
C -6.5791394207 -3.0647795128 -1.5690747263
O -7.2799941280 -3.7260810163 -0.5463065649
C -2.8323675767 -0.3664298281 -2.9193367182
O -1.5460138743 -0.3149452252 -3.5067400793
C -0.8233499863 2.6954813075 -4.7114203608
O -0.1309018926 1.4864753102 -4.9648144105
C 3.2576844243 1.7408925008 -3.6661857910
O 2.0935103979 0.9359445474 -3.6191619349
C 6.7656193567 -0.6877162311 -1.4838123060
O 7.8783089607 -0.4554879013 -0.6539483325

C	3.0178577617	-2.2214275792	-3.2580115721
O	2.0205149733	-1.7429369824	-4.1254021520
C	-0.9685773432	-3.9661335011	-4.5114266824
O	-0.5455405582	-2.6215052047	-4.4958378175
C	-4.0489287348	-6.7487323128	2.8823480188
C	1.0124185580	-4.6025573005	2.3303679311
C	5.3229335326	4.1825657325	4.0159166261
C	2.0185596229	9.8709640554	0.2222177469
C	-5.7197808595	7.8210363373	-2.1204658804
C	1.5023467600	-10.8474074852	-2.6147307007
C	-2.6685914247	-2.6360753514	5.8203853678
H	-4.5948220657	-5.2180992649	-2.3430057805
H	-3.1113527698	-7.1102767548	-1.9686245404
H	-1.3208106533	-5.1180776330	-0.5104471373
H	-0.7611511582	-6.4606934767	-3.1848175120
H	1.3881401296	-6.2310388917	-3.6988902107
H	3.5809161627	-6.4452622008	-2.4876055745
H	2.0762378305	-5.0201282915	-0.2579999950
H	4.4922797502	-4.0046662877	-1.7890405235
H	4.9071294964	-3.8810689256	0.7402404026
H	5.0922681056	-2.1123922117	2.4166624944
H	3.1180997184	-0.5043753073	0.7589660379
H	6.0997270802	0.0639884509	1.0664422598
H	6.5165992795	1.8133991134	-0.6805378751
H	5.9426878830	4.1555111657	-0.8287808011
H	3.1951513292	3.3677424995	0.1924502186
H	3.9546846697	4.2800151494	-2.6135526096
H	2.3664049295	5.3705663329	-3.4304267341
H	0.3210690879	6.6196838652	-2.9999026930
H	-0.2498670040	4.4846564154	-0.9074896376
H	-1.8019233230	4.9525991711	-3.4807004797
H	-3.7060567557	3.9058179580	-3.3667610628
H	-5.4715456105	3.1141841482	-1.8907608289
H	-3.3040744403	2.3718965837	0.1103458700
H	-5.1542684432	0.5955569175	-1.5416048877
H	-5.3567927637	0.0337842189	1.1825840713
H	-4.9785662103	-2.2276627142	2.1533473797
H	-2.6499123534	-2.2760513348	0.2118378063
H	-4.9291599832	-4.2313969287	0.0217149568
H	-4.7952046806	-1.9106232038	-1.8724836507
H	-2.1496485932	1.1846449513	-1.6483925336
H	0.0675433463	2.6552593408	-2.7622919101
H	3.0857800938	1.5456505046	-1.5550291776
H	4.6476728868	-1.0072405395	-1.3884323288
H	1.5734852593	-3.1030254044	-1.9645738396
H	-1.4476686567	-3.5624082806	-2.4766353179
H	0.1624797561	-6.9436949415	-0.7160210355
H	-2.2019950757	5.5378900615	-0.7318436105
H	-2.8858279210	-4.6768319591	1.1018828768
H	3.6888878504	-6.6746767915	0.2359979751
H	4.0306220067	1.1286093429	2.1968339252
H	2.7468363674	5.5750410068	-0.5015962831
H	-5.3269848360	3.0953220566	0.9074282027
H	-2.9355677058	-8.2625471862	-0.0350886217
H	-4.5938803100	-8.0042929562	0.5432790439
H	-2.8388565985	-8.4259502410	2.3296050940
H	-4.3567440904	-5.7748881842	2.4930073156
H	-3.5907747713	-6.5967352853	3.8631280517

H	-4.9362948245	-7.3754522827	3.0077869281
H	-1.3112303880	-6.9525514840	1.2266242268
H	3.7468129569	-3.3629273416	4.0779648977
H	3.7045355652	-4.4260896992	2.6514758288
H	1.9239519283	-4.9355553646	4.2465657754
H	0.0070052391	-4.9307715048	2.6099275625
H	1.5304205186	-5.4632855139	1.8964431258
H	0.9524567689	-3.8156865359	1.5728600904
H	0.1354422466	-3.1606005269	4.1394402621
H	5.9644974129	5.5761004025	0.9043303565
H	7.0777264853	4.7146820131	1.9823142002
H	5.5086315147	6.1554169706	3.1981719319
H	5.1209831954	3.1622154037	3.6762243251
H	4.6222461203	4.4324152859	4.8170633057
H	6.3381346835	4.2181506699	4.4221056395
H	3.7256269743	5.4698811234	1.5837352322
H	0.1604086924	8.0250559336	-0.5791357708
H	1.2098254606	8.4182777599	-1.9747589196
H	2.2035034242	7.8205877605	0.8405134771
H	1.0511119015	10.0309835002	0.7066134306
H	2.0563008100	10.4654264743	-0.6956954783
H	2.8074108453	10.2294459314	0.8867661456
H	3.7573225227	7.3644612739	-0.7491150951
H	-2.8844115226	-1.2076253190	-2.2196867636
H	-3.6195211562	-0.4904031082	-3.6783256611
H	-1.3100621879	-1.2035351574	-3.8572801088
H	-1.8854355880	2.4803913975	-4.5703345116
H	-0.7032862328	3.3560797698	-5.5766945993
H	-0.6721464051	0.7861806870	-4.5371279464
H	-6.1052276805	5.7290449495	-0.4047142388
H	-5.9884737190	5.1087833265	-2.0661292694
H	-4.1435952218	7.1750698223	-0.8121383691
H	-6.2880559093	7.4523079412	-2.9804602114
H	-5.2026074610	8.7328752263	-2.4271374654
H	-6.4234917768	8.0736346916	-1.3211428079
H	-2.9252992080	6.5399814537	-2.3765912433
H	3.0951958697	2.6048868639	-4.3203295563
H	4.0975728360	1.1631658736	-4.0716794275
H	1.3682883407	1.2984854980	-4.1873192273
H	3.2948636839	-9.0598001308	-1.6462638359
H	2.5470891985	-8.3609213916	-3.1032077948
H	0.9818576711	-9.6985088008	-0.8737962372
H	2.3661302839	-11.3405419601	-2.1593562090
H	1.7078474400	-10.6924768606	-3.6785496889
H	0.6395775051	-11.5118478158	-2.5346568115
H	-0.4363657297	-8.4655943420	-1.9051967931
H	6.9354884448	-1.5353300415	-2.1638356422
H	6.6212712257	0.2015526801	-2.0994837204
H	8.0460403271	-1.2733699283	-0.1720814333
H	-4.4021908325	-1.1795164492	4.1246968588
H	-2.7676445743	-0.5059788735	4.2434911909
H	-3.5417823385	-3.4509450570	4.0384889198
H	-2.3262155000	-3.6080651305	6.1835692503
H	-3.6161893562	-2.4010948949	6.3144512188
H	-1.9347996867	-1.8789989898	6.1194143279
H	-1.8130396133	-3.3070850970	2.8240828584
H	3.3078025829	-1.4406116477	-2.5496218352
H	3.9095838887	-2.5317091833	-3.8239162481

H	2.0153535293	-0.7642062761	-4.0442370393
H	-7.1971047905	-2.2991074755	-2.0603025800
H	-6.3204564271	-3.8130636481	-2.3244438080
H	-7.5144075317	-3.0459504130	0.0965935696
H	-0.1514227949	-4.6117045997	-4.8531853320
H	-1.7873358767	-4.0574736826	-5.2327762435
H	0.4223043903	-2.5352661601	-4.3618261018
H	2.6151604883	-0.1426682810	3.5839323802
H	1.6089625103	-1.4222435509	3.9596273530
H	1.5530768084	-0.8175667699	6.2830167884
H	2.7719718348	0.4433814436	5.9270398279
H	3.1445065320	-1.2727703824	5.6434315526
H	1.4848711156	5.6906182719	2.8284906760
H	-0.2843152357	7.4259751817	2.9999238018
H	-1.5563185690	2.6679260617	2.5456683553
H	-0.2036664995	-1.4516570449	2.2474858117
H	-0.2212836368	-1.3528607674	-0.2299899828
H	0.4725590746	0.7340687681	-1.3800156858
H	1.0484710025	2.7348946750	-0.0506188356
H	2.0619072613	3.4912668388	2.1360426560
H	1.7625609916	3.6103526423	4.6341630761
H	2.6603711431	2.2351542020	4.0275155580
H	-0.3314949393	2.1695980503	4.6952747988
H	0.8988982243	1.5944386130	5.7895678588
H	-0.2105245343	-0.2033522473	4.3773367494

2-HP-B-CD:trans-(1S,4R)-SRT_2_MD E(Ha)= -7253.91927192

C	-0.6454234574	-0.0187068503	3.7539859612
C	-0.3972225853	-0.0152971273	2.2612921946
C	-0.3067942088	-1.2063268710	1.5266972312
C	-0.3921431107	-2.5761173589	2.1748841270
C	-0.9864025876	-2.5119170024	3.5933793810
C	-0.3851884291	-1.3708559124	4.3962078859
C	-0.3277095902	1.2168752430	1.5990241293
C	-0.1760334999	1.2760732095	0.2213085462
C	-0.0913800836	0.0972009547	-0.5193628861
C	-0.1481393056	-1.1267738763	0.1361732451
C	0.9169373246	-3.3494981740	2.1558595182
C	0.8695559366	-4.7222483985	1.8900121976
C	2.0173181559	-5.5009826262	1.9147232832
C	3.2423119775	-4.9247727147	2.2382890458
C	3.3024929530	-3.5554265577	2.5153215415
C	2.1525817363	-2.7679673601	2.4462627636
Cl	4.6594116046	-5.9154644763	2.2644117951
Cl	4.8037974755	-2.8151607861	2.9531455037
N	-2.0678963682	0.4729227847	3.9535823948
C	-2.6184341662	0.3673762066	5.3199988645
C	-5.5897269025	0.4787601006	-1.0746257148
C	-5.1113549970	-0.4237099238	0.0607044098
C	-4.2192568345	0.2946044189	1.0631398518
C	-4.7616512846	1.6480198473	1.4669837609
C	-5.1338496361	2.4243823742	0.1913544647
O	-6.1001080559	1.6947329168	-0.5289753141
O	-3.9490179730	2.5964250858	-0.5365809872
C	-3.9578431227	3.5120443857	-1.6312698984
C	-3.8990879338	4.9449314447	-1.1123696573
C	-3.3257743481	5.9309576888	-2.1180660383
C	-2.0136193247	5.3795197563	-2.6699307918
O	-2.2782576137	4.1720245927	-3.3265569842
C	-2.6930668676	3.1420892878	-2.4282531612
O	-1.1680421420	5.1629466035	-1.5786831384
C	0.1223753855	5.7462002419	-1.4990107630
C	0.2670782126	5.9406611133	0.0082801365
C	1.6761756342	6.2732443350	0.4877198315
C	2.7393434278	5.5161458544	-0.3495274130
O	2.4420629508	5.5714119615	-1.7220608629
C	1.2356992545	4.8516598752	-2.0112200217
O	2.7351434838	4.1818806257	0.0521988455
C	3.8654274727	3.5743760740	0.6606388887
C	3.2183542362	2.5063710266	1.5139753806
C	4.2376373385	1.5576955840	2.1028651556
C	5.0317900579	0.9725057355	0.9239926377
O	5.6931584967	2.0329327080	0.2632351704
C	4.8383711807	2.9849160465	-0.3590085740
O	1.8824039892	5.8599842707	1.8311657921
C	1.1766739928	6.5746120650	2.8370120023
C	1.2527087455	5.8275993594	4.1647958885
O	0.5733257603	4.5719558986	4.0442049119
O	-0.6596332623	6.9275681925	0.4440811998
O	-3.1218249931	7.1351873529	-1.3973014728
C	-3.1290273778	8.3177104001	-2.1967201407
C	-2.2824730436	9.3901855391	-1.5270619481
O	-0.9241553468	9.0039343274	-1.5036842311

O -5.1877814313 5.3489889186 -0.6957950051
O -3.7570690971 2.2925320675 2.2227344534
C -4.2092750507 3.2384923576 3.1686122106
C -3.0413202455 4.1280357137 3.5593101489
O -2.0133200970 3.2959867146 4.0850753304
O -4.0540785941 -0.5299353076 2.2164670168
O -4.2585851286 -1.4621401525 -0.3809356019
C -4.7866982871 -2.5910877869 -1.0139773431
C -4.2585060248 -3.8074572735 -0.2393361226
C -2.7657733569 -3.9495423370 -0.4796281690
C -2.4461583005 -3.8822301340 -1.9687764469
C -2.9645735413 -2.5518364637 -2.5108622724
O -4.3912937230 -2.6067045269 -2.3607065553
O -4.5529450225 -3.5664286176 1.1225794424
C -4.8994641097 -4.7094726116 1.8818562544
C -5.2396452783 -4.2855709955 3.3038156554
O -4.1112857173 -3.7354116802 3.9712499488
O -2.2715794407 -5.1398162475 0.1040882294
O -1.0414287019 -4.0290039319 -2.0550548729
C -0.5131789042 -4.8861680601 -3.0387513333
C 0.4737798084 -5.8368237923 -2.3521758512
C 1.6242395632 -5.0231846324 -1.8040867854
C 2.2200743906 -4.1065230557 -2.8749780375
C 1.1475848512 -3.2892655414 -3.5989120833
O 0.1079869262 -4.1649634317 -4.0534506732
O -0.1960989219 -6.5301926488 -1.3169324844
C -0.5684171427 -7.8653762935 -1.6614895175
C -1.6811996349 -8.3524896266 -0.7473975706
O -2.8796078444 -7.6499869745 -0.9885433171
O 2.6338000511 -5.8670353491 -1.2826562309
O 3.1121511969 -3.3109763903 -2.1110370095
C 4.2129857943 -2.7212920460 -2.7372803377
C 5.3816344925 -2.7240473907 -1.7564297190
C 5.1039310512 -1.8149202238 -0.5651915302
C 4.6414893851 -0.4276991818 -1.0063502668
C 3.5049905796 -0.5770624970 -2.0338490330
O 3.9457326607 -1.3931223435 -3.1152845643
O 5.6608318593 -4.0096414744 -1.2476018546
C 6.5411344294 -4.8053808792 -2.0339746707
C 5.9401208736 -6.1734421160 -2.3175992343
O 4.7826289436 -6.0312050667 -3.1231313991
O 6.2754313000 -1.6713288332 0.2060073210
O 4.1145346276 0.3049801026 0.0930607324
O 3.5689818610 0.5731842248 2.8640499276
C 3.8417053434 0.5369432146 4.2527166728
C 3.2246545408 1.6853560704 5.0599671372
O 1.8552812672 1.8699458182 4.7261601930
O 2.4853216595 3.1310356952 2.5431556275
C 5.7052498400 4.0378265032 -1.0236261922
O 6.1698667296 4.9526935920 -0.0527269648
C 3.0287412888 0.7316025269 -2.6253883802
O 1.8478229543 0.5416925337 -3.3803783879
C 1.6191113263 -2.5495877804 -4.8462929990
O 0.8379800438 -1.3967653493 -5.0960592744
C -2.6063148824 -2.1994705546 -3.9562194125
O -1.5986890207 -1.2049830729 -3.9575193817
C -6.7114659656 -0.1137711004 -1.9100612472
O -7.7739043157 -0.6079475635 -1.1293667592

C	-2.8363687047	1.8874759103	-3.2604766258
O	-1.5866755921	1.5672668989	-3.8117008346
C	1.2005370525	4.4364353197	-3.4859052476
O	0.7809649196	3.0969740871	-3.6407069422
C	2.6755255676	5.6429765855	4.6634378409
C	-2.5403732690	4.9489889263	2.3856941840
C	-6.3415126946	-3.2461261174	3.3757477318
C	-1.9535365843	-9.8264037772	-0.9891747648
C	6.9414617803	-7.0632464742	-3.0351571522
C	-2.3868681329	10.7017953398	-2.2834394077
C	3.3269799747	1.4093171460	6.5461384884
H	3.7266284443	5.9702802144	-0.2161752070
H	1.8512883687	7.3540045887	0.3829303729
H	0.0069797090	4.9706898447	0.4597912432
H	0.1428323282	6.7177036156	-2.0114045345
H	-1.5563357241	6.0509382770	-3.4053896029
H	-4.0344955895	6.0798368102	-2.9438080920
H	-3.2097005268	4.9288719613	-0.2593678620
H	-4.8664844715	3.3798647550	-2.2359655167
H	-5.6009785409	3.3882116944	0.4139181461
H	-5.6763337977	1.5151074310	2.0626298251
H	-3.2428491112	0.4561532793	0.5883583468
H	-5.9886381721	-0.8343164126	0.5802652450
H	-5.8816943091	-2.5802284069	-1.0019720534
H	-4.7768341994	-4.7090732278	-0.5966083287
H	-2.2811929989	-3.0834563744	-0.0084198057
H	-2.9474416073	-4.7066130329	-2.4977036675
H	-1.3182871077	-5.4574602355	-3.5165372679
H	0.8529342616	-6.5420792842	-3.1032811312
H	1.2352543046	-4.3826693905	-1.0004190130
H	2.7863100753	-4.7123037459	-3.5969929899
H	4.4674954127	-3.2647545763	-3.6546406134
H	6.2558475023	-2.3185789673	-2.2862106320
H	4.2923819274	-2.2551265329	0.0333864673
H	5.4890358534	0.1105957506	-1.4546173639
H	5.8235206427	0.2976292223	1.2548390809
H	4.9581998049	2.1099531584	2.7217799738
H	2.5458370927	1.9124231703	0.8809751693
H	4.3957211781	4.2876810111	1.3023712528
H	4.2520763500	2.5047031830	-1.1492894029
H	2.6536873336	-1.0550204872	-1.5319236465
H	0.7320519484	-2.5566092647	-2.8947799196
H	-2.5615414752	-1.7337756215	-1.9018837616
H	-4.7401646293	0.6911489067	-1.7284983920
H	-1.8983416352	2.9664067982	-1.6946167524
H	1.2367492111	3.9124188077	-1.4501220273
H	-1.5092117432	6.6982846010	0.0255681920
H	3.2909935724	-5.2609599245	-0.9029554216
H	2.0328900868	3.9166118754	2.1828913272
H	-5.1030650233	6.2755500260	-0.4365999849
H	-3.9876763187	-1.4493135149	1.9007118074
H	-1.4190736497	-5.3422077350	-0.3328818159
H	6.4920960550	-2.5537093532	0.5316289743
H	0.1308215210	6.7092204231	2.5469537064
H	1.6169728028	7.5744451900	2.9694319072
H	0.7015734061	6.4514060957	4.8855328264
H	2.6787861821	5.1446706029	5.6385445504
H	3.1644958648	6.6134062359	4.7858389539

H	3.2566230551	5.0433758638	3.9593822586
H	1.0991057661	3.8828237041	4.4844741440
H	-4.6153950591	2.7278892819	4.0563292032
H	-5.0069330356	3.8735822465	2.7583917629
H	-3.4070507080	4.8022144092	4.3500947376
H	-2.2279582471	4.2835771755	1.5767331514
H	-1.6935932253	5.5741156387	2.6754129998
H	-3.3332426887	5.6073332496	2.0162392229
H	-1.1898145662	3.8190793304	4.1413339401
H	-4.0698388426	-5.4309347753	1.8899124659
H	-5.7732016306	-5.2110463380	1.4375477529
H	-5.5765499559	-5.1982942376	3.8220989174
H	-6.0112494824	-2.3077873004	2.9240490852
H	-6.5995276352	-3.0518122695	4.4194562691
H	-7.2381747334	-3.5926797266	2.8546878987
H	-3.4482505221	-4.4298518627	4.0468139613
H	0.3159120310	-8.5126775888	-1.5826196177
H	-0.9417489630	-7.9028193534	-2.6944542999
H	-1.3477051159	-8.2110977994	0.2948452078
H	-2.7614173656	-10.1608845620	-0.3350911920
H	-1.0685106939	-10.4390499408	-0.7954541502
H	-2.2730062522	-9.9859171541	-2.0238580383
H	-2.8145180793	-6.7841823487	-0.5553362332
H	2.8245222162	1.4149088550	-1.7944971254
H	3.8328765373	1.1559094579	-3.2465244175
H	1.4795144700	1.4311476038	-3.5599042714
H	2.6680839456	-2.2623581288	-4.7531818263
H	1.5124285568	-3.2244255281	-5.7015022654
H	1.2444517034	-0.6734207176	-4.5741140955
H	7.4914012404	-4.9179595108	-1.4942612090
H	6.7527320491	-4.3141300649	-2.9927812664
H	5.6748670636	-6.6287750356	-1.3514435291
H	7.2177575090	-6.6229688769	-3.9986739720
H	6.4958889309	-8.0411959232	-3.2298578349
H	7.8511908213	-7.2063626575	-2.4440701902
H	4.0065309356	-6.2155100837	-2.5718360937
H	-2.2721975758	-3.0784783668	-4.5174377091
H	-3.5170687264	-1.8186586733	-4.4358371479
H	-0.8049956019	-1.4691655779	-4.4762244614
H	-4.1651331294	8.6583871664	-2.3327394875
H	-2.6995644780	8.1128782175	-3.1862615817
H	-2.6616546501	9.5304407066	-0.5020904427
H	-2.0186723805	10.5808142997	-3.3071619394
H	-1.7697404382	11.4573792502	-1.7931465386
H	-3.4183597724	11.0637032307	-2.3227614958
H	-0.7652068908	8.4582462162	-0.7178071129
H	-7.0467579953	0.6616885160	-2.6135794519
H	-6.3238687942	-0.9484560909	-2.5006321532
H	-8.1587969348	0.1467096428	-0.6694432171
H	4.9257639636	0.5061912850	4.4409558079
H	3.4213298677	-0.4144480553	4.5973298638
H	3.7719559910	2.6114924028	4.8239985561
H	2.7642843540	0.5061737333	6.8034807483
H	2.9113304283	2.2433979851	7.1172853857
H	4.3675779054	1.2680691877	6.8519554500
H	1.8865587546	2.1238240096	3.7785690146
H	-3.1824345171	1.0875819494	-2.5957919303
H	-3.5971616373	2.0507920525	-4.0410406208

H	-1.5799618926	0.6038381304	-3.9841575468
H	6.5309278549	3.5178506486	-1.5275049321
H	5.0981915082	4.5444992457	-1.7896494061
H	6.8808541699	5.4708628817	-0.4402040888
H	0.5861594495	5.1126992472	-4.0933262791
H	2.2260384652	4.5054955074	-3.8626886742
H	-0.1836127890	3.0026031247	-3.7260373035
H	-2.7230663004	0.0173105248	3.2799964138
H	-2.0731039167	1.4827325927	3.7092301415
H	-3.5547052347	0.9243385260	5.3547334826
H	-1.9132267745	0.8032052666	6.0288231584
H	-2.8141529480	-0.6760188808	5.5657847829
H	-0.0812902362	-5.1867513129	1.6426005205
H	1.9759580085	-6.5565278180	1.6717052581
H	2.2502996478	-1.6952703628	2.5913671422
H	-0.3999039404	2.1375306525	2.1738621242
H	-0.1268321138	2.2390308646	-0.2776220954
H	0.0271620512	0.1410581133	-1.5981931543
H	-0.0840546435	-2.0479175042	-0.4411293701
H	-1.0878922630	-3.1736329943	1.5763183662
H	-0.8041526778	-3.4649798896	4.1006283627
H	-2.0758881937	-2.4034991904	3.5207589835
H	0.7036946945	-1.4847485095	4.4440544392
H	-0.7278507541	-1.3829313865	5.4350259988
H	-0.0104359098	0.7282037750	4.2442134254

2-HP-B-CD:trans-(1S,4R)-SRT_3_MD E(Ha)= -7253.91675574

C	-1.0005833157	-0.3193929450	4.1142066814
C	-0.7188515147	-0.3050284756	2.6293290965
C	-0.5531075155	-1.4980501711	1.9116004120
C	-0.5385678918	-2.8648032986	2.5722614787
C	-1.0352002864	-2.8284044500	4.0284693012
C	-0.5230456033	-1.6034195719	4.7709100367
C	-0.6547866532	0.9240029518	1.9601574127
C	-0.4512944731	0.9820519195	0.5881061728
C	-0.3143831708	-0.2024155377	-0.1362092656
C	-0.3565674840	-1.4215230970	0.5268623524
C	0.8148950036	-3.5462400050	2.4355746282
C	0.8490728862	-4.9080742036	2.1231032037
C	2.0515840851	-5.5831502295	1.9723256202
C	3.2551629161	-4.9077628656	2.1510597410
C	3.2348861788	-3.5487928686	2.4808287559
C	2.0237197629	-2.8714160967	2.6126844172
Cl	4.7424015593	-5.7623712233	1.9334144214
Cl	4.7117610961	-2.6725952595	2.7074332997
N	-2.4931202697	-0.0867646668	4.2939832726
C	-3.0776456992	-0.4294491942	5.6106792508
C	-4.7455111065	0.0673632026	-1.2735992942
C	-4.7879584544	-0.8651174686	-0.0711771550
C	-4.1060740533	-0.1888336906	1.1070820961
C	-4.8074420618	1.1133234191	1.4262941495
C	-4.9293602991	1.9761335086	0.1506340842
O	-5.4775482171	1.2404408088	-0.9094613843
O	-3.6523815845	2.4863602871	-0.1554755162
C	-3.6773343124	3.6246929638	-1.0096480880
C	-3.8201741838	4.9103759236	-0.1997736561
C	-3.7054667493	6.1231779736	-1.1127201363
C	-2.3647680234	6.0891094042	-1.8486650421
O	-2.3041039482	4.8719085612	-2.5689045687
C	-2.3363518249	3.7050732421	-1.7486961934
O	-1.3382648733	6.1909581319	-0.9197929735
C	-0.0742937003	6.7079066284	-1.3291993611
C	0.6535138766	6.8661323856	0.0014605786
C	2.1508712711	7.0607915543	-0.1385456134
C	2.7305266485	6.0073288499	-1.0824475605
O	2.0781664176	6.0896712159	-2.3188677200
C	0.6847217305	5.7628385079	-2.2754858020
O	2.5387720481	4.7397717327	-0.5138274313
C	3.6902841195	3.9506621745	-0.2348850342
C	3.2328718884	3.0303382616	0.8869458184
C	4.2984034063	1.9985754296	1.2131850063
C	4.7487118015	1.3007346158	-0.0763968145
O	5.1802491479	2.2530756861	-1.0248383003
C	4.1771400342	3.1722447927	-1.4492428165
O	2.6906736718	6.9425469813	1.1652488837
C	3.9371271934	7.6114110030	1.3505222512
C	4.6455883719	7.0266654338	2.5630116093
O	5.0595752698	5.6993463163	2.3206800070
O	0.0597765259	7.9466903483	0.6875387869
O	-3.8960245621	7.2489594678	-0.2920428503
C	-4.2391498111	8.4564245362	-0.9661478445
C	-3.2554032091	9.5535491085	-0.5893192826
O	-1.9448062025	9.1739857960	-0.9511257197

O -5.0537206976 4.9475113904 0.4868950109
O -4.1004221063 1.7600951849 2.4620166984
C -4.8623879824 2.7173491706 3.1731440100
C -3.9308845678 3.5068671451 4.0704614693
O -3.2626782047 2.5658044988 4.9155677628
O -4.1238499977 -1.0567055849 2.2406158026
O -4.0795832231 -2.0784474433 -0.2594119234
C -4.8120888992 -3.2349383561 -0.5657425956
C -4.2907282552 -4.3567049165 0.3421016001
C -2.8615879012 -4.6560406481 -0.0576538324
C -2.7268969946 -4.9128109135 -1.5570507632
C -3.3187361250 -3.7421829494 -2.3410483920
O -4.6811711417 -3.5774344739 -1.9147700637
O -4.4183352998 -3.8666050938 1.6614072979
C -4.3449286398 -4.8117440778 2.7236752238
C -5.1489602854 -4.2647098448 3.8968889835
O -4.6577967215 -2.9908889529 4.2971800464
O -2.3163979269 -5.7434233473 0.6678755460
O -1.3216182216 -5.0100030465 -1.6960405555
C -0.7343139644 -5.8558803687 -2.6441725659
C 0.4808898355 -6.4922868296 -1.9518394461
C 1.4847722142 -5.4012643303 -1.6361801148
C 1.7580393230 -4.4986238674 -2.8437442527
C 0.4534846994 -3.9960367470 -3.4605656605
O -0.3470726362 -5.1393240802 -3.7796153927
O 0.0606719613 -7.1228360134 -0.7573109431
C -0.1688843245 -8.5249116247 -0.8745099229
C -1.3490472532 -8.9353455590 -0.0062867087
O -2.5356166879 -8.3290001924 -0.4840771795
O 2.6926684652 -5.9625246127 -1.1641053822
C 2.5263421676 -3.4513442711 -2.2754571765
O 3.4998886081 -2.8212643268 -3.0543040304
C 4.7616021550 -2.6723289641 -2.2057141911
C 4.5497926352 -1.6834111341 -1.0630867148
C 4.0069857092 -0.3634024611 -1.6088362046
C 2.7278456125 -0.6917050834 -2.3950667278
O 3.0682862426 -1.5522410653 -3.4802148519
O 5.1567600892 -3.9100329018 -1.6535107757
C 6.1495151023 -4.6169115783 -2.3953320393
C 5.8298889395 -6.1032609982 -2.4344965757
O 4.6359287284 -6.3218730656 -3.1611015334
O 5.7686323473 -1.4664228655 -0.3927321133
O 3.6738133417 0.5382088921 -0.5613520050
O 3.8384095966 1.0212756558 2.1162567918
C 4.2428165307 1.1085106669 3.4748347010
C 3.0498920099 1.4901346672 4.3432773851
O 1.9383637914 0.6799633685 3.9778572015
O 2.9362832712 3.8144015985 2.0352318034
C 4.8325748910 4.0262222813 -2.5208326816
O 5.8285545535 4.8792997617 -2.0105691555
C 1.9964876489 0.5028600257 -2.9635313462
O 0.6889570799 0.1325654926 -3.3640924561
C 0.5476756281 -3.1404448081 -4.7218282150
O -0.4452417832 -2.1314025638 -4.7363227799
C -3.3218335098 -3.8634513013 -3.8611677431
O -3.2770411899 -2.6022303345 -4.4796801121
C -5.3428727395 -0.5147301225 -2.5486834003
O -6.4651100360 -1.3367310973 -2.3054466700

C	-2.0213217274	2.5324789242	-2.6567375545
O	-0.6508061455	2.4968272476	-3.0134897888
C	0.2513653459	5.8122043612	-3.7338900432
O	0.5543598442	4.5986480560	-4.4051645821
C	5.8847290377	7.8366773696	2.8969558245
C	-2.9409751372	4.3494687086	3.2878478235
C	-6.6407993498	-4.2043511890	3.6099711531
C	-1.5333013708	-10.4422727744	-0.0282686719
C	6.9562117080	-6.8740514084	-3.1011146958
C	-3.5915421546	10.8509691495	-1.3005788670
C	3.3303112724	1.2780787779	5.8142384750
H	3.7923885494	6.1850044540	-1.2835511811
H	2.3479936212	8.0589941303	-0.5549977114
H	0.4922694569	5.9277060906	0.5535919996
H	-0.2122184713	7.6962971384	-1.7919078116
H	-2.3031291725	6.8915655032	-2.5936698631
H	-4.4965381425	6.0659693144	-1.8767131739
H	-2.9875461987	4.9463881984	0.5169091769
H	-4.5007429939	3.5388468899	-1.7329439304
H	-5.6312262316	2.7976094691	0.3106347486
H	-5.8319234801	0.8797388689	1.7574193357
H	-3.0651934656	0.0250773915	0.8314044219
H	-5.8399051676	-1.0750836336	0.1608859269
H	-5.8804399831	-3.0724669740	-0.3915297877
H	-4.9232466276	-5.2457234648	0.2017813938
H	-2.2804123862	-3.7459100295	0.1517574354
H	-3.2105047274	-5.8621355465	-1.8318018467
H	-1.4430002846	-6.6238621877	-2.9760458715
H	0.9394379343	-7.2187978912	-2.6352649172
H	1.0488803108	-4.7692921211	-0.8491927457
H	2.3532745282	-5.0477785216	-3.5871932891
H	3.7037126223	-3.3997402350	-3.9626570525
H	5.5575270595	-2.2657136783	-2.8446383329
H	3.7922061956	-2.0858980443	-0.3738097449
H	4.7434606736	0.0995878395	-2.2809036655
H	5.6154155353	0.6652069745	0.1145421266
H	5.1782861395	2.5169159433	1.6214882320
H	2.3304830290	2.4916651480	0.5626594850
H	4.5018345233	4.5881369920	0.1400808372
H	3.3253298879	2.6430559244	-1.8939047429
H	2.0388590813	-1.2117328274	-1.7178683721
H	-0.0614974429	-3.3922996341	-2.7035589493
H	-2.7452281307	-2.8426231695	-2.0834201140
H	-3.7011013593	0.3382773035	-1.4803588297
H	-1.5411972249	3.7669511727	-0.9922625730
H	0.5611808786	4.7379883267	-1.9037360951
H	0.5510970529	8.0600522945	1.5096031313
H	3.2771517823	-5.2082102927	-0.9764827978
H	2.3965973079	4.5518137169	1.7082100367
H	-5.1866419432	5.8828527071	0.7012968448
H	-3.9441387255	-1.9568302121	1.8981222027
H	-1.4627447712	-5.9363568561	0.2304632516
H	6.0075170740	-2.3092889919	0.0118266454
H	3.7581054668	8.6886718178	1.4803237511
H	4.5870295259	7.4691349545	0.4766711178
H	3.9449612063	7.0656348316	3.4137700060
H	6.3905841427	7.3930989441	3.7569517950
H	5.6358463539	8.8749059094	3.1341752936

H	6.5828582164	7.8264290400	2.0540128610
H	4.2955551840	5.1013665835	2.3661440591
H	-5.6312663293	2.2115789453	3.7769050183
H	-5.3512737613	3.4236870404	2.4902030312
H	-4.5650986397	4.1582282308	4.6902071762
H	-2.2313845450	4.8493087694	3.9561889306
H	-3.4721045832	5.1210973649	2.7249291784
H	-2.3916316552	3.7258034068	2.5779604766
H	-2.6932151078	3.0609158755	5.5138510103
H	-3.2989313013	-4.9697049234	3.0092900609
H	-4.7574518915	-5.7776473436	2.4036680550
H	-4.9670219341	-4.9311045822	4.7486415807
H	-6.8365746777	-3.5771631722	2.7334871146
H	-7.1709699420	-3.7819815552	4.4667378879
H	-7.0472209555	-5.1999678017	3.4092442803
H	-4.9800867001	-2.3421977658	3.6559413061
H	0.7414756692	-9.0660529237	-0.5824386213
H	-0.4108117747	-8.7866603335	-1.9131878972
H	-1.1422023874	-8.6090802852	1.0254725785
H	-1.7551560063	-10.7803553912	-1.0454235993
H	-2.3757327489	-10.7217202410	0.6079321271
H	-0.6391015821	-10.9636689209	0.3258279039
H	-2.6846362623	-7.5241667492	0.0325604386
H	1.9426696781	1.2617873404	-2.1761511606
H	2.5707291423	0.9081573512	-3.8107323620
H	0.1525485187	0.9536157441	-3.3842246148
H	1.5364056419	-2.6810626582	-4.8052725611
H	0.3905470268	-3.7870488776	-5.5908420439
H	-0.0638088619	-1.3466867780	-4.3012438175
H	7.1322663967	-4.4433575301	-1.9351861934
H	6.1850518739	-4.2512582812	-3.4298142177
H	5.7145668276	-6.4515546739	-1.3963278003
H	6.7158664948	-7.9392304868	-3.1158968612
H	7.9067261056	-6.7372094729	-2.5767197802
H	7.0782362253	-6.5442906803	-4.1378763089
H	3.9150227727	-6.4257575158	-2.5193386919
H	-2.4793886147	-4.4874362549	-4.1774590808
H	-4.2491916862	-4.3654807813	-4.1619742632
H	-2.3369062464	-2.3826932298	-4.6184934666
H	-5.2638172326	8.7401020417	-0.6901439306
H	-4.2094382841	8.3118279169	-2.0538186787
H	-3.3197651302	9.7080299935	0.4990171179
H	-4.6078954746	11.1837761999	-1.0698172600
H	-3.5047098661	10.7227106835	-2.3843370941
H	-2.8918474268	11.6328171300	-0.9980538973
H	-1.5594257917	8.6504433213	-0.2332605827
H	-5.6431419818	0.3341262558	-3.1766333936
H	-4.5632437176	-1.0663309411	-3.0867285732
H	-6.1913598907	-2.2288206205	-2.5519373688
H	5.0610186740	1.8284214263	3.6030891887
H	4.6010975760	0.1137258929	3.7651257501
H	2.8079429988	2.5446220806	4.1481208571
H	3.5701121131	0.2281652213	6.0100290288
H	2.4553359736	1.5457615896	6.4129689326
H	4.1697934007	1.8963606308	6.1458970621
H	1.9108278117	0.7147129168	3.0102348447
H	-2.2234579847	1.6072542111	-2.1140903261
H	-2.6685296563	2.5674084557	-3.5435900938

H	-0.4121090231	3.2562698417	-3.5834071393
H	5.2322046258	3.3491239095	-3.2899959911
H	4.0808916137	4.6642397296	-2.9952091331
H	6.4885169604	4.3162720935	-1.5879208224
H	-0.8237705785	5.9315062305	-3.8341685043
H	0.7482546546	6.6638464574	-4.2158494584
H	1.5124576786	4.4905970335	-4.3873790669
H	-3.0318268405	-0.5657720227	3.5378308827
H	-2.6877776459	0.9181221332	4.1436137261
H	-4.0592006985	0.0405196909	5.6680861281
H	-2.4462830714	-0.0310470252	6.4059815495
H	-3.1862012506	-1.5095022200	5.7002123160
H	-0.0830191039	-5.4475739930	1.9802270598
H	2.0643715273	-6.6271186118	1.6820581019
H	2.0486066199	-1.8103782697	2.8437914040
H	-0.7622835070	1.8422900617	2.5326050963
H	-0.4084377147	1.9394109221	0.0787212827
H	-0.1565524777	-0.1745817804	-1.2121920252
H	-0.2191790441	-2.3429929481	-0.0354493842
H	-1.2398480433	-3.4997942840	2.0184734104
H	-0.7221321345	-3.7428643227	4.5413436557
H	-2.1337214305	-2.8357826307	4.0318325227
H	0.5711306291	-1.5576680575	4.7547738809
H	-0.8098090445	-1.6337326019	5.8263343684
H	-0.5007716221	0.5343125780	4.5815912775

255

2-HP-B-CD:trans-(1S,4R)-SRT_4_MD E(Ha)= -7253.9114221936

C	-0.30035618	0.76359268	-4.07150143
C	-0.17624391	0.72140852	-2.56185757
C	-0.31917405	1.87056696	-1.76989607
C	-0.47689857	3.24863240	-2.37641812
C	-1.05267055	3.15621544	-3.79987132
C	-0.24715211	2.17483046	-4.63988867
C	0.03896438	-0.52027715	-1.95376833
C	0.05855000	-0.64237333	-0.57343173
C	-0.11785968	0.48837125	0.22197750
C	-0.27760327	1.73229496	-0.37697144
C	0.81950464	4.04427352	-2.37674230
C	0.76466648	5.43924172	-2.28151043
C	1.91520980	6.20772265	-2.38654871
C	3.15326306	5.60104286	-2.59904849
C	3.22315221	4.20653382	-2.66028522
C	2.06546251	3.43859532	-2.53866038
Cl	4.56078440	6.58317483	-2.77109924
Cl	4.73488838	3.39505478	-2.89669840
N	-1.58058158	0.04402525	-4.43102378
C	-1.95510199	0.03600593	-5.85807486
O	2.78467044	-3.97166420	-1.98642149
C	3.35519201	-3.04163685	-1.06252025
C	4.20178007	-2.01120540	-1.78149886
C	4.86720118	-1.14562273	-0.69712935
O	5.69851551	-1.96249205	0.09331789
C	4.98804663	-2.90436331	0.88351714
C	4.11353228	-3.80524568	0.01085220
O	3.82308634	-0.55649085	0.03934414
C	4.17684202	0.28640195	1.12728088
C	4.49993488	1.69706165	0.66019246
C	4.64155296	2.66597450	1.83526958
C	3.49475217	2.56280020	2.85988043
O	3.31613349	1.20246231	3.17052519
C	2.96081664	0.39054452	2.05627110
O	2.35352820	3.17818177	2.34993948
C	1.45079834	3.81555479	3.26122721
C	0.93139432	5.04097136	2.49911870
C	-0.39537540	5.56689577	3.02372541
C	-1.37313089	4.44972806	3.35456414
O	-0.79427098	3.54377222	4.23304987
C	0.35762581	2.84075934	3.73587721
O	-1.76911960	3.80918062	2.15978838
C	-3.11934374	3.92674229	1.74086938
C	-3.06332418	4.17936317	0.23770620
C	-4.44656463	4.13846501	-0.38335768
C	-5.14269428	2.82681979	0.01907695
O	-5.18124325	2.71165627	1.41862856
C	-3.89286384	2.64182139	2.03411957
O	-4.42866618	1.79195395	-0.58183860
C	-5.06458440	0.58466556	-0.97634623
C	-3.99996731	-0.05307360	-1.86529905
C	-4.25280683	-1.51675392	-2.18053553
C	-4.62223447	-2.29274793	-0.90708249
O	-5.68517891	-1.64927094	-0.25711565
C	-5.42563029	-0.32391489	0.20227011
O	-4.29720221	4.22049645	-1.77892368

C	-5.42035124	4.72513844	-2.46211038
C	-5.37087880	4.22605483	-3.88940954
O	-5.43819504	2.80098642	-3.81646499
O	-2.44405436	5.40843465	-0.06084945
O	-1.01161398	6.38655880	2.04957628
C	-0.90793578	7.79381219	2.23872928
C	-1.57242202	8.48029201	1.05377998
O	-2.92597416	8.10655165	0.93742240
O	1.84782038	6.10378312	2.56111873
O	4.78040392	3.92883843	1.22483656
C	5.04901109	5.02919839	2.07406324
C	4.91228819	6.26171253	1.19317212
O	3.64956143	6.20142049	0.52974707
O	5.69587740	1.67823292	-0.08230091
O	3.37389445	-1.22363773	-2.60984929
C	3.57314720	-1.29285185	-4.00317996
C	2.94779010	-2.52517000	-4.66956837
O	1.64078805	-2.75479527	-4.15108411
O	3.05773334	-4.36052857	0.78052217
C	3.15253477	-5.60253340	1.41616931
C	2.29408649	-6.59342649	0.60809374
C	0.84594118	-6.14548487	0.65834218
C	0.37593647	-5.71967734	2.04856593
C	1.38903621	-4.81140655	2.73557060
O	2.65650275	-5.46915095	2.72264718
O	2.67987785	-6.56964929	-0.75435925
C	3.74245220	-7.45407687	-1.09993516
C	4.12749443	-7.22069701	-2.55361357
O	4.72978172	-5.95712072	-2.73492138
O	0.00736435	-7.15457320	0.13408865
O	-0.82181790	-5.01056230	1.75795853
C	-1.95987574	-5.10193955	2.56008180
C	-3.08655447	-5.65790079	1.69301495
C	-3.29407761	-4.73584387	0.50205485
C	-3.56467006	-3.31209656	0.97387356
C	-2.48225073	-2.86678139	1.96793382
O	-2.31723667	-3.82534636	3.02724295
O	-2.74766008	-6.93215587	1.17410115
C	-3.09164224	-8.02617622	2.03021343
C	-2.19042960	-9.21717304	1.73966519
O	-0.85929535	-8.93263864	2.10847920
O	-4.35681857	-5.20272695	-0.30056528
O	-3.47455908	-2.39263678	-0.10946874
O	-3.07732957	-1.99555485	-2.79800555
C	-3.21412075	-3.17359868	-3.56502622
C	-1.82251286	-3.69971685	-3.88981509
O	-1.11005364	-2.65723508	-4.54623220
O	-3.88875266	0.65550316	-3.09449722
C	-6.68845796	0.07134280	0.96537490
O	-6.60676489	-0.21962037	2.34472163
C	-2.75683150	-1.51662481	2.58913398
O	-4.04097545	-1.47136898	3.15115818
C	1.06126090	-4.40887124	4.17222722
O	0.27141076	-3.23686250	4.22954129
C	5.98621300	-3.68942659	1.71590343
O	6.54360803	-4.72855608	0.94117922
C	2.44249795	-0.92713987	2.59291014
O	1.15358380	-0.73425592	3.12583782

C	0.79178649	1.99784316	4.92725665
O	1.16758613	2.81147104	6.01404187
C	-4.13098482	2.38436705	3.51042160
O	-4.67636070	1.11096787	3.75722909
C	-6.51071164	4.78796349	-4.71879051
C	4.97896815	7.55185683	1.97961268
C	2.85988455	-2.34813399	-6.17055707
C	5.12640530	-8.26569388	-3.01485037
C	-2.64975912	-10.43122467	2.52800212
C	-1.51789814	9.98858031	1.21100670
C	-1.09452830	-4.19251594	-2.64938789
H	-6.19115213	2.82060965	-0.30686412
H	-5.04122404	4.97960932	0.00386670
H	-2.49252141	3.34939178	-0.20307651
H	-3.60177367	4.78466659	2.23276631
H	-2.25258025	4.85884584	3.86682086
H	-0.20648060	6.13832931	3.94186816
H	0.76247870	4.71864715	1.46111874
H	1.99517241	4.17176572	4.14648740
H	3.77779525	3.02325369	3.81479195
H	5.56596553	2.40212332	2.37360323
H	3.65622106	2.03803530	0.03821959
H	5.03821874	-0.12896412	1.66916566
H	5.52290475	-0.38521870	-1.12819508
H	5.00466276	-2.49619506	-2.35411157
H	2.54591000	-2.48846327	-0.57177262
H	4.72890470	-4.58296961	-0.45688595
H	4.19399963	-5.93280572	1.49963842
H	2.39289409	-7.60543893	1.02468059
H	0.77382862	-5.24324944	0.03214739
H	0.16339436	-6.60937679	2.65855808
H	-1.77967068	-5.72109387	3.44707933
H	-4.01291022	-5.71327474	2.28091702
H	-2.35869979	-4.71416977	-0.07456322
H	-4.55144601	-3.25203093	1.44887240
H	-5.01038962	-3.28580418	-1.14601028
H	-5.11098358	-1.58693178	-2.86688649
H	-3.05091167	0.00719362	-1.31401046
H	-5.96272680	0.80546597	-1.57643136
H	-4.57789646	-0.32430788	0.89792750
H	-1.53579133	-2.78674956	1.41844520
H	1.45218111	-3.87787022	2.16643724
H	4.32683866	-2.37934160	1.58094546
H	2.14611345	0.86725820	1.49742504
H	0.06183705	2.19256084	2.90261402
H	-3.32449107	1.80036795	1.61424318
H	-1.74909764	5.56059484	0.61237808
H	-0.90941680	-6.85753709	0.27369312
H	-4.24966487	1.55979014	-3.00556077
H	2.40822720	6.12446300	1.75981445
H	5.84643307	2.58398280	-0.37870247
H	2.49297817	-4.75082443	-1.47222585
H	-4.19654320	-6.14685597	-0.42546302
H	-5.42261650	5.82523774	-2.44884812
H	-6.36091397	4.37722575	-2.00971720
H	-4.40427517	4.52571773	-4.32303737
H	-7.47703255	4.49944335	-4.29337037
H	-6.46580828	4.41838589	-5.74906180

H	-6.46208092	5.87966590	-4.76424229
H	-5.63282371	2.46133950	-4.69576740
H	6.05618589	4.95775982	2.50971845
H	4.30790916	5.08746995	2.88178503
H	5.70578735	6.24044271	0.43144401
H	5.94523129	7.64680602	2.48357758
H	4.18495120	7.58445903	2.73204996
H	4.85707120	8.40608802	1.30938881
H	3.59880881	5.30536984	0.16491781
H	4.64220005	-1.24182396	-4.26098694
H	3.09453944	-0.39041584	-4.40261066
H	3.56561073	-3.40704061	-4.44599226
H	3.84976021	-2.17194296	-6.60157024
H	2.22227406	-1.49264501	-6.42096867
H	2.43744090	-3.24116390	-6.63739430
H	1.79819898	-3.12647698	-3.26239299
H	3.40809509	-8.49071909	-0.95225829
H	4.62514453	-7.27164749	-0.47019672
H	3.20728200	-7.30453655	-3.15605169
H	4.71132391	-9.27528285	-2.94818389
H	6.03570960	-8.21637668	-2.40763416
H	5.40543982	-8.07008494	-4.05242763
H	4.05938419	-5.26762938	-2.62273205
H	-1.97664854	-1.32774863	3.34172850
H	-2.62307346	-0.77029835	1.79036756
H	-4.14781030	-0.57794328	3.53639099
H	0.59206320	-5.23291298	4.72834307
H	2.00812423	-4.17918956	4.66904226
H	-0.63872378	-3.42978102	3.94907479
H	-4.14948340	-8.28157119	1.87699680
H	-2.95228319	-7.74321116	3.08176305
H	-2.25573912	-9.43848149	0.66196034
H	-3.67644370	-10.71318129	2.27704341
H	-2.59343107	-10.22948266	3.60244793
H	-1.99232474	-11.27587939	2.31204941
H	-0.42456625	-8.48096375	1.36625141
H	6.74763826	-2.98065342	2.06731262
H	5.46053507	-4.08861006	2.59776619
H	7.35444881	-5.02523879	1.36229405
H	0.14814330	8.07666873	2.31861784
H	-1.43145954	8.07972451	3.16298787
H	-1.01177838	8.19161353	0.14724337
H	-2.07145856	10.29546390	2.10395690
H	-1.98411259	10.46629868	0.34641532
H	-0.48746284	10.34598046	1.29620971
H	-2.95754002	7.20837063	0.57681177
H	2.42743884	-1.64765723	1.76356346
H	3.14824158	-1.29391417	3.35580840
H	0.88543604	-1.55635195	3.57453238
H	-3.76531868	-2.95883162	-4.49435344
H	-3.75994106	-3.95409878	-3.01683367
H	-1.95619978	-4.54041444	-4.58838681
H	-0.07319068	-4.49943732	-2.89382316
H	-1.60572968	-5.06693704	-2.23526270
H	-1.07151310	-3.40812749	-1.88780947
H	-0.14953433	-2.84575150	-4.54731837
H	-0.04003407	1.32715596	5.18777313
H	1.64593645	1.37842348	4.65559227

H	0.39479834	3.34437656	6.23277267
H	-6.87802519	1.14270635	0.89898351
H	-7.53126868	-0.45736942	0.49880830
H	-6.11254804	-1.04453738	2.46038296
H	-3.17316581	2.43182457	4.03770515
H	-4.78564551	3.17418908	3.90871482
H	-5.50700956	0.98409470	3.25817933
H	-2.39174365	0.39227661	-3.86522462
H	-1.46557496	-0.96020013	-4.16681965
H	-2.76560025	-0.68120477	-5.98875253
H	-1.10147592	-0.28005004	-6.45990399
H	-2.28876949	1.02451942	-6.17258985
H	-0.19328917	5.92565567	-2.11349247
H	1.87105793	7.28833331	-2.30522431
H	2.15750574	2.35641229	-2.56115141
H	0.20707024	-1.38894988	-2.58131350
H	0.22399783	-1.61204288	-0.11261344
H	-0.09275319	0.38800988	1.30393838
H	-0.37960502	2.61578334	0.24796292
H	-1.19240172	3.81787304	-1.77316565
H	-1.04412049	4.14694222	-4.26488368
H	-2.10347858	2.84552467	-3.73018113
H	0.80393406	2.48416137	-4.64379590
H	-0.55839381	2.18840513	-5.68870950
H	0.48849836	0.14743340	-4.52008701

255

2-HP-B-CD:trans-(1S,4R)-SRT_5_MD E(Ha)= -7253.9108353648

C	-0.23591181	-0.70156239	3.93957864
C	-0.17882424	-0.74173562	2.42718687
C	-0.24064405	-1.95000221	1.72062477
C	-0.23138410	-3.29754293	2.41210148
C	-0.67024779	-3.18403318	3.88249838
C	0.05584990	-2.04716449	4.58562497
C	-0.14763024	0.46996326	1.72797395
C	-0.21005390	0.50058576	0.34299029
C	-0.29988471	-0.69715546	-0.36379140
C	-0.29407348	-1.90340087	0.32324697
C	1.11264376	-3.99768068	2.28970600
C	1.15064952	-5.38157841	2.09748627
C	2.35779958	-6.06611620	2.04454900
C	3.56102934	-5.38275372	2.20603110
C	3.53622643	-3.99768537	2.39778529
C	2.32334559	-3.31211867	2.41220421
Cl	5.04677708	-6.26102518	2.14966733
Cl	4.99956751	-3.10438432	2.62992099
N	-1.60568606	-0.15527824	4.29623101
C	-2.07273259	-0.33156308	5.68687001
C	-5.14325116	0.61922585	-0.64458866
C	-4.86027751	-0.40355018	0.44875923
C	-3.80829200	0.12114459	1.41165152
C	-4.15523778	1.50105926	1.93934792
C	-4.55182185	2.43534920	0.77644908
O	-5.53603103	1.83630952	-0.02726702
O	-3.37794207	2.74352877	0.06996971
C	-3.49076434	3.77575438	-0.90794232
C	-3.56823094	5.16205945	-0.27355605
C	-3.44997335	6.24504447	-1.34077663
C	-2.14578630	6.06143673	-2.12051767
O	-2.18160253	4.77187130	-2.69837425
C	-2.20248363	3.71965651	-1.74262000
O	-1.09667025	6.21151533	-1.22906338
C	0.19438851	6.64420199	-1.65755717
C	0.89427983	6.82022709	-0.31338223
C	2.40849992	6.86937881	-0.37621545
C	2.93182053	5.76947330	-1.30056867
O	2.33137916	5.89928601	-2.54604809
C	0.92530857	5.61683783	-2.53811159
O	2.60336310	4.51568908	-0.74304156
C	3.64082560	3.67191343	-0.28479815
C	2.94308212	2.79396345	0.73543770
C	3.89742347	1.77471831	1.32106693
C	4.51449543	0.98927435	0.14715567
O	5.14959879	1.88150793	-0.74371468
C	4.27727310	2.81967153	-1.37614321
O	2.84214242	6.70100063	0.96475983
C	4.16815863	7.14390204	1.23137404
C	4.58951412	6.60440820	2.58989298
O	4.67618876	5.19338030	2.57353194
O	0.37242729	7.97114051	0.31305954
O	-3.54937132	7.46614470	-0.65054107
C	-3.85524517	8.60531621	-1.44673433
C	-2.87755792	9.72531764	-1.11954805
O	-1.55671232	9.31913289	-1.39124932

O	-4.77519262	5.33359900	0.43629191
O	-3.02719934	1.95706216	2.65428870
C	-3.22537666	3.08207398	3.48662842
C	-1.85938869	3.60443332	3.91479389
O	-1.16223273	2.52551252	4.53104070
O	-3.67300950	-0.79204573	2.50021493
O	-4.31032003	-1.60294383	-0.07585815
C	-5.13421978	-2.72121224	-0.27915788
C	-4.55708739	-3.87149580	0.55813345
C	-3.16802660	-4.19954871	0.03435882
C	-3.16435085	-4.41962489	-1.47511038
C	-3.87281563	-3.28292413	-2.20368002
O	-5.16585965	-3.08101239	-1.63096087
O	-4.54255815	-3.40614860	1.89308861
C	-4.47647264	-4.38579099	2.92545349
C	-4.97949332	-3.75230760	4.21791786
O	-4.18196389	-2.63308685	4.57684787
O	-2.63023875	-5.33504977	0.69251331
O	-1.78432915	-4.46548284	-1.81218104
C	-1.33276672	-5.36956532	-2.78779026
C	-0.28470439	-6.27709530	-2.12752409
C	0.89769812	-5.43116063	-1.70963545
C	1.41221835	-4.56369805	-2.85896551
C	0.28708745	-3.80740080	-3.57726378
O	-0.79780111	-4.69320634	-3.88406951
O	-0.86423625	-6.89419229	-0.99512366
C	-1.34446147	-8.21564580	-1.23781478
C	-2.38336354	-8.59301580	-0.19315314
O	-3.53949783	-7.79290583	-0.32684653
O	1.94084457	-6.24908588	-1.21804991
O	2.32535349	-3.69911239	-2.20275734
C	3.35143625	-3.10910540	-2.94534444
C	4.59302491	-2.97111176	-2.06813511
C	4.40778576	-1.93618566	-0.96031081
C	3.88162239	-0.61520691	-1.52030483
C	2.63465273	-0.92768677	-2.36002316
O	2.98778789	-1.83060440	-3.40900241
O	4.96443226	-4.18288873	-1.45402760
C	5.83729370	-5.01892942	-2.20541293
C	5.26039626	-6.41835064	-2.35378361
O	4.06739460	-6.36470828	-3.11723963
O	5.64658830	-1.71542710	-0.32801657
O	3.48196510	0.27126848	-0.48048230
O	3.21436663	0.91588972	2.20745307
C	3.57437949	0.96827906	3.57292388
C	2.98730197	2.15768045	4.34451782
O	1.60942608	2.32494147	4.01484729
O	2.39853737	3.63007674	1.75650166
C	5.12466784	3.61213399	-2.35460842
O	6.03589592	4.47222258	-1.70891835
C	1.95719349	0.26492429	-3.01104949
O	0.62037436	-0.01080583	-3.39507709
C	0.69991791	-3.20504779	-4.91567603
O	-0.02004257	-2.02787090	-5.23489520
C	-4.11172302	-3.54951926	-3.67797927
O	-4.74334972	-2.45955439	-4.29881168
C	-6.25066151	0.18475508	-1.58244751
O	-7.32204778	-0.33033713	-0.82102274

C	-1.97599554	2.42585969	-2.49783816
O	-0.62491363	2.39829197	-2.90534746
C	0.50823728	5.57292439	-4.00750579
O	0.75071909	4.31908002	-4.57922595
C	5.95105277	7.13968513	2.98809187
C	-1.07985241	4.19476120	2.75089548
C	-6.45292381	-3.38122805	4.15708346
C	-2.79369529	-10.04574726	-0.35634891
C	6.25313600	-7.34207562	-3.04012366
C	-3.17008705	10.95909415	-1.95299495
C	3.11140318	1.94701147	5.83865610
H	4.01302564	5.84931487	-1.45315219
H	2.72885356	7.84372116	-0.77217956
H	0.62741358	5.92122729	0.26646861
H	0.11182093	7.61504241	-2.16712514
H	-2.06814256	6.76596121	-2.95644582
H	-4.28094986	6.13159746	-2.05439082
H	-2.70582518	5.26683789	0.40152288
H	-4.37648187	3.60511707	-1.53645780
H	-5.02787935	3.34571820	1.14516608
H	-5.03109818	1.41802888	2.60301645
H	-2.85238569	0.19103090	0.87698022
H	-5.79238054	-0.60859414	0.98927550
H	-6.16757087	-2.50082332	0.00542521
H	-5.21783934	-4.74606832	0.46780752
H	-2.53792706	-3.32260752	0.23419991
H	-3.64288471	-5.38535012	-1.69844377
H	-2.16684375	-5.96739158	-3.17384180
H	0.04551066	-7.03209435	-2.85336005
H	0.56048527	-4.75451970	-0.91287740
H	1.94923407	-5.20079926	-3.57713287
H	3.57370351	-3.71373185	-3.83259696
H	5.40134771	-2.60269286	-2.71669011
H	3.66028937	-2.31126006	-0.24361441
H	4.65675698	-0.14478164	-2.14202255
H	5.30052374	0.31507581	0.49357131
H	4.72160963	2.29593553	1.82926935
H	2.12517900	2.25180298	0.24411559
H	4.42620035	4.25321614	0.21583320
H	3.48962010	2.30127632	-1.93565757
H	1.90246074	-1.40440472	-1.69768955
H	-0.06340890	-3.00184989	-2.91861687
H	-3.27727947	-2.36747610	-2.09615851
H	-4.23073160	0.76930660	-1.23868274
H	-1.36074859	3.83929879	-1.04614837
H	0.75955222	4.62204960	-2.10917688
H	0.83179164	8.06505282	1.15514809
H	2.57100775	-5.64204279	-0.80269788
H	2.01645651	4.38623480	1.27948849
H	-4.83886889	6.28825512	0.58175218
H	-3.71504719	-1.69459222	2.12282060
H	-1.87478155	-5.64438127	0.15290444
H	5.91046345	-2.56436110	0.04768350
H	4.20240950	8.24344676	1.22207917
H	4.86886372	6.76973441	0.47171903
H	3.83763136	6.93311039	3.32746969
H	6.70500467	6.85048737	2.24925030
H	6.24495936	6.71966743	3.95264891

H	5.94117545	8.22997721	3.07177640
H	3.80232800	4.82456257	2.37422190
H	-3.81881794	2.79948101	4.37070263
H	-3.75615456	3.88941249	2.96378447
H	-2.03804820	4.38881307	4.66610754
H	-1.55073632	5.12171047	2.41051143
H	-1.05602440	3.49507344	1.91103873
H	-0.05707855	4.43749891	3.05666653
H	-0.19944558	2.68360756	4.53204695
H	-3.44569448	-4.73702375	3.04342325
H	-5.10364668	-5.24907235	2.66286315
H	-4.82327453	-4.49307703	5.01173128
H	-6.63898153	-2.67983997	3.33674301
H	-6.76174020	-2.91297060	5.09481511
H	-7.07714189	-4.26452877	3.99179963
H	-4.44709488	-1.89247736	4.01368231
H	-0.49670702	-8.91439461	-1.21977021
H	-1.82384420	-8.27154159	-2.22535741
H	-1.93035448	-8.45475891	0.80244290
H	-3.24320969	-10.20495735	-1.34171544
H	-3.54135883	-10.30237902	0.39707663
H	-1.94006371	-10.72086380	-0.24728599
H	-3.39107722	-6.97016871	0.16399147
H	1.89166214	1.07293229	-2.27991423
H	2.55491864	0.61309968	-3.86449415
H	0.56858555	-0.64068913	-4.13929067
H	1.74242033	-2.89485815	-4.89259921
H	0.57537628	-3.97198739	-5.69116974
H	-0.95440044	-2.24510465	-5.32191890
H	6.80757940	-5.06432112	-1.69283192
H	6.00259753	-4.60238402	-3.20791473
H	5.04758979	-6.80026163	-1.34361681
H	6.47121821	-6.98093407	-4.05041984
H	5.82847351	-8.34466044	-3.12834420
H	7.19326378	-7.41068379	-2.48412624
H	3.32111508	-6.54409354	-2.52686105
H	-3.14834365	-3.69796762	-4.17586199
H	-4.69572150	-4.47795744	-3.78652134
H	-5.60755802	-2.37558696	-3.88152785
H	-4.89039664	8.91732409	-1.24868542
H	-3.77077978	8.36499804	-2.51454346
H	-2.99232805	9.97209356	-0.05140667
H	-2.47303984	11.75818712	-1.69142958
H	-4.19069518	11.31966432	-1.79339012
H	-3.04036659	10.73512552	-3.01683433
H	-1.23809766	8.76230672	-0.66656365
H	-6.54917877	1.06202857	-2.17180658
H	-5.84118648	-0.57193005	-2.26748151
H	-8.10107074	-0.37938812	-1.38103791
H	4.66778403	0.95789453	3.69830889
H	3.18457733	0.03801066	4.00327021
H	3.52767668	3.07307133	4.06249576
H	2.70889016	2.80664268	6.37999139
H	4.15827975	1.82047138	6.12952531
H	2.55955137	1.05337162	6.15064616
H	1.62917615	2.67962765	3.10669244
H	-2.20076316	1.59114501	-1.82125673
H	-2.66339517	2.38151145	-3.35624846

H	-0.36640881	1.50480441	-3.20609325
H	5.63706460	2.90062599	-3.01793670
H	4.47207310	4.23387390	-2.97519109
H	6.62028865	3.91719878	-1.18004023
H	-0.54282836	5.86892334	-4.11396694
H	1.11320546	6.30843028	-4.54912451
H	0.16478791	3.68726602	-4.12910680
H	-2.32196132	-0.50926171	3.62910468
H	-1.55564773	0.87481325	4.12960544
H	-2.36880105	-1.36627214	5.85758078
H	-2.94028647	0.31393253	5.83107331
H	-1.28686489	-0.02457481	6.37832675
H	0.22357791	-5.93457791	1.97167982
H	2.37824066	-7.13724548	1.87588737
H	2.34356405	-2.22885683	2.49377573
H	-0.08968620	1.39384942	2.29085771
H	-0.19800509	1.44514848	-0.19359079
H	-0.34411408	-0.68059689	-1.44913080
H	-0.34742010	-2.83472757	-0.23450216
H	-0.96152740	-3.94069969	1.90640025
H	-0.47487448	-4.13084644	4.39602374
H	-1.75540406	-3.02139078	3.92661020
H	1.13862933	-2.20589972	4.52644605
H	-0.17964985	-2.02682165	5.65378058
H	0.46441787	0.05729435	4.30728379

2-HP-B-CD:trans-(1S,4R)-SRT_6_MD E(Ha)= -7253.9091817336

C	-1.01365011	-0.08096597	4.01423610
C	-0.65708735	-0.18215968	2.54912218
C	-0.81884052	-1.38212132	1.84285815
C	-1.24351197	-2.68121007	2.50926190
C	-1.78988172	-2.47511765	3.93587633
C	-1.00298277	-1.42986200	4.71187544
C	-0.21302054	0.96598771	1.88004958
C	0.03668138	0.94615826	0.51525061
C	-0.14922345	-0.23672640	-0.20167148
C	-0.55714484	-1.38510771	0.46576495
C	-0.13979119	-3.72901323	2.46560045
C	-0.44063758	-5.02146415	2.02422030
C	0.52829922	-6.01786647	1.99869623
C	1.82409131	-5.74182551	2.42650378
C	2.13712020	-4.45074410	2.86064763
C	1.16762901	-3.45113208	2.87395540
Cl	3.01172486	-6.99467024	2.39897648
Cl	3.74271255	-4.07211093	3.39632823
N	-2.36511583	0.60468444	4.08597535
C	-3.01832062	0.64417578	5.41066118
C	-5.44461363	0.29205489	-1.25154389
C	-5.26081012	-0.44653726	0.07598275
C	-4.27173470	0.29492114	0.97113591
C	-4.65147056	1.74675150	1.15898931
C	-4.84072448	2.39623197	-0.22792701
O	-5.76712718	1.65866212	-0.98286075
O	-3.58432300	2.47830376	-0.83788308
C	-3.45468621	3.41188366	-1.90831331
C	-3.40130059	4.84374828	-1.37249879
C	-2.87799345	5.83078373	-2.40657367
C	-1.54244755	5.33419905	-2.95491042
O	-1.74070198	4.07477119	-3.52432969
C	-2.10337010	3.08712330	-2.55822805
O	-0.66035223	5.24932796	-1.87555610
C	0.59548069	5.90890600	-1.85636272
C	0.72947504	6.23996150	-0.36959135
C	2.11989779	6.68879033	0.06014971
C	3.18669030	5.83273300	-0.65741307
O	2.94264302	5.74652442	-2.03710748
C	1.73929194	5.01903983	-2.31873814
O	3.12625000	4.55812385	-0.09961362
C	4.25284672	3.91977283	0.48242135
C	3.57707072	3.03507999	1.52039465
C	4.53274088	1.99005400	2.05550452
C	5.11276881	1.23404973	0.85193022
O	5.85630884	2.13369280	0.06101126
C	5.08584573	3.16689003	-0.55169067
O	2.34599594	6.48394375	1.44563488
C	1.62255109	7.32188777	2.34377439
C	1.71550466	6.76445159	3.76106022
O	1.04096395	5.51389170	3.87572706
O	-0.24951782	7.21048051	-0.02441586
O	-2.73922741	7.07164243	-1.73402379
C	-2.85584513	8.21834542	-2.58148365
C	-2.06099007	9.37891430	-2.00121612
O	-0.67770611	9.10814935	-2.05804239

O	-4.67113203	5.26332520	-0.91446036
O	-3.63760523	2.36230394	1.92337993
C	-4.00945986	3.58787932	2.52391082
C	-2.77605078	4.27157296	3.08843225
O	-2.18229398	3.39083196	4.04885561
O	-4.22700025	-0.37353885	2.22924939
O	-4.65193714	-1.72933132	-0.01146554
C	-5.33136283	-2.78640331	-0.62916604
C	-4.82646595	-4.09767395	-0.02363850
C	-3.40686102	-4.39272479	-0.48521137
C	-3.18061917	-4.16346622	-1.98111675
C	-3.75225978	-2.81167970	-2.39366478
O	-5.13205728	-2.78951796	-2.01352451
O	-4.88327697	-3.97931127	1.38150994
C	-5.25559812	-5.16160075	2.08644469
C	-5.17580913	-4.81289672	3.56216958
O	-5.91472267	-3.63543471	3.82198892
O	-3.06266789	-5.70043054	-0.11208075
O	-1.76707072	-4.18146812	-2.09335520
C	-1.11152515	-4.86241022	-3.12322524
C	-0.05081907	-5.75159522	-2.45835410
C	0.96720863	-4.85795391	-1.77215607
C	1.49053779	-3.77878598	-2.71307243
C	0.33464785	-3.01697992	-3.36059948
O	-0.51043620	-3.96795842	-4.01684082
O	-0.67180967	-6.58418731	-1.49913851
C	-0.65922018	-7.98578988	-1.75881475
C	0.72275755	-8.61032736	-1.57180408
O	1.27556755	-8.21875915	-0.33971503
O	2.04122374	-5.63636467	-1.28149436
O	2.30174686	-2.93960956	-1.91299173
C	3.64887779	-2.75541146	-2.26375594
C	4.50462384	-2.89905297	-1.00665150
C	4.24831091	-1.76227931	-0.01980667
C	4.41888357	-0.42232705	-0.73077353
C	3.51528731	-0.41091919	-1.97522626
O	3.86818901	-1.49469974	-2.82996592
O	4.28654699	-4.14353717	-0.36040094
C	5.38038515	-5.06656238	-0.36302266
C	5.05907344	-6.33031299	-1.15654641
O	4.60089206	-5.99491980	-2.45395974
O	5.15887041	-1.82922987	1.05157122
O	4.05610341	0.65130080	0.13176564
O	3.91915710	1.06131495	2.91137898
C	3.78493942	1.46225943	4.26488646
C	3.20960831	0.25040094	4.98318427
O	2.01999564	-0.14463956	4.30478290
O	3.05276081	3.88987588	2.52290509
C	6.09092538	4.05759730	-1.26209493
O	6.94771753	4.71301719	-0.36028072
C	3.64405412	0.85838837	-2.79304677
O	2.86325914	0.79744572	-3.96783480
C	0.73237492	-1.95520478	-4.38057940
O	0.71619196	-0.69092747	-3.75866410
C	-3.68550099	-2.44823719	-3.86647769
O	-3.86832203	-1.06846839	-4.06831032
C	-6.60007069	-0.18114229	-2.12533686
O	-6.42609132	0.22863603	-3.46664309

C	-1.98321012	1.75181889	-3.25513702
O	-0.61192597	1.59345804	-3.52635537
C	1.73411014	4.58957109	-3.79271616
O	1.57064475	3.19857090	-3.95207722
C	3.13892068	6.68721916	4.29282014
C	-1.76573249	4.66792793	2.02873925
C	-5.71993174	-5.92404699	4.43594715
C	0.62925073	-10.12392461	-1.60073421
C	6.29626539	-7.20089641	-1.27973299
C	-2.32666934	10.64873840	-2.79106187
C	4.20963478	-0.89048105	5.06627917
H	4.17847438	6.28156609	-0.53628306
H	2.27003658	7.74513205	-0.20668496
H	0.52623637	5.30351497	0.17107501
H	0.55841151	6.83411643	-2.44878687
H	-1.15098381	5.98705537	-3.74349115
H	-3.60069939	5.91566134	-3.22973018
H	-2.68179995	4.82701899	-0.54352842
H	-4.28393217	3.30276207	-2.62184161
H	-5.29367817	3.38526492	-0.13817421
H	-5.61855692	1.80153285	1.68375462
H	-3.28339700	0.25642524	0.49162974
H	-6.23015710	-0.52863927	0.59479951
H	-6.41365475	-2.69053165	-0.47067834
H	-5.49217759	-4.89885333	-0.37414646
H	-2.75907875	-3.65524807	0.01722790
H	-3.63222423	-4.97997365	-2.56333625
H	-1.81566462	-5.46435105	-3.71021718
H	0.44321961	-6.34729352	-3.23684373
H	0.46274012	-4.36190825	-0.93213707
H	2.08965383	-4.24977641	-3.50775620
H	3.96209310	-3.49242785	-3.01144678
H	5.55220037	-2.82855093	-1.32493252
H	3.20950565	-1.82426864	0.33915798
H	5.46446891	-0.30593536	-1.05116351
H	5.81771189	0.46972184	1.18894514
H	5.37893424	2.47474205	2.56654482
H	2.76219371	2.49277545	1.02110098
H	4.89167266	4.65026805	0.99755365
H	4.40177064	2.74345594	-1.28849281
H	2.47055858	-0.52632434	-1.65798887
H	-0.23726615	-2.50177893	-2.58065588
H	-3.20552782	-2.03413694	-1.84417309
H	-4.51407748	0.21812120	-1.82945705
H	-1.36063601	3.08385117	-1.75141840
H	1.72700574	4.09358200	-1.73277734
H	-1.08450442	6.90650383	-0.42466781
H	2.64980266	-5.03344968	-0.80348909
H	2.74018259	4.67749036	2.03293023
H	-4.57882331	6.20681065	-0.72739044
H	-4.15927270	-1.31449242	2.00130597
H	-2.20368328	-5.90907806	-0.52665485
H	4.92958849	-2.61217660	1.56720872
H	0.57149368	7.37361877	2.04758590
H	2.04046557	8.33980952	2.31950435
H	1.14197556	7.46311638	4.38459724
H	3.73879991	5.98354375	3.70883334
H	3.13233784	6.35282201	5.33362265

H	3.62312885	7.66729455	4.25016070
H	1.66304545	4.81237870	3.63624999
H	-4.74218942	3.40818735	3.32637337
H	-4.46409546	4.27196897	1.79368588
H	-3.13370935	5.17045252	3.61285875
H	-2.15956459	5.48616795	1.41945394
H	-1.54433181	3.81495478	1.38077756
H	-0.84092542	5.02601438	2.49566038
H	-1.37488397	3.81833054	4.36105868
H	-4.58268777	-5.98829066	1.83514412
H	-6.28689255	-5.44001078	1.81930658
H	-4.11026264	-4.64861705	3.80384281
H	-5.14000340	-6.84344857	4.31124514
H	-6.76600936	-6.12729240	4.18767034
H	-5.67427072	-5.62766945	5.48662708
H	-5.81181814	-3.08277978	3.03816880
H	-1.05232247	-8.19712028	-2.76457894
H	-1.34962113	-8.41112507	-1.02383944
H	1.37609184	-8.28186727	-2.39875562
H	0.19243744	-10.48146655	-2.53821886
H	0.01355544	-10.47877442	-0.76824569
H	1.62524859	-10.55887438	-1.49350107
H	1.52981636	-7.28723567	-0.44002601
H	3.29891774	1.68341475	-2.16410923
H	4.70142246	1.02244265	-3.04897184
H	2.50601637	1.69725786	-4.12198801
H	1.72169685	-2.15933147	-4.80702024
H	-0.00086170	-1.99203905	-5.19643996
H	1.58029719	-0.22493808	-3.88401965
H	5.60649394	-5.32406942	0.67879696
H	6.26345943	-4.58395261	-0.79875220
H	4.27895132	-6.89140084	-0.62027212
H	6.70983601	-7.45049932	-0.29758441
H	7.06554536	-6.68329002	-1.86172961
H	6.04874185	-8.13008043	-1.79749894
H	3.63592566	-5.98638218	-2.39668082
H	-2.68781251	-2.69939794	-4.24147570
H	-4.41689146	-3.05362642	-4.42248206
H	-4.80702377	-0.83294057	-3.99749592
H	-3.91823314	8.47955435	-2.68679296
H	-2.45288681	7.99694802	-3.57809539
H	-2.38560764	9.52637622	-0.95833334
H	-1.74189570	11.46904161	-2.36986619
H	-3.38482869	10.92525387	-2.76918449
H	-2.01897912	10.51953164	-3.83363486
H	-0.42173527	8.62265842	-1.25805124
H	-6.65408062	-1.26622186	-2.16223299
H	-7.53436979	0.21264522	-1.70115051
H	-6.37954314	1.19118107	-3.47350564
H	3.11021716	2.32183556	4.34565655
H	4.76139516	1.74233841	4.68744540
H	2.90417018	0.55380167	5.99191407
H	3.74437910	-1.77415323	5.50864412
H	5.06957066	-0.60735970	5.68227464
H	4.56955630	-1.14549114	4.06543752
H	2.22730325	-0.05144911	3.36317930
H	-2.35841252	0.96458168	-2.59105507
H	-2.58911374	1.74071829	-4.17261580

H	-0.37737079	0.66849602	-3.74689751
H	6.64848936	3.44003649	-1.98168477
H	5.55961989	4.82673827	-1.83127310
H	7.42562188	4.02176882	0.11215016
H	0.97477862	5.13597216	-4.36738754
H	2.70962490	4.85231011	-4.21220584
H	0.64346569	2.91020069	-3.82743055
H	-3.01796246	0.19252174	3.38378171
H	-2.23875418	1.59233367	3.78926920
H	-3.86422370	1.32928963	5.35278262
H	-2.31020729	1.01046452	6.15554071
H	-3.37142098	-0.34855090	5.68822135
H	-1.44401287	-5.25877995	1.67666616
H	0.30297301	-7.00915537	1.61716376
H	1.45606113	-2.45755269	3.20582024
H	-0.06428289	1.88486517	2.44305960
H	0.37677245	1.84410998	0.00760148
H	0.03183188	-0.25963490	-1.27376357
H	-0.68166614	-2.31207414	-0.08928107
H	-2.06873372	-3.09681350	1.91825239
H	-1.77434832	-3.43069607	4.46835139
H	-2.84822183	-2.18344420	3.87986252
H	0.05036214	-1.71401627	4.79551448
H	-1.37049148	-1.34315284	5.73927760
H	-0.30719001	0.58865849	4.51421241

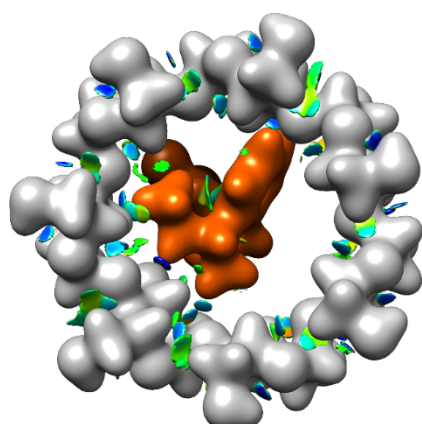
2.- Geometry differences between molecular dynamics candidates and optimized DFT structures

Table S1. Differences, in percent, between parameters involved in hydrogen bonds obtained from molecular dynamics and DFT optimizations. Donor (D), acceptor (A) and angle (θ) in a hydrogen bond.

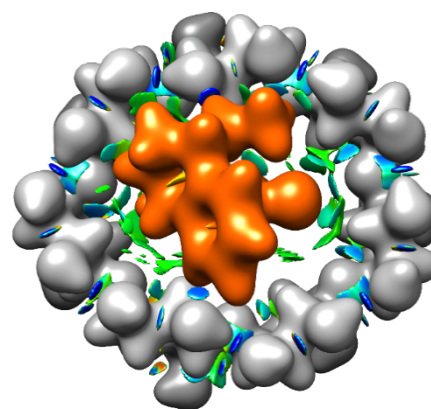
BCD:I_MD1				BCD:I_MD2				BCD:I_MD3			
H. Bond	θ	DA	HA	H. Bond	θ	DA	HA	H. Bond	θ	DA	HA
N-H...O	6.20	1.47	8.00	N-H...O	6.53	4.03	9.71	N-H...O	4.05	3.79	0.57
N-H...O	1.26	0.00	0.00	N-H...O	18.88	0.37	11.83	N-H...O	13.30	0.37	7.69
O-H...C	11.90	6.63	3.64	O-H...C	5.26	1.58	4.08	O-H...C	2.11	0.57	2.92
HPBCD:I_MD1				HPBCD:I_MD2				HPBCD:I_MD3			
N-H...O	5.04	2.56	2.94	N-H...O	4.21	0.74	1.20	N-H...O	4.81	8.77	11.35
N-H...O	1.16	7.64	13.68	N-H...O	3.15	4.29	6.78	N-H...O	4.49	10.38	19.83

3.- Non Covalent Interaction index

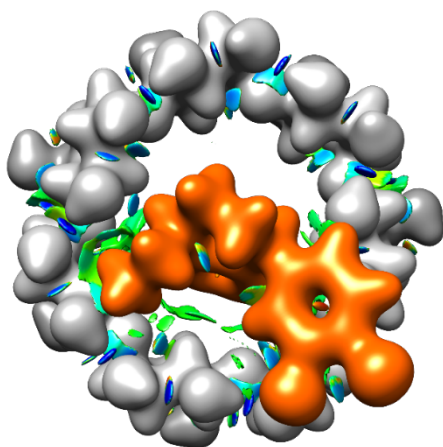
Electron density with an isosurface of 0.01 atomic units, in white for HPBCD and Orange for SRT. Non-covalent interactions index in green (weak interactions) and blue (strong interactions) isosurfaces.



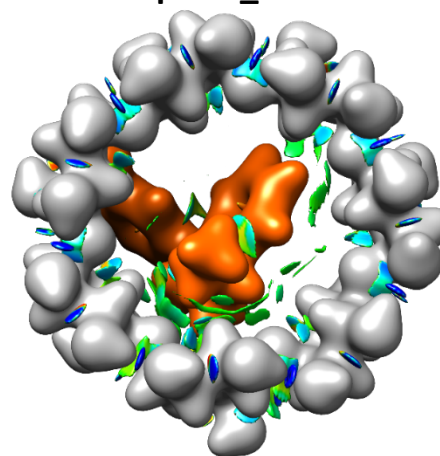
β CD:I_CI1



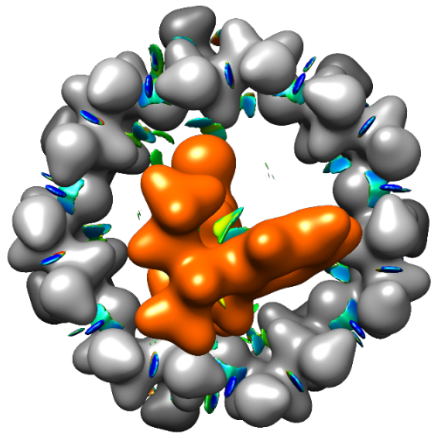
β CD:I_CI2



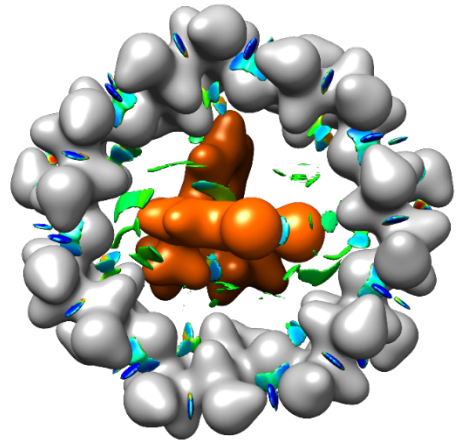
β CD:I_CI3



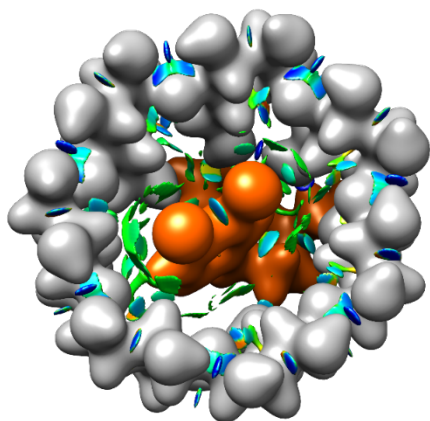
β CD:I_CI4



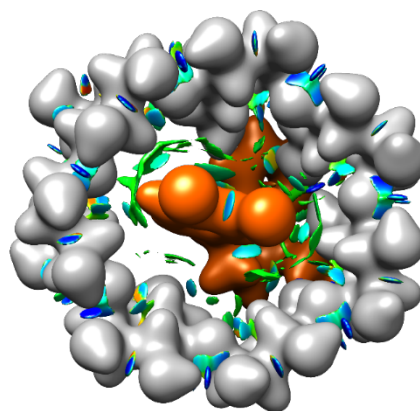
β CD:I_C15



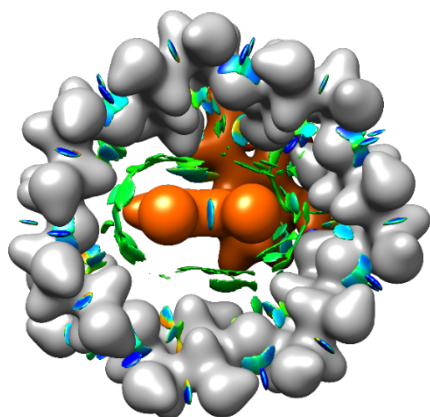
β CD:I_C16



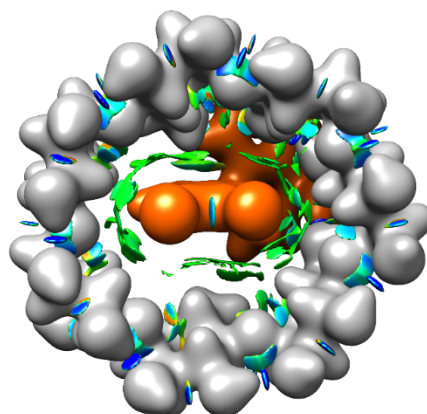
β CD:I_MD1



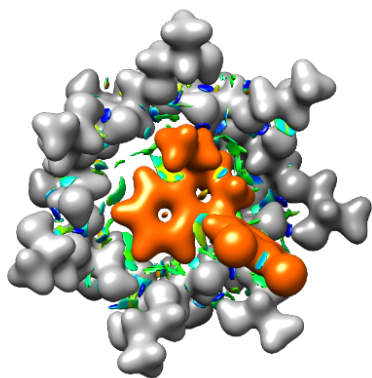
β CD:I_MD2



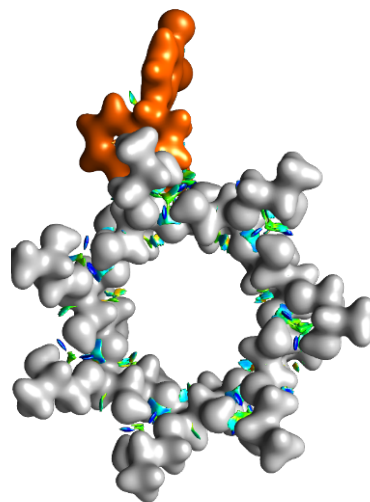
β CD:I_MD3



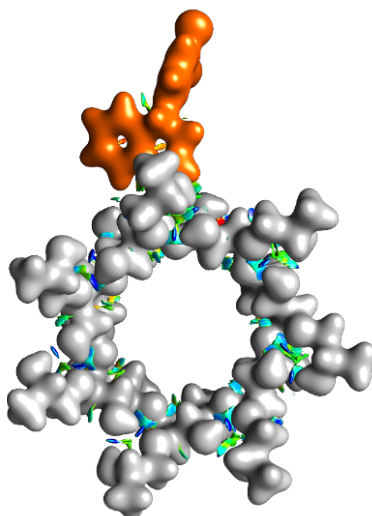
β CD:I_MD4



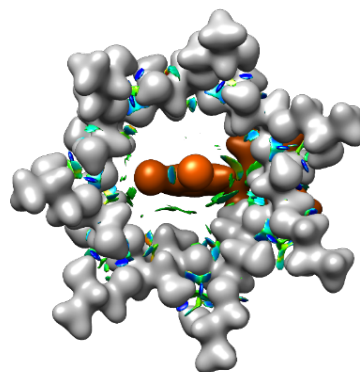
HPβCD:I_CI1



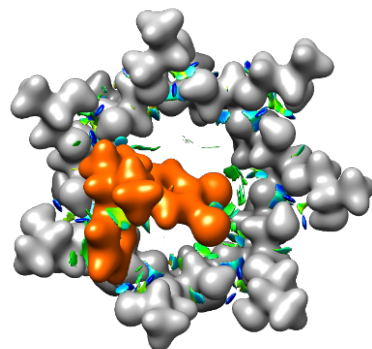
HPβCD:I_CI2



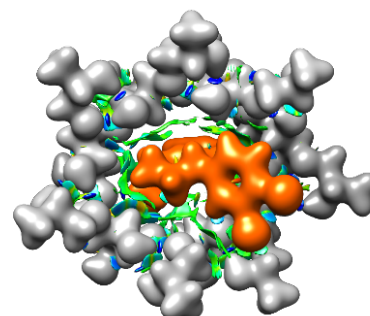
HPβCD:I_CI3



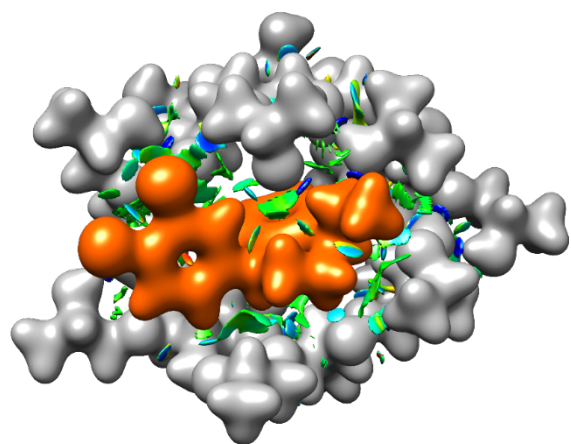
HPβCD:I_CI4



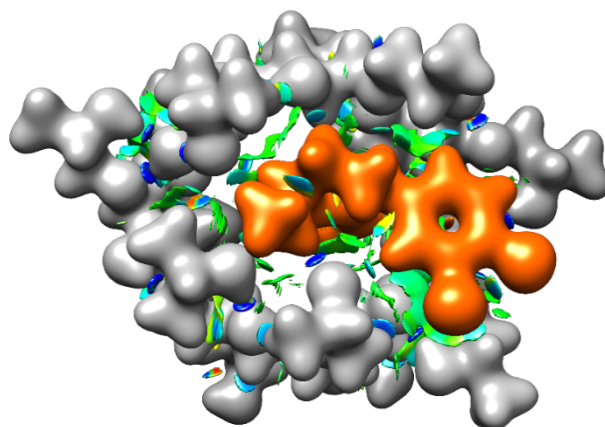
HPβCD:I_CI5



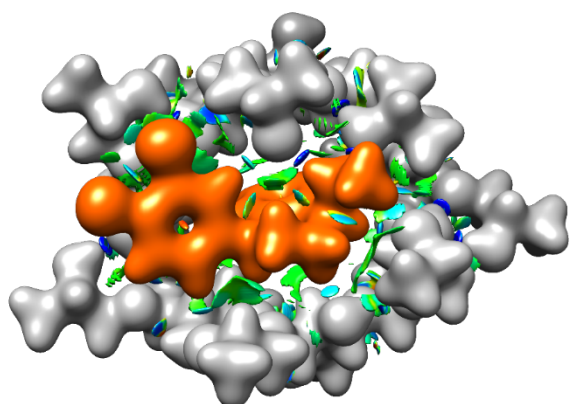
HPβCD:I_CI6



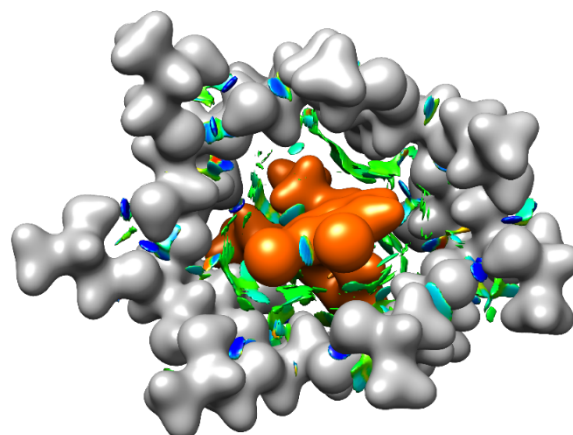
HPβCD:I_MD1



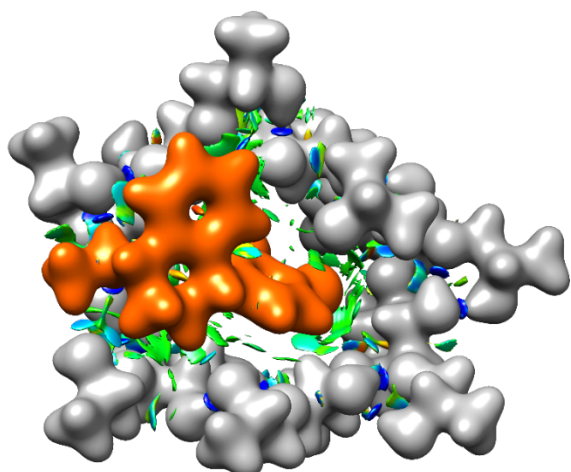
HPβCD:I_MD2



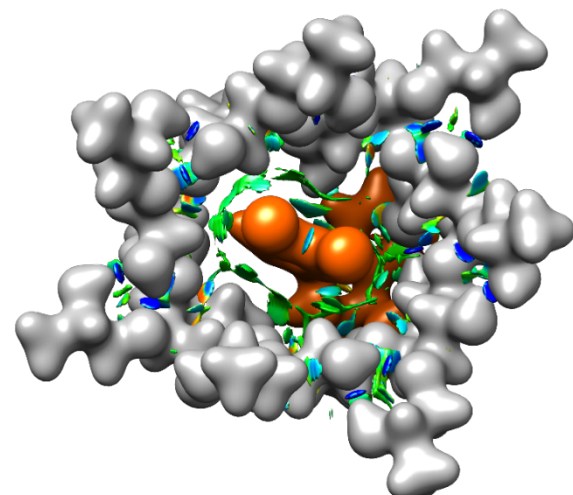
HPβCD:I_MD3



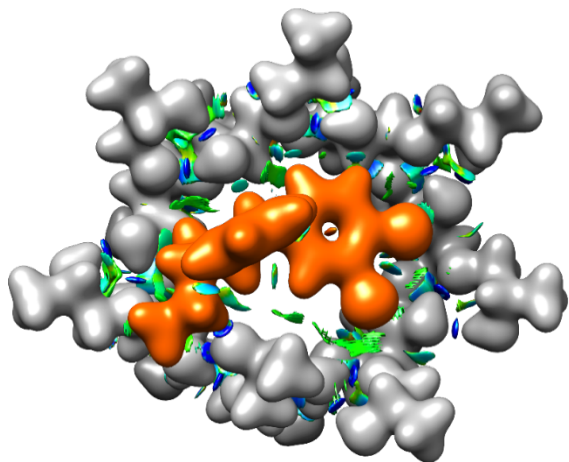
HPβCD:I_MD4



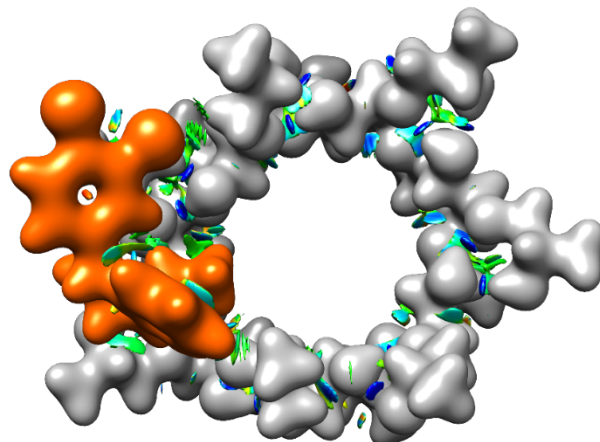
HPβCD:I_MD5



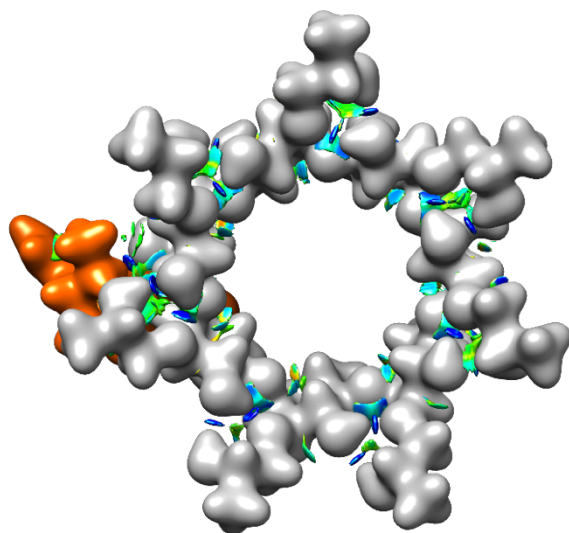
HPβCD:I_MD6



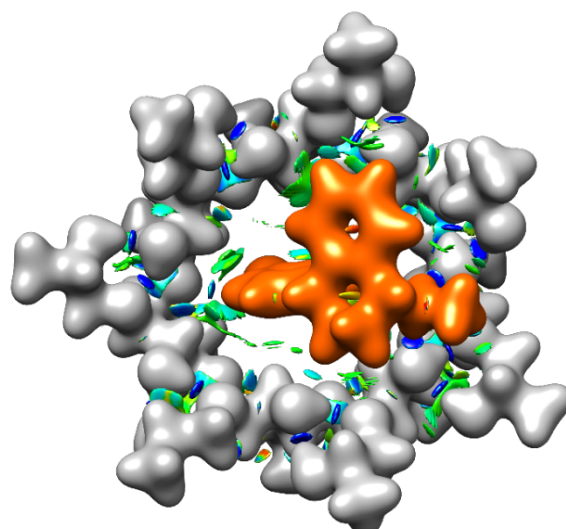
HPβCD:II_CI1



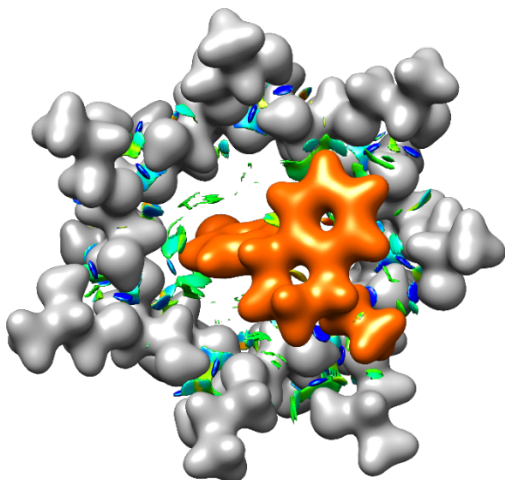
HPβCD:II_CI2



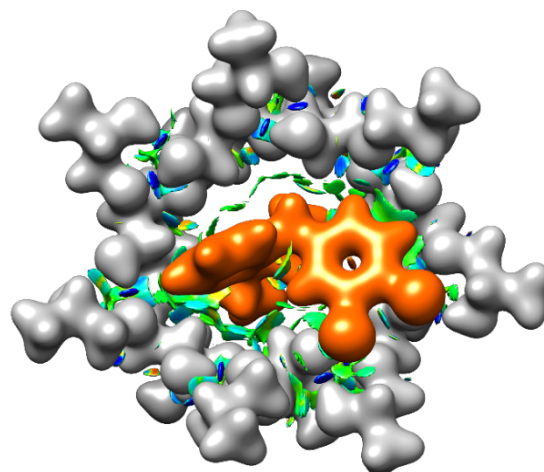
HPβCD:II_CI3



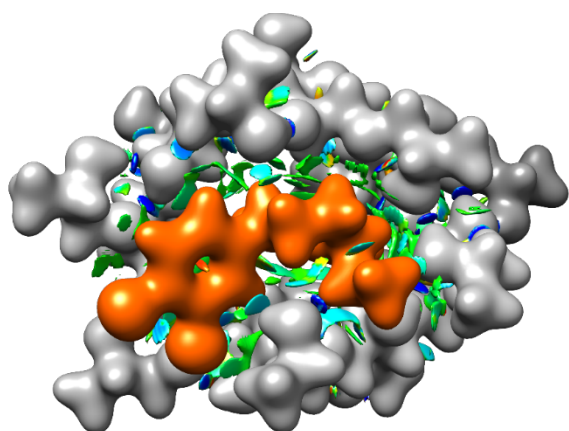
HPβCD:II_CI4



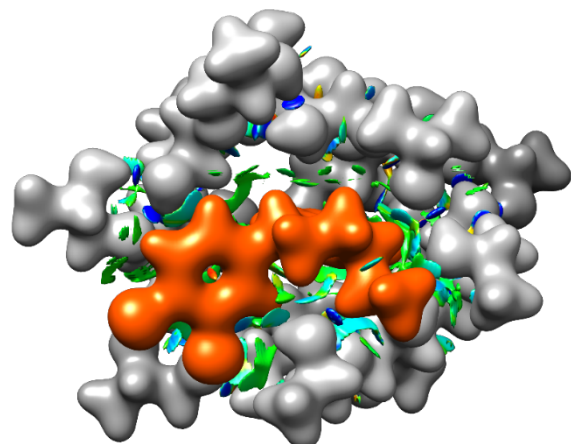
HPβCD:II_CI5



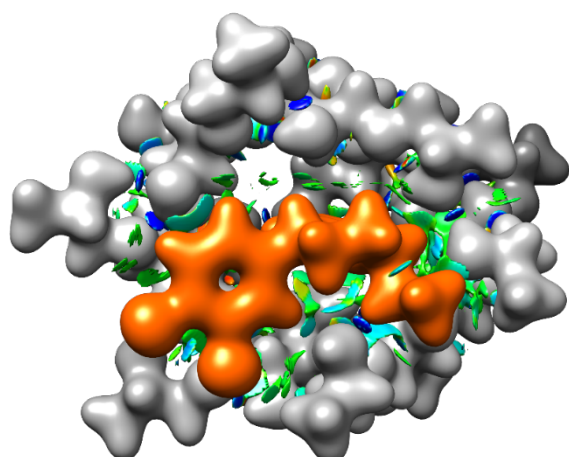
HPβCD:II_CI6



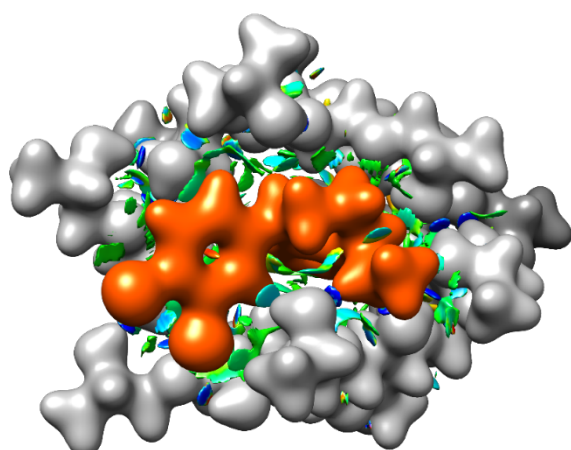
HPβCD:II_MD1



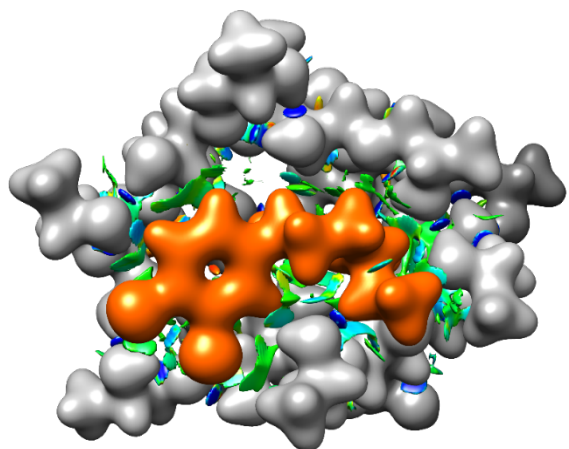
HPβCD:II_MD2



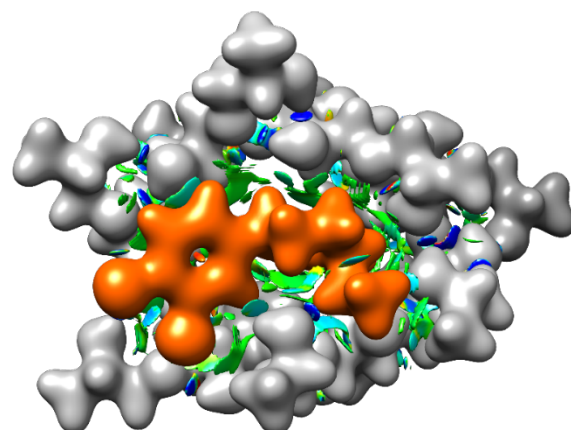
HPHPβCD:II_MD3



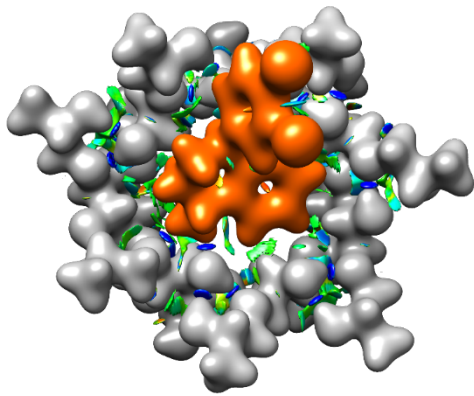
HPβCD:II_MD4



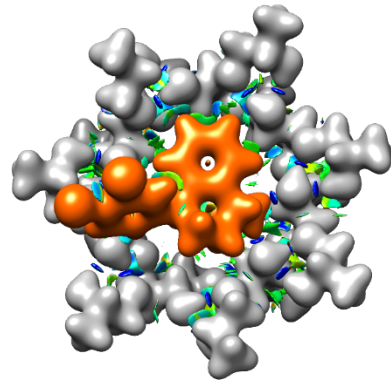
HPβCD:II_MD5



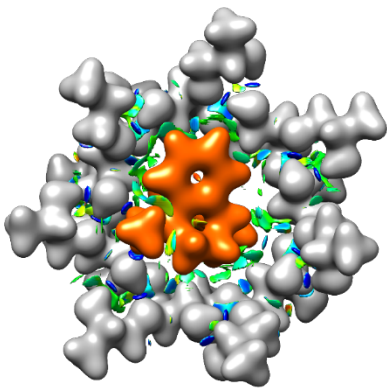
HPβCD:II_MD6



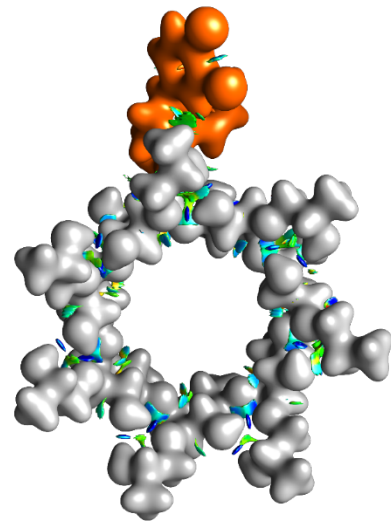
HPβCD:III_CI1



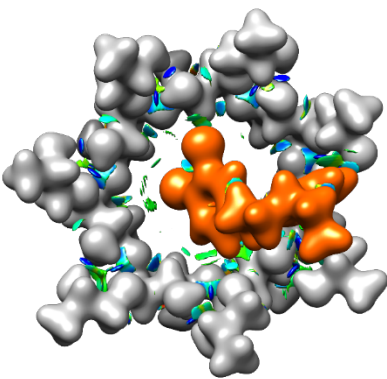
HPβCD:III_CI2



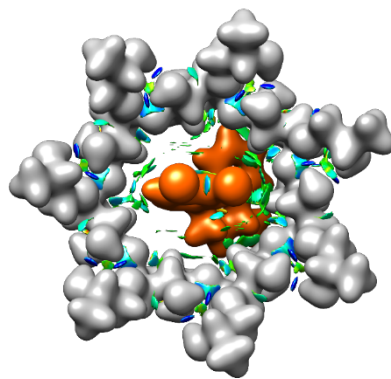
HPβCD:III_CI3



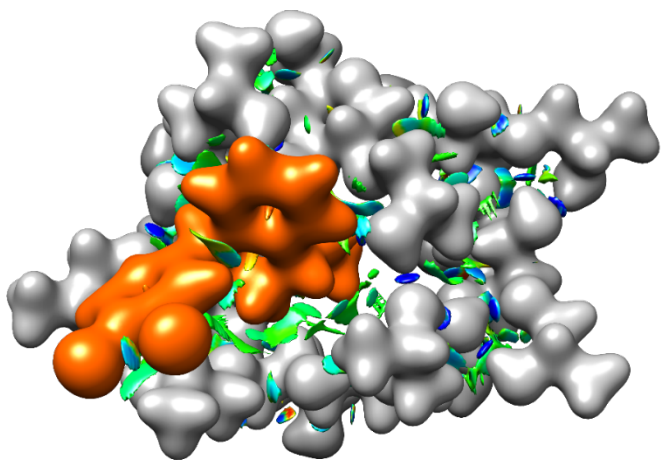
HPβCD:III_CI4



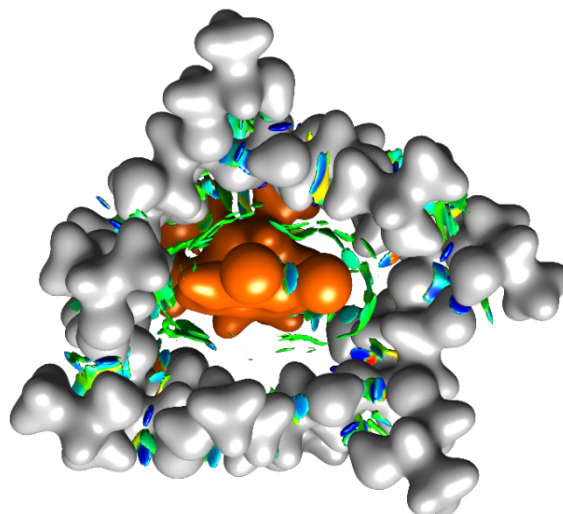
HPβCD:III_CI5



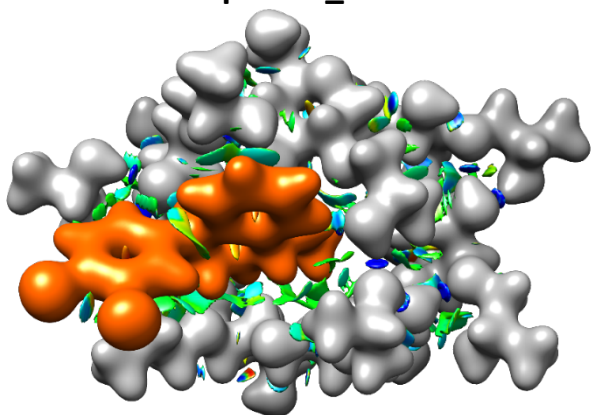
HPβCD:III_CI6



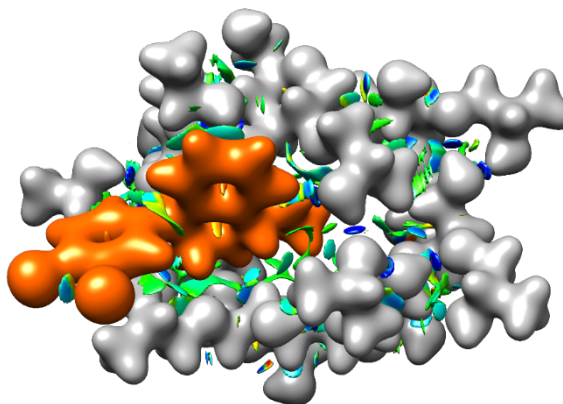
HPβCD:III_MD1



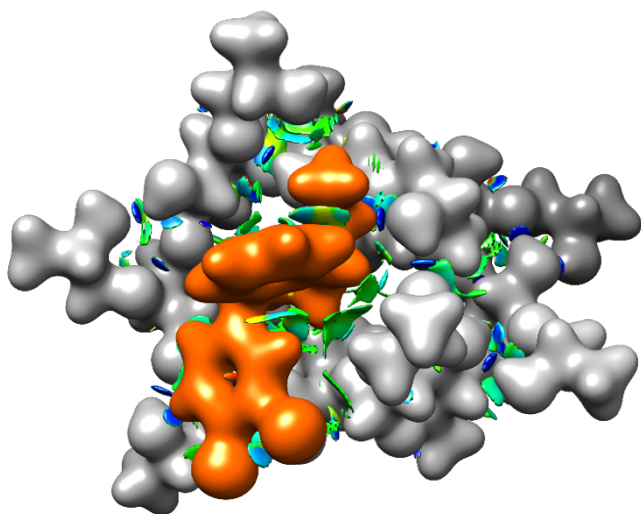
HPβCD:III_MD2



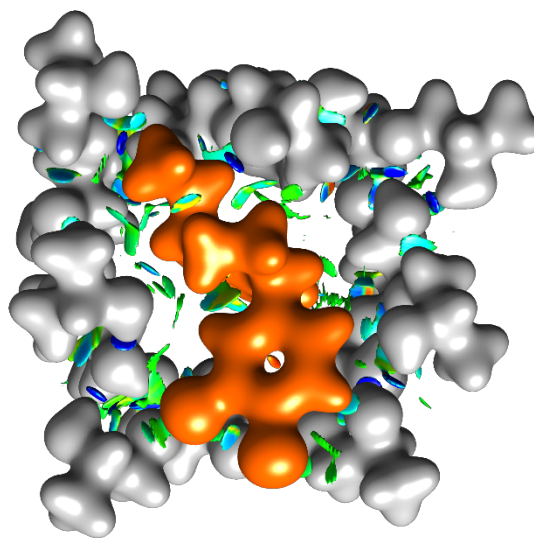
HPβCD:III_MD3



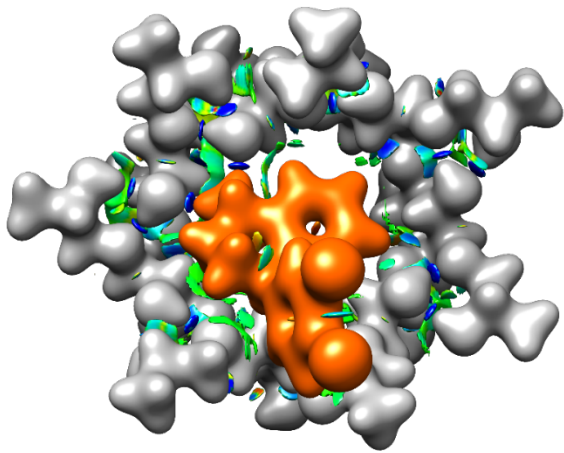
HPβCD:III_MD4



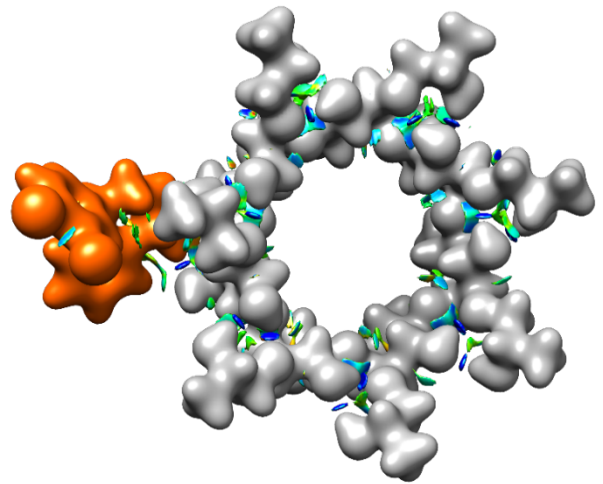
HPβCD:III_MD5



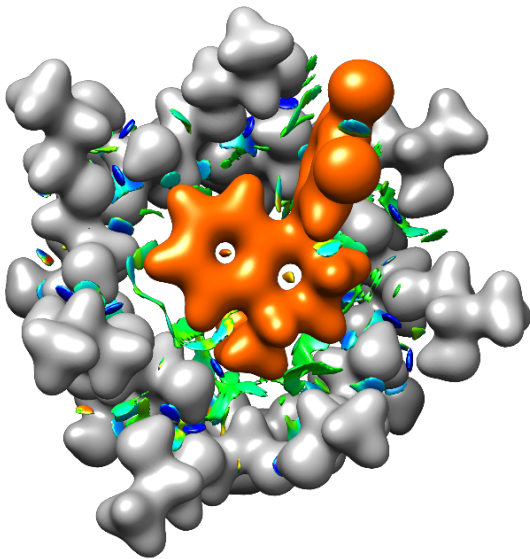
HPβCD:III_MD6



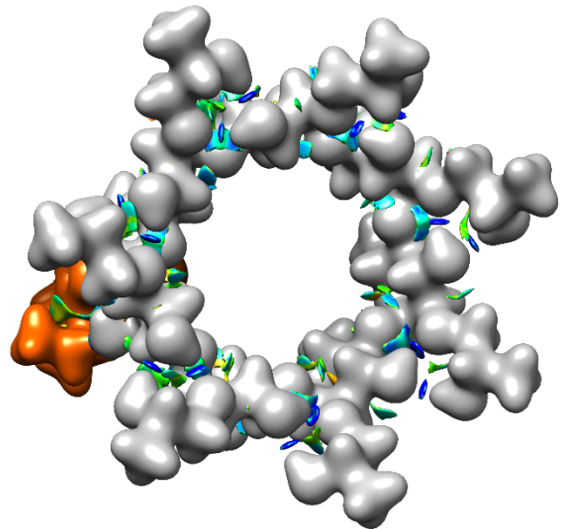
HPβCD:IV_CI1



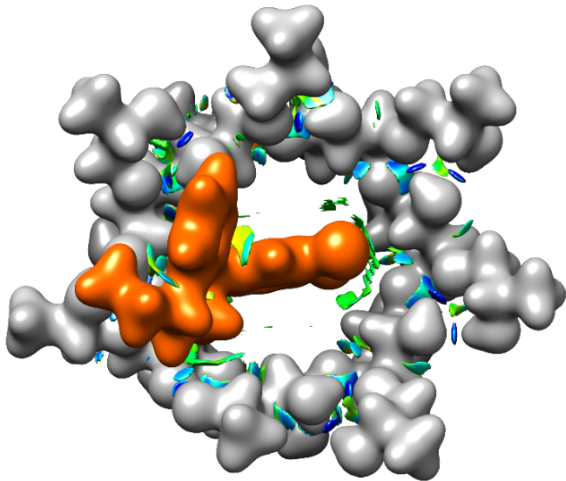
HPβCD:IV_CI2



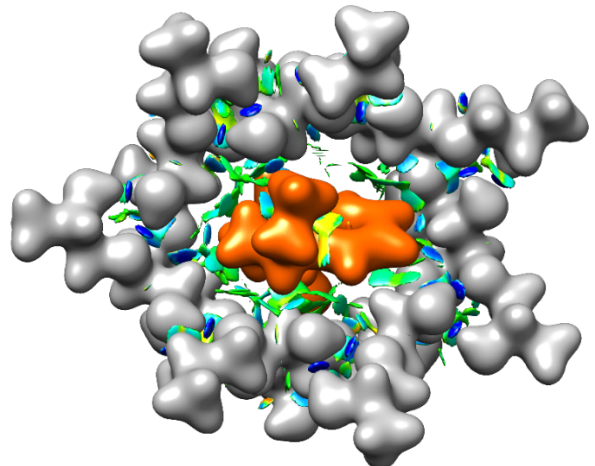
HPβCD:IV_CI3



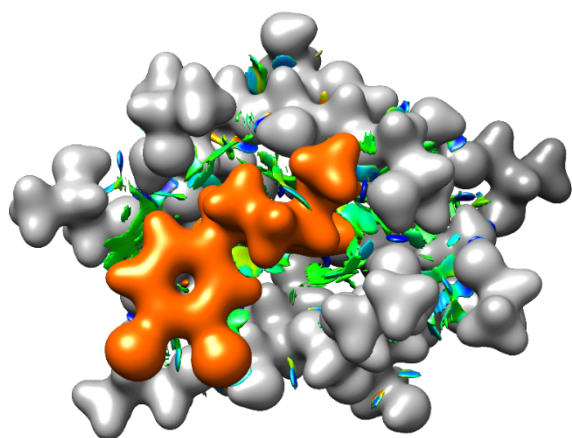
HPβCD:IV_CI4



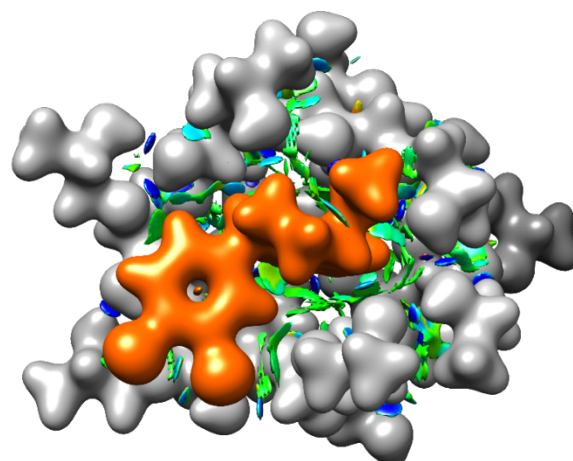
HPβCD:IV_CI5



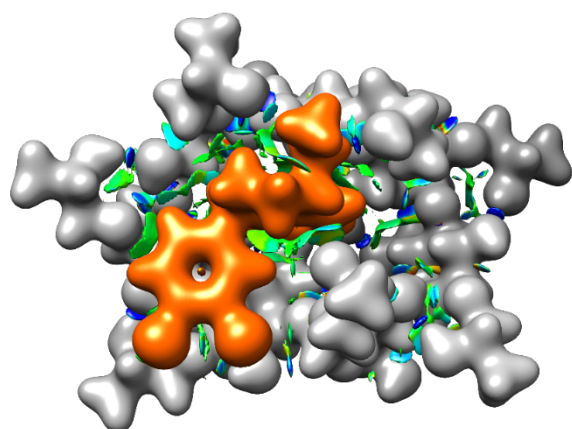
HPβCD:IV_CI6



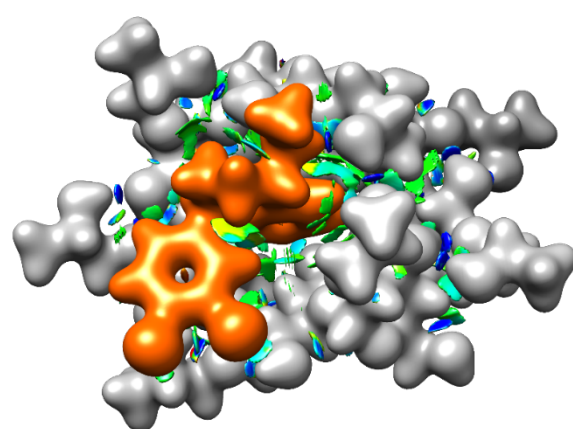
HPβCD:IV_MD1



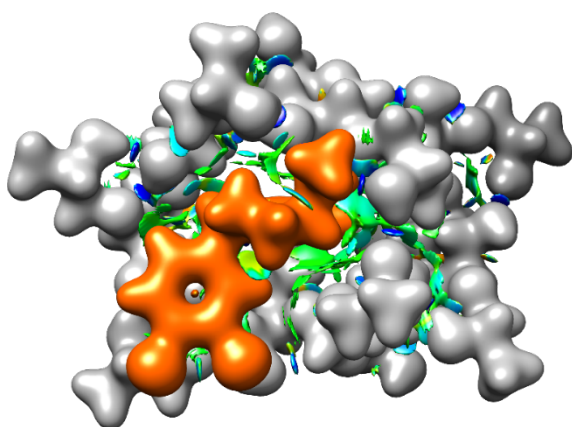
HPβCD:IV_MD2



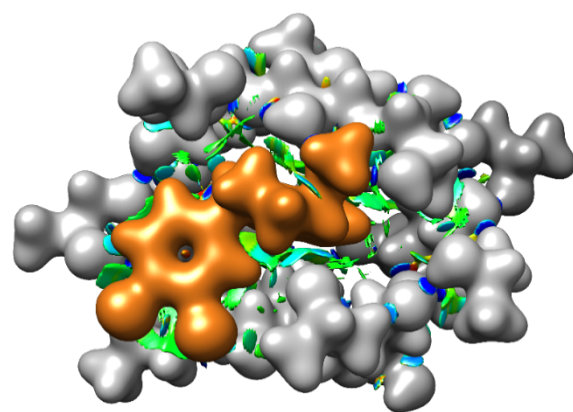
HPβCD:IV_MD3



HPβCD:IV_MD4



HPβCD:IV_MD5



HPβCD:IV_MD6