

Photochromic resorcin[4]arenes: stabilization of intramolecular anthracene dimers in solution

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Supplementary Material

Cartesian coordinates for the equilibrium [RI-BP86/SV(P)] head-to-head (**h2h**) and head-to-tail (**h2t**) dimer structures **9'-11'**, **13'**, and two adducts of **11'(h2t)** with a sodium cation **Na⁺@11'(h2t)**.

9'(h2h)

C	-1.2219112	-2.4581096	-5.6109937
C	-1.2393161	-1.1830900	-4.9940928
C	0.0001683	-0.5924919	-4.6951093
C	1.2393982	-1.1837721	-4.9938017
C	1.2214284	-2.4587898	-5.6106969
C	-0.0003858	-3.0994548	-5.9045076
C	-2.5633250	-0.4519636	-4.7609944
C	-2.8129980	0.5634557	-5.8984566
C	2.5637850	-0.4533788	-4.7604977
C	2.8144482	0.5614966	-5.8982369
O	2.4418250	-3.0102757	-5.9131416
C	2.4904099	-4.2847859	-6.5199982
O	-2.4425466	-3.0089305	-5.9137047
C	-2.4916796	-4.2833125	-6.5207816
C	-2.6837693	0.1521875	-3.3622279
C	-3.0231307	-0.6785511	-2.2705106
C	-3.1982322	-0.1722851	-0.9555109
C	-3.0734275	1.2285608	-0.7591439
C	-2.6906107	2.0891177	-1.8233745
C	-2.5024738	1.5230662	-3.0972323
C	-2.5804535	3.5893026	-1.5647657
C	-2.8953815	4.4586740	-2.8033893
O	-3.2884837	1.8339938	0.4563585
C	-4.5149900	1.5782365	1.1429766
C	-3.4559504	-1.1661398	0.1722907
O	-2.8067897	-0.9084612	1.4073249
C	-1.3882789	-0.9265655	1.3679922
C	-0.8481048	-1.2450314	2.7870096
C	-1.3715943	-0.1926250	3.7922113
C	-1.3771709	-0.5286087	5.1682848
C	-0.8129548	-1.8764928	5.5638457
C	-1.3823689	-2.9189444	4.6258219
C	-1.3777006	-2.6262465	3.2398494
C	-1.8731650	0.3765820	6.1216344
C	-2.3523667	1.6369064	5.7301371
C	-2.3243689	1.9868576	4.3720308
C	-1.8421348	1.0790802	3.4124516
C	-1.8692785	-3.6056051	2.3550242
C	-2.3693065	-4.8317542	2.8262593
C	-2.3913261	-5.1020656	4.2024536
C	-1.8915661	-4.1414763	5.0960480
O	-3.1499931	-2.0402892	-2.5017349
C	-4.4828783	-2.5177345	-2.6428637

C	0.8479374	-1.2449464	2.7871555
C	1.3711399	-0.1924937	3.7924777
C	1.3766293	-0.5285510	5.1685343
C	0.8123962	-1.8764527	5.5639730
C	1.3819974	-2.9188650	4.6260026
C	1.3776168	-2.6260908	3.2400454
C	1.8724483	0.3766426	6.1219718
C	2.3516047	1.6370153	5.7305791
C	2.3236822	1.9870466	4.3724910
C	1.8416283	1.0792641	3.4128254
C	1.8694628	-3.6053684	2.3552785
C	2.3694901	-4.8314974	2.8265668
C	2.3911950	-5.1018929	4.2027481
C	1.8911772	-4.1413817	5.0962839
C	1.3883425	-0.9263216	1.3682604
O	2.8068406	-0.9080209	1.4079005
C	3.4563356	-1.1658181	0.1730671
C	3.1984882	-0.1723708	-0.9550605
C	3.0235524	-0.6790944	-2.2699130
C	2.6841420	0.1512316	-3.3619255
C	2.5026164	1.5221725	-3.0973820
C	2.6905855	2.0886696	-1.8237027
C	3.0733821	1.2285107	-0.7591373
O	3.1506634	-2.0408880	-2.5006856
C	4.4836427	-2.5181694	-2.6415024
C	2.5804254	3.5889575	-1.5656121
C	2.8947062	4.4578573	-2.8047284
O	3.2881547	1.8343675	0.4561983
C	4.5145789	1.5790281	1.1431166
C	1.2416261	4.0222435	-0.9570737
C	1.2211788	5.0263754	0.0435605
C	0.0004656	5.5138457	0.5535803
C	-1.2204636	5.0265230	0.0439427
C	-1.2413683	4.0224075	-0.9567049
C	0.0000283	3.5449974	-1.4178348
O	2.4409049	5.4976537	0.4599661
C	2.4914121	6.4809887	1.4729298
O	-2.4400041	5.4979398	0.4607377
C	-2.4900842	6.4812147	1.4737843
H	0.0003776	0.3926030	-4.1963043
H	-0.0006022	-4.0899634	-6.3749965
H	-3.3522943	-1.2246085	-4.8448831
H	-3.7807704	1.0963116	-5.7615798
H	-2.8434035	0.0321988	-6.8742651
H	-2.0037708	1.3234409	-5.9653276
H	3.3522949	-1.2265447	-4.8438319
H	2.8449440	0.0298745	-6.8738446
H	3.7824563	1.0938778	-5.7611726
H	2.0056581	1.3218938	-5.9656915
H	3.5651463	-4.5200249	-6.6625579
H	1.9846342	-4.2928853	-7.5157717
H	2.0302172	-5.0718912	-5.8753036
H	-3.5665072	-4.5179138	-6.6637075
H	-2.0321287	-5.0707834	-5.8760750
H	-1.9856127	-4.2915475	-7.5164058
H	-2.2536276	2.1925563	-3.9339578
H	-3.3453058	3.8232585	-0.7984126
H	-3.8739202	4.1800478	-3.2552691
H	-2.9432451	5.5281724	-2.5050783
H	-2.1111280	4.3719483	-3.5873656
H	-4.7214800	2.4792656	1.7582489
H	-4.4266747	0.6965428	1.8138397
H	-5.3513125	1.4354108	0.4201118

H	-3.1637488	-2.1745645	-0.2084778
H	-4.5361034	-1.2117099	0.4366678
H	-1.0086375	0.0537047	1.0066934
H	-1.0407464	-1.6932440	0.6390614
H	-1.1231430	-2.1120204	6.6020754
H	-1.8774334	0.0889912	7.1872269
H	-2.7414737	2.3415355	6.4841101
H	-2.6884531	2.9749761	4.0442986
H	-1.8600680	1.3833317	2.3562686
H	-1.8713294	-3.4301264	1.2695080
H	-2.7502665	-5.5755858	2.1067003
H	-2.7924547	-6.0572875	4.5800823
H	-1.8927681	-4.3424787	6.1812599
H	-5.0671443	-2.4266768	-1.6951755
H	-4.4083274	-3.5900567	-2.9182900
H	-5.0308586	-1.9730955	-3.4481589
H	1.1224333	-2.1120074	6.6022420
H	1.8766295	0.0890078	7.1875529
H	2.7405910	2.3416324	6.4846255
H	2.6877096	2.9752134	4.0448438
H	1.8596134	1.3835726	2.3566596
H	1.8717356	-3.4298380	1.2697687
H	2.7506646	-5.5752649	2.1070547
H	2.7923144	-6.0571037	4.5804148
H	1.8921637	-4.3424332	6.1814862
H	1.0086372	0.0539117	1.0069322
H	1.0410755	-1.6930108	0.6392156
H	4.5364478	-1.2109562	0.4376712
H	3.1645348	-2.1744445	-0.2074674
H	2.2537589	2.1913539	-3.9343534
H	5.0678453	-2.4265397	-1.6938319
H	5.0315657	-1.9738259	-3.4470395
H	4.4092916	-3.5906421	-2.9164005
H	3.3456448	3.8232321	-0.7997200
H	3.8727571	4.1787151	-3.2573419
H	2.1097630	4.3712348	-3.5880268
H	2.9432560	5.5274198	-2.5067535
H	5.3510502	1.4360734	0.4204499
H	4.4262751	0.6975638	1.8142831
H	4.7208331	2.4803148	1.7580917
H	0.0006298	6.2847497	1.3333889
H	-0.0001330	2.7529940	-2.1871596
H	3.5665773	6.6913854	1.6471528
H	2.0335594	6.1218535	2.4258310
H	1.9845985	7.4267205	1.1627472
H	-1.9832616	7.4269106	1.1635081
H	-2.0319731	6.1219586	2.4265147
H	-3.5651713	6.6917227	1.6483524

9'(h2t)

C	3.5449935	-0.7635935	-0.9185376
C	2.8521344	-2.0039790	-0.8028486
C	3.7923424	0.0443117	0.2250032
C	3.4401151	-0.4836926	1.4988117
C	2.7247294	-1.6961446	1.6527608
C	2.4316104	-2.4125506	0.4747465
C	2.4726900	-2.2725408	3.0475424
C	1.0777769	-2.1036289	3.6695936
C	2.8866511	-3.7642995	3.1424118
C	1.0064022	-1.8796590	5.0709139
C	-0.2332041	-1.8107008	5.7370808
C	-1.4269368	-2.0080354	5.0161303

C	-1.4070660	-2.2431985	3.6168618
C	-0.1432731	-2.2729112	2.9859652
C	-2.7358818	-2.5799290	2.9192077
C	-2.9005784	-2.0623689	1.4912209
C	2.7528131	-2.9214250	-2.0206879
C	1.4166437	-2.9394089	-2.7672080
C	0.1654386	-3.0119876	-2.1293175
C	-1.0520205	-3.1822508	-2.8146306
C	1.4267136	-3.0191749	-4.1837912
C	0.2277743	-3.1543154	-4.9123121
C	-1.0008442	-3.2529434	-4.2291994
C	-2.3833384	-3.4430271	-2.1053976
C	-2.7249569	-2.5035149	-0.9488564
C	-2.4450312	-2.8205230	0.3939186
C	-3.4461520	-1.3106396	-1.1880634
C	-3.8808261	-0.4730914	-0.1318121
C	-3.6527960	-0.8872363	1.2087525
C	-2.9985868	-4.1040993	3.0337726
C	-2.4713767	-4.9373760	-1.7108875
C	3.1759232	-4.3765109	-1.6943351
O	-2.6642573	-1.9954781	5.6142498
O	2.2020074	-1.7508885	5.7316307
O	-2.1963149	-3.4472319	-4.8785101
O	2.6577347	-2.9822277	-4.7887474
C	-2.2135166	-3.5022333	-6.2896741
C	2.7371282	-3.0214022	-6.1977755
C	2.2037706	-1.4955454	7.1210583
C	-2.7586233	-1.7626578	7.0054768
C	4.4349696	1.4309052	0.1594895
C	-4.5519237	0.8549517	-0.4557225
O	3.9539559	-0.4328249	-2.1833543
O	3.8309190	0.2083522	2.6382470
O	-3.7086754	-0.9309232	-2.4946691
O	-4.3496077	-0.2165486	2.1988484
C	-0.8486156	1.7938581	-0.3063205
C	-1.6906697	3.2024157	-0.3845943
C	-1.2304350	4.2397221	0.6709063
C	0.0137064	4.8920810	0.4523782
C	0.8080843	4.4990242	-0.7805938
C	-0.1878421	4.5093602	-1.9364421
C	-1.4519405	3.8885797	-1.7404017
C	0.0770498	5.1833655	-3.1397958
C	-0.8915154	5.2475626	-4.1572919
C	-2.1358964	4.6298207	-3.9670821
C	-2.4121013	3.9513930	-2.7651490
C	0.4513599	5.8978234	1.3285504
C	-0.3228740	6.2746668	2.4394147
C	-1.5472515	5.6334888	2.6679679
C	-1.9936105	4.6278712	1.7893823
C	0.0652891	1.7926256	0.8918355
C	1.2753843	2.5137962	0.7892999
C	1.6318799	3.0865273	-0.5927149
C	1.1890268	2.1363547	-1.7157724
C	-0.0708130	1.5159485	-1.5725372
C	1.9025967	1.9494799	-2.9157602
C	1.3770547	1.1537671	-3.9460868
C	0.1279421	0.5348779	-3.7926537
C	-0.5967096	0.7209714	-2.6058611
C	1.9971046	2.7667411	1.9713188
C	1.5861704	2.2370451	3.2061783
C	0.4490481	1.4221793	3.2741063
C	-0.3092049	1.2110766	2.1119880
C	3.1527632	3.3829837	-0.7114040

O	3.9861315	2.2513258	-0.9212895
C	-3.1660760	2.8186570	-0.1219491
O	-3.6268454	1.8085884	-1.0045289
C	-3.6740857	0.5499935	3.1899979
C	-4.9695379	-1.3258622	-3.0227684
C	5.1858016	0.0093878	3.0210700
C	5.2787792	0.0289622	-2.4110562
H	1.9417116	-3.3945714	0.5709093
H	3.1457792	-1.7131099	3.7233610
H	3.9202029	-3.9165185	2.7583645
H	2.2034448	-4.4232196	2.5627849
H	2.8541022	-4.1017577	4.2012454
H	-0.2676793	-1.6299764	6.8179977
H	-0.1088471	-2.4320370	1.8948050
H	-3.5359752	-2.0969943	3.5140546
H	3.4891638	-2.5274228	-2.7450685
H	0.1355132	-2.9366799	-1.0290558
H	0.2535752	-3.2083911	-6.0072095
H	-3.1575830	-3.2764895	-2.8766773
H	-1.9125147	-3.7603428	0.6042527
H	-3.0391959	-4.3962128	4.1053026
H	-2.1938243	-4.7049540	2.5573817
H	-3.9674865	-4.3776855	2.5599516
H	-1.6500705	-5.2371661	-1.0235615
H	-2.3819914	-5.5696270	-2.6206714
H	-3.4417778	-5.1699529	-1.2171148
H	2.4412360	-4.8891688	-1.0348011
H	4.1688168	-4.4010647	-1.1915893
H	3.2459922	-4.9685173	-2.6330465
H	-1.6096186	-4.3558487	-6.6823302
H	-1.8406402	-2.5551567	-6.7488253
H	-3.2735971	-3.6496593	-6.5815929
H	2.3231042	-3.9717080	-6.6142346
H	3.8158947	-2.9605290	-6.4491718
H	2.2070017	-2.1594480	-6.6696496
H	3.2691340	-1.4188675	7.4200518
H	1.7257548	-2.3233463	7.6984004
H	1.6887477	-0.5365854	7.3697358
H	-2.2288973	-2.5486230	7.5953599
H	-3.8395770	-1.7958985	7.2516302
H	-2.3528318	-0.7620676	7.2897582
H	4.2679012	1.9280088	1.1364078
H	5.5392590	1.3410647	0.0221420
H	-5.0380107	1.2545823	0.4601263
H	-5.3411770	0.7216190	-1.2241636
H	-1.6157228	1.0050124	-0.1943816
H	1.5766998	5.2782442	-0.9730793
H	1.0555803	5.6741116	-3.2808342
H	-0.6705678	5.7827798	-5.0959035
H	-2.9026723	4.6698236	-4.7589190
H	-3.3781999	3.4416031	-2.6345395
H	1.4147316	6.3997856	1.1330325
H	0.0291689	7.0695908	3.1177366
H	-2.1725058	5.9171506	3.5309892
H	-2.9657824	4.1579508	1.9989749
H	2.8857412	2.4156520	-3.0641663
H	1.9589704	1.0126978	-4.8722000
H	-0.2879902	-0.0961568	-4.5947530
H	-1.5944490	0.2696864	-2.4948927
H	2.8955077	3.4019760	1.9577023
H	2.1808463	2.4435391	4.1104669
H	0.1434379	0.9572218	4.2254417
H	-1.2132296	0.5864254	2.1489943

H	3.5041448	3.9850423	0.1604171
H	3.3186343	4.0137374	-1.6116024
H	-3.8148332	3.7262828	-0.2032763
H	-3.2318818	2.4526280	0.9281143
H	-4.4348359	0.7945930	3.9603440
H	-3.2724154	1.4996370	2.7645407
H	-2.8394316	-0.0055623	3.6699305
H	-5.8219038	-0.9131027	-2.4316798
H	-5.0761358	-2.4362133	-3.0586815
H	-5.0174875	-0.9252563	-4.0562429
H	5.9022728	0.3519614	2.2356098
H	5.3975094	-1.0643059	3.2437560
H	5.3478525	0.6083486	3.9418684
H	6.0106827	-0.5001596	-1.7561911
H	5.3603065	1.1286534	-2.2643765
H	5.5112080	-0.2110902	-3.4706243

10'(h2h)

C	0.2275276	-0.6533811	-5.0482492
C	0.2684976	-1.6610426	-4.0546894
C	-0.8474262	-1.7828880	-3.2033682
C	-1.9999888	-0.9825645	-3.3024252
C	-1.9935051	0.0303360	-4.2990552
C	-0.8877931	0.2034756	-5.1547514
C	-2.8121351	-3.0490131	-0.7873026
C	-2.7611296	-3.5690663	0.5182791
C	-3.0538391	-2.6845019	1.5887798
C	-3.3819968	-1.3270477	1.3632834
C	-3.4395992	-0.8664544	0.0248746
C	-3.1475574	-1.7077521	-1.0738512
C	0.1291366	-4.8853492	0.7556034
C	1.4214056	-5.1584221	1.2368293
C	1.5137673	-5.7925585	2.5043960
C	0.3584674	-6.1436720	3.2290346
C	-0.9181553	-5.8892235	2.6866694
C	-1.0519657	-5.2421840	1.4347473
C	2.0834496	-3.7024106	-1.7211532
C	2.1549693	-2.6266640	-2.6250909
C	2.9294259	-1.5030424	-2.2415332
C	3.5914629	-1.4428507	-0.9953187
C	3.4967960	-2.5615436	-0.1278573
C	2.7419982	-3.7080259	-0.4726734
C	-2.4367165	-5.0371356	0.8114421
C	-3.2924112	-1.1933733	-2.5030885
C	1.4508993	-2.6343763	-3.9850534
C	2.7181190	-4.9194017	0.4541900
O	4.1500824	-2.5122083	1.0930608
C	5.4952228	-2.9740253	1.0783510
O	3.0070919	-0.4203206	-3.1089959
C	4.1319936	-0.4232495	-3.9804877
O	2.7820799	-6.0528070	2.9606138
C	2.9525406	-6.6170725	4.2448929
O	-2.0772804	-6.2652643	3.3182047
C	-2.0002816	-6.9161461	4.5695590
O	-2.9988674	-3.1655401	2.8856315
C	-4.2304361	-3.6448916	3.4098037
O	-3.7954604	0.4608109	-0.1986752
C	-5.1954032	0.6892963	-0.3405946
O	-3.1243173	0.8028347	-4.3856845
C	-3.1560791	1.8837824	-5.2967018
O	1.3048187	-0.5727600	-5.8942940

C	1.3106720	0.4062846	-6.9128873
C	-3.6033387	-0.3768239	2.5377066
C	4.2885880	-0.1738198	-0.5163816
C	-2.6200546	-5.9707897	-0.4041823
C	-4.2733031	-2.0716857	-3.3247792
C	3.1272411	-6.2179297	-0.2893528
C	1.0182399	-4.0384051	-4.4577162
O	3.4203615	0.6366139	0.2664423
C	2.6846653	1.6356308	-0.4489609
C	0.9826689	3.3279246	0.6465513
C	2.0957288	3.9834644	1.4976585
C	2.1459711	5.3991563	1.5671250
C	1.0723542	6.1781096	0.8356736
C	0.9201324	5.5760886	-0.5467351
C	0.8452879	4.1625559	-0.6442961
C	0.8553745	6.3737216	-1.7011807
C	0.6970488	5.7910735	-2.9698764
C	0.5932821	4.3965758	-3.0735247
C	0.6658645	3.5934933	-1.9207547
C	3.0781726	3.2490030	2.1932253
C	4.0853287	3.8991034	2.9292969
C	4.1334439	5.2994657	2.9815751
C	3.1588747	6.0434982	2.2965625
O	-2.4433014	0.3693271	2.8768094
C	-2.3667751	1.7380432	2.4729936
C	-0.5060946	3.3610777	1.5129263
C	-1.5276530	4.2152560	0.7295693
C	-1.4637423	5.6264728	0.8439402
C	-0.3297369	6.2076680	1.6579323
C	-0.2305862	5.4415167	2.9588495
C	-0.2695791	4.0269095	2.8880894
C	-2.5168397	3.6629121	-0.1099420
C	-3.4409473	4.4845231	-0.7812242
C	-3.3988900	5.8775903	-0.6226667
C	-2.4006727	6.4422167	0.1873215
C	-0.0684116	6.0926814	4.1934750
C	0.0849947	5.3554275	5.3784525
C	0.0902107	3.9541136	5.3153106
C	-0.0861726	3.3007239	4.0830078
C	-1.0455306	1.9183237	1.7050286
C	1.3584019	1.8643613	0.3077410
H	-0.8099253	-2.5527797	-2.4150617
H	-0.9055605	0.9896597	-5.9188380
H	-2.6227535	-3.7293194	-1.6314090
H	0.0302409	-4.3613980	-0.2096067
H	0.4526251	-6.6312160	4.2065579
H	1.5151118	-4.5983267	-2.0138644
H	-3.1598265	-5.3752577	1.5787430
H	-3.7489031	-0.1885416	-2.4293737
H	2.1847698	-2.2645218	-4.7277343
H	3.4876324	-4.7367538	1.2274432
H	5.5633052	-4.0514337	0.7920047
H	6.1315279	-2.3857781	0.3731393
H	5.8862510	-2.8485703	2.1095550
H	4.0422796	0.4784827	-4.6201374
H	5.0946132	-0.3774152	-3.4159811
H	4.1498207	-1.3294743	-4.6309052
H	4.0472014	-6.6984499	4.4045022
H	2.5010656	-7.6360430	4.3166634
H	2.5165943	-5.9705087	5.0435879
H	-3.0461066	-7.1230243	4.8764594
H	-1.5164009	-6.2743130	5.3443143
H	-1.4463806	-7.8837393	4.5037011

H	-4.9942345	-2.8326535	3.4850218
H	-4.6577863	-4.4689650	2.7904952
H	-4.0143234	-4.0334598	4.4260162
H	-5.3332465	1.7875000	-0.4216907
H	-5.6015753	0.1995424	-1.2573872
H	-5.7666101	0.3134829	0.5411829
H	-4.1415906	2.3739147	-5.1605164
H	-3.0679226	1.5398737	-6.3554179
H	-2.3502747	2.6262515	-5.0853005
H	0.4592649	0.2745012	-7.6233431
H	2.2627936	0.2724361	-7.4661504
H	1.2775375	1.4416829	-6.4964539
H	-3.8601406	-0.9719974	3.4375102
H	-4.4574773	0.3079943	2.3310038
H	4.6987389	0.4044927	-1.3745193
H	5.1340232	-0.4359100	0.1502609
H	-2.4894394	-7.0278374	-0.0865501
H	-3.6350589	-5.8654086	-0.8487789
H	-1.8708310	-5.7762342	-1.2028159
H	-3.8635286	-3.0905875	-3.5000564
H	-5.2481369	-2.1789755	-2.7978400
H	-4.4624487	-1.6077533	-4.3167592
H	4.1023673	-6.0876441	-0.8105988
H	3.2280770	-7.0554984	0.4340061
H	2.3689940	-6.5156329	-1.0465836
H	1.8740261	-4.7500209	-4.4543341
H	0.2105535	-4.4660960	-3.8239083
H	0.6222891	-3.9788821	-5.4945087
H	2.4931295	1.2907680	-1.4884618
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H	1.3933644	7.2350479	0.7370200
H	0.9287555	7.4706499	-1.6031759
H	0.6524114	6.4263649	-3.8702345
H	0.4616140	3.9179173	-4.0585079
H	0.5791735	2.5037332	-2.0398008
H	3.0988420	2.1507696	2.1452335
H	4.8432606	3.2961083	3.4567187
H	4.9262768	5.8133812	3.5503336
H	3.1814876	7.1466104	2.3289585
H	-3.2390234	2.0107965	1.8418664
H	-2.3961572	2.3790191	3.3844625
H	-0.5411557	7.2744734	1.8750012
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H	-4.2010104	4.0230736	-1.4340149
H	-4.1308667	6.5241171	-1.1349877
H	-2.3381523	7.5378092	0.3059426
H	-0.0538094	7.1959722	4.2228376
H	0.2094645	5.8738911	6.3436757
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H	-0.0785813	2.2006892	4.0725282
H	-1.1702163	1.4149069	0.7269361
H	-0.2993670	1.3082071	2.2502600
H	1.4421814	1.2758265	1.2408544
H	0.5377879	1.3851692	-0.2588274

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C	-2.0816193	3.0845763	-1.3073905
C	-2.2207441	2.3273626	-2.4988471
C	-0.8366713	3.6334197	-0.9196147
C	0.2859749	3.4356602	-1.7635613
C	0.1938773	2.6696322	-2.9514607
C	-1.0683571	2.1293497	-3.2795121

C	1.3744960	2.5876660	-3.9144670
C	2.0421421	1.2248342	-4.1466421
C	0.9891109	3.2123889	-5.2853312
C	3.3738072	1.2388842	-4.6462079
C	4.0332903	0.0486432	-5.0073276
C	3.3691522	-1.1865499	-4.8758218
C	2.0616753	-1.2548566	-4.3323598
C	1.4375073	-0.0374578	-3.9836069
C	1.3717791	-2.6237222	-4.2372329
C	0.6042551	-2.8918517	-2.9424141
C	-3.5997989	1.8067713	-2.9128330
C	-4.0577484	0.5733463	-2.1299624
C	-3.3269376	-0.6289599	-2.1505921
C	-3.7719199	-1.8264472	-1.5654446
C	-5.2973176	0.5747517	-1.4467964
C	-5.7657622	-0.5934748	-0.8099931
C	-5.0171737	-1.7849489	-0.8848844
C	-3.0676428	-3.1763294	-1.7282854
C	-1.5415023	-3.1563436	-1.7251064
C	-0.7953427	-2.7712592	-2.8547907
C	-0.8351574	-3.6751032	-0.6062234
C	0.5805365	-3.7974584	-0.6317963
C	1.2750113	-3.4266777	-1.8123588
C	0.5298940	-2.8643455	-5.5121417
C	-3.6293046	-3.9062949	-2.9764606
C	-3.7342279	1.5510419	-4.4303375
O	3.9431481	-2.3786095	-5.2429608
O	3.9653086	2.4723983	-4.7630726
O	-5.4469295	-2.9664623	-0.3331559
O	-6.0128134	1.7467623	-1.4625180
C	-6.6593563	-2.9902656	0.3904223
C	-7.2561046	1.8027173	-0.7954300
C	5.3079475	2.5587602	-5.1955837
C	5.2435057	-2.3798140	-5.7964850
C	-0.7078785	4.4107144	0.3743007
C	1.3898964	-4.2824895	0.5558403
O	-3.1955699	3.2815664	-0.5095527
O	1.4908398	4.0218242	-1.4063287
O	-1.6013943	-4.0233024	0.4809114
O	2.6243054	-3.7282121	-1.8934177
C	0.6929302	-0.7236811	2.7446527
C	1.3423299	-1.3236472	4.1339718
C	2.7365540	-0.7141679	4.3978339
C	2.7837366	0.6597988	4.7575121
C	1.4691368	1.4006128	4.9448283
C	0.5582327	0.4776368	5.7366881
C	0.4921314	-0.8890926	5.3540108
C	-0.1589481	0.9339139	6.8547760
C	-0.9557374	0.0556823	7.6091336
C	-1.0254498	-1.2936715	7.2384596
C	-0.3048479	-1.7582294	6.1219172
C	4.0157554	1.2738389	5.0375558
C	5.2171533	0.5474263	4.9743913
C	5.1761727	-0.8148934	4.6496841
C	3.9442260	-1.4363172	4.3698577
C	1.6309641	0.1976222	1.9932113
C	1.6961752	1.5525651	2.3861531
C	0.7944261	1.9769034	3.5590434
C	-0.5914344	1.3352380	3.3859140
C	-0.6256458	-0.0136524	2.9624225
C	-1.8085007	1.9822046	3.6666030
C	-3.0372315	1.3246188	3.4806506
C	-3.0641289	0.0045824	3.0069300

C	-1.8549844	-0.6632897	2.7534841
C	2.5905667	2.4077663	1.7176936
C	3.3881958	1.9388026	0.6617392
C	3.2918980	0.6016754	0.2495258
C	2.4107176	-0.2617125	0.9181416
C	0.7303902	3.5190038	3.7091911
O	-0.0357034	3.6514643	1.3677980
C	1.3738027	-2.8708727	4.0120627
O	0.9810916	-3.6035867	1.7420155
C	3.5691717	-2.6751950	-1.7042961
C	-1.4465236	-5.3026648	1.0822946
C	1.6964483	5.3361863	-1.9090910
C	-3.9324171	4.4684409	-0.7707930
C	0.0309086	4.3431826	2.5957751
C	1.9817322	-3.5181575	2.7518890
H	-1.1635161	1.5710408	-4.2237361
H	2.1720534	3.2238874	-3.4844935
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H	-4.3271679	2.6024341	-2.6634314
H	-2.3502287	-0.6282931	-2.6624281
H	-6.7231037	-0.5808825	-0.2755222
H	-3.3626380	-3.7760161	-0.8471511
H	-1.3442956	-2.4307726	-3.7461977
H	1.1870053	-2.8171378	-6.4072309
H	-0.2602036	-2.0926693	-5.6441599
H	0.0422889	-3.8643937	-5.4903862
H	-3.4367583	-3.3377553	-3.9129014
H	-4.7300233	-4.0288169	-2.8798684
H	-3.1743518	-4.9164317	-3.0848805
H	-3.1176186	0.6897860	-4.7692012
H	-3.4342247	2.4455650	-5.0212047
H	-4.7910007	1.3100605	-4.6767470
H	-7.5343527	-2.7232771	-0.2504960
H	-6.6335767	-2.3029369	1.2700727
H	-6.7843478	-4.0316275	0.7517311
H	-7.9922770	1.0783849	-1.2210157
H	-7.6417734	2.8324582	-0.9431100
H	-7.1512270	1.6097467	0.2992550
H	5.5698915	3.6364101	-5.1776216
H	5.4375486	2.1735085	-6.2356227
H	5.9998843	2.0060767	-4.5158429
H	5.2935307	-1.7876914	-6.7417406
H	5.4822766	-3.4392415	-6.0217472
H	6.0034312	-1.9828421	-5.0809683
H	-0.1534888	5.3689341	0.2030707
H	-1.7241051	4.6800432	0.7476472
H	2.4659709	-4.0961909	0.3487424
H	1.2897001	-5.3884640	0.7069934
H	0.5006768	-1.6091946	2.1138478
H	1.6732800	2.2969281	5.5650162
H	-0.0847917	1.9960472	7.1455888
H	-1.5118700	0.4258514	8.4864181
H	-1.6393447	-2.0005659	7.8213533
H	-0.3788310	-2.8246873	5.8645143
H	4.0327415	2.3387549	5.3269385
H	6.1770141	1.0423750	5.1970003
H	6.1047174	-1.4091005	4.6187081
H	3.9498913	-2.5122494	4.1425715

H	-1.8195144	3.0167516	4.0408535
H	-3.9780330	1.8583279	3.6964787
H	-4.0247133	-0.5068773	2.8308661
H	-1.8605130	-1.6996793	2.3756652
H	2.6637224	3.4699578	1.9917501
H	4.0651158	2.6345666	0.1402496
H	3.8922802	0.2359732	-0.5994927
H	2.3054546	-1.3095664	0.5955691
H	1.7730505	3.8800742	3.8414274
H	0.2185311	3.7581279	4.6679881
H	0.3297634	-3.2492138	4.0465806
H	1.8818066	-3.2875511	4.9095714
H	3.1984119	-1.7096800	-2.1102137
H	4.4936114	-2.9687323	-2.2439584
H	3.8110832	-2.5438065	-0.6218126
H	-0.6572855	-5.2915942	1.8665735
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H	-2.4205901	-5.5435144	1.5593229
H	0.8832080	6.0354972	-1.5980473
H	1.7626832	5.3535838	-3.0238321
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C	-3.2068112	-6.4041013	0.6201802
C	-3.4958241	-6.8062694	-0.7006214
C	0.0977028	-3.5254966	2.8347342
C	0.4842814	-2.1840257	3.0133145
C	-0.4969709	-1.1701954	2.8338494
C	-1.8320116	-1.5075528	2.4702946
C	-2.1675484	-2.8806977	2.3490986
C	-1.2155787	-3.9125547	2.5145516
C	2.9687819	-2.5738062	1.2569649
C	4.0144302	-2.5941647	0.3152362
C	5.1075550	-1.7225983	0.5311610
C	5.1310805	-0.8621961	1.6477704
C	4.0687861	-0.8831669	2.5733340
C	2.9606011	-1.7520583	2.3981189
C	1.8314158	-4.6230515	-1.7400540
C	0.6236477	-4.5906987	-2.4673654
C	0.2779627	-3.3773753	-3.1090360
C	1.1258443	-2.2448868	-3.0485422
C	2.3528940	-2.3494651	-2.3558381
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C	1.8853231	-1.8102965	3.4893059
C	-1.6506037	-5.3719600	2.3701509
C	-0.2897481	-5.8078294	-2.5825442
C	4.0227516	-3.5647184	-0.8700067
O	3.1995090	-1.2556524	-2.3195197
C	4.1440742	-1.1951351	-3.3794073
O	-0.9261456	-3.2920622	-3.7896738

C	-0.8435045	-3.5254783	-5.1899619
O	6.1240732	-1.7701658	-0.3926428
C	7.2391843	-0.9184693	-0.2326169
O	4.0433847	-0.0834289	3.6911894
C	5.1403871	0.7674796	3.9534846
O	-0.0613938	0.1155953	3.0255396
C	-0.8307053	1.0239300	3.8053188
O	-3.4674214	-3.2401236	2.0230305
C	-4.3677948	-3.3048491	3.1211039
O	-4.0677721	-6.6242126	1.6678687
C	-5.2967085	-7.2752338	1.4234484
O	-2.7591972	-6.9789495	-3.0242299
C	-3.9914148	-7.5721210	-3.3774995
C	-2.9008168	-0.4817012	2.1527471
C	0.6876080	-0.9039997	-3.5932823
C	2.3705192	-2.7126875	4.6527290
C	-0.6505936	-6.3850791	2.9670147
C	4.4405578	-4.9747226	-0.4027083
C	0.4943796	-7.1331294	-2.7480085
O	0.3957055	-0.0488288	-2.4982121
C	-0.0167396	1.2382900	-2.8901941
C	-0.7147395	4.4978715	-1.3488289
C	0.6965772	5.0651850	-1.7024762
C	0.9364304	6.4468953	-1.5015067
C	-0.1820947	7.2395401	-0.8809259
C	-1.4688745	6.8688584	-1.6164725
C	-1.7124429	5.5040449	-1.9116622
C	-2.3722472	7.8395716	-2.0805966
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C	-2.8316992	5.1350310	-2.6736141
C	1.6871092	4.3401712	-2.3968315
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C	2.1395234	7.0483377	-1.9029946
O	-2.4211551	0.4865866	1.2290951
C	-3.3692409	1.4978190	0.9652600
C	-1.1082637	4.3501358	0.3523907
C	-2.0847236	5.4061951	0.9580406
C	-1.6074101	6.7239116	1.1655620
C	-0.2013740	7.0056307	0.7092098
C	0.6832256	5.8669675	1.2155502
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C	-3.6707859	7.3775007	2.2896848
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C	2.6592307	5.0276143	2.3826984
C	2.1802897	3.7135203	2.2593565
C	0.9548697	3.4660778	1.6134173
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C	-0.1770353	2.0682546	-1.6156821
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H	-0.1408919	-5.0079077	0.0956657
H	-4.4482945	-7.2992065	-0.9292990
H	0.8514707	-4.3088999	3.0052728
H	2.1019307	-3.2331870	1.0822129
H	5.9749971	-0.1780800	1.7965651
H	2.1049773	-5.5576929	-1.2281169
H	1.8070522	-0.7820753	3.8921727
H	-2.5941288	-5.4860644	2.9403860

H	-0.8867434	-5.6749914	-3.5058327
H	4.8257160	-3.2078541	-1.5464763
H	4.8091451	-2.0912975	-3.4022712
H	3.6471952	-1.1042000	-4.3763655
H	4.7651371	-0.2930141	-3.2009919
H	-1.8757212	-3.4406619	-5.5894784
H	-0.1923469	-2.7751670	-5.7016867
H	-0.4474764	-4.5446258	-5.4178997
H	7.9180100	-1.1321892	-1.0837937
H	7.7839266	-1.1185935	0.7217010
H	6.9496235	0.1596138	-0.2627201
H	4.9077437	1.2881669	4.9049446
H	5.2801672	1.5298739	3.1498861
H	6.0908233	0.1940537	4.0765825
H	-1.5491754	1.5891057	3.1736165
H	-1.3651367	0.4965378	4.6293519
H	-0.1108926	1.7447264	4.2474346
H	-5.3292946	-3.6904842	2.7234646
H	-4.0010531	-3.9960109	3.9168244
H	-4.5404422	-2.3008371	3.5814540
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H	-5.1503431	-8.3058678	1.0185826
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H	-4.1614700	-8.5353409	-2.8382548
H	-3.9366099	-7.7765722	-4.4664782
H	-4.8533894	-6.8905618	-3.1794899
H	-3.2617116	0.0387691	3.0790642
H	-3.7765838	-1.0171032	1.7154786
H	-0.2196871	-1.0254400	-4.2314333
H	1.4875818	-0.4439302	-4.2283400
H	3.3227382	-2.3152534	5.0652111
H	1.6199355	-2.7404964	5.4742622
H	2.5606472	-3.7569381	4.3206276
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H	-0.4215194	-6.1533122	4.0313690
H	-1.0825165	-7.4081237	2.9212407
H	4.5072950	-5.6865753	-1.2559680
H	5.4388536	-4.9256348	0.0829056
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H	1.2283797	-7.0625516	-3.5820843
H	1.0457355	-7.4088317	-1.8226143
H	-0.2113158	-7.9610177	-2.9734653
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H	-2.9856392	4.0729276	-2.9153497
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H	3.6439759	4.3304132	-3.3301354
H	4.0820669	6.7691613	-2.8536489
H	2.2829787	8.1289419	-1.7310663
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H	-3.6777281	1.9996902	1.9208622
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H	-3.7314300	4.0681781	1.4901656
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H	-4.2842231	8.1417095	2.7948588
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H	2.7525063	2.8656698	2.6711860

H	0.5682151	2.4399467	1.5213816
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H	-0.7273355	1.4422989	-0.8837987

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C	3.4079757	2.6195310	0.8241805
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C	3.1034177	1.9695179	2.0337423
C	1.7012075	1.6156960	4.1510418
C	1.2907582	0.1400831	4.2236210
C	2.9191174	1.8544177	5.0821617
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C	0.0973363	-1.6127680	5.4786092
C	0.6896151	-2.6067877	4.6729229
C	1.5617964	-2.2556372	3.6113306
C	1.8219647	-0.8832070	3.4162725
C	2.2919044	-3.3582643	2.8324796
C	2.1422915	-3.3228251	1.3084823
C	4.7262218	2.4009374	0.0724432
C	4.6106413	1.4524735	-1.1276606
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C	4.3091720	-0.8467409	-2.0324355
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C	4.8474955	1.0306124	-3.5344381
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C	4.1867556	-2.3670514	-1.8592041
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C	3.1235779	-2.7887309	0.4513344
C	1.9851001	-3.6150394	-1.5139402
C	0.9655487	-4.1639948	-0.6992648
C	1.0395889	-3.9794726	0.7034839
C	3.7669896	-3.4262448	3.2902326
C	5.5660509	-2.9508757	-1.4556017
C	5.8906729	1.9699666	0.9912435
O	0.4679471	-3.9461908	4.8721386
O	-0.0877345	0.7483505	6.0561155
O	4.5794294	-1.2468228	-4.3582588
O	5.2284099	3.2379635	-2.5717903
C	4.7730201	-0.7972653	-5.6835347
C	5.5244910	3.7470215	-3.8554756
C	-1.0189040	0.4341675	7.0707456
C	-0.3828866	-4.3602325	5.9204744
C	0.2525657	4.7639548	0.3486504
C	-0.1844831	-4.9533564	-1.2883443
O	2.7181849	4.1713820	-0.8749835
O	-0.1220787	3.3785990	3.0117713
O	1.8969486	-3.7962061	-2.8861751
O	0.0803619	-4.5605502	1.5055415
C	-2.9515023	-0.4511203	-0.0518621
C	-3.6120966	-1.1842316	-1.3680880
C	-5.1070707	-0.8479745	-1.4818878
C	-5.4623450	0.4265950	-1.9901612
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C	-3.3617315	0.5356339	-3.2146928
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C	-2.8364895	0.9927223	-4.4341045

C	-1.8420005	0.2585000	-5.1023520
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C	-1.8714733	-1.3845075	-3.3003849
C	-6.8189002	0.7621747	-2.1336408
C	-7.8247821	-0.1472705	-1.7600775
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C	-6.1143546	-1.7401513	-1.0819792
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C	-3.5785599	2.0751327	-1.1120697
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C	0.2232979	1.8836334	-1.7570575
C	0.5533182	0.7012116	-1.0737524
C	-0.4564682	-0.0421016	-0.4443567
C	-5.3457353	2.3767693	0.7600424
C	-5.9799308	1.9122372	1.9252585
C	-5.5853805	0.6939935	2.5017713
C	-4.5863960	-0.0744082	1.8817828
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O	-1.0754329	4.2638312	0.3870045
C	-3.5676075	-3.5953061	-2.0266100
O	-1.2544438	-4.0751585	-1.6382298
C	-1.0843114	-3.7619462	1.7426115
C	2.5695931	-4.9435703	-3.3928370
C	-0.5107789	4.7060829	3.3311728
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O	-3.4011927	-2.5650879	-1.0600290
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H	4.0062832	-2.3124593	0.9058170
H	3.8117596	-3.6230323	4.3834367
H	4.3096260	-2.4719536	3.1096712
H	4.3144974	-4.2417297	2.7667321
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H	6.3377809	-2.6658157	-2.2038738
H	5.5285200	-4.0620767	-1.3968543
H	5.7553850	0.9441621	1.3988511
H	6.0030873	2.6673213	1.8512455
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H	5.7796053	-0.3344380	-5.8252602
H	3.9900556	-0.0638698	-5.9918735
H	4.6982935	-1.6962463	-6.3289358
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H	0.2793959	5.7817954	0.8261853
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H	0.1404438	-5.5223527	-2.1910705
H	-2.6109506	-1.3023014	0.5662264
H	-4.7207877	2.2160022	-2.9702675
H	-3.1960176	1.9492176	-4.8502645
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H	-1.4386758	-2.2832907	-2.8357243
H	-7.0911111	1.7502838	-2.5422190
H	-8.8864252	0.1252079	-1.8820929
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H	-5.8301708	-2.7084777	-0.6429041
H	-1.3651551	3.2645408	-2.3063506
H	1.0078526	2.4514528	-2.2822599
H	1.5950579	0.3435666	-1.0608473
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H	-5.6842668	3.3150068	0.2940834
H	-6.7908712	2.5054050	2.3801134
H	-6.0725622	0.3298840	3.4217551
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H	-3.5427774	4.0106616	0.6677577
H	-4.1089969	5.2616711	-0.4954940
H	-3.4417031	-3.2131397	-3.0616648
H	-4.5864674	-4.0508871	-1.9624649
H	-0.8260907	-2.8321815	2.3003901
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H	3.6720114	-4.8918055	-3.2245923
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C	-0.9502212	-3.8003994	-4.9726932
C	0.3302974	-3.6166126	-5.5299800
C	-2.4385427	-5.9194386	-0.9550852
C	-2.6319766	-6.0007672	0.4355915
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C	-3.1802351	-3.6217234	-1.0073228
C	-2.7076543	-4.7552990	-1.7075137
C	0.0757732	-6.7716557	1.7690462
C	1.2091280	-6.7447599	2.6001721
C	1.0206421	-7.1088584	3.9589692

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C	-1.2037062	-7.1627280	2.2052524
C	2.5141305	-5.7950914	-0.3736487
C	2.7174733	-4.9157596	-1.4482021
C	3.1638169	-3.5940138	-1.1635430
C	3.3576777	-3.1628550	0.1745224
C	3.1641529	-4.1102196	1.2192629
C	2.7420031	-5.4349164	0.9709107
C	-2.3868123	-7.2785159	1.2403876
C	-2.5458617	-4.7129484	-3.2239737
C	2.5732653	-5.3427056	-2.9087813
C	2.6299491	-6.4373238	2.1154446
O	3.3769410	-3.7141185	2.5331890
C	4.7320062	-3.7506304	2.9644955
O	3.3671891	-2.8044773	-2.2638623
C	4.5644955	-2.0515171	-2.3860916
O	2.1402742	-7.0821245	4.7544146
C	2.0154083	-7.3717325	6.1311549
O	-2.6040526	-7.9218110	3.9652828
C	-2.8083642	-8.3037517	5.3094619
O	-3.2635080	-4.8791840	2.4750656
C	-4.5884241	-5.1559643	2.9093794
O	-3.4709599	-2.4563449	-1.6983598
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O	2.7359141	-4.0036963	-5.3718203
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C	-3.6974564	-2.3589402	1.1296576
C	3.7257864	-1.7454898	0.5644992
C	-2.2433050	-8.5482322	0.3747061
C	-3.1297982	-5.9706189	-3.9160941
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C	-0.1413876	9.8403403	-3.4806772
C	0.4142605	8.5758328	-3.7294810
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C	2.8798415	7.8932862	1.4651948
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C	-0.5082959	6.6270523	0.5914452
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H	0.1899962	-6.4609693	0.7169832
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H	-3.2808686	-7.4320020	1.8777163
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H	4.4865487	-1.0724596	-1.8634206
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H	-5.5384404	-2.3899863	-1.2689684
H	-3.0410155	-2.4053241	-7.1027139
H	-1.5431380	-3.2794281	-7.6220635
H	-1.4133782	-1.7226589	-6.6946501
H	2.3775877	-3.9014950	-7.4415524
H	4.0103044	-3.4128435	-6.8303044
H	2.5959738	-2.3049467	-6.6032515
H	-3.8986054	-2.5732320	2.2060101
H	-4.6213243	-1.8935819	0.7002207
H	4.8216448	-1.5473081	0.4108570
H	3.5269185	-1.6360663	1.6563047
H	-2.1754501	-9.4419872	1.0317189
H	-3.1166768	-8.6824954	-0.3022449
H	-1.3211566	-8.5272517	-0.2467899
H	-2.5375728	-6.8833883	-3.6865478
H	-4.1811361	-6.1502229	-3.5966492
H	-3.1189108	-5.8339741	-5.0186271
H	4.4289681	-7.5624048	1.5016472
H	3.3877829	-8.4108911	2.7046793
H	2.8838113	-8.3301344	0.9849242
H	3.5207534	-7.3230667	-2.6633097
H	1.7188003	-7.3786251	-2.7012614

H	2.6316447	-7.0934146	-4.2126538
H	4.2643666	0.7632257	0.4533673
H	2.7276398	0.6225352	1.3830009
H	-0.3399792	10.9330838	0.4056070
H	-0.7877424	11.2489872	-1.9504981
H	-0.3975288	10.5123708	-4.3165567
H	0.5985214	8.2453003	-4.7653953
H	1.1976122	6.7425304	-2.8439321
H	3.3774930	6.9351800	1.2767958
H	4.4805240	8.5533458	2.7771319
H	3.4180482	10.7925064	3.2325521
H	1.2411373	11.3677221	2.1244979
H	-3.8571344	0.2250602	0.8965024
H	-3.0504875	-0.0332044	2.4905146
H	-2.1898638	10.0725429	1.3557302
H	-1.8302794	5.3242913	-1.4858358
H	-3.8909871	6.0729575	-2.6943026
H	-4.9583506	8.2754459	-2.1111745
H	-3.9007427	9.7451714	-0.3712242
H	-1.8239524	9.8442231	3.7599704
H	-1.0474549	8.4632826	5.7080134
H	0.0910844	6.2576268	5.2920597
H	0.3754276	5.4194301	2.9595908
H	-0.7987135	0.3842918	1.3906399
H	-1.6303797	0.5908073	-0.1935537
H	1.4482755	1.2441239	-0.7519077
H	3.0293862	1.5291977	-1.5713349
H	-1.0675525	2.8784543	-0.4556621
H	-0.0274218	2.7048986	1.0049379
H	1.0510434	3.7474552	-1.0010039
H	2.6961635	3.9387578	-1.7197270
H	1.8797785	5.0290081	1.0592835
H	3.4104630	5.3522051	0.1565230
H	-2.4030017	4.6764751	0.6923589
H	-1.4361598	4.4569310	2.1877818

13'(h2t)

C	2.3526294	2.8235999	-0.7617996
C	3.7569643	2.9848962	-0.8212690
C	1.6884226	2.5685270	0.4647289
C	2.4569586	2.5079401	1.6523582
C	3.8654230	2.6535426	1.6311316
C	4.4786838	2.8862575	0.3854418
C	4.6395812	2.5827705	2.9462209
C	4.6811044	1.1751607	3.5475074
C	6.0666853	3.1667224	2.8689565
C	4.5084139	1.0009174	4.9422832
C	4.5968393	-0.2795797	5.5258512
C	4.8885152	-1.3986556	4.7203382
C	5.0774838	-1.2632354	3.3201646
C	4.9572021	0.0298695	2.7780274
C	5.4791065	-2.4982092	2.5065987
C	5.0122143	-2.5232654	1.0532209
C	4.4236520	3.2716303	-2.1638658
C	4.7375064	2.0123984	-2.9774262
C	5.2385448	0.8332219	-2.4003373
C	5.6340096	-0.2936789	-3.1435739
C	4.6087493	2.0401992	-4.3889929
C	4.9675911	0.9231826	-5.1702131
C	5.4908992	-0.2313658	-4.5509687
C	6.2862539	-1.5106760	-2.4814826

C	5.4407551	-2.1100179	-1.3550512
C	5.7680125	-1.9572486	0.0052092
C	4.2966265	-2.8871318	-1.6702139
C	3.4891110	-3.4538850	-0.6569134
C	3.8496315	-3.2499785	0.6990730
C	7.0047337	-2.7363754	2.6374560
C	7.7342966	-1.1734318	-2.0638399
C	5.6881305	4.1543572	-2.0488351
O	5.0123761	-2.6685984	5.2268726
O	4.2626114	2.1361975	5.6736867
O	5.9020211	-1.3319978	-5.2618469
O	4.1368712	3.2087844	-4.9328793
C	5.7788810	-1.3284628	-6.6687858
C	3.9415652	3.2900598	-6.3293792
C	4.0598418	2.0284670	7.0673608
C	4.8017584	-2.8860022	6.6068514
C	0.2107744	2.2694185	0.4877337
C	2.3084790	-4.3343547	-0.9902700
O	1.6311321	2.8578874	-1.9385592
O	1.8426831	2.2400129	2.8598017
O	3.9584158	-3.0792526	-3.0000159
O	3.1036098	-3.8833868	1.6710064
C	-4.8552374	-0.9199222	0.1156521
C	-6.0721541	-1.8107922	-0.5640340
C	-7.3259823	-1.7921020	0.3273355
C	-8.0905198	-0.5994194	0.3552631
C	-7.6128478	0.5681510	-0.4934893
C	-7.2692193	-0.0036295	-1.8607209
C	-6.5221039	-1.2092092	-1.9105605
C	-7.7487977	0.5679910	-3.0505132
C	-7.5024203	-0.0455020	-4.2914051
C	-6.7866077	-1.2505522	-4.3378604
C	-6.3051382	-1.8318890	-3.1499154
C	-9.2705802	-0.5514389	1.1154094
C	-9.6949698	-1.6740500	1.8486443
C	-8.9337665	-2.8527095	1.8191970
C	-7.7520064	-2.9117379	1.0579092
C	-5.2361202	-0.3875121	1.4811117
C	-6.0503387	0.7686249	1.5348634
C	-6.4046648	1.4292937	0.1980448
C	-5.1990774	1.3987348	-0.7504424
C	-4.4141010	0.2251862	-0.7734493
C	-4.9330989	2.4349713	-1.6600298
C	-3.8641056	2.3255898	-2.5652550
C	-3.0419452	1.1867563	-2.5497704
C	-3.3201558	0.1401269	-1.6537864
C	-6.5660030	1.1852520	2.7755684
C	-6.2037951	0.5231457	3.9614140
C	-5.3341908	-0.5780225	3.9142459
C	-4.8684146	-1.0389584	2.6718714
C	-2.7248390	4.5238282	0.6499241
O	-0.5772272	3.4634630	0.6452433
C	-1.3077645	-3.8659646	-0.4630863
O	1.0669777	-3.7109571	-0.6548912
C	2.1229774	-3.0703249	2.3232413
C	4.5297789	-4.2270906	-3.6157086
C	1.1584999	3.3425425	3.4587318
C	0.9357435	4.0798985	-2.1957684
C	-1.9682864	3.1878163	0.5858516
C	-0.0190520	-4.5934086	-0.8354448
O	-6.9461520	2.7470984	0.3042880
O	-5.6817447	-3.1772454	-0.6741008
O	-4.1117557	4.4046557	0.3795958

C	-4.8574039	3.7938082	1.4176351
C	-6.3554581	3.7925514	1.0968540
O	-2.3748360	-4.7917339	-0.5908740
C	-3.6269694	-4.3280377	-0.1268644
C	-4.4125989	-3.5508812	-1.2011942
H	5.5696000	3.0255275	0.3543743
H	4.0815572	3.2035829	3.6766700
H	6.0600732	4.2080219	2.4756253
H	6.7324513	2.5531826	2.2229116
H	6.5177276	3.1845079	3.8843033
H	4.4511318	-0.4033726	6.6056961
H	5.0736670	0.1522634	1.6875696
H	4.9818899	-3.3624249	2.9929974
H	3.6895269	3.8398963	-2.7678304
H	5.3253020	0.7881500	-1.3007489
H	4.8547342	0.9580246	-6.2603861
H	6.3591800	-2.2786548	-3.2752161
H	6.6836174	-1.4048194	0.2653934
H	7.2721122	-2.8741161	3.7070040
H	7.5950870	-1.8756254	2.2537019
H	7.3142151	-3.6487069	2.0804685
H	7.7764578	-0.3307018	-1.3394126
H	8.3182721	-0.8643318	-2.9575927
H	8.2406540	-2.0521479	-1.6049419
H	6.5274632	3.6190990	-1.5530274
H	5.4792508	5.0846370	-1.4740797
H	6.0363889	4.4432406	-3.0638294
H	6.3815925	-0.5141374	-7.1390201
H	4.7158695	-1.2247725	-6.9944447
H	6.1673860	-2.3075740	-7.0169100
H	4.8974365	3.1633255	-6.8931111
H	3.5407057	4.3051796	-6.5280232
H	3.2056140	2.5325600	-6.6917685
H	3.8744300	3.0587615	7.4344492
H	4.9568388	1.6156168	7.5891607
H	3.1754099	1.3923434	7.3125806
H	5.5399765	-2.3304711	7.2342393
H	4.9364956	-3.9743969	6.7727806
H	3.7702980	-2.5964502	6.9218303
H	-0.0741129	1.7710859	-0.4688759
H	-0.0092505	1.5698060	1.3294206
H	2.3978768	-5.2925823	-0.4197860
H	2.3084620	-4.5745356	-2.0786527
H	-4.0163025	-1.6270766	0.2445949
H	-8.4181556	1.3205988	-0.5940365
H	-8.3366397	1.5001285	-3.0019970
H	-7.8865024	0.4112669	-5.2184973
H	-6.6074590	-1.7540308	-5.3023330
H	-5.7734203	-2.7921815	-3.2008224
H	-9.8694508	0.3749863	1.1257088
H	-10.6266644	-1.6272885	2.4366630
H	-9.2638014	-3.7400075	2.3848894
H	-7.1575793	-3.8352555	1.0139327
H	-5.5724336	3.3284166	-1.6598655
H	-3.6658805	3.1432044	-3.2778724
H	-2.1864456	1.1051965	-3.2401910
H	-2.6803866	-0.7590263	-1.6506397
H	-7.2778383	2.0214661	2.8198418
H	-6.6104230	0.8689626	4.9261859
H	-5.0372662	-1.0945362	4.8418458
H	-4.2209989	-1.9310124	2.6229755
H	-2.5548684	5.0142120	1.6431977
H	-2.3176257	5.1986302	-0.1332295

H	-1.2334268	-3.4920960	0.5895675
H	-1.4347959	-2.9726923	-1.1253766
H	2.5888642	-2.1926296	2.8282149
H	1.6396286	-3.7175389	3.0848038
H	1.3625524	-2.7217431	1.5893866
H	4.1463739	-5.1747279	-3.1641863
H	5.6431110	-4.2327049	-3.5426207
H	4.2398684	-4.1918079	-4.6860607
H	0.3872610	3.7612704	2.7729698
H	1.8718424	4.1533220	3.7433958
H	0.6760604	2.9503806	4.3782908
H	1.6493418	4.9260066	-2.3469127
H	0.2426349	4.3313209	-1.3615250
H	0.3615382	3.9235016	-3.1326774
H	-2.2307237	2.6664934	-0.3662433
H	-2.2617286	2.5104185	1.4278252
H	-0.0854667	-4.9476250	-1.8970545
H	0.0831107	-5.5054412	-0.1920549
H	-4.7270515	4.3827180	2.3643939
H	-4.5025592	2.7602512	1.6348176
H	-6.8977728	3.8458159	2.0685412
H	-6.5813682	4.7337752	0.5483366
H	-3.5072765	-3.6984802	0.7911335
H	-4.2203137	-5.2233101	0.1626653
H	-3.8345340	-2.6756907	-1.5687801
H	-4.5702295	-4.2260097	-2.0738386

Na⁺@11'(h2t) (first conformation)

1	1		
C	2.9716038	0.6864097	2.8898594
C	4.3625521	0.4914946	2.6971095
C	2.0644820	-0.4043923	2.8366238
C	2.5664209	-1.7060040	2.5941894
C	3.9453106	-1.9379597	2.3818258
C	4.8046662	-0.8222528	2.4417013
C	4.4425987	-3.3530071	2.0870046
C	3.9792411	-3.8358936	0.7125322
C	5.9682978	-3.5341297	2.2348430
C	3.4756186	-5.1490238	0.5360893
C	3.1154106	-5.6122292	-0.7474830
C	3.2796147	-4.7757376	-1.8709249
C	3.7832726	-3.4585770	-1.7267920
C	4.1117340	-3.0302555	-0.4293507
C	4.1004412	-2.6052224	-2.9551368
C	3.7804945	-1.1193611	-2.7661857
C	5.3292269	1.6715734	2.8052225
C	5.3875898	2.5574842	1.5572928
C	5.4222375	2.0423505	0.2503832
C	5.5943877	2.8400396	-0.8960008
C	5.5272107	3.9617941	1.7086365
C	5.6878761	4.7970009	0.5841800
C	5.7299096	4.2377770	-0.7097443
C	5.7015862	2.2362388	-2.3005608
C	4.5772172	1.2323065	-2.5482359
C	4.8044933	-0.1507482	-2.6780786
C	3.2331964	1.6738644	-2.5983996
C	2.1654357	0.7496165	-2.6536809
C	2.4522468	-0.6382237	-2.6779764
C	5.5517936	-2.8800704	-3.4125041
C	7.1190950	1.6819766	-2.5510847
C	6.7604286	1.2602854	3.2219430

O	2.9768096	-5.1732990	-3.1501954
O	3.3716740	-5.9155187	1.6637349
O	5.9057935	4.9887915	-1.8417721
O	5.5110197	4.4364670	2.9925428
C	6.1083409	6.3864170	-1.7234730
C	5.6657626	5.8260232	3.2230178
C	2.9301735	-7.2584774	1.5546572
C	2.5632018	-6.5111554	-3.3830058
C	0.5931324	-0.2006849	3.0933775
C	0.7309765	1.2253529	-2.6951833
O	2.4841356	1.9596095	3.1150610
O	1.6624157	-2.7556310	2.5166510
O	2.9358033	3.0221915	-2.5320998
O	1.3465959	-1.4846520	-2.5515733
C	-4.3938486	1.0834758	-0.1393135
C	-5.6030369	1.5358260	-1.1665627
C	-5.9673117	0.3886103	-2.1254135
C	-6.6962778	-0.7031643	-1.5888372
C	-7.0718674	-0.6527099	-0.1134622
C	-7.6238457	0.7455326	0.1302308
C	-6.9153334	1.8502226	-0.4155673
C	-8.8539874	0.9537875	0.7745038
C	-9.3995137	2.2450717	0.8821396
C	-8.7168210	3.3315906	0.3181074
C	-7.4851081	3.1311596	-0.3334263
C	-7.0982590	-1.7486374	-2.4360247
C	-6.7831034	-1.7208667	-3.8066094
C	-6.0614475	-0.6385375	-4.3328200
C	-5.6551096	0.4150226	-3.4929947
C	-3.8957134	-0.3036237	-0.4641876
C	-4.6347100	-1.3938127	0.0387226
C	-5.8610066	-1.0751483	0.9018778
C	-5.5931950	0.1112395	1.8316862
C	-4.8002768	1.1600018	1.3163426
C	-6.1880057	0.2636287	3.0972836
C	-5.8978159	1.3829857	3.8955035
C	-5.0181471	2.3720037	3.4265295
C	-4.4901328	2.2663097	2.1290416
C	-4.3145807	-2.6975697	-0.3793087
C	-3.2108689	-2.9269375	-1.2182321
C	-2.4330327	-1.8425548	-1.6638563
C	-2.7864372	-0.5296606	-1.3009528
C	-2.0993648	-1.9259380	2.5010013
O	-0.2089857	-0.4442619	1.9145087
C	-0.8561410	3.5481641	-1.3369821
O	0.1024240	1.2452522	-1.3890583
C	0.9885940	-2.3140938	-3.6761761
C	3.0218653	3.7387892	-3.7664307
C	1.4607620	-3.4960218	3.7223421
C	2.4030337	2.3622448	4.4837032
C	-1.6112206	-0.4968614	2.2250300
C	0.1010706	2.5263399	-0.7298016
O	-6.3321969	-2.2556059	1.5691235
O	-5.1341765	2.6086457	-1.9819709
O	-3.4819710	-1.8301522	2.7592505
C	-4.1925658	-3.0541729	2.7541600
C	-5.6989218	-2.7833062	2.7449228
O	-2.2063746	3.1701104	-1.1498262
C	-3.1216476	4.0283893	-1.8220332
C	-4.5709387	3.7793921	-1.4029239
Na	0.4007505	-0.8303854	-0.3068495
H	5.8822452	-0.9877596	2.3004209
H	3.9752275	-4.0336302	2.8259704

H	6.3210213	-3.2166483	3.2411986
H	6.5333516	-2.9610870	1.4676615
H	6.2294628	-4.6055990	2.1031977
H	2.7195791	-6.6271712	-0.8728610
H	4.5106029	-2.0081639	-0.3030574
H	3.4589958	-2.9751383	-3.7792564
H	4.9469442	2.3266002	3.6120377
H	5.3094271	0.9519536	0.1165064
H	5.7905396	5.8805991	0.7167713
H	5.5656236	3.0810955	-3.0050110
H	5.8452397	-0.5017201	-2.6967497
H	5.6609863	-3.9591824	-3.6502699
H	6.2921181	-2.6418760	-2.6185465
H	5.8106838	-2.3001185	-4.3259597
H	7.3896134	0.8836901	-1.8257662
H	7.8618259	2.4988093	-2.4311084
H	7.2245738	1.2733103	-3.5809356
H	7.2847887	0.6979186	2.4188095
H	6.7531279	0.6350661	4.1426943
H	7.3613471	2.1710343	3.4286808
H	7.0156105	6.6219206	-1.1188209
H	5.2254518	6.8972073	-1.2706605
H	6.2547062	6.7657235	-2.7549570
H	6.6453282	6.2010154	2.8431613
H	5.6303335	5.9622930	4.3226807
H	4.8423080	6.4174648	2.7568291
H	2.9576999	-7.6765509	2.5809406
H	3.6023690	-7.8609270	0.8995531
H	1.8864604	-7.3212311	1.1648307
H	3.3358858	-7.2412651	-3.0473487
H	2.4277684	-6.6054754	-4.4791121
H	1.5963098	-6.7409776	-2.8760397
H	0.4075319	0.8437741	3.4230282
H	0.2477690	-0.8861109	3.8999354
H	0.1137788	0.5426406	-3.3131248
H	0.6800333	2.2364460	-3.1443102
H	-3.5756908	1.7975549	-0.3360744
H	-7.8497406	-1.4100506	0.1044791
H	-9.4032234	0.0880233	1.1813954
H	-10.3681992	2.3951330	1.3861909
H	-9.1474959	4.3451260	0.3680038
H	-6.9901471	3.9927619	-0.8014316
H	-7.6782203	-2.5896275	-2.0198776
H	-7.1147933	-2.5415289	-4.4638880
H	-5.8228197	-0.6027922	-5.4088625
H	-5.1064465	1.2768808	-3.8985607
H	-6.9127307	-0.4805400	3.4584252
H	-6.3672532	1.4821218	4.8879327
H	-4.7713143	3.2426402	4.0562944
H	-3.8353185	3.0613286	1.7331415
H	-4.9566578	-3.5342378	-0.0661249
H	-2.9736356	-3.9530027	-1.5449183
H	-1.5866954	-2.0173715	-2.3494809
H	-2.2168067	0.3363025	-1.6769869
H	-1.9022759	-2.5676159	1.6042910
H	-1.5515344	-2.3829273	3.3661651
H	-0.6513224	4.5349550	-0.8444048
H	-0.6394219	3.6902837	-2.4264663
H	-0.1196734	-2.3814795	-3.6955946
H	1.4168565	-3.3341392	-3.5762717
H	1.3340187	-1.8490275	-4.6248845
H	4.0083904	3.5975911	-4.2621847
H	2.8924299	4.8115700	-3.5193677

H	2.2208206	3.4216075	-4.4768920
H	1.0220452	-2.8609786	4.5280974
H	2.4080780	-3.9410206	4.1023098
H	0.7537201	-4.3135637	3.4759306
H	3.3841139	2.2675014	5.0033055
H	1.6470681	1.7630051	5.0462359
H	2.0954781	3.4275639	4.4817496
H	-1.8419739	0.1617873	3.0920295
H	-2.1591010	-0.0975421	1.3487462
H	-0.1920803	2.3162465	0.3201146
H	1.1278462	2.9570379	-0.7340795
H	-3.9773549	-3.6376828	3.6886286
H	-3.8792633	-3.6884674	1.8918527
H	-6.2130432	-3.7566801	2.8983802
H	-5.9178818	-2.1493196	3.6316563
H	-3.0300329	3.9052943	-2.9305510
H	-2.8845007	5.0964576	-1.5806920
H	-4.6515729	3.7853897	-0.2942545
H	-5.1526173	4.6536698	-1.7803639

Na⁺@11'(h2t) (second conformation)

C	2.5742993	-2.7619248	0.2725861
C	3.9096591	-2.7170905	0.7302600
C	2.2511884	-2.6881958	-1.1097632
C	3.2993451	-2.4966263	-2.0412642
C	4.6389296	-2.3057711	-1.6095379
C	4.9067094	-2.4603981	-0.2388304
C	5.6962668	-1.8695049	-2.6233141
C	5.2926796	-0.5298167	-3.2480450
C	7.1338731	-1.8228576	-2.0700712
C	5.3219708	-0.3567055	-4.6519030
C	4.9038737	0.8592018	-5.2306529
C	4.4671032	1.9172061	-4.4094862
C	4.4650200	1.7934141	-2.9927361
C	4.8741642	0.5592746	-2.4606409
C	4.0470040	3.0090287	-2.1583386
C	3.6346626	2.7210101	-0.7160820
C	4.2677481	-2.9760736	2.1934210
C	4.4605413	-1.7246131	3.0539975
C	4.7760816	-0.4561472	2.5397462
C	5.0176871	0.6735696	3.3427531
C	4.3704580	-1.8455026	4.4678524
C	4.6258686	-0.7426461	5.3067388
C	4.9571568	0.5097657	4.7469174
C	5.3341896	2.0372076	2.7224317
C	4.2904524	2.3697310	1.6548662
C	4.6026101	2.5127103	0.2905665
C	2.9262226	2.4771672	2.0200804
C	1.9036375	2.5955654	1.0493577
C	2.2732922	2.7148006	-0.3208835
C	5.1418995	4.1090039	-2.2070628
C	6.7943857	2.1066035	2.2338832
C	5.4980079	-3.9139578	2.3137995
O	4.0218252	3.1111803	-4.9090171
O	5.7537380	-1.4262072	-5.3888127
O	5.2191588	1.6196899	5.5021948
O	4.0279894	-3.0823223	4.9437980
C	5.2422890	1.5102553	6.9158457
C	3.9178855	-3.2846523	6.3433847
C	5.8488315	-1.3062946	-6.7983497
C	3.9582263	3.2991726	-6.3131176

C	0.8208783	-2.7636370	-1.5941795
C	0.4473447	2.5526432	1.4750322
O	1.5203126	-2.7740371	1.1943698
O	2.9933033	-2.4176044	-3.3800292
O	2.5631968	2.4140304	3.3555142
O	1.2752808	2.8052836	-1.2746444
C	-4.5569452	0.0584954	0.6971877
C	-5.9536693	0.6889089	1.3179290
C	-6.4858301	1.8338914	0.4365090
C	-7.0914222	1.4816951	-0.7949722
C	-7.1670158	0.0044825	-1.1488107
C	-7.6695141	-0.7061815	0.0993130
C	-7.0928887	-0.3525111	1.3488067
C	-8.7457758	-1.6071390	0.0553236
C	-9.2675613	-2.1622524	1.2367665
C	-8.7192159	-1.7925299	2.4725949
C	-7.6424849	-0.8872041	2.5257132
C	-7.6449931	2.4844269	-1.6075040
C	-7.6001688	3.8325195	-1.2096655
C	-6.9976183	4.1777965	0.0096822
C	-6.4427219	3.1797410	0.8317046
C	-4.1076247	0.8269788	-0.5231096
C	-4.7327768	0.5196806	-1.7504048
C	-5.7749177	-0.6058654	-1.7516234
C	-5.3344476	-1.7591986	-0.8452629
C	-4.6763072	-1.4118827	0.3575465
C	-5.6524869	-3.1081107	-1.0835584
C	-5.2231325	-4.1146447	-0.2018005
C	-4.4814262	-3.7775200	0.9419090
C	-4.2288557	-2.4245879	1.2260010
C	-4.4978216	1.3395662	-2.8670493
C	-3.5852460	2.4062730	-2.7897506
C	-2.9096857	2.6664902	-1.5855990
C	-3.1809229	1.8826314	-0.4511768
C	-1.7513304	-1.4841743	-2.8862670
O	0.1096992	-1.5632590	-1.2269402
C	-1.4528945	1.4828945	3.7890484
O	0.0042110	1.1948698	1.7564408
C	0.8351822	4.1293443	-1.5912234
C	2.6373041	3.6590811	4.0574981
C	3.1526623	-3.6303311	-4.1200863
C	1.0015287	-4.0560858	1.5806046
C	-1.3088261	-1.6435541	-1.4254396
C	-0.2146422	0.8708999	3.1438402
O	-6.1205135	-0.9885612	-3.0918046
O	-5.6717093	1.2751975	2.5868174
O	-3.1241367	-1.8036810	-2.8951709
C	-3.8112701	-1.5122073	-4.0953784
C	-5.2984756	-1.8211803	-3.9196836
O	-2.6432598	0.8862685	3.3145674
C	-3.7681702	1.2162196	4.1238340
C	-5.0487177	0.5447752	3.6328913
H	5.9481357	-2.3728266	0.1036499
H	5.6986550	-2.6052707	-3.4538573
H	7.4519723	-2.8087828	-1.6636593
H	7.2476120	-1.0590656	-1.2695917
H	7.8351220	-1.5512600	-2.8870980
H	4.9089717	0.9782578	-6.3206194
H	4.8448658	0.4254641	-1.3658726
H	3.1596583	3.4232725	-2.6770085
H	3.4172606	-3.5209496	2.6501520
H	4.8298980	-0.3335120	1.4441215
H	4.5633754	-0.8570298	6.3955452

H	5.2380322	2.7785802	3.5417276
H	5.6600861	2.4759320	-0.0105078
H	5.3259395	4.4089234	-3.2589161
H	6.1052062	3.7517006	-1.7833282
H	4.8253840	5.0109453	-1.6373945
H	7.0103197	1.3444615	1.4532999
H	7.4798104	1.9100883	3.0852919
H	7.0422918	3.1100458	1.8221484
H	6.4326509	-3.4161296	1.9773558
H	5.3566378	-4.8372302	1.7094853
H	5.6381936	-4.2097409	3.3736728
H	6.0050510	0.7725271	7.2587378
H	4.2451736	1.2232177	7.3265925
H	5.5143705	2.5144636	7.2984945
H	4.8863091	-3.0984475	6.8640773
H	3.6340592	-4.3474701	6.4796171
H	3.1292898	-2.6362032	6.7931938
H	6.2458215	-2.2745768	-7.1642123
H	6.5499337	-0.4914270	-7.0956337
H	4.8533235	-1.1213352	-7.2672621
H	4.9666188	3.2309958	-6.7848868
H	3.5564483	4.3204810	-6.4690573
H	3.2760442	2.5609990	-6.7968902
H	0.2849829	-3.6367015	-1.1529731
H	0.8205524	-2.8752081	-2.6978693
H	-0.2053125	2.9224133	0.6612961
H	0.2804188	3.1816752	2.3733870
H	-3.8070512	0.2008318	1.4970510
H	-7.8797883	-0.1488702	-1.9817693
H	-9.1952129	-1.8626642	-0.9190871
H	-10.1161115	-2.8642468	1.1897905
H	-9.1373180	-2.1961943	3.4094004
H	-7.2572986	-0.5871218	3.5091934
H	-8.1277708	2.2045016	-2.5589273
H	-8.0468526	4.6106169	-1.8503895
H	-6.9681922	5.2313138	0.3340924
H	-5.9861225	3.4397174	1.7970064
H	-6.2696062	-3.3818004	-1.9512978
H	-5.4781946	-5.1670120	-0.4087806
H	-4.1327544	-4.5641934	1.6316592
H	-3.6887698	-2.1451130	2.1473321
H	-5.0627795	1.1599702	-3.7940343
H	-3.4154686	3.0462003	-3.6715494
H	-2.1998619	3.5072442	-1.5197536
H	-2.6953338	2.0990129	0.5148395
H	-1.5693205	-0.4367578	-3.2338316
H	-1.1765859	-2.1689734	-3.5637759
H	-1.3500772	1.3107852	4.8929627
H	-1.4781012	2.5942266	3.6448405
H	0.3273658	4.6125721	-0.7225894
H	0.1158318	4.0298778	-2.4283574
H	1.6829288	4.7778599	-1.9105257
H	3.6536013	4.1083368	3.9944251
H	2.4054090	3.4390695	5.1188639
H	1.8987785	4.3954374	3.6596321
H	2.4088963	-4.3997231	-3.8012008
H	4.1757790	-4.0552095	-4.0055624
H	2.9824271	-3.3743036	-5.1847851
H	1.7708578	-4.6541971	2.1178758
H	0.6443158	-4.6353514	0.6997727
H	0.1487921	-3.8600283	2.2610667
H	-1.6965823	-2.6151793	-1.0376078
H	-1.7592878	-0.8293613	-0.8205291

H	-0.3200899	-0.2355474	3.1757235
H	0.6840607	1.1617729	3.7309756
H	-3.4437214	-2.1706489	-4.9275101
H	-3.6348053	-0.4560319	-4.4074408
H	-5.7762451	-1.7396293	-4.9200595
H	-5.3695704	-2.8863788	-3.6054968
H	-3.9295085	2.3226876	4.1503267
H	-3.5756935	0.8790143	5.1754846
H	-4.8407559	-0.5126383	3.3578407
H	-5.7476739	0.5289294	4.5026940
Na	1.0570064	-0.3850416	0.4637434

Table S1. The calculated (RI-BP86/SV(P)) total energy values (E), energy correction magnitudes for vibrations at 0K (ZPE), corrected energy values (E+ZPE), lowest vibration frequencies (ν);calculated (RI-BP86/TZVP// RI-BP86/SV(P)) total energy values (E(TZVP)), corrected energy values (E(TZVP)+ZPE) and relative energies, calculated at the two levels of approximation (ΔE and $\Delta E(\text{TZVP})$).

Dimer	Structure	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE , kcal/mol	ν , cm^{-1}	E(TZVP)	E(TZVP)+ZPE, a.u.	$\Delta E(\text{TZVP})$, kcal/mol
9'	h2h	-3,536.604119	1.2478175	-3,535.356302	0.0	11.4	-3,540.399300	-3,539.151483	0.0
9'	h2t	-3,536.576691	1.2469858	-3,535.329705	+16.7	11.4	-3540.371705	-3,539.124719	+16.8
10'	h2h	-3,765.461820	-	-	0.0 ^a	-	-3769.518603	-	0.0 ^a
10'	h2t	-3,765.467826	-	-	-3.8 ^a	-	-3769.521202	-	-1.6 ^a
11'	h2h	-4,072.904869	-	-	0.0 ^a	-	-4077.311929	-	0.0 ^a
11'	h2t	-4,072.915549	-	-	-6.7 ^a	-	-4077.322411	-	-6.6 ^a
12'	h2h	-3,615.146658	1.3032344	-3,613.843424	0.0	9.3	-3619.036312	-3,617.733077	0.0
12'	h2t	-3,615.144306	1.3022098	-3,613.842096	0.8	8.6	-3619.030459	-3,617.728250	3.0
Na⁺@11'	h2t	-4,235.077584	-	-	-	-	-4239.531649	-	-
Na⁺@11'	h2t	-4,235.071440	-	-	-	-	-4239.526031	-	-

^a The frequency analysis has not been carried out, due to the extremely large size of the molecule. The relative energies have been calculated using uncorrected total energy values.