

Supplementary material for

Mechanistic insight into light-
driven molecular rotors: a
conformational search in
overcrowded alkenes by a pseudo-
random approach.

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Cartesian coordinates (in Angström) of the B3LYP/6-31G* structures used in Figures 5 and 8.

4a

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.527585
C	1.453379	0.000000	2.066665
S	2.713000	-0.814282	0.969739
C	1.690132	-1.781861	-0.122857
C	2.207658	-3.018973	-0.586552
C	1.474829	-3.788922	-1.454183
C	0.169330	-3.396342	-1.853232
C	-0.624998	-4.223850	-2.690303
C	-1.908305	-3.863444	-3.031556
C	-2.451981	-2.654902	-2.537246
C	-1.703347	-1.823432	-1.733875
C	-0.366549	-2.153102	-1.378123
C	0.452076	-1.310006	-0.550773
C	-0.329509	1.073243	-0.765233
C	-0.828583	2.370679	-0.220569
C	-0.155270	3.101211	0.771937
C	-0.674832	4.293137	1.274265
C	-1.875890	4.796280	0.771359
C	-2.527682	4.126884	-0.262554
C	-2.000786	2.933445	-0.766152
S	-2.824947	2.130204	-2.131986
C	-1.379752	1.522476	-2.991238
C	-1.372300	1.504920	-4.389180
C	-0.250949	1.034077	-5.069407
C	0.870372	0.607053	-4.354146
C	0.858687	0.625006	-2.961492
C	-0.275917	1.052276	-2.255280
C	-0.816196	-1.171502	2.109712
H	-0.465640	0.922440	1.884158
H	1.491209	-0.491538	3.043554
H	1.818357	1.023153	2.191896
H	3.184717	-3.346681	-0.243543
H	1.874008	-4.732426	-1.818836
H	-0.200040	-5.158984	-3.048062
H	-2.507879	-4.507479	-3.669101
H	-3.472182	-2.379713	-2.791082
H	-2.139450	-0.905305	-1.356897
H	0.796392	2.732918	1.141725
H	-0.136827	4.831743	2.049305
H	-2.286837	5.725385	1.156368
H	-3.432268	4.539614	-0.699924
H	-2.234240	1.874844	-4.937036
H	-0.245201	1.023928	-6.155898
H	1.756042	0.263295	-4.880971
H	1.731223	0.298445	-2.405030
H	-1.841234	-1.158039	1.724349
H	-0.864272	-1.084429	3.201402
H	-0.376505	-2.142935	1.866073

4b

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.537159
C	1.453355	0.000000	2.055426
S	2.627900	1.005469	1.022338
C	1.505549	1.944612	0.000000
C	1.888878	3.262309	-0.361648
C	1.066636	4.026422	-1.151042
C	-0.201359	3.540285	-1.567507
C	-1.094234	4.351935	-2.315868
C	-2.341938	3.892273	-2.670393
C	-2.749506	2.594748	-2.281189
C	-1.902500	1.776838	-1.566614
C	-0.599843	2.212503	-1.198376
C	0.314909	1.388623	-0.460480
C	-0.169263	-1.038729	-0.855956
C	-0.417785	-2.458237	-0.468825
C	0.459221	-3.192145	0.343746
C	0.193881	-4.519008	0.678643
C	-0.950486	-5.147456	0.182573
C	-1.794749	-4.463285	-0.690318
C	-1.516667	-3.136405	-1.032576
S	-2.535442	-2.302246	-2.240830
C	-1.231775	-1.410452	-3.084007
C	-1.291502	-1.257022	-4.472042
C	-0.272087	-0.578182	-5.137270
C	0.817473	-0.079212	-4.419884
C	0.871530	-0.230153	-3.035930
C	-0.166427	-0.866965	-2.340645
C	-0.865929	-1.011355	2.307266
H	-0.411519	0.983571	1.795678
H	1.859020	-1.015498	2.060360
H	1.485862	0.385178	3.079330
H	2.834268	3.656997	-0.000848
H	1.362804	5.033186	-1.435986
H	-0.774758	5.353611	-2.594469
H	-3.018137	4.524926	-3.238972
H	-3.741878	2.240121	-2.546650
H	-2.231104	0.787171	-1.269215
H	1.361290	-2.711386	0.709313
H	0.882975	-5.063051	1.318562
H	-1.164345	-6.180993	0.440464
H	-2.651206	-4.963784	-1.132788
H	-2.121997	-1.684817	-5.026243
H	-0.316978	-0.463301	-6.216805
H	1.627541	0.425957	-4.938292
H	1.718609	0.156053	-2.478691
H	-1.871234	-1.062496	1.876698
H	-0.454687	-2.021190	2.318427
H	-0.963011	-0.675775	3.346559

4c

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.532143
C	1.483201	0.000000	1.972547
S	2.607512	-1.162873	1.054022
C	1.517499	-1.943550	-0.110892
C	1.902118	-3.226765	-0.584249
C	1.084604	-3.925442	-1.434586
C	-0.189582	-3.415205	-1.800699
C	-1.091265	-4.172628	-2.593566
C	-2.351209	-3.700974	-2.885782
C	-2.761844	-2.444239	-2.383441
C	-1.902605	-1.676591	-1.627006
C	-0.583708	-2.120709	-1.326541
C	0.337339	-1.344486	-0.543083
C	-0.030779	1.155524	-0.720127
C	-0.413525	2.454703	-0.091357
C	-1.650651	2.633717	0.549887
C	-1.983690	3.845713	1.151027
C	-1.087317	4.916504	1.102528
C	0.124668	4.778487	0.429380
C	0.454971	3.558779	-0.171674
S	2.000659	3.389544	-1.038731
C	1.457555	2.302739	-2.350734
C	2.045134	2.462201	-3.609304
C	1.657097	1.647459	-4.670207
C	0.657838	0.695009	-4.474637
C	0.075103	0.535400	-3.218226
C	0.482214	1.306284	-2.119131
C	-0.816410	-1.131254	2.176845
H	-0.401973	0.947823	1.896411
H	1.904554	0.997095	1.825262
H	1.563876	-0.262245	3.032501
H	2.847101	-3.649869	-0.255391
H	1.385671	-4.903254	-1.802767
H	-0.769365	-5.146227	-2.956287
H	-3.033909	-4.294018	-3.487913
H	-3.765106	-2.082418	-2.592814
H	-2.229505	-0.714286	-1.246116
H	-0.708868	-0.198491	-3.092829
H	0.323795	0.072961	-5.300384
H	2.115018	1.776268	-5.647072
H	2.791543	3.237707	-3.755758
H	0.809915	5.617762	0.351759
H	-1.342135	5.866138	1.564866
H	-2.942867	3.956981	1.648869
H	-2.350773	1.802984	0.576733
H	-0.424994	-2.121674	1.928483
H	-1.860962	-1.092119	1.848049
H	-0.803304	-1.026449	3.267891

4d

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.540695
C	1.489268	0.000000	1.959401
S	2.583048	1.186974	1.040218
C	1.422411	2.023865	-0.014506
C	1.724414	3.359375	-0.391337
C	0.843580	4.077131	-1.159481
C	-0.408809	3.524759	-1.538752
C	-1.369921	4.286442	-2.254023
C	-2.603411	3.762051	-2.568140
C	-2.926831	2.443886	-2.169337
C	-2.010213	1.673072	-1.487544
C	-0.718153	2.175422	-1.163205
C	0.261429	1.399306	-0.458462
C	0.085182	-1.073776	-0.828205
C	-0.200345	-2.481968	-0.423730
C	-1.481564	-2.915248	-0.051938
C	-1.714629	-4.241003	0.309557
C	-0.667958	-5.165984	0.281470
C	0.597232	-4.772996	-0.152818
C	0.822963	-3.443704	-0.523334
S	2.409400	-2.942265	-1.166146
C	1.817168	-1.823236	-2.434198
C	2.498618	-1.781926	-3.653577
C	2.050891	-0.944522	-4.673440
C	0.903894	-0.175062	-4.480352
C	0.227765	-0.213786	-3.261092
C	0.688619	-1.006312	-2.201160
C	-0.737094	-1.070371	2.359286
H	-0.425741	0.964388	1.842163
H	1.910441	-0.995862	1.795527
H	1.574713	0.248861	3.021863
H	2.654806	3.807128	-0.053940
H	1.078731	5.097642	-1.452123
H	-1.114723	5.304147	-2.540788
H	-3.331515	4.358527	-3.110793
H	-3.908224	2.037399	-2.399417
H	-2.268682	0.663105	-1.185714
H	-2.295353	-2.196189	-0.037543
H	-2.711662	-4.552769	0.607982
H	-0.843745	-6.200774	0.562374
H	1.402044	-5.498024	-0.233243
H	3.363931	-2.420711	-3.805417
H	2.580852	-0.916585	-5.621572
H	0.528010	0.457733	-5.279561
H	-0.666301	0.382340	-3.132022
H	-0.675062	-0.803972	3.421417
H	-1.796655	-1.115373	2.091881
H	-0.311931	-2.068098	2.237425

4e

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.556779
C	1.463838	0.000000	2.065700
S	2.560702	-1.105250	1.071999
C	2.476733	-0.011685	-0.332600
C	3.659061	0.386761	-1.000802
C	3.621293	1.420298	-1.904149
C	2.422294	2.150235	-2.118156
C	2.398267	3.301561	-2.950015
C	1.249263	4.041856	-3.108176
C	0.068449	3.655763	-2.431061
C	0.052679	2.532073	-1.634206
C	1.217226	1.731523	-1.459336
C	1.240614	0.556766	-0.629226
C	-0.975759	-0.578710	-0.763685
C	-2.333918	-0.882213	-0.231043
C	-3.135714	0.129103	0.321175
C	-4.400914	-0.154560	0.831660
C	-4.895405	-1.460692	0.780028
C	-4.136957	-2.470486	0.189089
C	-2.870538	-2.178607	-0.326125
S	-1.889462	-3.453925	-1.081736
C	-1.140787	-2.467042	-2.371494
C	-0.920077	-3.090894	-3.603424
C	-0.377420	-2.373570	-4.665795
C	-0.093991	-1.019169	-4.499429
C	-0.307147	-0.400390	-3.268480
C	-0.790239	-1.111598	-2.158269
C	-0.723657	-1.179385	2.238525
H	-0.445151	0.940127	1.919618
H	1.913101	0.995765	2.026654
H	1.503842	-0.351536	3.099682
H	4.593423	-0.115129	-0.767451
H	4.525616	1.730415	-2.422216
H	3.317094	3.596157	-3.451815
H	1.247665	4.925047	-3.740868
H	-0.833940	4.251516	-2.540083
H	-0.862265	2.240122	-1.130052
H	-2.745937	1.142500	0.365524
H	-5.000697	0.640308	1.266179
H	-5.881195	-1.689231	1.175686
H	-4.529794	-3.480279	0.111416
H	-1.199603	-4.132993	-3.729551
H	-0.211272	-2.862076	-5.621981
H	0.290703	-0.432756	-5.329260
H	-0.101181	0.655121	-3.177154
H	-0.351458	-2.133522	1.850023
H	-1.803591	-1.156476	2.115767
H	-0.519732	-1.147732	3.315160

4f

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.533951
C	1.409098	0.000000	2.135263
S	2.350199	-1.472251	1.591632
C	2.291204	-1.082485	-0.138335
C	3.377535	-1.572265	-0.908306
C	3.541167	-1.189281	-2.211461
C	2.708901	-0.178807	-2.761863
C	3.005147	0.383438	-4.030557
C	2.293970	1.457005	-4.515611
C	1.267328	2.015065	-3.725235
C	0.932469	1.458935	-2.508133
C	1.606191	0.321725	-1.992982
C	1.282749	-0.282042	-0.704021
C	-1.189773	0.185016	-0.688360
C	-2.376742	0.973228	-0.202609
C	-2.876191	1.021981	1.117848
C	-3.911373	1.871364	1.503855
C	-4.518803	2.709813	0.573825
C	-4.096633	2.655671	-0.749505
C	-3.057104	1.802665	-1.137474
S	-2.624329	1.879630	-2.863474
C	-2.040978	0.221910	-3.088992
C	-2.232929	-0.401989	-4.326653
C	-1.775341	-1.700265	-4.528990
C	-1.154043	-2.385720	-3.481113
C	-0.972665	-1.760983	-2.252465
C	-1.376772	-0.429283	-2.034782
C	-0.782323	-1.216046	2.097142
H	-0.485863	0.924738	1.875425
H	1.974049	0.891552	1.845078
H	1.361554	-0.043985	3.227461
H	4.086317	-2.247286	-0.436311
H	4.360044	-1.585796	-2.806577
H	3.832240	-0.035475	-4.599218
H	2.538032	1.889581	-5.482038
H	0.732157	2.895039	-4.071657
H	0.150707	1.922152	-1.920930
H	-2.476319	0.368328	1.873772
H	-4.243959	1.862661	2.538160
H	-5.327850	3.374312	0.863373
H	-4.583844	3.266783	-1.504148
H	-2.751248	0.130163	-5.119345
H	-1.926546	-2.183497	-5.490275
H	-0.821361	-3.410734	-3.618425
H	-0.501865	-2.300803	-1.437509
H	-1.716690	-1.396175	1.563089
H	-1.008487	-1.068035	3.161106
H	-0.182027	-2.125855	2.007623

TS1			
C	0.079741	-0.067184	0.027994
C	0.029746	-0.147077	1.417280
C	1.212457	-0.166580	2.161208
C	2.443998	-0.127888	1.510211
C	2.488825	-0.047961	0.115907
S	4.067103	0.012584	-0.720754
C	3.636821	-1.035264	-2.101726
C	4.594781	-1.941611	-2.565431
C	4.254902	-2.889311	-3.527636
C	2.934329	-2.968796	-3.967131
C	1.988170	-2.050149	-3.513007
C	2.328362	-1.003846	-2.640685
C	1.307430	0.012422	-0.646734
C	1.387639	0.059422	-2.137319
C	0.732477	0.994016	-2.900108
C	0.040730	2.167864	-2.264297
C	0.620716	2.935862	-1.177010
C	2.008223	2.923276	-0.881989
C	2.538538	3.688978	0.134502
C	1.706604	4.501736	0.935028
C	0.361643	4.573872	0.652791
C	-0.201739	3.835065	-0.420146
C	-1.553742	4.033876	-0.806692
C	-2.013945	3.498048	-1.980170
C	-1.197899	2.620859	-2.738895
S	-1.725526	2.262374	-4.397408
C	-0.006381	2.140860	-5.039179
C	0.665232	0.896741	-4.446197
C	-0.084872	-0.345425	-5.022845
H	-0.838470	-0.049895	-0.551273
H	-0.932050	-0.198225	1.919954
H	1.177457	-0.233547	3.245103
H	3.369363	-0.173867	2.077181
H	5.592334	-1.927922	-2.135674
H	5.000844	-3.595035	-3.882446
H	2.630403	-3.754232	-4.653646
H	0.960875	-2.167769	-3.820236
H	2.670248	2.318744	-1.488974
H	3.609946	3.666126	0.315832
H	2.131321	5.086180	1.746666
H	-0.289596	5.229622	1.226290
H	-2.183711	4.693527	-0.214908
H	-2.997515	3.757551	-2.361948
H	-0.069689	2.061624	-6.127769
H	0.512512	3.069512	-4.782568
H	1.702100	0.872348	-4.812397
H	0.612223	-1.048580	-5.480606
H	-0.795372	-0.043098	-5.797737
H	-0.663014	-0.869677	-4.258066

TS2			
C	-0.047595	-0.052646	-0.026008
C	-0.112193	0.054605	1.509069
S	1.529004	-0.091748	2.311401
C	2.108150	1.432680	1.602907
C	2.848467	2.316607	2.421130
C	3.294326	3.514046	1.921172
C	2.948032	3.918661	0.605570
C	3.330020	5.197933	0.120887
C	2.950808	5.627665	-1.129091
C	2.153836	4.787993	-1.938421
C	1.782924	3.534100	-1.502403
C	2.181299	3.037281	-0.230382
C	1.825891	1.716098	0.260584
C	1.151712	0.733765	-0.629989
C	1.642829	0.495888	-1.923794
C	3.118763	0.493803	-2.166830
C	0.732555	0.242525	-3.078657
C	4.032164	0.453330	-1.081806
C	-0.668470	0.434524	-2.962829
C	3.721039	0.383794	-3.442963
C	1.172881	-0.045861	-4.395679
C	5.115945	0.424675	-3.614301
C	0.266853	-0.312375	-5.438145
C	5.407672	0.480788	-1.241654
C	-1.566552	0.194232	-3.990295
C	5.964443	0.506360	-2.523702
C	-1.100324	-0.225906	-5.239160
C	-0.019917	-1.543049	-0.420537
H	1.162578	2.919088	-2.141178
H	1.822267	5.134838	-2.913485
H	3.245630	6.610424	-1.486776
H	3.922284	5.838928	0.769930
H	3.880505	4.186837	2.542364
H	3.059200	2.028667	3.447050
H	-0.535058	1.011648	1.828227
H	-0.743589	-0.745743	1.905775
H	-1.009967	0.370729	-0.340505
H	3.645577	0.382696	-0.078032
H	6.045963	0.460235	-0.363071
H	7.040552	0.540649	-2.667756
H	5.523500	0.365294	-4.620470
H	0.659285	-0.562819	-6.420572
H	-1.787650	-0.436983	-6.053220
H	-2.627686	0.352771	-3.820757
H	-1.066289	0.816698	-2.037306
H	0.006137	-1.690138	-1.500750
H	0.863284	-2.026813	0.010123
H	-0.911947	-2.050525	-0.033665
S	2.843850	0.046383	-4.930620

TS3

C	-0.009000	-0.018000	-0.031000
C	-0.067000	0.031000	1.518000
S	1.637000	-0.021000	2.292000
C	2.594000	0.595000	0.915000
C	3.532000	1.641000	1.131000
C	4.101000	2.293000	0.067000
C	3.697000	1.989000	-1.263000
C	4.167000	2.737000	-2.375000
C	3.724000	2.469000	-3.651000
C	2.788000	1.431000	-3.870000
C	2.326000	0.675000	-2.814000
C	2.766000	0.924000	-1.485000
C	2.308000	0.139000	-0.370000
C	1.214000	-0.903000	-0.456000
C	1.400000	-2.274000	-0.559000
C	2.750000	-2.855000	-0.957000
C	0.307000	-3.277000	-0.247000
C	3.801000	-2.054000	-1.466000
C	-0.975000	-2.881000	0.190000
C	3.089000	-4.229000	-0.882000
C	0.458000	-4.687000	-0.307000
C	4.381000	-4.710000	-1.161000
C	-0.615000	-5.572000	-0.091000
C	5.075000	-2.518000	-1.761000
C	-2.038000	-3.741000	0.430000
C	5.390000	-3.863000	-1.581000
C	-1.872000	-5.114000	0.258000
C	-1.389000	-0.091000	-0.761000
H	1.618000	-0.132000	-2.983000
H	2.434000	1.228000	-4.877000
H	4.087000	3.055000	-4.491000
H	4.880000	3.539000	-2.197000
H	4.821000	3.091000	0.230000
H	3.768000	1.934000	2.150000
H	-0.570000	0.947000	1.842000
H	-0.590000	-0.823000	1.954000
H	0.332000	0.981000	-0.302000
H	3.628000	-1.019000	-1.662000
H	5.814000	-1.818000	-2.140000
H	6.384000	-4.248000	-1.792000
H	4.571000	-5.775000	-1.059000
H	-0.431000	-6.639000	-0.183000
H	-2.689000	-5.810000	0.421000
H	-2.989000	-3.330000	0.757000
H	-1.158000	-1.849000	0.375000
H	-1.387000	-0.825000	-1.570000
H	-2.227000	-0.329000	-0.096000
H	-1.610000	0.886000	-1.203000
S	1.976000	-5.533000	-0.517000

TS4

C	-2.204295	-0.268132	0.813920
C	-2.451091	-0.873717	2.055110
C	-3.752838	-1.055337	2.519148
C	-4.833731	-0.614363	1.750923
C	-4.608143	0.043957	0.542771
C	-3.299648	0.233070	0.088019
S	-2.984350	1.123798	-1.422163
C	-1.526232	2.008882	-0.877378
C	-1.358923	3.326612	-1.313255
C	-0.270895	4.075518	-0.871164
C	0.624774	3.513984	0.038074
C	0.461530	2.196452	0.464490
C	-0.585486	1.397094	-0.017288
C	-0.817880	-0.052815	0.308890
C	0.075268	-1.046837	0.040963
C	1.502880	-0.711439	-0.279647
C	2.451051	-0.319767	0.723180
C	2.145248	-0.310433	2.113574
C	3.082438	0.070487	3.048567
C	4.379269	0.469224	2.645732
C	4.713460	0.460278	1.310794
C	3.776359	0.058538	0.321605
C	4.128011	0.005658	-1.053586
C	3.243818	-0.478351	-1.986759
C	1.943118	-0.870150	-1.588074
S	0.866144	-1.756714	-2.697552
C	0.514579	-3.056449	-1.435796
C	-0.244089	-2.548178	-0.161902
C	-1.716252	-2.974307	-0.291451
H	-1.607855	-1.221546	2.646120
H	-3.924117	-1.538156	3.477267
H	-5.850992	-0.753997	2.106291
H	-5.440843	0.432041	-0.036793
H	-2.097574	3.767574	-1.976498
H	-0.146371	5.100794	-1.208728
H	1.454231	4.100318	0.423732
H	1.157217	1.787202	1.183773
H	1.151029	-0.607684	2.430989
H	2.825461	0.063322	4.104525
H	5.108219	0.773714	3.391622
H	5.710604	0.753748	0.990710
H	5.128482	0.309968	-1.351735
H	3.535966	-0.588034	-3.026899
H	-0.077075	-3.822949	-1.942428
H	1.479690	-3.496426	-1.172518
H	0.197331	-3.102621	0.681127
H	-1.750079	-4.039791	-0.546861
H	-2.288092	-2.843001	0.625034
H	-2.218061	-2.419708	-1.091520

TS5

C	-2.372065	-1.832365	-0.504513
C	-1.680548	-0.675825	-0.077170
C	-0.223285	-0.831446	0.325511
C	0.842093	0.031993	0.440898
C	2.255792	-0.470484	0.637891
C	2.775604	-1.001776	1.828342
C	4.092894	-1.454473	1.896572
C	4.924850	-1.362995	0.778139
C	4.452691	-0.767973	-0.391334
C	3.136527	-0.302113	-0.450618
S	2.561688	0.629297	-1.875885
C	1.762078	1.907244	-0.905135
C	1.994424	3.260921	-1.165605
C	1.545576	4.223143	-0.262119
C	0.909050	3.828404	0.918771
C	0.655015	2.479905	1.159871
C	1.009968	1.503054	0.215095
C	-2.529725	0.514188	0.046871
C	-2.051093	1.844220	-0.004402
C	-2.865479	2.945338	0.178323
C	-4.243633	2.791432	0.416310
C	-4.777007	1.523628	0.363773
C	-3.961024	0.387926	0.129504
C	-4.569030	-0.865970	-0.124146
C	-3.794883	-1.915031	-0.517939
S	-1.682727	-3.354847	-1.106402
C	0.032998	-3.211330	-0.525342
C	0.113531	-2.296475	0.695004
C	-0.656335	-2.813822	1.925104
H	2.129582	-1.081139	2.698805
H	4.469369	-1.877083	2.824035
H	5.950753	-1.717122	0.827547
H	5.110550	-0.631446	-1.244733
H	2.565068	3.550808	-2.042984
H	1.736533	5.275058	-0.455800
H	0.607318	4.572347	1.650808
H	0.130815	2.174890	2.060455
H	-1.026833	2.014989	-0.266821
H	-2.429017	3.938624	0.113491
H	-4.879177	3.656774	0.582460
H	-5.849405	1.369494	0.459478
H	-5.650339	-0.960250	-0.064925
H	-4.252736	-2.858641	-0.800846
H	0.671784	-2.830488	-1.327947
H	0.362959	-4.224187	-0.271042
H	1.161613	-2.335155	0.973089
H	-0.456676	-2.167401	2.787236
H	-1.737660	-2.849171	1.778504
H	-0.315622	-3.825636	2.176441

TS6

C	-0.916254	1.302221	-0.582552
C	-0.850728	-0.196199	-0.471515
C	0.200857	-1.065921	-0.324663
C	1.693180	-0.772108	-0.193351
C	2.322969	0.548800	-0.100828
C	1.957544	1.650848	-0.905652
C	2.534031	2.899437	-0.769153
C	3.540058	3.122003	0.189636
C	4.024529	2.044820	0.898792
C	3.485719	0.745923	0.720341
C	4.174635	-0.385620	1.228913
C	3.802311	-1.628052	0.807203
C	2.597426	-1.826594	0.071862
S	2.443922	-3.503861	-0.486587
C	0.697545	-3.444808	-0.976904
C	-0.048639	-2.560730	0.040211
C	-0.876398	2.008042	-1.795351
C	-1.046055	3.389873	-1.824195
C	-1.292396	4.090040	-0.638847
C	-1.468198	3.391317	0.554657
C	-1.330844	2.000837	0.568197
C	-2.292490	-0.568734	-0.253717
C	-3.105197	-1.208759	-1.195777
C	-4.443727	-1.481796	-0.910821
C	-4.991917	-1.098235	0.314986
C	-4.220976	-0.378068	1.230371
C	-2.890096	-0.084844	0.929369
S	-1.919450	1.026866	1.959713
C	-1.422033	-3.200781	0.312668
H	1.261763	1.487843	-1.707194
H	2.217407	3.704507	-1.426433
H	3.972682	4.110320	0.317939
H	4.874450	2.159542	1.567650
H	5.046324	-0.246086	1.863016
H	4.394514	-2.500665	1.068706
H	0.335537	-4.476251	-0.956566
H	0.592614	-3.062671	-1.998233
H	0.474693	-2.676519	0.997604
H	-0.679541	1.465499	-2.716970
H	-0.990192	3.921170	-2.770452
H	-1.414720	5.169518	-0.655350
H	-1.769044	3.911954	1.459013
H	-4.661539	-0.009037	2.152039
H	-6.032178	-1.315676	0.541068
H	-5.057709	-1.996820	-1.644647
H	-2.673451	-1.520441	-2.143287
H	-2.014967	-2.658941	1.049392
H	-2.029201	-3.340596	-0.582944
H	-1.215312	-4.195725	0.727968

TS7

C	-0.910433	1.323454	0.680469
C	-0.918589	-0.124784	0.377628
C	0.224796	-0.923627	0.501669
C	1.606070	-0.744578	-0.063025
C	2.407176	0.454933	-0.329707
C	1.903585	1.780644	-0.392800
C	2.712352	2.881538	-0.598465
C	4.103478	2.742173	-0.757195
C	4.632648	1.473387	-0.779584
C	3.814816	0.325841	-0.614895
C	4.389631	-0.953839	-0.804478
C	3.594519	-2.062103	-0.786508
C	2.220320	-1.970154	-0.442361
S	1.429824	-3.558305	-0.703804
C	-0.077531	-3.465690	0.340381
C	0.138325	-2.267265	1.265756
C	-0.271315	1.755599	1.861795
C	-0.273888	3.094764	2.238647
C	-0.940252	4.039495	1.453620
C	-1.625917	3.632399	0.309862
C	-1.621382	2.285178	-0.062549
C	-2.283030	-0.637637	-0.008980
C	-2.879904	-1.874564	0.322785
C	-4.092350	-2.302043	-0.212873
C	-4.786586	-1.503427	-1.117323
C	-4.252400	-0.265870	-1.454762
C	-3.035176	0.165931	-0.914930
S	-2.475980	1.750763	-1.513159
C	-0.677453	-2.197432	2.581328
H	0.847585	1.951042	-0.329429
H	2.254380	3.865712	-0.648979
H	4.736790	3.613702	-0.897610
H	5.694033	1.319056	-0.959947
H	5.453260	-1.035080	-1.013057
H	4.011093	-3.040382	-1.007677
H	-0.144698	-4.405061	0.899828
H	-0.952438	-3.376339	-0.304871
H	1.156095	-2.416440	1.640308
H	0.242200	1.018112	2.470092
H	0.240285	3.401233	3.145020
H	-0.949773	5.086465	1.743739
H	-2.178973	4.351807	-0.287271
H	-4.785218	0.391326	-2.136116
H	-5.733788	-1.826066	-1.539480
H	-4.490399	-3.266769	0.089585
H	-2.403266	-2.536949	1.023306
H	-0.082907	-1.666877	3.333523
H	-1.630245	-1.673975	2.514918
H	-0.863149	-3.206332	2.969787

TS8

S	1.939915	0.996911	1.869072
C	1.438921	2.056362	0.512301
C	1.006222	1.434997	-0.674133
C	0.894366	-0.056911	-0.676167
C	2.301800	-0.537824	-0.398702
C	2.861677	-0.149789	0.836467
C	1.597923	3.442746	0.580343
C	1.402801	4.216584	-0.563200
C	1.106220	3.597841	-1.781900
C	0.926020	2.217265	-1.837617
C	4.141454	-0.568759	1.211325
C	4.902675	-1.340153	0.334174
C	4.400753	-1.651636	-0.931655
C	3.118531	-1.242275	-1.296384
C	-0.176589	-0.923244	-0.678816
C	-1.661057	-0.706429	-0.471793
C	-2.516644	-1.828859	-0.381312
S	-2.275889	-3.430999	-1.101087
C	-0.551856	-3.256169	-1.631623
C	0.233803	-2.413503	-0.628814
C	-3.747499	-1.792727	0.338064
C	-4.182266	-0.652239	0.943071
C	-3.508647	0.568494	0.683629
C	-2.315981	0.559509	-0.118186
C	-4.077035	1.792069	1.117690
C	-3.576205	3.003469	0.694899
C	-2.515355	3.004496	-0.229031
C	-1.918341	1.820009	-0.617890
C	0.237264	-2.984956	0.802573
H	-1.168543	1.857465	-1.383080
H	-2.166741	3.938113	-0.662120
H	-4.028361	3.935946	1.021139
H	-4.954602	1.749108	1.758778
H	-5.080897	-0.650899	1.554633
H	-4.312533	-2.715723	0.435858
H	-0.509827	-2.809945	-2.631350
H	-0.139739	-4.268768	-1.689194
H	1.259294	-2.485982	-0.977537
H	0.682610	1.735143	-2.781288
H	1.018338	4.191146	-2.687936
H	1.537555	5.293632	-0.514778
H	1.915913	3.904157	1.510690
H	4.549019	-0.260567	2.169779
H	5.900299	-1.659669	0.622264
H	5.009078	-2.209511	-1.638255
H	2.735087	-1.483384	-2.284769
H	0.968396	-2.443920	1.410732
H	-0.735143	-2.904749	1.293023
H	0.524050	-4.043553	0.787115

TS9

C	-0.810337	-0.921045	-1.013822
C	-0.894541	0.371360	-0.265007
C	0.270911	1.114426	-0.094906
C	1.606820	0.491660	0.096449
C	1.796001	-0.573274	1.070050
C	0.753504	-1.072817	1.898623
C	0.968759	-2.095956	2.797943
C	2.243483	-2.687294	2.930323
C	3.287412	-2.208483	2.173039
C	3.099228	-1.146591	1.250731
C	4.199675	-0.622857	0.522460
C	4.032417	0.438643	-0.324370
C	2.745312	0.997977	-0.538009
S	2.727972	2.321616	-1.723542
C	1.022017	2.974130	-1.550830
C	0.327397	2.641735	-0.212317
C	0.268401	-1.146646	-1.904396
C	0.427367	-2.327021	-2.614184
C	-0.527628	-3.341856	-2.505362
C	-1.656564	-3.117430	-1.733197
C	-1.809286	-1.918470	-1.018519
C	-2.225970	0.817477	0.242730
C	-2.408960	2.028853	0.958900
C	-3.644421	2.473133	1.408363
C	-4.785873	1.696470	1.201530
C	-4.636819	0.446895	0.620886
C	-3.379982	-0.007737	0.187144
S	-3.359904	-1.729086	-0.206333
C	0.963903	3.376612	0.979144
H	-0.233050	-0.633565	1.835639
H	0.145124	-2.444541	3.415360
H	2.399503	-3.499365	3.635119
H	4.284841	-2.629796	2.276570
H	5.184101	-1.061538	0.665763
H	4.882588	0.855803	-0.857798
H	0.420034	2.593867	-2.380412
H	1.106796	4.060919	-1.661063
H	-0.680130	3.027962	-0.369659
H	1.000521	-0.364878	-2.048006
H	1.284988	-2.444705	-3.270184
H	-0.417185	-4.273411	-3.053208
H	-2.449485	-3.859899	-1.693663
H	-5.495374	-0.211371	0.516280
H	-5.764093	2.036942	1.528322
H	-3.708331	3.417897	1.940726
H	-1.552680	2.629010	1.218963
H	0.409411	3.183840	1.904497
H	1.995793	3.056272	1.144947
H	0.967905	4.459238	0.805825

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C	-1.652192	-0.210838	0.264972
C	-0.674645	0.884377	0.077457
C	-1.520167	2.160998	-0.044792
C	-2.793364	1.628272	-0.761812
C	-2.897067	0.206109	-0.256632
C	-1.553521	-1.426750	0.975623
C	-2.701705	-2.231915	1.013582
C	-3.898588	-1.852027	0.407925
C	-4.030399	-0.607595	-0.224198
C	0.674661	0.884374	-0.077407
C	1.520189	2.160993	0.044822
C	2.793412	1.628262	0.761793
C	2.897093	0.206099	0.256610
C	1.652198	-0.210845	-0.264947
C	1.553492	-1.426761	-0.975583
C	2.701670	-2.231932	-1.013584
C	3.898580	-1.852045	-0.407977
C	4.030421	-0.607610	0.224135
C	1.870901	2.786432	-1.318075
C	5.346496	-0.159849	0.814625
C	0.330372	-1.841076	-1.756481
C	-1.870924	2.786429	1.318097
C	-5.346450	-0.159830	-0.814739
C	-0.330445	-1.841061	1.756591
H	1.016044	2.913656	0.658330
H	2.654878	1.655753	1.853032
H	3.684569	2.227047	0.537696
H	4.759879	-2.514236	-0.465964
H	2.660393	-3.173786	-1.556737
H	0.970498	3.098479	-1.858526
H	2.508651	3.669159	-1.185990
H	2.408410	2.070079	-1.949517
H	5.253853	0.074748	1.882746
H	6.110984	-0.936258	0.709384
H	5.724192	0.746567	0.323273
H	-0.413837	-2.357998	-1.139996
H	-0.174456	-0.972388	-2.191167
H	0.612933	-2.517532	-2.570271
H	-1.016000	2.913664	-0.658279
H	-2.654787	1.655762	-1.853045
H	-3.684527	2.227059	-0.537749
H	-4.759894	-2.514213	0.465884
H	-2.660455	-3.173763	1.556747
H	-0.970540	3.098472	1.858581
H	-2.508670	3.669156	1.185996
H	-2.408456	2.070072	1.949516
H	-5.724161	0.746588	-0.323402
H	-5.253766	0.074764	-1.882857
H	-6.110945	-0.936236	-0.709525
H	0.174370	-0.972370	2.191284
H	-0.613056	-2.517496	2.570382
H	0.413788	-2.358006	1.140156

7b

C	1.955617	-0.235786	-0.242642
C	0.590616	0.334950	-0.436027
C	0.753155	1.831223	-0.151826
C	1.782699	1.797528	1.015301
C	2.639675	0.598827	0.669243
C	2.613762	-1.335220	-0.823999
C	3.916177	-1.607418	-0.378248
C	4.551252	-0.823504	0.582405
C	3.929798	0.313799	1.117869
C	-0.590612	-0.334918	-0.436033
C	-0.753139	-1.831197	-0.151863
C	-1.782659	-1.797524	1.015286
C	-2.639653	-0.598827	0.669254
C	-1.955619	0.235800	-0.242636
C	-2.613795	1.335217	-0.823992
C	-3.916206	1.607395	-0.378220
C	-4.551253	0.823474	0.582447
C	-3.929773	-0.313820	1.117900
C	-1.338662	-2.631483	-1.331920
C	-4.635634	-1.199860	2.116892
C	-2.030534	2.161308	-1.945367
C	1.338654	2.631535	-1.331878
C	4.635687	1.199825	2.116853
C	2.030457	-2.161318	-1.945345
H	0.192195	-2.277428	0.167799
H	-1.266306	-1.652693	1.975776
H	-2.358270	-2.727746	1.094882
H	-5.562032	1.076142	0.895781
H	-4.453404	2.446561	-0.815611
H	-0.709168	-2.573739	-2.223332
H	-1.445434	-3.688695	-1.059597
H	-2.331383	-2.252661	-1.599490
H	-4.077131	-1.274928	3.058732
H	-5.632950	-0.814289	2.351316
H	-4.755366	-2.223190	1.737699
H	-1.536735	3.071774	-1.584855
H	-1.289968	1.590791	-2.513175
H	-2.820100	2.477167	-2.636350
H	-0.192170	2.277452	0.167865
H	1.266361	1.652690	1.975799
H	2.358320	2.727744	1.094898
H	5.562032	-1.076188	0.895725
H	4.453352	-2.446598	-0.815641
H	0.709148	2.573801	-2.223283
H	1.445421	3.688743	-1.059538
H	2.331375	2.252726	-1.599467
H	4.755432	2.223154	1.737662
H	4.077197	1.274900	3.058701
H	5.632998	0.814237	2.351264
H	1.289886	-1.590797	-2.513142
H	2.819999	-2.477203	-2.636343
H	1.536650	-3.071769	-1.584803

7c

C	1.609617	-0.208217	0.329289
C	0.684643	0.901777	0.020072
C	1.571738	2.123385	-0.305087
C	2.898286	1.465366	-0.787745
C	2.906814	0.114991	-0.126048
C	1.419766	-1.361565	1.130464
C	2.535155	-2.187991	1.330200
C	3.789677	-1.896125	0.797880
C	4.007981	-0.718447	0.071213
C	-0.684659	0.901770	-0.020034
C	-1.571774	2.123372	0.305096
C	-2.898329	1.465341	0.787725
C	-2.906828	0.114965	0.126029
C	-1.609615	-0.208232	-0.329267
C	-1.419724	-1.361582	-1.130427
C	-2.535098	-2.188021	-1.330197
C	-3.789641	-1.896164	-0.797920
C	-4.007980	-0.718485	-0.071263
C	-1.044441	3.096055	1.367335
C	-5.377150	-0.358386	0.454991
C	-0.132306	-1.698887	-1.838687
C	1.044363	3.096052	-1.367320
C	5.377130	-0.358335	-0.455085
C	0.132385	-1.698877	1.838788
H	-1.799326	2.679561	-0.616799
H	-3.777125	2.073237	0.541822
H	-2.883027	1.367751	1.884887
H	-4.620809	-2.573376	-0.982530
H	-2.417242	-3.078247	-1.944344
H	-0.172254	3.667354	1.043136
H	-1.827555	3.817619	1.630890
H	-0.768393	2.553408	2.279136
H	-5.751466	0.573228	0.010086
H	-6.104709	-1.145760	0.233846
H	-5.368280	-0.208042	1.542137
H	-0.332658	-2.353405	-2.693655
H	0.366063	-0.794958	-2.204451
H	0.588477	-2.209810	-1.190073
H	1.799305	2.679584	0.616798
H	3.777083	2.073271	-0.541865
H	2.882959	1.367773	-1.884907
H	4.620859	-2.573328	0.982468
H	2.417330	-3.078213	1.944359
H	0.172174	3.667338	-1.043104
H	1.827459	3.817626	-1.630899
H	0.768302	2.553393	-2.279110
H	5.368225	-0.207995	-1.542231
H	5.751450	0.573285	-0.010195
H	6.104705	-1.145700	-0.233959
H	-0.365976	-0.794950	2.204567
H	-0.588423	-2.209815	1.190215
H	0.332787	-2.353384	2.693754

7d

C	1.949333	-0.229589	0.240938
C	0.595857	0.336091	0.047471
C	0.811195	1.810375	-0.355372
C	2.209746	1.760715	-1.043723
C	2.903068	0.596032	-0.390161
C	2.378008	-1.294786	1.066037
C	3.756251	-1.547740	1.113374
C	4.679786	-0.775654	0.410139
C	4.272584	0.333331	-0.344153
C	-0.595853	-0.335933	0.047419
C	-0.811025	-1.810214	-0.355476
C	-2.209596	-1.760713	-1.043793
C	-2.903046	-0.596124	-0.390200
C	-1.949392	0.229626	0.240853
C	-2.378180	1.294810	1.065910
C	-3.756453	1.547599	1.113272
C	-4.679914	0.775368	0.410099
C	-4.272595	-0.333591	-0.344166
C	0.223753	-2.448617	-1.287301
C	-5.272837	-1.213370	-1.055878
C	-1.453533	2.097554	1.948166
C	-0.223493	2.449016	-1.287134
C	5.272918	1.212979	-1.055899
C	1.453303	-2.097277	1.948467
H	-0.920648	-2.433392	0.544486
H	-2.755454	-2.705939	-0.939799
H	-2.079909	-1.588255	-2.123662
H	-5.739216	1.013057	0.480697
H	-4.117121	2.358976	1.742124
H	1.199101	-2.595208	-0.820907
H	-0.138832	-3.428669	-1.621479
H	0.372741	-1.825352	-2.176871
H	-5.238379	-2.247084	-0.687361
H	-6.293985	-0.845113	-0.914769
H	-5.079784	-1.256107	-2.135480
H	-1.991465	2.463166	2.829350
H	-0.605628	1.494226	2.287802
H	-1.038350	2.976439	1.438221
H	0.920949	2.433502	0.544606
H	2.755724	2.705872	-0.939730
H	2.080015	1.588285	-2.123590
H	5.739063	-1.013457	0.480735
H	4.116839	-2.359107	1.742284
H	-1.198777	2.595828	-0.820682
H	0.139292	3.428989	-1.621326
H	-0.372666	1.825790	-2.176701
H	5.079846	1.255725	-2.135496
H	5.238596	2.246702	-0.687395
H	6.294024	0.844599	-0.914808
H	0.605530	-1.493767	2.288106
H	1.037928	-2.976153	1.438666
H	1.991247	-2.462871	2.829651

TS1

C	-4.294253	0.282545	-0.538035
C	-2.935423	0.544839	-0.349717
C	-1.962270	-0.441366	-0.016346
C	-2.391195	-1.802412	-0.077898
C	-3.763971	-2.046857	-0.239432
C	-4.708407	-1.044296	-0.425036
C	-0.642645	0.262729	0.187102
C	-0.956216	1.762381	0.130858
C	-2.304372	1.890049	-0.579710
C	0.626849	-0.174945	0.451471
C	1.965703	0.436207	0.071583
C	2.803673	-0.665970	-0.261318
C	2.168972	-1.982154	0.117117
C	1.003514	-1.538226	1.013714
C	4.064211	-0.535963	-0.846179
C	4.535124	0.760792	-1.064350
C	3.785430	1.852957	-0.644646
C	2.516026	1.739490	-0.052836
C	1.436655	-1.394188	2.489657
C	1.947982	3.039593	0.485963
C	4.889802	-1.747330	-1.208976
C	-1.119084	2.291936	1.576354
C	-1.532860	-3.050912	-0.108982
C	-5.268498	1.384427	-0.881730
H	-0.174103	2.312734	-0.387203
H	-2.184834	2.060527	-1.660575
H	-2.899080	2.726883	-0.194934
H	-5.758275	-1.302568	-0.543705
H	-4.097183	-3.082095	-0.252153
H	-0.274644	2.018538	2.214262
H	-1.227683	3.383612	1.583816
H	-2.019407	1.860782	2.030455
H	-5.013319	1.868097	-1.833768
H	-6.286730	0.992966	-0.971633
H	-5.280414	2.173905	-0.119403
H	-2.099764	-3.860569	-0.579695
H	-0.622545	-2.913588	-0.699020
H	-1.244992	-3.413328	0.885758
H	0.183294	-2.237735	0.999403
H	1.800177	-2.519208	-0.771005
H	2.872733	-2.653793	0.624774
H	5.511365	0.915936	-1.518412
H	4.210464	2.848925	-0.750638
H	0.619323	-0.987196	3.095182
H	1.709122	-2.374521	2.900344
H	2.300623	-0.728988	2.595194
H	5.162304	-2.333885	-0.321530
H	4.346040	-2.424309	-1.880088
H	5.818056	-1.454904	-1.710067
H	1.374938	3.603792	-0.259913
H	1.311376	2.892396	1.356241
H	2.774669	3.687636	0.796547

TS2

C	-3.358316	-0.394054	1.349111
C	-2.454331	0.335824	0.579215
C	-1.670738	-0.253652	-0.442553
C	-1.994587	-1.545041	-0.885892
C	-2.895608	-2.286056	-0.099891
C	-3.523908	-1.747502	1.017295
C	-0.699672	0.814091	-0.891615
C	-1.614055	2.065550	-0.828639
C	-2.254417	1.834640	0.570604
C	0.658680	0.776634	-0.822747
C	1.551981	-0.328155	-0.312458
C	2.296600	0.232986	0.753275
C	2.137936	1.736938	0.759006
C	1.541380	2.021575	-0.649368
C	3.124289	-0.528890	1.576489
C	3.257566	-1.888634	1.258285
C	2.669980	-2.408543	0.110620
C	1.843780	-1.637887	-0.726619
C	2.630059	2.154220	-1.728005
C	1.526874	-2.183221	-2.098175
C	3.876951	0.088053	2.731635
C	-1.184232	3.514024	-1.075683
C	-1.641935	-2.079650	-2.253374
C	-4.154818	0.248994	2.459940
H	-2.411165	1.864298	-1.559929
H	-3.195652	2.383223	0.702375
H	-1.561528	2.180928	1.353216
H	-4.210876	-2.360882	1.596514
H	-3.142622	-3.299911	-0.409515
H	-0.605827	3.626875	-1.998711
H	-2.089399	4.125194	-1.182121
H	-0.611343	3.944669	-0.248554
H	-4.824215	1.031882	2.078810
H	-4.774267	-0.489481	2.978975
H	-3.505293	0.723572	3.206200
H	-2.567064	-2.211836	-2.829664
H	-1.009496	-1.389536	-2.811352
H	-1.151868	-3.057417	-2.219570
H	0.972540	2.942634	-0.635162
H	1.439440	2.078518	1.537992
H	3.090563	2.254464	0.930253
H	3.888493	-2.524422	1.875879
H	2.891477	-3.433737	-0.180335
H	2.181539	2.289480	-2.719040
H	3.266952	3.023821	-1.524727
H	3.270796	1.266778	-1.767096
H	4.597135	0.843458	2.389417
H	3.202498	0.590667	3.436355
H	4.435432	-0.671107	3.288588
H	0.920460	-3.093307	-2.068731
H	1.020637	-1.445750	-2.721117
H	2.465897	-2.446538	-2.601699