

Violations. How Nature Circumvents the Woodward-Hoffmann Rules and Promotes the Forbidden Conrotatory $4n+2$ Electron Electrocyclization of Prinzbach's Vinylogous Sesquifulvalene

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1. DFT Calculations

Density functional theory (DFT) calculations were performed with Gaussian 16.¹ Optimization of molecular geometries and subsequent frequency calculations were performed with the ω B97X-D functional,² and the 6-31G(d) basis set.³ Frequency calculations were used to confirm the optimized structures as minima (zero imaginary frequencies) or transition states (one imaginary frequency) on the potential energy surface. Transition state structures were confirmed by intrinsic reaction coordinate (IRC) calculations to connect the appropriate starting geometries and products. Single point energies were calculated for each structure using the ω B97X-D/6-311++G(d,p) level of theory, and were supplemented by quasi-harmonic corrections from the GoodVibes program.⁴ PyMol 2.3.5.⁵ was used to render 3D-like visualizations of optimized geometries. Initial structures were generated in GaussView 6.0.16.⁶

1.1 Summary of Energies

Structure	E_SPC (au)	qh-H_SPC (au)	T.qh-S (au)	qh- G(T)_SPC (au)	qh- G(T)_SPC (kcal/mol)
Figure 1a					
s-trans-1	-540.54672	-540.31948	0.05046	-540.36994	-339087.0
s-cis-1	-540.54227	-540.31509	0.04920	-540.36429	-339083.5
2-trans	-540.57089	-540.34252	0.04640	-540.38892	-339098.9
2-cis	-540.57668	-540.34819	0.04606	-540.39425	-339102.3
Figure 2					
9	-1000.28574	-999.93013	0.06108	-999.99120	-627503.5
9-TS	-1000.25954	-999.90765	0.05950	-999.96715	-627488.4
10	-1000.31689	-999.96000	0.05846	-1000.01845	-627520.6
des-Ph-11	-1076.49994	-1076.13091	0.06231	-1076.19322	-675320.9
des-Ph-11-conTS	-1076.46800	-1076.10311	0.06029	-1076.16340	-675302.2
des-Ph-11-disTS	-1076.45698	-1076.08928	0.06089	-1076.15017	-675293.9
des-Ph-12	-1076.52990	-1076.15945	0.05995	-1076.21941	-675337.4
des-Ph-12-synprod	-1076.51109	-1076.14074	0.06052	-1076.20125	-675326.0
Figure 3a					
13	-233.36871	-233.24090	0.03772	-233.27861	-146384.4
TS-1a	-233.29178	-233.16942	0.03541	-233.20483	-146338.1
TS-1b	-233.32055	-233.19385	0.03508	-233.22893	-146353.3
14	-233.39901	-233.26883	0.03430	-233.30313	-146399.8
Figure 3b					
15	-540.64022	-540.41126	0.04816	-540.45942	-339143.1
TS-2a	-540.54544	-540.32160	0.04632	-540.36792	-339085.7
TS-2b	-540.55064	-540.32368	0.04599	-540.36967	-339086.8

16	-540.58156	-540.35306	0.04570	-540.39876	-339105.1
17	-540.57033	-540.34178	0.04628	-540.38806	-339098.4
Figure 5					
TS-3a	-540.50671	-540.28171	0.04714	-540.32885	-339061.2
TS-3b	-540.48844	-540.26343	0.04753	-540.31096	-339050.0
Figure 6/7					
TS-4	-540.53550	-540.30965	0.04846	-540.35811	-339079.6
TS-5a	-540.49441	-540.26866	0.04684	-540.31549	-339052.8
TS-5b	-540.49352	-540.26883	0.04732	-540.31615	-339053.2
TS-6a	-540.50539	-540.28053	0.04690	-540.32742	-339060.3
18	-540.50961	-540.28349	0.04756	-540.33105	-339062.6
19	-540.55781	-540.33027	0.04717	-540.37744	-339091.7
20	-540.54340	-540.31615	0.04662	-540.36277	-339082.5
Figure 8					
21	-540.61985	-540.39087	0.04651	-540.43738	-339129.3
Figure 9a					
s-trans-22	-463.14555	-462.95569	0.04593	-463.00162	-290537.7
s-cis-22	-463.14069	-462.95080	0.04547	-462.99627	-290534.3
TS-7a	-463.11108	-462.92282	0.04310	-462.96593	-290515.3
TS-7b	-463.06529	-462.87733	0.04228	-462.91961	-290486.2
Figure 9b					
s-trans-23	-617.94354	-617.67945	0.05380	-617.73325	-387633.2
s-cis-23	-617.94338	-617.67944	0.05280	-617.73224	-387632.5
TS-8a	-617.90257	-617.64060	0.05044	-617.69104	-387606.7
TS-8b	-617.86290	-617.60205	0.05072	-617.65277	-387582.7
Figure 10					
24	-540.48884	-540.27003	0.04916	-540.31919	-339055.2
Figure 11					
SOSP	-540.49715	-540.27082	0.04627	-540.31709	-339053.8
Figure 15					
s-trans-25	-385.66788	-385.51619	0.04311	-385.55930	-241941.9
s-cis-25	-385.66426	-385.51245	0.04280	-385.55525	-241939.4
TS-9a	-385.62661	-385.47654	0.04020	-385.51674	-241915.2
TS-9b	-385.61289	-385.46241	0.04042	-385.50283	-241906.5
Figure 16					
s-cis-26	-436.33333	-436.16764	0.04727	-436.21492	-273728.8
TS-10a	-436.28486	-436.12090	0.04408	-436.16498	-273697.5
TS-10b	-436.28508	-436.12089	0.04441	-436.16530	-273697.7

1.2 Coordinates

Fig1a-s-trans-1

C	-4.236077	0.873081	0.044703
C	-4.417061	-0.464750	0.058338
C	-3.403056	-1.492044	0.005671
C	-2.985841	1.594337	-0.028281
C	-2.056831	-1.382738	-0.031677
C	-1.712516	1.142749	-0.060724
C	-1.179272	-0.215650	-0.029522
H	-5.126834	1.495222	0.084929
H	-5.441241	-0.826421	0.109112
H	-3.789860	-2.508625	0.000517
H	-3.095770	2.676196	-0.060782
H	-1.515511	-2.326898	-0.063030
H	-0.959835	1.922617	-0.121028
C	0.170015	-0.459118	-0.015457
C	1.234617	0.500851	-0.000032
H	0.477590	-1.501984	-0.009359
C	2.560570	0.202682	0.005620
C	3.639563	1.192461	0.027098
C	3.210673	-1.110315	-0.007870
C	4.819553	0.530661	0.026358
C	4.549446	-0.909318	0.004345
H	5.808399	0.973598	0.039698
H	5.312300	-1.679375	-0.001261
H	0.981840	1.559083	0.014179
H	3.484377	2.264662	0.041055
H	2.701853	-2.065406	-0.025459

Fig1a-s-cis-1

C	2.957913	1.667559	-0.194922
C	3.764804	0.727879	0.342659
C	3.509746	-0.691237	0.447141
C	1.657354	1.468660	-0.794546
C	2.365931	-1.379033	0.244132
C	0.844704	0.391180	-0.758540
C	1.026962	-0.907910	-0.113475
H	3.332116	2.688345	-0.222693
H	4.733679	1.054816	0.712654
H	4.367016	-1.284600	0.758286
H	1.274031	2.326921	-1.342337
H	2.425098	-2.454106	0.407721
H	-0.102423	0.494354	-1.281693
C	-0.007163	-1.788676	0.033270
C	-1.416801	-1.603769	-0.240675
H	0.257339	-2.800216	0.340364
C	-2.208638	-0.526781	-0.010217
C	-3.627053	-0.447767	-0.383730
C	-1.901251	0.727796	0.686011
C	-4.106385	0.745020	0.032039
C	-3.028263	1.474721	0.709499
H	-5.116386	1.115763	-0.097204
H	-3.139726	2.449922	1.169432
H	-1.916215	-2.485336	-0.646596
H	-4.160744	-1.224669	-0.917770
H	-0.944953	0.972956	1.127958

Fig1a-2-trans

C	-1.181348	-0.568363	0.391746
C	-2.058612	0.617719	0.107466

C	-1.523779	1.931083	0.379139
C	-0.186253	2.100284	0.429431
C	0.764605	1.042038	0.090897
C	0.283981	-0.399153	-0.051639
C	-1.971821	-1.720190	-0.158857
C	-3.165237	-1.263550	-0.586092
C	-3.228807	0.188962	-0.416561
H	-2.193865	2.777073	0.507203
H	0.225778	3.089989	0.611925
H	-1.634081	-2.749739	-0.146254
H	-4.071774	0.809830	-0.699931
H	-3.968974	-1.865136	-0.996329
C	2.024574	1.387600	-0.277693
C	1.169343	-1.313765	0.763128
H	0.694203	-1.855520	1.579678
H	2.268396	2.449326	-0.271946
C	2.471402	-1.529948	0.519356
C	3.075003	0.517812	-0.750731
H	2.986825	-2.293847	1.098976
C	3.274920	-0.783058	-0.422822
H	3.833397	0.997088	-1.367249
H	4.177353	-1.264612	-0.793554
H	0.371923	-0.670622	-1.114752
H	-1.177006	-0.668658	1.491640

Fig1a-2-cis

C	1.887013	-1.587710	0.884245
C	3.045417	-1.118546	0.161392
C	3.203664	0.128969	-0.370263
C	0.625281	-1.168408	0.660237

C	2.253324	1.206159	-0.288252
C	0.307414	-0.306940	-0.527621
C	0.902934	1.057796	-0.224525
H	2.068627	-2.307686	1.680001
H	3.917176	-1.770187	0.161819
H	4.191286	0.382355	-0.751416
H	-0.186700	-1.458335	1.323584
H	2.667542	2.210413	-0.205810
C	0.033076	2.148647	0.195619
C	-1.290578	1.984638	0.409755
H	0.507793	3.099326	0.426673
C	-1.904921	0.713888	0.103319
C	-3.019217	0.099353	0.563525
C	-1.190296	-0.210752	-0.845218
C	-3.078968	-1.253113	0.007975
C	-2.011747	-1.466065	-0.787478
H	-3.873319	-1.962197	0.214217
H	-1.789334	-2.364126	-1.351249
H	-1.885998	2.784755	0.841027
H	-3.742529	0.516169	1.256213
H	0.836354	-0.719510	-1.397101
H	-1.285279	0.221529	-1.854208

Fig2-9

C	-5.672786	-0.035778	-0.473684
C	-5.098408	-1.149466	0.084273
C	-3.718028	-1.163613	0.420554
C	-2.923214	-0.021738	0.127630
C	-3.554224	1.145220	-0.397113
C	-4.903486	1.122954	-0.695475

C	-2.752119	2.342721	-0.536417
C	-1.428627	2.350062	-0.279905
C	-0.695034	1.138132	0.040860
C	-1.523335	-0.027059	0.415147
C	0.695044	1.138128	-0.040802
C	1.428647	2.350058	0.279940
C	1.523332	-0.027064	-0.415107
C	1.015592	-1.092847	-1.145618
C	-1.015624	-1.092840	1.145679
C	-1.804249	-2.209394	1.460662
C	-3.121887	-2.267571	1.073688
C	2.923217	-0.021747	-0.127630
C	3.554244	1.145211	0.397096
C	2.752146	2.342714	0.536420
C	3.718019	-1.163625	-0.420574
C	5.098409	-1.149481	-0.084331
C	5.672805	-0.035794	0.473608
C	4.903514	1.122940	0.695420
C	3.121855	-2.267582	-1.073688
C	1.804204	-2.209404	-1.460620
H	0.022876	-1.080687	1.456788
H	-1.359174	-3.033326	2.010227
H	3.728470	-3.141176	-1.296956
H	1.359108	-3.033339	-2.010164
H	3.243375	3.249313	0.879952
H	5.377624	2.018282	1.089128
H	6.729999	-0.032702	0.721288
H	5.695997	-2.032447	-0.294852
H	-3.728513	-3.141162	1.296941
H	-3.243338	3.249320	-0.879967

H	-5.377582	2.018297	-1.089197
H	-6.729973	-0.032684	-0.721393
H	-5.696006	-2.032429	0.294779
H	-0.022923	-1.080693	-1.456683
H	0.875566	3.263297	0.466878
H	-0.875538	3.263298	-0.466840

Fig2-9-TS

C	-2.847146	2.365191	-0.556857
C	-1.473441	2.406636	-0.455970
C	-0.741043	1.293164	-0.010997
C	-1.422559	0.123415	0.369877
C	-2.826440	0.035806	0.171762
C	-3.554940	1.174322	-0.272589
C	1.473441	2.406636	0.455970
C	0.741043	1.293164	0.010997
C	2.847146	2.365191	0.556857
C	3.554940	1.174322	0.272589
C	2.826440	0.035806	-0.171762
C	1.422559	0.123415	-0.369877
C	3.511684	-1.202153	-0.385080
C	2.745883	-2.354898	-0.786708
C	1.408499	-2.268560	-1.029098
C	0.688606	-1.050383	-0.836655
C	4.959754	1.068268	0.447334
C	5.606862	-0.124868	0.219553
C	4.886669	-1.260856	-0.184848
C	-3.511684	-1.202153	0.385080
C	-2.745883	-2.354898	0.786708
C	-1.408499	-2.268560	1.029098

C	-0.688606	-1.050383	0.836655
H	0.177345	-0.889220	1.469687
H	-0.863832	-3.135241	1.392947
H	3.272513	-3.294093	-0.935371
H	0.863832	-3.135241	-1.392947
H	-0.177345	-0.889220	-1.469687
H	3.397251	3.237522	0.899195
H	5.514638	1.942882	0.776117
H	6.680988	-0.195646	0.362575
H	5.406495	-2.202476	-0.341090
H	-3.272513	-3.294093	0.935371
C	-4.886669	-1.260856	0.184848
C	-4.959754	1.068268	-0.447334
H	-3.397251	3.237522	-0.899195
C	-5.606862	-0.124868	-0.219553
H	-5.514638	1.942882	-0.776117
H	-6.680988	-0.195646	-0.362575
H	-5.406495	-2.202476	0.341090
H	-0.938701	3.305762	-0.749830
H	0.938701	3.305762	0.749830

Fig2-10

C	-0.353713	2.842946	-2.434413
C	-0.306248	1.475341	-2.447805
C	-0.035508	0.738602	-1.267124
C	0.166929	1.417353	-0.074668
C	0.083044	2.833053	-0.035670
C	-0.163447	3.561008	-1.228909
C	0.306248	-1.475341	-2.447805
C	0.035508	-0.738602	-1.267124

C	0.353713	-2.842946	-2.434413
C	0.163447	-3.561008	-1.228909
C	-0.083044	-2.833053	-0.035670
C	-0.166929	-1.417353	-0.074668
C	-0.206231	-3.539812	1.201461
C	-0.377355	-2.767065	2.429794
C	-0.468321	-1.435264	2.429841
C	-0.475100	-0.611273	1.174337
C	0.232353	-4.978682	-1.174303
C	0.083044	-5.638014	0.017179
C	-0.127000	-4.913575	1.211574
C	0.206231	3.539812	1.201461
C	0.377355	2.767065	2.429794
C	0.468321	1.435264	2.429841
C	0.475100	0.611273	1.174337
H	1.495676	0.199292	1.071411
H	0.621291	0.909525	3.367965
H	-0.428176	-3.319717	3.365055
H	-0.621291	-0.909525	3.367965
H	-1.495676	-0.199292	1.071411
H	0.559223	-3.393328	-3.348720
H	0.410888	-5.530147	-2.093638
H	0.137860	-6.721908	0.052286
H	-0.218319	-5.447625	2.153966
H	0.428176	3.319717	3.365055
C	0.127000	4.913575	1.211574
C	-0.232353	4.978682	-1.174303
H	-0.559223	3.393328	-3.348720
C	-0.083044	5.638014	0.017179
H	-0.410888	5.530147	-2.093638

H	-0.137860	6.721908	0.052286
H	0.218319	5.447625	2.153966
H	0.498363	-0.946816	-3.376081
H	-0.498363	0.946816	-3.376081

Fig2-des-Ph-11

C	5.654375	-0.247744	0.502205
C	5.086772	-1.396956	0.012602
C	3.711244	-1.431744	-0.342491
C	2.913459	-0.276226	-0.125905
C	3.539188	0.928971	0.315307
C	4.886588	0.926168	0.627684
C	2.750068	2.136611	0.314860
C	1.413058	2.140924	0.075512
C	0.684772	0.876559	-0.084322
C	1.518276	-0.299165	-0.421618
C	-0.684857	0.876645	0.084462
C	-1.412913	2.141034	-0.075442
C	-0.667632	3.385207	-0.059368
C	0.667783	3.385126	0.059932
C	-1.518229	-0.299248	0.421725
C	-1.018797	-1.396255	1.106913
C	1.018752	-1.396011	-1.107121
C	1.811943	-2.526984	-1.357055
C	3.122273	-2.568298	-0.944173
C	-2.913511	-0.276199	0.126055
C	-3.538922	0.928995	-0.315393
C	-2.749896	2.136605	-0.315018
C	-3.711434	-1.431622	0.342496
C	-5.086838	-1.396763	-0.012759

C	-5.654222	-0.247468	-0.502611
C	-4.886322	0.926270	-0.628139
C	-3.122573	-2.568201	0.944355
C	-1.812318	-2.526970	1.357278
H	-0.016556	-1.400232	-1.428686
H	1.374062	-3.376693	-1.871969
H	-3.730107	-3.453688	1.111297
H	-1.374610	-3.376602	1.872468
H	-3.258819	3.077925	-0.510869
H	-5.360152	1.848651	-0.953766
H	-6.707865	-0.228017	-0.764280
H	-5.686587	-2.291705	0.129909
H	3.729530	-3.454083	-1.110529
H	1.227132	4.314592	0.123066
H	-1.226898	4.314736	-0.122110
H	3.258965	3.077984	0.510503
H	5.360654	1.848630	0.952737
H	6.708019	-0.228394	0.763861
H	5.686306	-2.292036	-0.130138
H	0.016401	-1.400648	1.428672

Fig2-des-Ph-11-conTS

C	-0.177195	2.819037	-2.184431
C	-0.083618	1.427657	-2.200981
C	0.053598	0.722265	-0.977412
C	0.326236	1.437412	0.213481
C	0.138335	2.836330	0.236501
C	-0.138335	3.538406	-0.977236
C	-0.073211	0.672203	-3.433106
C	0.073211	-0.672203	-3.433106

C	0.083618	-1.427657	-2.200981
C	-0.053598	-0.722265	-0.977412
C	0.177195	-2.819037	-2.184431
C	0.138335	-3.538406	-0.977236
C	-0.138335	-2.836330	0.236501
C	-0.326236	-1.437412	0.213481
C	-0.221240	-3.555967	1.472105
C	-0.536100	-2.825407	2.671306
C	-0.845523	-1.497875	2.631661
C	-0.766121	-0.747200	1.419668
C	0.330464	-4.945995	-0.922841
C	0.267731	-5.618347	0.276492
C	-0.003934	-4.930373	1.471854
C	0.221240	3.555967	1.472105
C	0.536100	2.825407	2.671306
C	0.845523	1.497875	2.631661
C	0.766121	0.747200	1.419668
H	1.465659	-0.074156	1.299760
H	1.175832	0.988579	3.532746
H	-0.590167	-3.374374	3.607894
H	-1.175832	-0.988579	3.532746
H	-1.465659	0.074156	1.299760
H	0.296110	-3.358920	-3.121066
H	0.535172	-5.482328	-1.845467
H	0.426133	-6.692301	0.303553
H	-0.052090	-5.476596	2.410176
H	0.590167	3.374374	3.607894
C	0.003934	4.930373	1.471854
H	-0.138356	1.219217	-4.369961
H	0.138356	-1.219217	-4.369961

C	-0.330464	4.945995	-0.922841
H	-0.296110	3.358920	-3.121066
C	-0.267731	5.618347	0.276492
H	-0.535172	5.482328	-1.845467
H	-0.426133	6.692301	0.303553
H	0.052090	5.476596	2.410176

Fig2-des-Ph-11-disTS

C	5.051298	-0.211445	1.574863
C	4.475941	-1.426302	1.208768
C	3.316466	-1.463412	0.432789
C	2.688312	-0.240721	0.058803
C	3.284381	0.993877	0.434877
C	4.473654	0.984557	1.179175
C	2.645939	2.201019	0.028515
C	1.394474	2.195558	-0.521128
C	0.713305	0.943354	-0.803492
C	1.496052	-0.249731	-0.728765
C	-0.713305	0.943354	-0.803491
C	-1.394473	2.195558	-0.521127
C	-0.670534	3.440915	-0.714859
C	0.670535	3.440915	-0.714860
C	-1.496052	-0.249730	-0.728765
C	-1.126876	-1.469499	-1.363473
C	1.126875	-1.469500	-1.363472
C	1.744545	-2.699041	-0.937362
C	2.751127	-2.701951	-0.033325
C	-2.688312	-0.240721	0.058803
C	-3.284380	0.993878	0.434879
C	-2.645938	2.201020	0.028517

C	-3.316467	-1.463411	0.432788
C	-4.475942	-1.426301	1.208767
C	-5.051298	-0.211444	1.574863
C	-4.473653	0.984557	1.179177
C	-2.751129	-2.701950	-0.033328
C	-1.744546	-2.699040	-0.937365
H	0.900218	-1.403230	-2.414593
H	1.403670	-3.629205	-1.383471
H	-3.208561	-3.634338	0.287291
H	-1.403673	-3.629204	-1.383475
H	-3.131996	3.149450	0.246142
H	-4.931164	1.931270	1.454177
H	-5.962277	-0.202791	2.165715
H	-4.940480	-2.361300	1.510912
H	3.208559	-3.634339	0.287295
H	1.237072	4.367055	-0.758494
H	-1.237070	4.367055	-0.758492
H	3.131998	3.149449	0.246139
H	4.931165	1.931269	1.454174
H	5.962278	-0.202792	2.165714
H	4.940479	-2.361301	1.510914
H	-0.900219	-1.403228	-2.414594

Fig2-des-Ph-12

C	0.101952	2.814279	2.206296
C	0.069027	1.431370	2.207880
C	-0.003093	0.728404	0.968610
C	-0.130001	1.426704	-0.226057
C	-0.065338	2.836235	-0.226452
C	0.063883	3.541935	1.004272

C	0.049737	0.671745	3.441808
C	-0.049737	-0.671745	3.441808
C	-0.069027	-1.431370	2.207880
C	0.003093	-0.728404	0.968610
C	-0.101952	-2.814279	2.206296
C	-0.063883	-3.541935	1.004272
C	0.065338	-2.836235	-0.226452
C	0.130001	-1.426704	-0.226057
C	0.090881	-3.570389	-1.456340
C	0.162961	-2.818926	-2.706664
C	0.284411	-1.489686	-2.736793
C	0.419594	-0.648427	-1.497680
C	-0.130001	-4.965038	0.979057
C	-0.088949	-5.643819	-0.206966
C	0.013662	-4.941665	-1.432564
C	-0.090881	3.570389	-1.456340
C	-0.162961	2.818926	-2.706664
C	-0.284411	1.489686	-2.736793
C	-0.419594	0.648427	-1.497680
H	-1.476647	0.325976	-1.445015
H	-0.363623	0.987496	-3.696071
H	0.117300	-3.385188	-3.633972
H	0.363623	-0.987496	-3.696071
H	1.476647	-0.325976	-1.445015
H	-0.151606	-3.352313	3.150402
H	-0.217352	-5.499937	1.920992
H	-0.143103	-6.728269	-0.217324
H	0.025119	-5.495422	-2.367862
H	-0.117300	3.385188	-3.633972
C	-0.013662	4.941665	-1.432564

H	0.089555	1.221705	4.378410
H	-0.089555	-1.221705	4.378410
C	0.130001	4.965038	0.979057
H	0.151606	3.352313	3.150402
C	0.088949	5.643819	-0.206966
H	0.217352	5.499937	1.920992
H	0.143103	6.728269	-0.217324
H	-0.025119	5.495422	-2.367862

Fig2-des-Ph-12-synprod

C	5.561433	-0.351845	0.443439
C	4.782731	-1.527316	0.574988
C	3.428958	-1.506453	0.332654
C	2.813175	-0.275124	-0.067294
C	3.564515	0.929917	-0.055538
C	4.969155	0.850448	0.160365
C	2.877617	2.152211	-0.198129
C	1.496081	2.187923	-0.266060
C	0.758250	0.966021	-0.363406
C	1.433535	-0.242421	-0.358652
C	-0.697655	0.992624	-0.278346
C	-1.357751	2.228956	-0.014872
C	-0.577981	3.451537	-0.031422
C	0.761337	3.434335	-0.176461
C	-1.425528	-0.186473	-0.347075
C	-0.774672	-1.422234	-0.929185
C	0.756046	-1.559908	-0.658436
C	1.255786	-2.632058	0.284722
C	2.542843	-2.631908	0.648674
C	-2.798641	-0.188335	-0.026295

C	-3.455568	1.037858	0.282542
C	-2.717167	2.234102	0.243150
C	-3.539149	-1.414971	0.016148
C	-4.872895	-1.391071	0.347133
C	-5.529599	-0.170409	0.634656
C	-4.842893	1.012148	0.602885
C	-2.834970	-2.661032	-0.278103
C	-1.564618	-2.678305	-0.689569
H	1.169904	-1.862457	-1.633700
H	0.593922	-3.439635	0.580935
H	-3.389774	-3.589621	-0.167189
H	-1.088872	-3.623069	-0.940785
H	-3.224294	3.176724	0.436931
H	-5.344572	1.949907	0.826506
H	-6.586038	-0.180656	0.885581
H	-5.431637	-2.322564	0.388500
H	2.952012	-3.440820	1.248770
H	1.328373	4.361564	-0.171109
H	-1.106854	4.393255	0.090040
H	3.439475	3.083242	-0.170884
H	5.559078	1.762451	0.123364
H	6.631875	-0.401684	0.619141
H	5.256266	-2.448253	0.905622
H	-0.833125	-1.247682	-2.016813

Fig3a-13

C	2.882112	-0.319210	0.000009
C	1.548272	-0.404650	0.000003
C	0.673080	0.761493	0.000000
C	-0.673080	0.761493	-0.000002

C	-1.548272	-0.404650	-0.000003
C	-2.882112	-0.319210	-0.000008
H	3.389262	0.642983	0.000014
H	3.510318	-1.204189	0.000011
H	-3.389262	0.642983	-0.000012
H	-3.510318	-1.204189	-0.000009
H	1.086652	-1.389619	-0.000002
H	1.180921	1.725021	0.000001
H	-1.180921	1.725021	-0.000003
H	-1.086652	-1.389619	0.000001

Fig3a-TS-1a

C	-1.061857	1.136709	0.480883
C	-1.477970	-0.071765	-0.145390
C	-0.690435	-1.217663	-0.187543
C	0.690435	-1.217663	0.187543
C	1.477970	-0.071765	0.145390
C	1.061857	1.136709	-0.480883
H	-0.512595	1.099169	1.415543
H	-1.612260	2.054056	0.291288
H	0.512595	1.099169	-1.415543
H	1.612260	2.054056	-0.291288
H	-2.438761	-0.084626	-0.658055
H	-1.140199	-2.152289	-0.515664
H	1.140199	-2.152289	0.515664
H	2.438761	-0.084625	0.658055

Fig3a-TS-1b

C	-1.137664	-1.200283	0.061503
C	-1.473455	0.124777	-0.193362

C	-0.698428	1.233148	0.162581
C	0.700455	1.232333	0.161508
C	1.473775	0.122608	-0.193684
C	1.135616	-1.201648	0.062474
H	-1.632289	-1.978723	-0.518503
H	-0.931371	-1.491002	1.078524
H	0.928082	-1.490417	1.079816
H	1.629657	-1.981638	-0.515930
H	-2.311835	0.327822	-0.861036
H	-1.170471	2.213063	0.117189
H	1.173637	2.211637	0.114951
H	2.312797	0.323654	-0.861135

Fig3a-14

C	-1.190663	-0.725139	0.249175
C	0.112021	-1.420130	-0.063295
C	1.255481	-0.725911	-0.108276
C	1.255468	0.725976	0.108254
C	0.111956	1.420121	0.063299
C	-1.190699	0.725085	-0.249181
H	-1.339337	-0.740009	1.340830
H	-2.036110	-1.269656	-0.184268
H	-1.339394	0.739998	-1.340834
H	-2.036175	1.269540	0.184283
H	0.111545	-2.499515	-0.191447
H	2.203394	-1.226189	-0.287706
H	2.203324	1.226328	0.287752
H	0.111366	2.499498	0.191526

Fig3b-15

C	0.670009	1.917537	-0.019032
C	-0.669949	1.917639	0.019214
H	-1.161124	2.889891	-0.000931
H	1.161270	2.889782	0.000353
C	1.590636	0.763372	-0.098917
C	2.792621	0.793233	0.617191
C	1.325491	-0.345961	-0.911833
C	3.689964	-0.267709	0.552245
H	3.020168	1.656182	1.238316
C	2.223656	-1.403815	-0.981621
H	0.409490	-0.373008	-1.493313
C	3.406538	-1.371973	-0.246049
H	4.613403	-0.229341	1.122714
H	2.001585	-2.255143	-1.618418
H	4.107288	-2.199688	-0.302496
C	-1.590629	0.763462	0.099037
C	-1.325817	-0.345596	0.912360
C	-2.792300	0.793134	-0.617669
C	-2.224028	-1.403455	0.982062
H	-0.410019	-0.372451	1.494171
C	-3.689654	-0.267781	-0.552800
H	-3.019511	1.655896	-1.239165
C	-3.406560	-1.371814	0.245967
H	-2.002235	-2.254599	1.619198
H	-4.612843	-0.229640	-1.123690
H	-4.107335	-2.199516	0.302345

Fig3b-TS-2a

C	0.674937	2.155073	-0.077996
C	-0.674963	2.155070	0.077914

H	-1.218733	3.097101	0.089863
H	1.218683	3.097118	-0.089899
C	1.435023	0.922637	-0.202732
C	2.755555	0.834661	0.208152
C	0.700866	-0.294337	-0.599625
C	3.426410	-0.392531	0.261907
H	3.267650	1.740316	0.525767
C	1.463546	-1.530069	-0.579472
C	2.757853	-1.573660	-0.125217
H	4.457374	-0.434512	0.597886
H	0.975164	-2.436242	-0.927392
H	3.289606	-2.520896	-0.099945
C	-1.435027	0.922626	0.202722
C	-0.700834	-0.294347	0.599562
C	-2.755592	0.834645	-0.208057
C	-1.463496	-1.530090	0.579393
H	-0.081167	-0.176080	1.491796
C	-3.426445	-0.392550	-0.261789
H	-3.267711	1.740302	-0.525626
C	-2.757836	-1.573682	0.125233
H	-0.975075	-2.436272	0.927243
H	-4.457408	-0.434540	-0.597768
H	-3.289576	-2.520925	0.099974
H	0.081207	-0.176051	-1.491863

Fig3b-TS-2b

C	0.798291	2.059716	0.365757
C	-0.587415	2.133545	0.180663
H	-0.982690	3.065170	-0.219612
H	1.369610	2.958574	0.140560

C	1.494658	0.846027	0.375374
C	2.713990	0.769386	-0.370125
C	0.894866	-0.397620	0.868991
C	3.187093	-0.419197	-0.837360
H	3.202103	1.700637	-0.648133
C	1.406824	-1.630485	0.270990
C	2.481613	-1.633152	-0.553331
H	4.076090	-0.448166	-1.459676
H	0.926975	-2.566126	0.544504
H	2.847075	-2.568161	-0.968778
C	-1.392760	0.997514	0.154794
C	-0.994518	-0.160820	0.945825
C	-2.489307	0.884966	-0.753868
C	-1.723148	-1.402213	0.698964
H	-0.947176	0.094291	2.000441
C	-3.101427	-0.311960	-0.971893
H	-2.786321	1.766769	-1.316470
C	-2.693663	-1.477983	-0.242358
H	-1.472318	-2.272841	1.299849
H	-3.901632	-0.393201	-1.701074
H	-3.209447	-2.417646	-0.419734
H	0.907150	-0.465648	1.953579

Fig3b-16

C	-0.003130	0.720627	2.065670
C	0.003130	-0.720627	2.065670
H	-0.053794	-1.246101	3.016183
H	0.053794	1.246101	3.016183
C	-0.106345	1.427558	0.916119
C	-0.116180	2.877067	0.901965

C	-0.324954	0.696668	-0.400788
C	0.003130	3.566622	-0.249977
H	-0.170251	3.395364	1.856450
C	0.090467	1.532947	-1.587681
C	0.192213	2.866230	-1.513969
H	0.020948	4.652351	-0.242648
H	0.259566	1.031459	-2.536320
H	0.446073	3.446676	-2.396581
C	0.106345	-1.427558	0.916119
C	0.324954	-0.696668	-0.400788
C	0.116180	-2.877067	0.901965
C	-0.090467	-1.532947	-1.587681
H	1.421755	-0.538349	-0.485108
C	-0.003130	-3.566622	-0.249977
H	0.170251	-3.395364	1.856450
C	-0.192213	-2.866230	-1.513969
H	-0.259566	-1.031459	-2.536320
H	-0.020948	-4.652351	-0.242648
H	-0.446073	-3.446676	-2.396581
H	-1.421755	0.538349	-0.485108

Fig3b-17

C	0.899872	2.002708	0.117873
C	-0.508361	2.063553	-0.213863
H	-0.884816	2.960942	-0.698925
H	1.504434	2.896744	-0.019667
C	1.512434	0.825705	0.380139
C	2.952732	0.634520	0.247224
C	0.726993	-0.447828	0.584389
C	3.407133	-0.514748	-0.296123

H	3.626038	1.459649	0.466364
C	1.171393	-1.479959	-0.429664
C	2.467161	-1.527243	-0.774462
H	4.468687	-0.654870	-0.477950
H	0.458178	-2.212203	-0.796575
H	2.836182	-2.304525	-1.437801
C	-1.316438	0.991476	-0.047303
C	-0.793581	-0.171269	0.774019
C	-2.664799	0.927448	-0.566579
C	-1.632107	-1.414031	0.678783
H	-0.866255	0.177277	1.819412
C	-3.390901	-0.207443	-0.500312
H	-3.062126	1.811580	-1.059589
C	-2.842626	-1.414894	0.104662
H	-1.235834	-2.317137	1.138228
H	-4.389063	-0.244603	-0.926268
H	-3.439490	-2.322462	0.083560
H	1.050637	-0.858359	1.556505

Fig5-TS-3a

C	2.328727	-1.702195	0.351332
C	3.286400	-0.854631	-0.222505
C	3.166733	0.510311	-0.423628
C	1.056861	-1.402511	0.798074
C	2.076736	1.361531	-0.215180
C	0.313445	-0.207665	0.679205
C	0.774537	1.084392	0.214154
H	2.649853	-2.729403	0.514135
H	4.238312	-1.305817	-0.487727
H	4.050854	1.001835	-0.825401

H	0.522583	-2.207293	1.295119
H	2.250683	2.401412	-0.483829
H	-0.565784	-0.168321	1.313029
C	-0.193499	2.154406	0.246846
C	-1.538064	1.925698	0.117592
H	0.180385	3.168996	0.359628
C	-2.056942	0.658453	-0.268019
C	-3.148842	0.001891	0.337808
C	-1.283029	-0.347414	-0.962175
C	-3.057083	-1.368153	0.048693
C	-1.939611	-1.576650	-0.777187
H	-3.745410	-2.132658	0.389981
H	-1.659176	-2.517122	-1.237496
H	-2.230363	2.738906	0.334391
H	-3.867753	0.467186	1.003373
H	-0.542397	-0.142498	-1.725274

Fig5-TS-3b

C	-2.206304	-1.790350	-0.050925
C	-3.101831	-0.936733	-0.721102
C	-3.106396	0.442082	-0.744854
C	-1.166529	-1.439232	0.782698
C	-2.137299	1.332400	-0.248127
C	-0.590122	-0.179575	1.037989
C	-0.932867	1.085331	0.392044
H	-2.426866	-2.852783	-0.115744
H	-3.916759	-1.427211	-1.248391
H	-3.933634	0.909277	-1.273275
H	-0.710040	-2.256314	1.336977
H	-2.321741	2.381659	-0.476728

C	0.036105	2.139150	0.416230
C	1.375406	1.909117	0.211561
H	-0.328491	3.156604	0.294770
C	2.019625	0.650212	0.090358
C	2.854136	0.316350	-0.983242
C	1.721535	-0.598003	0.809951
C	3.030242	-1.081134	-0.986825
C	2.373512	-1.634808	0.113992
H	3.596592	-1.634609	-1.728705
H	2.442297	-2.665051	0.443256
H	1.958086	2.776447	-0.099713
H	3.166883	0.998683	-1.765826
H	-0.177089	-0.043712	2.026170
H	1.635487	-0.631840	1.888714

Fig6-TS-4

C	3.589482	1.385436	0.206534
C	4.130640	0.167677	0.411633
C	3.463443	-1.118708	0.380214
C	2.207341	1.705822	-0.091375
C	2.188666	-1.424290	0.068466
C	1.155811	0.893327	-0.316048
C	1.069249	-0.571126	-0.342966
H	4.254332	2.242443	0.285807
H	5.193122	0.130084	0.640814
H	4.098899	-1.962214	0.641740
H	1.994709	2.771796	-0.140814
H	1.931375	-2.481676	0.114441
H	0.206731	1.388492	-0.509202
C	-0.085559	-1.170522	-0.717601

C	-1.306195	-0.475442	-1.177257
H	-0.134967	-2.259183	-0.708889
C	-2.361260	-0.179139	-0.399352
C	-3.605427	0.479217	-0.831751
C	-2.507856	-0.428793	1.042868
C	-4.404143	0.603281	0.247789
C	-3.716795	0.036885	1.419898
H	-5.393753	1.044620	0.270259
H	-4.132547	0.010804	2.420520
H	-1.358632	-0.203356	-2.234177
H	-3.811221	0.792169	-1.847911
H	-1.752422	-0.895735	1.661093

Fig6-TS-5a

C	1.871703	-1.830231	-0.381773
C	3.042540	-1.110820	0.077755
C	3.163993	0.211844	0.328935
C	0.654583	-1.361447	-0.720049
C	2.162343	1.248981	0.247408
C	0.144367	0.010454	-0.695301
C	0.878437	1.180013	-0.183763
H	2.018318	-2.900224	-0.513786
H	3.931123	-1.721040	0.219558
H	4.141970	0.554537	0.659935
H	-0.071603	-2.076256	-1.098975
H	2.491704	2.228819	0.588468
H	-0.407379	0.242177	-1.601899
C	-0.027504	2.333804	-0.112848
C	-1.332942	2.046176	0.008114
H	0.361356	3.347441	-0.094397

C	-1.748778	0.639844	0.098072
C	-2.848846	0.024255	-0.542284
C	-1.209375	-0.346984	1.042636
C	-2.953930	-1.275793	-0.054860
C	-1.960894	-1.505810	0.926221
H	-3.686340	-2.006035	-0.382842
H	-1.808896	-2.420719	1.483546
H	-2.089511	2.824814	0.053104
H	-3.464101	0.480776	-1.307650
H	-0.430814	-0.140009	1.765365

Fig6-TS-5b

C	-1.694776	-1.936591	0.193562
C	-2.960266	-1.337822	0.325089
C	-3.325387	-0.022506	0.097398
C	-0.574915	-1.395661	-0.411321
C	-2.486251	1.080774	-0.137602
C	-0.375936	-0.078418	-0.839603
C	-1.118435	1.086039	-0.350442
H	-1.632795	-2.986034	0.470062
H	-3.760888	-2.000817	0.645839
H	-4.376786	0.213012	0.243019
H	0.254510	-2.069860	-0.631240
H	-2.954756	2.059689	-0.035572
H	0.187705	0.063039	-1.747696
C	-0.321105	2.196784	0.048502
C	0.934304	1.906404	0.522949
H	-0.804661	3.138965	0.294816
C	1.626412	0.680564	0.254840
C	2.154658	-0.199961	1.273738

C	2.267295	0.270754	-0.993810
C	2.941736	-1.138173	0.663114
C	3.038132	-0.827162	-0.746527
H	3.422237	-1.980137	1.149140
H	3.641814	-1.362459	-1.469528
H	1.337550	2.567813	1.291024
H	1.881216	-0.161190	2.321301
H	2.172068	0.807835	-1.930489

Fig6-TS-6a

C	-2.080495	-1.455199	0.558642
C	-2.775159	-0.768443	-0.381806
C	-2.654821	0.631147	-0.695179
C	-1.066355	-0.949617	1.444484
C	-1.629563	1.468314	-0.415205
C	-0.339659	0.185520	1.316267
C	-0.361694	1.158673	0.231496
H	-2.357269	-2.496122	0.711289
H	-3.555596	-1.305262	-0.915737
H	-3.480152	1.053018	-1.265168
H	-0.844339	-1.570496	2.308481
H	-1.711449	2.490584	-0.783242
H	0.409464	0.379805	2.077637
C	0.664475	2.186988	0.234065
C	1.944462	1.713145	0.198114
H	0.393012	3.240942	0.227257
C	2.001301	0.351294	-0.220906
C	2.639236	-0.778747	0.290876
C	0.965069	-0.117614	-1.172168
C	1.985800	-1.904273	-0.245631

C	0.997031	-1.506372	-1.166854
H	2.222462	-2.932727	0.009338
H	0.412375	-2.165552	-1.795394
H	2.821307	2.302415	0.454899
H	3.381546	-0.789879	1.079740
H	0.570876	0.504376	-1.966262

Fig6-18

C	-3.169710	0.679741	-0.041510
C	-3.169641	-0.679822	-0.041521
C	-2.116924	-1.516935	-0.570292
C	-2.117070	1.516978	-0.570219
C	-0.807420	-1.201222	-0.609220
C	-0.807527	1.201385	-0.609129
C	-0.252000	0.000019	0.108045
H	-4.088050	1.181553	0.257303
H	-4.087942	-1.181724	0.257258
H	-2.430389	-2.462528	-1.009356
H	-2.430641	2.462523	-1.009314
H	-0.117894	-1.835601	-1.159972
H	-0.118063	1.835774	-1.159938
C	-0.405470	-0.000102	1.625736
H	-1.292180	-0.000157	2.248603
C	0.903887	-0.000108	1.862413
H	1.518379	-0.000164	2.756715
C	1.320917	-0.000015	0.395045
C	2.145324	1.174310	-0.059870
C	2.145294	-1.174287	-0.060055
H	1.863236	2.204524	0.122007
C	3.265270	0.735997	-0.655999

H	1.863177	-2.204524	0.121656
C	3.265249	-0.735907	-0.656120
H	4.059664	1.350834	-1.064280
H	4.059627	-1.350701	-1.064498

Fig6-19

C	3.109766	-1.186568	0.270676
C	3.301522	0.147934	0.408360
C	2.395043	1.202087	0.012258
C	1.965896	-1.831973	-0.345839
C	1.054401	1.094242	-0.088704
C	0.709167	-1.362033	-0.401151
C	0.242720	-0.124891	0.324284
H	3.934905	-1.839805	0.547764
H	4.269584	0.474462	0.784014
H	2.843318	2.171453	-0.200164
H	2.166049	-2.790850	-0.821518
H	-0.033843	-1.926903	-0.957136
C	0.124149	2.151253	-0.459526
H	0.440665	3.142534	-0.767370
C	-1.143468	1.743500	-0.335119
H	-2.031517	2.334492	-0.532119
C	-1.251981	0.282068	0.064645
C	-2.168645	0.077229	1.249419
C	-1.998118	-0.450197	-1.032273
H	-1.940254	0.465075	2.235572
C	-3.254289	-0.618414	0.879559
H	-1.646673	-0.489032	-2.056755
C	-3.152512	-0.937941	-0.552331
H	-4.083114	-0.905308	1.516849

H	-3.907268	-1.472768	-1.118167
H	0.386242	-0.281126	1.403490

Fig6-20

C	-0.754995	-0.121268	-0.702232
C	-2.136080	0.217339	-0.208368
C	-2.836497	-0.912568	0.014787
H	-3.842840	-0.994699	0.409461
C	-0.721755	-1.617319	-0.619035
H	0.113388	-2.230299	-0.929799
C	-1.952017	-2.049749	-0.270610
H	-2.260881	-3.088052	-0.204842
C	-2.148019	1.623354	0.163317
H	-3.032717	2.219293	0.357704
C	-0.878918	2.042360	0.279832
C	2.718768	-0.671041	-0.590866
C	2.324373	-1.215972	0.584820
C	1.514456	-0.570730	1.594763
C	2.414210	0.668607	-1.045285
C	0.612693	0.410076	1.409956
C	1.345256	1.411823	-0.708426
C	0.141309	0.923331	0.062244
H	3.417684	-1.239801	-1.200895
H	2.727601	-2.192249	0.846618
H	1.670417	-0.916604	2.615109
H	3.152516	1.122179	-1.704674
H	0.141401	0.850182	2.285861
H	1.309393	2.444950	-1.051851
H	-0.687125	0.149886	-1.768104
H	-0.565533	3.045763	0.556032

Fig8-21

C	1.145137	-0.399744	-0.084078
C	1.971959	0.712461	0.096047
C	1.426303	1.994819	0.121368
C	0.056094	2.126131	-0.030544
C	-0.800376	1.018370	-0.176869
C	-0.243899	-0.287439	-0.210405
C	2.001512	-1.641954	-0.089062
C	3.389197	-1.090212	0.113933
C	3.357267	0.247043	0.216303
H	2.055415	2.871278	0.248050
H	-0.386972	3.118998	-0.029437
H	4.210439	0.900069	0.363767
H	4.274181	-1.713893	0.162571
C	-2.229973	1.298030	-0.368148
C	-1.024855	-1.506347	-0.459286
H	-0.510692	-2.285688	-1.019223
H	-2.456092	2.243786	-0.858317
C	-2.278420	-1.740377	-0.056562
C	-3.252035	0.527344	0.020527
H	-2.759104	-2.672998	-0.343068
C	-3.061564	-0.761393	0.780295
H	-4.267008	0.840604	-0.212557
H	1.715390	-2.343503	0.705705
H	1.924256	-2.197017	-1.034705
H	-4.027214	-1.185727	1.066550
H	-2.510670	-0.556310	1.709538

Fig9a-s-trans-22

C	-1.851541	0.200775	0.000111
C	-0.529988	0.490372	0.000448
C	0.530021	-0.489413	0.000471
H	-0.239036	1.538579	0.000702
C	1.851600	-0.200811	0.000197
C	2.932336	-1.196036	0.000212
C	2.506509	1.116580	-0.000239
C	4.108654	-0.535591	-0.000114
C	3.840533	0.911492	-0.000406
H	5.097663	-0.977871	-0.000154
H	4.606693	1.677852	-0.000731
H	0.237980	-1.537332	0.000733
H	2.773972	-2.267209	0.000493
H	1.998382	2.071648	-0.000440
C	-2.506354	-1.116722	-0.000464
C	-3.840408	-0.911763	-0.000197
H	-1.998139	-2.071782	-0.000871
C	-4.108845	0.535340	-0.000127
H	-4.606279	-1.678427	-0.000401
C	-2.932421	1.195842	0.000170
H	-5.098039	0.977140	-0.000103
H	-2.773778	2.267013	0.000404

Fig9a-s-cis-22

C	-1.601933	0.554464	-0.034384
C	-0.697889	1.541403	-0.209380
C	0.697888	1.541403	0.209381
H	-1.048364	2.466894	-0.667373
C	1.601933	0.554465	0.034384
C	1.454300	-0.724341	-0.681878

C	2.993459	0.599811	0.510596
C	2.637051	-1.369823	-0.614006
C	3.597852	-0.546929	0.138483
H	2.866788	-2.333191	-1.053809
H	4.623170	-0.831335	0.343471
H	1.048363	2.466894	0.667374
H	0.554028	-1.048164	-1.185337
H	3.417035	1.418288	1.079224
C	-1.454299	-0.724342	0.681876
C	-2.637051	-1.369824	0.614006
H	-0.554026	-1.048167	1.185332
C	-3.597853	-0.546929	-0.138480
H	-2.866788	-2.333192	1.053808
C	-2.993459	0.599811	-0.510596
H	-4.623171	-0.831333	-0.343467
H	-3.417034	1.418288	-1.079225

Fig9a-TS-7a

C	-1.408733	0.737118	0.089880
C	-0.697858	1.918656	-0.058687
C	0.697999	1.918655	0.058792
H	-1.230515	2.842036	-0.274676
C	1.408832	0.737098	-0.089760
C	0.836615	-0.498702	-0.737149
C	2.696731	0.392949	0.371144
C	1.785241	-1.497380	-0.599322
C	2.896165	-0.955624	0.094225
H	1.721698	-2.496204	-1.009865
H	3.786749	-1.515110	0.362432
H	1.230621	2.842128	0.274469

H	0.089924	-0.452124	-1.520350
H	3.354036	1.037992	0.939933
C	-0.836816	-0.498680	0.737461
C	-1.785463	-1.497282	0.599407
H	-0.090242	-0.452181	1.520775
C	-2.896157	-0.955470	-0.094487
H	-1.722116	-2.496090	1.010020
C	-2.696531	0.393050	-0.371405
H	-3.786702	-1.514905	-0.362930
H	-3.353610	1.038129	-0.940415

Fig9a-TS-7b

C	-0.830720	-1.286973	-0.000080
C	-2.173573	-0.660550	-0.000142
C	-2.166575	0.681406	0.000207
H	-3.093127	-1.240255	-0.000561
C	-0.817225	1.293619	0.000523
C	0.031602	1.266449	1.115944
C	0.031027	1.267482	-1.115362
C	1.412154	1.499602	0.675823
C	1.411758	1.500545	-0.675951
H	2.262962	1.617086	1.334385
H	2.262243	1.618571	-1.334831
H	-3.080032	1.270652	0.000387
H	-0.296309	1.273642	2.149267
H	-0.297825	1.273581	-2.148383
C	0.018237	-1.267920	1.115469
C	1.396803	-1.512384	0.675625
H	-0.309759	-1.270673	2.148777
C	1.396664	-1.512528	-0.676196

H	2.245857	-1.641173	1.334336
C	0.018180	-1.267500	-1.115756
H	2.245945	-1.639395	-1.334988
H	-0.309955	-1.269513	-2.149017

Fig9b-s-trans-23

C	4.855360	-0.912104	-0.187430
C	5.051246	0.407876	-0.383651
C	4.093730	1.480779	-0.207155
C	3.642276	-1.565770	0.262366
C	2.761829	1.415232	0.000103
C	2.393063	-1.073225	0.391722
C	1.866797	0.264022	0.106477
H	5.706825	-1.570564	-0.343480
H	6.047570	0.721975	-0.686915
H	4.514450	2.481524	-0.277743
H	3.767894	-2.612423	0.532695
H	2.249436	2.373921	0.075683
H	1.657033	-1.772631	0.779645
C	0.522878	0.494952	0.023061
C	-0.522852	-0.494868	0.023059
H	0.220502	1.531415	-0.112258
H	-0.220392	-1.531304	-0.112310
C	-1.866774	-0.263987	0.106468
C	-2.761782	-1.415223	0.000026
C	-2.393079	1.073283	0.391604
C	-4.093689	-1.480812	-0.207188
H	-2.249352	-2.373894	0.075580
C	-3.642322	1.565768	0.262283
H	-1.657051	1.772766	0.779393

C	-5.051260	-0.407953	-0.383563
H	-4.514376	-2.481570	-0.277773
H	-3.767963	2.612443	0.532521
H	-6.047604	-0.722089	-0.686728
C	-4.855425	0.912028	-0.187351
H	-5.706946	1.570438	-0.343306

Fig9b-s-cis-23

C	-3.994285	-1.076884	0.260814
C	-3.025681	-1.851537	-0.272244
C	-1.798276	-1.410499	-0.902219
C	-4.024603	0.368895	0.339346
C	-1.203927	-0.201239	-0.852211
C	-3.021254	1.253025	0.159447
C	-1.609364	1.016422	-0.145169
H	-4.878161	-1.580875	0.645819
H	-3.196245	-2.925913	-0.281866
H	-1.284724	-2.170182	-1.487953
H	-4.990224	0.791035	0.610144
H	-0.276282	-0.096084	-1.411033
H	-3.276531	2.303164	0.299130
C	-0.717845	2.020222	0.098681
C	0.717842	2.020223	-0.098677
H	-1.133193	2.968418	0.442539
H	1.133191	2.968420	-0.442531
C	1.609362	1.016421	0.145169
C	3.021252	1.253026	-0.159447
C	1.203925	-0.201242	0.852206
C	4.024602	0.368898	-0.339345
H	3.276527	2.303165	-0.299132

C	1.798277	-1.410501	0.902215
H	0.276277	-0.096090	1.411024
C	3.994289	-1.076881	-0.260811
H	4.990222	0.791040	-0.610144
H	1.284723	-2.170186	1.487946
H	4.878167	-1.580871	-0.645812
C	3.025686	-1.851536	0.272245
H	3.196253	-2.925911	0.281869

Fig9b-TS-8a

C	3.735010	-1.155051	-0.146876
C	2.628490	-1.900068	0.263593
C	1.405623	-1.416398	0.718174
C	3.863653	0.226053	-0.250902
C	0.841280	-0.139945	0.655792
C	2.874089	1.201335	-0.116786
C	1.504508	1.088595	0.129974
H	4.630429	-1.729589	-0.377335
H	2.772688	-2.975771	0.329955
H	0.751688	-2.163927	1.168930
H	4.851185	0.594993	-0.516120
H	0.107067	0.070042	1.434705
H	3.211999	2.221568	-0.302454
C	0.696634	2.228324	-0.029163
C	-0.696699	2.228417	0.029273
H	1.200054	3.186270	-0.148070
H	-1.200022	3.186422	0.148195
C	-1.504644	1.088738	-0.130320
C	-2.874257	1.201343	0.116419
C	-0.841355	-0.139897	-0.655806

C	-3.863776	0.225898	0.250616
H	-3.212202	2.221561	0.302081
C	-1.405454	-1.416397	-0.717783
H	-0.106892	0.070013	-1.434498
C	-3.734935	-1.155237	0.146949
H	-4.851373	0.594716	0.515770
H	-0.751537	-2.163866	-1.168661
H	-4.630259	-1.729889	0.377499
C	-2.628250	-1.900156	-0.263223
H	-2.772335	-2.975873	-0.329583

Fig9b-TS-8b

C	3.551402	-1.349919	-0.198138
C	2.473734	-1.824578	-0.930556
C	1.315714	-1.011976	-0.944617
C	3.775922	-0.000762	0.270146
C	1.083516	-0.337116	0.247528
C	2.942768	1.097849	0.320292
C	1.507235	1.078777	0.253007
H	4.439704	-1.980658	-0.164793
H	2.614042	-2.684525	-1.584335
H	0.809025	-0.738194	-1.869291
H	4.824723	0.209913	0.473716
H	1.451121	-0.872598	1.126702
H	3.418876	2.076558	0.382115
C	0.731573	2.198029	0.040017
C	-0.660833	2.180822	-0.231171
H	1.251320	3.146215	-0.086709
H	-1.076995	3.052406	-0.733622
C	-1.507484	1.122179	0.033127

C	-2.820793	1.127585	-0.519359
C	-1.044462	0.080534	0.970634
C	-3.725459	0.107518	-0.665158
H	-3.117683	2.082689	-0.953268
C	-1.581334	-1.165611	1.192936
C	-3.603937	-1.247243	-0.263902
H	-4.640956	0.356671	-1.195791
H	-1.094501	-1.741774	1.978079
H	-4.403406	-1.903809	-0.601954
C	-2.650853	-1.822216	0.538775
H	-2.782543	-2.874109	0.779397
H	-0.412985	0.467980	1.768395

Fig10-24

C	3.043646	1.066015	0.676679
C	3.043629	1.066037	-0.676681
C	2.225320	0.281940	-1.577455
C	2.225345	0.281875	1.577441
C	1.266671	-0.644992	-1.262400
C	1.266702	-0.645032	1.262380
C	0.799552	-1.097966	-0.000027
H	3.745357	1.740378	1.163097
H	3.745330	1.740419	-1.163087
H	2.395533	0.459364	-2.635852
H	2.395581	0.459264	2.635842
H	0.771932	-1.110463	-2.114011
H	0.771975	-1.110537	2.113979
C	-0.272467	-2.137476	-0.000026
C	-1.570200	-1.832205	-0.000002
H	0.027115	-3.187133	-0.000030

C	-2.053633	-0.438802	0.000009
C	-2.330321	0.358662	-1.166243
C	-2.330281	0.358656	1.166272
C	-2.745918	1.585689	-0.736897
C	-2.745802	1.585717	0.736945
H	-3.024839	2.429637	-1.356207
H	-3.024653	2.429678	1.356267
H	-2.318875	-2.625565	0.000003
H	-2.208989	0.023132	-2.187579
H	-2.208918	0.023121	2.187603

Fig11-SOSP

C	2.422721	-1.560218	0.453647
C	3.197409	-0.738823	-0.300915
C	2.939152	0.641519	-0.585812
C	1.166575	-1.269612	1.072689
C	1.840881	1.400370	-0.337785
C	0.325523	-0.211489	0.893802
C	0.537230	1.049653	0.205550
H	2.805090	-2.563191	0.633397
H	4.133526	-1.136775	-0.683028
H	3.756202	1.163390	-1.081099
H	0.783180	-2.050739	1.723622
H	1.907802	2.435516	-0.667477
H	-0.586974	-0.247906	1.480926
C	-0.385705	2.104673	0.296618
C	-1.755509	1.817015	0.337595
H	-0.017541	3.126196	0.246152
C	-2.090089	0.578870	-0.165829
C	-3.129666	-0.337489	0.210075

C	-1.081845	-0.175103	-0.917380
C	-2.741922	-1.584754	-0.216957
C	-1.512464	-1.479393	-0.958413
H	-3.286200	-2.506988	-0.043734
H	-1.039311	-2.292127	-1.496202
H	-2.488103	2.508840	0.746943
H	-3.975039	-0.099111	0.843680
H	-0.386384	0.251583	-1.624478

Fig15-s-trans-25

C	1.100147	0.177652	0.000006
C	-0.234578	0.421888	-0.000015
C	-1.289315	-0.555121	0.000041
H	-0.553056	1.465336	-0.000100
C	-2.582469	-0.191608	-0.000042
C	-3.984011	-0.471069	-0.000061
C	-3.619154	0.797670	-0.000168
H	-1.043959	-1.612166	0.000150
C	1.791232	-1.111122	0.000085
C	3.124960	-0.867266	0.000148
H	1.309991	-2.081110	0.000112
C	3.347200	0.577316	0.000118
H	3.912037	-1.612877	0.000237
C	2.144530	1.201411	-0.000116
H	4.320796	1.053578	0.000166
H	1.955959	2.268658	-0.000259
H	-3.910100	1.836932	-0.000282
H	-4.782912	-1.196850	-0.000006

Fig15-s-cis-25

C	0.908858	0.560967	-0.063362
C	-0.086107	1.486830	-0.061420
C	-1.502599	1.307029	-0.276640
H	0.216409	2.515731	0.138342
C	-2.170293	0.169039	-0.017269
C	-2.247547	-1.173554	0.464504
C	-3.372297	-0.597253	0.080353
H	-2.082464	2.174986	-0.577098
C	0.874126	-0.851006	-0.443219
C	2.119334	-1.361460	-0.270878
H	0.022129	-1.362398	-0.871011
C	3.001570	-0.311370	0.230492
H	2.431068	-2.375834	-0.493730
C	2.290068	0.837032	0.334797
H	4.051136	-0.444044	0.465638
H	2.643197	1.800551	0.683275
H	-1.731871	-2.038655	0.852022
H	-4.440265	-0.667863	-0.061591

Fig15-TS-9a

C	0.628259	0.847057	0.300282
C	-0.477123	1.733650	0.166132
C	-1.778046	1.264125	0.101165
H	-0.300180	2.807955	0.109794
C	-1.879905	-0.113787	-0.152255
C	-0.961578	-1.094030	-0.588765
C	-2.254546	-1.420231	-0.214171
H	-2.648458	1.902055	0.193831
C	0.561561	-0.472085	0.892082
C	1.719308	-1.165459	0.491741

H	-0.048431	-0.728370	1.751071
C	2.436208	-0.365245	-0.413854
H	2.018413	-2.146137	0.844468
C	1.793731	0.877968	-0.500500
H	3.347034	-0.644280	-0.929555
H	2.083460	1.698622	-1.148507
H	-2.987468	-2.177082	0.018458
H	-0.191586	-1.264538	-1.330705

Fig15-TS-9b

C	-0.706931	0.711176	-0.313980
C	0.356973	1.636026	-0.298094
C	1.711257	1.362544	-0.166632
H	0.075417	2.678656	-0.149962
C	2.024239	0.017368	0.041816
C	1.502777	-1.275757	-0.234646
C	2.404943	-1.052595	0.787448
H	2.395948	2.145044	0.138737
C	-0.686685	-0.718797	-0.668350
C	-1.882747	-1.268336	-0.160950
H	-0.302935	-1.040050	-1.629148
C	-2.589772	-0.274707	0.522420
H	-2.230635	-2.278381	-0.346076
C	-1.899829	0.939887	0.397708
H	-3.521509	-0.413481	1.059324
H	-2.159839	1.871965	0.888637
H	2.961392	-1.437323	1.629392
H	1.376816	-1.987278	-1.031343

Fig16-s-cis-26

C	-2.722910	0.363818	0.020586
C	-1.373604	0.207611	-0.111423
C	-0.708811	-1.063350	-0.149323
C	0.625604	-1.312072	-0.141133
C	1.654293	-0.310079	-0.025740
C	2.977272	-0.577148	-0.052503
H	-0.785008	1.113317	-0.219326
H	-1.348853	-1.943189	-0.226458
H	0.958140	-2.343963	-0.226084
H	1.348767	0.726020	0.101389
C	3.958978	0.448092	0.075948
N	4.763552	1.279638	0.178917
N	-3.365025	1.567676	-0.214003
H	-4.072199	1.809092	0.468602
H	-2.754027	2.341118	-0.434883
N	-3.610217	-0.626336	0.402056
H	-4.464802	-0.663200	-0.138021
H	-3.211370	-1.535328	0.581206
H	3.346246	-1.591945	-0.173686

Fig16-TS-10a

C	-0.002731	1.179604	0.131210
C	-1.426226	1.181701	-0.300054
C	-2.224829	0.089492	-0.264885
C	-1.877820	-1.257401	0.149106
C	-0.603841	-1.750822	0.102922
C	0.425659	-1.107840	-0.643067
H	0.166592	-0.674165	-1.603672
H	-1.842729	2.167357	-0.486645
H	-3.275443	0.272290	-0.487234

H	-2.684760	-1.863597	0.551153
H	-0.374272	-2.657316	0.666118
C	1.763977	-1.037121	-0.263732
N	2.842299	-0.746178	0.102467
N	0.929007	1.772070	-0.637049
H	0.706333	1.815786	-1.621682
H	1.899233	1.524672	-0.440463
N	0.264223	1.022881	1.439423
H	1.233251	0.851194	1.692388
H	-0.402046	0.436696	1.927151

Fig16-TS-10b

C	0.438754	-1.021599	0.424228
C	-0.577318	-1.864899	-0.056985
C	-1.887885	-1.441690	0.000957
C	-2.242240	-0.066738	-0.049561
C	-1.461214	1.053813	-0.223176
C	-0.037533	1.260884	-0.018880
H	-0.337363	-2.815322	-0.532783
H	-2.689792	-2.150094	-0.186489
H	-3.303097	0.111761	-0.223798
H	-1.922925	1.874063	-0.773068
H	0.258744	-0.580493	1.393297
C	1.806714	-1.112510	0.064548
N	2.924528	-1.029528	-0.254810
N	0.689510	1.686016	-1.093718
N	0.434295	1.707422	1.199129
H	1.632839	2.011557	-0.930754
H	0.582334	1.137433	-1.933651
H	1.400082	1.481855	1.415141

H -0.194825 1.538310 1.971099

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