

Supporting information for

Predicting Pathways for Terpene Formation from First Principles – Routes to Known and New Sesquiterpenes

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Tables S1-S69: Cartesian coordinates of critical points (in Å).

Figures S1-S33: Sketches of IRC paths

Complete citation of Ref 12

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Table S1. Cartesian coordinate of **A1**.

C	3.22803543	0.13792122	0.54760424
H	3.89456607	0.79129908	-0.02353523
H	3.11122300	0.57845897	1.54089939
H	3.67905585	-0.85102261	0.62637836
C	1.88635808	0.11647146	-0.31034154
C	1.09017231	-0.53484671	0.72011770
C	1.09036591	-1.97285042	1.08639912
H	1.72985984	-2.10026500	1.97374565
C	-0.37229622	-2.33390914	1.38414284
H	-0.49187998	-3.41997605	1.42270010
C	-1.19834895	-1.70020565	0.27526910
C	-1.85111497	-0.53593968	0.51067406
C	-2.64857742	0.29588028	-0.44659329
H	-2.42440753	0.03128577	-1.48274073
H	-3.71292553	0.06386656	-0.30778534
C	-2.44879929	1.80374440	-0.20407404
C	-0.99706043	2.21811267	-0.08625025
C	1.41923454	1.57050270	-0.58045031
H	1.69454584	2.20823042	0.26373140
H	1.97187010	1.94022275	-1.45165456
C	-1.24426969	-2.45608816	-1.01761870
H	-1.91383641	-3.31692311	-0.90403383
H	-1.61735419	-1.86239050	-1.85187688
H	-0.26671812	-2.86403607	-1.29162787
H	0.62391211	0.13570737	1.44316174
C	2.13072720	-0.66644861	-1.59911295
H	2.90358040	-0.16191287	-2.18221693
H	1.22482863	-0.70443377	-2.20726268
H	2.46959528	-1.68793933	-1.41939741
H	-1.83459591	-0.15710904	1.53395261
H	-0.66920316	-1.93524850	2.35809367
H	1.50672537	-2.59197217	0.29111195
C	-0.06249316	1.56303951	-0.79005636
H	-0.40442584	0.82700053	-1.51497123
C	-0.72261341	3.32659369	0.88677827
H	-1.33694615	4.19728564	0.63339449
H	-1.00603463	3.04198067	1.90697411
H	0.31634388	3.65740287	0.89293215
H	-2.95673041	2.08020451	0.72705254
H	-2.95646384	2.37134753	-0.99221666
H	-2.95646384	2.37134753	-0.99221666

Table S2. Cartesian coordinate of **A2**.

C	2.99485223	-0.70972467	-1.45751749
H	3.57330519	-1.61447995	-1.26097009
H	2.24354594	-0.94914723	-2.21186478
H	3.66989107	0.03999306	-1.87801647
C	2.33263703	-0.22559180	-0.16723063
C	1.87637436	1.14092464	-0.20816699
C	0.84227952	1.79329378	0.56061541
H	1.24339863	2.68707794	1.04790963
C	-0.24982964	2.30406217	-0.52347883
H	-0.29394672	3.38967896	-0.41306756
C	-1.55274035	1.61700182	-0.25217493
C	-1.90882673	0.59632916	-1.04956961
C	-2.93983346	-0.45577726	-0.81512420
H	-3.52272792	-0.25643838	0.08632092
H	-3.64984147	-0.51268483	-1.64695330
C	-2.21349836	-1.82787168	-0.69841455
H	-1.86211715	-2.12432220	-1.69134247
H	-2.93485447	-2.58468547	-0.37440727
C	-1.04203722	-1.74580308	0.25282404
C	0.19433779	-1.57962899	-0.24380076
C	1.45715655	-1.28900250	0.51817802
H	2.08138915	-2.18813429	0.60311816
H	1.23435424	-0.98240311	1.54330125
C	-2.30245560	2.08789379	0.96031359
H	-2.59210992	3.13716252	0.83930978
H	-3.21498357	1.51842916	1.13343697
H	-1.69786415	2.03399547	1.87334552
H	2.43565416	1.79236745	-0.88414502
C	3.50843078	0.21554716	0.85639385
H	4.04860801	-0.72825241	0.98405198
H	3.13333048	0.53779415	1.82748081
H	4.20832209	0.94604144	0.44843965
C	-1.38990414	-1.76814949	1.71089102
H	-1.83303093	-2.73597459	1.96856575
H	-0.53571328	-1.61949663	2.37254097
H	-2.14445718	-1.01139610	1.94941376
H	-1.27206978	0.40506839	-1.91384337
H	0.08446794	2.09816854	-1.54420559
H	0.30676824	-1.64379282	-1.32465830
H	0.37097755	1.14016823	1.29219425

Table S3. Cartesian coordinate of **A3**.

C	1.96686209	0.31351415	1.38522259
H	2.56148668	1.18534993	1.66745578
H	0.92010550	0.56744258	1.55000891
H	2.24869628	-0.50180168	2.05635874
C	2.25705333	-0.02996182	-0.07338606
C	1.63549410	-1.30443613	-0.57164500
C	0.60326171	-2.13784834	-0.12661259
H	0.41046550	-2.96809053	-0.80650115
C	-0.30219494	-2.09756370	1.07946754
H	-0.43338781	-3.13388087	1.40892354
C	-1.62322166	-1.47483510	0.62541771
C	-1.81946264	-0.18395059	0.92761236
C	-2.79708035	0.78973784	0.35142931
H	-3.72053349	0.31528782	0.01274390
H	-3.07957030	1.51904997	1.11561633
C	-2.14306012	1.52313885	-0.86349135
C	-0.68700070	1.84679115	-0.62503712
C	1.74755744	1.11536938	-1.03462626
H	2.10701945	2.05072804	-0.59847106
H	2.25565308	1.00724094	-1.99907972
C	-2.53016903	-2.33004034	-0.20970580
H	-2.83326746	-3.22133076	0.34989707
H	-3.43652929	-1.79776071	-0.49724161
H	-2.05473657	-2.68441381	-1.13203206
H	2.03205125	-1.61696400	-1.53997001
C	3.77744058	-0.19907229	-0.26822984
H	4.26927733	0.74693431	-0.03023448
H	4.03688726	-0.45793589	-1.29837239
H	4.18610399	-0.96367851	0.39705913
H	-1.08708695	0.27289703	1.58948217
H	0.13491324	-1.52875676	1.89711762
H	0.33333985	-1.08727024	-0.84883026
C	0.26180885	1.11886031	-1.24649905
H	-0.09782669	0.43821560	-2.02412269
C	-0.41120573	2.94784359	0.35363078
H	-0.84999592	3.88120672	-0.01446404
H	-0.88419868	2.75131035	1.32209758
H	0.65040839	3.12323582	0.52551045
H	-2.71454286	2.43349101	-1.07282740
H	-2.22854548	0.87581662	-1.74108136

Table S4. Cartesian coordinate of **B**.

C	2.16384800	0.45887387	1.27711079
H	2.84060181	1.30688924	1.14871947
H	1.18434185	0.85648085	1.55067652
H	2.53975543	-0.13177292	2.11771607
C	2.11648376	-0.38933093	-0.00004454
C	1.20297645	-1.62287936	0.29686352
C	-0.15854481	-1.86918184	-0.23154019
H	1.67758722	-2.50944863	-0.17377251
C	-1.17675541	-2.58669147	0.51428568
H	-1.67917365	-3.40971574	0.00946573
C	-1.92134925	-1.27214354	0.27406441
C	-1.60593847	-0.16732373	1.01312917
C	-2.23402569	1.18175702	0.88815881
H	-3.32420288	1.08075483	0.85134103
H	-1.99388521	1.76083819	1.78225334
C	-1.77684331	1.98016110	-0.37901547
C	-0.27664412	1.97633333	-0.52006160
C	1.69103687	0.47641995	-1.22146492
H	2.39223081	1.31688866	-1.26215515
H	1.86279407	-0.09626358	-2.13973831
C	-2.96981991	-1.31206975	-0.79783339
H	-3.80781584	-1.92601353	-0.45236176
H	-3.35123848	-0.32583245	-1.05424335
H	-2.59529782	-1.77875368	-1.71389305
H	1.22721875	-1.84039805	1.36845228
C	3.53154758	-0.92281201	-0.27027075
H	4.23527466	-0.09494729	-0.38808854
H	3.56692049	-1.52246575	-1.18517307
H	3.89059298	-1.54234527	0.55709762
H	-0.82638652	-0.28089791	1.76290040
H	-0.93123907	-2.81191406	1.54969563
H	-0.30103522	-1.77935361	-1.30494994
C	0.27049181	0.94739239	-1.18888255
H	-0.43524719	0.32287663	-1.73320274
C	0.46610104	3.08176920	0.16834730
H	0.13736690	4.04429702	-0.23817946
H	0.26211685	3.11538889	1.24468821
H	1.54468171	3.01479574	0.03258258
H	-2.18020209	2.99138665	-0.27679022
H	-2.23681563	1.53727549	-1.26559822

Table S5. Cartesian coordinate of **C**.

C	2.05930918	0.82794929	1.25918925
H	2.31882137	1.87069295	1.09298559
H	1.33229262	0.75491336	2.07071828
H	2.96769193	0.32364535	1.60420289
C	1.59524151	0.10601465	0.02410594
C	1.48946140	-1.40960991	0.22894838
C	0.40160935	-2.25732659	-0.46100639
H	0.83018113	-3.25531567	-0.59237426
C	-0.90897115	-2.43147705	0.33973590
H	-1.42678018	-3.31311862	-0.05043836
C	-1.81814075	-1.23300411	0.26884414
C	-1.65000986	-0.20926913	1.12041927
C	-2.25678681	1.15456996	0.99430911
H	-3.34739557	1.11450839	0.91347260
H	-2.03617366	1.74987030	1.88333274
C	-1.77703024	1.95018909	-0.27717011
C	-0.29600134	1.99429632	-0.41522635
C	1.80734934	0.70194517	-1.28471382
H	2.39013859	1.61652791	-1.33926059
H	1.94091556	0.04033070	-2.13615406
C	-2.81015422	-1.23546415	-0.85753004
H	-3.43551231	-2.13197530	-0.79454360
H	-3.47747750	-0.37294226	-0.85209259
H	-2.31717023	-1.28313788	-1.83740916
H	1.35514699	-1.54717461	1.30749884
C	2.88500248	-1.96217799	-0.14002927
H	3.70089003	-1.37415041	0.28678281
H	3.02065339	-1.99141008	-1.22434852
H	2.98208329	-2.98164939	0.23899988
H	-0.92626637	-0.33763188	1.92324413
H	-0.65182485	-2.65639628	1.38019545
H	0.20044066	-1.90746633	-1.48117270
C	0.33483800	0.86483250	-0.92323279
H	-0.31431194	0.09447571	-1.31066835
C	0.38477477	3.24108976	0.00513612
H	-0.10636935	4.08650619	-0.48917864
H	0.23641681	3.40576008	1.08055525
H	1.44796846	3.28043817	-0.21971446
H	-2.18801784	2.96026859	-0.22017421
H	-2.20227486	1.45664364	-1.15466860
H	-2.20227486	1.45664364	-1.15466860

Table S6. Cartesian coordinate of **D**.

C	3.64112902	0.70295822	0.59798435
H	4.37945243	1.27511541	0.02845295
H	3.32004710	1.32003800	1.44238162
H	4.14884068	-0.18017647	0.99835777
C	2.46738783	0.30885707	-0.28442653
C	1.22418989	-0.27675205	0.46248856
C	0.93453765	-1.75888040	0.55831922
H	1.63435636	-2.25961165	1.23334170
C	-0.49122555	-2.02379240	1.13746817
H	-0.66042670	-3.10669084	1.14428294
C	-1.52446451	-1.38222014	0.29263298
C	-2.10346700	-0.15664519	0.68987714
C	-3.16501657	0.56441435	-0.14614929
H	-3.81682935	-0.08039258	-0.73746998
H	-3.79777753	1.17888891	0.49474459
C	-2.13374546	1.39288021	-0.92947901
C	-0.99275513	1.08927497	0.05645345
C	1.53764871	1.47101877	-0.75090653
H	1.59579629	2.31520992	-0.05951934
H	1.65877755	1.84003807	-1.77180164
C	-1.87105602	-2.03610313	-0.98587227
H	-2.76665160	-2.64448285	-0.77876180
H	-2.15789312	-1.33539623	-1.77008181
H	-1.09701758	-2.71651375	-1.34109055
H	1.20925262	0.15893364	1.46969665
C	2.94172760	-0.54424180	-1.45774071
H	3.67206439	0.01411711	-2.04971206
H	2.13009227	-0.82996420	-2.13400043
H	3.43209499	-1.45914926	-1.11241900
H	-2.11490965	-0.02087259	1.77045870
H	-0.53858430	-1.65320202	2.16398698
H	1.03446295	-2.23910613	-0.41977866
C	0.31957162	0.55755529	-0.47243766
H	0.11629980	-0.02615135	-1.37852667
C	-0.87685438	2.11182912	1.16555941
H	-0.44146922	3.02094729	0.73725846
H	-1.85043321	2.38415029	1.57724539
H	-0.23079160	1.78117835	1.98090433
H	-2.35508649	2.45722305	-1.03439835
H	-1.92797968	0.98938725	-1.92369663

Table S7. Cartesian coordinate of E.

C	1.76793006	1.26000660	1.36513039
H	2.57845107	1.98225288	1.23760494
H	0.83559066	1.82088736	1.39415130
H	1.90778547	0.78278843	2.34040954
C	1.79926261	0.22029274	0.24042091
C	0.78157623	-0.92676816	0.56272388
C	0.87863685	-2.09505864	-0.45177715
H	1.67379475	-2.79174167	-0.18814174
C	-0.48394708	-2.77862461	-0.47292637
H	-0.80010249	-3.20110699	-1.43378560
C	-1.44729710	-1.78942140	0.02522750
C	-0.79894159	-0.72373923	0.76413785
C	-1.64606653	0.56235673	1.01177981
H	-2.56421921	0.26490578	1.53210492
H	-1.10192935	1.18461141	1.72437295
C	-1.99993882	1.39973594	-0.24202817
C	-0.69727976	1.94489540	-0.75697787
C	1.57517245	0.90605806	-1.15234154
H	2.10091199	1.86458930	-1.14804290
H	2.03063435	0.30634729	-1.94634056
C	-2.88918133	-1.96464008	-0.15274403
H	-3.17223660	-3.01898646	-0.18933101
H	-3.49903157	-1.40696644	0.55695586
H	-3.11053672	-1.55701726	-1.15339054
H	1.12880529	-1.30104049	1.53280770
C	3.20405798	-0.40770287	0.24248114
H	3.95102025	0.37440796	0.08267779
H	3.33834456	-1.14573746	-0.55207496
H	3.43225799	-0.88662883	1.20004435
H	-0.99473710	-1.27612682	1.73267244
H	-0.55130675	-3.63087506	0.22784473
H	1.10587462	-1.71574437	-1.45138309
C	0.10557905	1.03967472	-1.33532535
H	-0.38256293	0.12294114	-1.67815321
C	-0.31731595	3.33548193	-0.34924494
H	-0.93734624	4.04909453	-0.90393813
H	-0.50250352	3.53016006	0.71297175
H	0.72550577	3.56826894	-0.56514589
H	-2.70506746	2.18151943	0.05545776
H	-2.50365044	0.78005956	-0.99184639

Table S8. Cartesian coordinate of **E2**.

C	2.99118285	-0.00808412	0.41855858
H	3.75981752	0.45279616	-0.20712422
H	3.05722093	0.45511345	1.40766235
H	3.25230817	-1.06557584	0.51188644
C	1.61327189	0.21373734	-0.22734231
C	0.47344940	-0.15457227	0.79752669
C	0.74071982	-1.39526573	1.68155296
H	0.21785611	-1.27812722	2.63764858
C	0.12665138	-2.56779937	0.92246899
H	0.82515753	-2.98870498	0.17763606
C	-0.96560941	-1.99318560	0.13407588
C	-1.00173088	-0.54697707	0.26921792
C	-1.96895552	0.20156387	-0.67479120
H	-1.60187369	0.09516289	-1.69903252
H	-2.93066320	-0.32471684	-0.64505094
C	-2.20477996	1.69533212	-0.37514626
C	-0.86635441	2.34775332	-0.11141272
C	1.53263043	1.74790545	-0.55721080
H	1.83336561	2.30975311	0.33159356
H	2.25851467	1.97040969	-1.34555152
C	-1.89478835	-2.80362193	-0.65464339
H	-2.91796135	-2.64558620	-0.28655096
H	-1.91576488	-2.43765331	-1.68914775
H	-1.66361148	-3.86739724	-0.62956722
H	0.36070781	0.71327222	1.44761982
C	1.54752554	-0.61384230	-1.51677664
H	2.30880566	-0.27308479	-2.22362306
H	0.58333744	-0.53613473	-2.02782202
H	1.75394092	-1.67235398	-1.33180933
H	-1.51574645	-0.57664648	1.27041059
H	-0.19880207	-3.43720239	1.50721698
H	1.78996631	-1.55427717	1.91613180
C	0.12861354	2.02165712	-0.95009744
H	-0.15456034	1.57034829	-1.89912335
C	-0.71286414	3.09467465	1.17851811
H	-1.38221976	3.96261645	1.17558809
H	-1.00666084	2.49386911	2.04932721
H	0.29939843	3.46798545	1.33700103
H	-2.85381220	1.80737431	0.49946231
H	-2.75027389	2.13728809	-1.21586624

Table S9. Cartesian coordinate of **F**.

C	3.49402453	0.54381589	0.79466590
H	4.37168895	1.03894572	0.36917554
H	3.13267084	1.15985043	1.62339684
H	3.82422971	-0.41538848	1.20343391
C	2.42626964	0.34959215	-0.27205125
C	1.05217486	-0.12588440	0.27665210
C	0.57579517	-1.56875213	0.24282532
H	0.98091874	-2.05220634	1.14091419
C	-1.76451447	-2.21684318	1.34526139
H	-2.65764122	-2.78040392	1.09352748
C	-0.94448467	-1.70591241	0.18408313
C	-1.72888018	-0.74677738	1.05277878
C	-2.81200283	0.13963189	0.48860010
H	-3.61593369	-0.41946052	0.00523454
H	-3.27552433	0.73424191	1.28054221
C	-2.18339196	1.07373624	-0.59977884
C	-0.83129944	1.53685265	-0.20417844
C	1.73472804	1.63476770	-0.78603375
H	1.80978353	2.45777997	-0.07246665
H	2.03708014	1.99387519	-1.77251700
C	-1.46247456	-2.10621887	-1.18662986
H	-2.55303503	-2.08772506	-1.24171489
H	-1.07262841	-1.47615735	-1.99245783
H	-1.15021449	-3.13130865	-1.40684207
H	0.91424341	0.30388058	1.27246881
C	2.95452559	-0.50006042	-1.42368401
H	3.80700116	0.00312107	-1.88801483
H	2.20900489	-0.66688116	-2.20711757
H	3.29963025	-1.47646523	-1.07406721
H	-1.11216743	-0.20674688	1.77180077
H	-1.26724306	-2.55481174	2.24869090
H	1.01697775	-2.08901337	-0.61110143
C	0.34742275	0.96034232	-0.77831363
H	0.13266772	0.41582324	-1.69766619
C	-0.74765424	2.60828028	0.80372317
H	-0.69967697	3.55187940	0.23467726
H	-1.63654380	2.66455705	1.43319848
H	0.15913327	2.57363932	1.40892694
H	-2.82660450	1.95430118	-0.72385032
H	-2.13310485	0.53653490	-1.54640156

Table S10. Cartesian coordinate of **G**.

C	-3.54577643	0.00826380	-0.62882167
H	-4.20873195	0.64803427	-0.04073646
H	-3.44003695	0.46242095	-1.61913936
H	-4.04196112	-0.95905871	-0.75187053
C	-2.18544021	-0.14665781	0.06782296
C	-1.27591350	-0.94714478	-0.90504833
C	-0.18347617	-1.83548383	-0.37112483
C	0.77308767	-2.49935255	-1.20942348
H	1.07820653	-3.51696747	-0.98287992
C	1.49927073	-1.50054829	-0.23903346
C	1.81727353	-0.26420411	-0.75118237
C	2.86121618	0.66163222	-0.24409159
H	3.66652650	0.12429241	0.26100905
H	3.28665634	1.19506678	-1.09891371
C	2.20181199	1.68182957	0.73691950
C	0.80311714	2.01716922	0.26601598
C	-1.64135215	1.28178191	0.33287269
H	-1.77061912	1.87709121	-0.57565012
H	-2.28683395	1.74087009	1.09292777
C	2.18692521	-2.08695409	0.96667413
H	3.21807494	-2.35921086	0.72489875
H	2.20277447	-1.38643894	1.80375848
H	1.68425609	-2.99546916	1.30294326
H	-1.92009179	-1.68381365	-1.41104490
C	-2.39963212	-0.89996276	1.38520005
H	-3.15946347	-0.39171752	1.98403481
H	-1.49719033	-0.95987313	2.00092855
H	-2.75907167	-1.91950889	1.20995932
H	1.26134924	0.06946750	-1.62393975
H	0.80680217	-2.24117046	-2.26338193
H	-0.38622343	-2.30239323	0.58942553
C	-0.21915000	1.31461453	0.78322331
H	0.01843377	0.65353985	1.61713829
C	0.70444346	3.04638685	-0.82061403
H	1.03308165	4.01837623	-0.43668038
H	1.36292520	2.81628682	-1.66690310
H	-0.30720932	3.17295390	-1.20465888
H	2.84816212	2.56156567	0.79923219
H	2.16233515	1.23215881	1.73182793
H	-0.91461748	-0.30102685	-1.71192695

Table S11. Cartesian coordinate of **G2**.

C	2.01949909	0.23683189	1.41136565
H	2.71023876	1.03411985	1.69810027
H	1.02391658	0.57395131	1.70924575
H	2.28383129	-0.64090182	2.00896547
C	2.15494701	-0.03837744	-0.08874781
C	1.44625240	-1.33597041	-0.57245832
C	0.24308619	-2.05969780	-0.02465022
H	-0.04840037	-2.84499094	-0.72082631
C	-0.25860810	-2.26589418	1.30750805
H	-0.54043191	-3.27560296	1.59604881
C	-1.39747602	-1.59759447	0.47720749
C	-1.51741968	-0.23773448	0.61616719
C	-2.63766892	0.63845085	0.20448827
H	-3.49308906	0.07878616	-0.17527158
H	-2.96435744	1.16211331	1.11398108
C	-2.15251344	1.68593732	-0.84877013
C	-0.70172217	2.05135420	-0.61159209
C	1.69806700	1.19274751	-0.93355839
H	2.07593536	2.09547449	-0.44588126
H	2.20692042	1.13502269	-1.90328249
C	-2.47677234	-2.47298506	-0.10463491
H	-3.32864522	-2.52137588	0.57906314
H	-2.83091937	-2.10127245	-1.06820003
H	-2.12435568	-3.49575453	-0.25068057
H	2.17049596	-2.16075991	-0.43749890
C	3.65193675	-0.24512143	-0.38356752
H	4.20399914	0.68321405	-0.21525227
H	3.81884750	-0.54401268	-1.42286309
H	4.08463471	-1.01240617	0.26561628
H	-0.70102878	0.26773795	1.11632821
H	0.13657380	-1.66565364	2.11864483
H	1.32255943	-1.27567094	-1.65805752
C	0.22635485	1.26458947	-1.17892094
H	-0.14687374	0.52790479	-1.89224624
C	-0.43733152	3.16306466	0.35713918
H	-0.86900305	4.09692907	-0.01862268
H	-0.91438565	2.97750714	1.32784223
H	0.62462040	3.33311830	0.53274706
H	-2.81459200	2.55426017	-0.80695525
H	-2.26211645	1.23927569	-1.84005798

Table S12. Cartesian coordinate of **H**.

C	-3.42399633	0.18057495	-0.87661799
H	-4.23346697	0.65591389	-0.31603742
H	-3.21296783	0.80746298	-1.74833959
H	-3.78981156	-0.78728476	-1.23195273
C	-2.18631294	0.02158666	0.01981110
C	-1.04952088	-0.49381010	-0.90367601
C	0.17605720	-1.12537672	-0.16407008
C	0.53414808	-2.59423266	-0.58670591
H	0.23398951	-3.42294644	0.04737812
C	1.77993868	-1.91934713	-0.26433077
C	1.66462881	-0.61323689	-0.82840587
C	2.54387838	0.56003656	-0.41267090
H	3.52880418	0.17671021	-0.12728819
H	2.71390422	1.16440744	-1.30584346
C	2.01030397	1.47940896	0.71069673
C	0.62226614	1.95813980	0.37821012
C	-1.83846227	1.42168788	0.61935100
H	-2.02570535	2.17949893	-0.14584973
H	-2.53310190	1.62343506	1.44154447
C	2.59822209	-2.26873836	0.91522537
H	3.41105789	-2.89551715	0.51955623
H	3.05240357	-1.40978694	1.40669551
H	2.05306535	-2.88428203	1.63259666
H	-1.46133873	-1.26677499	-1.55848975
C	-2.51623246	-0.98220176	1.13047652
H	-3.43536245	-0.68351632	1.64049679
H	-1.74013466	-1.04707347	1.89916841
H	-2.68126429	-1.98594124	0.72538113
H	1.37073286	-0.60592171	-1.87806195
H	0.29710642	-2.73738512	-1.63915710
H	0.13160440	-0.99364441	0.91080554
C	-0.41686363	1.46329166	1.06818860
H	-0.18673074	0.88512381	1.96404927
C	0.50938756	2.87309969	-0.81010873
H	1.21405739	3.70448305	-0.70491657
H	0.75786332	2.37837501	-1.75735387
H	-0.48627330	3.30246790	-0.91674926
H	2.72207573	2.30640682	0.80907403
H	2.00458643	0.94771990	1.66787266
H	-0.71368245	0.32522683	-1.54197378

Table S13. Cartesian coordinate of **11**.

C	-3.41412986	0.16160341	-0.75384229
H	-3.85962902	1.03474598	-0.26743166
H	-3.30822999	0.38415842	-1.82022104
H	-4.12158249	-0.66593108	-0.65787392
C	-2.06499212	-0.21320488	-0.12080780
C	-1.47168815	-1.39760239	-0.91859904
C	-0.34818329	-2.15248960	-0.24294001
C	0.86291413	-2.61870068	-1.00202161
H	1.27466481	-3.59620501	-0.77515073
C	1.00326175	-1.53255692	0.03616058
C	1.20827724	-0.10858541	-0.45644293
C	2.61905039	0.47254226	-0.26282060
H	3.03578808	0.17794022	0.70339160
H	3.32072432	0.15602758	-1.03479594
C	2.38771481	1.98516084	-0.26266152
C	1.03021855	2.18392280	0.24095733
C	-1.17983727	1.04665615	-0.23272336
H	-1.14892112	1.35939048	-1.28463011
H	-1.67202085	1.85244970	0.32298895
C	1.67022224	-1.90004179	1.34507269
H	2.76051471	-1.93411234	1.26008141
H	1.41674813	-1.20551257	2.15592300
H	1.34524338	-2.89111537	1.66853271
H	-2.27830378	-2.11197926	-1.11773879
C	-2.28829002	-0.57706118	1.34897022
H	-2.77991317	0.24166418	1.88382872
H	-1.35616278	-0.81512778	1.87142944
H	-2.93357224	-1.45563823	1.43562101
H	0.96440262	-0.06516141	-1.52569650
H	0.93803821	-2.33946110	-2.04914591
H	-0.68659125	-2.83160503	0.53565151
C	0.28616139	0.92654280	0.24096335
H	0.27657918	0.69266607	1.33327792
C	0.48259372	3.48516523	0.61581608
H	1.24831751	4.22273542	0.85476573
H	-0.07121300	3.85057543	-0.26612617
H	-0.26446218	3.40765946	1.40983305
H	2.29324982	2.35243198	-1.30863805
H	3.14219671	2.63171188	0.19455611
H	-1.15860680	-1.03728105	-1.90629736

Table S14. Cartesian coordinate of **I2**.

C	2.87962220	-0.54221590	-1.13744565
H	3.38594811	-1.43935058	-0.76790412
H	2.20627271	-0.83947347	-1.95033809
H	3.64128324	0.10502394	-1.58065731
C	2.14042445	0.18911885	-0.01318960
C	1.55439130	1.51450868	-0.56778273
C	0.33940953	2.04092412	0.16516036
H	2.34115780	2.27629043	-0.54936026
C	-0.78449153	2.69849405	-0.58293503
H	-1.29625486	3.53521112	-0.11980632
C	-0.99480010	1.32851390	0.02023425
C	-0.97488413	0.13898699	-0.92249095
C	-2.33231997	-0.50563918	-1.26982966
H	-3.15745576	0.20655201	-1.23338453
H	-2.30495159	-0.91478563	-2.28339865
C	-2.49995660	-1.64856624	-0.26411573
H	-3.02468713	-2.54856680	-0.60889294
H	-3.07260436	-1.33928409	0.63046253
C	-1.16269614	-1.95240754	0.25352404
C	-0.16783793	-1.03583184	-0.28422624
C	1.05385568	-0.72608832	0.59482795
H	1.53496792	-1.66652485	0.88562505
H	0.68273835	-0.26751701	1.51753022
C	-1.86778553	1.21829059	1.24898795
H	-1.76574546	2.10734332	1.87478379
H	-2.92962714	1.12541794	0.99594593
H	-1.59295114	0.36216388	1.88143391
H	1.31379362	1.38852755	-1.62794087
C	3.13018212	0.49754185	1.12069041
H	3.52721090	-0.41916414	1.56748289
H	2.66171065	1.08341757	1.91744477
H	3.97806465	1.07223681	0.73951840
C	-0.89059409	-3.02238501	1.21286190
H	-1.72271785	-3.71310346	1.34070561
H	0.03046871	-3.55838751	0.96061967
H	-0.67473860	-2.54280438	2.18075515
H	-0.48130004	0.44142439	-1.84501214
H	-0.69851412	2.77584277	-1.66282208
H	0.16249830	-1.66926119	-1.14713009
H	0.53558279	2.43788236	1.15893556

Table S15. Cartesian coordinate of **I3**.

C	2.13029681	-0.24950161	1.70514976
H	2.66788149	0.61496756	2.10687673
H	1.15126370	-0.27030590	2.18300020
H	2.66715246	-1.14650345	2.02502515
C	2.08598607	-0.17672130	0.17125732
C	1.65047309	-1.49558030	-0.49409980
C	0.31141349	-2.17179288	-0.23697775
H	0.19720357	-2.98866874	-0.94721011
C	-0.33367741	-2.47628224	1.08704597
H	-0.75087517	-3.46797341	1.22940129
C	-1.02552327	-1.54935136	0.11430882
C	-1.07125731	-0.05760376	0.46530120
C	-2.47165007	0.58492486	0.47936585
H	-3.09721034	0.19954975	-0.32847337
H	-3.00687833	0.42233549	1.41523516
C	-2.19435742	2.06933067	0.21751201
C	-0.99573610	2.09516999	-0.61691637
C	1.25693066	1.04110035	-0.31375418
H	1.40471092	1.85373963	0.40739990
H	1.67204122	1.38952458	-1.26457481
C	-2.22384753	-2.10765511	-0.62944042
H	-3.14214056	-2.04834470	-0.03733014
H	-2.39923961	-1.60191450	-1.58637323
H	-2.05998173	-3.16292150	-0.85695645
H	2.42419846	-2.23708293	-0.26056646
C	3.52924474	0.09660135	-0.29579402
H	3.88057581	1.07239904	0.05353816
H	3.61060824	0.07524054	-1.38669264
H	4.20934693	-0.65922765	0.10569311
H	-0.63460654	0.09339515	1.45730628
H	0.08432462	-2.04878941	1.99028630
H	1.72559216	-1.34527166	-1.58022372
C	-0.27389563	0.82834539	-0.52085808
H	-0.39844588	0.39539990	-1.53769842
C	-0.54677390	3.25795988	-1.37814413
H	0.10441581	2.99559659	-2.21325428
H	-1.36934306	3.90318905	-1.68987309
H	0.07290551	3.85331568	-0.68477042
H	-1.83366855	2.54867413	1.15401174
H	-3.01539167	2.69930374	-0.13400580

Table S16. Cartesian coordinate of **14**.

C	3.04769156	-0.61691361	1.13828708
H	3.50300592	0.23378942	1.65482763
H	2.54405725	-1.23598574	1.88361015
H	3.85803400	-1.21177550	0.70871277
C	2.08923685	-0.14271354	0.03930952
C	1.39962361	-1.34557860	-0.65013796
C	0.24757283	-2.09563319	-0.00022439
H	0.15588224	-3.09084864	-0.42962214
C	-0.14667912	-2.02731300	1.45010986
H	-0.39902678	-2.95122988	1.96034509
C	-1.10288231	-1.52555822	0.39555171
C	-1.40477976	-0.02942674	0.34366946
C	-2.51245833	0.41508104	-0.62323905
H	-2.35520637	-0.01909574	-1.61722751
H	-3.51462720	0.14271516	-0.29478178
C	-2.31530059	1.93294869	-0.69097334
C	-0.87813558	2.15174890	-0.48308009
C	1.08578181	0.86881894	0.64958804
H	0.86435996	0.62046172	1.69174682
H	1.55776263	1.85635484	0.67604447
C	-2.31636449	-2.40099041	0.14262539
H	-3.12591312	-2.17208176	0.84373238
H	-2.70368375	-2.29552894	-0.87499264
H	-2.05904417	-3.45294936	0.28240371
H	2.19229200	-2.07782214	-0.83927664
C	2.90527309	0.58143444	-1.04168084
H	3.51509575	1.37957176	-0.60782908
H	2.26268046	1.02448841	-1.81367537
H	3.58022546	-0.11148655	-1.55096678
H	-1.70130138	0.29044538	1.35551977
H	0.34073959	-1.30401982	2.09246098
H	1.07631569	-1.04144315	-1.65806216
C	-0.24777488	0.91520841	-0.08018066
H	-0.06247277	0.64121523	-1.16729524
C	-0.20305819	3.43543830	-0.66648789
H	0.83953009	3.31608859	-0.97046304
H	-0.73977097	4.11204615	-1.33107273
H	-0.16654376	3.90496307	0.33094092
H	-2.76807421	2.40619102	0.20444183
H	-2.73251658	2.47198713	-1.54602734

Table S17. Cartesian coordinate of J.

C	3.317890165	0.728345794	0.885077019
H	3.34440897	1.789627419	0.61992833
H	3.336822469	0.653480097	1.976830557
H	4.235812018	0.270719364	0.507065845
C	2.081933439	0.030865274	0.29562086
C	2.175125823	-1.455103236	0.686076248
C	1.040428639	-2.371911188	0.244093366
H	1.303421946	-3.394989434	0.527943392
C	-0.295679646	-2.031207412	0.901216395
H	-0.931988787	-2.925694815	0.927927121
C	-1.183706862	-1.002403088	0.227324729
C	-1.844280496	-0.05410186	1.079257148
C	-3.073210263	0.675564996	0.578239663
H	-3.848524029	-0.031912656	0.27392817
H	-3.492231627	1.290343342	1.376266874
C	-2.581744649	1.557353161	-0.57629228
C	-1.091260366	1.542004473	-0.507363849
C	0.844049096	0.725001708	0.937851443
H	0.784934586	0.408450582	1.98501371
H	1.04850375	1.799911785	0.982032116
C	-1.734773149	-1.446096619	-1.103364596
H	-2.353982598	-2.331203178	-0.924073681
H	-2.358497906	-0.710830831	-1.604810041
H	-0.935833605	-1.742067947	-1.784127885
H	3.114800181	-1.845754478	0.280683783
C	2.119801667	0.176444413	-1.230094623
H	2.310946269	1.209376279	-1.532983871
H	1.198001042	-0.156327974	-1.716541635
H	2.938027952	-0.421672544	-1.640702813
H	-1.69492475	-0.154760155	2.151453884
H	-0.130199243	-1.759681283	1.948059537
H	0.948741556	-2.385632139	-0.846604936
C	-0.542706629	0.579617665	0.332840107
H	2.270733959	-1.523056075	1.77791135
C	-0.348711396	2.6401202	-1.161191031
H	-0.793382007	2.866468596	-2.135292236
H	-0.47428591	3.551027259	-0.559396759
H	0.713401452	2.447285266	-1.274912024
H	-2.922554024	2.593052175	-0.465058353
H	-2.927267529	1.263413232	-1.576122493

Table S18. Cartesian coordinate of K.

C	-3.88994733	0.22143925	-0.44365696
H	-4.40707659	1.01861135	0.09815017
H	-3.72253296	0.56621395	-1.46865839
H	-4.56322798	-0.63952669	-0.48289362
C	-2.57623979	-0.13798589	0.24759076
C	-1.78470700	-1.19039948	-0.55705367
C	-0.35804071	-1.06530408	-0.01054199
C	0.72622723	-1.57893679	-1.03962607
H	0.61402065	-2.64812954	-1.22170591
C	1.98594292	-1.20704501	-0.42013255
C	2.23267805	0.21734678	-0.32005902
C	2.81058040	0.89077345	0.95309474
H	2.58765315	0.32397795	1.85967857
H	3.87180769	1.13787570	0.94278326
C	1.81335427	2.04396657	0.69815771
C	0.99037077	1.17233473	-0.29499601
C	-1.58231513	1.04209103	0.25499006
H	-1.66731230	1.56506569	-0.70122738
H	-1.80608502	1.77047400	1.03907877
C	2.87503528	-2.20115282	0.18567389
H	3.80485841	-1.78235921	0.56765210
H	2.33079394	-2.67152615	1.02060920
H	3.06374555	-3.02053498	-0.51686405
H	-2.18870158	-2.20161415	-0.45855200
C	-2.86604432	-0.62910043	1.67118004
H	-3.40877789	0.13563838	2.23348386
H	-1.95801165	-0.86217523	2.23609060
H	-3.48702728	-1.52930968	1.65483536
H	2.86991118	0.44877475	-1.19443190
H	0.57219064	-1.01329523	-1.96411085
C	-0.17675065	0.42538330	0.41212165
H	0.08092506	0.41731127	1.47782336
C	0.63391417	1.85987249	-1.60498415
H	0.01185610	2.73879352	-1.42075863
H	1.53658661	2.21041921	-2.11279399
H	0.08774565	1.21398063	-2.29878333
H	2.29321065	2.88287589	0.18908969
H	1.27443749	2.41985678	1.56985226
H	-1.80942717	-0.92326795	-1.62041842
H	-0.26562365	-1.70152809	0.87515711

Table S19. Cartesian coordinate of **K2**.

C	2.746530696	0.181536763	1.324243703
H	3.251800403	1.139091359	1.477465798
H	1.822023228	0.212137986	1.906497832
H	3.379504721	-0.598914408	1.756361124
C	2.516827572	-0.072342624	-0.171676331
C	1.782966643	-1.405465709	-0.417874016
C	0.27317252	-1.09989173	-0.40486782
H	-0.226339716	-1.739547085	-1.140044467
C	-0.381510645	-1.436289395	1.005065492
H	-0.168843658	-2.46458068	1.297658903
C	-1.774712744	-1.174354882	0.71990218
C	-2.11521767	0.205923515	0.434309859
C	-2.962469159	0.596334272	-0.811217421
H	-2.842441221	-0.118510173	-1.628576634
H	-4.024764978	0.778021318	-0.650207307
C	-2.039373305	1.825530464	-0.947490704
C	-0.978167223	1.187259641	0.000408174
C	1.560884699	0.971572747	-0.799477172
H	1.64166449	1.93498515	-0.294269534
H	1.859554606	1.148231513	-1.836596022
C	-2.752500871	-2.260841901	0.59893536
H	-2.906734003	-2.670147139	1.609238562
H	-3.709027437	-1.952863179	0.180582866
H	-2.330390514	-3.097232408	0.028837623
H	2.072638712	-2.18894881	0.288135588
C	3.87868839	-0.068136431	-0.870999129
H	4.378615389	0.896587502	-0.743969575
H	3.777229018	-0.253553658	-1.944405718
H	4.537618817	-0.836697791	-0.456656968
H	-2.610924083	0.577722909	1.349369292
H	0.027555729	-0.727942374	1.728549699
H	2.030048585	-1.77656949	-1.418411261
C	0.117933344	0.397791071	-0.79512346
H	-0.23297283	0.394354242	-1.831837358
C	-0.469008908	2.130676744	1.080890147
H	0.05442561	2.981302534	0.638804188
H	-1.306615245	2.538619782	1.653495842
H	0.21717637	1.653636938	1.784554871
H	-2.489622152	2.713747515	-0.498273743
H	-1.703349924	2.072149283	-1.956167433

Table S20. Cartesian coordinate of L.

C	3.58820038	0.57149164	0.40157778
H	4.30696424	1.17104980	-0.16513172
H	3.37162652	1.10443704	1.33155650
H	4.07942349	-0.37332432	0.65578907
C	2.32855570	0.33962879	-0.41663252
C	1.12261995	-0.27513018	0.37809798
C	0.84259510	-1.80496313	0.31755238
H	1.20356920	-2.26393275	1.24940217
C	-1.47942543	-1.36765964	1.22447038
H	-2.36815882	-1.98544200	1.38847571
C	-0.60822598	-2.00036141	0.24992573
C	-2.02620854	0.04028621	0.72194972
C	-2.76891213	0.25044812	-0.60723867
H	-2.39254143	-0.35573403	-1.43431572
H	-3.85600111	0.16094009	-0.58298611
C	-2.15951478	1.67261204	-0.62506085
C	-1.06225267	1.21091528	0.38067117
C	1.40978645	1.57444711	-0.65678932
H	1.56905639	2.33980833	0.10616388
H	1.46571458	2.04292081	-1.64193368
C	-1.18376107	-2.79726808	-0.83588816
H	-2.27067038	-2.77086475	-0.88749999
H	-0.72632548	-2.54444023	-1.79883603
H	-0.86315992	-3.83723290	-0.64999624
H	1.21165534	0.02769816	1.42529237
C	2.65543599	-0.37976636	-1.72055150
H	3.32588660	0.24113352	-2.32059565
H	1.76902298	-0.57649947	-2.33211622
H	3.17171378	-1.32873160	-1.54360030
H	-2.67832205	0.33970082	1.54849379
H	-0.96094696	-1.17850059	2.16752042
H	1.34972480	-2.28666772	-0.51963496
C	0.17668744	0.69365928	-0.35770402
H	-0.14594733	0.23221220	-1.30100198
C	-0.74352458	2.16207244	1.52218304
H	-0.31730573	3.09570520	1.14679339
H	-1.65259376	2.42053249	2.07116493
H	-0.03405743	1.73892867	2.24075325
H	-2.83177732	2.40835518	-0.17854334
H	-1.81183410	2.05276891	-1.58804300

Table S21. Cartesian coordinate of **M**.

C	3.28455158	0.24197708	-1.32314445
H	3.73010938	-0.69803758	-1.66122550
H	2.81173536	0.71829997	-2.18814208
H	4.09984966	0.88878949	-0.98686156
C	2.27886192	-0.00231106	-0.19878134
C	1.58483670	1.29897503	0.24361376
C	0.28859431	0.84358276	0.91697471
H	0.47147621	0.55951220	1.95630908
C	-0.84673218	1.86823797	0.81942790
H	-1.63711667	1.67682637	1.57302661
C	-1.50619028	1.59684261	-0.46178162
C	-1.24743869	0.23924293	-0.89681390
C	-2.59430957	-0.59994406	-0.73988655
H	-3.29356692	-0.11105805	-0.05380527
H	-3.09102234	-0.70958120	-1.70414882
C	-2.07240641	-1.89144391	-0.12262766
H	-1.62509953	-2.52701183	-0.89519918
H	-2.87726536	-2.45800821	0.35359073
C	-1.00214609	-1.43073386	0.86696821
C	-0.18407415	-0.37504321	0.06650056
C	1.08396074	-0.87117674	-0.67411767
H	0.95899983	-0.75524503	-1.75649862
H	1.27665332	-1.93231728	-0.50493535
C	-2.30302996	2.57360656	-1.19798026
H	-2.81819990	3.27812888	-0.54035176
H	-1.56680438	3.17719078	-1.75800893
H	-2.97789890	2.12681241	-1.92822005
H	1.35286935	1.90333109	-0.64650038
C	2.99998912	-0.65210569	0.98837026
H	3.43668062	-1.61115009	0.69646235
H	2.33366386	-0.83951659	1.83447169
H	3.81242709	-0.01141444	1.34290074
H	2.21170835	1.91761346	0.89239451
C	-0.23525003	-2.56298121	1.53337380
H	0.23608211	-3.22716437	0.80503908
H	0.54245122	-2.18954779	2.20336767
H	-0.91619488	-3.17057687	2.13432181
H	-0.98621833	0.21380835	-1.96251450
H	-0.58459326	2.92259660	0.95988364
H	-1.52618844	-0.88053161	1.66488134

Table S22. Cartesian coordinate of **M2**.

C	-3.157791091	-1.15315578	-0.983900409
H	-3.678751558	-0.472554122	-1.663582254
H	-2.58270239	-1.858091311	-1.59414813
H	-3.917511152	-1.725493779	-0.444193347
C	-2.259226703	-0.382259632	-0.013387194
C	-1.452028657	-1.344319929	0.912650288
C	0.036891725	-0.982396033	0.782606825
C	0.858063587	-1.893243743	-0.148843556
H	1.369226237	-2.749562575	0.303119036
C	1.727139718	-1.023370868	-0.95227946
C	1.40926458	0.358829129	-0.710396041
C	2.543296383	0.695619453	0.380000742
H	3.068937812	-0.192461354	0.749618371
H	3.293684551	1.31056525	-0.118540172
C	1.778431671	1.393828787	1.525290759
C	0.312555314	1.575442241	1.083785491
C	-1.171051642	0.407548288	-0.780168468
H	-0.954833175	-0.109994614	-1.724652056
H	-1.503558766	1.409578774	-1.060153895
C	2.724877605	-1.503145697	-1.912674165
H	2.18253048	-1.635137806	-2.863724338
H	3.504889538	-0.765826143	-2.109960453
H	3.147452841	-2.473253081	-1.648308993
H	-1.777450403	-1.23564635	1.950205022
C	-3.133309435	0.559795728	0.824398002
H	-3.686426405	1.251973471	0.182995777
H	-2.545866563	1.153701061	1.530155207
H	-3.865061023	-0.00902975	1.405125557
H	1.523567334	1.031347524	-1.562055139
H	0.20230188	-2.341638484	-0.922952619
C	0.095094223	0.411866293	0.089298155
H	-0.347729119	1.455255389	1.948302517
C	0.069175204	2.957902356	0.48140669
H	-0.975489266	3.104473289	0.200887701
H	0.318756528	3.733207555	1.209630177
H	0.682972064	3.135904134	-0.40820993
H	2.250475911	2.354325909	1.748105919
H	1.847676001	0.791314857	2.432989889
H	-1.62647553	-2.393059598	0.651285377
H	0.529191232	-0.970081731	1.759182375

Table S23. Cartesian coordinate of **N**.

C	3.57715190	0.35253695	-1.17954635
H	3.94232020	-0.52207708	-1.72510301
H	3.16955469	1.06027852	-1.90800064
H	4.44003099	0.82462233	-0.70194310
C	2.53532458	-0.04237622	-0.13589421
C	1.96949223	1.18705763	0.63374108
C	0.45959304	0.93769207	0.81767562
H	0.12198813	1.08168096	1.84534067
C	-0.39568688	1.94152890	-0.13354972
H	-0.42868481	2.91144890	0.36559490
C	-1.77188036	1.36501790	-0.38853583
C	-1.86699515	0.36466881	-1.32977615
C	-2.61183102	-0.95024428	-1.23235484
H	-3.49131925	-0.88841228	-0.58929794
H	-2.93493324	-1.31633161	-2.20761334
C	-1.56487604	-2.00411312	-0.61806243
H	-0.86446027	-2.30310847	-1.40062094
H	-2.10577130	-2.88942170	-0.28147529
C	-0.86435427	-1.28042581	0.52351391
C	0.23176925	-0.46886724	0.27067609
C	1.27522342	-0.66672102	-0.79683103
H	1.03608786	-0.10818015	-1.71104291
H	1.41201334	-1.71425150	-1.07288946
C	-2.84115819	1.68874673	0.60379051
H	-2.47475992	1.68160494	1.63330397
H	-3.16157772	2.71778167	0.40051898
H	-3.72165706	1.05260831	0.51911823
H	2.14265859	2.11326214	0.07798210
C	3.13899671	-1.04451336	0.85493489
H	3.46909821	-1.95287955	0.34287225
H	2.42262243	-1.33849423	1.62953245
H	4.00778229	-0.61022147	1.35646265
H	2.46983289	1.30255478	1.59799030
C	-1.62897763	-1.22274395	1.81155687
H	-1.53187181	-2.21481693	2.26847815
H	-1.23533906	-0.49671087	2.52089314
H	-2.69813353	-1.05528888	1.66670847
H	-1.07858757	0.35600650	-2.08414648
H	0.15585421	2.05912486	-1.06979088
H	-1.02855501	-0.06656774	-0.22608886

Table S24. Cartesian coordinate of **O**.

C	3.62070448	-0.18008545	-1.07633346
H	4.17973515	-1.11985459	-1.05082355
H	3.05537796	-0.14925899	-2.01362258
H	4.34676563	0.63755800	-1.10160451
C	2.70400905	-0.05320683	0.14210453
C	1.94107712	1.31343140	0.11039432
C	0.48742986	0.94088563	0.37892469
H	0.39686314	0.71258807	1.44853042
C	-0.63121486	1.95539878	0.02456862
H	-0.63182661	2.77853417	0.74289590
C	-1.94132805	1.22128967	0.04183122
C	-2.13017360	0.34684664	-1.01949091
C	-3.04297266	-0.82648263	-1.27846069
H	-3.76648577	-1.01238096	-0.48397785
H	-3.56445615	-0.78734597	-2.23467776
C	-1.83187725	-1.78408053	-1.21224454
H	-1.31388665	-1.82575630	-2.17349807
H	-2.03654534	-2.79965520	-0.86447063
C	-1.04229901	-0.94066495	-0.19001143
C	0.33780247	-0.37643764	-0.39393079
C	1.57549615	-1.13903195	0.10324449
H	1.83611352	-1.98272258	-0.54051639
H	1.39810153	-1.53253029	1.10940373
C	-2.85977138	1.37984673	1.19031484
H	-2.32752436	1.37636088	2.14594194
H	-3.30471975	2.38024137	1.09750166
H	-3.67429256	0.65731907	1.20659654
H	2.02800569	1.77880142	-0.87836480
C	3.52698945	-0.19722686	1.42381517
H	3.97350075	-1.19372614	1.49211568
H	2.91156766	-0.04582619	2.31684414
H	4.34101461	0.53261036	1.45048574
H	2.33990465	2.02266773	0.83968558
C	-1.39104576	-1.36929610	1.21371227
H	-0.92755732	-2.35427452	1.34577638
H	-1.01247119	-0.71918365	2.00078089
H	-2.46309077	-1.51406206	1.35562411
H	-1.51223541	0.56829188	-1.88842413
H	-0.44212258	2.36756732	-0.97213903
H	0.47667115	-0.17605239	-1.46443651

Table S25. Cartesian coordinate of **P**.

C	3.37966651	-1.06626463	-0.73691039
H	3.93324707	-1.69884096	-0.03730384
H	2.74544062	-1.71538334	-1.34944195
H	4.10688363	-0.59139222	-1.40187014
C	2.55850804	-0.00984300	0.00551611
C	1.80820357	0.91489524	-1.00775361
C	0.37297748	0.98010903	-0.49392934
H	0.37341418	1.63894118	0.38839055
C	-0.74872195	1.43431798	-1.43075041
H	-0.85733294	2.52055787	-1.42450793
C	-1.89364956	0.52559434	0.44119214
C	-2.11737011	0.74945974	-0.99694061
C	-2.31815044	-0.66753068	-1.58626880
H	-3.32897247	-0.78345636	-1.98014292
H	-1.63429691	-0.84115725	-2.41928310
C	-2.05558250	-1.63762717	-0.41291521
H	-1.47645720	-2.51898361	-0.69650883
H	-2.99497619	-1.99457808	0.02004254
C	-1.29921082	-0.78978199	0.63679009
C	0.17675006	-0.45882305	0.00004389
C	1.41799243	-0.68717077	0.84595429
H	1.62345044	-1.74221681	1.04014227
H	1.32734864	-0.18339016	1.81413424
C	-2.16473126	1.51413968	1.47659980
H	-1.50035130	1.43393404	2.33872656
H	-2.23001882	2.53469844	1.09706495
H	-3.17097251	1.24604767	1.84869175
H	1.81444089	0.46800715	-2.00946790
C	3.47302271	0.80307609	0.92395956
H	3.91438944	0.16885111	1.69843064
H	2.92844993	1.61107857	1.42361210
H	4.29288327	1.25239207	0.35645896
H	2.27548264	1.89924881	-1.09048310
C	-1.25824252	-1.37147752	2.03897829
H	-0.74925251	-2.33657363	2.02573401
H	-0.73184338	-0.73291860	2.75020148
H	-2.27150957	-1.54058510	2.41317331
H	-2.93621746	1.44330039	-1.20082206
H	-0.57077708	1.12429293	-2.46442483
H	0.21786219	-1.11753892	-0.87575400

Table S26. Cartesian coordinate of **Q**.

C	1.65611207	1.33528579	1.32654351
H	2.36586878	2.08373954	0.96226488
H	0.68750057	1.82925082	1.41286314
H	1.96557700	1.06045198	2.33844267
C	1.66016580	0.10802696	0.40310641
C	0.83409359	-1.07408938	0.98237288
C	0.92355609	-2.34475230	0.11174012
H	0.67941718	-3.21164859	0.73123224
C	-0.14900817	-2.16649497	-0.98730321
H	0.27874717	-2.02685191	-1.98521673
C	-1.00405660	-0.95570520	-0.54661296
C	-0.70671473	-0.87384039	0.96315960
C	-1.35625911	0.32413553	1.66878016
H	-2.30827698	0.01300193	2.10495453
H	-0.74157787	0.65267400	2.50985279
C	-1.62924900	1.53154183	0.76006004
C	-0.96838317	1.57335946	-0.54268253
C	1.13316493	0.46095331	-0.99414058
H	1.49082798	1.44223578	-1.31988047
H	1.49562555	-0.25915903	-1.73153013
C	-2.47331369	-1.15649111	-0.91884993
H	-2.86264764	-2.05458381	-0.43293346
H	-3.12390685	-0.32716806	-0.62669368
H	-2.58539741	-1.29364686	-1.99853634
H	1.19129637	-1.26711618	1.99962359
C	3.14158175	-0.28846679	0.24960924
H	3.72837422	0.56074590	-0.11175012
H	3.29609240	-1.11135762	-0.44907464
H	3.55522834	-0.58645028	1.21716015
H	-1.12035493	-1.77525859	1.42935199
H	-0.78772751	-3.05001828	-1.05855300
H	1.91670564	-2.53411235	-0.29349695
C	-0.46004987	0.35761706	-1.15328601
H	-0.61785868	0.41736255	-2.23823308
C	-0.86718029	2.86589726	-1.24285347
H	-1.81363205	3.41276788	-1.16591995
H	-0.13710839	3.49040100	-0.70931519
H	-0.56679581	2.77479775	-2.28574752
H	-1.57973736	2.49855241	1.27080668
H	-2.68267069	1.48858519	0.40701134

Table S27. Cartesian coordinate of **R**.

C	1.82738954	1.34593186	1.22771341
H	2.50811153	2.11963231	0.86067878
H	0.83950226	1.80852484	1.35546459
H	2.16033174	1.05682580	2.22816632
C	1.80899457	0.13842737	0.28326967
C	0.78558179	-0.91714392	0.79583354
C	0.91422762	-2.35417159	0.22463943
H	0.80421974	-3.07114325	1.04302185
C	-0.24336020	-2.53418891	-0.76000448
H	0.01516757	-2.15090950	-1.75636979
C	-1.35915750	-1.69512473	-0.14515642
C	-0.62536149	-0.41989972	0.33266749
C	-1.44307436	0.39763903	1.36932978
H	-2.33748626	-0.13900299	1.69172941
H	-0.85729526	0.60091398	2.26882929
C	-1.80524577	1.71944225	0.68432989
C	-0.89902905	1.86349713	-0.45491357
C	1.23058774	0.55911579	-1.07587195
H	1.62523021	1.51088616	-1.44277466
H	1.43734889	-0.19735264	-1.83597766
C	-2.58817459	-1.49497416	-1.02050738
H	-3.06659407	-2.45561184	-1.22519606
H	-3.34364224	-0.86356522	-0.54097176
H	-2.34322857	-1.06012312	-1.99617113
H	0.84255765	-0.95471408	1.88822735
C	3.24418967	-0.37565111	0.13884613
H	3.91581941	0.43945224	-0.14483192
H	3.33541454	-1.15276484	-0.62188199
H	3.60498834	-0.78537634	1.08627571
H	-1.68224736	-2.20692374	0.77227395
H	-0.52888631	-3.58037374	-0.89387226
H	1.88616810	-2.55608500	-0.22587071
C	-0.30422801	0.58646317	-0.81467852
H	-0.80147100	0.35111036	-1.77720016
C	-0.67848732	3.12070890	-1.16658520
H	-1.54011027	3.78979167	-1.11145376
H	0.13504235	3.63056931	-0.62320114
H	-0.33648184	2.98129699	-2.19278626
H	-1.87496070	2.61763505	1.30756024
H	-2.79762636	1.65623304	0.19142194

Table S28. Cartesian coordinate of **S**.

C	3.85271401	0.80473958	0.39288875
H	4.57017918	1.42061799	-0.15705956
H	3.55938239	1.35676191	1.29101203
H	4.37214933	-0.10485375	0.70939040
C	2.65087493	0.46925614	-0.47550247
C	1.41092541	-0.13142467	0.27817107
C	0.69157547	-1.46455624	0.47803132
H	0.84104366	-1.89721954	1.47160201
C	-1.81579748	-1.30148913	1.37667746
H	-2.42815751	-2.20091049	1.22221820
C	-0.82205306	-1.08701459	0.21101110
C	-2.76982384	-0.14626332	1.41828119
C	-3.31937451	0.38497540	0.12507183
H	-3.86500394	-0.44771744	-0.33564318
H	-4.05166346	1.17175478	0.31261067
C	-2.14691302	0.86278597	-0.78478704
C	-0.86597009	0.49929924	-0.03938504
C	1.68280452	1.67833843	-0.80659825
H	1.72217539	2.42897236	-0.01195337
H	1.79388690	2.16838074	-1.77561387
C	-1.29429180	-1.89102531	-1.00996570
H	-2.35104284	-1.75146232	-1.25001110
H	-0.71064191	-1.65949703	-1.90360909
H	-1.15118931	-2.95521490	-0.80364575
H	1.44549559	0.38635543	1.24554727
C	3.08942132	-0.30473674	-1.71361087
H	3.79297774	0.28989203	-2.30273729
H	2.26082875	-0.57607414	-2.37372313
H	3.59963876	-1.22821517	-1.42533398
H	-3.40550115	-0.06528571	2.30625505
H	-1.33534024	-1.42877522	2.35159670
H	1.00464558	-2.21922533	-0.24830154
C	0.52674681	0.66438408	-0.65153056
H	0.46748542	0.13663276	-1.60919412
C	-0.99116288	1.19296438	1.29394467
H	-1.17500578	2.26922665	1.23912752
H	-2.01979119	0.89481367	1.86341455
H	-0.29087882	0.91857337	2.08200907
H	-2.21989632	1.94399529	-0.93097078
H	-2.18588585	0.40718330	-1.77386446

Table S29. Cartesian coordinate of T.

C	3.20546429	0.02780435	0.60591770
H	3.80577835	0.83361587	0.17224658
H	3.08114010	0.23426830	1.67355709
H	3.77904342	-0.89766432	0.51029750
C	1.85457726	-0.10373995	-0.10655541
C	0.96424635	-1.09358595	0.64623469
C	1.06098222	-2.60459975	0.92427879
H	1.69228962	-2.92267328	1.75490807
C	-0.47635478	-2.54002467	1.16661597
H	-1.07946269	-3.39916992	0.86587934
C	-0.51658689	-1.29326309	0.23339138
C	-1.22921787	0.02072923	0.54549883
C	-2.66114439	0.33144466	0.10528825
H	-2.86012042	-0.06142232	-0.89654400
H	-3.41956568	-0.06933879	0.77786153
C	-2.67155173	1.86798735	0.06609338
C	-1.29133223	2.28216307	-0.22860213
C	1.09573798	1.25371051	0.02964460
H	1.24513128	1.63587669	1.04747352
H	1.53080233	1.99124533	-0.65417957
C	-0.80900027	-1.77791118	-1.18872973
H	-1.80489101	-2.23060986	-1.22066886
H	-0.79084045	-0.99207095	-1.95110284
H	-0.09851908	-2.54001444	-1.51185981
H	0.89314800	-0.66127267	1.65786616
C	2.11210552	-0.44568918	-1.57696558
H	2.84883119	0.24237960	-2.00200270
H	1.21762082	-0.39395823	-2.20088480
H	2.51731979	-1.45619703	-1.67272892
H	-1.13947229	0.21638457	1.62368087
H	-0.69950424	-2.29132488	2.20813669
H	1.30780435	-3.20411536	0.04525265
C	-0.41511283	1.13406139	-0.19628461
H	-0.58784871	0.87770666	-1.28320913
C	-0.87810308	3.66070760	-0.47970340
H	-1.70445106	4.33247245	-0.70738768
H	-0.38403037	4.00948687	0.44243863
H	-0.09824907	3.71237275	-1.24579847
H	-2.83551097	2.27037346	1.08654122
H	-3.42216199	2.36765714	-0.55465229

Table S30. Cartesian coordinate of **U**.

C	3.42079569	-0.56951876	-1.23545602
H	4.23177722	-1.23354100	-0.92338823
H	2.85670180	-1.08410374	-2.01931875
H	3.87191919	0.32231335	-1.68042848
C	2.54648971	-0.19623404	-0.04027832
C	1.22339539	0.50107152	-0.51875914
C	0.68421108	1.60919330	0.36816959
H	1.40690692	2.43027032	0.36871412
C	-0.65049727	2.23723400	-0.11714541
H	-0.84773091	3.13903354	0.46671068
C	-1.80999050	1.30771695	-0.00678051
C	-1.87421102	0.20458455	-0.86851468
C	-2.92809576	-0.88515792	-0.97630626
H	-3.67687738	-0.84196534	-0.18512989
H	-3.43867369	-0.91612738	-1.93924621
C	-1.87701229	-1.97669698	-0.72870978
H	-1.43374391	-2.32754120	-1.66307435
H	-2.19618776	-2.83834675	-0.13793304
C	-0.91040438	-1.03075305	0.02187532
C	0.52203823	-0.90049516	-0.43672014
C	1.68977138	-1.39191271	0.45246893
H	2.06401881	-2.39935961	0.25444417
H	1.47134236	-1.30537592	1.51967176
C	-2.79422279	1.57470562	1.05922400
H	-2.29735775	1.75820386	2.01837157
H	-3.28142113	2.52683344	0.80223633
H	-3.56688215	0.81790881	1.16980262
H	1.28652563	0.88568791	-1.54461082
C	3.38480485	0.50063576	1.02145158
H	4.18615916	-0.16533435	1.35454672
H	2.80433830	0.77509674	1.90639240
H	3.85824497	1.40601535	0.62954764
C	-1.14852410	-1.09834175	1.51258862
H	-0.75174897	-2.06354928	1.84526139
H	-0.64165581	-0.32365076	2.08798260
H	-2.20985501	-1.09518727	1.76686215
H	-1.27773684	0.31033743	-1.77443285
H	-0.52496861	2.53137376	-1.16557736
H	0.59158026	-1.36221061	-1.42551088
H	0.58982632	1.29360301	1.41114765

Table S31. Cartesian coordinate of **V**.

C	3.51719594	0.74167636	0.80488373
H	4.29427993	1.35794968	0.34653107
H	3.05690795	1.32736135	1.60569225
H	4.00445837	-0.12778099	1.25452867
C	2.49913777	0.31627786	-0.24223691
C	1.22915522	-0.27934941	0.36290180
C	0.36299608	-1.14842825	-0.27758465
H	-0.49004821	-3.38797134	1.06768715
C	-0.93523265	-2.44118511	1.38353399
H	-1.93875617	-2.65524565	1.75871143
C	-1.03733925	-1.44135884	0.21079124
C	-1.65041423	-0.09043511	0.71508504
C	-3.01854120	0.36379731	0.14421893
H	-3.65836413	-0.39298653	-0.30807885
H	-3.60553810	0.88715450	0.90080232
C	-2.29293915	1.33056555	-0.81152295
C	-0.99358500	1.15718624	0.02876829
C	1.62002949	1.46234404	-0.81070162
H	1.61455514	2.32295888	-0.14134572
H	1.86299002	1.78828995	-1.82322180
C	-1.81880199	-2.10636630	-0.93068656
H	-2.80629525	-2.41964910	-0.58928458
H	-1.95563445	-1.44773225	-1.79276033
H	-1.29747077	-3.00461880	-1.27273255
H	0.96141434	0.07924559	1.35593535
C	3.14379864	-0.53325130	-1.33271673
H	3.98459736	0.01322158	-1.76574478
H	2.46289509	-0.76882102	-2.15564151
H	3.53028672	-1.47114596	-0.92509167
H	-1.58957768	-0.06244761	1.80730143
H	-0.34315652	-2.03916914	2.20961447
H	0.72151454	-1.68909222	-1.15135880
C	0.25377833	0.71761670	-0.72224936
H	0.00568201	0.31123365	-1.70769391
C	-0.76465167	2.32098138	0.98321225
H	-0.49700862	3.23394602	0.44434249
H	-1.68273447	2.53084945	1.53670076
H	0.01495064	2.11534954	1.72411427
H	-2.67826341	2.34985958	-0.87728968
H	-2.20193944	0.93490368	-1.82716951

Table S32. Cartesian coordinate of **W**.

C	2.59669885	0.10750340	1.20883579
H	3.38256361	0.85955977	1.31465645
H	1.75960903	0.40590280	1.83634681
H	2.97969379	-0.83754401	1.60436392
C	2.22790821	-0.07418509	-0.26293518
C	1.37601121	-1.34556424	-0.52603231
C	0.11384211	-1.79486934	0.22600441
H	0.02451043	-2.86000095	0.02061201
C	-0.32941029	-1.46934897	1.62806400
H	-0.51154510	-2.28063650	2.32612877
C	-1.29092699	-1.25505584	0.48860170
C	-1.82861019	0.13609483	0.22401449
C	-2.58268917	0.46003541	-1.07986318
H	-2.20695796	-0.09460785	-1.94356805
H	-3.66701034	0.35520194	-1.05909744
C	-2.03178971	1.88249123	-0.99809352
C	-0.87424161	1.39789394	0.03244056
C	1.57310272	1.33347399	-0.79441172
H	1.84661217	2.13321327	-0.10843143
H	1.98575409	1.50655434	-1.79028046
C	-2.41643664	-2.26666889	0.34605052
H	-3.26937671	-1.99028038	0.97462450
H	-2.76769748	-2.34186201	-0.68717918
H	-2.09170047	-3.26092011	0.66014013
H	2.08707993	-2.15746989	-0.33481762
C	3.51654040	-0.23089657	-1.08244755
H	4.14592987	0.65889872	-1.00370369
H	3.30758987	-0.41712390	-2.13926407
H	4.08912378	-1.08014623	-0.69810418
H	-2.47200429	0.42015779	1.06578398
H	0.06980086	-0.57948047	2.09914250
H	1.17933242	-1.41629567	-1.60359221
C	0.17341989	1.04721918	-0.86417164
H	-0.13251748	0.42468391	-1.70390243
C	-0.56743544	2.30530612	1.20369622
H	-0.15053233	3.25917231	0.86915799
H	-1.48552287	2.52235638	1.75262991
H	0.13439970	1.85628808	1.90817243
H	-2.66035437	2.55224822	-0.40731823
H	-1.71838813	2.39833484	-1.90644611

Table S33. Cartesian coordinate of **X**.

C	2.596698851	0.107503399	1.208835786
H	3.382563606	0.859559771	1.314656446
H	1.759609027	0.405902797	1.836346812
H	2.979693787	-0.837544008	1.604363915
C	2.227908209	-0.074185086	-0.262935176
C	1.376011207	-1.345564239	-0.526032314
C	0.113842115	-1.79486934	0.226004407
H	0.024510431	-2.86000095	0.020612009
C	-0.329410286	-1.469348965	1.628064
H	-0.511545096	-2.280636505	2.326128769
C	-1.29092699	-1.255055843	0.488601695
C	-1.828610187	0.13609483	0.224014487
C	-2.582689172	0.460035413	-1.079863177
H	-2.206957955	-0.094607845	-1.943568052
H	-3.667010342	0.355201937	-1.059097437
C	-2.031789709	1.88249123	-0.998093524
C	-0.87424161	1.397893943	0.032440558
C	1.573102723	1.333473991	-0.794411724
H	1.846612171	2.133213265	-0.108431432
H	1.98575409	1.506554344	-1.790280464
C	-2.416436636	-2.266668889	0.346050516
H	-3.269376705	-1.990280377	0.974624499
H	-2.767697475	-2.341862012	-0.687179185
H	-2.091700474	-3.26092011	0.660140126
H	2.087079928	-2.157469891	-0.334817625
C	3.516540397	-0.230896569	-1.082447546
H	4.145929868	0.65889872	-1.003703695
H	3.307589874	-0.417123896	-2.139264072
H	4.08912378	-1.080146227	-0.698104176
H	-2.472004289	0.420157789	1.065783979
H	0.069800856	-0.579480474	2.099142495
H	1.179332421	-1.41629567	-1.603592205
C	0.173419893	1.047219176	-0.864171643
H	-0.132517481	0.424683914	-1.703902431
C	-0.567435439	2.30530612	1.203696216
H	-0.150532329	3.25917231	0.869157989
H	-1.485522872	2.522356378	1.75262991
H	0.134399697	1.856288081	1.908172426
H	-2.660354366	2.552248217	-0.407318234
H	-1.718388128	2.398334835	-1.906446114

Table S34. Cartesian coordinate of Y.

C	-3.82970593	-0.83938731	-1.22373071
H	-4.42604797	0.05675019	-1.41588755
H	-3.46897734	-1.22139517	-2.18347742
H	-4.49760660	-1.59144939	-0.79623009
C	-2.67670599	-0.54090383	-0.26905857
C	-1.77330203	-1.78373229	-0.03670743
C	-0.40213725	-1.19745223	0.34122010
C	0.96345157	-1.82816436	0.02164440
H	1.30616176	-2.51718047	0.79564552
C	1.92385171	-0.61792636	-0.15824649
C	0.98493162	0.58377164	-0.53802094
C	2.57594661	-0.16263623	1.16939306
H	1.97501035	-0.48839268	2.02720072
H	3.57155530	-0.59360380	1.29895439
C	2.58534682	1.35751711	1.10061682
C	1.20140319	1.73472626	0.56084500
C	-1.66772347	0.46994777	-0.88079699
H	-1.58218303	0.31341667	-1.97497541
H	-1.89400662	1.53825509	-0.77828888
C	2.97411486	-0.88407953	-1.23236988
H	3.66693628	-0.04430860	-1.33524404
H	3.56398304	-1.76830363	-0.97558684
H	2.51417269	-1.06296680	-2.20894644
H	-2.17315863	-2.45398685	0.72570827
C	-3.22254177	0.00563241	1.05558400
H	-3.81071659	0.91187694	0.88701614
H	-2.43375486	0.25550476	1.77287515
H	-3.87805474	-0.72861655	1.52974971
H	1.16877179	1.03609113	-1.51808728
H	0.88139270	-2.39756616	-0.91009727
C	-0.35508218	0.08034063	-0.37685050
H	0.47536922	1.59606034	1.37310915
C	1.05733350	3.13534912	-0.00364494
H	0.05422899	3.32733494	-0.39431247
H	1.24293161	3.87181934	0.78249187
H	1.77680623	3.31212127	-0.80774351
H	3.35485099	1.71171941	0.40589962
H	2.76902389	1.83491125	2.06697149
H	-1.67502345	-2.35941562	-0.96407433
H	-0.42522997	-0.91402327	1.41135534

Table S35. Cartesian coordinate of **Z**.

C	-2.30043609	-0.89665627	-1.73094577
H	-2.53701756	-0.07984548	-2.41893482
H	-1.51027331	-1.50137936	-2.18191262
H	-3.18964614	-1.52826747	-1.66141853
C	-1.93548589	-0.36170118	-0.34843303
C	-1.52937184	-1.46681881	0.67554932
C	-0.23421471	-0.97212510	1.34993228
C	1.03688062	-1.61781544	0.67908682
H	1.94408947	-1.26827071	1.17785848
C	1.05449846	-1.31281072	-0.82347189
C	0.63493152	0.13443596	-1.15540276
C	1.66485323	1.24515277	-0.94586390
H	2.54886276	1.04535985	-1.55946758
H	1.24521645	2.18007439	-1.33116442
C	2.08871830	1.41350103	0.50909522
C	0.86341386	1.40963029	1.50791332
C	-0.71940591	0.59039578	-0.32954725
H	0.29797306	-1.95479186	-1.28467564
H	-0.92497244	1.60504768	-0.67091039
C	2.39686089	-1.69245653	-1.45532664
H	2.39705903	-1.50205483	-2.53120093
H	3.22957491	-1.14053139	-1.01130638
H	2.59483399	-2.75677338	-1.31105660
H	-2.31744094	-1.61355845	1.41783592
C	-3.12637980	0.43568497	0.20583057
H	-3.38489218	1.27747182	-0.44321141
H	-2.91905762	0.83352598	1.20554463
H	-4.00650414	-0.20782420	0.28210253
H	0.28419061	0.16411997	-2.19349567
H	0.97596396	-2.69489756	0.86137766
C	-0.08264543	0.43492734	0.94742932
H	1.21971276	1.06100675	2.48149609
C	0.25825853	2.81564792	1.65447465
H	-0.64513337	2.80519061	2.26769570
H	0.98752471	3.46029194	2.14838424
H	0.01483130	3.26003326	0.68757073
H	2.62192586	2.35579031	0.65920732
H	2.77259111	0.61526591	0.80233460
H	-1.37084890	-2.43410783	0.19267678
H	-0.16780681	-1.12995863	2.42928161

Table S36. Cartesian coordinate of α .

C	3.84938975	0.66491469	0.45660903
H	4.56310370	1.20604693	-0.17124819
H	3.58959325	1.31231050	1.29918562
H	4.36106608	-0.21785558	0.85221411
C	2.62049899	0.26859797	-0.34653996
C	1.40697801	-0.25727490	0.49466577
C	0.91018964	-1.65755637	0.77075300
H	1.48646046	-2.19872805	1.52447596
C	-0.55647413	-1.51047104	1.29913722
H	-1.07014659	-2.46852415	1.40487675
C	-1.39008006	-0.53306517	0.58469527
C	-2.77650398	-0.77625719	0.16980057
C	-3.28407251	0.58337271	-0.33564296
H	-4.04879248	0.47644537	-1.10667490
H	-3.73408764	1.14566922	0.48739570
C	-2.00995844	1.27037474	-0.84384790
C	-0.90385675	0.79389956	0.12585617
C	1.67221630	1.44478148	-0.77765043
H	1.75288392	2.28359540	-0.08081249
H	1.75121227	1.81507638	-1.80144804
C	-2.67286386	-1.83296461	-0.98392830
H	-2.27538057	-2.78511637	-0.63190474
H	-3.68815156	-1.99356911	-1.35077180
H	-2.06392741	-1.47579406	-1.81593585
H	1.46552552	0.28211494	1.44868119
C	3.01083694	-0.63066188	-1.51556651
H	3.71513298	-0.10978626	-2.16975794
H	2.15964308	-0.93323346	-2.13239632
H	3.50507139	-1.53886264	-1.15837412
H	-3.36622682	-1.24355738	0.96718711
H	-0.48892219	-1.08532979	2.31848085
H	0.89596836	-2.26859726	-0.13710382
C	0.49484878	0.50396001	-0.45318156
H	0.33275292	-0.11817137	-1.34333751
C	-0.86633371	1.73393960	1.36981592
H	-0.52359023	2.70914444	1.01752113
H	-1.85661691	1.86303646	1.81109069
H	-0.18405201	1.38251285	2.14342724
H	-2.09107286	2.35817272	-0.86564770
H	-1.77155623	0.94600473	-1.86190789

Table S37. Cartesian coordinate of **A1D**.

C	3.46468176	0.34549223	0.64629083
H	4.15727148	0.94825185	0.05265035
H	3.28674633	0.86772279	1.58921323
H	3.94117786	-0.61564486	0.85080373
C	2.16464361	0.17731113	-0.19654137
C	1.19920432	-0.48762828	0.71093133
C	0.91875690	-1.91740603	0.77085013
H	1.67577990	-2.23248920	1.52623084
C	-0.48475462	-2.32865570	1.26519170
H	-0.50353660	-3.41939365	1.34581197
C	-1.49626898	-1.79773945	0.27612506
C	-2.11134706	-0.64225539	0.55753738
C	-2.83778085	0.26752978	-0.38371158
H	-2.64387140	-0.00611386	-1.42464857
H	-3.92341846	0.19949328	-0.24801099
C	-2.43376765	1.72498635	-0.11961423
C	-0.96383494	2.05857817	-0.04062608
C	1.50070181	1.54121523	-0.49958911
H	1.72196437	2.23718800	0.31235166
H	1.92727218	1.96600601	-1.41533321
C	-1.62321894	-2.55206992	-1.01442807
H	-2.02131169	-3.55380737	-0.81853129
H	-2.29937198	-2.06968564	-1.71975131
H	-0.65924297	-2.69806623	-1.51643807
H	0.83117072	0.11784024	1.54049516
C	2.47076537	-0.60231580	-1.47514993
H	3.16719937	-0.02339721	-2.08515958
H	1.57277004	-0.77450382	-2.07407334
H	2.94320048	-1.56607085	-1.27174478
H	-1.98682581	-0.24336542	1.56580140
H	-0.66476507	-1.92004922	2.26367307
H	1.19515172	-2.42529807	-0.15393481
C	0.01074959	1.29723151	-0.60355229
H	-0.29409702	0.47425385	-1.24910095
C	-0.68305684	3.32714576	0.70734448
H	-1.40090068	4.09797299	0.41039557
H	-0.83171438	3.17736734	1.78416468
H	0.31773957	3.72647350	0.54945910
H	-2.88734457	2.04870684	0.82593842
H	-2.88261228	2.37823033	-0.88002384

Table S35. Cartesian coordinate of **A1E2**.

C	3.04467198	-0.01853857	0.35007626
H	3.78967734	0.48662662	-0.27024890
H	3.09535569	0.42874451	1.34696416
H	3.33673492	-1.06760212	0.41880418
C	1.65879861	0.18801600	-0.31403971
C	0.64901314	-0.33850261	0.71235809
C	0.96021224	-1.71491159	1.34216369
H	1.54250114	-1.60435770	2.26006231
C	-0.39514684	-2.39128488	1.54402708
H	-0.34083993	-3.47969430	1.53481153
C	-1.06343394	-1.81326514	0.33395726
C	-1.33775737	-0.44273457	0.37798425
C	-2.13803662	0.26331006	-0.70249442
H	-1.69682003	0.08680493	-1.68511284
H	-3.12869650	-0.21252522	-0.72072451
C	-2.28070392	1.77848175	-0.45994023
C	-0.91213901	2.30692729	-0.09426338
C	1.49960913	1.72376929	-0.54215377
H	1.78078836	2.24622478	0.37656874
H	2.21375670	2.02560086	-1.31478617
C	-1.23354415	-2.66534232	-0.85672097
H	-2.08822572	-3.32121986	-0.62707007
H	-1.46146453	-2.12324364	-1.77161454
H	-0.38266224	-3.33614377	-1.00379015
H	0.44282438	0.41398597	1.47092696
C	1.62587650	-0.58126063	-1.63764430
H	2.41894595	-0.21941092	-2.29629703
H	0.67729099	-0.45661299	-2.16382067
H	1.79685977	-1.65156743	-1.49151942
H	-1.55126748	-0.06704331	1.37795681
H	-0.89001360	-2.06676829	2.46311074
H	1.55490486	-2.31457358	0.65040550
C	0.08993141	1.98508204	-0.92480986
H	-0.18599385	1.60544592	-1.90702118
C	-0.76111357	2.94339360	1.25389311
H	-1.40431822	3.82834105	1.31277953
H	-1.09442974	2.28310503	2.06645887
H	0.25799036	3.26833001	1.46555145
H	-2.99431248	1.96590494	0.34827763
H	-2.69504471	2.25055246	-1.35595509

Table S39. Cartesian coordinate of **A1J**.

C	3.591510894	0.033592486	0.659328528
H	4.30806132	0.651045765	0.111126049
H	3.635272167	0.316189909	1.714925117
H	3.925859205	-1.003346544	0.574548138
C	2.183190924	0.187541567	0.091510061
C	1.133892619	-0.600629368	0.905161803
C	0.942420605	-2.088001012	0.694849011
H	1.646615998	-2.624640133	1.340571825
C	-0.490677374	-2.591173485	1.020890325
H	-0.510307591	-3.673202062	0.862697771
C	-1.491042397	-1.884852515	0.147846462
C	-2.09313675	-0.786458483	0.633494148
C	-2.873617081	0.247226628	-0.10644708
H	-2.797246344	0.119575189	-1.188700788
H	-3.941801869	0.194904695	0.139738584
C	-2.427277372	1.662419521	0.286364315
C	-0.9972867	2.070886513	0.001692622
C	1.647332132	1.62272407	0.28069896
H	1.916991116	2.017355045	1.267512756
H	2.024648578	2.318361775	-0.480268175
C	-1.639541728	-2.400704686	-1.252459795
H	-2.095931811	-3.396167146	-1.227469775
H	-2.269033914	-1.771295836	-1.881418216
H	-0.670595694	-2.518593595	-1.748707834
H	1.215355588	-0.354601353	1.970882016
C	2.157523552	-0.172653044	-1.395305838
H	2.795897733	0.511559108	-1.960677468
H	1.148068026	-0.120287391	-1.815490368
H	2.541260795	-1.180446064	-1.564901559
H	-1.955821221	-0.574604467	1.695404462
H	-0.708270327	-2.412431788	2.078319794
H	1.184434704	-2.358018404	-0.335487733
C	0.185025533	1.566927833	0.164460282
H	0.1440041	-0.086538107	0.587747786
C	-0.838294155	3.506372344	-0.543687513
H	-1.357213484	3.55182865	-1.5038847
H	-1.322853367	4.179045828	0.168468624
H	0.191550929	3.83069754	-0.683231462
H	-2.570946841	1.806310533	1.364539528
H	-3.068241468	2.396124115	-0.207529676

Table S40. Cartesian coordinate of **A1T**.

C	3.108753878	0.007685757	0.481185454
H	3.805660425	0.630130465	-0.087367111
H	3.022013026	0.439690994	1.482134419
H	3.5375088	-0.992881353	0.56226211
C	1.755299174	0.002931813	-0.287141772
C	0.851523691	-0.681675373	0.711426327
C	1.099805023	-2.072018265	1.262499879
H	1.707545069	-2.068800104	2.171495426
C	-0.377444918	-2.410628249	1.428036067
H	-0.635964383	-3.464699226	1.310608715
C	-0.886323633	-1.553761963	0.26137437
C	-1.671666617	-0.428024775	0.497182904
C	-2.575495189	0.293620635	-0.438562808
H	-2.391723374	0.017800224	-1.477505892
H	-3.58930643	-0.076677283	-0.2105849
C	-2.499413122	1.810693924	-0.20811097
C	-1.050028889	2.233452348	-0.061382731
C	1.346303476	1.486870773	-0.528781248
H	1.637401986	2.088725406	0.336390781
H	1.92727052	1.853826882	-1.382797027
C	-0.924944491	-2.261509272	-1.068299594
H	-1.792379459	-2.93046249	-1.075768603
H	-1.016254262	-1.588330162	-1.92021989
H	-0.043067459	-2.885600295	-1.217149758
H	0.531502341	0.007538156	1.493622169
C	1.954286463	-0.735023976	-1.612260463
H	2.792558455	-0.285216953	-2.149124174
H	1.079211404	-0.667841276	-2.260411101
H	2.193567706	-1.790876368	-1.466875185
H	-1.719319805	-0.076945645	1.529002886
H	-0.771085951	-2.062241448	2.385793043
H	1.581526232	-2.720272222	0.528364463
C	-0.119557704	1.5659993	-0.765941924
H	-0.473131621	0.881553725	-1.533864607
C	-0.773736274	3.326239634	0.924686806
H	-1.337184528	4.222536304	0.641971252
H	-1.113159339	3.058447504	1.931882305
H	0.278264332	3.606991017	0.972785038
H	-3.031582978	2.062308723	0.715494484
H	-3.017452551	2.348486745	-1.008938152

Table S41. Cartesian coordinate of **A2U**.

C	3.12826750	-0.93500920	-1.28956161
H	3.72042699	-1.78191581	-0.93745982
H	2.42979941	-1.31004090	-2.04021074
H	3.81032714	-0.23384917	-1.77792294
C	2.40862681	-0.27964626	-0.10504132
C	1.67237172	0.92427330	-0.52673826
C	0.87308737	1.80837731	0.27933180
H	1.61680105	2.63467295	0.38140949
C	-0.37804574	2.48290800	-0.39583457
H	-0.47160764	3.48485948	0.02817498
C	-1.60726329	1.65693840	-0.12182584
C	-1.94421585	0.69700277	-0.99623869
C	-2.93178088	-0.41260787	-0.83669257
H	-3.51521330	-0.30400562	0.07983667
H	-3.64702811	-0.42423192	-1.66584258
C	-2.16431903	-1.76069575	-0.83045254
H	-1.76571460	-1.94659801	-1.83279987
H	-2.86393461	-2.57247058	-0.60728901
C	-1.03310420	-1.73648689	0.17016669
C	0.22528456	-1.50329823	-0.24948212
C	1.44453803	-1.26300174	0.60659046
H	2.01017042	-2.18242063	0.80402538
H	1.16409155	-0.85820563	1.58239724
C	-2.30991732	1.95472146	1.17102598
H	-2.70319730	2.97691026	1.15870041
H	-3.14867255	1.28574719	1.35902217
H	-1.63360538	1.89180851	2.03147928
H	1.86125191	1.28542463	-1.54343860
C	3.48114451	0.24704650	0.91042563
H	4.06473381	-0.62205550	1.22399062
H	3.02325380	0.69704100	1.79250927
H	4.16519678	0.96233122	0.44861484
C	-1.42377009	-1.91675012	1.60430133
H	-1.84043514	-2.92006716	1.74570627
H	-0.59485164	-1.80569600	2.30369142
H	-2.21331833	-1.21441066	1.89067988
H	-1.33995440	0.62263083	-1.90278400
H	-0.19292447	2.59651040	-1.46732238
H	0.39248895	-1.49041012	-1.32605018
H	0.66329653	1.42898660	1.27992783

Table S42. Cartesian coordinate of **A3G2**.

C	1.99230307	0.31150992	1.38187495
H	2.64456089	1.13387381	1.68566869
H	0.96729382	0.62522603	1.58305505
H	2.23547813	-0.54301059	2.01898918
C	2.23676202	0.00454162	-0.09397560
C	1.46334114	-1.20683482	-0.62775559
C	0.57083061	-2.13674705	-0.06718622
H	0.31276325	-2.93805329	-0.76222869
C	-0.28154325	-2.11261820	1.14642733
H	-0.41634183	-3.14322146	1.49166783
C	-1.61213315	-1.52471140	0.63288373
C	-1.77130544	-0.20442539	0.80955184
C	-2.77153726	0.74309143	0.22681602
H	-3.65794090	0.23820749	-0.16150076
H	-3.11505578	1.42772626	1.00822935
C	-2.10294537	1.55248267	-0.92722603
C	-0.65842583	1.88258987	-0.62025576
C	1.80873226	1.21721144	-0.99267952
H	2.15015588	2.13202291	-0.50208772
H	2.35078111	1.15883048	-1.94272533
C	-2.55832506	-2.45749977	-0.06059121
H	-2.89321978	-3.23777148	0.63099206
H	-3.44420689	-1.93458367	-0.42043609
H	-2.10814975	-2.96795967	-0.91892213
H	1.83823287	-1.53814733	-1.59775490
C	3.72936978	-0.29547912	-0.30289784
H	4.31754658	0.58698223	-0.03869398
H	3.95517632	-0.54299246	-1.34379820
H	4.06521836	-1.12154526	0.32950753
H	-1.00371783	0.29017053	1.39854746
H	0.12996098	-1.50865172	1.95113012
H	0.35929942	-0.79069179	-0.88515249
C	0.32921926	1.23246988	-1.27391197
H	0.01420274	0.64356028	-2.14012164
C	-0.43404303	2.91040945	0.44612478
H	-0.86335206	3.86419859	0.12014634
H	-0.94967060	2.65152982	1.37760966
H	0.61797461	3.07761371	0.67378261
H	-2.68220554	2.46477944	-1.10413221
H	-2.14922879	0.95528962	-1.84242963

Table S43. Cartesian coordinate of **BC**.

C	3.108753878	0.007685757	0.481185454
H	3.805660425	0.630130465	-0.087367111
H	3.022013026	0.439690994	1.482134419
H	3.5375088	-0.992881353	0.56226211
C	1.755299174	0.002931813	-0.287141772
C	0.851523691	-0.681675373	0.711426327
C	1.099805023	-2.072018265	1.262499879
H	1.707545069	-2.068800104	2.171495426
C	-0.377444918	-2.410628249	1.428036067
H	-0.635964383	-3.464699226	1.310608715
C	-0.886323633	-1.553761963	0.26137437
C	-1.671666617	-0.428024775	0.497182904
C	-2.575495189	0.293620635	-0.438562808
H	-2.391723374	0.017800224	-1.477505892
H	-3.58930643	-0.076677283	-0.2105849
C	-2.499413122	1.810693924	-0.20811097
C	-1.050028889	2.233452348	-0.061382731
C	1.346303476	1.486870773	-0.528781248
H	1.637401986	2.088725406	0.336390781
H	1.92727052	1.853826882	-1.382797027
C	-0.924944491	-2.261509272	-1.068299594
H	-1.792379459	-2.93046249	-1.075768603
H	-1.016254262	-1.588330162	-1.92021989
H	-0.043067459	-2.885600295	-1.217149758
H	0.531502341	0.007538156	1.493622169
C	1.954286463	-0.735023976	-1.612260463
H	2.792558455	-0.285216953	-2.149124174
H	1.079211404	-0.667841276	-2.260411101
H	2.193567706	-1.790876368	-1.466875185
H	-1.719319805	-0.076945645	1.529002886
H	-0.771085951	-2.062241448	2.385793043
H	1.581526232	-2.720272222	0.528364463
C	-0.119557704	1.5659993	-0.765941924
H	-0.473131621	0.881553725	-1.533864607
C	-0.773736274	3.326239634	0.924686806
H	-1.337184528	4.222536304	0.641971252
H	-1.113159339	3.058447504	1.931882305
H	0.278264332	3.606991017	0.972785038
H	-3.031582978	2.062308723	0.715494484
H	-3.017452551	2.348486745	-1.008938152

Table S44. Cartesian coordinate of **BG1**.

C	2.52155962	0.47112391	1.20018868
H	3.27826336	1.21141694	0.92845742
H	1.65006557	1.00525116	1.58675930
H	2.93521547	-0.13284771	2.01382965
C	2.16487199	-0.41037687	-0.00487095
C	1.15350609	-1.48250098	0.52234621
C	-0.11595297	-1.86268384	-0.13780448
H	1.65881961	-2.46804540	0.47989920
C	-1.16273516	-2.57623040	0.56310907
H	-1.61800722	-3.42380335	0.05513265
C	-1.90681059	-1.27872225	0.21724647
C	-1.69486863	-0.15869253	0.96977366
C	-2.36446948	1.16269911	0.81070091
H	-3.44079403	1.02892613	0.66167906
H	-2.22980123	1.73006214	1.73388097
C	-1.80660800	1.99782772	-0.39310095
C	-0.29996176	1.96672017	-0.46033552
C	1.67397871	0.47484103	-1.19299750
H	2.37141561	1.31685374	-1.25642483
H	1.81014901	-0.08656030	-2.12380348
C	-2.87352499	-1.36753918	-0.92687097
H	-3.76070760	-1.92253171	-0.60511581
H	-3.19225004	-0.39090994	-1.28658316
H	-2.44814152	-1.91619415	-1.77183378
H	0.97498920	-1.34942568	1.59411604
C	3.43928895	-1.12903553	-0.47443406
H	4.17991604	-0.40499885	-0.82404808
H	3.23254025	-1.81539455	-1.30182373
H	3.89857968	-1.70125081	0.33733199
H	-0.95029179	-0.22820833	1.75880077
H	-0.99402736	-2.75468607	1.62260894
H	-0.15813605	-1.85203052	-1.22410139
C	0.25393530	0.94445884	-1.13293267
H	-0.44672470	0.33338157	-1.69948639
C	0.43375927	3.04472849	0.27888739
H	0.12472350	4.02354543	-0.10328122
H	0.20100497	3.04565683	1.35030380
H	1.51500621	2.97043942	0.16913167
H	-2.19239500	3.01404438	-0.27552574
H	-2.22667722	1.60095862	-1.32027241

Table S45. Cartesian coordinate of **BG2**.

C	1.99234836	0.38810394	1.38782132
H	2.58842339	1.26743778	1.64599172
H	0.95157062	0.64495222	1.58403848
H	2.29127634	-0.41336786	2.07009426
C	2.24704946	0.01113545	-0.06990695
C	1.65910967	-1.40165836	-0.43891095
C	0.29794992	-1.94521603	-0.23323673
H	-0.19880325	-2.28471078	-1.14078164
C	-0.35483726	-2.37208737	0.99649887
H	-0.55387013	-3.44643569	1.04791243
C	-1.61116481	-1.60474260	0.58593360
C	-1.65332666	-0.27745293	0.86542404
C	-2.66955382	0.72636668	0.47185062
H	-3.63442163	0.28169135	0.22335121
H	-2.82858899	1.41571745	1.30656432
C	-2.14394635	1.53352344	-0.76838062
C	-0.68870921	1.89427169	-0.63269838
C	1.70478474	1.08580226	-1.05469090
H	2.07773392	2.05345505	-0.70580951
H	2.17135386	0.91080822	-2.03110190
C	-2.67307415	-2.38417671	-0.12425041
H	-3.21972020	-2.99326219	0.60438583
H	-3.38787596	-1.74679676	-0.64303890
H	-2.25266816	-3.08153948	-0.85534271
H	2.26528694	-2.10961149	0.15294714
C	3.76286980	-0.10716439	-0.28369227
H	4.23271930	0.87093774	-0.15385180
H	4.00552558	-0.45857488	-1.29054638
H	4.21970089	-0.79109097	0.43723525
H	-0.80162917	0.12270146	1.40348485
H	0.12467095	-2.02377855	1.91087269
H	1.89330914	-1.55513778	-1.49571645
C	0.22116176	1.09229025	-1.21349642
H	-0.17147467	0.31478576	-1.87003039
C	-0.37555681	3.06992099	0.24435289
H	-0.82568766	3.97758125	-0.17107924
H	-0.80173826	2.94867944	1.24751941
H	0.69314917	3.24948140	0.35683668
H	-2.77579065	2.42078711	-0.87009669
H	-2.29255028	0.91698755	-1.65859389

Table S46. Cartesian coordinate of **CD**.

C	2.40050859	1.15046799	1.21982450
H	3.09884843	1.93205040	0.91461357
H	1.47589958	1.62988595	1.54452867
H	2.83902723	0.62973327	2.07575575
C	2.14491940	0.19077530	0.05284730
C	1.27781967	-0.91373882	0.49363596
C	0.79450304	-2.08416082	-0.23520817
H	1.63650344	-2.79713103	-0.08129899
C	-0.48472362	-2.66331871	0.38758484
H	-0.71852407	-3.61166087	-0.10156003
C	-1.62244650	-1.66522809	0.23650298
C	-1.70172650	-0.61123931	1.06845091
C	-2.57182382	0.60540816	0.89540396
H	-3.62527904	0.31366023	0.81865580
H	-2.49789328	1.22357350	1.79369195
C	-2.23207218	1.46815310	-0.35414201
C	-0.76936569	1.82186918	-0.45625223
C	1.54988933	0.92896480	-1.17870284
H	1.99523172	1.92712193	-1.20676640
H	1.85373691	0.42790813	-2.10210968
C	-2.52703737	-1.89727202	-0.93080414
H	-2.96243086	-2.90091656	-0.86840515
H	-3.34655235	-1.18192988	-0.98496667
H	-1.97746763	-1.86451748	-1.88140299
H	1.14946244	-0.99958457	1.57685354
C	3.48705984	-0.54181806	-0.30503971
H	4.19728157	0.24598649	-0.57053294
H	3.37203871	-1.21180277	-1.15830478
H	3.90306599	-1.09193092	0.54250944
H	-1.04958966	-0.60611547	1.94306415
H	-0.30897754	-2.88708835	1.44553315
H	0.72736954	-1.93117937	-1.31438802
C	0.04358313	0.95687245	-1.09367579
H	-0.44661013	0.12548730	-1.59358580
C	-0.34358989	3.10596593	0.18813367
H	-0.89413314	3.93755273	-0.26436194
H	-0.59190454	3.12303045	1.25549342
H	0.72065783	3.31601075	0.07965949
H	-2.84406971	2.37414344	-0.31179135
H	-2.53533384	0.92538464	-1.25290241

Table S47. Cartesian coordinate of **CE**.

C	1.89614392	1.19098690	1.29694470
H	2.60286942	1.99886019	1.09590129
H	0.91515378	1.63656146	1.46098141
H	2.21117994	0.70137502	2.22335331
C	1.87669614	0.19844732	0.13005261
C	1.03023565	-0.98825713	0.49145038
C	0.84522023	-2.18872362	-0.39912017
H	1.72363402	-2.83768201	-0.29002360
C	-0.44236646	-2.87718773	0.03363310
H	-0.76266147	-3.63645436	-0.68106515
C	-1.44181669	-1.75243153	0.14758017
C	-1.10876558	-0.67136823	0.94743838
C	-1.94798291	0.59861461	1.03208321
H	-2.93851995	0.30089606	1.40455406
H	-1.52676558	1.22788895	1.82090148
C	-2.10890185	1.45814438	-0.24662938
C	-0.74061725	1.93423713	-0.65479023
C	1.51477342	0.89780997	-1.21524848
H	2.04320365	1.85445800	-1.24199286
H	1.89366243	0.30941020	-2.05646671
C	-2.63458315	-1.82416674	-0.72045837
H	-3.07741761	-2.82224408	-0.61869889
H	-3.38799756	-1.06868468	-0.51073845
H	-2.33598630	-1.75265874	-1.77661614
H	1.19890838	-1.27699315	1.52804343
C	3.29843855	-0.43379153	0.01308872
H	3.99723979	0.38919301	-0.16290802
H	3.37770448	-1.12617185	-0.82686246
H	3.61003762	-0.94100542	0.92996205
H	-0.63517852	-0.93744884	1.89242218
H	-0.32928316	-3.37446618	1.00561754
H	0.78746589	-1.89725631	-1.45108725
C	0.03166184	1.03423870	-1.27916523
H	-0.47783880	0.14916269	-1.65709825
C	-0.31316797	3.28592055	-0.16889833
H	-0.90907185	4.05133096	-0.67857415
H	-0.49591042	3.42177549	0.90304114
H	0.73702148	3.50037648	-0.36811745
H	-2.78695756	2.28462793	-0.01515940
H	-2.57360500	0.88204914	-1.05078920

Table S48. Cartesian coordinate of $\mathbf{D} \alpha$.

C	3.74514445	0.62069737	0.49769478
H	4.47907272	1.16876179	-0.10050258
H	3.46028302	1.25609549	1.34149381
H	4.24471776	-0.26750679	0.89693586
C	2.53941817	0.23522782	-0.34455978
C	1.29895047	-0.29393941	0.44189142
C	0.84176663	-1.70207674	0.77317365
H	1.45308195	-2.15923657	1.55623585
C	-0.61921788	-1.60711968	1.28460446
H	-1.03255854	-2.61054900	1.43075882
C	-1.51576847	-0.82719843	0.31657444
C	-2.79612326	-0.35368722	0.71449280
C	-3.36194921	0.68161927	-0.17498106
H	-4.14260250	0.23957866	-0.81628052
H	-3.90272776	1.42231944	0.42417025
C	-2.12870269	1.25717608	-0.90574852
C	-0.97619071	0.76318176	-0.00425452
C	1.60762620	1.41715254	-0.79227168
H	1.65970619	2.24151101	-0.07625439
H	1.72302334	1.80853511	-1.80548471
C	-1.68743605	-1.62725041	-1.01737247
H	-2.13719970	-2.58959922	-0.76474535
H	-2.31630060	-1.14144844	-1.75935817
H	-0.71292546	-1.82060931	-1.45940598
H	1.31067201	0.27371804	1.38074186
C	2.96766210	-0.64817972	-1.51297150
H	3.69027519	-0.11959595	-2.14080657
H	2.13583778	-0.94702771	-2.15759419
H	3.45215582	-1.55968788	-1.15104642
H	-3.27327771	-0.60953339	1.66394618
H	-0.62357430	-1.12099547	2.26574066
H	0.90598576	-2.36483094	-0.09585021
C	0.40665738	0.46600541	-0.54694811
H	0.29347718	-0.11814742	-1.46240402
C	-0.92846230	1.63833590	1.25599437
H	-0.45109147	2.58559642	0.99289219
H	-1.91844716	1.88288483	1.65148131
H	-0.35292075	1.19833168	2.06916448
H	-2.16692541	2.34702916	-0.95514986
H	-2.03314726	0.89298336	-1.92927931

Table S49. Cartesian coordinate of **DF**.

C	3.62718638	0.58146955	0.59757816
H	4.43061066	1.10782989	0.07273678
H	3.34136837	1.18926033	1.46063290
H	4.03893730	-0.36356990	0.96497254
C	2.45317285	0.34984097	-0.33857800
C	1.12171802	-0.12978637	0.36790870
C	0.62366336	-1.53707368	0.48237960
H	0.92672829	-2.01403109	1.41701515
C	-1.47815505	-2.38793398	1.34892159
H	-2.07828254	-3.28422625	1.18137877
C	-1.03588933	-1.54998153	0.31134220
C	-1.63774627	-0.10517679	0.75233142
C	-2.98991271	0.26839517	0.10359621
H	-3.57410566	-0.52151970	-0.36783933
H	-3.63714419	0.76723817	0.82827242
C	-2.25665546	1.24698041	-0.82962778
C	-0.97177058	1.15787255	0.04602055
C	1.63432497	1.61288535	-0.76152515
H	1.72987954	2.40706237	-0.01648019
H	1.83132488	2.02773044	-1.75203761
C	-1.42764525	-2.04316317	-1.08184335
H	-2.50843232	-2.14213688	-1.18707614
H	-1.07478129	-1.37231839	-1.86321145
H	-0.98480816	-3.02465225	-1.26718206
H	1.11924433	0.33709925	1.35936700
C	2.86764207	-0.50584027	-1.52875243
H	3.64289256	0.01133022	-2.10078760
H	2.04318975	-0.71177397	-2.21753344
H	3.28769225	-1.46272129	-1.20407329
H	-1.61665458	-0.03074068	1.84477527
H	-1.22868529	-2.16130227	2.38342787
H	0.94149467	-2.18417750	-0.33789113
C	0.34817188	0.77977086	-0.58609139
H	0.16632493	0.25182641	-1.52678151
C	-0.87518138	2.31529920	1.03111378
H	-0.64260201	3.23792953	0.49215417
H	-1.82083705	2.47176091	1.55733201
H	-0.09712205	2.16006769	1.78394236
H	-2.68476166	2.24816598	-0.91585071
H	-2.10554391	0.84407573	-1.83398288

Table S50. Cartesian coordinate of **DV**.

C	3.56076097	0.42807823	0.75086904
H	4.40754891	0.96966303	0.32024407
H	3.24045972	0.97282416	1.64383051
H	3.92808641	-0.55515811	1.06314487
C	2.43532272	0.30594360	-0.26350517
C	1.06142966	-0.17119520	0.30180269
C	0.42244952	-1.52319198	0.13335673
H	0.78810364	-2.19852571	1.05464081
C	-0.60153079	-2.27213924	1.32897878
H	-0.65028147	-3.35698699	1.26534370
C	-1.14644140	-1.45403765	0.24035659
C	-1.70731712	-0.06076556	0.62021695
C	-3.01068551	0.39774171	-0.08863975
H	-3.59200948	-0.35179743	-0.62548595
H	-3.68190990	0.88381149	0.62124500
C	-2.21104869	1.40189690	-0.93895701
C	-0.99607201	1.22527852	0.00728243
C	1.67853515	1.62799898	-0.63198578
H	1.75829294	2.36187880	0.17410540
H	1.94466883	2.10370612	-1.57753483
C	-1.85060028	-2.22776689	-0.86283450
H	-2.87276635	-2.46820935	-0.56645989
H	-1.89345854	-1.64105720	-1.78203136
H	-1.33740672	-3.16693477	-1.08454326
H	0.98292013	0.15011911	1.34696576
C	2.89609932	-0.46329692	-1.49768620
H	3.73084548	0.06081143	-1.97009807
H	2.11336109	-0.56577672	-2.25552751
H	3.25386884	-1.46425586	-1.23403761
H	-1.76987696	-0.01092494	1.71165283
H	-0.50386274	-1.83951631	2.32263980
H	0.72807925	-2.17861863	-0.68133286
C	0.34536159	0.84455316	-0.58789990
H	0.18655916	0.39451844	-1.57572795
C	-0.90512756	2.33972221	1.04106453
H	-0.61044024	3.27813088	0.56412353
H	-1.87031172	2.50642264	1.52709908
H	-0.17643314	2.11787496	1.82801246
H	-2.61724666	2.41173950	-1.02493790
H	-2.00907576	1.02920662	-1.94769604

Table S51. Cartesian coordinate of **EQ**.

C	1.77942680	1.38060944	1.11075371
H	2.35462724	2.17595317	0.62925810
H	0.81001713	1.78870259	1.39209607
H	2.29423406	1.12299221	2.04069136
C	1.69212994	0.13616825	0.21434742
C	0.81902303	-0.93519885	0.94599771
C	0.91947889	-2.32714032	0.30013854
H	0.61966787	-3.08993292	1.02540241
C	-0.09914228	-2.28724328	-0.84540655
H	0.35059264	-2.02539843	-1.80730928
C	-1.12379710	-1.27259064	-0.40530293
C	-0.75530281	-0.78351985	0.96180153
C	-1.55966562	0.42756045	1.48303575
H	-2.43031531	0.06751778	2.03919136
H	-0.95796477	0.98157211	2.20679730
C	-2.08562298	1.40660997	0.37949492
C	-0.93224876	1.70803146	-0.50578602
C	1.15626684	0.49165273	-1.21679134
H	1.65191199	1.40632469	-1.55696206
H	1.44545093	-0.27645410	-1.93573116
C	-2.53237194	-1.53979662	-0.84267616
H	-2.78625646	-2.51842251	-0.41367576
H	-3.27604084	-0.83133425	-0.49145552
H	-2.61829582	-1.65355419	-1.92631806
H	1.17827002	-0.97203398	1.97912181
C	3.13450149	-0.36845272	0.04797034
H	3.77883389	0.45491096	-0.27327210
H	3.22969846	-1.15840973	-0.70007001
H	3.53429350	-0.74481842	0.99404165
H	-1.07175948	-1.62661953	1.60802970
H	-0.60002676	-3.24539380	-1.01974419
H	1.92138535	-2.58978734	-0.03263370
C	-0.32670005	0.67428980	-1.17213787
H	-0.98537117	-0.06453144	-1.66506182
C	-0.38974488	3.09771407	-0.48680413
H	-1.11578616	3.72082508	-1.02616253
H	-0.33577629	3.50816175	0.52521443
H	0.57440333	3.20755544	-0.97797129
H	-2.48047922	2.31031038	0.84737395
H	-2.91008950	0.94780695	-0.16505564

Table S52. Cartesian coordinate of **ER**.

C	1.78088566	1.27227326	1.34419975
H	2.57947127	2.00216128	1.18873225
H	0.84410585	1.82369504	1.39680670
H	1.95359504	0.80388577	2.31833471
C	1.79451571	0.22366120	0.22670063
C	0.77003846	-0.91409172	0.57126922
C	0.90007543	-2.13637680	-0.37293299
H	1.68033152	-2.82048043	-0.04105495
C	-0.46695312	-2.81770960	-0.42875095
H	-0.74959606	-3.19366829	-1.41872413
C	-1.44163222	-1.78781176	0.00329932
C	-0.80049747	-0.69269189	0.65990842
C	-1.63904561	0.55392164	1.01615369
H	-2.54757986	0.23048438	1.53713068
H	-1.08336053	1.15195139	1.74001852
C	-2.00869373	1.42864010	-0.20993119
C	-0.70071537	1.96195309	-0.73356749
C	1.55732085	0.90065584	-1.16790990
H	2.10038507	1.84947397	-1.18003000
H	1.98828313	0.28621871	-1.96423805
C	-2.89039823	-1.97293182	-0.18711509
H	-3.18326546	-3.01816147	-0.06628293
H	-3.51015358	-1.32036716	0.42542321
H	-3.08585002	-1.71698555	-1.23924271
H	1.06937106	-1.22298627	1.58083633
C	3.19499337	-0.41263545	0.22350985
H	3.94524888	0.36660857	0.06583997
H	3.32440455	-1.14806126	-0.57392382
H	3.42273066	-0.89612520	1.17888055
H	-1.09028992	-1.44246169	1.52045849
H	-0.56218346	-3.68893306	0.23557744
H	1.17507975	-1.80089259	-1.37636097
C	0.08621463	1.05408828	-1.33084882
H	-0.41379615	0.14960265	-1.68437430
C	-0.30233581	3.34450347	-0.31762837
H	-0.91935450	4.06802400	-0.86301535
H	-0.47813527	3.53420200	0.74708238
H	0.74105030	3.56777179	-0.54055906
H	-2.69466340	2.21526271	0.11649183
H	-2.53504944	0.82919955	-0.96054378

Table S53. Cartesian coordinate of **FL**.

C	3.64381055	0.60139580	0.62069035
H	4.43576815	1.16781945	0.12229720
H	3.32885363	1.17266073	1.49907143
H	4.08168872	-0.33951392	0.96798526
C	2.48273213	0.35019812	-0.32774705
C	1.17007218	-0.18481002	0.32628500
C	0.65658412	-1.61826473	0.36703421
H	0.95643362	-2.12579898	1.28736180
C	-1.71439058	-1.87903907	1.33390612
H	-2.70683244	-2.29391857	1.18341438
C	-0.86125997	-1.66758670	0.22142430
C	-1.72581737	-0.28784264	0.89889132
C	-2.99815162	0.23714886	0.21660597
H	-3.63149475	-0.52595541	-0.23710959
H	-3.61548751	0.77992862	0.93601696
C	-2.25961168	1.14664424	-0.77160256
C	-0.94900853	1.11197103	0.02094544
C	1.63436086	1.59965066	-0.72904973
H	1.69635484	2.38052314	0.03268579
H	1.81588511	2.04038271	-1.71125640
C	-1.37496812	-2.06007273	-1.14082617
H	-2.45736281	-1.98558827	-1.23652768
H	-0.89631975	-1.51109962	-1.95059660
H	-1.11361284	-3.11619000	-1.26832353
H	1.13105223	0.23608924	1.33894771
C	2.94054843	-0.45337290	-1.54061524
H	3.71333394	0.09740804	-2.08351935
H	2.13289858	-0.65945747	-2.24984655
H	3.37543587	-1.41077743	-1.23791688
H	-1.50314203	0.08790213	1.89449119
H	-1.29065117	-2.02942736	2.32085656
H	1.07183431	-2.18583635	-0.47102325
C	0.35753507	0.72515529	-0.59513330
H	0.18154388	0.23158259	-1.55363063
C	-0.86470557	2.22153513	1.04398002
H	-0.64372739	3.14568529	0.49892242
H	-1.80845534	2.37463248	1.57139431
H	-0.06965711	2.06995523	1.77700478
H	-2.66711184	2.15096085	-0.90651722
H	-2.14985397	0.68305920	-1.75419454

Table S54. Cartesian coordinate of **FS**.

C	3.82369283	0.71753038	0.37167945
H	4.57883477	1.23584997	-0.22619830
H	3.57557326	1.35839351	1.22283911
H	4.28206030	-0.19767402	0.75879713
C	2.59682974	0.39930719	-0.46761285
C	1.32302286	-0.03965947	0.33052340
C	0.55321500	-1.30807166	0.73592841
H	0.62443504	-1.49789164	1.80956501
C	-2.03673850	-1.90353649	1.25060465
H	-2.52432686	-2.63390992	0.61723075
C	-0.90308435	-1.00491223	0.27014940
C	-2.36325201	-0.54934225	1.20109002
C	-3.22730960	0.19572657	0.20168513
H	-3.85870538	-0.48414777	-0.37186983
H	-3.89821718	0.85187457	0.76249529
C	-2.23358211	0.98423000	-0.69834224
C	-0.88786394	0.78624090	-0.00112468
C	1.70714791	1.63629460	-0.88770824
H	1.79817764	2.44334077	-0.15632690
H	1.83699049	2.03604819	-1.89485766
C	-1.21598654	-1.68164400	-1.08391133
H	-2.26544906	-1.61806009	-1.37006933
H	-0.62783651	-1.25926556	-1.89515165
H	-0.95475984	-2.73992826	-1.02161572
H	1.38723177	0.58004559	1.22984485
C	2.97511720	-0.49487002	-1.64345257
H	3.71097006	0.00753494	-2.27705722
H	2.12716318	-0.76079771	-2.28095012
H	3.42942502	-1.42437077	-1.28834220
H	-2.05082676	0.01592111	2.07083191
H	-1.55618006	-2.28965108	2.14257776
H	0.88029163	-2.21878890	0.22692487
C	0.47229702	0.71872580	-0.66623231
H	0.39113132	0.15541501	-1.59348450
C	-0.83086368	1.70189274	1.23177771
H	-0.31410186	2.61594663	0.92570839
H	-1.81940152	2.00978648	1.57750005
H	-0.28292402	1.29396786	2.08200510
H	-2.48016703	2.04659079	-0.76401964
H	-2.23692640	0.59359488	-1.71665485

Table S55. Cartesian coordinate of **G1H**.

C	-3.42519521	0.19918744	-0.87609174
H	-4.22835645	0.68997724	-0.31977371
H	-3.19818611	0.82127615	-1.74730618
H	-3.80769947	-0.76173693	-1.23267655
C	-2.19544599	0.01706761	0.02582967
C	-1.06109464	-0.51828435	-0.89306836
C	0.11334365	-1.20815503	-0.14682652
C	0.55034248	-2.60071847	-0.61704428
H	0.30753319	-3.46060810	0.00002472
C	1.77516968	-1.87124140	-0.26868432
C	1.71030717	-0.59034477	-0.84201868
C	2.57835488	0.57867739	-0.42177085
H	3.56031141	0.19633960	-0.12535602
H	2.74970305	1.18648080	-1.31257436
C	2.02903679	1.48898953	0.70361112
C	0.63468216	1.94844736	0.37324122
C	-1.82407863	1.40895644	0.62888090
H	-2.01223390	2.17349689	-0.12925667
H	-2.50644011	1.61418892	1.46049425
C	2.56988714	-2.22545691	0.93322225
H	3.32527434	-2.94575502	0.59255742
H	3.08398002	-1.37959718	1.38570858
H	1.96612460	-2.74314318	1.68166799
H	-1.48647059	-1.27325142	-1.56156077
C	-2.55151654	-0.97963037	1.13549446
H	-3.47543308	-0.66835962	1.62907014
H	-1.78987791	-1.04855607	1.91829645
H	-2.72100661	-1.98380685	0.73329173
H	1.32418856	-0.54897302	-1.85805994
H	0.34282018	-2.75232715	-1.67465940
H	0.06958777	-1.10019656	0.93042047
C	-0.39730806	1.43809134	1.06275365
H	-0.15899199	0.85205379	1.95126396
C	0.51077256	2.86865651	-0.80995106
H	1.21148783	3.70337793	-0.70575020
H	0.75731634	2.37821004	-1.76018180
H	-0.48760417	3.29281926	-0.91123383
H	2.72861341	2.32579832	0.80412267
H	2.03161344	0.95161874	1.65715152
H	-0.70785546	0.30099140	-1.52044584

Table S56. Cartesian coordinate of **G111**.

C	-3.570757286	0.065528551	-0.541902854
H	-4.138308631	0.773664916	0.068010627
H	-3.497854805	0.478393846	-1.553033902
H	-4.149981478	-0.860018836	-0.600583687
C	-2.182391223	-0.19505267	0.060674395
C	-1.418003556	-1.113439748	-0.926229199
C	-0.277016851	-1.941904726	-0.375495149
C	0.813261109	-2.427447016	-1.222479214
H	1.264961917	-3.397608044	-1.042872568
C	1.138287457	-1.394512238	-0.063947759
C	1.502021967	-0.130246105	-0.604121172
C	2.775766551	0.6046938	-0.242983516
H	3.51122996	-0.062154702	0.209292494
H	3.212638987	1.012436023	-1.158496307
C	2.335110827	1.728103204	0.709248362
C	0.921389729	2.016966391	0.23490027
C	-1.495592484	1.186662811	0.199669187
H	-1.578828215	1.709340763	-0.75753593
H	-2.088427158	1.77412029	0.915401325
C	1.832925353	-1.932310708	1.165747342
H	2.911825848	-2.027870846	1.024558838
H	1.656762287	-1.29106292	2.034308027
H	1.450889765	-2.923901716	1.413782333
H	-2.128127777	-1.845039152	-1.331315455
C	-2.362136341	-0.858109385	1.430606084
H	-2.99180561	-0.236502629	2.0729605
H	-1.417901417	-1.021460784	1.958363165
H	-2.857934227	-1.828750398	1.334061942
H	1.02474275	0.150113064	-1.53802186
H	0.889416878	-2.069748512	-2.243693268
H	-0.572039604	-2.624758378	0.417069858
C	-0.07887098	1.203979748	0.677839721
H	0.143288825	0.581570249	1.542878073
C	0.781803908	3.076955548	-0.805755614
H	0.971047084	4.047819243	-0.331675247
H	1.538751853	2.974844282	-1.590759691
H	-0.203419226	3.121324661	-1.266678994
H	2.991661209	2.59781215	0.650018112
H	2.331219173	1.378160445	1.744566639
H	-1.093950818	-0.526030188	-1.793563806

Table S57. Cartesian coordinate of **G1K**.

C	-3.84632436	0.15844116	-0.62651303
H	-4.43955743	0.88446145	-0.06477470
H	-3.67958540	0.56759886	-1.62738064
H	-4.44779530	-0.74920397	-0.72673998
C	-2.52694012	-0.12396898	0.09543757
C	-1.66029480	-1.05115322	-0.77933283
C	-0.34964953	-1.39985892	-0.23902985
C	0.77749861	-1.93417420	-1.03261480
H	0.70936793	-3.03338260	-0.94389126
C	2.05774489	-1.40812420	-0.40543275
C	2.47028701	-0.22452748	-0.87020525
C	3.21370913	0.81881360	-0.10967006
H	4.02184010	0.42998730	0.51286402
H	3.65003380	1.56610990	-0.77539268
C	2.14033473	1.46617765	0.83384422
C	0.79307393	1.63135788	0.19404134
C	-1.71986146	1.18723187	0.24933205
H	-1.75351232	1.73314331	-0.69687371
H	-2.23215885	1.81826605	0.98701422
C	2.59093842	-2.13358175	0.78975016
H	2.89996667	-3.14617189	0.50850371
H	3.45830734	-1.63271150	1.21966229
H	1.84458279	-2.24634058	1.58555758
H	-2.16844645	-2.03564148	-0.84178208
C	-2.82588727	-0.75697013	1.45898349
H	-3.48046582	-0.10065902	2.03760375
H	-1.93524482	-0.93099361	2.06933663
H	-3.34408145	-1.71330041	1.34383800
H	1.96926383	0.14691324	-1.76400995
H	0.68898153	-1.68002295	-2.09129315
H	-0.29428041	-1.60400089	0.82733488
C	-0.30565658	0.96815440	0.68563176
H	-0.16215667	0.46748525	1.64193761
C	0.71814522	2.59765767	-0.94596692
H	0.45607339	3.58890159	-0.55459559
H	1.67887144	2.70536438	-1.45219000
H	-0.04073223	2.33768611	-1.68495414
H	2.50260897	2.45396726	1.14804587
H	2.04740990	0.84559720	1.72814979
H	-1.58075259	-0.69396809	-1.81141350

Table S58. Cartesian coordinate of **G2I3**.

C	2.12026460	0.17104746	1.46852747
H	2.71074716	1.06744451	1.67808657
H	1.12620081	0.35120099	1.88061432
H	2.56585534	-0.65011152	2.03761057
C	2.14880128	-0.13825354	-0.03399889
C	1.60480555	-1.53715452	-0.39340478
C	0.25412121	-2.12481730	0.00185800
H	0.07985717	-3.00199795	-0.61791497
C	-0.37087703	-2.26900969	1.31824648
H	-0.85703990	-3.20413833	1.57855939
C	-1.13492617	-1.45431623	0.20178950
C	-1.26121164	-0.07583045	0.58034914
C	-2.57118094	0.69044560	0.44869009
H	-3.41800019	0.02548739	0.28082634
H	-2.75144262	1.22451425	1.38595920
C	-2.35812577	1.66917009	-0.71232650
C	-0.87461229	1.95791392	-0.58901018
C	1.48114407	0.98319170	-0.87756008
H	1.83505225	1.94453751	-0.49667314
H	1.88074113	0.90100802	-1.89614370
C	-2.28624585	-2.12592245	-0.51913116
H	-3.21199779	-2.09626559	0.05952941
H	-2.47227119	-1.66496398	-1.49395574
H	-2.05649238	-3.17682629	-0.70070749
H	2.32812136	-2.27265728	-0.01800907
C	3.63267841	-0.15269543	-0.44728475
H	4.07728870	0.84015170	-0.33531671
H	3.75669435	-0.45852626	-1.49026788
H	4.20557573	-0.84401647	0.17653850
H	-0.58149298	0.27895601	1.34236709
H	-0.00049144	-1.70165600	2.16363156
H	1.65900027	-1.62407359	-1.48518042
C	-0.01298505	0.99128848	-1.02714539
H	-0.42045534	0.25871112	-1.72116835
C	-0.49758882	3.16146182	0.20007740
H	-0.75902300	4.05071069	-0.38753573
H	-1.08539070	3.23159724	1.12166091
H	0.55993157	3.21781122	0.44990799
H	-2.97754193	2.56278721	-0.62297143
H	-2.58248223	1.19440959	-1.67126109

Table S59. Cartesian coordinate of **I2O**.

C	3.410157789	-0.465794987	-1.278311022
H	4.090541907	-1.276668558	-1.006252523
H	2.76755937	-0.82566156	-2.0877198
H	4.016717864	0.354399781	-1.673078545
C	2.601097465	-0.013384285	-0.057263261
C	1.734189667	1.200969291	-0.4743293
C	0.427958312	1.327324828	0.169700609
H	2.245157689	2.135641019	-0.161782985
C	-0.635362335	2.243649628	-0.292388448
H	-0.583124575	3.151028491	0.331657551
C	-1.926545959	1.479826245	-0.052178642
C	-2.286342426	0.617791932	-1.014041799
C	-3.061721549	-0.631310867	-0.826931776
H	-3.626723725	-0.643437563	0.106640338
H	-3.760996902	-0.835143101	-1.641784208
C	-1.991196862	-1.781508248	-0.836445813
H	-1.602247668	-1.871416212	-1.853902078
H	-2.512607255	-2.716169271	-0.60055116
C	-0.856165642	-1.596693483	0.128185766
C	0.364723609	-1.170869116	-0.325125708
C	1.657378004	-1.145135641	0.42778486
H	2.177171231	-2.102454389	0.297944193
H	1.480157841	-1.050012474	1.50387701
C	-2.537076218	1.621953632	1.306670938
H	-1.821863885	1.420816668	2.11301978
H	-2.879448695	2.653112859	1.447973883
H	-3.397161957	0.969339021	1.451420694
H	1.630679226	1.306384041	-1.559902121
C	3.558521225	0.361770454	1.079016495
H	4.098438204	-0.521749589	1.429614411
H	3.025815847	0.782989907	1.938339226
H	4.302263079	1.092178295	0.748650811
C	-1.139162885	-1.939180902	1.554379354
H	-1.171436821	-3.030258594	1.663334762
H	-0.391453059	-1.567015516	2.254849392
H	-2.123704523	-1.573477537	1.85899412
H	-1.750371292	0.678510826	-1.961776183
H	-0.49465295	2.540620376	-1.334044279
H	0.450382509	-1.046372468	-1.404307803
H	0.328454347	0.967631066	1.192370264

Table S60. Cartesian coordinate of **I2U**.

C	3.324570201	-0.708122817	-1.212387676
H	4.032666002	-1.46758516	-0.875206772
H	2.753043019	-1.133326411	-2.042271651
H	3.904550868	0.13757754	-1.593554043
C	2.416154374	-0.292760509	-0.047711214
C	1.439664369	0.741365671	-0.556606845
C	0.746730747	1.711792814	0.167249529
H	1.882485898	2.019718168	-0.336181959
C	-0.384989319	2.524360675	-0.403684327
H	-0.408749985	3.517196983	0.050822994
C	-1.638905108	1.71434246	-0.075475757
C	-1.959230965	0.721201277	-0.917769992
C	-2.937783108	-0.394468534	-0.747393048
H	-3.483093311	-0.312461882	0.19506751
H	-3.685504353	-0.38100933	-1.547542619
C	-2.1692999	-1.742302059	-0.81738029
H	-1.83184092	-1.905691455	-1.845708935
H	-2.862059591	-2.554867107	-0.574391467
C	-0.984604594	-1.750573801	0.118961652
C	0.267528653	-1.681863644	-0.369691731
C	1.530893334	-1.500996417	0.426410033
H	2.174099803	-2.387854784	0.373328777
H	1.292045321	-1.343916777	1.47970675
C	-2.344240274	2.072830942	1.198291872
H	-2.730923736	3.095927281	1.139606501
H	-3.19027692	1.416489737	1.399913119
H	-1.677490723	2.038569054	2.067551566
H	1.228116978	0.729857749	-1.627181303
C	3.261205019	0.212702262	1.126833462
H	3.893282016	-0.602440183	1.48522213
H	2.65541688	0.540393126	1.976024566
H	3.924233005	1.030612321	0.827697907
C	-1.333275754	-1.778757021	1.578618431
H	-1.985271009	-2.634342688	1.782363615
H	-0.470479631	-1.864983319	2.238357558
H	-1.896243983	-0.88596963	1.870924372
H	-1.354037493	0.629521573	-1.82185592
H	-0.266775095	2.639599229	-1.484119277
H	0.387066523	-1.754583558	-1.451126112
H	0.913607761	1.749135222	1.243308594

Table S61. Cartesian coordinate of **I4W**.

C	-3.65915691	0.69873639	-0.71942848
H	-4.40394845	1.12035120	-0.03949093
H	-3.31666096	1.49833422	-1.38268025
H	-4.16259268	-0.05286355	-1.33295370
C	-2.50243506	0.07284297	0.05459991
C	-1.42813396	-0.51571390	-0.89196250
C	-0.06045049	-0.51955996	-0.20144232
C	0.79167214	-1.82659238	-0.47177965
H	0.36469425	-2.66621013	0.08428616
C	2.23568032	-1.53971271	-0.21723637
C	2.69491956	-0.57656230	-1.03369024
C	3.25224195	0.70000609	-0.48883873
H	4.15568171	0.60419099	0.11791063
H	3.46446359	1.42452000	-1.27730333
C	2.07824227	1.13982790	0.42721018
C	0.61034390	0.92990812	-0.07605642
C	-1.77448610	1.13870255	0.93762760
H	-1.83198861	2.12563085	0.46893033
H	-2.23988400	1.20637882	1.92234872
C	2.83374051	-1.94350920	1.09372242
H	3.80342594	-1.47429034	1.26683546
H	2.18185230	-1.72440017	1.94927114
H	2.99221295	-3.02777718	1.10628211
H	-1.68876798	-1.54767646	-1.14020498
C	-3.03116508	-1.03861399	0.97195737
H	-3.75958834	-0.64203042	1.68338324
H	-2.23929401	-1.52490811	1.55590540
H	-3.52463784	-1.81730207	0.38544554
H	2.14937968	-0.44475066	-1.96932322
H	0.60874560	-2.00898518	-1.53662854
H	-0.39472757	-0.69559859	0.92965067
C	-0.32715339	0.77661186	1.06140838
H	0.12191883	0.64462088	2.04656033
C	0.27856413	1.91315437	-1.18737538
H	0.56970355	2.91929710	-0.87719650
H	0.85365349	1.66889258	-2.08322291
H	-0.77203656	1.94837553	-1.46815677
H	2.14471791	2.20654745	0.67325037
H	2.19924091	0.59729672	1.36862509
H	-1.37233177	0.02739095	-1.83742774

Table S62. Cartesian coordinate of **KM**.

C	-3.94175796	-0.21656805	-0.64818890
H	-4.53605118	0.64775559	-0.33810826
H	-3.81728114	-0.17081741	-1.73421132
H	-4.52191520	-1.11356215	-0.41675465
C	-2.59389393	-0.24904832	0.06787610
C	-1.69677180	-1.38746163	-0.41651009
C	-0.25264970	-1.00439279	-0.05833724
C	0.77298205	-1.78746030	-0.91022719
H	0.48550141	-2.84283563	-0.86000971
C	2.10138659	-1.48258855	-0.29954673
C	2.66026001	-0.34378798	-0.72185000
C	3.23776394	0.67661990	0.18761371
H	3.37424492	0.28929460	1.19900475
H	4.18998835	1.11577777	-0.12746064
C	2.19634413	1.80533079	0.16577921
C	0.68447662	1.65150871	0.02052333
C	-1.72981142	0.96189485	-0.30105797
H	-1.80499205	1.15436880	-1.38137665
H	-2.05414697	1.86992880	0.20585863
C	2.50886112	-2.25441264	0.91792658
H	3.39343233	-1.84151050	1.40367701
H	1.71001610	-2.33885474	1.66360616
H	2.75652739	-3.27896537	0.61949281
H	-1.96057433	-2.35514873	0.01768101
C	-2.81166603	-0.30940601	1.58429161
H	-3.39956925	0.54616009	1.92871450
H	-1.87357791	-0.31576698	2.15097151
H	-3.35723491	-1.21595900	1.85784231
H	2.32349492	0.04998506	-1.68257971
H	0.71648336	-1.47354002	-1.95669453
C	-0.26923749	0.57388858	-0.04452233
H	0.03816727	0.94650411	1.09178588
C	0.08472900	3.04519439	-0.05348661
H	-0.63120565	3.23613268	0.74807453
H	0.85890484	3.80704031	0.01138032
H	-0.44843757	3.16855914	-1.00007578
H	2.39461672	2.40968064	-0.73342673
H	2.34977159	2.51554983	0.98899053
H	-1.78349279	-1.48563297	-1.50544610
H	-0.07856137	-1.29592189	0.98369162

Table S63. Cartesian coordinate of **M2Z**.

C	-2.57651132	-1.49975259	-1.19409575
H	-2.90178176	-0.98343280	-2.10110778
H	-1.82862821	-2.24731951	-1.47069515
H	-3.43846715	-2.02788495	-0.78127057
C	-2.03137813	-0.51478773	-0.15249812
C	-1.43713271	-1.18426575	1.12096968
C	0.07661559	-0.93785668	1.04599537
C	0.79404761	-1.86770596	0.03832456
H	1.75432346	-2.22492140	0.42628948
C	1.08365704	-0.95805223	-1.14054624
C	1.44729472	0.39681599	-0.51706999
C	2.59755162	0.61862043	0.46171127
H	2.88494398	-0.31226199	0.95797772
H	3.49443935	1.01168382	-0.01952373
C	1.99494159	1.61933865	1.49229997
C	0.44059216	1.67157090	1.29172259
C	-0.88921146	0.30799065	-0.64017872
H	-0.08633400	-0.64418737	-1.46387474
H	-1.00425417	1.00033974	-1.47796078
C	1.75709967	-1.48911785	-2.36589122
H	1.78678864	-0.75639404	-3.17417780
H	2.79616129	-1.71718676	-2.09294337
H	1.30179922	-2.41351458	-2.72594888
H	-1.85012333	-0.71184595	2.01691746
C	-3.14106194	0.51451848	0.19577348
H	-3.53298242	1.00940703	-0.69567667
H	-2.79730918	1.27161815	0.90380914
H	-3.95983357	-0.03529925	0.66861489
H	1.43487580	1.18550791	-1.27754693
H	0.21935132	-2.75398858	-0.23918466
C	0.20857267	0.46699435	0.36370576
H	-0.07402113	1.51385652	2.24469448
C	-0.01756086	3.00444179	0.70361493
H	-1.10128434	3.04422523	0.56083791
H	0.24969081	3.82073743	1.37850471
H	0.46157804	3.21324534	-0.25820714
H	2.40840692	2.62058731	1.34815283
H	2.25380458	1.32474574	2.51129490
H	-1.68161430	-2.24741127	1.18034965
H	0.54770807	-0.96727001	2.02997573

Table S64. Cartesian coordinate of **MY**.

C	-3.57575303	-0.60895188	-1.22999790
H	-4.12201878	0.30161483	-1.49194322
H	-3.21766862	-1.06684629	-2.15688018
H	-4.28863135	-1.29885785	-0.77021673
C	-2.42375165	-0.30597278	-0.27421714
C	-1.58942455	-1.56277606	0.04456765
C	-0.23142436	-1.05143980	0.53862665
C	1.00607895	-1.89141763	0.15800032
H	1.43711141	-2.44865632	0.99221703
C	2.01401602	-0.87227335	-0.42189710
C	1.15263760	0.15602303	-0.96310590
C	2.63795936	0.00311025	0.81373554
H	2.46012360	-0.61514302	1.69639504
H	3.71388769	0.05960132	0.64258855
C	2.05523166	1.40479828	0.98680525
C	0.52948126	1.50287741	0.80534350
C	-1.38033294	0.62524377	-0.93264859
H	-1.28440213	0.36934677	-1.99304907
H	-1.66105479	1.67679907	-0.88529443
C	3.12474333	-1.43017738	-1.29919935
H	3.75270808	-0.63787464	-1.71374278
H	3.76296730	-2.09146859	-0.70933269
H	2.71254254	-2.01556347	-2.12419645
H	-2.08255385	-2.21761924	0.76754687
C	-2.97530861	0.32560865	1.01034537
H	-3.52435830	1.24482147	0.78704457
H	-2.19229770	0.57565470	1.73274755
H	-3.66764704	-0.35979380	1.50640857
H	1.45871692	0.84995310	-1.74822226
H	0.75372845	-2.62011825	-0.61895811
C	-0.04857086	0.30844948	-0.20784368
H	0.02933897	1.20555233	1.73203594
C	0.11242255	2.91131223	0.42716246
H	-0.96451397	3.06437862	0.49503413
H	0.57976721	3.61060872	1.12733540
H	0.44409556	3.19045289	-0.57722900
H	2.53880966	2.08914203	0.28014249
H	2.31382647	1.77452836	1.98340357
H	-1.45162881	-2.14383958	-0.87605956
H	-0.26409909	-0.88929914	1.61968595

Table S65. Cartesian coordinate of **NM**.

C	3.52670660	0.36578387	-1.23199314
H	3.88795145	-0.50773081	-1.78179850
H	3.05654857	1.04716446	-1.94752504
H	4.39962528	0.87319951	-0.81270788
C	2.56167849	-0.03942822	-0.12142574
C	1.98854060	1.18602433	0.65476059
C	0.48764129	0.91565667	0.84114089
H	0.11146661	1.10837788	1.84839292
C	-0.38598649	1.87199966	-0.17597888
H	-0.38372902	2.85063767	0.30878340
C	-1.77572970	1.33486879	-0.42280306
C	-1.91553949	0.40337192	-1.41735471
C	-2.65579763	-0.90239130	-1.32222669
H	-3.54750771	-0.83620537	-0.69434644
H	-2.95445007	-1.29567720	-2.29491770
C	-1.60796406	-1.90571238	-0.65102487
H	-0.87095169	-2.20379943	-1.40010148
H	-2.13503818	-2.80583082	-0.33006578
C	-0.96034029	-1.16752015	0.53106816
C	0.26674191	-0.48161106	0.35162137
C	1.29042062	-0.73691366	-0.68868691
H	0.99134337	-0.24861453	-1.63008499
H	1.41943334	-1.79932807	-0.91056935
C	-2.84826046	1.69853731	0.56683762
H	-2.51099266	1.60804871	1.60377149
H	-3.10919185	2.75125278	0.41450522
H	-3.75976128	1.11475725	0.43703346
H	2.14874081	2.11689787	0.10364060
C	3.25459501	-0.99619882	0.85585437
H	3.58320591	-1.90854139	0.34983799
H	2.59393398	-1.29081321	1.67919962
H	4.13693499	-0.52194326	1.29316995
H	2.49123623	1.30091062	1.61774116
C	-1.58743908	-1.35603826	1.90505390
H	-1.34404321	-2.36442871	2.25183133
H	-1.20685169	-0.64818027	2.64199424
H	-2.67447754	-1.27220041	1.86298991
H	-1.09245912	0.36396204	-2.13412209
H	0.17853786	1.94853142	-1.10824700
H	-1.34584572	-0.09069340	0.19136104

Table S66. Cartesian coordinate of **NO**.

C	3.72622701	0.27713629	-0.98706004
H	4.13577133	-0.63732027	-1.42493859
H	3.45674799	0.95394143	-1.80316454
H	4.52446737	0.75059733	-0.40888915
C	2.52622374	-0.02890490	-0.09229963
C	1.90144891	1.25326044	0.51332995
C	0.39075378	0.97198564	0.68754916
H	0.08042106	1.01637354	1.73332322
C	-0.49969854	2.03194448	-0.14257704
H	-0.52636045	2.97617323	0.40441956
C	-1.85493924	1.41425882	-0.34895956
C	-1.96541598	0.44196647	-1.32436833
C	-2.65002780	-0.88930158	-1.16044184
H	-3.45344455	-0.85894129	-0.42402787
H	-3.06447040	-1.26834113	-2.09543201
C	-1.56122626	-2.00596554	-0.68118239
H	-0.93448371	-2.24566892	-1.54384952
H	-2.10645026	-2.89771255	-0.37075835
C	-0.78338159	-1.36513953	0.41984252
C	0.17285285	-0.40101038	0.03317286
C	1.35669258	-0.63307193	-0.91037166
H	1.24241337	-0.07742580	-1.84874517
H	1.50406708	-1.68673085	-1.15585645
C	-2.84459080	1.60520743	0.74767655
H	-2.39262165	1.52024751	1.74073675
H	-3.20518184	2.63994158	0.67688982
H	-3.71503518	0.95405734	0.67859129
H	2.05549662	2.10208348	-0.16044233
C	2.93839710	-0.99681675	1.02178572
H	3.30135379	-1.94147253	0.60683497
H	2.11052173	-1.22585510	1.70116823
H	3.74392701	-0.56600785	1.62214650
H	2.37688355	1.51485418	1.46161055
C	-1.37666303	-1.43511852	1.77636241
H	-1.14985503	-2.44644618	2.14665714
H	-0.95569767	-0.72358169	2.48394235
H	-2.46840774	-1.36917991	1.76966088
H	-1.35534983	0.56453372	-2.22288180
H	0.00297904	2.20234211	-1.09979860
H	-0.73239137	-0.04592481	-0.69695455

Table S67. Cartesian coordinate of **NX**.

C	3.64438537	0.39050349	-1.07869396
H	4.05869105	-0.47927013	-1.59599352
H	3.28343051	1.09395160	-1.83536609
H	4.46394788	0.87129497	-0.53747706
C	2.53089252	-0.02127379	-0.11753570
C	1.89773086	1.20129570	0.60346203
C	0.39309544	0.88416789	0.76884547
H	0.05066220	0.95924627	1.80124384
C	-0.48123014	1.99280146	-0.09061943
H	-0.48270702	2.92247002	0.47921567
C	-1.82597769	1.42466928	-0.33386586
C	-1.85979082	0.38112969	-1.29718973
C	-2.61010038	-0.93918321	-1.16674590
H	-3.43714691	-0.88028268	-0.45748956
H	-3.02243244	-1.27148258	-2.11997427
C	-1.55960942	-2.04248369	-0.66106545
H	-0.90898659	-2.30840315	-1.49861791
H	-2.10148775	-2.93543748	-0.34540321
C	-0.80268931	-1.37130439	0.45474186
C	0.20653465	-0.48100532	0.13923661
C	1.32991977	-0.64946662	-0.87206168
H	1.15343057	-0.08495710	-1.79857491
H	1.49864981	-1.69257582	-1.14718162
C	-2.89306474	1.69294912	0.65219468
H	-2.51558298	1.74701718	1.67743128
H	-3.26104639	2.70591449	0.42573555
H	-3.74270832	1.01561253	0.58703804
H	2.04680843	2.11437599	0.01926641
C	3.07113841	-1.01755988	0.91393211
H	3.45903615	-1.91502723	0.42377614
H	2.29906404	-1.33126257	1.62359217
H	3.88825965	-0.57076319	1.48656996
H	2.36726095	1.37276280	1.57536046
C	-1.50322015	-1.36430701	1.77223541
H	-1.43162691	-2.38249094	2.17740767
H	-1.06251675	-0.69125875	2.50599839
H	-2.57616191	-1.16430277	1.68584953
H	-1.42149590	0.62518037	-2.26945150
H	0.06338853	2.13886599	-1.02767977
H	-0.82828212	-0.01868666	-0.81904872

Table S68. Cartesian coordinate of **OP**.

C	3.47315582	-0.76584218	-1.16995873
H	4.00698482	-1.65658194	-0.82616009
H	2.79349672	-1.06941984	-1.97346635
H	4.21052622	-0.08265739	-1.60158059
C	2.72069243	-0.09561395	-0.01784058
C	2.00283933	1.20597601	-0.52036190
C	0.58696234	1.09098690	0.02786255
H	0.60071306	1.34065353	1.09785765
C	-0.62517579	1.76050005	-0.60932133
H	-0.79372228	2.78499259	-0.27167128
C	-1.79799758	0.83396120	-0.20096690
C	-2.44656913	0.16395249	-1.28321590
C	-3.11332473	-1.10405539	-0.99042061
H	-3.93234128	-0.96773926	-0.27387264
H	-3.48144003	-1.63521503	-1.86613060
C	-1.90284622	-1.77751880	-0.27222931
H	-1.27201448	-2.29163267	-1.00137639
H	-2.26045077	-2.52468757	0.43941856
C	-1.10779716	-0.61973148	0.41480426
C	0.31144965	-0.40481610	-0.10061537
C	1.56610762	-1.02377103	0.50277162
H	1.72141978	-2.06773071	0.21688004
H	1.52219866	-0.98517646	1.59612083
C	-2.75728002	1.47577387	0.82542036
H	-2.18109092	1.78328138	1.69837308
H	-3.20847451	2.36519145	0.38137286
H	-3.55134654	0.80250820	1.14760796
H	1.97510452	1.22607646	-1.61644153
C	3.69678222	0.22053638	1.11758635
H	4.12177358	-0.69718624	1.53524737
H	3.20435079	0.76088281	1.93269340
H	4.52612064	0.83708112	0.75951657
H	2.52128507	2.11046956	-0.19304642
C	-1.21630256	-0.70941075	1.92467167
H	-0.75563702	-1.65775117	2.22402206
H	-0.68894527	0.08989526	2.44794942
H	-2.25022420	-0.73213721	2.27332129
H	-2.22857237	0.43894086	-2.31883459
H	-0.50830952	1.78988803	-1.69927302
H	0.30128715	-0.62737599	-1.18226177

Table S69. Cartesian coordinate of **WK2**.

C	2.57617459	0.34181731	1.24029186
H	3.05287403	1.32417030	1.29026585
H	1.66632714	0.38043317	1.83566087
H	3.24827718	-0.37391367	1.72154419
C	2.34467872	-0.07896136	-0.21119182
C	1.64656895	-1.42871611	-0.34229480
C	0.15831041	-1.60764796	0.02848253
H	-0.12212684	-2.50934129	-0.51400297
C	-0.37060336	-1.60192618	1.45207751
H	-0.49814345	-2.56063133	1.95274647
C	-1.40602975	-1.16999556	0.50186380
C	-1.97226689	0.23846680	0.44736195
C	-2.87513539	0.65133567	-0.74336113
H	-2.77777066	0.00056509	-1.61462646
H	-3.93771001	0.76555873	-0.52852671
C	-2.05935787	1.94870127	-0.87387973
C	-0.94136021	1.31775571	0.05119027
C	1.42193257	0.91626199	-1.00059471
H	1.61358840	1.93314366	-0.64521148
H	1.69668984	0.84830700	-2.05629724
C	-2.40495610	-2.22218123	0.08983744
H	-3.30794013	-2.07325485	0.69406264
H	-2.70101551	-2.14117027	-0.95775483
H	-2.04585865	-3.23535309	0.27677039
H	2.18901542	-2.18305610	0.24033930
C	3.70782572	-0.14055189	-0.90794024
H	4.20521166	0.83258121	-0.88243113
H	3.61833121	-0.44936403	-1.95317107
H	4.36183641	-0.85470769	-0.40011720
H	-2.46442821	0.46034513	1.40139776
H	0.06262115	-0.83500028	2.08560850
H	1.72484035	-1.74237741	-1.38872167
C	-0.01228367	0.60900887	-0.86048872
H	-0.49207704	0.13670016	-1.71306753
C	-0.37386455	2.23612361	1.11542703
H	0.21404619	3.04870003	0.67972571
H	-1.20092965	2.69669511	1.65994984
H	0.24770302	1.72016412	1.84636311
H	-2.51156536	2.79214129	-0.34886811
H	-1.76705428	2.27880765	-1.87261263

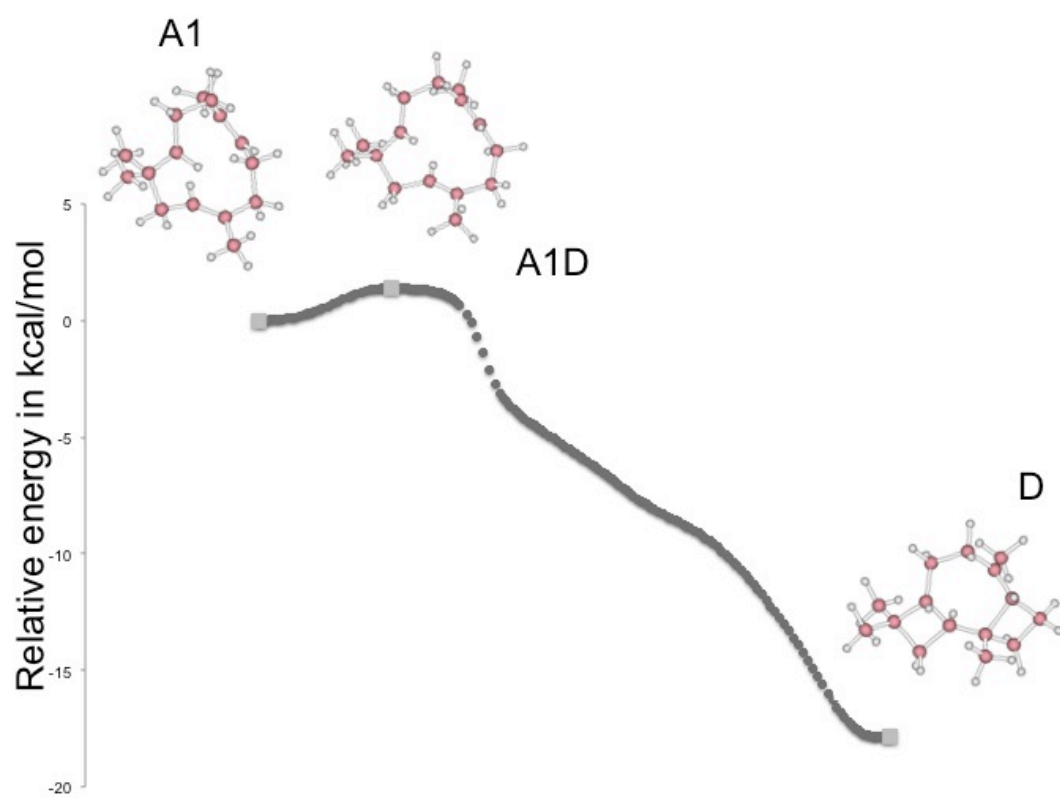


Fig. S1: IRC path from A1 to D.

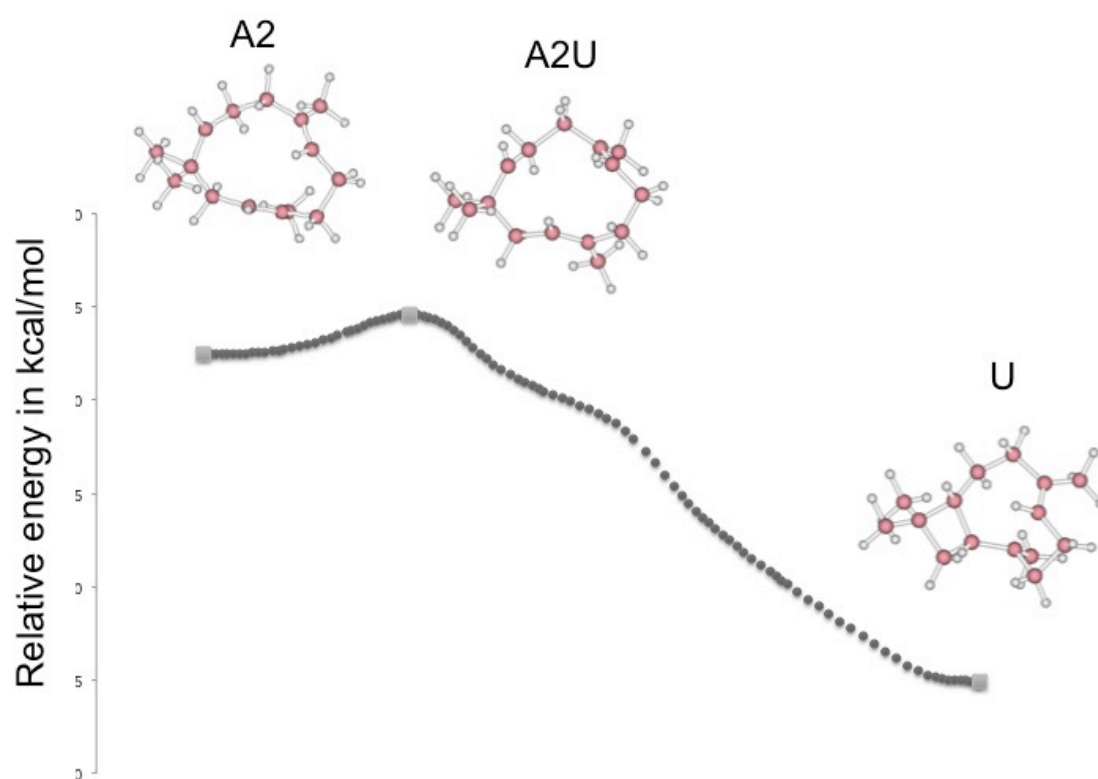


Fig. S2: IRC path from A2 to U.

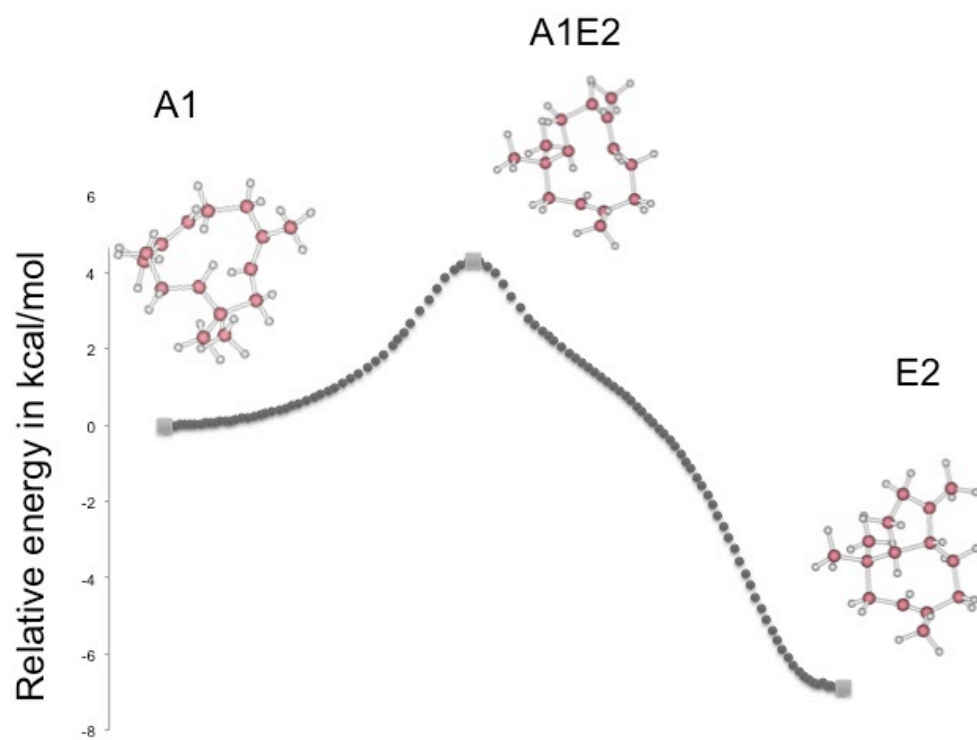


Fig. S3: IRC path from A1 to E2.

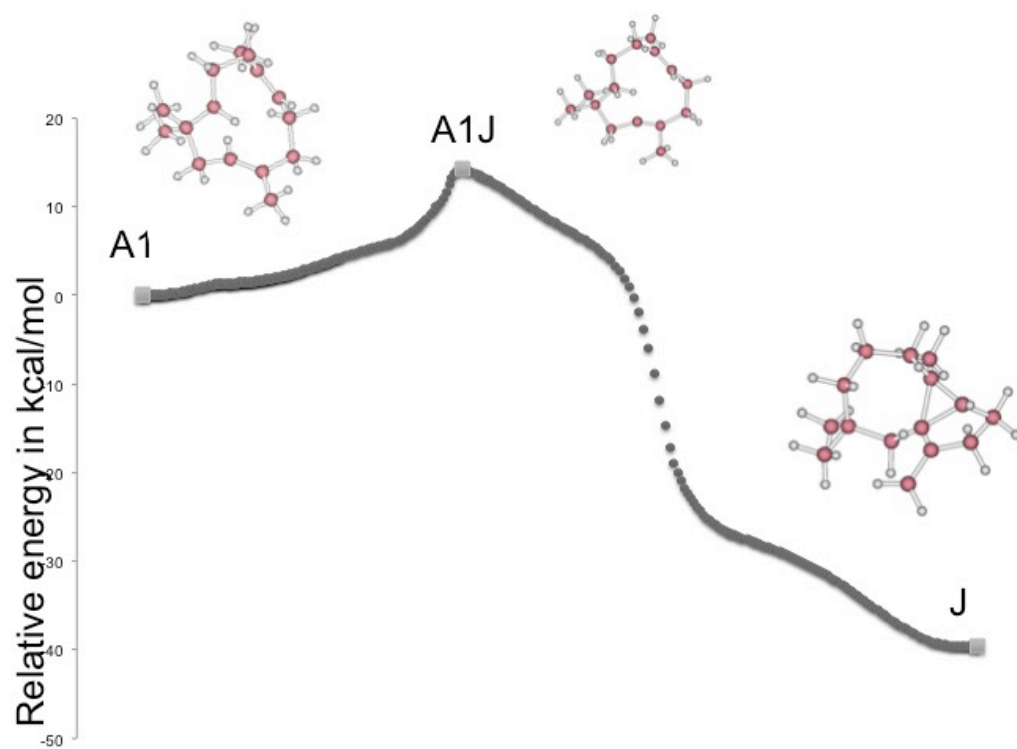


Fig. S4: IRC path from A1 to J.

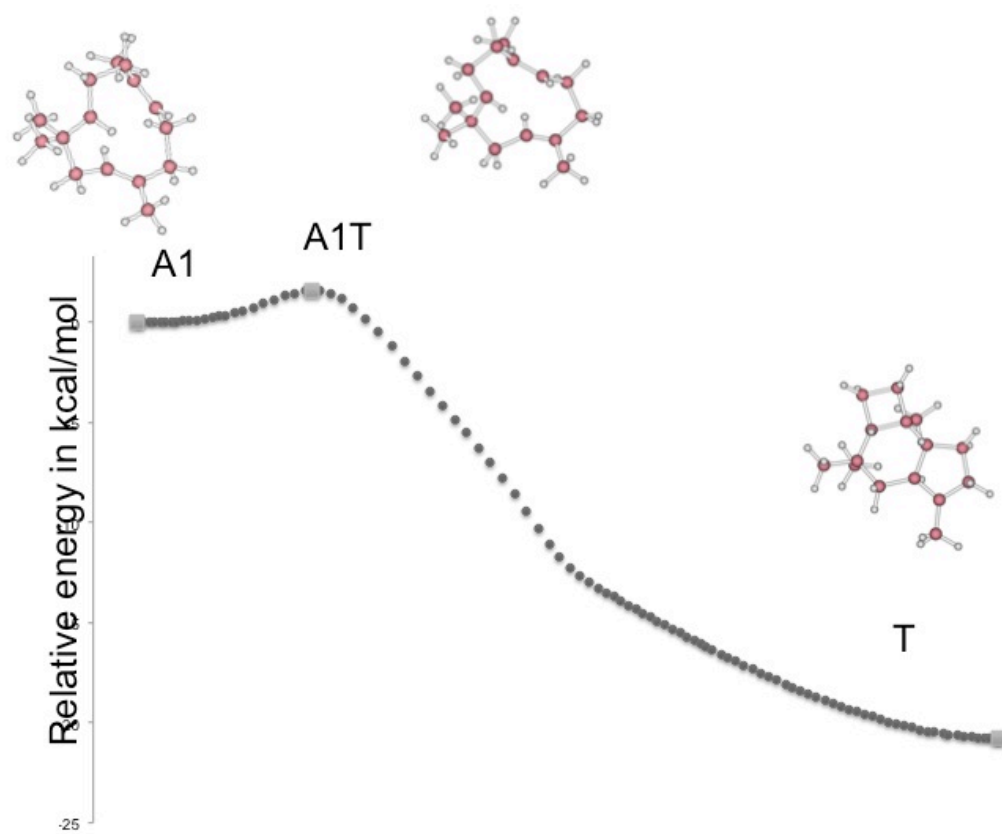


Fig. S5: IRC path from A1 to T.

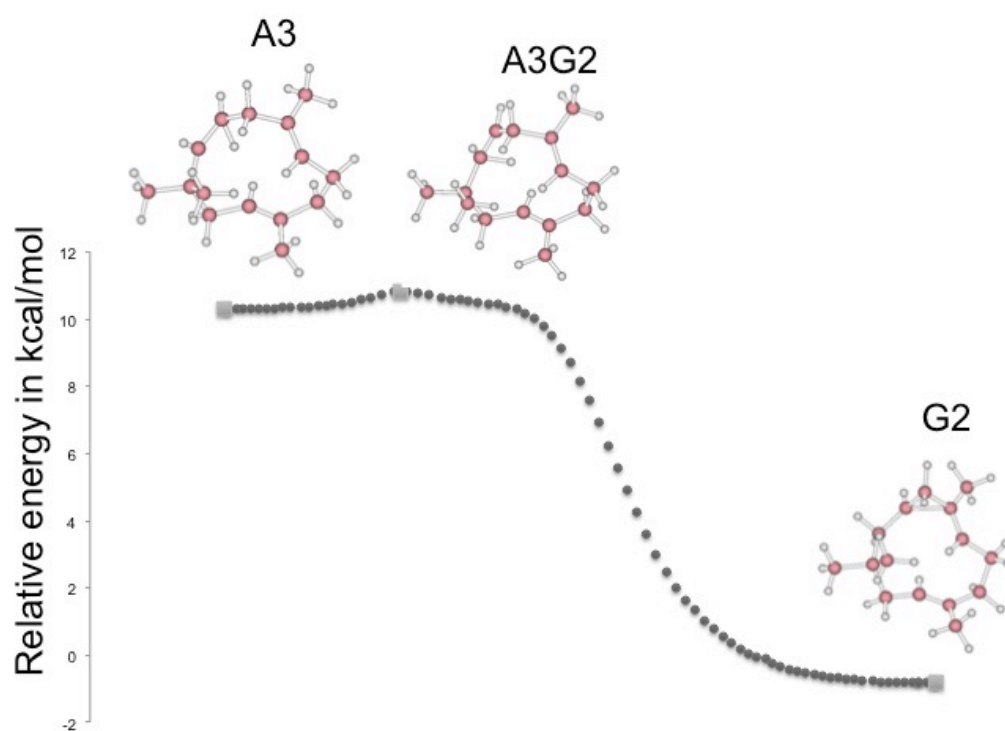


Fig. S6: IRC path from A3 to G2.

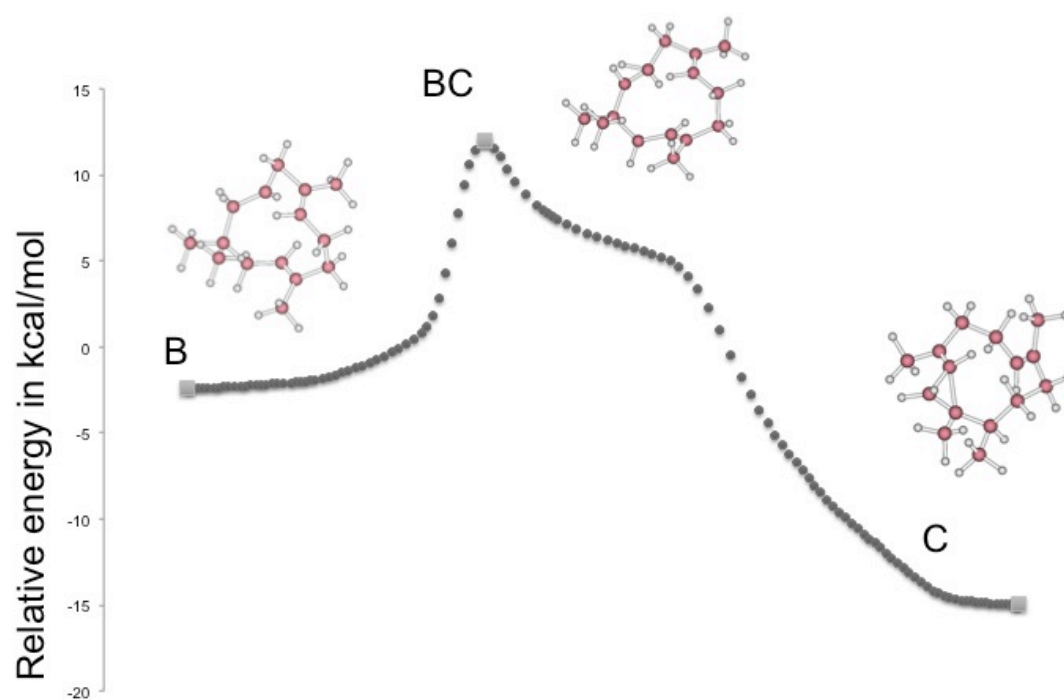


Fig. S7: IRC path from B to C.

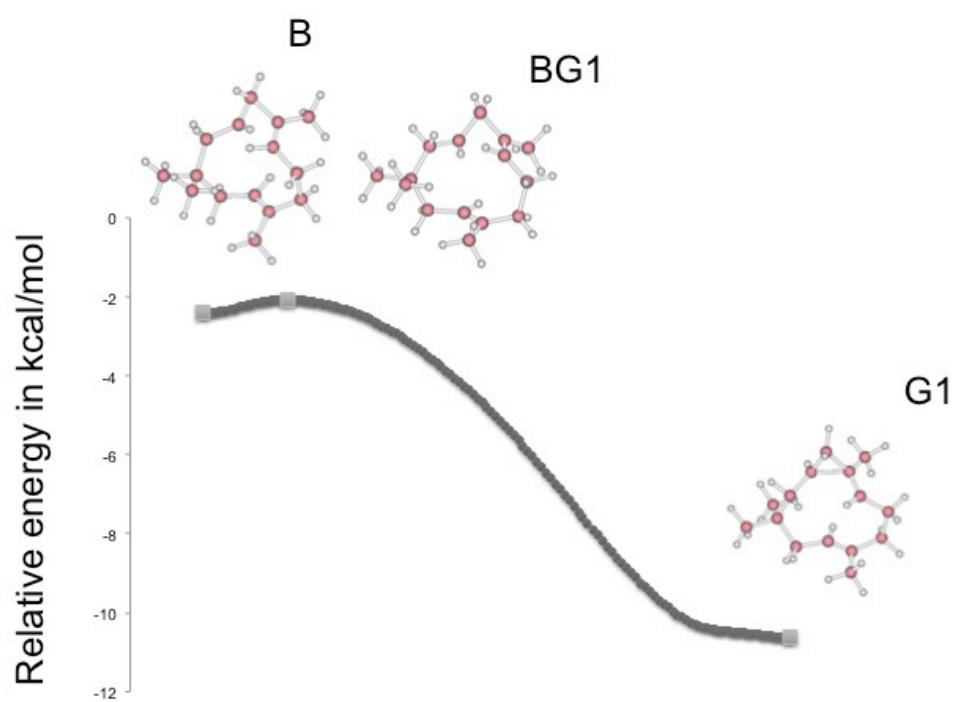


Fig. S8: IRC path from B to G1.

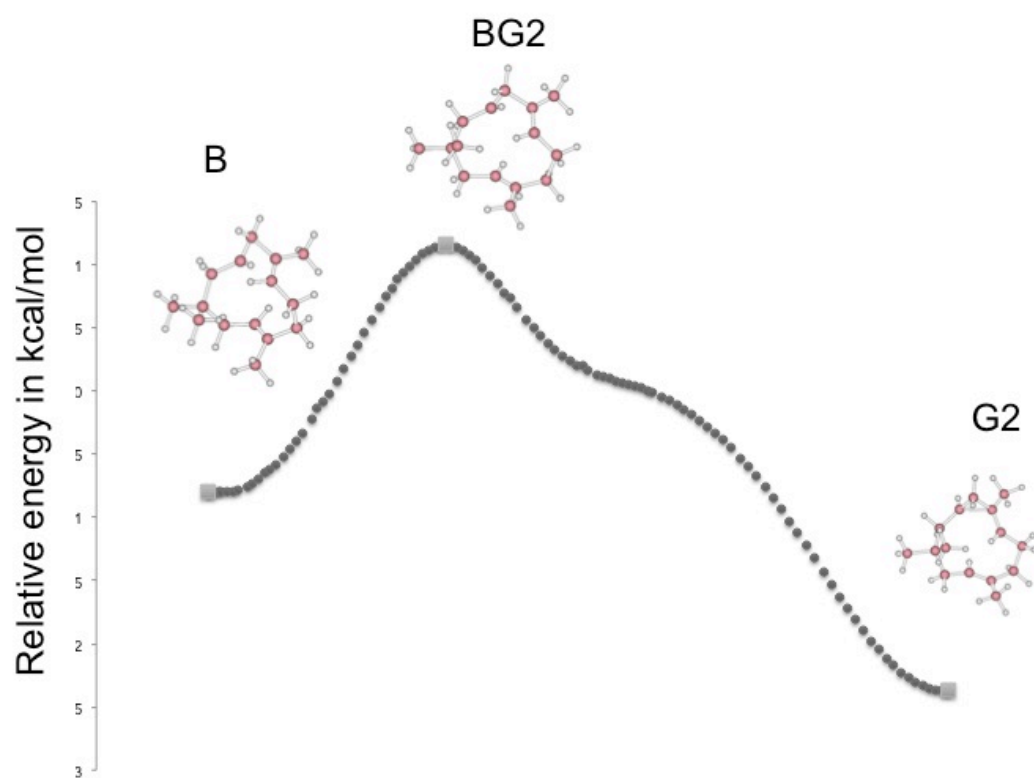


Fig. S9: IRC path from B to G2.

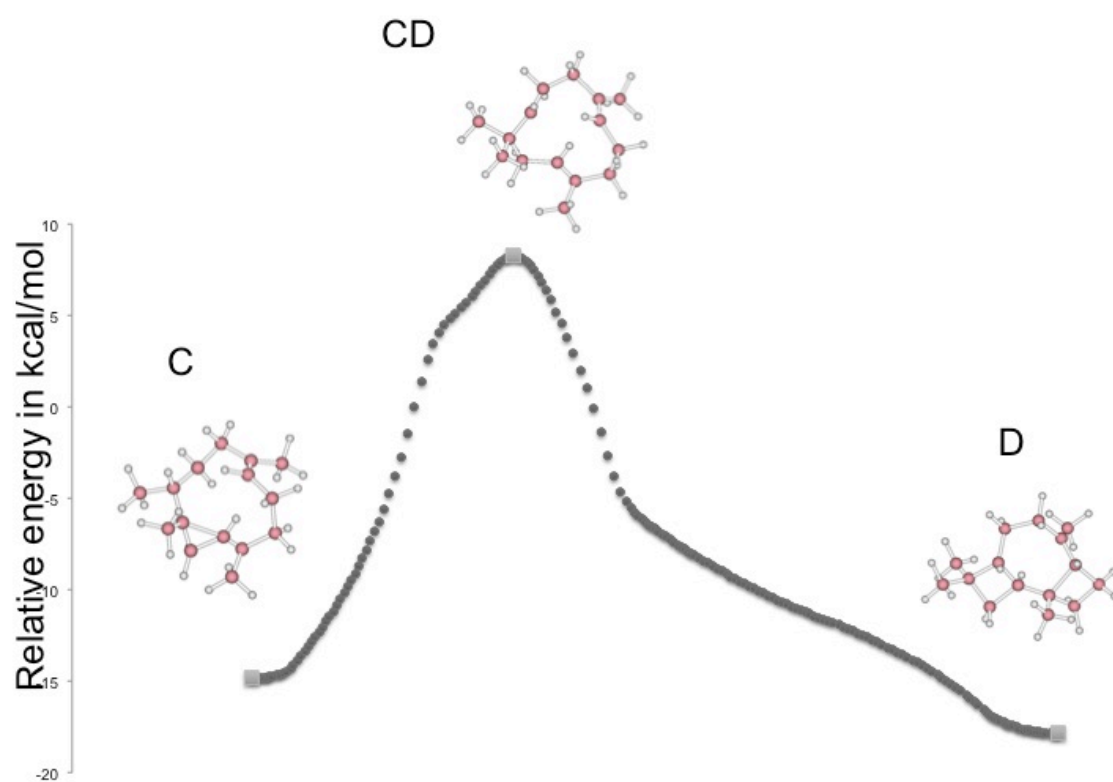


Fig. S10: IRC path from C to D.

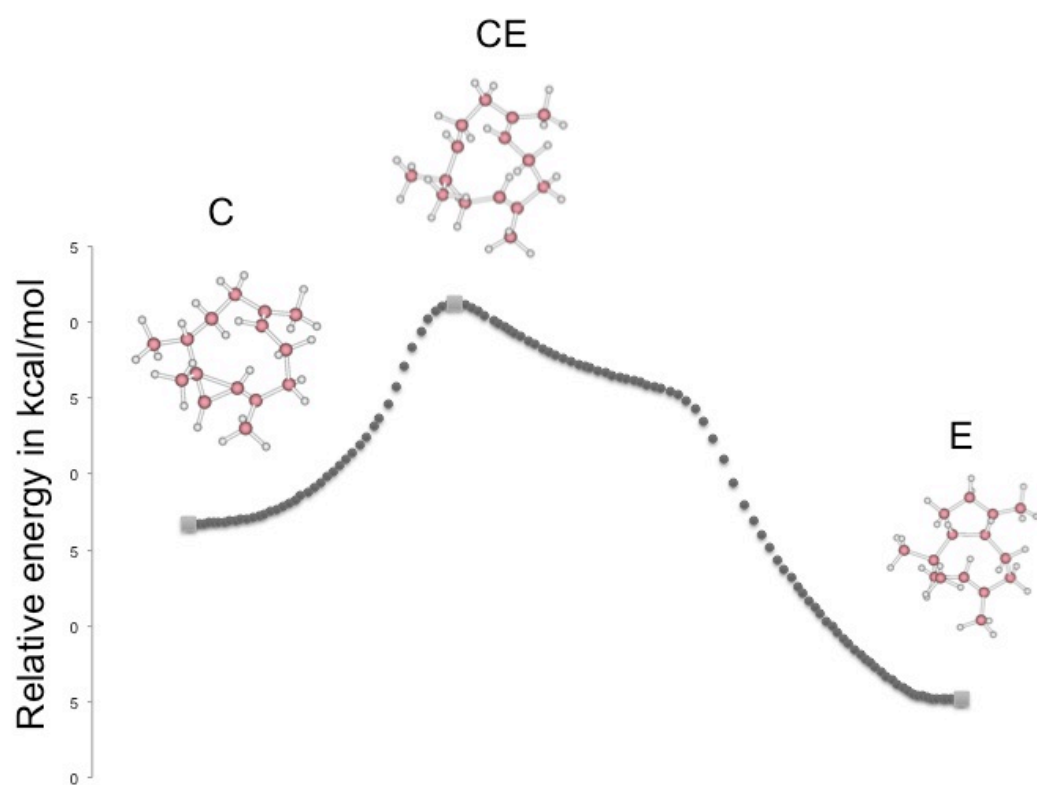


Fig. S11: IRC path from C to E.

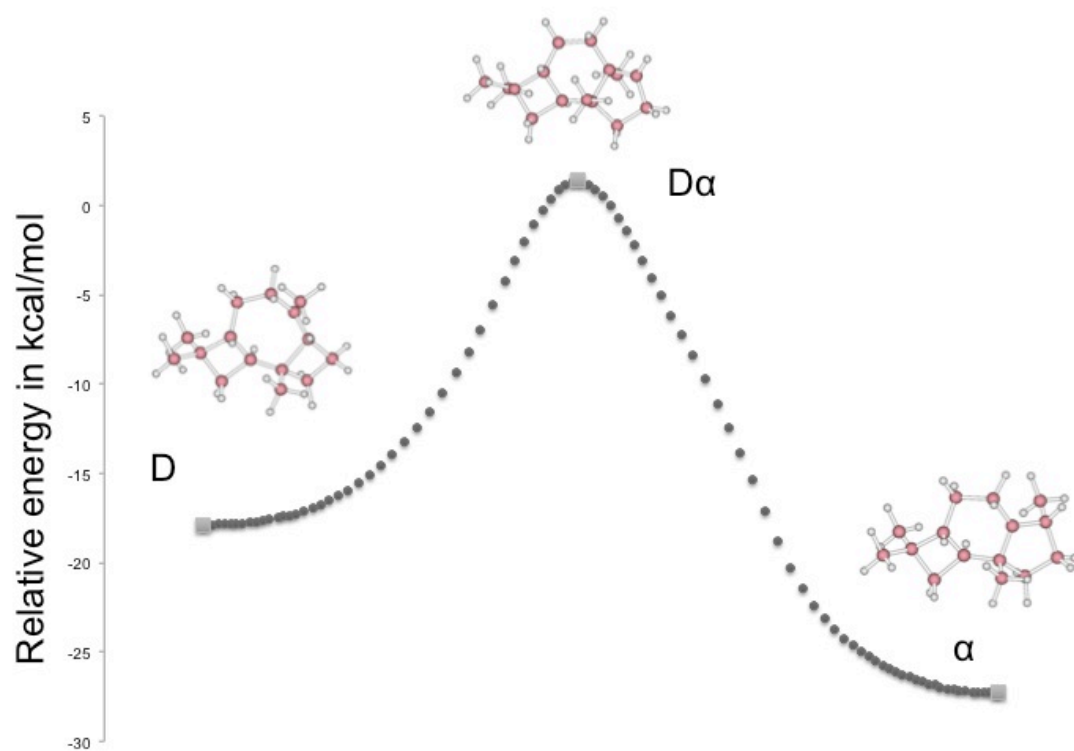


Fig. S12: IRC path from D to α .

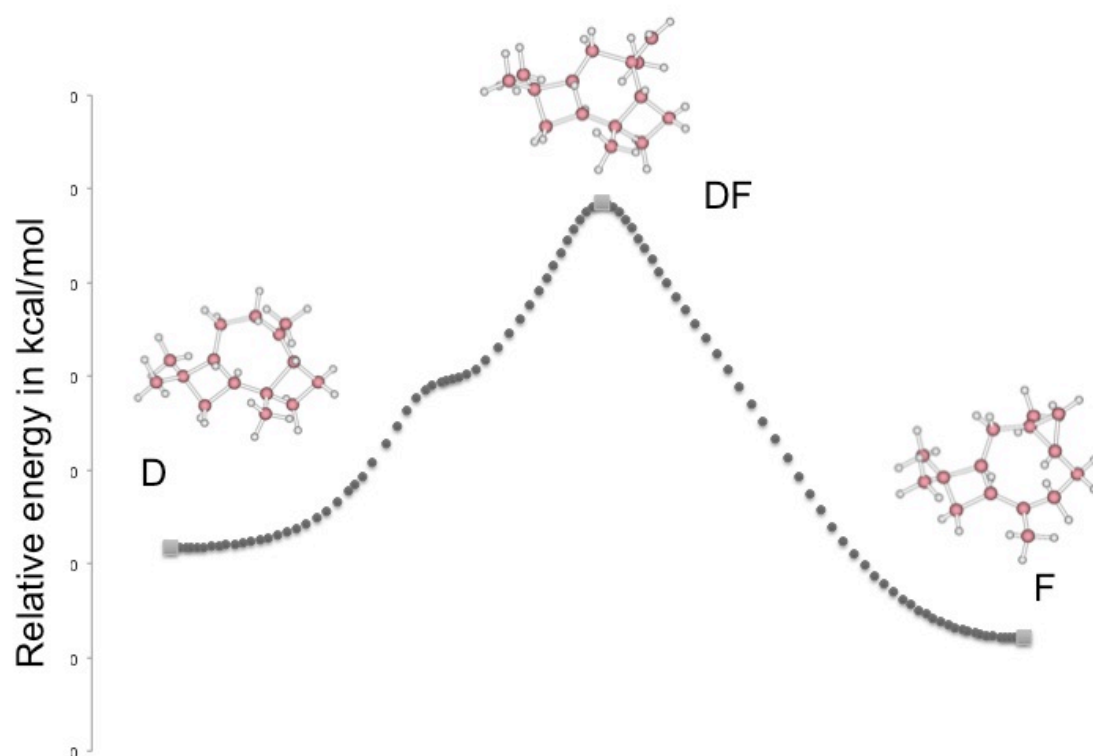


Fig. S13: IRC path from D to F.

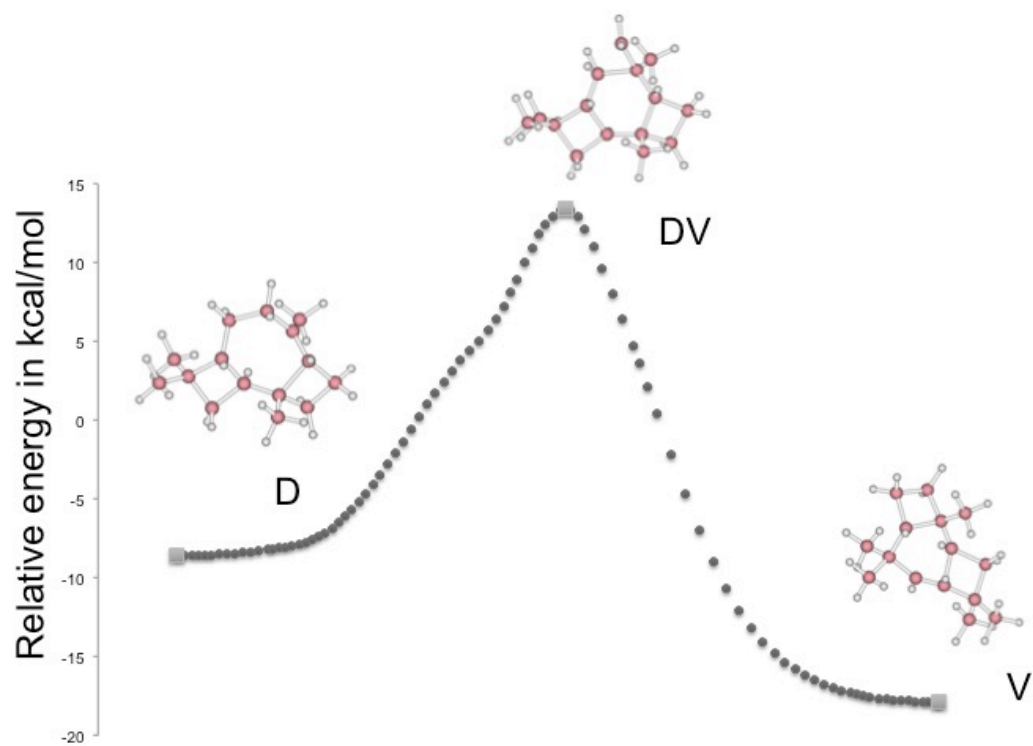


Fig. S14: IRC path from D to V.

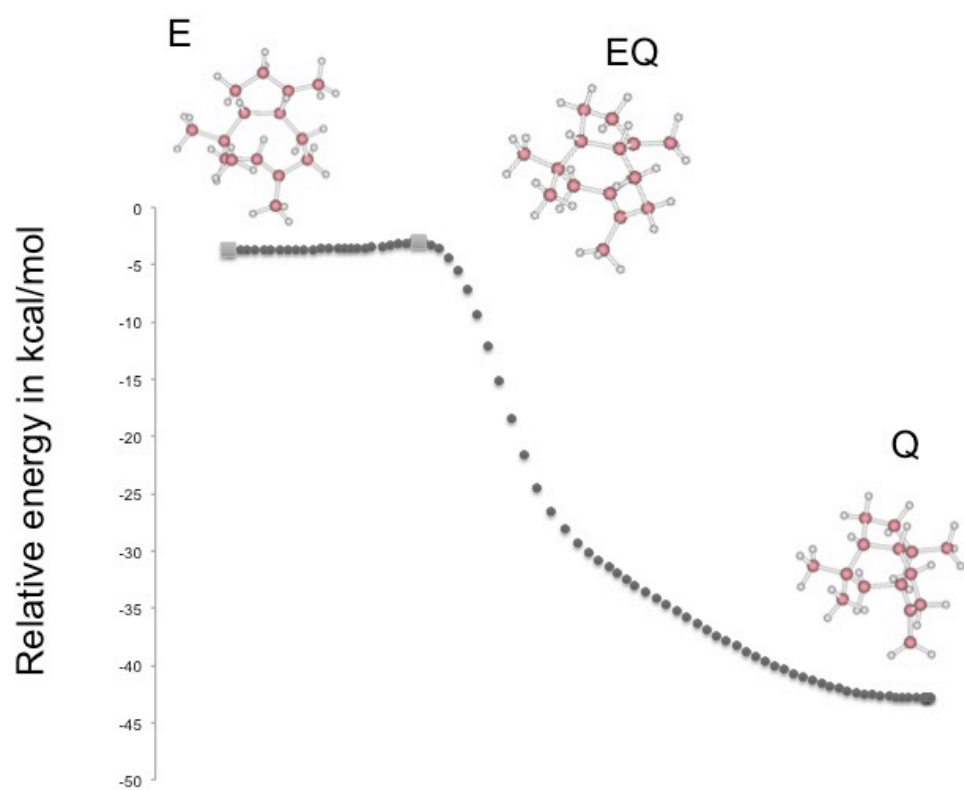


Fig. S15: IRC path from E to Q.

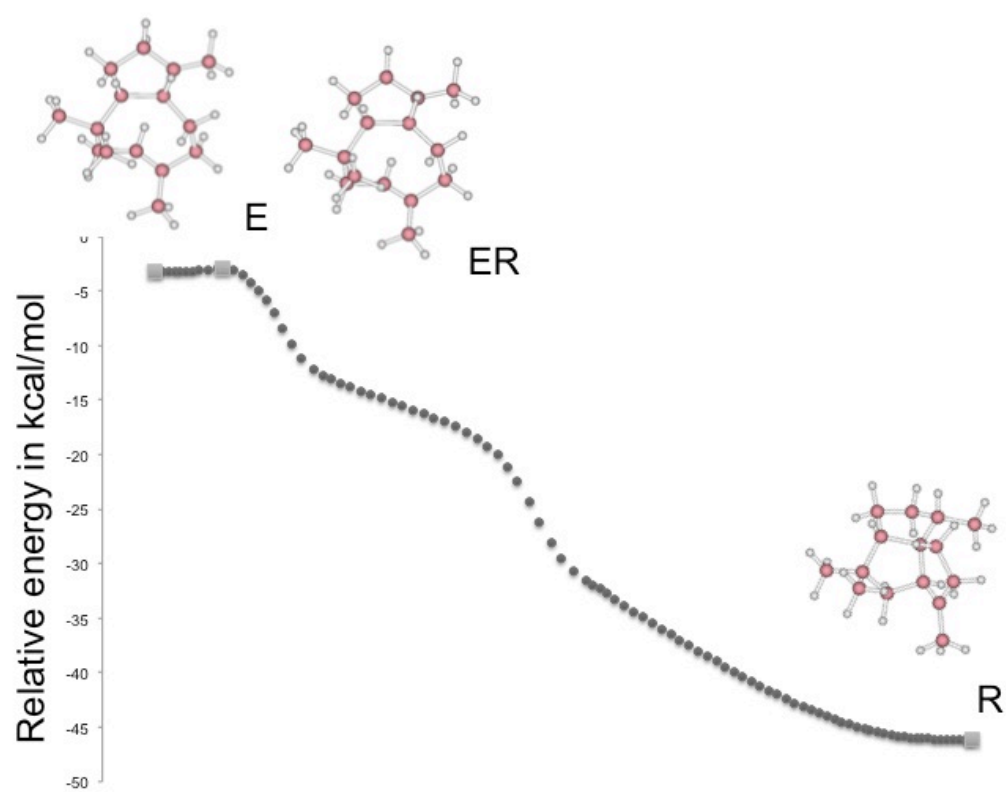


Fig. S16: IRC path from E to R.

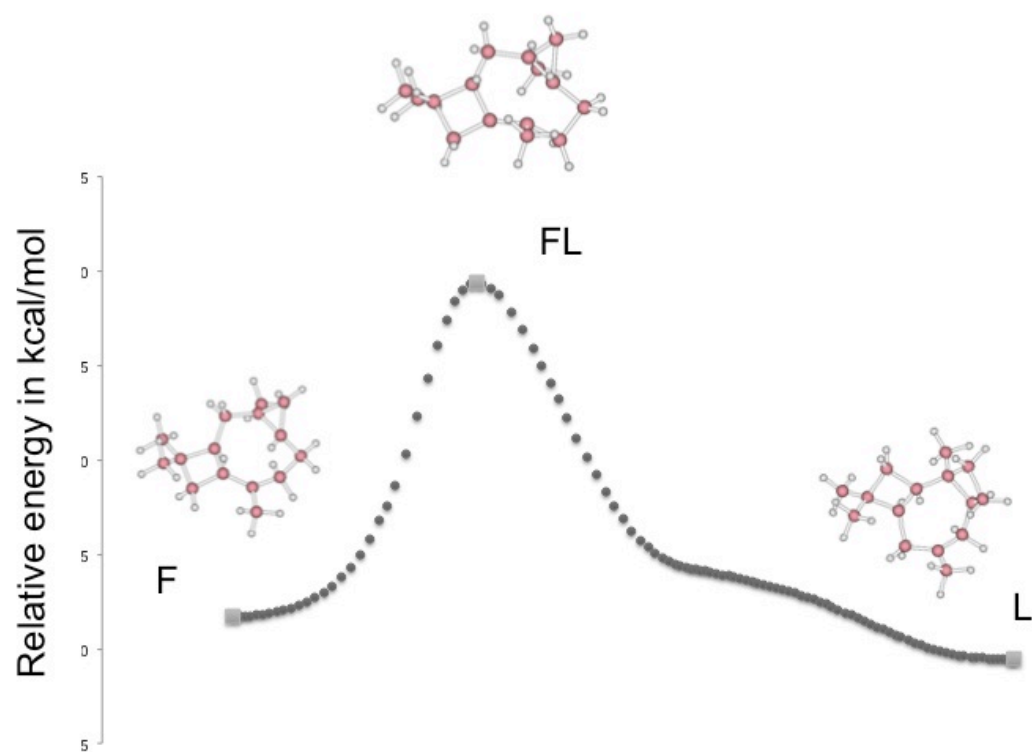


Fig. S17: IRC path from F to L.

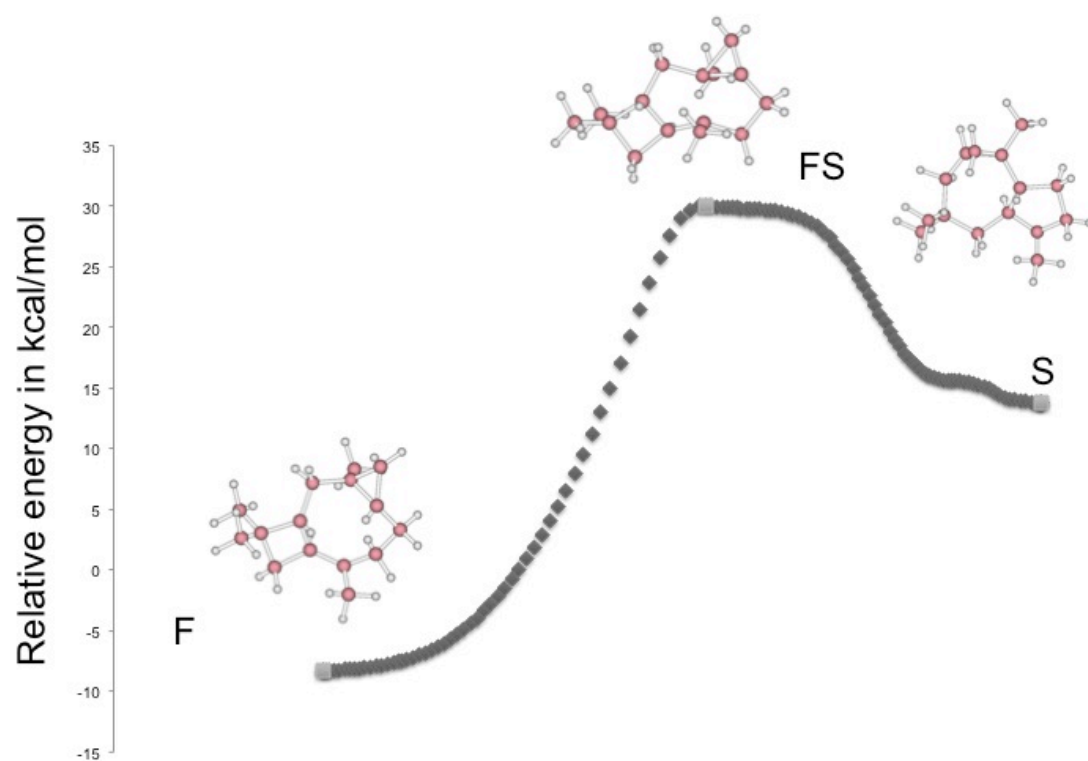


Fig. S18: IRC path from F to S.

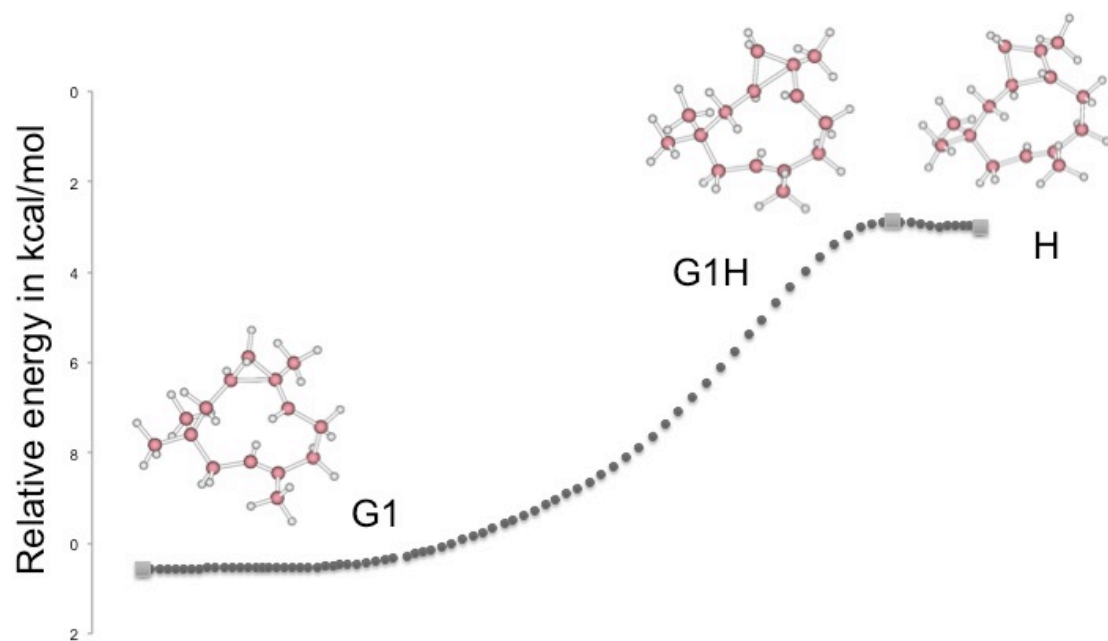


Fig. S19: IRC path from G1 to H.

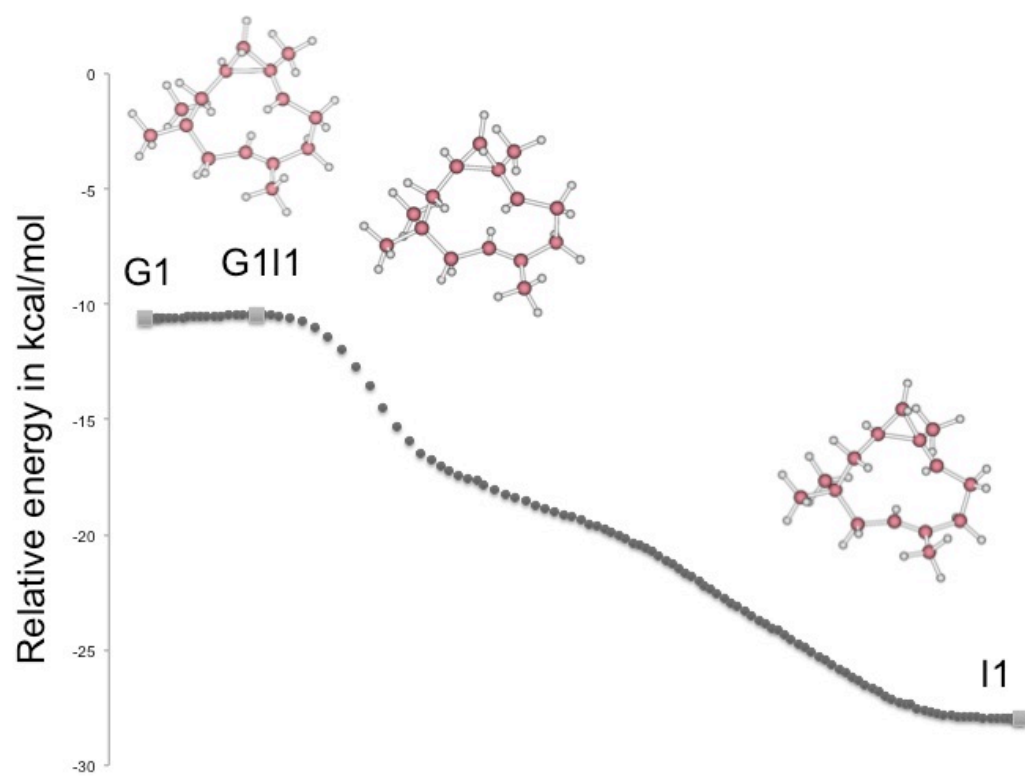


Fig. S20: IRC path from G1 to I1.

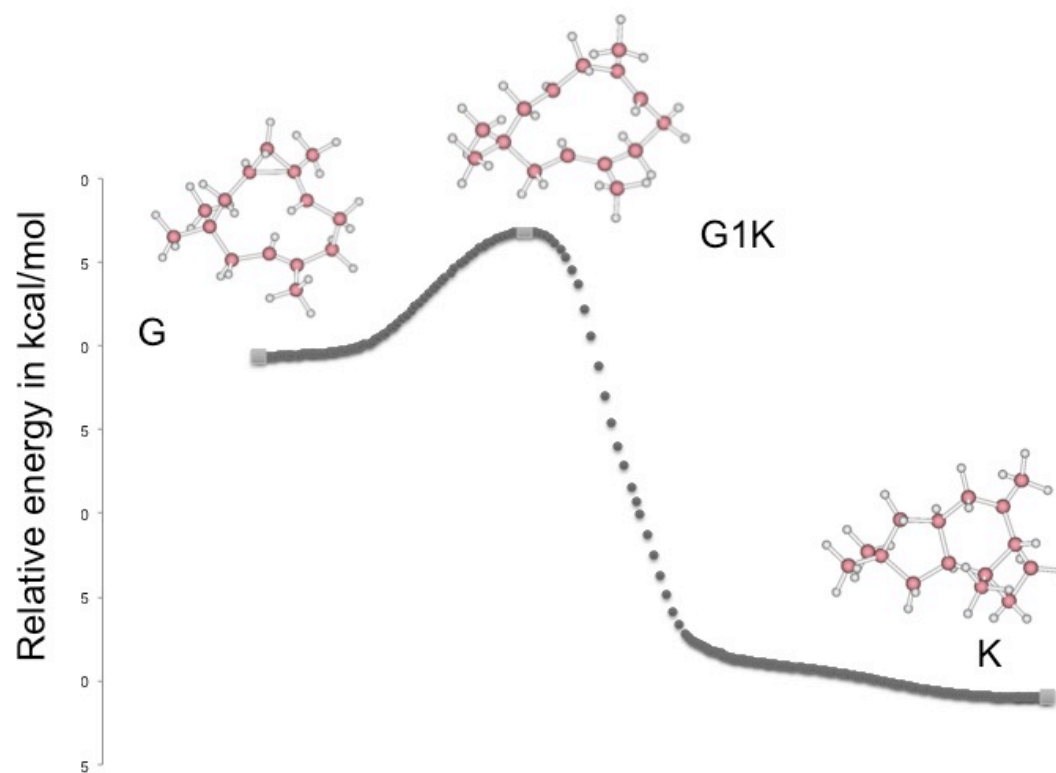


Fig. S21: IRC path from G to K.

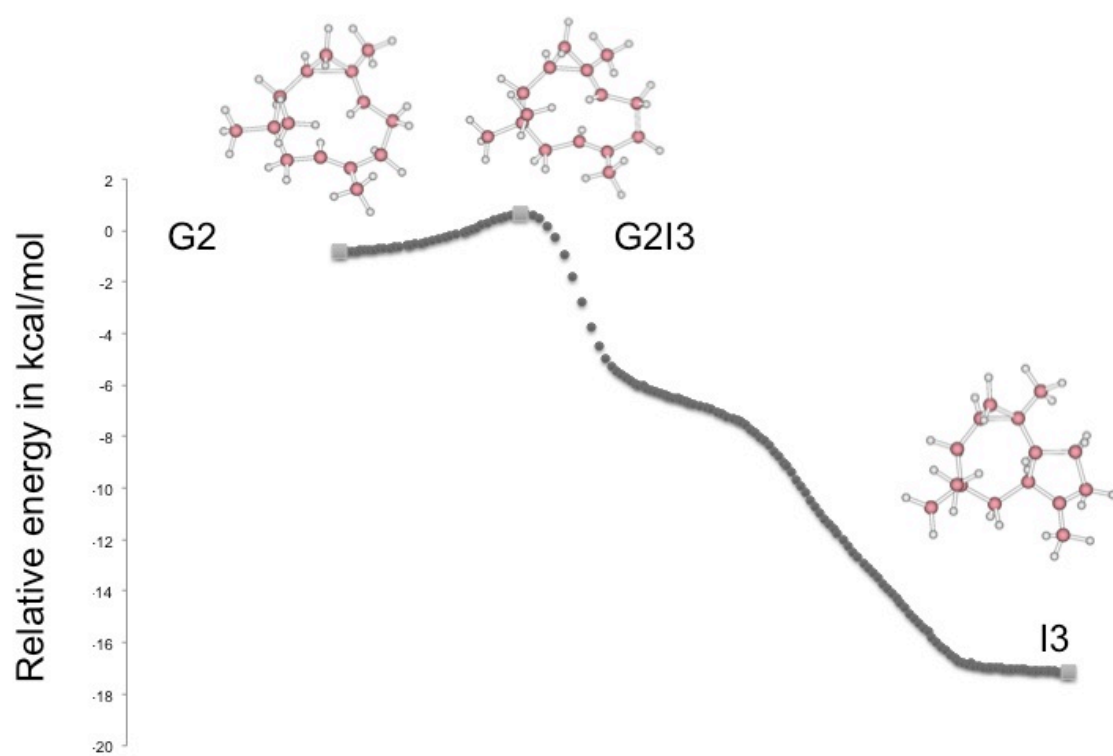


Fig. S22: IRC path from G2 to I3.

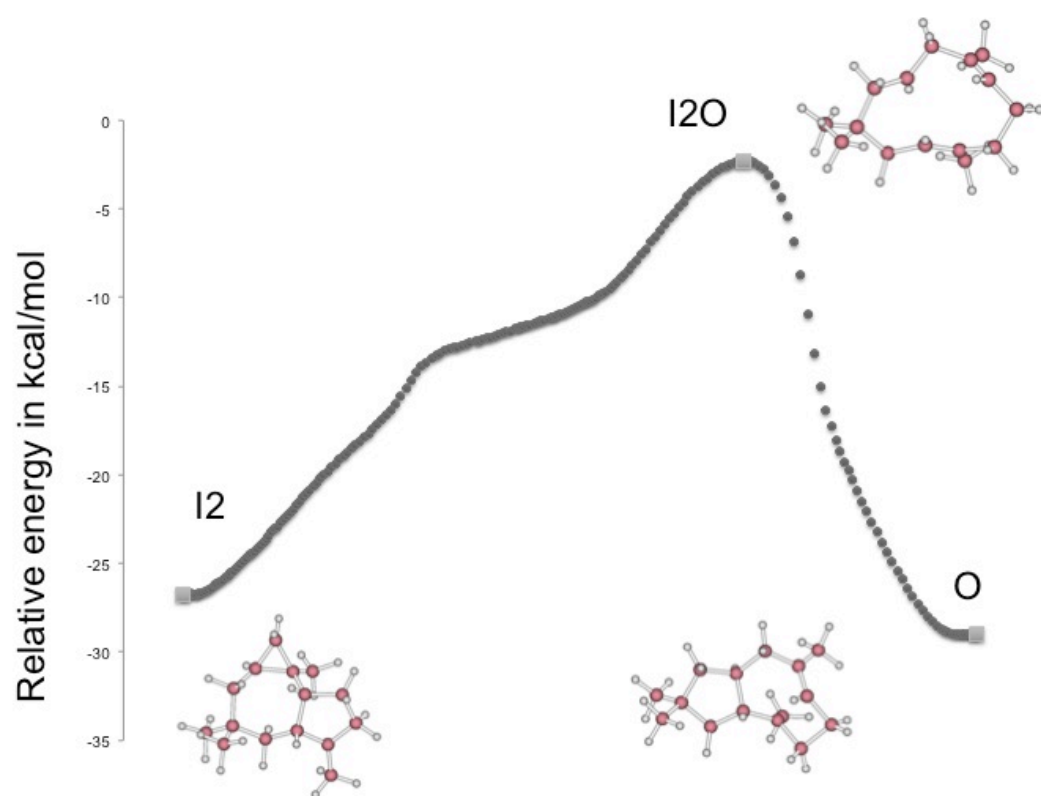


Fig. S23: IRC path from I2 to O.

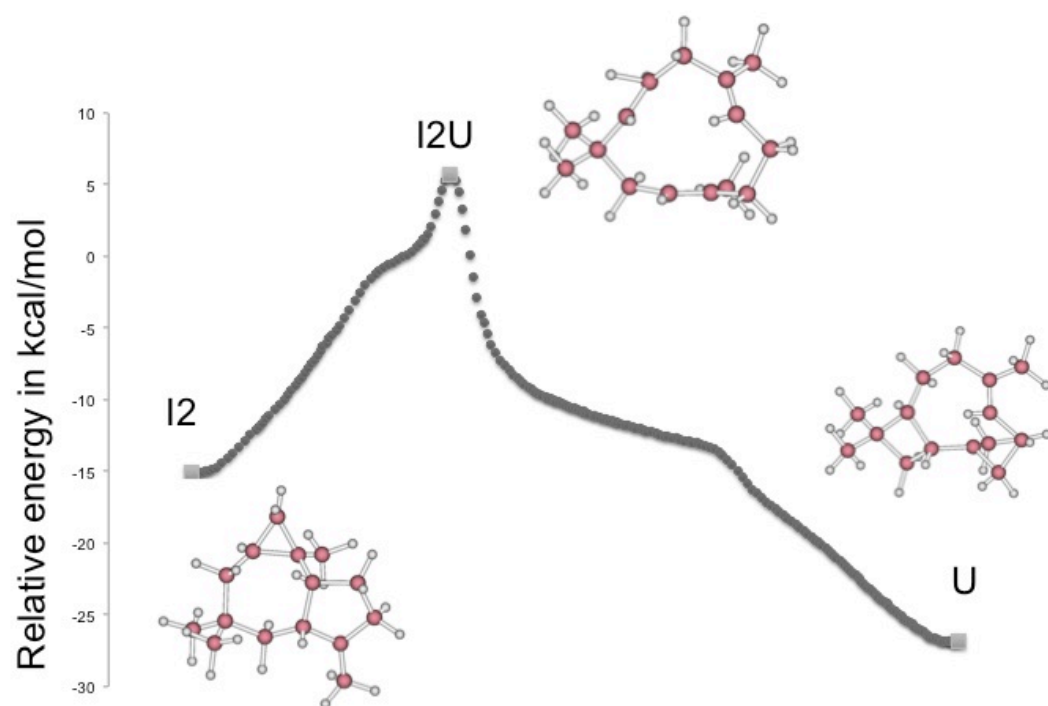


Fig. S24: IRC path from I2 to U.

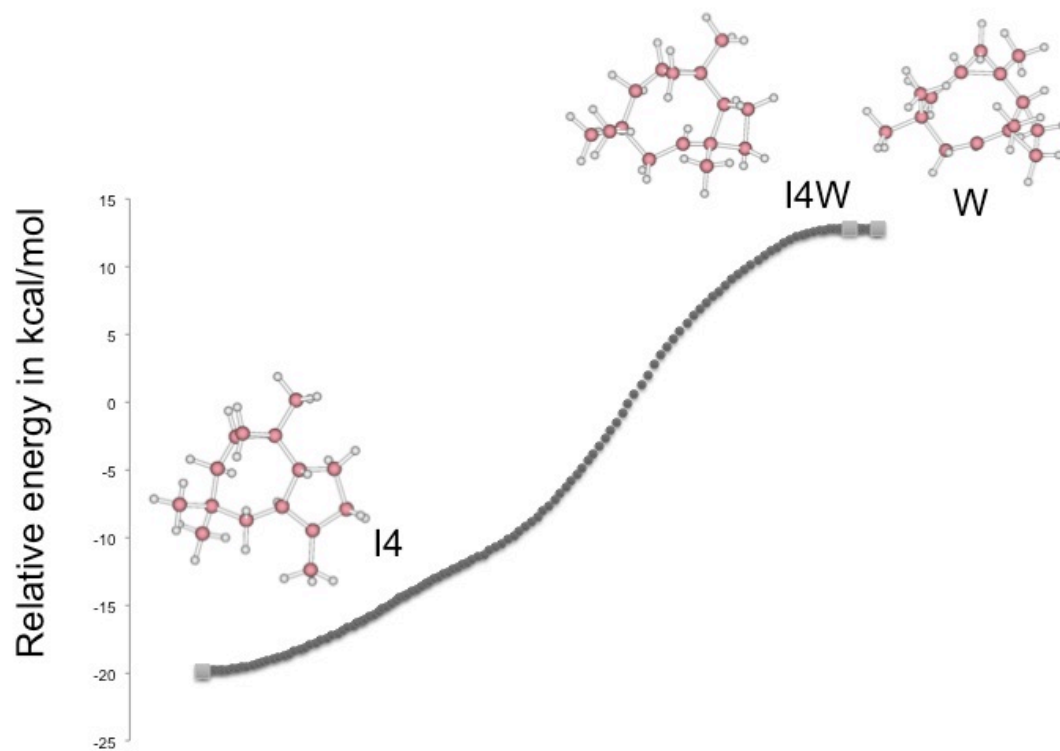


Fig. S25: IRC path from I4 to W.

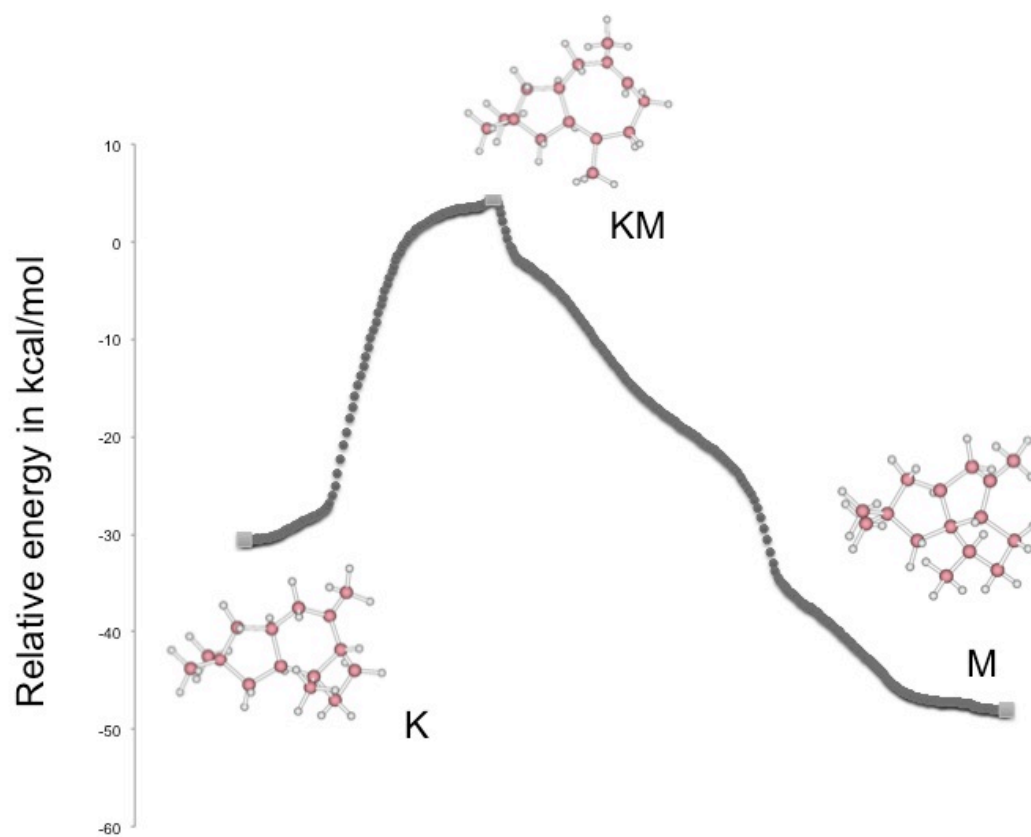


Fig. S26: IRC path from K to M.

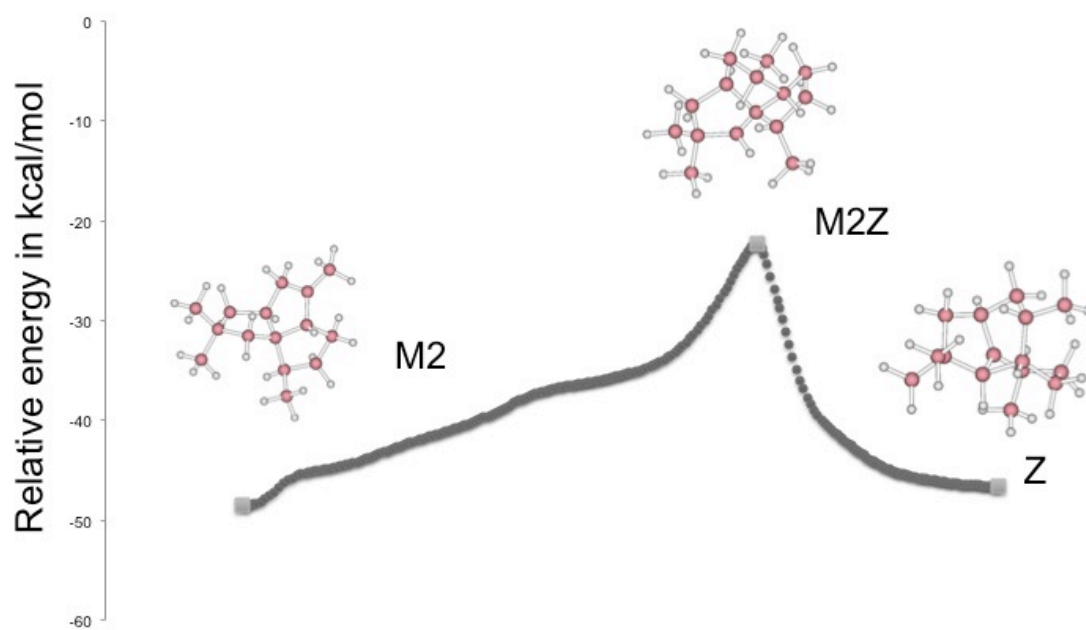


Fig. S27: IRC path from M2 to Z.

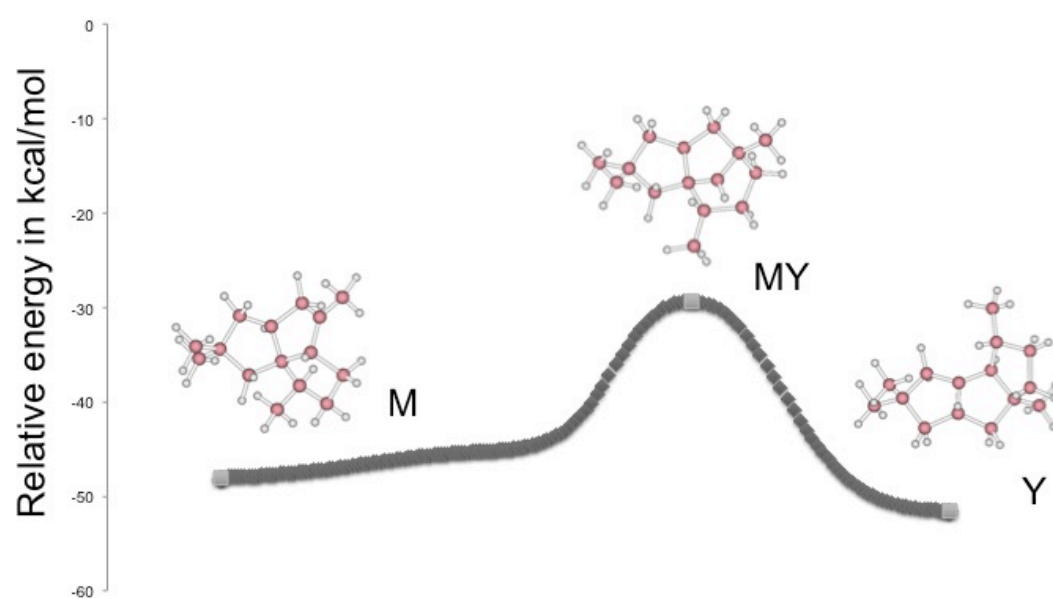


Fig. S28: IRC path from M to Y.

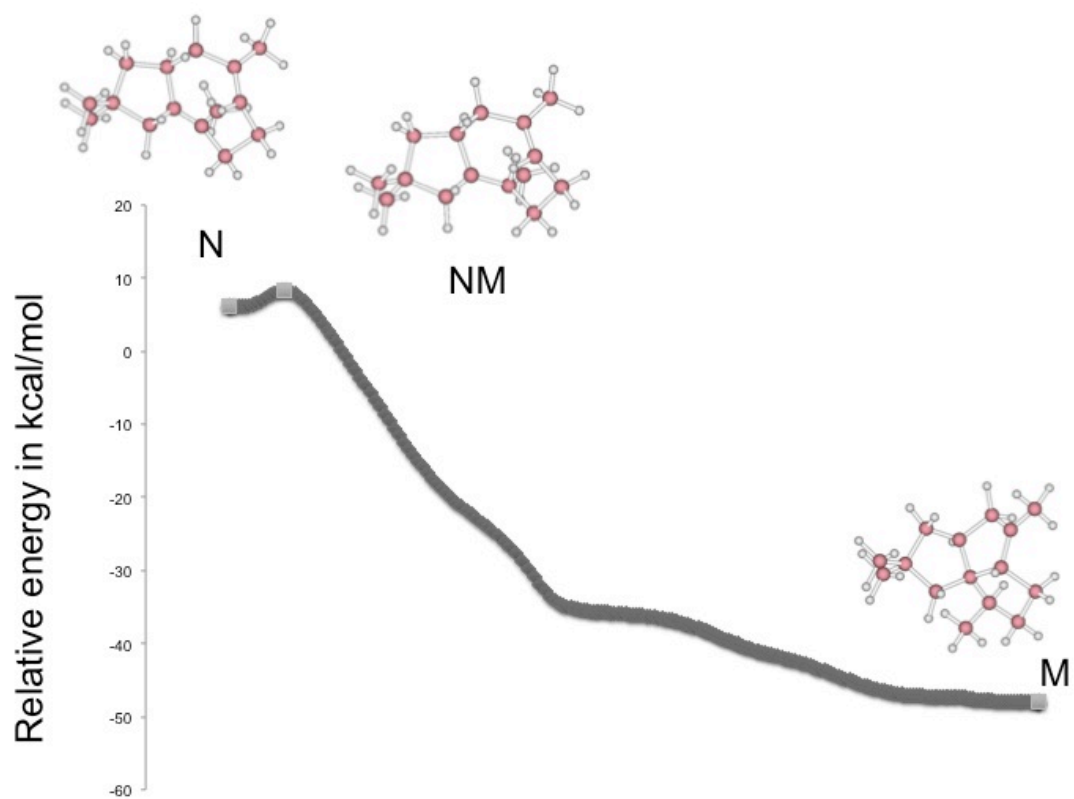


Fig. S29: IRC path from N to M.

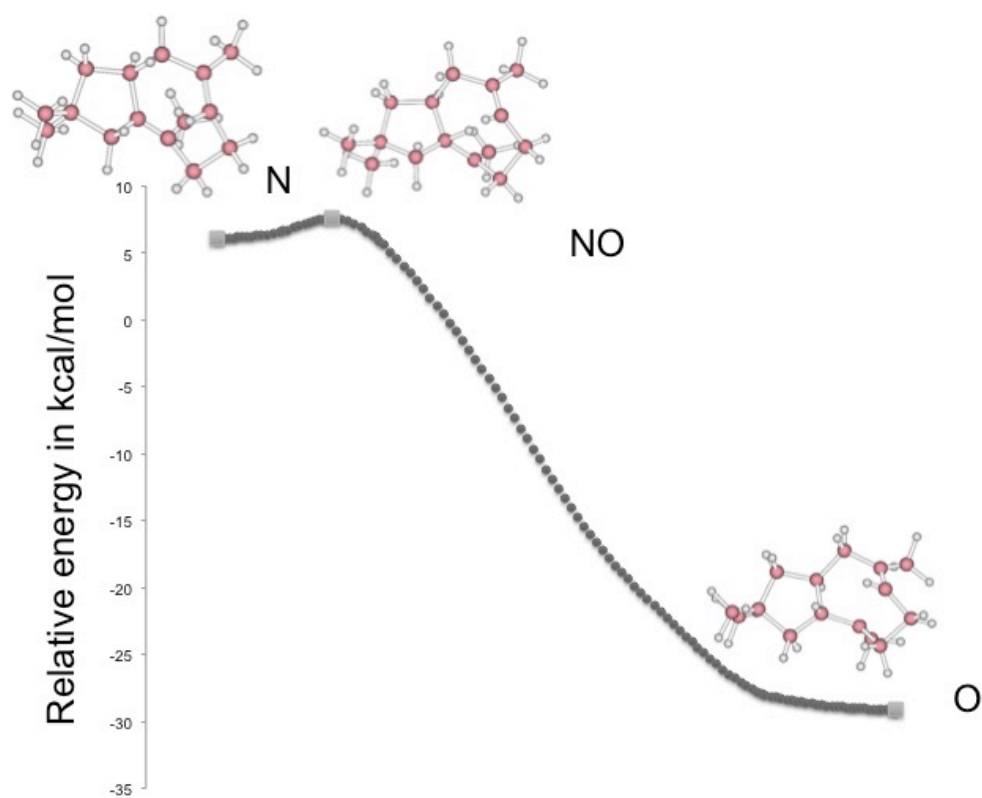


Fig. S30: IRC path from N to O.

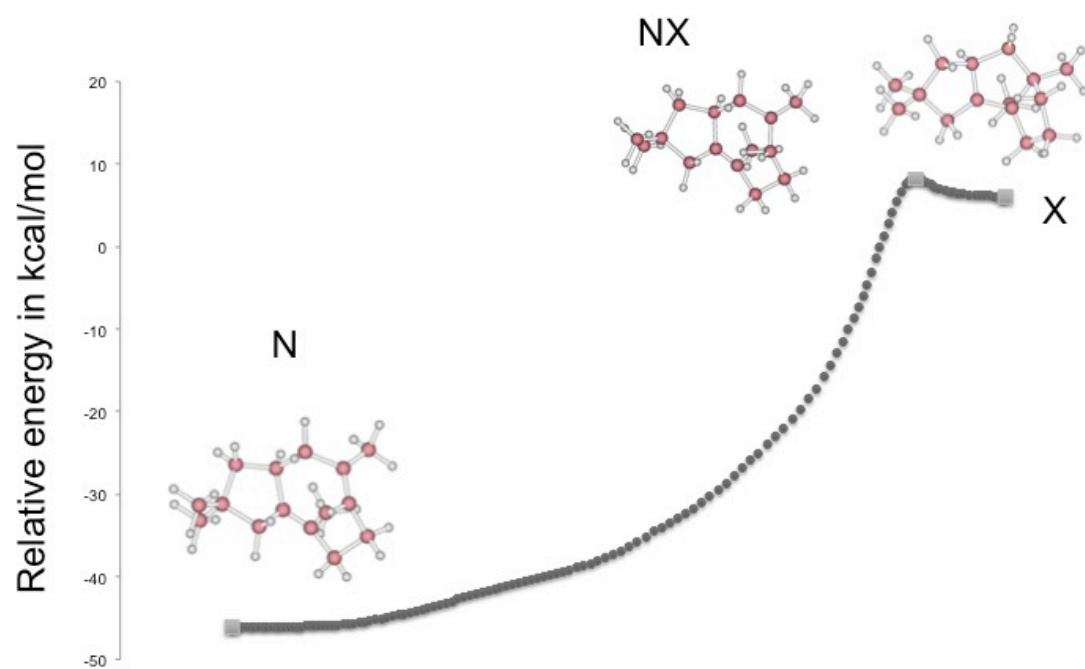


Fig. S31: IRC path from N to X.

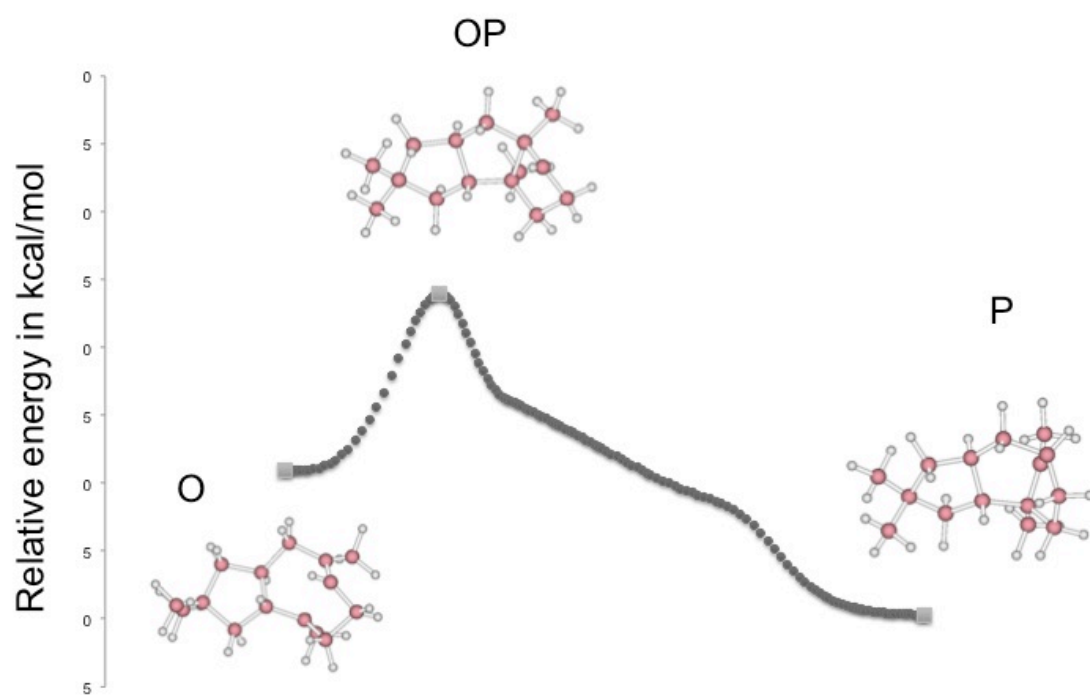


Fig. S32: IRC path from O to P.

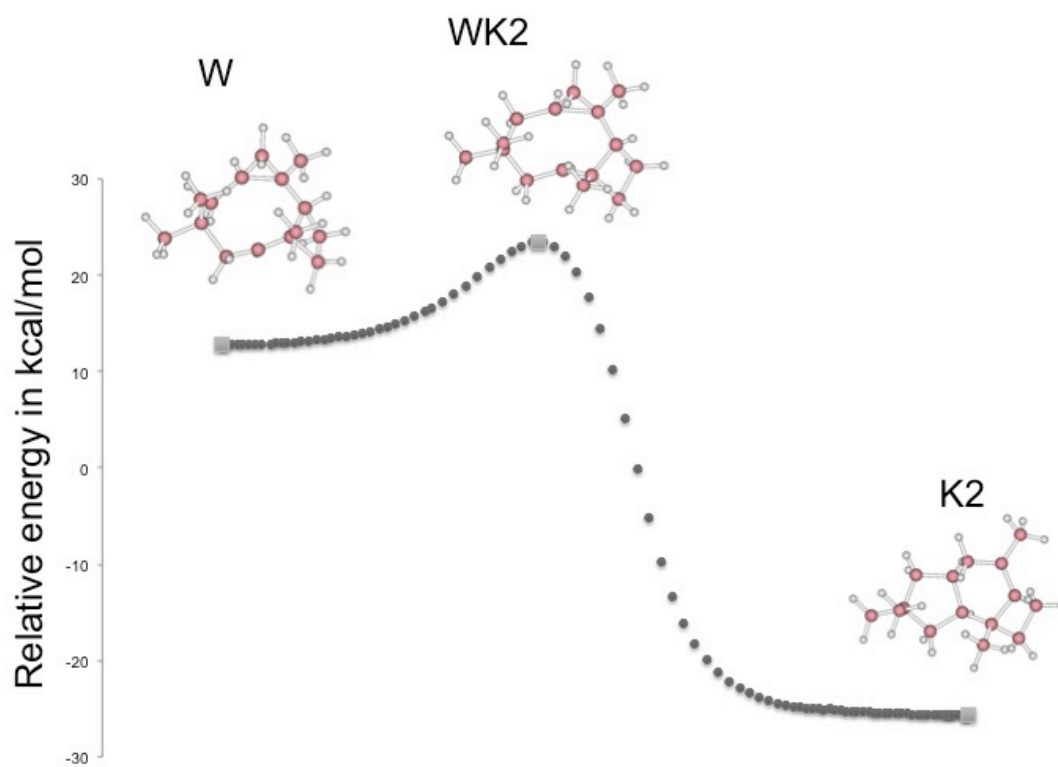


Fig. S33: IRC path from W to K2.