1. Computational Details

All calculations were carried out with Gaussian 16 program suite.[S1] The M06-2X[S2] method, which have been shown to give reliable kinetic and thermochemistry for main-group chemistry,[S2] was combined with the 6-31G* basis set to optimize all transition state structures in the gas phase. Then, vibration frequency calculations were carried out at the same level of theory to verify the optimized transition states and get their free energy correction. All 3D images of the optimized structures were illustrated by CYLview.[S3]

References:

(S1) Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

(S2) (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

(S3) C. Y. Legault, CYL View, version 1.0 b; Universite de Sherbrooke, Sherbrooke, Quebec, Canada, **2009**; http://www.cylview.org.

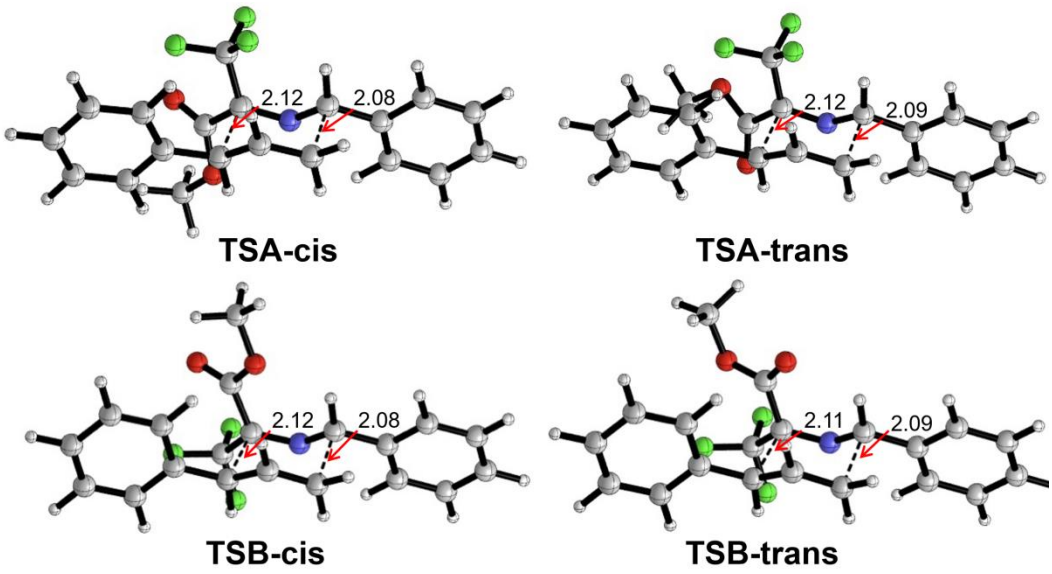

Figure S1. The optimized transition state structures (**TSA** & **TSB**; the CF_3 and CO_2Me groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method. The key bond lengths (Å, in italics) are given.

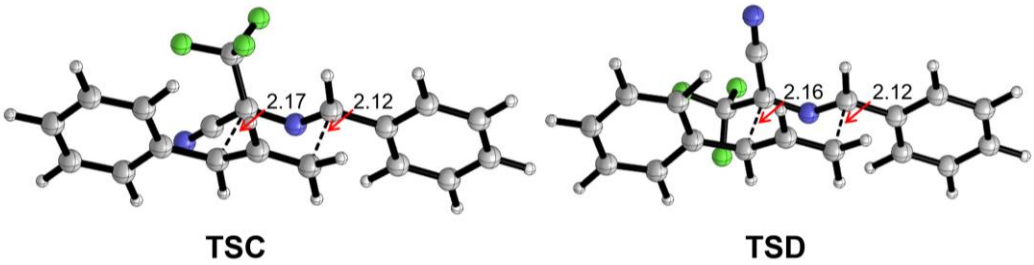

Figure S2. The optimized transition state structures (**TSC** & **TSD**; the CF_3 and CN groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method. The key bond lengths (Å, in italics) are given.

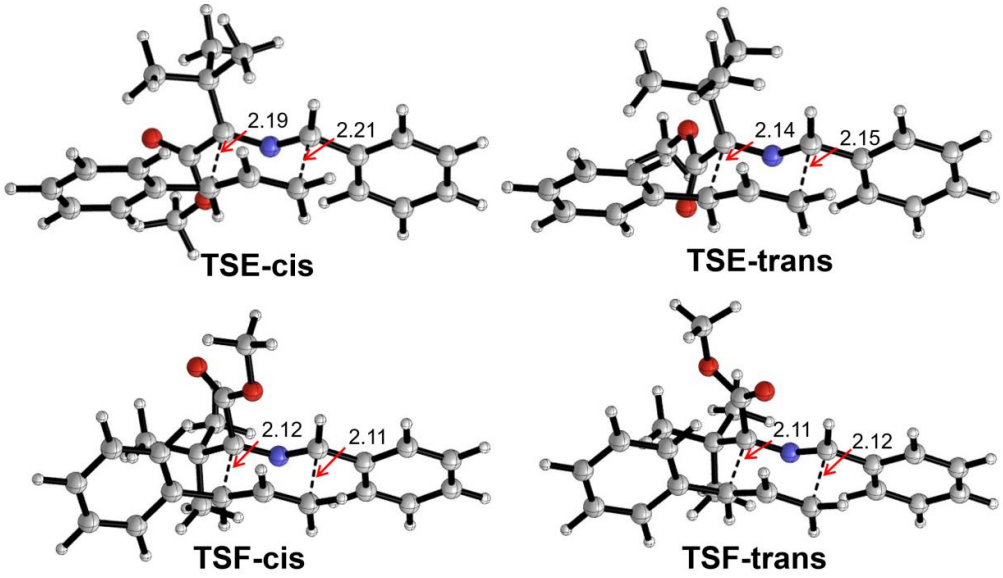

Figure S3. The optimized transition state structures (**TSE** & **TSF**; the t-Bu and CO_2Me groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method. The key bond lengths (Å, in italics) are given.

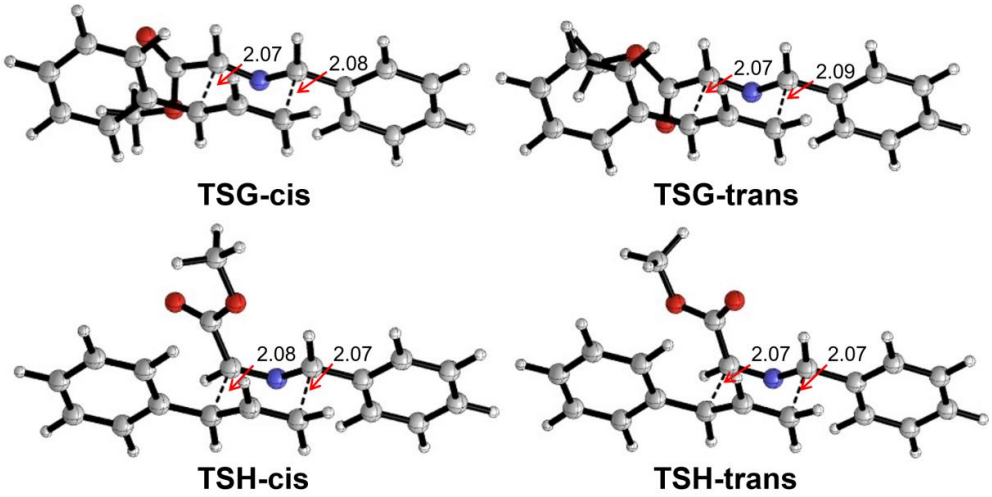

Figure S4. The optimized transition state structures (**TSG** & **TSH**; the H and CO_2Me groups at the reacting carbon center) for the 2-aza-Cope rearrangement by the M06-2X method. The key bond lengths (Å, in italics) are given.

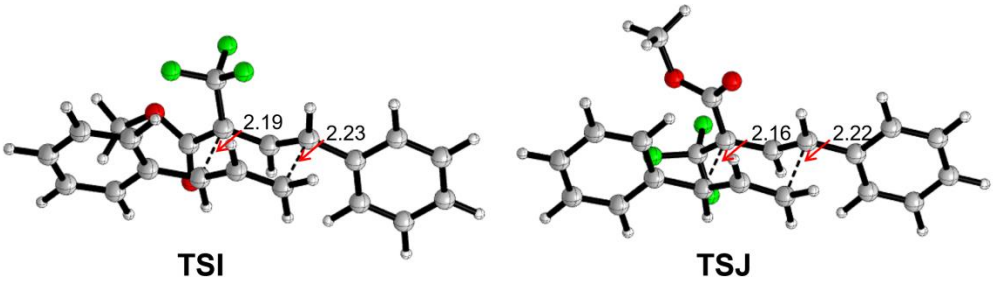

Figure S5. The optimized transition state structures (**TSI** & **TSJ**; the CF_3 and CO_2Me groups at the quaternary carbon center) for the Cope rearrangement by the M06-2X method. The key bond lengths (Å, in italics) are given.

Steric and electronic effects were proposed to enhance the observed high diastereoselectivity in our 2-aza-Cope rearrangement reaction. First, a lager repulsion in the classical chair-like transition state should be experienced, when a more bulky trifluoromethyl group (instead of the ester group) was positioned at the axial position. When using a more bulkier t-butyl group in **TSE** and **TSF**, the diastereoselectivity was computed to be further increased (8.7 kcal/mol). Whereas, when using a hydrogen atom to replace the trifluoromethyl group in **TSG** and **TSH**, the diastereoselectivity was computed to be lost (0.1 kcal/mol). Therefore, steric repulsion of the trifluoromethyl group at the axial position partly accounts the diastereoselectivity. In addition, anomeric effect was found to an additional factor to increase the diastereoselectivity. For instance, as the anomeric effect is eliminated by replacing the aza-nitrogen atom by the C-H group in **TSI** and **TSJ**, the computed diastereoselectivity was significantly reduced from 3.1 kcal/mol to 1.3 kcal/mol. Moreover, the nearly same energy for **TSG** and **TSH** (with the ester and H groups at the reacting carbon) should further support the electronic effect of the ester group at the axial position.

Table S1. The absolute and relative (free) energies for the transition state structures **TSA** & **TSB** (the CF_3 and CO_2Me groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method.

	CO_2Me	E/a.u	E+ZPE/a.u	G/a.u	ΔG(kcal/mol)
TSA	cis	-1277.122786	-1276.777805	-1276.830556	4.3
	trans	-1277.123440	-1276.778558	-1276.832332	**3.1**
TSB	cis	-1277.124538	-1276.779655	-1276.832172	3.2
	trans	-1277.130076	-1276.785081	-1276.837343	**0.0**

Table S2. The absolute and relative (free) energies for the transition state structures **TSC** & **TSD** (the CF_3 and CN groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method.

	E/a.u	E+ZPE/a.u	G/a.u	ΔG/(kcal/mol)
TSC	-1141.544863	-1141.245322	-1141.294641	**3.4**
TSD	-1141.549967	-1141.250507	-1141.300126	**0.0**

Table S3. The absolute and relative (free) energies for the transition state structures **TSE** & **TSF** (the CF_3 and t-Bu groups at the quaternary carbon center) for the 2-aza-Cope rearrangement by the M06-2X method.

	CO_2Me	E/a.u	E+ZPE/a.u	G/a.u	ΔG(kcal/mol)
TSE	cis	-1097.347764	-1096.893734	-1096.947313	**8.7**
	trans	-1097.348019	-1096.893876	-1096.947170	8.8
TSF	cis	-1097.358660	-1096.904967	-1096.958269	1.9
	trans	-1097.362008	-1096.908040	-1096.961249	**0.0**

Table S4. The absolute and relative (free) energies for the transition state structures **TSG** & **TSH** (the CF_3 and H groups at the reacting carbon center) for the 2-aza-Cope rearrangement by the M06-2X method.

	CO_2Me	E/a.u	E+ZPE/a.u	G/a.u	ΔG(kcal/mol)
TSG	cis	-940.191003	-939.851395	-939.900133	1.1
	trans	-940.192686	-939.853102	-939.901763	**0.1**
TSH	cis	-940.187676	-939.847796	-939.896361	3.5
	trans	-940.193389	-939.853209	-939.901948	**0.0**

Table S5. The absolute and relative (free) energies for the transition state structures **TSA** & **TSB** (the CF_3 and CO_2Me groups at the quaternary carbon center) for the Cope rearrangement by the M06-2X method.

	E/a.u	E+ZPE/a.u	G/a.u	ΔG/(kcal/mol)
TSI	-1261.084050	-1260.727268	-1260.780408	**1.3**
TSJ	-1261.086815	-1260.730029	-1260.782406	**0.0**

Cartesian coordinates of all optimized structures

TSA-cis

C	-0.178004	0.306735	0.644627
C	1.944790	-0.545417	0.210143
C	-0.938680	-0.336565	-1.223493
C	-2.407298	-0.475173	-1.092077
C	-0.064135	-1.411577	-1.441450
C	1.287024	-1.179960	-1.656424
C	-3.024653	-1.670184	-0.702277
C	-4.407429	-1.750170	-0.607368
C	-5.198935	-0.637684	-0.891172
C	-4.596488	0.558093	-1.269045
C	-3.211063	0.636820	-1.367543
H	-0.625781	0.616180	-1.643949
H	-0.393719	-2.423404	-1.224176
H	1.602914	-0.248984	-2.116947
H	-2.420235	-2.535233	-0.445814
H	-4.871609	-2.682890	-0.302533
H	-6.279452	-0.703862	-0.812581
H	-5.204285	1.430073	-1.489687
H	-2.736710	1.567067	-1.671799
C	-0.634859	-0.776504	1.626298
F	-0.049798	-0.582061	2.815340
F	-0.279814	-2.016939	1.224786
F	-1.950662	-0.801466	1.811913
N	1.105880	0.478430	0.347638
C	-0.943251	1.599954	0.826537
O	-1.691647	1.831688	1.740817
O	-0.679709	2.472137	-0.157693
H	1.962651	-2.017516	-1.808696
H	1.777706	-1.501802	0.709875
C	3.371645	-0.244753	-0.075101
C	4.326495	-1.254803	0.058018
C	3.771102	1.026948	-0.496880
C	5.665542	-1.001373	-0.223639
H	4.016075	-2.243645	0.389014
C	5.108514	1.278926	-0.777254
H	3.018837	1.804592	-0.586037
C	6.058919	0.266756	-0.642705
H	6.401074	-1.792029	-0.112587
H	5.414394	2.269614	-1.099560
H	7.103053	0.467860	-0.861429
C	-1.345445	3.727104	-0.018281
H	-1.043323	4.215579	0.910285
H	-1.043652	4.318721	-0.881037
H	-2.428542	3.581232	-0.004640

TSA-trans

C	-0.140447	0.562997	0.325792
C	2.008028	-0.346209	0.378754
C	-0.841480	-0.888515	-1.049130
C	-2.310969	-0.996132	-0.889466
C	0.056804	-1.921108	-0.741559
C	1.408503	-1.775847	-1.016488
C	-2.912278	-1.915486	-0.020577
C	-4.294870	-1.986275	0.085732
C	-5.103353	-1.135193	-0.666883
C	-4.517259	-0.210836	-1.526259
C	-3.131552	-0.142291	-1.636881
H	-0.535280	-0.210639	-1.843067
H	-0.260977	-2.735529	-0.096780
H	1.721833	-1.141389	-1.839702
H	-2.296008	-2.562597	0.596633
H	-4.745369	-2.703933	0.764351
H	-6.183873	-1.192717	-0.580315
H	-5.138414	0.454778	-2.117940
H	-2.670943	0.577929	-2.308292
C	-0.616496	0.043758	1.683929
F	-0.095350	0.793510	2.665614
F	-0.216153	-1.224180	1.917046
F	-1.940989	0.050771	1.824855
N	1.150915	0.602761	0.014911
C	-0.894416	1.753318	-0.237772
O	-0.777216	2.123478	-1.379471
O	-1.687247	2.341519	0.659142
H	2.102903	-2.571770	-0.760587
H	1.840488	-0.978840	1.252736
C	3.437309	-0.172045	0.013202
C	4.403210	-0.982785	0.612612
C	3.828512	0.774662	-0.938641
C	5.745673	-0.851349	0.270307
H	4.098686	-1.717696	1.354911
C	5.169369	0.904976	-1.279078
H	3.067279	1.403993	-1.389374
C	6.131017	0.093124	-0.677374
H	6.489779	-1.483266	0.745154
H	5.468656	1.644573	-2.015479
H	7.177700	0.198839	-0.945378
C	-2.463484	3.428096	0.153017
H	-3.119429	3.074225	-0.645821
H	-3.045706	3.791717	0.997411
H	-1.810538	4.210954	-0.237264

TSB-cis

C	-0.156598	0.566568	0.557237
C	1.889107	-0.504732	0.130451
C	-0.987215	-0.039600	-1.293916
C	-2.446129	-0.258157	-1.129698
C	-0.119324	-1.106841	-1.577661
C	1.231426	-0.906286	-1.801445
C	-2.967433	-1.454136	-0.620620
C	-4.340861	-1.637337	-0.504689
C	-5.217918	-0.629267	-0.896545
C	-4.711126	0.565018	-1.403134
C	-3.338319	0.748589	-1.514053
H	-0.719196	0.927369	-1.716124
H	-0.468429	-2.121460	-1.404026
H	1.582594	0.050236	-2.176790
H	-2.294602	-2.248530	-0.310673
H	-4.727226	-2.570647	-0.106330
H	-6.289913	-0.772318	-0.804650
H	-5.386618	1.357790	-1.708685
H	-2.944372	1.687035	-1.894681

C	-0.690242	1.991257	0.704221
F	-2.021621	2.062702	0.639370
F	-0.206493	2.768066	-0.277589
F	-0.307978	2.529379	1.866803
N	1.153238	0.581927	0.324847
C	-0.859866	-0.396706	1.479836
O	-1.689947	-0.064445	2.285004
O	-0.447150	-1.670298	1.330858
H	1.875807	-1.752603	-2.023028
H	1.601037	-1.477726	0.531533
C	3.348272	-0.324281	-0.088682
C	4.194629	-1.433063	-0.023952
C	3.884762	0.933679	-0.379392
C	5.561339	-1.291456	-0.244023
H	3.776977	-2.411688	0.203672
C	5.249792	1.074032	-0.597974
H	3.215720	1.787773	-0.416778
C	6.091317	-0.036522	-0.532214
H	6.211842	-2.158742	-0.187661
H	5.662151	2.053931	-0.818294
H	7.157313	0.077420	-0.702986
C	-1.072490	-2.592708	2.227765
H	-2.156181	-2.570800	2.090933
H	-0.666474	-3.571125	1.975543
H	-0.840231	-2.331073	3.261871

TSB-trans

C	-0.099531	0.638590	0.314228
C	1.958653	-0.467331	0.338186
C	-0.881942	-0.577981	-1.227221
C	-2.347095	-0.734066	-1.038761
C	-0.012852	-1.671360	-1.076101
C	1.342390	-1.558294	-1.329148
C	-2.887549	-1.645471	-0.122019
C	-4.265761	-1.785046	0.007473
C	-5.127010	-1.021533	-0.776767
C	-4.599797	-0.111975	-1.690394
C	-3.223291	0.031826	-1.815320
H	-0.597058	0.172725	-1.962994
H	-0.369144	-2.549845	-0.544623
H	1.703863	-0.805758	-2.023590
H	-2.229329	-2.239265	0.506183
H	-4.667797	-2.496671	0.722761
H	-6.201944	-1.133850	-0.675886
H	-5.261935	0.489811	-2.305004
H	-2.814229	0.752594	-2.518278
C	-0.662357	2.016789	-0.027147
F	-0.127196	2.461324	-1.172180
F	-0.366112	2.906112	0.929699
F	-1.989233	2.028291	-0.189123
N	1.216481	0.609265	0.108750
C	-0.739174	-0.092107	1.463940
O	-0.384113	-1.181747	1.857492
O	-1.742502	0.596344	2.005276
H	1.992071	-2.419745	-1.202545
H	1.651449	-1.232198	1.052274
C	3.421961	-0.361502	0.102402
C	4.268375	-1.358414	0.592163
C	3.963672	0.707435	-0.617874
C	5.640439	-1.290559	0.369959
H	3.846042	-2.188515	1.154455
C	5.333890	0.774366	-0.838728
H	3.294052	1.479450	-0.984188
C	6.175497	-0.223556	-0.346970
H	6.291102	-2.067817	0.758606
H	5.750248	1.608911	-1.394647
H	7.245631	-0.167393	-0.520897
C	-2.424390	-0.056928	3.076596
H	-1.726863	-0.290787	3.882976
H	-3.184382	0.646576	3.410324
H	-2.886137	-0.978690	2.715124

TSC

C	-0.247752	0.755490	0.588515
C	1.803648	-0.250222	0.242062
C	-1.102108	-0.062868	-1.233496
C	-2.558495	-0.187984	-1.019817
C	-0.231320	-1.153869	-1.375232
C	1.115165	-0.962822	-1.630427
C	-3.152060	-1.356862	-0.522684
C	-4.527239	-1.428017	-0.347270
C	-5.333610	-0.332921	-0.655689
C	-4.754651	0.835872	-1.139842
C	-3.377537	0.907297	-1.320278
H	-0.802472	0.854587	-1.736642
H	-0.567229	-2.142633	-1.077048
H	1.451498	-0.057883	-2.126907
H	-2.538176	-2.210468	-0.253951
H	-4.972791	-2.339720	0.038138
H	-6.408175	-0.391513	-0.513892
H	-5.373101	1.695646	-1.376332
H	-2.925932	1.823069	-1.691005
C	-0.766338	-0.202701	1.662290
F	-0.058602	-0.043310	2.788909
F	-0.648070	-1.498768	1.322826
F	-2.046323	0.028428	1.942796
N	1.042303	0.837250	0.273792
H	1.777973	-1.818032	-1.728497
H	1.538723	-1.154298	0.796680
C	3.250892	-0.097796	-0.040895
C	4.109528	-1.175693	0.186542
C	3.767200	1.098766	-0.547683
C	5.469063	-1.062974	-0.086504
H	3.708110	-2.105350	0.584350
C	5.125224	1.209422	-0.819627
H	3.092023	1.933322	-0.708411
C	5.979093	0.130306	-0.591330
H	6.129621	-1.904294	0.098084
H	5.522249	2.142206	-1.207960
H	7.039686	0.221472	-0.803706
C	-0.961047	2.021426	0.586276
N	-1.548159	3.016127	0.527186

TSD

C	-0.228677	0.596570	0.608391
C	1.861862	-0.339066	0.516433
C	-1.048603	-0.722886	-0.895512
C	-2.509935	-0.774929	-0.690179
C	-0.184548	-1.792793	-0.619026
C	1.160275	-1.711759	-0.932774
C	-3.104671	-1.604356	0.269448
C	-4.485826	-1.620559	0.423072
C	-5.292399	-0.813839	-0.376953
C	-4.709996	0.018067	-1.330071
C	-3.329028	0.041123	-1.480199
H	-0.723879	-0.034603	-1.673126
H	-0.524966	-2.590218	0.037987
H	1.486946	-1.069256	-1.744849
H	-2.489537	-2.223107	0.915160
H	-4.933665	-2.262904	1.174573
H	-6.370750	-0.830026	-0.253743
H	-5.331323	0.653511	-1.953179
H	-2.871504	0.702411	-2.211132
C	-1.024389	1.871106	0.380681
F	-1.039417	2.209936	-0.914382
F	-0.487373	2.894096	1.053064
F	-2.285605	1.732254	0.794323
N	1.044545	0.666001	0.229726
H	1.827710	-2.536270	-0.698358
H	1.647754	-0.999388	1.363966
C	3.290207	-0.241680	0.135212
C	4.209078	-1.139563	0.683005
C	3.729157	0.722206	-0.777802
C	5.552632	-1.076360	0.327043
H	3.867610	-1.887105	1.395768
C	5.071465	0.784314	-1.131079
H	3.007297	1.421042	-1.188809
C	5.985881	-0.114291	-0.581570
H	6.260664	-1.774952	0.761598
H	5.408554	1.538055	-1.835892
H	7.033856	-0.062113	-0.859631
C	-0.629164	-0.161386	1.783088
N	-0.882135	-0.821880	2.699613

TSE-cis

C	-0.187258	0.194360	0.799530
C	1.972092	-0.674976	0.296759
C	-0.935927	-0.430690	-1.157545
C	-2.416532	-0.465458	-1.168372
C	-0.128512	-1.567798	-1.356431
C	1.211518	-1.430915	-1.633984
C	-3.151018	-1.659479	-1.188496
C	-4.539359	-1.642105	-1.199254
C	-5.228631	-0.429992	-1.199855
C	-4.513842	0.763468	-1.210760
C	-3.123116	0.742887	-1.203744
H	-0.524903	0.492337	-1.558281
H	-0.520806	-2.555080	-1.123384
H	1.581751	-0.515069	-2.082079
H	-2.635601	-2.615317	-1.190170
H	-5.087690	-2.579122	-1.210878
H	-6.313960	-0.418608	-1.204959
H	-5.037579	1.714122	-1.228025
H	-2.568783	1.676587	-1.234373
C	-0.709188	-0.700239	1.965077
N	1.101941	0.298927	0.438081
C	-0.839781	1.573582	0.759657
O	-1.740866	1.956801	1.469657
O	-0.312109	2.368216	-0.192535
H	1.849904	-2.302595	-1.749241
H	1.874932	-1.663098	0.742965
C	3.357207	-0.322897	-0.104032
C	4.360725	-1.292723	-0.049191
C	3.671458	0.963942	-0.554413
C	5.662200	-0.986000	-0.435276
H	4.117365	-2.293835	0.301192
C	4.970766	1.268680	-0.939952
H	2.878661	1.705557	-0.584661
C	5.969877	0.296208	-0.882072
H	6.435476	-1.746469	-0.385310
H	5.209947	2.269842	-1.285939
H	6.984371	0.538860	-1.183021
C	-0.840252	3.690788	-0.215579
H	-0.658068	4.190066	0.738673
H	-0.319084	4.202573	-1.023291
H	-1.918080	3.677829	-0.399002
C	-2.233910	-0.913849	1.956605
H	-2.795562	-0.011889	1.717640
H	-2.513588	-1.698054	1.249971
H	-2.535353	-1.250841	2.955246
C	-0.304667	0.018911	3.272850
H	0.769882	0.231676	3.279978
H	-0.853632	0.952618	3.402160
H	-0.527834	-0.634557	4.124104
C	-0.082376	-2.104187	2.024903
H	-0.112085	-2.618630	1.059970
H	0.945807	-2.088369	2.393873
H	-0.664121	-2.702256	2.734745

TSE-trans

C	-0.200383	0.572491	0.306616
C	1.923548	-0.440003	0.448415
C	-0.966448	-1.029704	-0.888038
C	-2.448225	-1.127003	-0.770289
C	-0.111441	-2.072959	-0.478169
C	1.233247	-2.062280	-0.783412
C	-3.092247	-2.124002	-0.022503
C	-4.478631	-2.171497	0.070492
C	-5.261142	-1.231946	-0.595966
C	-4.639349	-0.261315	-1.376497
C	-3.252205	-0.213843	-1.469063
H	-0.646851	-0.472456	-1.763030
H	-0.462734	-2.800151	0.248917
H	1.588684	-1.523320	-1.655390
H	-2.513044	-2.887493	0.487059
H	-4.948773	-2.952570	0.660318
H	-6.343465	-1.267818	-0.521162

H	-5.236645	0.462373	-1.923056
H	-2.774829	0.542871	-2.081507
C	-0.734214	0.449785	1.770905
N	1.096535	0.466834	-0.033859
C	-0.701693	1.776520	-0.506424
O	-0.935854	1.781185	-1.690500
O	-0.725679	2.904724	0.222542
H	1.881589	-2.862044	-0.434931
H	1.755303	-0.954189	1.397266
C	3.348663	-0.397964	0.033489
C	4.291513	-1.159710	0.727289
C	3.762423	0.379241	-1.053167
C	5.630017	-1.146361	0.346674
H	3.971208	-1.764963	1.572910
C	5.098810	0.391414	-1.432828
H	3.019512	0.971279	-1.578477
C	6.036634	-0.370529	-0.735498
H	6.354912	-1.739482	0.895733
H	5.413868	0.999135	-2.275744
H	7.080172	-0.357544	-1.034522
C	-1.064715	4.084886	-0.506297
H	-2.061996	3.989420	-0.941085
H	-1.036143	4.896909	0.218430
H	-0.342639	4.254209	-1.307367
C	0.181116	1.300266	2.676236
H	1.194564	0.889855	2.722503
H	0.244904	2.329565	2.318319
H	-0.225961	1.309005	3.693697
C	-0.762649	-0.980128	2.336723
H	-1.551161	-1.572001	1.870514
H	0.180401	-1.519444	2.237725
H	-0.992287	-0.916567	3.406159
C	-2.176915	0.980423	1.891549
H	-2.231736	2.057972	1.732352
H	-2.853334	0.483731	1.189885
H	-2.541287	0.773917	2.903755

TSF-cis

C	-0.211192	0.553063	0.587732
C	1.874498	-0.492479	0.140998
C	-0.980136	-0.161396	-1.251490
C	-2.455813	-0.307125	-1.172535
C	-0.161795	-1.284914	-1.470020
C	1.184047	-1.138517	-1.741162
C	-3.069807	-1.324411	-0.432611
C	-4.455960	-1.427346	-0.381210
C	-5.255127	-0.521783	-1.074578
C	-4.655965	0.483573	-1.829866
C	-3.270389	0.588075	-1.876789
H	-0.654510	0.744853	-1.754765
H	-0.548377	-2.268986	-1.217807
H	1.544166	-0.227233	-2.208929
H	-2.455719	-2.036966	0.109747
H	-4.914217	-2.216918	0.206623
H	-6.336628	-0.601056	-1.029270
H	-5.268619	1.189352	-2.382326
H	-2.806927	1.375900	-2.465596
C	-0.765101	1.993505	0.829695
N	1.100070	0.568556	0.288385
C	-0.733945	-0.481516	1.575032
O	-1.362088	-0.223310	2.572682
O	-0.369461	-1.751387	1.291447
H	1.813789	-2.011848	-1.887323
H	1.653690	-1.448662	0.617971
C	3.315880	-0.271030	-0.155378
C	4.206751	-1.342668	-0.061539
C	3.797067	0.983503	-0.541419
C	5.557430	-1.168819	-0.347293
H	3.834642	-2.319666	0.240327
C	5.146129	1.157555	-0.826360
H	3.098149	1.812091	-0.600545
C	6.030343	0.083142	-0.731601
H	6.240448	-2.008977	-0.267425
H	5.512702	2.136157	-1.121486
H	7.083675	0.222737	-0.954210
C	-0.780398	-2.714525	2.262834
H	-1.869016	-2.715371	2.357933
H	-0.423156	-3.675504	1.895193
H	-0.343813	-2.483929	3.236573
C	0.037472	2.576279	2.010111
H	-0.069354	1.948586	2.899557
H	1.097875	2.652298	1.753537
H	-0.340638	3.576215	2.251472
C	-0.502181	2.870419	-0.403898
H	-0.584597	3.924775	-0.120028
H	0.500270	2.699019	-0.805944
H	-1.242760	2.691328	-1.190622
C	-2.261040	2.088860	1.177601
H	-2.893448	1.530975	0.484798
H	-2.465460	1.736658	2.187726
H	-2.554870	3.143193	1.115554

TSF-trans

C	-0.163399	0.699026	0.125802
C	1.930684	-0.355718	0.450559
C	-0.875933	-0.974095	-0.948295
C	-2.352719	-1.063769	-0.817710
C	-0.050767	-1.987808	-0.424795
C	1.299825	-2.012409	-0.703924
C	-2.974647	-1.472273	0.369689
C	-4.361748	-1.529708	0.458254
C	-5.153742	-1.192769	-0.637267
C	-4.545956	-0.807120	-1.829562
C	-3.159531	-0.743802	-1.916329
H	-0.540595	-0.548262	-1.890356
H	-0.438232	-2.622344	0.367621
H	1.673874	-1.553644	-1.614373
H	-2.368053	-1.738935	1.230782
H	-4.827131	-1.841758	1.388723
H	-6.235797	-1.236677	-0.564077
H	-5.152262	-0.553198	-2.693670
H	-2.689308	-0.438114	-2.847883
C	-0.721434	2.001929	-0.533212
N	1.161230	0.573585	-0.088857

C	-0.678416	0.288100	1.492317
O	-0.328266	-0.705387	2.094937
O	-1.550837	1.155083	2.020153
H	1.936421	-2.782519	-0.277494
H	1.669189	-0.852357	1.386003
C	3.384188	-0.327718	0.135457
C	4.260762	-1.116691	0.884077
C	3.892395	0.458195	-0.903209
C	5.623807	-1.122467	0.603984
H	3.866829	-1.727587	1.693670
C	5.253647	0.452876	-1.182985
H	3.203737	1.074844	-1.472542
C	6.123529	-0.337352	-0.431806
H	6.295459	-1.737227	1.195394
H	5.641088	1.068953	-1.988977
H	7.186492	-0.339045	-0.652637
C	-2.067735	0.794010	3.299651
H	-1.256852	0.680388	4.021521
H	-2.733357	1.606224	3.586966
H	-2.619375	-0.146888	3.230260
C	0.037501	3.177702	0.112479
H	-0.106388	3.183770	1.198038
H	1.107834	3.108833	-0.099402
H	-0.344208	4.125173	-0.284928
C	-2.232070	2.273188	-0.382303
H	-2.844040	1.377867	-0.500223
H	-2.469330	2.719636	0.583219
H	-2.529238	2.984651	-1.161297
C	-0.394941	1.992021	-2.035918
H	-0.481411	3.010190	-2.429627
H	0.621720	1.634754	-2.218416
H	-1.102638	1.370530	-2.594743

TSG-cis

C	-0.273489	0.303777	0.837043
C	1.845101	-0.441274	0.616141
C	-0.992330	-0.760985	-0.780828
C	-2.442406	-0.886375	-0.509674
C	-0.085744	-1.826286	-0.696623
C	1.257470	-1.629798	-0.983764
C	-2.950440	-1.773650	0.445756
C	-4.314990	-1.830880	0.702282
C	-5.194550	-0.994878	0.017223
C	-4.699186	-0.098794	-0.925763
C	-3.333348	-0.043527	-1.183401
H	-0.738090	0.033145	-1.480662
H	-0.381901	-2.725546	-0.158419
H	1.542907	-0.873177	-1.708559
H	-2.272774	-2.413139	1.005439
H	-4.693318	-2.522577	1.448530
H	-6.259111	-1.037047	0.224366
H	-5.376729	0.558924	-1.461799
H	-2.943232	0.658170	-1.917133
N	0.977062	0.558248	0.470594
C	-1.279330	1.413629	0.842806
O	-2.141981	1.514699	1.679469
O	-1.149482	2.242454	-0.203612
H	1.960741	-2.452171	-0.883099
H	1.664454	-1.214255	1.373879
C	3.276366	-0.213013	0.296148
C	4.238453	-1.132162	0.720264
C	3.674635	0.903058	-0.445991
C	5.581783	-0.941519	0.411592
H	3.929694	-2.000257	1.299056
C	5.016833	1.093060	-0.752283
H	2.917314	1.614368	-0.760506
C	5.973903	0.172185	-0.326448
H	6.321982	-1.660184	0.749650
H	5.320572	1.964783	-1.324005
H	7.021437	0.324191	-0.567394
C	-2.122372	3.284962	-0.244674
H	-2.043428	3.915399	0.643581
H	-1.903843	3.859428	-1.143666
H	-3.128302	2.859000	-0.287837
H	-0.504260	-0.439208	1.608721

TSG-trans

C	0.226702	0.541568	-0.595982
C	-1.893934	-0.238645	-0.622410
C	0.903953	-0.869167	0.762039
C	2.355999	-0.965981	0.485264
C	-0.013577	-1.880225	0.445587
C	-1.360854	-1.727989	0.736134
C	2.860843	-1.670422	-0.614296
C	4.226599	-1.702816	-0.868212
C	5.112883	-1.024752	-0.032782
C	4.621429	-0.312290	1.057658
C	3.253180	-0.278622	1.310719
H	0.650787	-0.227514	1.604731
H	0.285410	-2.659580	-0.253697
H	-1.660592	-1.120591	1.584831
H	2.179509	-2.183368	-1.288020
H	4.601393	-2.252354	-1.726265
H	6.179274	-1.049830	-0.233927
H	5.303305	0.221383	1.713087
H	2.866806	0.293100	2.150695
N	-1.039178	0.703329	-0.233332
C	1.195595	1.621156	-0.217329
O	1.145713	2.287343	0.786163
O	2.176787	1.704100	-1.128748
H	-2.068504	-2.503844	0.456480
H	-1.676484	-0.843132	-1.512466
C	-3.337949	-0.079225	-0.319550
C	-4.276880	-0.888677	-0.962489
C	-3.771101	0.860799	0.620801
C	-5.632425	-0.762648	-0.674669
H	-3.940491	-1.619328	-1.695301
C	-5.125423	0.986243	0.906118
H	-3.030916	1.490143	1.105105
C	-6.059516	0.175475	0.261544
H	-6.354623	-1.394097	-1.182964
H	-5.456306	1.721590	1.633256
H	-7.116589	0.276789	0.487051
C	3.215165	2.626158	-0.805395

H	3.668077	2.359277	0.152226
H	3.944845	2.544270	-1.609415
H	2.816826	3.641429	-0.744521
H	0.498385	-0.008849	-1.503370

TSH-cis

C	-0.324584	-0.212615	-1.157146
C	1.708051	0.249094	-0.120283
C	-1.089013	-1.168432	0.518995
C	-2.554311	-0.958940	0.433927
C	-0.279959	-0.583604	1.504084
C	1.086447	-0.817998	1.534794
C	-3.194878	0.130506	1.038209
C	-4.566124	0.312070	0.901727
C	-5.324159	-0.586803	0.154694
C	-4.698387	-1.670011	-0.455709
C	-3.326590	-1.850533	-0.317872
H	-0.754479	-2.130754	0.135893
H	-0.667341	0.255752	2.075118
H	1.480356	-1.754820	1.151422
H	-2.619101	0.846567	1.617822
H	-5.045514	1.161043	1.379954
H	-6.394282	-0.441355	0.046888
H	-5.278491	-2.375478	-1.042411
H	-2.839843	-2.695321	-0.799625
N	0.988735	-0.394132	-1.038602
C	-1.079431	1.086554	-1.060143
O	-1.978770	1.362210	-1.813587
O	-0.683548	1.904453	-0.063482
H	1.699132	-0.344111	2.296916
H	1.400484	1.221163	0.270322
C	3.175889	0.009446	-0.087705
C	3.995385	0.863302	0.653871
C	3.750286	-1.068826	-0.767221
C	5.368775	0.648323	0.717202
H	3.550024	1.704010	1.181924
C	5.122100	-1.282756	-0.704746
H	3.103973	-1.718694	-1.348522
C	5.935388	-0.426792	0.037678
H	5.996213	1.321075	1.293811
H	5.561907	-2.119463	-1.239179
H	7.006674	-0.596516	0.083759
C	-1.413393	3.130930	0.009030
H	-2.478129	2.925346	0.142975
H	-1.008439	3.667276	0.866035
H	-1.277813	3.708488	-0.907649
H	-0.806876	-0.826072	-1.919015

TSH-trans

C	-0.267380	0.193947	-1.043181
C	1.783443	0.326531	0.020396
C	-0.981616	-1.268231	0.242205
C	-2.453836	-1.089192	0.239185
C	-0.168900	-0.987929	1.350434
C	1.200745	-1.196361	1.291246
C	-3.109989	-0.236442	1.136936
C	-4.489324	-0.070504	1.075539
C	-5.239423	-0.745865	0.114726
C	-4.597398	-1.591132	-0.786071
C	-3.218194	-1.757694	-0.723213
H	-0.628787	-2.053500	-0.423993
H	-0.559155	-0.362023	2.148355
H	1.599179	-1.971788	0.643231
H	-2.539533	0.317303	1.877234
H	-4.981140	0.591623	1.782327
H	-6.315866	-0.613927	0.069478
H	-5.170716	-2.122309	-1.539605
H	-2.719336	-2.416761	-1.429913
N	1.048480	-0.012229	-1.039683
C	-0.938613	1.365799	-0.387699
O	-0.611727	1.901266	0.649258
O	-1.997155	1.752519	-1.112113
H	1.822207	-0.954693	2.149059
H	1.467707	1.124313	0.694701
C	3.252630	0.107901	-0.051486
C	4.084115	0.716716	0.891211
C	3.817335	-0.714130	-1.031210
C	5.460247	0.512216	0.857535
H	3.645608	1.358338	1.652570
C	5.191663	-0.917809	-1.064959
H	3.160959	-1.173247	-1.763701
C	6.017127	-0.306862	-0.121095
H	6.097400	0.994285	1.592667
H	5.623932	-1.553995	-1.831527
H	7.090446	-0.467512	-0.150592
C	-2.749990	2.827555	-0.554793
H	-2.128873	3.721862	-0.469290
H	-3.577993	2.995210	-1.241388
H	-3.122965	2.552606	0.434503
H	-0.787221	-0.121539	-1.947726

TSI

C	-0.185546	0.651637	0.402906
C	2.157187	-0.198516	0.450001
C	-0.819085	-0.959971	-0.939384
C	-2.291636	-1.048991	-0.849471
C	0.073436	-1.961715	-0.524022
C	1.414275	-1.858912	-0.833806
C	-2.949347	-1.953897	-0.006365
C	-4.336014	-2.008116	0.027328
C	-5.094722	-1.157750	-0.776823
C	-4.453795	-0.253040	-1.617739
C	-3.063728	-0.201567	-1.654750
H	-0.478268	-0.337220	-1.765228
H	-0.243958	-2.694359	0.212459
H	1.727260	-1.302523	-1.711775
H	-2.373498	-2.607169	0.642047
H	-4.829696	-2.714630	0.687319
H	-6.178863	-1.203661	-0.747391
H	-5.035041	0.408851	-2.252967
H	-2.560954	0.502912	-2.313682
C	-0.613481	0.172503	1.771071
F	-0.326100	1.091518	2.707970
F	0.027724	-0.958603	2.134031

F	-1.917015	-0.095682	1.871794
C	-1.009288	1.726091	-0.229576
O	-0.764477	2.186396	-1.324302
O	-2.059725	2.097435	0.504419
H	2.124137	-2.604195	-0.486375
H	2.016794	-0.789603	1.347081
C	3.561708	-0.089129	0.000317
C	4.575415	-0.629111	0.800437
C	3.920018	0.504957	-1.217242
C	5.908991	-0.558275	0.411731
H	4.309794	-1.100878	1.743259
C	5.252027	0.576616	-1.606920
H	3.151184	0.907033	-1.871752
C	6.252736	0.047709	-0.793502
H	6.679990	-0.976722	1.051345
H	5.510225	1.042002	-2.553198
H	7.292186	0.103000	-1.101013
C	-2.913522	3.064806	-0.104439
H	-3.343026	2.658629	-1.023138
H	-3.694522	3.266053	0.626305
H	-2.354026	3.972672	-0.337995
C	1.181139	0.710406	0.076008
H	1.411809	1.409664	-0.724965

TSJ

C	-0.166331	0.715437	0.331771
C	2.067659	-0.365620	0.354492
C	-0.892158	-0.569655	-1.244280
C	-2.349948	-0.761392	-1.051938
C	0.001835	-1.648418	-1.103770
C	1.340522	-1.515903	-1.393602
C	-2.862115	-1.683032	-0.128772
C	-4.235118	-1.860580	0.006030
C	-5.120261	-1.126093	-0.779623
C	-4.621903	-0.206570	-1.699540
C	-3.250525	-0.024549	-1.829377
H	-0.632509	0.188098	-1.982379
H	-0.326743	-2.528086	-0.557754
H	1.680842	-0.749103	-2.083465
H	-2.183517	-2.252677	0.500186
H	-4.614823	-2.578930	0.726859
H	-6.191298	-1.268333	-0.674752
H	-5.302919	0.372827	-2.315117
H	-2.864365	0.703983	-2.537509
C	-0.812943	2.050193	0.025603
F	-0.299427	2.558258	-1.116702
F	-0.576091	2.954356	0.988575
F	-2.133948	1.992277	-0.149067
C	-0.742890	-0.071704	1.456447
O	-0.325504	-1.146850	1.832100
O	-1.801007	0.530779	2.008318
H	2.022721	-2.350290	-1.259912
H	1.736847	-1.143480	1.034345
C	3.522872	-0.310423	0.097688
C	4.375762	-1.135226	0.840388
C	4.084112	0.515388	-0.885273
C	5.750361	-1.118111	0.628628
H	3.950586	-1.787736	1.598696
C	5.457265	0.533262	-1.098481
H	3.441442	1.142308	-1.497962
C	6.296787	-0.281286	-0.340632
H	6.395099	-1.759587	1.221501
H	5.873966	1.180333	-1.864242
H	7.368801	-0.267734	-0.510061
C	-2.428793	-0.188537	3.067791
H	-1.714141	-0.386054	3.869126
H	-3.236759	0.451885	3.416475
H	-2.825450	-1.135664	2.694811
C	1.233087	0.716503	0.144364
H	1.635835	1.570697	-0.394922