Cartesian coordinates, electronic energy (E, in a.u.) and the smallest vibrational frequency (v, in cm^{-1}) for all the stable molecules calculated by M06-2X/6-311++G method**

A1
E= -126.977969555 a.u.
υ= 333.8675

B	0.000000	0.000000	1.275959
C	0.000000	0.742229	0.000000
C	0.000000	-0.742229	0.000000
B	0.000000	0.000000	-1.275959
H	0.000000	0.000000	2.447650
H	0.000000	0.000000	-2.447650

A2
E= -205.627134943 a.u.
υ= 38.6426

B	0.000000	1.281955	0.000000
C	0.000000	0.000000	0.741541
C	0.000000	0.000000	-0.741541
B	0.000000	-1.281955	0.000000
C	0.030605	2.824369	0.000000
H	-0.432612	3.247603	0.891913
H	1.079102	3.143331	0.000000
H	-0.432612	3.247603	-0.891913
C	-0.030605	-2.824369	0.000000
H	-1.079102	-3.143331	0.000000
H	0.432612	-3.247603	-0.891913
H	0.432612	-3.247603	0.891913

A3
E= -708.322958076 a.u.
υ= 37.6349

B	1.288577	0.011162	-0.015677
C	-0.000008	0.746724	-0.000053
C	0.000010	-0.725494	-0.000058
B	-1.288575	0.011125	0.015575
H	3.827355	1.259381	-0.540027
H	3.716592	-0.162473	1.406937
H	3.791867	-1.144073	-0.795661
H	-3.716753	-0.165250	-1.406517
H	-3.791741	-1.142530	0.798002
H	-3.827337	1.260416	0.537684
Si	3.282003	-0.005159	-0.000927
Si	-3.282003	-0.005147	0.000981

A4
E= -237.801824835 a.u.
υ= 133.5090

B	0.000000	0.000000	1.281132
C	0.000000	0.737553	0.000000
C	0.000000	-0.737553	0.000000
B	0.000000	0.000000	-1.281132
N	0.000000	0.000000	2.666860
H	0.000000	-0.848336	3.208604
H	0.000000	0.848336	3.208604
N	0.000000	0.000000	-2.666860
H	0.000000	-0.848336	-3.208604
H	0.000000	0.848336	-3.208604

A5
E= -810.877128753 a.u.
υ= 82.2559

B	-1.283341	0.000227	-0.029371
C	0.000046	0.735871	-0.000030
C	-0.000043	-0.735642	-0.000007
B	1.283348	0.000058	0.029333
H	-3.397983	1.056137	-0.787967
H	-3.397513	-1.056273	-0.788161
H	3.397693	-1.056311	0.788061
H	3.397836	1.056134	0.788060
P	3.157247	-0.000070	-0.117042
P	-3.157252	-0.000095	0.117070

A6

E= -277.554407665 a.u.
υ= 139.3394

B	0.008100	1.270656	0.000000
C	0.746691	-0.007450	0.000000
C	-0.746691	0.007450	0.000000
B	-0.008100	-1.270656	0.000000
O	-0.008100	2.608276	0.000000
H	0.868233	3.002147	0.000000
O	0.008100	-2.608276	0.000000
H	-0.868233	-3.002147	0.000000

A7

E= -923.432211191 a.u.
υ= 78.6553

B	-0.017301	1.277049	0.000000
C	-0.736438	-0.010202	0.000000
C	0.736438	0.010202	0.000000
B	0.017301	-1.277049	0.000000
S	0.017301	3.044795	0.000000
H	-1.317975	3.197748	0.000000
S	-0.017301	-3.044795	0.000000
H	1.317975	-3.197748	0.000000

A8

E= -923.432211191 a.u.
υ= 78.6553

B	0.000000	0.000000	1.257527
C	0.000000	0.754220	0.000000
C	0.000000	-0.754220	0.000000
B	0.000000	0.000000	-1.257527
F	0.000000	0.000000	-2.560667
F	0.000000	0.000000	2.560667

A9

E= -1046.27672083 a.u.
υ= 87.7410

B	0.000000	0.000000	1.265908
C	0.000000	0.746004	0.000000
C	0.000000	-0.746004	0.000000
B	0.000000	0.000000	-1.265908
Cl	0.000000	0.000000	-2.977329
Cl	0.000000	0.000000	2.977329

A10

E= -5274.21137871 a.u.
υ= 76.5304

B	0.000000	0.000000	1.267495
C	0.000000	0.744877	0.000000
C	0.000000	-0.744877	0.000000
B	0.000000	0.000000	-1.267495
Br	0.000000	0.000000	3.133719
Br	0.000000	0.000000	-3.133719

A11

E= -589.044304471 a.u.
υ= 35.4980

B	0.000000	0.000000	1.279871
C	0.000000	0.741463	0.000000
C	0.000000	-0.741463	0.000000
B	0.000000	0.000000	-1.279871
C	0.000000	0.000000	-2.806478
C	0.000000	1.206784	-3.520701
C	0.000000	-1.206784	-3.520701
C	0.000000	1.208345	-4.909774
H	0.000000	2.144867	-2.975444
C	0.000000	-1.208345	-4.909774
H	0.000000	-2.144867	-2.975444
C	0.000000	0.000000	-5.602168
H	0.000000	2.145659	-5.454433
H	0.000000	-2.145659	-5.454433
H	0.000000	0.000000	-6.686767
C	0.000000	0.000000	2.806478
C	0.000000	-1.206784	3.520701
C	0.000000	1.206784	3.520701

C	0.000000	-1.208345	4.909774
H	0.000000	-2.144867	2.975444
C	0.000000	1.208345	4.909774
H	0.000000	2.144867	2.975444
C	0.000000	0.000000	5.602168
H	0.000000	-2.145659	5.454433
H	0.000000	2.145659	5.454433
H	0.000000	0.000000	6.686767

A12

E= -441.441726950 a.u.

υ= 12.1981

B	0.217018	1.263666	0.000000
C	0.000000	0.000000	0.742153
C	0.000000	0.000000	-0.742153
B	-0.217018	-1.263666	0.000000
C	-0.546598	-2.781131	0.000000
C	0.546598	2.781131	0.000000
C	0.000000	-3.467038	1.259974
H	-0.382432	-2.991351	2.165959
H	-0.296838	-4.521118	1.272373
H	1.091821	-3.426030	1.294457
C	0.000000	-3.467038	-1.259974
H	-0.296838	-4.521118	-1.272373
H	-0.382432	-2.991351	-2.165959
H	1.091821	-3.426030	-1.294457
C	-2.088678	-2.872285	0.000000
H	-2.519685	-2.399680	-0.886518
H	-2.386807	-3.926009	0.000000
H	-2.519685	-2.399680	0.886518
C	2.088678	2.872285	0.000000
H	2.519685	2.399680	-0.886518
H	2.386807	3.926009	0.000000
H	2.519685	2.399680	0.886518
C	0.000000	3.467038	-1.259974
H	-1.091821	3.426030	-1.294457
H	0.296838	4.521118	-1.272373
H	0.382432	2.991351	-2.165959
C	0.000000	3.467038	1.259974
H	-1.091821	3.426030	1.294457
H	0.382432	2.991351	2.165959
H	0.296838	4.521118	1.272373

A13

E= -311.477557358 a.u.

υ= 69.9530

B	0.000000	0.000000	1.266882
C	0.000000	0.743778	0.000000
C	0.000000	-0.743778	0.000000
B	0.000000	0.000000	-1.266882
C	0.000000	0.000000	-2.775366
C	0.000000	0.000000	2.775366
N	0.000000	0.000000	-3.925100
N	0.000000	0.000000	3.925100

A14

E= -535.970296575 a.u.

υ= 40.2039

B	-1.253900	0.000000	0.000000
C	0.000000	0.000000	0.747536
C	0.000000	0.000000	-0.747536
B	1.253900	0.000000	0.000000
N	-2.753711	0.000000	0.000000
N	2.753711	0.000000	0.000000
O	-3.295337	1.084208	0.000000
O	-3.295337	-1.084208	0.000000
O	3.295337	1.084208	0.000000
O	3.295337	-1.084208	0.000000

B1

E= -332.600256467 a.u.

υ= 158.6112

C	0.390615	1.183706	0.051198
C	1.644762	0.743350	-0.066425
C	1.644761	-0.743350	-0.066424
C	0.390614	-1.183706	0.051199
H	0.044697	2.207453	0.091202
H	2.534817	1.352972	-0.146628
H	2.534817	-1.352972	-0.146627
H	0.044696	-2.207452	0.091203
C	-0.554987	0.000000	0.065105
C	-1.495894	0.000000	-1.131459
H	-2.130029	-0.887877	-1.102151
H	-2.130027	0.887878	-1.102152
H	-0.921392	-0.000002	-2.059263
F	-1.344090	0.000000	1.217250

B2

E= -2866.86356600 a.u.

υ= 135.3068

C	0.651449	0.918304	1.191724
C	0.651449	2.174341	0.744388
C	0.651449	2.174341	-0.744388
C	0.651449	0.918304	-1.191724
H	0.652034	0.551670	2.207067
H	0.646908	3.068308	1.352530
H	0.646908	3.068308	-1.352530
H	0.652034	0.551670	-2.207067
C	0.626766	-0.003811	0.000000
Br	-1.051422	-1.033402	0.000000
F	1.645167	-0.906640	0.000000

B3

E= -752.891309909 a.u.

υ= 149.8621

C	0.280623	0.593617	1.192371
C	0.280623	1.848413	0.745436
C	0.280623	1.848413	-0.745436
C	0.280623	0.593617	-1.192371
H	0.278764	0.226488	2.207744
H	0.277052	2.742868	1.352887
H	0.277052	2.742868	-1.352887
H	0.278764	0.226488	-2.207744
C	0.260217	-0.333487	0.000000
Cl	-1.245486	-1.316202	0.000000
F	1.307263	-1.207412	0.000000

B4

E= -692.963870439 a.u.

υ= 143.8019

C	0.661396	0.022137	1.179989
C	1.878958	-0.310516	0.740328
C	1.878958	-0.310517	-0.740328
C	0.661396	0.022136	-1.179989
H	0.318368	0.106582	2.201635
H	2.737305	-0.550487	1.353144
H	2.737305	-0.550489	-1.353144
H	0.318368	0.106580	-2.201635
C	-0.232297	0.313865	0.000000
C	-0.770683	1.740453	-0.000001
H	-1.380237	1.916610	-0.887263
H	-1.380236	1.916611	0.887263
H	0.071683	2.436566	-0.000001
Cl	-1.640525	-0.838078	0.000000

B5

E= -2806.93792900 a.u.

υ= 125.7222

C	1.121023	0.011727	1.179204
C	2.216233	-0.618518	0.739368
C	2.216233	-0.618517	-0.739368
C	1.121023	0.011728	-1.179204
H	0.812232	0.182727	2.200839
H	2.985790	-1.066399	1.353119
H	2.985791	-1.066397	-1.353120

H	0.812232	0.182729	-2.200839
C	0.331824	0.512720	0.000000
C	0.115566	2.020714	0.000001
H	-0.438507	2.329509	-0.887008
H	-0.438507	2.329508	0.887009
H	1.092790	2.511785	0.000001
Br	-1.444092	-0.380645	0.000000

B6

E= -3227.22258128 a.u.

υ= 127.7476

C	0.393110	1.055673	1.187065
C	0.393110	2.314130	0.741172
C	0.393110	2.314130	-0.741172
C	0.393110	1.055673	-1.187065
H	0.395302	0.688207	2.202080
H	0.390609	3.204980	1.353772
H	0.390609	3.204980	-1.353772
H	0.395302	0.688207	-2.202080
C	0.386979	0.130664	0.000000
Br	-1.258483	-0.937071	0.000000
Cl	1.806975	-0.953558	0.000000

B7

E= -233.363120591 a.u.

υ= 162.9159

C	-0.206580	-1.173388	0.190474
C	-1.421106	-0.735988	-0.176757
C	-1.421110	0.735983	-0.176757
C	-0.206585	1.173390	0.190470
H	0.979063	0.000005	1.524817
H	0.112786	-2.203538	0.278722
H	-2.272647	-1.350549	-0.437862
H	-2.272656	1.350540	-0.437858
H	0.112774	2.203541	0.278720
C	0.695567	0.000002	0.462424
C	1.972044	0.000001	-0.389297
H	2.576966	0.884527	-0.179801
H	2.576909	-0.884584	-0.179883
H	1.713422	0.000058	-1.450200

B8

E= -2767.63022270 a.u.

υ= 126.1447

C	0.729890	0.912445	1.182297
C	0.729890	2.175903	0.738782
C	0.729890	2.175903	-0.738782
C	0.729890	0.912445	-1.182297
H	1.642965	-0.659701	0.000000
H	0.719385	0.564030	2.204459
H	0.724667	3.067074	1.351622
H	0.724667	3.067074	-1.351622
H	0.719385	0.564030	-2.204459
C	0.766049	-0.010170	0.000000
Br	-0.761278	-1.245762	0.000000

B9

E= -653.655383899 a.u.

υ= 142.9188

C	0.396198	0.472086	1.183006
C	0.396198	1.734394	0.739655
C	0.396198	1.734394	-0.739655
C	0.396198	0.472086	-1.183006
H	1.370765	-1.042499	0.000000
H	0.383795	0.122666	2.204960
H	0.391480	2.625961	1.352020
H	0.391480	2.625961	-1.352020
H	0.383795	0.122666	-2.204960
C	0.449529	-0.453829	0.000000
Cl	-0.889838	-1.659384	0.000000

B10

E= -293.290033203 a.u.

υ= 189.0113

C	0.130968	0.129988	1.185925
C	0.130968	1.390662	0.741983
C	0.130968	1.390662	-0.741983
C	0.130968	0.129988	-1.185925
H	1.228283	-1.265951	0.000000
H	0.121396	-0.216591	2.209142
H	0.127687	2.285123	1.350431
H	0.127687	2.285123	-1.350431
H	0.121396	-0.216591	-2.209142
C	0.234611	-0.794892	0.000000
F	-0.697482	-1.816618	0.000000

TS-B1-anti

E= -658.182177952 a.u.

υ= 369.0929i

C	1.363232	-0.149373	-0.000014
C	0.600015	-0.728259	-1.174212
C	0.072156	-1.918123	-0.708889
C	0.072174	-1.918097	0.708962
C	0.600040	-0.728212	1.174226
H	0.840774	-0.493059	-2.201631
H	-0.368701	-2.688806	-1.326187
H	-0.368667	-2.688756	1.326301
H	0.840842	-0.492984	2.201629
C	-1.148098	0.666555	-0.794604
C	-1.148075	0.666524	0.794591
B	-0.650928	1.825908	0.000006
B	-2.071525	-0.157025	-0.000013
C	2.820735	-0.623447	-0.000019
H	3.321691	-0.233516	-0.886795
H	3.321709	-0.233482	0.886732
H	2.870577	-1.710451	0.000001
F	-2.915999	-1.161195	-0.000018
F	-0.325486	3.095038	0.000030
F	1.437147	1.242960	-0.000042

TS-B1-syn

E= -658.160569506 a.u.

υ= 370.7523i

C	-1.427994	-0.125810	-0.000034
C	-0.637231	-0.712248	1.176199
C	-0.090128	-1.886603	0.711892
C	-0.090141	-1.886713	-0.711720
C	-0.637289	-0.712451	-1.176193
H	-0.875397	-0.483279	2.205793
H	0.374147	-2.646857	1.325668
H	0.374132	-2.647057	-1.325385
H	-0.875420	-0.483599	-2.205820
C	1.177358	0.648062	0.803552
C	1.177390	0.648134	-0.803585
B	0.842874	1.848086	0.000024
B	2.055408	-0.222174	-0.000046
C	-1.830747	1.342537	-0.000189
H	-1.480595	1.865763	-0.890331
H	-2.919108	1.389263	-0.000478
H	-1.481044	1.865825	0.890096
F	0.515376	3.117969	0.000090
F	2.856043	-1.258756	-0.000067
F	-2.644245	-0.845775	0.000092

TS-B2-anti

E= -3192.43818125 a.u.

υ= 390.1576i

C	0.586658	0.199476	0.000276
C	0.006260	-0.546208	-1.180728
C	-0.245640	-1.820211	-0.708123
C	-0.245482	-1.820403	0.708247
C	0.006733	-0.546654	1.181142
H	0.205900	-0.254903	-2.201072
H	-0.502208	-2.669972	-1.325017
H	-0.501918	-2.670348	1.324944

H	0.206178	-0.255427	2.201538
C	-2.018000	0.403857	-0.797963
C	-2.018564	0.404073	0.797977
B	-1.845637	1.650035	-0.000010
B	-2.723721	-0.613743	-0.000099
Br	2.544104	-0.041001	-0.000177
F	-1.775948	2.954649	-0.000176
F	-3.307262	-1.786519	-0.000215
F	0.412477	1.549718	0.000545

TS-B2-syn

E= -3192.42207326 a.u.

υ= 401.8113i

C	-0.416091	-1.084905	-0.000003
C	0.541206	-0.983430	1.186278
C	1.698158	-1.561833	0.712614
C	1.698179	-1.561814	-0.712574
C	0.541239	-0.983385	-1.186257
H	0.193331	-0.963528	2.208249
H	2.535614	-1.868393	1.324592
H	2.535651	-1.868357	-1.324537
H	0.193391	-0.963482	-2.208238
C	1.053577	1.204663	0.795619
C	1.053566	1.204648	-0.795608
B	0.025242	1.938034	0.000012
B	2.285758	1.086058	-0.000006
Br	-1.987936	0.049233	-0.000002
F	3.552812	0.749227	-0.000019
F	-0.887299	2.879136	0.000009
F	-0.938205	-2.359864	-0.000038

TS-B3-anti

E= -1078.46566628 a.u.

υ= 390.9006i

C	1.084675	0.150840	0.000014
C	0.469937	-0.574839	-1.181995
C	0.180081	-1.838408	-0.709473
C	0.180145	-1.838389	0.709623
C	0.470076	-0.574836	1.182083
H	0.679686	-0.289724	-2.202263
H	-0.103858	-2.680450	-1.325042
H	-0.103746	-2.680415	1.325235
H	0.679853	-0.289656	2.202325
C	-1.522510	0.445377	-0.797704
C	-1.522586	0.445389	0.797706
B	-1.302305	1.684192	0.000019
B	-2.258795	-0.549912	-0.000035
F	0.943404	1.507239	0.000012
F	-1.190553	2.985735	0.000018
F	-2.870732	-1.708102	-0.000068
Cl	2.863270	-0.122695	-0.000079

TS-B3-syn

E= -1078.45392739 a.u.

υ= 400.0951i

C	-0.873082	-0.986565	-0.000001
C	0.089782	-0.977122	1.185767
C	1.195452	-1.647875	0.712515
C	1.195457	-1.647885	-0.712494
C	0.089785	-0.977149	-1.185765
H	-0.257335	-0.929649	2.207219
H	2.004501	-2.021732	1.324976
H	2.004511	-2.021750	-1.324945
H	-0.257320	-0.929679	-2.207221
C	0.767505	1.163146	0.796454
C	0.767503	1.163159	-0.796457
B	-0.218646	1.949757	0.000005
B	1.988219	0.959355	-0.000007
F	-1.520567	-2.201049	0.000014
F	-1.102427	2.916621	0.000015
F	3.228939	0.537022	-0.000012
Cl	-2.187655	0.208567	-0.000017

TS-B4-anti

E= -1018.53282578 a.u.

υ= 387.8106i

C	0.934044	-0.933001	-0.000011
C	-0.020578	-1.011428	-1.174423
C	-1.078271	-1.773459	-0.707541
C	-1.078269	-1.773382	0.707590
C	-0.020633	-1.011208	1.174391
H	0.312031	-0.936752	-2.200141
H	-1.850664	-2.208349	-1.326754
H	-1.850656	-2.208217	1.326848
H	0.312051	-0.936635	2.200094
C	-0.820819	1.060682	-0.784716
C	-0.820767	1.060501	0.784670
B	0.208550	1.837514	0.000015
B	-2.035950	0.815721	-0.000022
C	1.903395	-2.130997	0.000153
H	2.536856	-2.100102	-0.886889
H	2.536675	-2.100005	0.887322
H	1.327886	-3.055247	0.000144
F	-3.261438	0.338786	-0.000027
F	0.815150	3.024538	0.000137
Cl	1.990635	0.534292	-0.000133

TS-B4-syn

E= -1018.52166160 a.u.

υ= 393.5701i

C	-1.123530	0.291594	0.090929
C	-0.602592	-0.593056	1.204910
C	-0.309666	-1.822032	0.652209
C	-0.269714	-1.708679	-0.754035
C	-0.470893	-0.382389	-1.122973
H	-0.771333	-0.376611	2.250321
H	-0.058972	-2.713994	1.209552
H	0.010460	-2.502152	-1.433248
H	-0.674883	-0.039394	-2.128172
C	1.644524	0.349487	0.813439
C	1.513398	0.268114	-0.797165
B	1.610998	1.551749	-0.045093
B	2.211831	-0.752019	0.020909
C	-1.099202	1.804628	0.277158
H	-0.965246	2.315160	-0.678098
H	-2.041427	2.139961	0.705839
H	-0.321237	2.108906	0.974284
F	1.651853	2.860531	-0.132830
F	2.739874	-1.951797	0.024818
Cl	-2.912412	-0.138538	-0.117311

TS-B5-anti

E= -3132.50153410 a.u.

υ= 398.4750i

C	0.384573	1.153949	-0.000010
C	-0.563628	1.015255	1.174036
C	-1.758061	1.541880	0.707028
C	-1.758084	1.541794	-0.707057
C	-0.563652	1.015058	-1.174029
H	-0.224397	1.013628	2.200346
H	-2.604843	1.805699	1.325903
H	-2.604879	1.805530	-1.325949
H	-0.224425	1.013443	-2.200345
C	-0.953687	-1.171431	0.785628
C	-0.953718	-1.171315	-0.785606
B	0.176132	-1.789726	-0.000024
B	-2.193559	-1.157631	0.000038
C	1.048339	2.548447	-0.000140
H	1.671604	2.668181	0.886335
H	1.671580	2.668018	-0.886654
H	0.271833	3.312388	-0.000200
F	-3.487698	-0.923406	0.000050
F	0.959351	-2.867447	-0.000111
Br	1.874094	-0.122122	0.000055

TS-B5-syn

E= -3132.49568503 a.u.

υ= 381.9618i

C	-0.605250	0.366811	-0.004505
C	-0.068362	-0.439907	1.165351
C	0.120374	-1.735789	0.704818
C	0.119675	-1.739679	-0.702731
C	-0.071669	-0.447004	-1.169958
H	-0.238585	-0.147312	2.192000
H	0.347264	-2.588937	1.329160
H	0.346122	-2.596289	-1.322468
H	-0.239664	-0.159136	-2.198278
C	2.064369	0.241860	0.807479
C	2.069764	0.244551	-0.807149
B	2.173571	1.484603	0.002200
B	2.643795	-0.850483	-0.000089
C	-0.489223	1.891026	-0.010971
H	0.046486	2.232149	-0.897878
H	-1.464801	2.368368	-0.025973
H	0.025588	2.241629	0.884669
F	2.308642	2.790281	0.005541
F	3.117285	-2.072551	-0.000045
Br	-2.588019	-0.036339	0.002421

TS-B6-anti

E= -3552.78570608 a.u.

υ= 401.6839i

C	-0.602511	0.136570	-0.000077
C	-0.023922	-0.621943	1.178427
C	0.173020	-1.909361	0.706816
C	0.173009	-1.909807	-0.705615
C	-0.023916	-0.622693	-1.178075
H	-0.210464	-0.323104	2.199155
H	0.402028	-2.765205	1.326352
H	0.401946	-2.766067	-1.324604
H	-0.210368	-0.324534	-2.199016
C	2.067753	0.165192	0.796431
C	2.067810	0.165588	-0.796513
B	2.080939	1.429525	0.000239
B	2.685889	-0.908078	-0.000323
Br	-2.561913	-0.184182	0.000001
F	2.348107	2.715051	0.000644
F	3.167766	-2.127690	-0.000590
Cl	-0.422391	1.900619	-0.000609

TS-B6-syn

E= -3552.78080178 a.u.

υ= 404.7550i

C	0.644073	0.747354	-0.000031
C	-0.274060	1.016595	1.181301
C	-1.165501	1.960250	0.708518
C	-1.165401	1.960401	-0.708519
C	-0.273849	1.016975	-1.181410
H	0.052980	0.881695	2.201488
H	-1.839179	2.537264	1.326528
H	-1.838972	2.537594	-1.326481
H	0.053170	0.882058	-2.201593
C	-1.478973	-0.862341	0.787460
C	-1.479098	-0.862544	-0.787548
B	-0.689154	-1.875913	-0.000043
B	-2.612306	-0.358335	-0.000016
Br	1.554465	-0.974414	-0.000051
F	-3.702746	0.373055	0.000020
F	-0.354359	-3.160339	0.000106
Cl	1.961401	1.980150	0.000140

TS-B7-anti

E= -558.937708954 a.u.

υ= 388.9061i

C	-1.474399	0.240986	0.000035
C	-0.801453	-0.454849	1.164058
C	-0.416766	-1.709595	0.703778

C	-0.416652	-1.709471	-0.703851
C	-0.801233	-0.454620	-1.164004
H	-1.381932	1.326393	0.000180
H	-1.005084	-0.209838	2.197620
H	-0.061269	-2.520467	1.325446
H	-0.061044	-2.520232	-1.325601
H	-1.004748	-0.209458	-2.197555
C	1.133230	0.603901	0.811947
C	1.133257	0.603947	-0.811900
B	0.809286	1.796090	0.000049
B	1.963622	-0.309303	0.000010
C	-2.990431	-0.066565	-0.000115
H	-3.458295	0.370529	0.883547
H	-3.458197	0.370763	-0.883714
H	-3.171256	-1.141281	-0.000261
F	0.346372	3.026209	0.000052
F	2.714070	-1.384293	-0.000012

TS-B7-syn

E= -558.933215046 a.u.

υ= 369.6235i

C	0.574282	-1.570723	0.000077
C	-0.289953	-1.155412	-1.163580
C	-1.605285	-1.179124	-0.702135
C	-1.605360	-1.179044	0.702028
C	-0.290062	-1.155094	1.163602
H	0.011904	-1.264854	-2.196646
H	-2.486201	-1.096973	-1.324552
H	-2.486349	-1.096874	1.324339
H	0.011643	-1.264512	2.196717
H	0.409489	-2.662120	0.000311
C	0.077786	1.053424	-0.806130
C	0.077700	1.053286	0.806106
B	1.296326	1.301294	0.000131
B	-1.088435	1.460951	-0.000022
C	2.083637	-1.330365	0.000070
H	2.626414	-2.275595	0.000039
H	2.403571	-0.779145	-0.885951
H	2.403672	-0.779156	0.886054
F	2.578968	1.586994	-0.000101
F	-2.364531	1.767041	-0.000020

TS-B8-anti

E= -3093.20171349 a.u.

υ= 392.7066i

C	0.599394	0.293830	-0.000049
C	-0.004166	-0.443851	-1.172389
C	-0.341746	-1.705159	-0.705206
C	-0.341817	-1.705226	0.704804
C	-0.004323	-0.443940	1.172169
H	0.529162	1.375328	-0.000017
H	0.204091	-0.179547	-2.198360
H	-0.657763	-2.532264	-1.325901
H	-0.657896	-2.532395	1.325381
H	0.203876	-0.179768	2.198185
C	-1.969931	0.580855	-0.810983
C	-1.969836	0.580904	0.811042
B	-1.687510	1.785601	-0.000026
B	-2.764108	-0.366397	0.000111
Br	2.553027	0.000276	0.000085
F	-1.256821	3.024752	-0.000071
F	-3.468153	-1.469365	0.000183

TS-B8-syn

E= -3093.20009011 a.u.

υ= 391.0356i

C	0.360207	-1.260801	-0.000010
C	-0.564672	-1.104720	-1.176056
C	-1.787721	-1.571755	-0.704877
C	-1.787758	-1.571778	0.704724
C	-0.564736	-1.104753	1.175988
H	-0.227648	-1.114892	-2.202222

H	-2.645317	-1.798580	-1.323743
H	-2.645388	-1.798630	1.323533
H	-0.227776	-1.114963	2.202175
H	0.649970	-2.317181	-0.000016
C	-0.894707	1.105588	-0.796659
C	-0.894649	1.105607	0.796662
B	0.186614	1.753474	-0.000043
B	-2.132322	1.102941	0.000051
Br	2.054096	-0.331709	0.000044
F	-3.434277	0.935438	0.000104
F	1.182670	2.607633	-0.000096

TS-B9-anti

E= -979.226726172 a.u.

υ= 390.0671i

C	-1.135590	0.279362	0.000214
C	-0.519227	-0.456710	1.173465
C	-0.179469	-1.713794	0.706078
C	-0.179671	-1.713229	-0.707555
C	-0.519586	-0.455788	-1.173806
H	-1.049625	1.360384	0.000684
H	-0.727772	-0.192948	2.199688
H	0.139263	-2.541498	1.324773
H	0.138900	-2.540424	-1.327014
H	-0.728419	-0.191155	-2.199748
C	1.443414	0.590797	0.809637
C	1.443543	0.590670	-0.809434
B	1.148699	1.793113	-0.000021
B	2.239870	-0.354977	0.000270
Cl	-2.925598	0.002259	0.000386
F	2.944012	-1.457625	0.000402
F	0.711487	3.029704	-0.000156

TS-B9-syn

E= -979.229442163 a.u.

υ= 380.8582i

C	-0.532970	-1.425447	0.000068
C	0.353633	-1.115777	1.176231
C	1.638423	-1.357983	0.705821
C	1.638591	-1.358342	-0.705092
C	0.353969	-1.116466	-1.175944
H	0.021687	-1.182896	2.201964
H	2.522843	-1.427453	1.324376
H	2.523171	-1.428165	-1.323375
H	0.022263	-1.183679	-2.201738
H	-0.638741	-2.516600	0.000377
C	0.264510	1.119967	0.796268
C	0.264260	1.120210	-0.796484
B	-0.927468	1.529008	0.000055
B	1.480999	1.347924	-0.000274
Cl	-2.200680	-0.815835	-0.000318
F	2.791211	1.422789	-0.000368
F	-2.090080	2.135694	0.000333

TS-B10-anti

E= -618.861018640 a.u.

υ= 382.8998i

C	-1.441959	0.353335	0.000386
C	-0.862685	-0.423649	1.178858
C	-0.618433	-1.694500	0.711475
C	-0.618462	-1.693779	-0.712783
C	-0.862694	-0.422461	-1.178905
H	-1.281896	1.429871	0.001109
H	-1.044221	-0.147388	2.207016
H	-0.364570	-2.548943	1.324616
H	-0.364622	-2.547607	-1.326790
H	-1.044074	-0.145031	-2.206777
C	1.167689	0.538890	0.805722
C	1.168160	0.539038	-0.805590
B	0.931699	1.756148	0.000033
B	1.892658	-0.463526	0.000160
F	-2.822925	0.188855	0.000270

F	0.579237	3.018622	0.000024
F	2.509011	-1.616951	0.000249

TS-B10-syn

E= -618.874612286 a.u.

υ= 366.3245i

C	0.304142	-1.595400	-0.000018
C	-0.477615	-1.077961	-1.177737
C	-1.775286	-0.963677	-0.707906
C	-1.775282	-0.963706	0.707908
C	-0.477610	-1.078014	1.177726
H	-0.177036	-1.229109	-2.204132
H	-2.649193	-0.801585	-1.323824
H	-2.649186	-0.801637	1.323838
H	-0.177024	-1.229205	2.204113
H	0.196527	-2.688124	-0.000042
C	0.310233	1.019515	-0.795176
C	0.310223	1.019478	0.795184
B	1.565448	0.920896	0.000007
B	-0.765561	1.631308	0.000006
F	1.657495	-1.333260	-0.000013
F	2.872846	0.968398	0.000014
F	-1.981047	2.123443	0.000010

P-B1-anti

E= -658.247604708 a.u.

υ= 124.2089

C	-1.357852	-0.063028	0.000048
C	-0.417906	-0.492449	1.159233
C	-0.099315	-1.893460	0.670978
C	-0.099341	-1.893492	-0.670866
C	-0.417983	-0.492512	-1.159177
H	-0.834925	-0.394597	2.159146
H	0.174658	-2.720089	1.313308
H	0.174603	-2.720154	-1.313167
H	-0.835069	-0.394716	-2.159068
C	0.835074	0.391796	0.856734
C	0.835013	0.391752	-0.856813
B	0.670110	1.643030	-0.000066
B	1.911371	-0.225261	-0.000062
C	-2.764540	-0.617638	0.000112
H	-3.294185	-0.262013	0.885399
H	-3.294244	-0.262070	-0.885164
H	-2.760710	-1.705282	0.000147
F	2.954948	-1.022685	-0.000079
F	0.608027	2.952629	-0.000099
F	-1.487023	1.334975	0.000016

P-B1-syn

E= -658.234347588 a.u.

υ= 122.7278

C	1.360106	-0.232426	0.000007
C	0.361463	-0.532020	-1.159221
C	-0.166914	-1.874840	-0.669605
C	-0.166943	-1.874826	0.669582
C	0.361433	-0.532008	1.159212
H	0.793775	-0.498739	-2.156753
H	-0.557980	-2.650353	-1.314471
H	-0.558039	-2.650326	1.314446
H	0.793723	-0.498740	2.156755
C	-0.765606	0.503382	-0.862896
C	-0.765621	0.503401	0.862867
B	-0.545287	1.732227	-0.000025
B	-1.900640	0.001573	-0.000032
C	2.053121	1.126279	0.000025
H	3.128525	0.956171	0.000131
H	1.811591	1.715083	-0.887719
H	1.811437	1.715061	0.887746
F	-0.263396	3.014423	-0.000011
F	-3.053836	-0.624543	0.000034
F	2.359496	-1.198637	0.000014

P-B2-anti

E= -3192.50624318 a.u.

υ= 107.5238

C	-0.582174	0.299295	0.000000
C	0.212186	-0.339622	1.166413
C	0.212186	-1.774910	0.670174
C	0.212186	-1.774910	-0.670174
C	0.212186	-0.339622	-1.166413
H	-0.185943	-0.146105	2.158502
H	0.276561	-2.640082	1.315670
H	0.276561	-2.640082	-1.315670
H	-0.185943	-0.146105	-2.158502
C	1.629892	0.237483	0.859691
C	1.629892	0.237483	-0.859691
B	1.784895	1.487341	0.000000
B	2.528557	-0.621322	0.000000
Br	-2.481537	-0.098999	0.000000
F	1.982783	2.778896	0.000000
F	3.377995	-1.619224	0.000000
F	-0.477759	1.666556	0.000000

P-B2-syn

E= -3192.50101090 a.u.

υ= 94.3435

C	-1.051714	-0.282202	0.000000
C	-0.211118	-0.864104	1.166428
C	-0.211118	-2.307799	0.670054
C	-0.211118	-2.307799	-0.670054
C	-0.211118	-0.864104	-1.166428
H	-0.614392	-0.676147	2.157890
H	-0.146999	-3.172214	1.316959
H	-0.146999	-3.172214	-1.316959
H	-0.614392	-0.676147	-2.157890
C	1.196643	-0.291861	0.857421
C	1.196643	-0.291861	-0.857421
B	1.418918	0.956758	0.000000
B	2.087489	-1.160426	0.000000
Br	-1.179953	1.670073	0.000000
F	2.925883	-2.168945	0.000000
F	1.881192	2.185441	0.000000
F	-2.328573	-0.736399	0.000000

P-B3-anti

E= -1078.53545202 a.u.

υ= 118.9537

C	-1.058011	0.271345	0.000000
C	-0.259707	-0.363580	1.165955
C	-0.259707	-1.799591	0.670138
C	-0.259707	-1.799591	-0.670138
C	-0.259707	-0.363580	-1.165955
H	-0.661317	-0.169248	2.156696
H	-0.191712	-2.664527	1.315655
H	-0.191712	-2.664527	-1.315655
H	-0.661317	-0.169248	-2.156696
C	1.156168	0.215728	0.860016
C	1.156168	0.215728	-0.860016
B	1.305478	1.466471	0.000000
B	2.059029	-0.638079	0.000000
F	-0.953993	1.640384	0.000000
F	1.495726	2.759432	0.000000
F	2.911421	-1.633335	0.000000
Cl	-2.793403	-0.095970	0.000000

P-B3-syn

E= -1078.53162176 a.u.

υ= 118.5507

C	-1.256334	0.048945	0.000000
C	-0.420993	-0.541658	1.166037
C	-0.420993	-1.983835	0.670080
C	-0.420993	-1.983835	-0.670080
C	-0.420993	-0.541658	-1.166037
H	-0.825472	-0.351828	2.156747

H	-0.355139	-2.848415	1.316488
H	-0.355139	-2.848415	-1.316488
H	-0.825472	-0.351828	-2.156747
C	0.988995	0.031051	0.858032
C	0.988995	0.031051	-0.858032
B	1.199690	1.277457	0.000000
B	1.881170	-0.835758	0.000000
F	-2.535882	-0.399703	0.000000
F	1.572676	2.533583	0.000000
F	2.722239	-1.841409	0.000000
Cl	-1.358853	1.835258	0.000000

P-B4-anti

E= -1018.60141948 a.u.

υ= 118.3101

C	1.069022	0.739835	0.000049
C	0.029051	0.730031	1.156847
C	-0.819204	1.894430	0.670336
C	-0.819174	1.894485	-0.670221
C	0.029096	0.730121	-1.156790
H	0.448878	0.808338	2.157790
H	-1.400523	2.538661	1.316748
H	-1.400465	2.538768	-1.316608
H	0.448962	0.808505	-2.157710
C	-0.765970	-0.571939	0.848550
C	-0.765937	-0.571872	-0.848621
B	-0.081754	-1.669758	-0.000065
B	-2.005239	-0.445005	-0.000055
C	2.114309	1.838563	0.000114
H	2.746178	1.761875	0.886255
H	2.746228	1.761936	-0.885996
H	1.627511	2.812227	0.000134
F	-3.278584	-0.120884	-0.000067
F	0.111064	-2.988278	-0.000114
Cl	1.958748	-0.857410	0.000001

P-B4-syn

E= -1018.58996617 a.u.

υ= 103.4547

C	-1.078223	0.368148	0.000001
C	-0.282489	-0.315980	1.157345
C	-0.297242	-1.759810	0.669204
C	-0.297248	-1.759811	-0.669197
C	-0.282508	-0.315985	-1.157354
H	-0.664522	-0.120965	2.156509
H	-0.223305	-2.623055	1.316704
H	-0.223327	-2.623066	-1.316687
H	-0.664553	-0.120976	-2.156513
C	1.167220	0.185347	0.860908
C	1.167202	0.185339	-0.860935
B	1.481591	1.396056	-0.000020
B	1.994644	-0.744408	-0.000030
C	-1.102261	1.899276	0.000043
H	-2.123835	2.269345	0.000028
H	-0.613524	2.305942	0.889172
H	-0.613485	2.305962	-0.889049
F	1.791260	2.671389	-0.000016
F	2.806809	-1.775351	0.000027
Cl	-2.800232	-0.213819	-0.000007

P-B5-anti

E= -3132.57111705 a.u.

υ= 109.7249

C	0.450771	1.088633	0.000049
C	-0.536332	0.756871	1.157264
C	-1.689392	1.624531	0.670312
C	-1.689338	1.624644	-0.670209
C	-0.536311	0.756971	-1.157209
H	-0.160029	0.952546	2.159316
H	-2.430512	2.073908	1.318208
H	-2.430417	2.074114	-1.318088
H	-0.159983	0.952719	-2.159237

C	-0.928654	-0.715168	0.847698
C	-0.928654	-0.715094	-0.847758
B	0.008219	-1.607988	-0.000068
B	-2.156261	-0.933245	-0.000039
C	1.098051	2.462810	0.000111
H	1.722387	2.589147	0.885628
H	1.722384	2.589232	-0.885396
H	0.331213	3.236081	0.000150
F	-3.469825	-0.983092	-0.000043
F	0.508855	-2.842762	-0.000119
Br	1.924373	-0.246688	-0.000004

P-B5-syn

E= -3132.56131452 a.u.

υ= 104.8506

C	-0.577143	0.450691	-0.000046
C	0.172274	-0.280448	1.157502
C	0.082147	-1.721205	0.669196
C	0.082123	-1.721203	-0.669304
C	0.172289	-0.280452	-1.157602
H	-0.195536	-0.065535	2.157641
H	0.111396	-2.587269	1.316506
H	0.111347	-2.587286	-1.316591
H	-0.195482	-0.065498	-2.157744
C	1.649826	0.138700	0.860498
C	1.649852	0.138680	-0.860529
B	2.035595	1.329357	0.000009
B	2.421164	-0.838449	-0.000019
C	-0.512210	1.980094	-0.000049
H	-1.504804	2.420679	-0.000834
H	0.001804	2.353096	0.890066
H	0.003043	2.353023	-0.889461
F	2.422075	2.583426	0.000048
F	3.174465	-1.913282	0.000086
Br	-2.494268	-0.072462	0.000036

P-B6-anti

E= -3552.85776263 a.u.

υ= 71.8033

C	-0.596250	0.144399	0.000000
C	0.222899	-0.480224	1.163977
C	0.222899	-1.918509	0.669537
C	0.222899	-1.918509	-0.669537
C	0.222899	-0.480224	-1.163977
H	-0.175704	-0.291074	2.157203
H	0.293271	-2.780839	1.318145
H	0.293271	-2.780839	-1.318145
H	-0.175704	-0.291074	-2.157203
C	1.629553	0.101908	0.854063
C	1.629553	0.101908	-0.854063
B	1.763434	1.380273	0.000000
B	2.543285	-0.745126	0.000000
Br	-2.481426	-0.308359	0.000000
F	2.330867	2.576567	0.000000
F	3.394336	-1.742709	0.000000
Cl	-0.457197	1.938321	0.000000

P-B6-syn

E= -3552.85630587 a.u.

υ= 94.2196

C	-0.918682	-0.229261	0.000000
C	-0.085470	-0.836739	1.163710
C	-0.085470	-2.277748	0.669517
C	-0.085470	-2.277748	-0.669517
C	-0.085470	-0.836739	-1.163710
H	-0.485247	-0.648855	2.156874
H	-0.015519	-3.139600	1.318908
H	-0.015519	-3.139600	-1.318908
H	-0.485247	-0.648855	-2.156874
C	1.318888	-0.258050	0.852389
C	1.318888	-0.258050	-0.852389
B	1.476544	1.023010	0.000000

B	2.230767	-1.108585	0.000000
Br	-0.798613	1.734353	0.000000
F	3.079393	-2.108864	0.000000
F	2.136106	2.175766	0.000000
Cl	-2.634491	-0.673745	0.000000

P-B7-anti

E= -558.993958421 a.u.

υ= 120.9504

C	-1.406228	0.516899	0.000043
C	-0.620417	-0.175813	1.155031
C	-0.674333	-1.617603	0.670029
C	-0.674440	-1.617624	-0.669928
C	-0.620509	-0.175854	-1.154980
H	-1.232981	1.599628	0.000014
H	-0.979914	0.018510	2.163003
H	-0.601691	-2.485885	1.312408
H	-0.601886	-2.485928	-1.312288
H	-0.980082	0.018442	-2.162931
C	0.845215	0.309716	0.862234
C	0.845153	0.309672	-0.862305
B	1.037884	1.536863	-0.000073
B	1.698967	-0.589862	-0.000042
C	-2.910347	0.280093	0.000104
H	-3.364740	0.736777	0.882307
H	-3.364812	0.736776	-0.882062
H	-3.155546	-0.782221	0.000115
F	2.492846	-1.636118	-0.000042
F	1.050800	2.850782	-0.000109

P-B7-syn

E= -558.992183800 a.u.

υ= 136.8139

C	-0.725833	-1.471641	-0.000020
C	0.129177	-0.869222	1.154132
C	1.506675	-1.298394	0.670810
C	1.506904	-1.297951	-0.670615
C	0.129298	-0.869316	-1.154157
H	-0.153619	-1.164246	2.162291
H	2.362750	-1.459595	1.313505
H	2.363162	-1.458880	-1.313142
H	-0.153270	-1.164337	-2.162374
H	-0.566084	-2.551852	0.000189
C	0.034817	0.670244	0.858736
C	0.034840	0.670204	-0.858887
B	-1.058679	1.271759	-0.000011
B	1.138646	1.236550	-0.000155
C	-2.220741	-1.150854	-0.000147
H	-2.809684	-2.068246	-0.002666
H	-2.521177	-0.583421	0.885504
H	-2.520434	-0.579501	-0.883509
F	-2.229887	1.869433	0.000166
F	2.366298	1.707247	0.000047

P-B8-anti

E= -3093.26196418 a.u.

υ= 94.1734

C	-0.587563	0.454873	0.000000
C	0.187569	-0.217374	1.161660
C	0.187569	-1.658285	0.669243
C	0.187569	-1.658285	-0.669243
C	0.187569	-0.217374	-1.161660
H	-0.536836	1.543954	0.000000
H	-0.196483	-0.028695	2.159721
H	0.279202	-2.521212	1.314873
H	0.279202	-2.521212	-1.314873
H	-0.196483	-0.028695	-2.159721
C	1.625678	0.333409	0.865140
C	1.625678	0.333409	-0.865140
B	1.775592	1.567973	0.000000
B	2.510990	-0.535857	0.000000
Br	-2.496194	0.059229	0.000000

F	1.731255	2.878621	0.000000
F	3.359950	-1.534174	0.000000

P-B8-syn

E= -3093.26677523 a.u.

υ= 103.2151

C	-1.218504	-0.342764	0.000000
C	-0.368234	-0.911044	1.161414
C	-0.368234	-2.353785	0.671098
C	-0.368234	-2.353785	-0.671098
C	-0.368234	-0.911044	-1.161414
H	-0.750822	-0.729475	2.162064
H	-0.292327	-3.219226	1.316342
H	-0.292327	-3.219226	-1.316342
H	-0.750822	-0.729475	-2.162064
H	-2.233007	-0.732513	0.000000
C	1.047633	-0.332684	0.853627
C	1.047633	-0.332684	-0.853627
B	1.266230	0.915119	0.000000
B	1.940595	-1.198049	0.000000
Br	-1.382081	1.597334	0.000000
F	2.762302	-2.223225	0.000000
F	1.708260	2.152626	0.000000

P-B9-anti

E= -979.289493944 a.u.

υ= 106.1825

C	-1.108627	0.456600	0.000000
C	-0.327272	-0.210896	1.161409
C	-0.327272	-1.651988	0.669273
C	-0.327272	-1.651988	-0.669273
C	-0.327272	-0.210896	-1.161409
H	-1.053890	1.546166	0.000000
H	-0.714368	-0.021913	2.158487
H	-0.235956	-2.515244	1.314559
H	-0.235956	-2.515244	-1.314559
H	-0.714368	-0.021913	-2.158487
C	1.107017	0.344909	0.865118
C	1.107017	0.344909	-0.865118
B	1.251231	1.580017	0.000000
B	1.997798	-0.518204	0.000000
Cl	-2.856175	0.075652	0.000000
F	2.852139	-1.511901	0.000000
F	1.201911	2.890691	0.000000

P-B9-syn

E= -979.295838656 a.u.

υ= 120.3687

C	-1.485961	0.000156	0.000000
C	-0.641742	-0.578118	1.161152
C	-0.641742	-2.019130	0.671086
C	-0.641742	-2.019130	-0.671086
C	-0.641742	-0.578118	-1.161152
H	-1.025777	-0.395206	2.161133
H	-0.564204	-2.884900	1.315613
H	-0.564204	-2.884900	-1.315613
H	-1.025777	-0.395206	-2.161133
H	-2.503839	-0.382094	0.000000
C	0.773656	0.004436	0.854367
C	0.773656	0.004436	-0.854367
B	0.973536	1.252656	0.000000
B	1.671346	-0.855134	0.000000
Cl	-1.596892	1.785368	0.000000
F	2.498963	-1.875117	0.000000
F	1.349953	2.510254	0.000000

P-B10-anti

E= -618.929355040 a.u.

υ= 121.4999

C	-1.429373	0.430723	0.000000
C	-0.635605	-0.215282	1.162509
C	-0.635605	-1.655788	0.669659
C	-0.635605	-1.655788	-0.669659

C	-0.635605	-0.215282	-1.162509
H	-1.415063	1.525878	0.000000
H	-1.028294	-0.028524	2.158230
H	-0.550525	-2.521347	1.312980
H	-0.550525	-2.521347	-1.312980
H	-1.028294	-0.028524	-2.158230
C	0.785618	0.363249	0.866399
C	0.785618	0.363249	-0.866399
B	0.910988	1.599790	0.000000
B	1.692617	-0.479114	0.000000
F	-2.749009	0.048307	0.000000
F	0.850120	2.910571	0.000000
F	2.560892	-1.461099	0.000000

P-B10-syn

E= -618.939087595 a.u.

υ= 129.6035

C	-1.599724	0.200195	0.000000
C	-0.778264	-0.396700	1.162254
C	-0.778264	-1.832240	0.671479
C	-0.778264	-1.832240	-0.671479
C	-0.778264	-0.396700	-1.162254
H	-1.165131	-0.212518	2.161022
H	-0.708153	-2.700685	1.313193
H	-0.708153	-2.700685	-1.313193
H	-1.165131	-0.212518	-2.161022
H	-2.643985	-0.111053	0.000000
C	0.629223	0.213349	0.857628
C	0.629223	0.213349	-0.857628
B	0.737575	1.467006	0.000000
B	1.553118	-0.613580	0.000000
F	-1.559187	1.585712	0.000000
F	0.894876	2.766647	0.000000
F	2.404656	-1.612775	0.000000

C1

E= -1284.60034497 a.u.

υ= 12.8949

N	-5.833412	-0.436496	-0.072918
C	-6.937672	0.248874	-0.337418
C	-6.919183	1.627397	-0.551584
N	-5.793276	2.329828	-0.499212
C	-4.700225	0.261215	-0.036194
C	-4.683408	1.641258	-0.243530
C	-3.442657	-0.508844	0.294243
O	-3.434871	-1.416905	1.098850
N	-2.328953	-0.093229	-0.360320
C	-1.046706	-0.692048	-0.077052
C	0.042712	0.248533	-0.584098
O	-0.247430	1.191999	-1.282319
C	-0.930397	-2.104070	-0.714821
C	0.165537	-2.954506	-0.123939
C	1.241236	-3.397004	-0.891803
C	2.258809	-4.156715	-0.320517
C	2.209878	-4.481745	1.030467
C	1.129402	-4.060139	1.801821
C	0.112695	-3.307016	1.227113
C	1.472558	-0.085371	-0.225373
C	2.396814	1.136236	-0.176247
C	3.873479	0.699494	0.040853
C	1.906735	2.081559	0.932225
C	2.638983	3.416475	1.104912
C	2.566841	4.264896	-0.165383
C	2.032154	4.180693	2.282999
C	4.285845	-0.608197	-0.593589
C	5.371187	-0.424334	-1.360376
C	5.755887	0.993322	-1.315320
C	4.908805	1.653256	-0.511220
H	-7.867801	-0.308400	-0.378770
H	-7.833961	2.170280	-0.764982

H	-3.759572	2.208411	-0.180094
H	-2.346228	0.647379	-1.048313
H	-0.942502	-0.797280	1.008410
H	-1.894281	-2.588093	-0.539876
H	-0.800633	-1.997409	-1.795894
H	1.285540	-3.142452	-1.946578
H	3.089111	-4.491993	-0.931555
H	3.002494	-5.068696	1.478983
H	1.076045	-4.325680	2.851225
H	-0.740186	-2.995068	1.823690
H	1.503486	-0.655202	0.710214
H	1.804368	-0.778096	-1.006442
H	2.322468	1.634299	-1.147039
H	4.032912	0.600388	1.127871
H	0.851626	2.315247	0.747949
H	1.947503	1.531473	1.882476
H	3.688359	3.217071	1.348184
H	3.058943	5.229659	-0.017743
H	3.035914	3.775706	-1.021197
H	1.521310	4.457626	-0.427031
H	2.553875	5.125882	2.450541
H	2.082742	3.596634	3.205428
H	0.979837	4.409749	2.086669
H	3.792969	-1.552487	-0.400307
H	5.900919	-1.190363	-1.911290
H	6.596692	1.422531	-1.843917
H	4.950100	2.708097	-0.282728

C2

E= -1089.29470268 a.u.

υ= 18.7339

O	2.846021	1.506654	0.894627
O	-0.069466	-1.985675	-0.526625
N	5.179291	-0.091434	1.171631
N	1.884667	-0.291361	-0.084253
N	5.778498	-1.567807	-1.130427
C	-1.821664	-0.673551	0.383371
C	-0.950604	2.165518	-0.661950
C	-4.167330	-1.381278	0.549790
C	-2.128379	2.068141	-1.400543
C	-3.253739	2.804276	-1.041117
C	-3.211099	3.647938	0.064017
C	-6.573878	-1.900485	0.795122
C	-2.034756	3.761078	0.800743
C	6.659733	-1.406480	-0.149731
C	-0.438310	-0.926386	-0.057797
C	6.360052	-0.669574	0.996178
C	0.547257	0.230808	0.071933
C	2.948338	0.410794	0.383967
C	4.589421	-0.996982	-0.950342
C	4.286999	-0.265187	0.198933
C	-5.180518	-2.244373	0.352842
C	-5.049960	-3.588880	-0.302519
C	-0.911718	3.026882	0.437157
C	0.259941	1.329709	-0.987231
C	-2.786985	-1.581780	0.162835
H	1.959224	-1.261621	-0.362657
H	-2.039229	0.270244	0.872215
H	-4.386962	-0.433930	1.036734
H	-2.169526	1.398221	-2.253372
H	-4.163878	2.717451	-1.623193
H	-4.086618	4.221186	0.345664
H	-6.622971	-0.915856	1.259760
H	-7.258819	-1.918956	-0.058630
H	-6.941325	-2.643519	1.509990
H	-1.991549	4.424952	1.656306
H	7.633170	-1.869009	-0.275690
H	7.095102	-0.543705	1.784387
H	0.452097	0.680592	1.066545
H	3.864462	-1.107500	-1.750713

H	-5.418131	-4.366056	0.374022
H	-5.679348	-3.626427	-1.197188
H	-4.031577	-3.840657	-0.588994
H	0.009669	3.116704	1.006219
H	0.158590	0.855274	-1.967233
H	1.147748	1.965849	-1.008266
H	-2.496558	-2.497998	-0.342539

C3

E= -1127.39591398 a.u.

υ= 12.7025

O	1.648626	-1.442701	-1.598639
O	-0.306620	0.435782	2.391714
N	4.334121	-1.773759	-0.708946
N	1.225712	-0.566734	0.444411
N	5.319495	0.495235	0.602778
C	-2.187306	0.874164	0.980978
C	-2.134507	-2.320583	0.128369
C	-2.010771	2.264045	-1.156465
C	-3.101818	-2.510506	1.114136
C	-4.449944	-2.598374	0.776915
C	-4.843673	-2.495493	-0.552584
C	-3.882945	-2.316675	-1.545484
C	6.121824	-0.471419	0.171470
C	-0.865034	0.224385	1.341186
C	5.629506	-1.601059	-0.482412
C	-0.208972	-0.671955	0.295729
C	2.051475	-0.988344	-0.549129
C	4.018395	0.318006	0.384666
C	3.525077	-0.814193	-0.264837
C	-2.537937	-2.232180	-1.206191
C	-0.681143	-2.138141	0.476504
C	-1.874677	2.101181	0.171810
C	-1.538160	3.600572	-1.536742
C	-1.107952	4.255788	-0.443135
C	-0.553528	5.640009	-0.351476
C	-1.280704	3.356261	0.753143
H	1.574908	-0.327912	1.362938
H	-2.802870	0.191560	0.392025
H	-2.701905	1.127251	1.910625
H	-2.412453	1.526823	-1.842158
H	-2.797081	-2.580823	2.153757
H	-5.191891	-2.745184	1.553206
H	-5.892575	-2.561015	-0.816153
H	-4.183312	-2.248454	-2.584622
H	7.185795	-0.347432	0.344132
H	6.301053	-2.378645	-0.831447
H	-0.479962	-0.332237	-0.707355
H	3.351912	1.108584	0.715443
H	-1.785951	-2.097687	-1.978845
H	-0.484070	-2.440026	1.508981
H	-0.056691	-2.744723	-0.183434
H	-1.541626	3.992001	-2.546106
H	-0.505584	6.106363	-1.336321
H	-1.171759	6.269781	0.295259
H	0.454350	5.633681	0.073697
H	-1.945892	3.804925	1.501644
H	-0.328974	3.162389	1.263725

C4

E= -1722.16138202 a.u.

υ= 7.3676i

O	1.487097	-2.012468	1.046924
Cl	6.355916	-1.318331	-0.743431
N	-3.397917	-0.841851	0.190455
O	-2.039138	0.860980	-0.451215
Cl	1.506306	2.357815	0.666652
N	0.215779	-0.391315	0.154344
C	4.985530	-0.315016	-0.367687
C	-8.226144	-0.738377	-0.065970
C	2.653130	-0.118176	0.228613

C	4.032533	1.855220	-0.055743
C	3.771347	-0.903029	-0.064114
C	-0.997775	-1.116489	0.419400
C	5.127844	1.066714	-0.369470
C	2.805092	1.269779	0.237795
C	-2.178346	-0.253185	0.004449
C	1.401746	-0.911045	0.533713
C	-7.018631	1.297107	-0.822220
C	-5.801258	-0.763503	0.051036
C	-4.600362	-0.202727	-0.121650
C	-7.067249	-0.101484	-0.268600
H	-3.432291	-1.775394	0.574439
H	0.116008	0.530861	-0.249481
H	-9.175186	-0.268093	-0.293337
H	-8.253736	-1.746379	0.332737
H	4.123689	2.933292	-0.030270
H	3.664133	-1.979949	-0.037521
H	-1.072213	-1.365250	1.483874
H	-1.015913	-2.063943	-0.131002
H	6.083976	1.517493	-0.602025
H	-6.528214	1.977145	-0.120107
H	-6.453210	1.326520	-1.757762
H	-8.023832	1.669639	-1.016000
H	-5.867926	-1.772099	0.453243
H	-4.456491	0.794268	-0.518134

C5

E= -1218.84636398 a.u.

υ= 16.7147

C	-3.791705	2.399309	1.076399
C	-3.805526	2.683848	-0.254973
S	-3.782777	1.254794	-1.213719
C	-3.753625	0.242883	0.190727
C	-3.760215	0.996014	1.331113
C	-3.662451	-1.246333	0.074023
C	-2.261742	-1.827345	-0.097966
O	-2.122378	-2.991968	-0.444922
N	-1.224574	-1.000566	0.187757
C	0.149270	-1.324851	0.124626
C	3.459749	0.205806	0.620064
C	2.502485	-0.684992	0.343010
C	1.083337	-0.397021	0.393721
C	4.920497	-0.115116	0.574860
C	5.722490	0.902919	-0.199940
O	5.344092	1.984395	-0.552767
O	6.976148	0.463170	-0.436653
O	0.449834	-2.586255	-0.201619
H	-3.810359	3.156068	1.848121
H	-3.837653	3.650901	-0.732499
H	-3.749981	0.558016	2.321559
H	-4.070445	-1.709052	0.977467
H	-4.248983	-1.630061	-0.762718
H	-1.447265	-0.048489	0.447266
H	3.196754	1.224557	0.891414
H	2.776805	-1.697679	0.057775
H	0.758478	0.602846	0.656969
H	5.105607	-1.103577	0.148486
H	5.358471	-0.130455	1.581929
H	7.442407	1.167072	-0.907355
H	-0.374342	-3.078356	-0.389495

C6

E= -1143.61534148 a.u.

υ= 17.5981

C	4.060532	-2.135695	1.080488
C	4.051316	-2.435066	-0.247552
S	3.868733	-1.026047	-1.217713
C	3.801492	-0.001083	0.176482
C	3.915430	-0.736976	1.322338
C	3.581109	1.473678	0.047153
C	2.134667	1.933162	-0.148465

O	1.884351	3.048974	-0.543943
N	1.166348	1.024545	0.190526
C	-0.191884	1.312403	0.098071
C	-3.568480	-0.047030	0.617579
C	-2.571723	0.783762	0.302663
C	-1.162683	0.446049	0.410461
C	-5.015444	0.319773	0.518950
C	-5.836768	-0.727188	-0.195565
O	-5.478830	-1.835737	-0.477317
O	-7.077234	-0.273707	-0.467314
H	4.174134	-2.878307	1.858023
H	4.151480	-3.402231	-0.715597
H	3.902346	-0.288127	2.307800
H	3.936233	1.970548	0.954733
H	4.145737	1.901055	-0.783117
H	1.456814	0.105101	0.494697
H	-0.394127	2.317430	-0.254055
H	-3.347392	-1.052390	0.965225
H	-2.803998	1.783916	-0.060055
H	-0.910120	-0.552884	0.758415
H	-5.467289	0.423880	1.514104
H	-5.160101	1.279687	0.018356
H	-7.559548	-0.993700	-0.895825

TS-C1-anti

E= -1610.17755412 a.u.

υ= 380.1379i

N	-6.466036	0.057318	1.703403
C	-7.639711	0.656594	1.554857
C	-8.061770	1.162541	0.324614
N	-7.311050	1.068763	-0.766824
C	-5.703034	-0.022643	0.615299
C	-6.128450	0.476850	-0.616033
C	-4.378469	-0.733433	0.770501
O	-4.256198	-1.727377	1.452088
N	-3.348236	-0.177177	0.077998
C	-2.037953	-0.792873	0.081014
C	-1.005966	0.266250	-0.300244
O	-1.262995	1.057289	-1.176372
C	-1.986598	-1.952201	-0.944697
C	-0.632110	-2.604299	-1.050277
C	0.236066	-2.274570	-2.092729
C	1.493252	-2.864870	-2.183764
C	1.902994	-3.784937	-1.224209
C	1.051030	-4.107581	-0.170651
C	-0.208992	-3.522891	-0.086985
C	0.301223	0.234761	0.449252
C	1.407591	1.102137	-0.154105
C	2.758830	0.692088	0.517405
C	1.121646	2.603574	0.052608
C	1.561115	3.517251	-1.101992
C	0.623483	3.392582	-2.303689
C	1.625812	4.968051	-0.624645
C	3.181698	-0.692170	0.065758
C	3.992284	-0.508899	-1.048973
C	4.443164	0.824496	-1.086162
C	3.919785	1.515180	0.000502
H	-8.268959	0.737283	2.434976
H	-9.027132	1.646902	0.223375
H	-5.514432	0.376704	-1.505948
H	-3.464061	0.665996	-0.467028
H	-1.837184	-1.184503	1.081652
H	-2.741848	-2.678573	-0.635263
H	-2.281995	-1.539482	-1.912885
H	-0.081547	-1.557415	-2.843537
H	2.149734	-2.606775	-3.006677
H	2.880780	-4.247399	-1.292991
H	1.364202	-4.823331	0.580326
H	-0.878458	-3.788280	0.725811
H	0.075654	0.556298	1.477263

H	0.595448	-0.816217	0.532390
H	1.472763	0.883771	-1.224452
H	2.581879	0.793621	1.589789
H	0.047786	2.756318	0.202162
H	1.608558	2.924911	0.982462
H	2.563107	3.216316	-1.426469
H	0.971340	4.021879	-3.126694
H	0.550045	2.364988	-2.663229
H	-0.387257	3.710433	-2.031526
H	1.909527	5.639300	-1.438549
H	2.349148	5.090960	0.186114
H	0.647734	5.289646	-0.252412
H	4.323444	-1.297411	-1.712181
H	5.176645	1.214547	-1.779471
H	2.618218	-1.592764	0.266018
H	4.022854	2.577273	0.171620
C	4.791162	-0.830898	1.595563
C	5.317225	0.704451	1.566894
B	4.456960	0.162317	2.638851
B	6.040096	-0.412114	0.925746
F	3.723263	0.432306	3.695802
F	6.993146	-0.756181	0.093524

TS-C1-syn

E= -1610.17862523 a.u.

υ= 361.7815i

N	-6.507294	0.638458	0.415332
C	-7.617753	0.000790	0.760865
C	-7.689674	-1.392094	0.798436
N	-6.648947	-2.156842	0.488344
C	-5.457016	-0.124330	0.119428
C	-5.530983	-1.517549	0.151939
C	-4.198073	0.595098	-0.305570
O	-4.227682	1.592758	-0.995752
N	-3.042212	0.026642	0.121763
C	-1.768511	0.594071	-0.254476
C	-0.692893	-0.467030	-0.026692
O	-0.936565	-1.444449	0.639390
C	-1.470936	1.893937	0.546820
C	-0.450042	2.791269	-0.106364
C	0.764183	3.080762	0.513611
C	1.719935	3.868127	-0.123275
C	1.462602	4.385484	-1.388137
C	0.242816	4.118912	-2.007735
C	-0.706809	3.328789	-1.370987
C	0.662979	-0.200888	-0.639808
C	1.676366	-1.326605	-0.432470
C	3.098053	-0.861077	-0.794082
C	1.273005	-2.552965	-1.271386
C	2.112198	-3.820215	-1.071329
C	2.107966	-4.275928	0.389533
C	1.574810	-4.932501	-1.973728
C	3.525740	0.594518	-0.859637
C	4.921284	0.578108	-0.921749
C	5.395902	-0.666244	-0.480296
C	4.315291	-1.481775	-0.157111
H	-8.479620	0.609400	1.013587
H	-8.608696	-1.894730	1.080552
H	-4.678164	-2.131532	-0.120764
H	-3.026259	-0.765474	0.749955
H	-1.806459	0.849213	-1.317750
H	-2.423660	2.424056	0.613281
H	-1.161079	1.626104	1.560993
H	0.976504	2.668983	1.494856
H	2.665383	4.063160	0.369844
H	2.202912	4.999710	-1.887127
H	0.030263	4.532251	-2.986790
H	-1.663433	3.131903	-1.847108
H	0.522171	0.019934	-1.706126
H	1.016715	0.737485	-0.202509

H	1.632432	-1.632549	0.614756
H	3.241995	-1.139246	-1.855666
H	0.234146	-2.801463	-1.033830
H	1.299859	-2.268728	-2.332014
H	3.144974	-3.617053	-1.378739
H	2.638222	-5.225017	0.499829
H	2.578197	-3.552133	1.059791
H	1.079207	-4.421284	0.734263
H	2.180489	-5.837331	-1.886217
H	1.570376	-4.627069	-3.023082
H	0.548389	-5.187428	-1.692491
H	2.906864	1.386197	-1.264581
H	5.539235	1.435350	-1.153319
H	6.435587	-0.914882	-0.315425
H	4.388240	-2.520091	0.132272
C	3.822039	-0.462884	1.900709
C	3.418866	0.982579	1.298544
B	2.447510	0.077058	1.956971
B	4.755828	0.674381	1.855997
F	1.190353	-0.070661	2.318860
F	5.991155	1.089398	2.005275

TS-C2-anti

E= -1414.86363679 a.u.

υ= 404.6516i

O	-3.389019	1.656115	-0.580409
O	-0.642717	-2.166004	-0.058785
N	-5.851068	0.617309	0.433592
N	-2.473577	-0.307423	0.056670
N	-6.331948	-1.996365	-0.448373
C	1.215335	-0.803289	-0.588895
C	0.289521	2.217009	0.451692
C	3.225803	-1.918389	-1.585352
C	1.519114	2.404312	1.079188
C	2.425360	3.351224	0.606033
C	2.101226	4.129292	-0.499316
C	5.682962	-1.642540	-1.373021
C	0.862445	3.967336	-1.117259
C	-7.291146	-1.245355	0.080594
C	-0.208006	-1.049530	-0.234540
C	-7.049995	0.056381	0.520116
C	-1.124873	0.164628	-0.146236
C	-3.523639	0.503495	-0.222852
C	-5.125560	-1.439153	-0.523640
C	-4.883550	-0.138071	-0.081553
C	4.285249	-1.110568	-1.173173
C	4.230049	0.399831	-1.146568
C	-0.038420	3.020665	-0.644851
C	-0.687219	1.178685	0.946537
C	1.853632	-1.779878	-1.329857
H	-2.589450	-1.270984	0.340209
H	3.513986	-2.903799	-1.944569
H	1.764701	1.807446	1.949968
H	3.380496	3.473458	1.103701
H	2.802695	4.866538	-0.871989
H	5.707165	-2.731471	-1.342085
H	6.064044	-1.308862	-2.344676
H	6.352761	-1.256494	-0.603431
H	0.595115	4.585661	-1.966385
H	-8.280697	-1.683852	0.156450
H	-7.847019	0.656022	0.947461
H	-1.084869	0.675541	-1.115231
H	-4.336180	-2.036836	-0.969792
H	5.053078	0.803324	-0.554018
H	4.356814	0.754480	-2.175204
H	3.299748	0.828740	-0.779668
H	-1.014590	2.911968	-1.109388
H	-0.273592	0.643843	1.806144
H	-1.600262	1.682953	1.271124
H	1.252422	-2.661632	-1.538887

H	1.545525	0.222577	-0.544500
C	2.425269	-1.092377	1.414805
C	3.919720	-1.487600	0.953083
B	3.579245	-0.189063	1.578468
B	2.879874	-2.491294	1.276033
F	4.042773	0.985894	1.937603
F	2.543104	-3.751340	1.231617

TS-C2-syn

E= -1414.86753950 a.u.

υ= 407.3574i

O	3.008081	1.302695	1.315382
O	0.646646	-1.164829	-2.050328
N	5.678272	0.773861	0.470401
N	2.350596	0.075073	-0.466487
N	6.077099	-1.912396	-0.209559
C	-1.323449	-0.487974	-0.911299
C	-0.539768	2.557422	-0.524852
C	-3.483489	-1.644771	-1.362733
C	-1.462202	2.899450	-1.513006
C	-2.702844	3.433130	-1.173691
C	-3.038942	3.622861	0.162514
C	-5.565333	-1.979738	-0.050820
C	-2.127611	3.277673	1.157606
C	7.092553	-1.082700	0.001020
C	0.129951	-0.466326	-1.205502
C	6.892440	0.255401	0.340559
C	0.972289	0.494823	-0.375376
C	3.271166	0.522484	0.424553
C	4.858354	-1.390656	-0.089661
C	4.657803	-0.050646	0.244748
C	-4.290606	-1.216591	-0.310985
C	-4.351726	0.214373	0.167963
C	-0.885810	2.753928	0.815227
C	0.799114	1.955909	-0.870128
C	-2.162687	-1.279707	-1.667712
H	2.596694	-0.517976	-1.247853
H	-3.836396	-2.531209	-1.886142
H	-1.208408	2.744536	-2.556683
H	-3.405999	3.698221	-1.954755
H	-4.004758	4.036205	0.428707
H	-5.472953	-3.027673	-0.335374
H	-5.832163	-1.927465	1.005710
H	-6.383842	-1.530041	-0.624116
H	-2.381017	3.420019	2.201543
H	8.093845	-1.488799	-0.097477
H	7.734083	0.918097	0.513571
H	0.656267	0.438439	0.671026
H	4.019774	-2.063346	-0.241556
H	-5.125933	0.716198	-0.424466
H	-4.656208	0.270873	1.214296
H	-3.440241	0.789020	0.028899
H	-0.170094	2.500532	1.592339
H	0.971135	1.984735	-1.949615
H	1.592043	2.530147	-0.385197
H	-1.667477	-1.868581	-2.436109
H	-1.671216	0.309170	-0.277708
C	-1.390757	-1.659519	1.075975
C	-2.945159	-2.021650	1.291636
B	-1.956689	-2.994740	0.785406
B	-2.272875	-0.891489	1.971797
F	-1.766435	-4.161382	0.229947
F	-2.417856	0.175636	2.718697

TS-C3-anti

E= -1452.97516534 a.u.

υ= 396.1372i

O	-2.976841	1.104106	-1.166197
O	-0.813055	-1.480474	2.158208
N	-5.230081	-0.592245	-1.500446
N	-2.452186	-0.139887	0.646373

N	-6.531268	-1.190690	0.904676
C	1.218574	-0.336916	1.682243
C	-0.007582	2.692809	0.608982
C	2.188790	0.304593	-0.628469
C	1.056538	3.217378	1.339247
C	2.046234	3.971336	0.711792
C	1.971665	4.215338	-0.654793
C	0.897435	3.714542	-1.388163
C	-7.090684	-1.431363	-0.275472
C	-0.280025	-0.564293	1.579144
C	-6.441293	-1.131196	-1.473537
C	-1.105062	0.379520	0.707938
C	-3.289508	0.270269	-0.341686
C	-5.311577	-0.658971	0.878658
C	-4.659053	-0.365248	-0.319236
C	-0.085638	2.958708	-0.761760
C	-1.073739	1.839324	1.250056
C	1.905844	-0.630620	0.373538
C	2.612799	-0.358756	-1.786730
C	2.610364	-1.742393	-1.579266
C	2.804627	-2.789450	-2.632376
C	1.760989	-1.953070	-0.347226
H	-2.649352	-0.959010	1.207208
H	1.427104	0.698339	1.961890
H	1.583134	-0.999344	2.467492
H	2.208343	1.377808	-0.480011
H	1.115787	3.036374	2.408322
H	2.873209	4.364825	1.290895
H	2.742173	4.797930	-1.145588
H	0.826502	3.914090	-2.451046
H	-8.083080	-1.869891	-0.274566
H	-6.916133	-1.329244	-2.428934
H	-0.678696	0.388692	-0.302369
H	-4.850458	-0.441299	1.836991
H	-0.926039	2.563909	-1.326553
H	-0.969298	1.834655	2.339107
H	-2.050909	2.267391	1.018348
H	3.007990	0.126174	-2.670808
H	3.555261	-2.465780	-3.354261
H	3.134924	-3.731041	-2.192570
H	1.867360	-2.969111	-3.168430
H	1.931515	-2.861501	0.231264
H	0.722313	-1.997120	-0.709863
C	4.488719	-1.814397	-0.391959
C	3.981284	-1.052643	0.949792
B	4.134091	-2.521952	0.855272
B	4.866562	-0.426091	-0.057086
F	3.899997	-3.683354	1.425563
F	5.404538	0.689695	-0.485792

TS-C3-syn

E= -1452.97812157 a.u.

υ= 390.9088i

O	2.322693	1.714424	1.539012
O	-0.239532	0.058198	-2.191863
N	4.952458	1.250467	0.606520
N	1.589271	0.797471	-0.393318
N	5.290019	-1.251453	-0.602862
C	-2.132878	0.327887	-0.780933
C	-1.223852	3.355194	-0.223590
C	-3.350350	-1.566449	0.473773
C	-2.116977	3.639393	-1.256078
C	-3.411368	4.069561	-0.976959
C	-3.825946	4.220521	0.341880
C	-2.936750	3.951439	1.379992
C	6.323884	-0.501354	-0.239524
C	-0.673291	0.515066	-1.160491
C	6.154238	0.745192	0.363429
C	0.239245	1.279351	-0.213209
C	2.543761	1.073759	0.533514

C	4.082100	-0.741258	-0.368423
C	3.912787	0.507918	0.230814
C	-1.644521	3.524135	1.098009
C	0.146781	2.800360	-0.507365
C	-2.372690	-1.111417	-0.414071
C	-3.412532	-2.965206	0.433581
C	-2.471822	-3.463719	-0.477246
C	-2.389546	-4.879274	-0.962521
C	-2.088575	-2.276356	-1.332045
H	1.805537	0.344155	-1.271439
H	-2.416128	0.974599	0.050701
H	-2.737244	0.599156	-1.653507
H	-3.884960	-0.935098	1.172642
H	-1.796927	3.517222	-2.286506
H	-4.094362	4.288112	-1.789582
H	-4.832813	4.555240	0.561108
H	-3.249878	4.079483	2.409563
H	7.315989	-0.898474	-0.426963
H	7.011088	1.342826	0.656550
H	-0.067101	1.092627	0.819443
H	3.229829	-1.352897	-0.645931
H	-0.949275	3.315260	1.905891
H	0.424884	2.964338	-1.551956
H	0.894152	3.280580	0.127671
H	-4.005702	-3.580571	1.098968
H	-2.581666	-5.573992	-0.144107
H	-3.132125	-5.057991	-1.746270
H	-1.401571	-5.095316	-1.370395
H	-2.846321	-2.220988	-2.126995
H	-1.118219	-2.298665	-1.826475
C	-0.603593	-1.620817	0.879818
C	-0.725590	-3.237715	0.808231
B	0.264784	-2.462017	0.029932
B	-1.106630	-2.446125	1.998325
F	1.173675	-2.484966	-0.922890
F	-1.727074	-2.451982	3.152138

TS-C4-anti

E= -2047.73612601 a.u.

υ= 408.6393i

O	-2.691549	-2.045592	1.177777
Cl	-7.632738	-1.184120	-0.388515
N	2.143312	-1.410624	-0.306435
O	0.865929	0.337080	-0.984761
Cl	-2.465597	2.239227	0.383880
N	-1.405796	-0.630781	-0.000274
C	-6.176811	-0.253003	-0.188073
C	-3.801847	-0.172421	0.238663
C	-5.065027	1.863400	-0.129929
C	-4.985714	-0.898817	0.089264
C	-0.220803	-1.402913	0.258513
C	-6.228160	1.130528	-0.303155
C	-3.860679	1.218784	0.135005
C	0.958588	-0.722231	-0.409720
C	-2.584099	-1.017580	0.534242
C	4.528585	-1.538911	-0.684198
C	3.341497	-0.854794	-0.727852
C	5.786699	-0.974041	-1.006042
C	7.014471	-1.749527	-0.597682
C	3.960367	0.911008	0.900660
C	5.437559	1.330853	0.377491
B	4.205033	2.127548	0.122195
F	3.704565	3.126715	-0.561142
B	5.193241	0.417006	1.522492
F	5.730495	-0.444647	2.354081
H	2.168211	-2.254419	0.248795
H	-1.287672	0.233696	-0.512089
H	-5.083765	2.943594	-0.193606
H	-4.948615	-1.974541	0.204772
H	-0.330110	-2.425170	-0.119689

H	-0.035034	-1.480254	1.336300
H	-7.166693	1.626310	-0.514719
H	4.529476	-2.526205	-0.227002
H	3.195252	0.044107	-1.308739
H	6.889000	-2.813165	-0.809556
H	7.901410	-1.394446	-1.121413
H	7.190600	-1.646496	0.478599
C	5.921427	0.339578	-1.415733
H	6.909884	0.731899	-1.619422
H	5.118860	0.835346	-1.949216

TS-C4-syn

E= -2047.73616084 a.u.

υ= 407.9267i

O	2.699140	-2.198509	-0.943043
Cl	7.352674	-1.274762	1.284841
N	-2.198963	-0.833401	-1.033290
O	-0.903883	0.910899	-0.379541
Cl	2.792443	2.168214	-1.237752
N	1.380307	-0.450718	-0.445751
C	6.060251	-0.332536	0.600498
C	3.816958	-0.213853	-0.285800
C	5.206497	1.768566	-0.156660
C	4.873221	-0.951729	0.254227
C	0.186542	-1.195034	-0.742835
C	6.237646	1.030921	0.402188
C	4.004896	1.153931	-0.495134
C	-1.001141	-0.252571	-0.692843
C	2.587789	-1.032948	-0.608527
C	-4.600073	-0.691957	-1.277796
C	-3.399156	-0.153717	-0.894072
C	-5.856789	-0.077125	-1.058767
C	-7.084170	-0.934714	-1.242463
C	-3.903089	-0.009788	1.530760
C	-5.391790	0.635235	1.514808
B	-4.153310	1.403983	1.821538
F	-3.659931	2.604970	1.994569
B	-5.118497	-0.813133	1.697695
F	-5.638271	-2.017923	1.728743
H	-2.222116	-1.826444	-1.218146
H	1.263843	0.520270	-0.187542
H	5.328284	2.828137	-0.340111
H	4.742122	-2.018249	0.384919
H	0.036636	-2.007955	-0.022203
H	0.261369	-1.657167	-1.732795
H	7.172518	1.505042	0.671631
H	-4.605458	-1.720981	-1.631112
H	-3.254895	0.898799	-0.698554
H	-7.209700	-1.610219	-0.389285
H	-7.984400	-0.327137	-1.328520
H	-6.994854	-1.551288	-2.139017
C	-5.977298	1.153213	-0.439814
H	-6.963844	1.564992	-0.267851
H	-5.186872	1.890209	-0.520563

TS-C5-anti

E= -1544.42761926 a.u.

υ= 438.2390i

C	2.229691	-2.465729	-0.149376
C	3.152846	-2.138602	-1.095922
S	3.738269	-0.532511	-0.888270
C	2.728092	-0.282861	0.497457
C	1.988038	-1.399322	0.766223
C	2.640219	1.048646	1.176853
C	1.559424	1.985257	0.649560
O	1.409215	3.100509	1.111456
N	0.757199	1.491577	-0.345978
C	-0.289962	2.196702	-0.952247
C	-1.196364	-0.780251	-0.956798
C	-1.465290	0.209044	-1.902547
C	-1.128727	1.566563	-1.860842

C	-1.784457	-2.160277	-1.137359
C	-1.974994	-2.892610	0.168026
O	-2.966657	-3.469298	0.507556
O	-0.854198	-2.871384	0.928573
O	-0.220662	3.522692	-0.932469
C	-1.922795	1.643827	0.837650
C	-2.201960	0.042612	0.648623
B	-3.188615	1.115501	0.317648
F	-4.331085	1.370006	-0.269189
B	-1.212494	0.615754	1.597129
F	-0.194703	0.325083	2.388990
H	1.731884	-3.423887	-0.096823
H	3.536311	-2.749912	-1.898133
H	1.275234	-1.447983	1.578916
H	2.406546	0.910848	2.235758
H	3.580263	1.602772	1.130437
H	0.990441	0.589605	-0.741020
H	-2.244682	-0.033346	-2.621727
H	-1.680392	2.250477	-2.495004
H	-1.110802	-2.771990	-1.750491
H	-2.755976	-2.118893	-1.628562
H	-1.065175	-3.337453	1.749275
H	0.291658	3.794073	-0.146194
H	-0.274515	-0.795402	-0.391097

TS-C5-syn

E= -1544.41051233 a.u.

υ= 443.3564i

C	3.563174	-0.309481	-1.568223
C	3.806835	0.533671	-0.526633
S	3.063569	-0.012672	0.921678
C	2.397888	-1.398448	0.132141
C	2.753930	-1.421626	-1.188979
C	1.537844	-2.376467	0.872530
C	0.076011	-2.453060	0.456629
O	-0.659945	-3.291029	0.944226
N	-0.365109	-1.547167	-0.473220
C	-1.664835	-1.538807	-1.000489
C	-1.131712	1.703357	-1.015574
C	-1.892337	0.856241	-1.821304
C	-2.151481	-0.522441	-1.805862
C	0.321340	1.562897	-0.595756
C	0.935547	2.836656	-0.053225
O	2.112670	3.077301	-0.071502
O	0.038336	3.672832	0.488827
O	-2.311376	-2.701435	-1.001350
C	-2.128090	1.259994	0.802047
C	-2.634036	-0.288123	0.963977
B	-3.542810	0.823896	0.648206
F	-4.741365	1.188001	0.263381
B	-1.413412	0.216646	1.585088
F	-0.287873	-0.089619	2.212544
H	3.942539	-0.147496	-2.567530
H	4.351321	1.464372	-0.526551
H	2.455151	-2.213846	-1.865449
H	1.924333	-3.393960	0.769365
H	1.520862	-2.159929	1.943596
H	0.316929	-0.927597	-0.890841
H	-1.402681	2.745309	-1.146799
H	-2.652246	1.391465	-2.386062
H	-3.031856	-0.840660	-2.353578
H	0.955002	1.263546	-1.437735
H	0.494908	0.833679	0.196607
H	0.525373	4.433230	0.834515
H	-1.994680	-3.230872	-0.242920

TS-C6-anti

E= -1469.19091730 a.u.

υ= 398.8246i

C	-5.118152	-1.319287	-1.433431
C	-5.068126	-1.686081	-0.123386

S	-4.336634	-0.471332	0.853172
C	-4.086719	0.560105	-0.515357
C	-4.551239	-0.028900	-1.657366
C	-3.379837	1.872536	-0.377338
C	-1.857743	1.798040	-0.266956
O	-1.210297	2.694172	0.218684
N	-1.274557	0.668338	-0.796932
C	0.083811	0.439454	-0.670148
C	2.942286	-0.252360	-0.257820
C	2.053978	-0.982709	-1.024795
C	0.698070	-0.666321	-1.216716
C	4.363856	-0.702548	-0.078392
C	5.314195	0.033619	-0.994346
O	5.050476	0.996970	-1.656813
O	6.543315	-0.517334	-0.965652
H	-5.546607	-1.937593	-2.209835
H	-5.426984	-2.596739	0.330633
H	-4.495417	0.451642	-2.626269
H	-3.598683	2.491094	-1.252739
H	-3.716274	2.431814	0.496780
H	-1.877968	-0.089121	-1.089233
H	2.368687	-1.973090	-1.345031
H	0.068339	-1.415228	-1.688764
H	4.705786	-0.519372	0.944919
H	4.470835	-1.776098	-0.249333
H	7.110557	0.010001	-1.544420
H	0.629159	1.326931	-0.379745
H	2.798295	0.820287	-0.172406
C	0.469851	-0.130035	1.609124
C	2.040204	-0.511292	1.671761
B	0.951271	-1.517657	1.647538
B	1.492748	0.808430	2.085330
F	0.655107	-2.785575	1.501639
F	1.800856	2.035436	2.419485

TS-C6-syn

E= -1469.19180185 a.u.

υ= 408.5236i

C	5.302371	-1.556351	0.583072
C	5.638539	-1.307827	-0.712536
S	4.956528	0.168506	-1.276378
C	4.199243	0.471498	0.250632
C	4.474695	-0.533620	1.134853
C	3.321264	1.665700	0.459835
C	1.879826	1.535993	-0.029976
O	1.178866	2.505251	-0.196353
N	1.426397	0.252505	-0.229901
C	0.100028	-0.003290	-0.528503
C	-2.748671	-0.679225	-0.967688
C	-1.708271	-1.585925	-1.041411
C	-0.354986	-1.269479	-0.827507
C	-4.177966	-1.108324	-1.144117
C	-5.141057	0.006388	-0.817340
O	-4.881546	1.176405	-0.832102
O	-6.371093	-0.465429	-0.544281
H	5.634905	-2.428271	1.129027
H	6.257339	-1.900635	-1.368370
H	4.102148	-0.534893	2.151826
H	3.256307	1.880878	1.530642
H	3.724073	2.561269	-0.015662
H	2.049346	-0.517196	-0.024624
H	-1.959864	-2.643577	-1.070894
H	0.347099	-2.093943	-0.739580
H	-4.374422	-1.379456	-2.189583
H	-4.417774	-1.982416	-0.536815
H	-6.941300	0.297624	-0.378414
H	-0.446567	0.893260	-0.787488
H	-2.564187	0.362196	-1.213111
C	-1.147844	0.276938	1.496680
C	-2.644524	-0.184957	1.104998

B	-1.682929	-1.048076	1.831194
B	-2.223204	1.239864	1.209520
F	-1.422278	-2.264117	2.247516
F	-2.554541	2.482744	0.992125

P-C1-anti

E= -1610.23425998 a.u.

υ= 7.2970

N	6.606477	-0.339464	1.021099
C	7.740482	-0.935937	0.679499
C	7.998747	-1.338684	-0.631166
N	7.123618	-1.142043	-1.610699
C	5.719326	-0.156137	0.045407
C	5.981804	-0.550900	-1.267020
C	4.434152	0.541241	0.424595
O	4.398224	1.425588	1.253145
N	3.333233	0.118683	-0.253827
C	2.036979	0.672699	0.063758
C	0.967190	-0.321130	-0.387042
O	1.266488	-1.258208	-1.089790
C	1.865443	2.065874	-0.599719
C	0.710887	2.876330	-0.065910
C	-0.330988	3.288613	-0.897033
C	-1.410386	4.004319	-0.386236
C	-1.460461	4.315649	0.968227
C	-0.416078	3.925055	1.802836
C	0.663523	3.216622	1.287985
C	-0.450125	-0.041875	0.050509
C	-1.409420	-1.219867	-0.106374
C	-2.871910	-0.800904	0.174347
C	-1.002264	-2.370990	0.827546
C	-1.807240	-3.667617	0.679647
C	-1.610413	-4.296159	-0.701001
C	-1.395745	-4.656369	1.771347
C	-3.255370	0.696417	-0.058081
C	-3.209273	0.725856	-1.579362
C	-3.584913	-0.476586	-2.038470
C	-3.902491	-1.375739	-0.849428
H	8.470653	-1.098803	1.465469
H	8.933239	-1.825172	-0.890241
H	5.265091	-0.367689	-2.061471
H	3.336324	-0.736995	-0.794129
H	1.962755	0.798710	1.149424
H	2.799773	2.599142	-0.406499
H	1.776310	1.931053	-1.681584
H	-0.299405	3.040675	-1.954041
H	-2.212895	4.316405	-1.045004
H	-2.302487	4.866450	1.370015
H	-0.439831	4.179161	2.856165
H	1.485326	2.930111	1.938021
H	-0.442984	0.350961	1.074281
H	-0.780323	0.793388	-0.576790
H	-1.323834	-1.557630	-1.142259
H	-3.115179	-1.098354	1.202756
H	0.052488	-2.612074	0.657282
H	-1.084420	-2.015751	1.863568
H	-2.872524	-3.443318	0.818663
H	-2.158683	-5.238102	-0.780178
H	-1.946459	-3.644763	-1.510607
H	-0.549620	-4.506676	-0.869834
H	-1.966415	-5.585137	1.698875
H	-1.554991	-4.236421	2.767594
H	-0.334303	-4.906778	1.676926
H	-3.028362	1.614261	-2.172409
H	-3.764957	-0.740737	-3.072973
H	-2.662693	1.443229	0.465681
H	-3.859577	-2.447484	-1.025376
C	-4.775499	0.688970	0.327582
C	-5.260692	-0.853778	-0.265714
B	-5.296766	-0.439670	1.188171

B	-5.765988	0.467867	-0.791048
F	-5.409293	-0.879889	2.420896
F	-6.437467	1.049694	-1.758026

P-C1-syn

E= -1610.23090651 a.u.

υ= 12.5711

N	-6.380877	-0.095186	0.297823
C	-7.362921	-0.983610	0.370804
C	-7.229808	-2.276284	-0.137100
N	-6.111942	-2.687322	-0.724615
C	-5.252755	-0.508881	-0.275401
C	-5.122107	-1.799981	-0.788925
C	-4.139348	0.506423	-0.386024
O	-4.351987	1.674892	-0.632659
N	-2.890479	0.001525	-0.213281
C	-1.727941	0.852361	-0.322967
C	-0.511778	-0.049132	-0.543323
O	-0.564904	-1.217489	-0.242359
C	-1.584413	1.748166	0.939144
C	-0.578185	2.863010	0.799373
C	0.529977	2.952636	1.640607
C	1.482694	3.952630	1.463550
C	1.330891	4.885145	0.443862
C	0.210209	4.825829	-0.381484
C	-0.737845	3.825554	-0.202174
C	0.693948	0.572063	-1.204519
C	2.000032	-0.235635	-1.144780
C	2.657821	-0.018008	0.224961
C	2.873563	0.265866	-2.314381
C	4.230645	-0.396941	-2.579818
C	4.124990	-1.920364	-2.632794
C	4.799172	0.142585	-3.894538
C	1.821872	-0.290985	1.522091
C	2.875622	0.101849	2.548750
C	4.079902	-0.234604	2.065209
C	3.892741	-0.861597	0.687569
H	-8.285652	-0.663598	0.843728
H	-8.045719	-2.988190	-0.068977
H	-4.208858	-2.118988	-1.282160
H	-2.728535	-0.955035	0.072727
H	-1.855037	1.504739	-1.192546
H	-2.577449	2.173008	1.107103
H	-1.346373	1.112605	1.797415
H	0.653242	2.236006	2.445304
H	2.341572	3.999317	2.123102
H	2.072216	5.662311	0.300802
H	0.072314	5.564392	-1.162587
H	-1.617099	3.792516	-0.839120
H	0.386589	0.710985	-2.250396
H	0.848910	1.584540	-0.817307
H	1.750730	-1.283783	-1.333125
H	2.953441	1.037781	0.261202
H	2.279388	0.146646	-3.230066
H	3.025270	1.346501	-2.190593
H	4.929721	-0.111802	-1.788488
H	5.081811	-2.365571	-2.916378
H	3.827628	-2.352770	-1.675586
H	3.382352	-2.222196	-3.379409
H	5.799742	-0.254917	-4.079498
H	4.863306	1.233720	-3.883309
H	4.162152	-0.149297	-4.735449
H	0.864809	0.215966	1.596468
H	2.660538	0.465477	3.546086
H	5.023480	-0.190117	2.594132
H	4.768394	-0.862571	0.048445
C	3.276840	-2.277793	0.958498
C	1.747135	-1.853751	1.593806
B	1.946913	-2.735200	0.382270
B	2.843249	-2.523754	2.382914

F	1.389744	-3.435570	-0.578457
F	3.243458	-2.884935	3.583261

P-C2-anti

E= -1414.96188828 a.u.

υ= 11.5977

O	2.898075	1.076933	1.586311
O	0.370389	-0.370494	-2.246781
N	5.535197	0.539497	0.620504
N	2.176993	0.283380	-0.406356
N	5.734567	-2.006604	-0.528372
C	-1.555376	-0.073952	-0.840917
C	-0.565848	2.926487	-0.260874
C	-3.052963	-2.064059	-1.495932
C	-1.294796	3.480350	-1.312687
C	-2.591881	3.944689	-1.111315
C	-3.175970	3.855281	0.147549
C	-3.116421	-4.142564	-0.136158
C	-2.450203	3.318793	1.208197
C	6.808252	-1.304150	-0.184888
C	-0.078218	0.065267	-1.215578
C	6.707483	-0.035718	0.387458
C	0.838286	0.803818	-0.239716
C	3.116634	0.475088	0.557275
C	4.557710	-1.425936	-0.305180
C	4.457217	-0.155653	0.263714
C	-3.487725	-2.652683	-0.158935
C	-5.009946	-2.495144	-0.025703
C	-1.152886	2.863658	1.005830
C	0.799624	2.333405	-0.490292
C	-2.265540	-1.025066	-1.785908
H	2.411546	-0.107099	-1.309027
H	-3.473426	-2.602927	-2.344257
H	-0.847324	3.538327	-2.299866
H	-3.146100	4.371587	-1.939102
H	-4.188557	4.207043	0.304533
H	-2.037982	-4.278720	-0.244411
H	-3.429605	-4.593266	0.808651
H	-3.614916	-4.672984	-0.951963
H	-2.898103	3.250262	2.192412
H	7.777230	-1.759015	-0.362430
H	7.596041	0.522166	0.664272
H	0.522906	0.612407	0.788256
H	3.670149	-1.995282	-0.563709
H	-5.522301	-3.006684	-0.844862
H	-5.352081	-2.927445	0.917843
H	-5.297295	-1.441191	-0.047409
H	-0.589094	2.448873	1.836353
H	1.135493	2.522239	-1.513548
H	1.530532	2.769151	0.195699
H	-2.091490	-0.805352	-2.834201
H	-1.994237	0.923810	-0.971354
C	-1.734524	-0.524905	0.590617
C	-2.767343	-1.907349	0.946010
B	-1.286484	-1.837978	1.168352
B	-2.994098	-0.494420	1.403646
F	-0.209241	-2.562892	1.397222
F	-3.895967	0.314306	1.923450

P-C2-syn

E= -1414.95635008 a.u.

υ= 14.8992

O	-1.699372	-1.895485	1.947643
O	1.899124	-0.476162	1.750922
N	-4.190445	-2.584618	0.710409
N	-0.915741	-1.599334	-0.148639
N	-4.904192	-0.766126	-1.296259
C	0.003174	0.820123	1.051516
C	2.810787	-2.075100	-0.674311
C	0.819594	3.212853	1.562430
C	3.779825	-1.086447	-0.824570

C	5.111063	-1.349932	-0.517044
C	5.484964	-2.606719	-0.056616
C	1.857563	4.624570	-0.198713
C	4.522625	-3.601552	0.092995
C	-5.774486	-1.631769	-0.789774
C	0.894477	-0.427060	1.095751
C	-5.418749	-2.534423	0.213756
C	0.475705	-1.647929	0.262335
C	-1.914616	-1.766580	0.763011
C	-3.668857	-0.819116	-0.802607
C	-3.310171	-1.731893	0.189341
C	0.544714	3.986676	0.278116
C	-0.489715	5.082480	0.573669
C	3.194912	-3.335546	-0.215929
C	1.362559	-1.796853	-0.990515
C	0.610501	1.933429	1.882253
H	-1.134040	-1.584766	-1.133336
H	1.264472	3.837898	2.335617
H	3.489127	-0.104475	-1.181538
H	5.855365	-0.571393	-0.636413
H	6.521263	-2.812636	0.184074
H	2.614748	3.861051	-0.391514
H	1.691043	5.189452	-1.119146
H	2.246600	5.309223	0.559483
H	4.808163	-4.584599	0.448306
H	-6.784928	-1.608223	-1.184143
H	-6.146369	-3.228159	0.621986
H	0.624510	-2.510617	0.918762
H	-2.954331	-0.096504	-1.186457
H	-0.114071	5.766474	1.339194
H	-0.698116	5.659284	-0.330782
H	-1.426417	4.649258	0.932191
H	2.447437	-4.114829	-0.098495
H	1.279675	-0.895386	-1.604924
H	0.952698	-2.630387	-1.570999
H	0.911901	1.610768	2.873500
H	-0.939046	0.522363	1.529508
C	-0.257156	1.305875	-0.357864
C	0.018994	3.012643	-0.754949
B	0.746114	1.840995	-1.340559
B	-1.300621	2.304657	-0.774599
F	1.806071	1.496298	-2.051668
F	-2.607043	2.484291	-0.822762

P-C3-anti

E= -1453.02322969 a.u.

υ= 11.1503

O	-2.599886	0.739616	-1.731964
O	-0.451893	0.340251	2.535723
N	-4.751773	-1.065152	-1.238233
N	-2.094136	0.504137	0.459780
N	-6.177851	-0.426164	1.084909
C	1.572729	0.462042	1.292597
C	0.441152	3.298157	-0.018800
C	1.760523	-0.510627	-1.140861
C	1.162908	3.958731	0.974276
C	2.418316	4.494427	0.701540
C	2.965737	4.374406	-0.571334
C	2.245723	3.729492	-1.574268
C	-6.656979	-1.266757	0.175017
C	0.080586	0.619857	1.487199
C	-5.945708	-1.583227	-0.982799
C	-0.779049	1.091212	0.315727
C	-2.912521	0.378577	-0.617739
C	-4.975180	0.086137	0.834465
C	-4.260714	-0.235186	-0.320171
C	0.990465	3.198710	-1.299524
C	-0.877122	2.637563	0.283711
C	1.887812	-0.715898	0.365978
C	1.624814	-1.705526	-1.730870

C	1.652197	-2.797478	-0.666014
C	1.024072	-4.129075	-1.017174
C	1.014419	-1.993720	0.496800
H	-2.337494	0.133738	1.368612
H	2.011076	1.373340	0.876014
H	2.003499	0.282077	2.278747
H	1.906053	0.446735	-1.629432
H	0.742977	4.044684	1.971675
H	2.968611	5.003491	1.484205
H	3.944649	4.787189	-0.783784
H	2.661944	3.644355	-2.571480
H	-7.633817	-1.699776	0.363616
H	-6.355318	-2.268956	-1.717238
H	-0.348403	0.749040	-0.629605
H	-4.579783	0.788769	1.561785
H	0.424105	2.701236	-2.082516
H	-1.273288	2.977407	1.244401
H	-1.608508	2.876877	-0.492463
H	1.625669	-1.902423	-2.796584
H	1.551733	-4.595804	-1.851527
H	1.069496	-4.810640	-0.164943
H	-0.021861	-3.995052	-1.302958
H	1.087811	-2.483351	1.474594
H	-0.035895	-1.777625	0.277672
C	3.157608	-2.852072	-0.184527
C	3.329639	-1.323460	0.570450
B	3.447738	-2.651267	1.284838
B	4.075939	-1.756792	-0.668642
F	3.456440	-3.233249	2.461260
F	4.835821	-1.351354	-1.658716

P-C3-syn

E= -1453.02711275 a.u.

υ= 17.3939

O	-2.406813	-1.481319	1.612835
O	0.146750	-0.193369	-2.276541
N	-5.037747	-0.990427	0.680486
N	-1.680644	-0.724502	-0.390726
N	-5.303334	1.439660	-0.683539
C	2.025785	-0.389013	-0.827706
C	1.017825	-3.401064	-0.185754
C	3.530419	1.432004	0.257394
C	1.862823	-3.748797	-1.239216
C	3.149092	-4.219681	-0.991345
C	3.604080	-4.347252	0.316708
C	2.763153	-4.012990	1.375695
C	-6.357948	0.749179	-0.265761
C	0.578035	-0.591024	-1.219394
C	-6.224303	-0.460894	0.415248
C	-0.351469	-1.263827	-0.217327
C	-2.626025	-0.903351	0.569937
C	-4.110837	0.905626	-0.425244
C	-3.978104	-0.308917	0.249751
C	1.478332	-3.545689	1.125014
C	-0.338414	-2.799383	-0.440659
C	2.179743	1.045328	-0.329726
C	3.655336	2.765026	0.207934
C	2.403019	3.363907	-0.422487
C	2.523605	4.743036	-1.035329
C	2.042790	2.188908	-1.369241
H	-1.908539	-0.344426	-1.299546
H	2.315190	-1.087082	-0.038935
H	2.659178	-0.553439	-1.702586
H	4.199997	0.732023	0.743371
H	1.511699	-3.643859	-2.261359
H	3.794148	-4.487594	-1.820057
H	4.605167	-4.713283	0.511324
H	3.108339	-4.121073	2.397270
H	-7.338286	1.166778	-0.470949
H	-7.098029	-1.009312	0.752185

H	-0.015706	-1.049910	0.801693
H	-3.239587	1.471118	-0.739293
H	0.821322	-3.285448	1.949843
H	-0.664695	-2.994687	-1.465886
H	-1.080331	-3.216558	0.243760
H	4.451444	3.354335	0.648399
H	3.295993	4.753188	-1.808012
H	1.576030	5.046355	-1.485722
H	2.787453	5.480573	-0.274343
H	2.790513	2.080064	-2.157936
H	1.048142	2.265128	-1.820391
C	1.108091	1.499702	0.743693
C	1.272828	3.202625	0.673530
B	0.018453	2.449630	0.299292
B	1.594313	2.361514	1.884392
F	-1.137032	2.536161	-0.323419
F	2.170608	2.353285	3.062371

P-C4-anti

E= -2047.83290058 a.u.

υ= 8.3663

O	2.524019	-1.826823	1.295160
Cl	7.519694	-1.434214	-0.289651
N	-2.241766	-0.962401	-0.339070
O	-0.818210	0.604933	-1.134155
Cl	2.591533	2.378753	0.146164
N	1.344801	-0.439010	-0.021172
C	6.128644	-0.393968	-0.181439
C	3.762126	-0.120256	0.211079
C	5.162680	1.789584	-0.307009
C	4.895118	-0.933762	0.134222
C	0.103336	-1.102824	0.276846
C	6.274600	0.968904	-0.407613
C	3.916011	1.250612	-0.004011
C	-1.016485	-0.390836	-0.468073
C	2.487395	-0.854895	0.561716
C	-4.530202	-1.341879	-0.994682
C	-3.430566	-0.300020	-0.873176
C	-5.740752	-1.401253	-0.423298
C	-6.643317	-2.575533	-0.698945
C	-3.890550	0.858253	-0.024795
C	-5.469118	0.796394	0.752264
B	-5.030473	1.793366	-0.283988
F	-5.487232	2.702493	-1.119558
B	-4.147117	0.809141	1.453872
F	-3.558350	0.559172	2.607344
H	-2.370800	-1.710359	0.327673
H	1.289944	0.377466	-0.616464
H	5.254715	2.857347	-0.457534
H	4.784466	-1.991432	0.336721
H	-0.098650	-1.078931	1.353624
H	0.143337	-2.156292	-0.018074
H	7.245736	1.381667	-0.648217
H	-4.248638	-2.168670	-1.642984
H	-3.159597	0.050382	-1.871986
H	-6.173004	-3.301044	-1.362362
H	-6.910497	-3.079162	0.234616
H	-7.576561	-2.238137	-1.159312
C	-6.374903	-0.383786	0.517324
H	-6.615090	-0.897368	1.453890
H	-7.329851	-0.073558	0.081383

P-C4-syn

E= -2047.83294079 a.u.

υ= 7.4218

O	2.523960	-1.699408	-1.526778
Cl	7.250570	-1.717280	0.774972
N	-2.291107	-0.122897	-0.876552
O	-0.843697	1.241878	0.199399
Cl	2.877710	2.536899	-0.564680
N	1.323799	-0.127129	-0.459707

C	6.010010	-0.551635	0.413463
C	3.769023	-0.066120	-0.342561
C	5.277031	1.721303	0.296640
C	4.784404	-0.983040	-0.060333
C	0.072972	-0.678292	-0.909461
C	6.267477	0.800794	0.599447
C	4.036913	1.292728	-0.166850
C	-1.050978	0.246171	-0.464079
C	2.486641	-0.688730	-0.847736
C	-4.619082	0.282912	-1.353091
C	-3.476087	0.587611	-0.399049
C	-5.805052	-0.300725	-1.133373
C	-6.763203	-0.506148	-2.277623
C	-3.853670	0.219710	1.013436
C	-5.398262	-0.565276	1.326282
B	-4.966881	0.778686	1.843822
F	-5.423990	1.880414	2.401023
B	-4.047493	-1.176955	1.529381
F	-3.419060	-2.324857	1.694970
H	-2.418724	-1.022704	-1.317697
H	1.272923	0.721162	0.089733
H	5.460711	2.781498	0.412780
H	4.590804	-2.034519	-0.230216
H	-0.087929	-1.678999	-0.492506
H	0.069192	-0.780998	-1.999109
H	7.232051	1.127759	0.965602
H	-4.397763	0.583300	-2.374828
H	-3.236210	1.651913	-0.458665
H	-6.349733	-0.150327	-3.221074
H	-7.010008	-1.566561	-2.383329
H	-7.701308	0.023673	-2.087933
C	-6.358239	-0.810443	0.191902
H	-6.577316	-1.876793	0.075670
H	-7.318472	-0.315098	0.367401

P-C5-anti

E= -1544.51158940 a.u.

υ= 4.1690

C	-4.227284	-2.516131	-0.224190
C	-4.969801	-1.977062	0.782179
S	-4.892888	-0.258061	0.779638
C	-3.844689	-0.246722	-0.598088
C	-3.580362	-1.520843	-1.015301
C	-3.297058	1.032177	-1.149785
C	-1.995653	1.531870	-0.526652
O	-1.581481	2.653884	-0.764419
N	-1.311637	0.667081	0.258965
C	0.004842	1.050008	0.783425
C	2.480668	-1.074220	0.458125
C	1.455842	-0.939598	1.570766
C	0.458375	-0.065940	1.713406
C	3.890059	-1.054302	1.071715
C	4.978993	-1.213608	0.039441
O	5.997117	-0.584593	0.000456
O	4.688069	-2.183914	-0.852230
O	-0.093038	2.200840	1.576450
C	0.986346	1.205212	-0.356587
C	2.286359	0.037914	-0.544835
B	2.448893	1.514243	-0.268976
F	3.325849	2.419568	0.097517
B	1.144529	0.238562	-1.491958
F	0.479797	-0.315671	-2.487244
H	-4.148645	-3.579461	-0.402855
H	-5.567645	-2.488568	1.520422
H	-2.945243	-1.736017	-1.866071
H	-3.081875	0.905686	-2.214805
H	-4.011570	1.853175	-1.070513
H	-1.703304	-0.237920	0.477998
H	1.588622	-1.659570	2.376066
H	-0.149122	-0.109859	2.613854

H	3.995517	-1.875725	1.788495
H	4.075657	-0.117411	1.599533
H	5.426221	-2.234839	-1.474436
H	-0.409178	2.906275	0.993957
H	2.335135	-2.047718	-0.020187

P-C5-syn

E= -1544.51495704 a.u.

υ= 34.9086

C	-3.730558	0.033973	1.524754
C	-3.518774	0.978366	0.566763
S	-2.754659	0.315479	-0.825509
C	-2.704448	-1.264882	-0.118932
C	-3.260719	-1.254964	1.129568
C	-2.006472	-2.397685	-0.806298
C	-0.487990	-2.425707	-0.622469
O	0.230284	-3.061208	-1.373288
N	0.006980	-1.719837	0.424231
C	1.458468	-1.588390	0.621585
C	1.655302	1.559599	0.968589
C	1.732381	0.505809	2.064074
C	1.656236	-0.819234	1.919192
C	0.215674	2.080020	0.880297
C	0.072102	3.196246	-0.122361
O	0.973144	3.800698	-0.630321
O	-1.224574	3.463784	-0.383662
O	2.058989	-2.838987	0.787905
H	-4.206559	0.241568	2.473114
H	-3.765407	2.028678	0.588805
H	-3.327797	-2.143073	1.746204
H	-2.388782	-3.349371	-0.426254
H	-2.175576	-2.394869	-1.884329
H	-0.625965	-1.253558	1.058464
H	2.310759	2.391815	1.237413
H	1.836693	0.891977	3.074776
H	1.708524	-1.464310	2.791213
H	-0.133403	2.459099	1.846905
H	-0.474534	1.276171	0.601818
H	-1.243398	4.187441	-1.025066
H	1.905428	-3.327721	-0.032675
C	2.119724	0.945732	-0.337712
C	2.050659	-0.787648	-0.527032
B	1.289483	0.213762	-1.347165
B	3.306918	0.027790	-0.486893
F	0.255121	0.337200	-2.155693
F	4.612817	-0.030767	-0.365056

P-C6-anti

E= -1469.28453496 a.u.

υ= 8.6876

C	-3.585043	-2.490655	-1.010994
C	-3.245758	-2.765341	0.278868
S	-3.197655	-1.340022	1.242445
C	-3.638580	-0.343234	-0.102388
C	-3.807975	-1.098296	-1.228828
C	-3.722249	1.144912	0.035407
C	-2.389926	1.899052	-0.014387
O	-2.288980	3.018144	0.441071
N	-1.366502	1.262859	-0.648263
C	-0.036829	1.855196	-0.686998
C	2.778106	0.172132	-0.918199
C	1.822790	0.633330	-2.006623
C	0.680088	1.320634	-1.916387
C	2.896316	-1.353059	-0.960261
C	3.961686	-1.853209	-0.016852
O	4.754549	-1.168065	0.564983
O	3.935722	-3.194435	0.090677
H	-3.682173	-3.248329	-1.776262
H	-3.033373	-3.724178	0.725818
H	-4.089772	-0.668668	-2.182129
H	-4.334224	1.547241	-0.777046

H	-4.201040	1.443248	0.969088
H	-1.474036	0.287240	-0.890494
H	-0.188526	2.931286	-0.804177
H	3.766041	0.591544	-1.134393
H	2.131484	0.338359	-3.007557
H	0.147474	1.527765	-2.840848
H	1.946691	-1.830321	-0.699648
H	3.157576	-1.705797	-1.963676
H	4.643599	-3.451687	0.696908
C	2.294049	0.666669	0.422301
C	0.785920	1.578330	0.547590
B	1.061536	0.237049	1.161087
B	2.158217	2.095076	0.861869
F	0.473676	-0.814247	1.700819
F	2.845615	3.198479	1.068182

P-C6-syn

E= -1469.28480592 a.u.

υ= 10.0129

C	3.228381	-2.620877	0.605958
C	3.924040	-2.523032	-0.560913
S	4.331471	-0.889622	-0.921405
C	3.557760	-0.313470	0.515764
C	3.018106	-1.351594	1.222130
C	3.473028	1.148329	0.827185
C	2.230707	1.888612	0.320652
O	2.110943	3.082108	0.499387
N	1.298652	1.137608	-0.324252
C	0.015299	1.707923	-0.709605
C	-2.720742	-0.083788	-1.035892
C	-1.610015	0.195062	-2.035586
C	-0.499355	0.927717	-1.908958
C	-2.807734	-1.590924	-0.784921
C	-3.996540	-1.943666	0.073913
O	-4.882115	-1.195714	0.378837
O	-3.963240	-3.232929	0.458635
H	2.883178	-3.559492	1.017101
H	4.233270	-3.315561	-1.224481
H	2.486624	-1.208635	2.154942
H	3.479730	1.294156	1.910263
H	4.332744	1.696972	0.437205
H	1.409941	0.133157	-0.344902
H	-1.756070	-0.298434	-2.994434
H	0.172794	0.968097	-2.761905
H	-2.906560	-2.145964	-1.723927
H	-1.901008	-1.963128	-0.298372
H	-4.752478	-3.397050	0.992618
H	0.216653	2.738703	-1.011222
H	-3.667231	0.237941	-1.482243
C	-1.006679	1.674913	0.400099
C	-2.464496	0.689698	0.233725
B	-1.365565	0.476881	1.229401
B	-2.415896	2.184733	0.376836
F	-0.846963	-0.415385	2.055507
F	-3.141221	3.273687	0.237187