

Supporting Information

Revisiting the Formation Mechanism of 1,3,4-Oxadiazole-2(3*H*)-ones from Hydrazonyl Chloride and Carbon Dioxide

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Table of Contents

1. Formation of nitrile imine and its 1,3-dipolar cycloaddition for reaction 2	S2
2. Mechanism resulting from the conformational analysis of 3-TS₃ of the reaction 3	S3
3. Mechanism resulting from the conformational analysis of 6-TS₂ of the reaction 6	S4
4. Cartesian coordinates of all the structures	S5

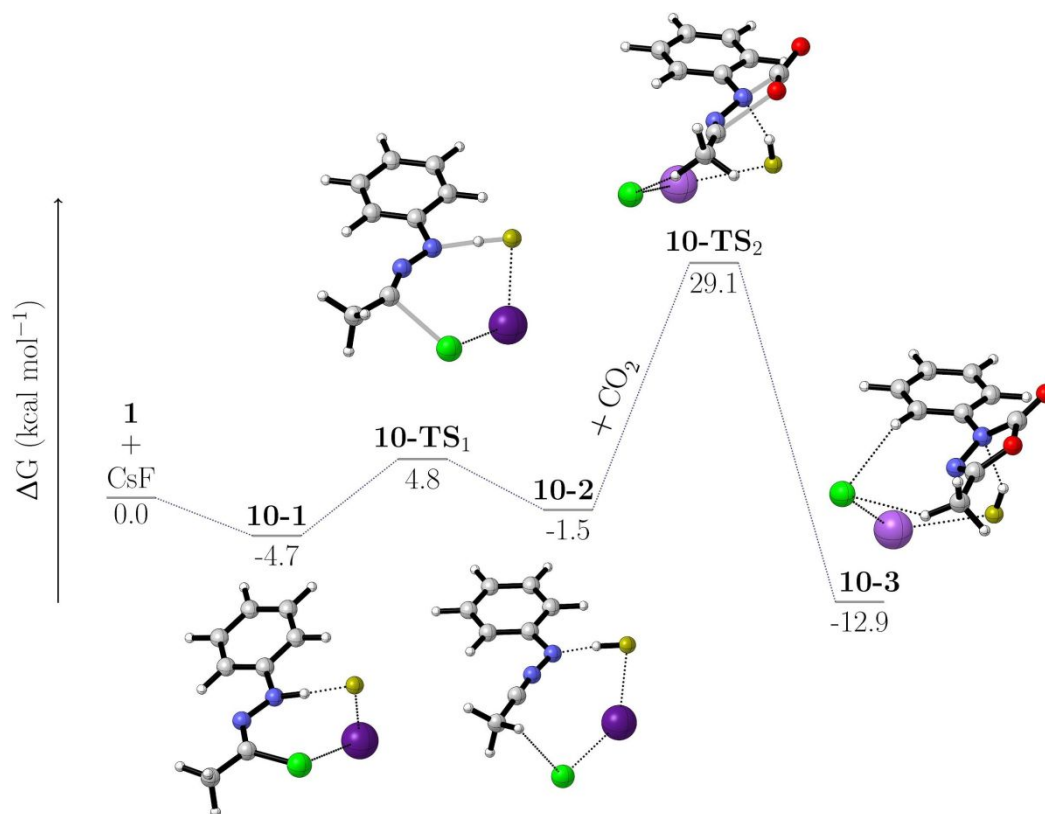


Figure 1-SI. Formation of nitrile imine and its 1,3-dipolar cycloaddition for reaction 2. Gibbs free energies in kcal mol^{-1} computed at the SMD/M06-2X/def2-TZVP level.

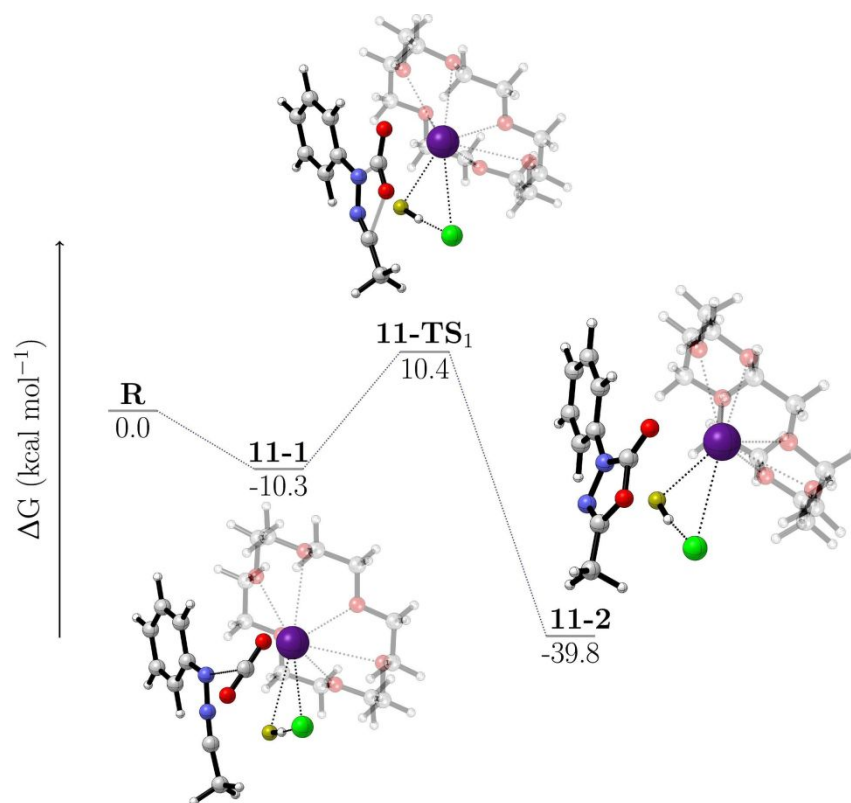


Figure 2-SI. Mechanism resulting from the conformational analysis of the transition state **3-TS₃** of the reaction 3.

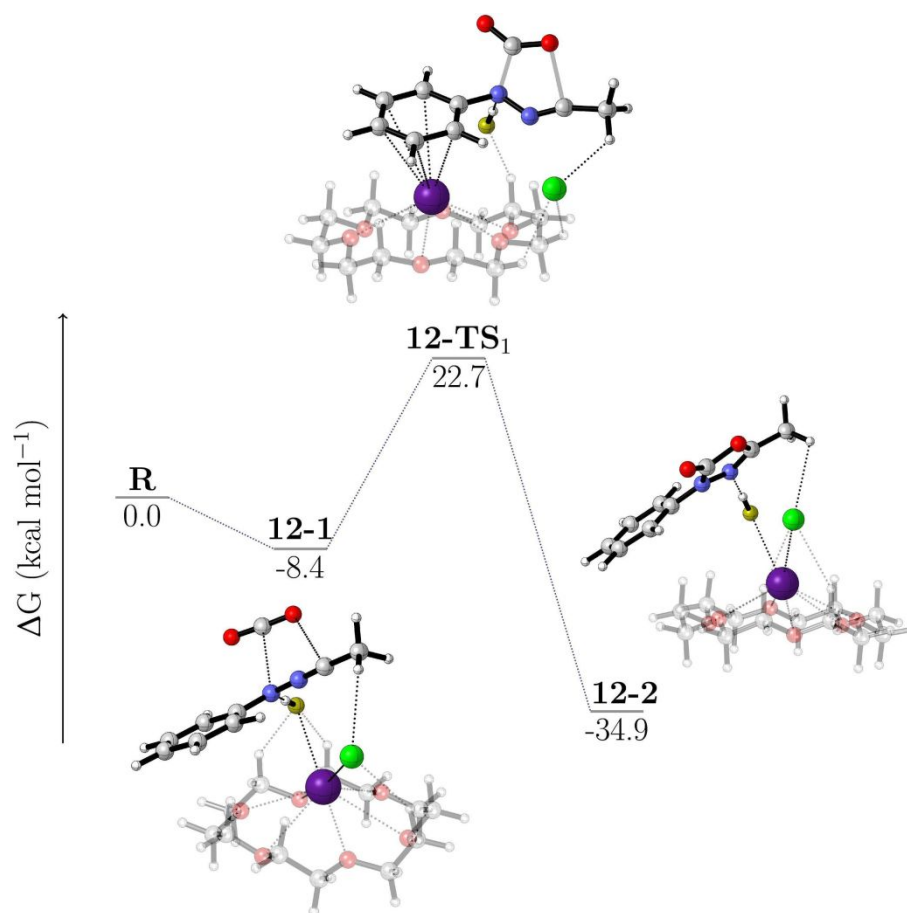


Figure 3-SI. Mechanism resulting from the conformational analysis of the transition state **6-TS₂** of the reaction 6.

2. Cartesian coordinates of all the structures.

Cartesian coordinates for the structures of 1, CO₂, COS, CsF, and 18C6

1 $G = -879.801398$ a.u. in the gas phase

N	0.0000000	0.4311920	0.0000000
H	-0.1943530	1.4231030	0.0000000
N	1.2678680	0.0230580	0.0000000
C	-1.0521270	-0.4767300	0.0000000
C	2.2304620	0.8339250	0.0000000
C	-2.3561280	0.0189200	0.0000000
C	-0.8362380	-1.8536330	0.0000000
H	-2.5226860	1.0898430	0.0000000
H	0.1756610	-2.2311930	0.0000000
Cl	1.9676890	2.5806320	0.0000000
C	3.6587520	0.4183080	0.0000000
C	-3.4296040	-0.8546650	0.0000000
C	-1.9227600	-2.7139390	0.0000000
H	3.7081540	-0.6681860	0.0000000
H	4.1691920	0.8080990	0.8816530
C	-3.2231460	-2.2278060	0.0000000
H	4.1691920	0.8080990	-0.8816530
H	-4.4361600	-0.4564370	0.0000000
H	-1.7463460	-3.7821260	0.0000000
H	-4.0637160	-2.9079770	0.0000000

1 $G = -879.811779$ a.u. in solution

N	0.0000000	0.4347010	0.0000000
H	-0.1915510	1.4280550	0.0000000
N	1.2651400	0.0132290	0.0000000
C	-1.0570950	-0.4647290	0.0000000
C	2.2394780	0.8100080	0.0000000
C	-2.3576670	0.0429380	0.0000000
C	-0.8543440	-1.8442390	0.0000000
H	-2.5120030	1.1158810	0.0000000
H	0.1530910	-2.2349460	0.0000000
Cl	1.9983110	2.5614380	0.0000000
C	3.6613010	0.3769470	0.0000000

C	-3.4389530	-0.8208850	0.0000000
C	-1.9494980	-2.6948680	0.0000000
H	3.6992820	-0.7106990	0.0000000
H	4.1767670	0.7594600	0.8825080
C	-3.2454320	-2.1967870	0.0000000
H	4.1767670	0.7594600	-0.8825080
H	-4.4419650	-0.4129980	0.0000000
H	-1.7820810	-3.7647950	0.0000000
H	-4.0923150	-2.8696920	0.0000000

CO₂ G= -188.606257 a.u. in the gas phase

O	0.0000000	0.0000000	1.1547650
C	0.0000000	0.0000000	-0.0000370
O	0.0000000	0.0000000	-1.1547370

CO₂ G= -188.606493 a.u. in solution

O	0.0000000	0.0000000	1.1545150
C	0.0000000	0.0000000	-0.0000270
O	0.0000000	0.0000000	-1.1544950

COS G= -511.553864 a.u. in solution

O	0.0000000	0.0000000	-1.6740310
C	0.0000000	0.0000000	-0.5258620
S	0.0000000	0.0000000	1.0342140

CsF G= -120.042933 a.u. in solution

Cs	0.0000000	0.0000000	0.3547800
F	0.0000000	0.0000000	-2.1680970

18C6 G= -922.656898 a.u. in solution

C	0.6381060	3.5341310	-0.2944390
C	-0.7480720	3.5126960	0.2948410
O	-1.4729620	2.4414100	-0.2503380
H	-1.2495900	4.4654350	0.0714200
H	-0.6771790	3.4145580	1.3862250
C	-2.7651850	2.3298290	0.2862030

C	-3.4431800	1.1152030	-0.2913330
H	-3.3586070	3.2230700	0.0427890
H	-2.7224410	2.2382060	1.3795130
H	-3.3249050	1.1184710	-1.3829390
H	-4.5186020	1.1606310	-0.0663110
O	-2.8773340	-0.0442810	0.2614250
C	-3.4067510	-1.2214700	-0.2900710
C	-2.6903380	-2.4138960	0.2873900
H	-3.2893120	-1.2217820	-1.3817900
H	-4.4800100	-1.3006600	-0.0640440
O	-1.3955420	-2.4846210	-0.2498130
H	-3.2552000	-3.3255060	0.0441950
H	-2.6498820	-2.3210690	1.3806840
C	-0.6381360	-3.5344710	0.2930400
C	0.7480890	-3.5123520	-0.2961000
H	-1.1102110	-4.5016490	0.0673170
H	-0.5705060	-3.4367290	1.3846570
O	1.4729700	-2.4417070	0.2503500
H	0.6772770	-3.4129300	-1.3873740
H	1.2495690	-4.4653670	-0.0737740
C	2.7654060	-2.3298420	-0.2856280
C	3.4429810	-1.1151780	0.2923300
H	3.3588520	-3.2230370	-0.0421120
H	2.7231190	-2.2380410	-1.3789390
O	2.8773120	0.0442470	-0.2607250
H	4.5185240	-1.1605020	0.0678640
H	3.3241290	-1.1184790	1.3838750
C	3.4065980	1.2215250	0.2907360
C	2.6904680	2.4138360	-0.2873070
H	3.2887380	1.2220820	1.3824000
H	4.4799570	1.3005770	0.0651230
O	1.3955790	2.4849520	0.2496160
H	2.6502240	2.3205580	-1.3805730
H	3.2553910	3.3254840	-0.0443930
H	1.1101850	4.5015980	-0.0699760
H	0.5703700	3.4350200	-1.3859270

Cartesian coordinates for the structures of the Figure 1 in the gas phase

1-TS₁ **G= -1068.314484 a.u.** **□v_{min}= 431*i* cm⁻¹**

N	-0.0786190	-0.1064730	-0.2808650
H	-0.3243850	-0.6675370	-1.1097460
N	-0.8450340	1.0672820	-0.2152190
C	1.3626960	0.0869890	-0.2444580
C	-2.0590820	0.6676320	0.0315390
C	2.1662100	-0.9890410	-0.5816380
C	1.8914130	1.3007780	0.1529380
C	-0.6506390	-1.0345310	0.9765160
H	1.7220870	-1.9330390	-0.8705550
H	1.2275870	2.1158190	0.3997550
O	0.0397270	-1.9299660	1.3291420
O	-1.7675430	-0.5530140	1.2682970
Cl	-2.8605790	-0.5106730	-1.1834940
C	-3.0828190	1.6075250	0.5604370
C	3.5428060	-0.8409890	-0.5215090
C	3.2716890	1.4345100	0.2058070
H	-2.6227280	2.2493910	1.3083700
H	-3.9028830	1.0433200	0.9973680
C	4.0962310	0.3697950	-0.1284830
H	-3.4668000	2.2073160	-0.2636160
H	4.1808620	-1.6749260	-0.7810630
H	3.7018350	2.3797230	0.5094610
H	5.1713360	0.4835320	-0.0843970

1-1 $G = -1068.319925$ a.u.

N	-0.0654110	-0.1317870	-0.2495610
H	-0.3405370	-0.7355790	-1.0483360
N	-0.8398590	1.0635110	-0.3287490
C	1.3865050	0.0464140	-0.2346980
C	-2.0001960	0.6527190	0.1599040
C	2.1777570	-1.0629670	-0.4742400
C	1.9154540	1.2922250	0.0382390
C	-0.6178280	-0.8828150	0.9818440
H	1.7270810	-2.0271900	-0.6729290
H	1.2510970	2.1276080	0.2036740
O	-0.0471800	-1.7616800	1.5160620
O	-1.7736080	-0.3315590	1.2132910
Cl	-2.9144150	-0.6448830	-1.1908130
C	-3.0574000	1.6371460	0.5126960
C	3.5550910	-0.9140740	-0.4382620

C	3.2968170	1.4244980	0.0688750
H	-2.6895640	2.2738430	1.3180530
H	-3.9586030	1.1183480	0.8259760
C	4.1133460	0.3277780	-0.1662130
H	-3.2714380	2.2400960	-0.3659090
H	4.1901810	-1.7697030	-0.6235650
H	3.7336690	2.3928920	0.2730930
H	5.1890900	0.4410000	-0.1417580

1-TS₂ **G= -1068.318823 a.u.** $\square v_{\min} = 92i \text{ cm}^{-1}$

N	-0.0723140	-0.1138110	-0.2131290
H	-0.3824170	-0.7353640	-0.9901300
N	-0.8421400	1.0820630	-0.3409070
C	1.3801380	0.0468010	-0.2202080
C	-1.9885280	0.7016210	0.1725300
C	2.1545240	-1.0795110	-0.4338750
C	1.9269980	1.2943150	0.0062390
C	-0.6310680	-0.8171050	1.0379120
H	1.6898720	-2.0435020	-0.5983780
H	1.2763920	2.1441350	0.1523820
O	-0.0711190	-1.6766500	1.6106650
O	-1.7890760	-0.2506890	1.2395230
Cl	-2.8538230	-0.7476500	-1.2152540
C	-3.0977120	1.6529430	0.4233390
C	3.5338130	-0.9458660	-0.4196680
C	3.3099030	1.4109690	0.0154580
H	-2.8017080	2.3344290	1.2225800
H	-3.9923910	1.1080990	0.7088760
C	4.1100710	0.2972960	-0.1948120
H	-3.2850660	2.2107860	-0.4899020
H	4.1563690	-1.8144810	-0.5859870
H	3.7605670	2.3800290	0.1830720
H	5.1872630	0.3981010	-0.1879440

1-2 **G= -1068.400393 a.u.**

N	-0.0018220	-0.7932280	0.0190660
H	-1.6677970	1.7617830	-0.1644650
N	-1.1807320	-0.0845540	0.0889440

C	1.2542940	-0.1398040	0.0332390
C	-2.1027900	-0.9693260	0.1017830
C	2.4022040	-0.8307690	-0.3416700
C	1.3208330	1.1936910	0.4218200
C	-0.2465020	-2.1405790	-0.0022950
H	2.3403020	-1.8663450	-0.6386630
H	0.4271230	1.7216420	0.7213170
O	0.4818390	-3.0817480	-0.0512230
O	-1.6292120	-2.2304470	0.0503970
Cl	-2.1915630	2.9464210	-0.2699800
C	-3.5610380	-0.7455600	0.1570090
C	3.6204930	-0.1696190	-0.3207130
C	2.5475850	1.8374090	0.4281520
H	-3.7616810	0.3229690	0.1780400
H	-3.9745470	-1.2156390	1.0493980
C	3.7018880	1.1617640	0.0597280
H	-4.0376820	-1.1927620	-0.7153000
H	4.5135650	-0.7073070	-0.6110210
H	2.5954170	2.8757790	0.7288270
H	4.6569380	1.6695110	0.0697440

Cartesian coordinates for the structures of the Figure 1 in solution

1-TS₁ ***G* = -1068.330592 a.u.** □ ***v*_{min} = 429i cm⁻¹**

N	-0.0787870	-0.1957290	-0.2683600
H	-0.3085280	-0.9473730	-0.9364580
N	-0.8425090	0.9627500	-0.5020850
C	1.3615390	0.0149150	-0.2715570
C	-2.0562220	0.6641940	-0.1441060
C	2.1738040	-1.0239970	-0.6857970
C	1.8762030	1.2117390	0.1935310
C	-0.6308300	-0.7679170	1.1675790
H	1.7400060	-1.9538950	-1.0341870
H	1.2072920	2.0008070	0.5069830
O	0.0563540	-1.5629330	1.7209090
O	-1.7345900	-0.2152110	1.3709690
Cl	-2.8972990	-0.7839330	-0.9868470
C	-3.0571460	1.7229660	0.1431560
C	3.5502450	-0.8553730	-0.6426990
C	3.2534220	1.3674500	0.2294750

H	-2.5778960	2.5259620	0.6999360
H	-3.8822350	1.3059530	0.7159400
C	4.0891510	0.3388400	-0.1865430
H	-3.4451680	2.1057470	-0.8008340
H	4.1977880	-1.6593890	-0.9663370
H	3.6738570	2.2984060	0.5866820
H	5.1629370	0.4697540	-0.1554630

1-2 $G = -1068.414769$ a.u.

N	-0.1136690	-0.7893340	0.0397380
H	-1.4174840	1.8692140	-0.1859560
N	-1.2231620	0.0172490	0.1723500
C	1.1948920	-0.2505490	0.0661160
C	-2.2210080	-0.7817100	0.1658900
C	2.2475310	-0.9518860	-0.5106650
C	1.4029190	0.9864530	0.6652470
C	-0.4784650	-2.1035950	-0.0344850
H	2.0736970	-1.9118520	-0.9736550
H	0.5778180	1.5139000	1.1235830
O	0.1644400	-3.1041630	-0.1384560
O	-1.8567680	-2.0753940	0.0462270
Cl	-1.6942770	3.1213090	-0.4305040
C	-3.6519030	-0.4399070	0.2554050
C	3.5185910	-0.3986990	-0.4803380
C	2.6782220	1.5281960	0.6754150
H	-3.7619760	0.6372080	0.3570070
H	-4.1001630	-0.9369290	1.1163010
C	3.7400860	0.8395740	0.1058010
H	-4.1709490	-0.7775760	-0.6425340
H	4.3400810	-0.9416990	-0.9296550
H	2.8382410	2.4937630	1.1376260
H	4.7346920	1.2654980	0.1187580

Cartesian coordinates for the structures of the Figure 2 in solution

2-1 $G = -1188.461288$ a.u.

H	0.41623	-0.02912	-0.82999
N	1.29141	0.41969	-0.39782
F	-0.63673	-0.86311	-1.43530

C	2.41477	-0.40520	-0.33282
Cs	-2.87094	-0.94489	-0.09713
N	1.52378	1.73325	-0.58097
O	0.95930	1.22942	2.48769
H	1.23450	-2.14965	-0.70631
C	2.22916	-1.78416	-0.48160
C	0.62346	2.60238	-0.55541
C	0.24284	0.37701	2.19344
Cl	-1.08572	2.19731	-0.20549
C	3.69434	0.08713	-0.06932
H	3.83960	1.15129	0.05288
C	3.30755	-2.64467	-0.36967
O	-0.50582	-0.48214	1.97897
C	4.76458	-0.78938	0.03424
C	0.84492	4.05542	-0.78146
H	3.14938	-3.70938	-0.49330
C	4.58442	-2.15803	-0.11094
H	1.90592	4.22389	-0.95478
H	0.51776	4.63332	0.08444
H	0.27951	4.39843	-1.64953
H	5.75251	-0.39262	0.23578
H	5.42397	-2.83552	-0.02656

2-TS₁ **G= -1188.446920 a.u.** $\square$ **v_{min}= 236.5i cm⁻¹**

H	0.2110630	-0.0222070	-0.9437130
N	1.0746040	0.4469220	-0.2022240
F	-0.6174320	-0.5280300	-1.6242080
C	2.2513690	-0.3692710	-0.2186230
Cs	-2.6621500	-1.0483710	-0.0097960
N	1.3656100	1.7655520	-0.4741250
O	0.8136440	1.1773670	2.1777400
H	1.1612270	-2.0553070	-0.9477790
C	2.1226820	-1.6992550	-0.6018980
C	0.4749410	2.6410030	-0.4463230
C	0.3986040	0.2742500	1.5406950
Cl	-1.2362670	2.2970530	-0.0779260
C	3.4809010	0.1213910	0.2062930
H	3.5604530	1.1556200	0.5106700
C	3.2286860	-2.5351100	-0.5631050
O	-0.2742060	-0.7228640	1.5289620

C	4.5807770	-0.7218070	0.2358570
C	0.7229570	4.0831140	-0.7196200
H	3.1276320	-3.5681630	-0.8705820
C	4.4609390	-2.0513680	-0.1462960
H	1.7793020	4.2216550	-0.9352050
H	0.4398630	4.6778200	0.1493540
H	0.1233350	4.4146790	-1.5676590
H	5.5373330	-0.3377040	0.5669440
H	5.3233170	-2.7046370	-0.1216740

2-2 $G = -1188.448598$ a.u.

H	0.1201300	-0.0472900	-1.0932800
N	1.0699110	0.4501220	-0.1176620
F	-0.5858840	-0.4318790	-1.7425280
C	2.2576130	-0.3777350	-0.1522910
Cs	-2.6653100	-1.0496980	0.0217800
N	1.3992320	1.7780200	-0.3507220
O	0.5672090	1.1012240	2.1167660
H	1.1929840	-2.0275320	-0.9972610
C	2.1458920	-1.6773270	-0.6247650
C	0.5160290	2.6608050	-0.3718210
C	0.3694050	0.2194530	1.3247080
Cl	-1.2218070	2.3390680	-0.1611970
C	3.4716620	0.0935960	0.3300800
H	3.5345880	1.1056960	0.7044760
C	3.2581800	-2.5066990	-0.6204880
O	-0.2499160	-0.8472990	1.3117140
C	4.5787720	-0.7407380	0.3261370
C	0.8081620	4.1039720	-0.5921590
H	3.1707790	-3.5185830	-0.9946970
C	4.4770960	-2.0417280	-0.1482320
H	1.8752090	4.2244230	-0.7606690
H	0.5065000	4.6752310	0.2863150
H	0.2472650	4.4764540	-1.4493080
H	5.5247600	-0.3731000	0.7028110
H	5.3443100	-2.6891670	-0.1493400

2-TS₂ $G = -1188.444648$ a.u. $\square \nu_{\min} = 49.5i \text{ cm}^{-1}$

H	0.1478100	-0.0618640	-1.1315440
N	1.0717330	0.4606400	-0.0614560
F	-0.5233730	-0.4693810	-1.7713510
C	2.2929790	-0.3211140	-0.1063520
Cs	-2.6280700	-1.0596980	0.0350360
N	1.3603250	1.8118610	-0.1727220
O	0.1050070	1.0065840	2.0364400
H	1.2945640	-1.9977090	-0.9792390
C	2.2349220	-1.6126910	-0.6110790
C	0.4565620	2.6671210	-0.2745810
C	0.2578570	0.0950760	1.2613160
Cl	-1.2811900	2.3001080	-0.3766070
C	3.4915520	0.1888420	0.3752360
H	3.5211500	1.1959140	0.7655050
C	3.3810530	-2.3932570	-0.6352120
O	-0.1151260	-1.0816370	1.2099340
C	4.6335650	-0.5977980	0.3425630
C	0.7300110	4.1293210	-0.3526720
H	3.3316370	-3.3991890	-1.0318230
C	4.5841140	-1.8897620	-0.1611790
H	1.8052250	4.2872900	-0.3428570
H	0.2755410	4.6297450	0.5029710
H	0.2954290	4.5475410	-1.2605550
H	5.5662120	-0.1974670	0.7193610
H	5.4777450	-2.4998230	-0.1842670

2-3 $G = -1188.447568$ a.u.

H	-0.1632630	-0.0567850	1.2931560
N	-1.0872190	0.4205440	-0.0362440
F	0.4596230	-0.4773570	1.9122190
C	-2.3334210	-0.3094710	0.0226530
Cs	2.6791640	-1.0008030	-0.1210870
N	-1.3333060	1.7679630	-0.2432490
O	0.6656120	0.6279590	-1.5636500
H	-1.4991020	-1.8399240	1.2645440
C	-2.3853380	-1.4875140	0.7547970
C	-0.5078950	2.6632220	0.0482580
C	-0.0733500	-0.1818820	-1.0059340
Cl	1.0352170	2.4261000	0.8725060
C	-3.4671450	0.1448900	-0.6384290

H	-3.4206800	1.0694680	-1.1974570
C	-3.5662990	-2.2096640	0.8176590
O	-0.0500060	-1.4146010	-0.9818080
C	-4.6457690	-0.5814990	-0.5662970
C	-0.7754850	4.0936920	-0.2515620
H	-3.5970680	-3.1291180	1.3914030
C	-4.7020550	-1.7614120	0.1598040
H	-1.7749380	4.1934540	-0.6714220
H	-0.0397290	4.4594810	-0.9716970
H	-0.6835330	4.6971470	0.6536560
H	-5.5257990	-0.2197290	-1.0864300
H	-5.6258040	-2.3258890	0.2158800

2-TS₃ **G= -1188.417980 a.u.** **□ v_{min}= 444.2i cm⁻¹**

H	-0.2741820	-0.4203280	1.3853420
N	-1.1862370	0.5258550	-0.0238450
F	0.2488050	-1.1246950	1.7424200
C	-2.4833960	-0.0840160	-0.0006770
Cs	2.5613960	-1.0353460	-0.1270350
N	-1.1934060	1.9187800	-0.0389620
O	0.6376250	0.9858250	-1.2919170
H	-1.7056400	-2.0739370	0.1816870
C	-2.5951240	-1.4662680	0.1246460
C	-0.0285970	2.3724950	-0.1119400
C	-0.1883610	0.0704070	-0.9943640
Cl	1.3452170	1.8283940	1.2438310
C	-3.6272290	0.7046840	-0.0569470
H	-3.5274040	1.7768770	-0.1327830
C	-3.8521400	-2.0486950	0.1637760
O	-0.1442120	-1.1091610	-1.3206340
C	-4.8777900	0.1068530	-0.0082610
C	0.3867860	3.7146620	-0.5779850
H	-3.9315090	-3.1243730	0.2562310
C	-4.9990920	-1.2701570	0.0960560
H	-0.3806540	4.1157600	-1.2363240
H	1.3256230	3.6180450	-1.1193040
H	0.5485460	4.3692480	0.2770830
H	-5.7627750	0.7288810	-0.0519840
H	-5.9768360	-1.7321280	0.1342750

2-4 **G= -1188.504799 a.u.**

H	1.3299970	0.9213320	1.5470160
N	-1.7033570	0.6341510	-0.5691410
F	0.5434530	0.3270740	1.6073100
C	-2.8927450	0.0226900	-0.1289380
Cs	2.4775500	-1.3035170	-0.0285310
N	-1.5047750	1.9849480	-0.4048640
O	0.2889920	1.0657190	-1.2796710
H	-2.4734070	-1.8725910	-1.0476650
C	-3.1729700	-1.3008290	-0.4553190
C	-0.3169020	2.1943070	-0.8247160
C	-0.5942760	0.0423270	-1.0749790
Cl	2.9509570	1.6635070	1.1003970
C	-3.7866790	0.7673080	0.6327650
H	-3.5499980	1.7935600	0.8766820
C	-4.3540500	-1.8705280	-0.0070310
O	-0.3231440	-1.1114280	-1.3180310
C	-4.9627650	0.1806200	1.0671210
C	0.4359330	3.4538110	-0.8484320
H	-4.5705370	-2.9015290	-0.2624540
C	-5.2536050	-1.1388800	0.7529490
H	-0.1825560	4.2487110	-0.4369180
H	0.7279000	3.7056310	-1.8706120
H	1.3450420	3.3310030	-0.2502930
H	-5.6556120	0.7641710	1.6623050
H	-6.1749320	-1.5931310	1.0977260

Cartesian coordinates for the structures of the Figure 3 in solution**3-1** **G= -2111.140036 a.u.**

N	-2.0269560	-0.7897360	-1.5443430
H	-1.0618350	-0.5312280	-2.1701800
N	-2.5229690	-2.0139040	-1.3268900
Cs	0.6128310	0.2058810	0.0871190
C	-2.8434470	0.2713810	-1.2027670
O	-1.8023180	-1.4734660	1.5715400
F	-0.0493240	-0.0204720	-2.6993280
C	-1.8184400	-3.0580960	-1.3714810
C	-2.4042220	1.5701470	-1.5162540

H	-1.4787190	1.6850530	-2.0680410
C	-2.7719650	-2.1022020	1.5092910
Cl	-0.0722400	-3.0112210	-1.6613680
C	-4.0618600	0.1272970	-0.5215720
H	-4.4325400	-0.8648150	-0.3042600
O	-3.7317360	-2.7416330	1.5023690
C	-2.3746480	-4.4273880	-1.1773460
C	-3.1605960	2.6715890	-1.1546890
H	-3.4345260	-4.3450010	-0.9457770
H	-1.8588880	-4.9446340	-0.3658540
C	-4.8014490	1.2447740	-0.1658340
C	-4.3619380	2.5270090	-0.4692130
H	-2.2456990	-5.0243480	-2.0820720
H	-2.8068180	3.6609630	-1.4232950
H	-5.7438860	1.1065990	0.3506880
H	-4.9502550	3.3922390	-0.1943170
C	1.7564900	3.4627480	-1.7835180
C	2.0202400	2.2614850	-2.6524970
O	2.7951230	1.3272830	-1.9249570
H	2.5728750	2.5853690	-3.5449230
H	1.0777560	1.7954940	-2.9628460
C	3.0448290	0.1537110	-2.6757400
C	3.8780680	-0.7878070	-1.8468400
H	3.6052310	0.4081790	-3.5856480
H	2.0950540	-0.3156830	-2.9599420
H	4.7548870	-0.2638180	-1.4455910
H	4.2242820	-1.6154820	-2.4792120
O	3.0953150	-1.2930220	-0.7861060
C	3.7896970	-2.1806380	0.0511810
C	2.8553860	-2.6631340	1.1304050
H	4.6558290	-1.6827240	0.5057020
H	4.1487240	-3.0450020	-0.5233440
O	2.5477650	-1.5894950	1.9927590
H	3.3376700	-3.4728420	1.6935370
H	1.9383830	-3.0584480	0.6725320
C	1.6743950	-1.9646530	3.0314410
C	1.3883630	-0.7670540	3.9003470
H	2.1293260	-2.7556610	3.6423130
H	0.7313500	-2.3475380	2.6185140
O	0.6064390	0.1464660	3.1713310
H	2.3309060	-0.3000120	4.2120970

H	0.8489100	-1.0945710	4.7990580
C	0.2500270	1.2946190	3.9028130
C	-0.5538030	2.2098630	3.0155200
H	-0.3528670	1.0139790	4.7762750
H	1.1483730	1.8176200	4.2536540
O	0.2906940	2.7565890	2.0301370
H	-0.9931900	3.0103480	3.6251960
H	-1.3752590	1.6483940	2.5481410
C	-0.3861730	3.6639640	1.1851530
C	0.5625450	4.1601010	0.1248660
H	-1.2457720	3.1743910	0.7094370
H	-0.7545800	4.5169230	1.7702290
O	0.8582630	3.1049380	-0.7551360
H	1.4815620	4.5367050	0.5920680
H	0.0877260	4.9872400	-0.4198040
H	1.3209100	4.2630160	-2.3959290
H	2.6954560	3.8287640	-1.3492070

3-TS₁ **G= -2111.125773 a.u.** $\square$ **v_{min}= 243i cm⁻¹**

H	-1.8775600	0.9434220	0.7954330
N	-2.8578290	1.0050940	-0.1045940
F	-1.1124770	0.8527530	1.5764930
C	-3.7407980	-0.0882980	0.1059310
Cs	1.1156080	0.0712990	-0.0321940
N	-3.5033730	2.2147460	-0.0483160
O	-2.7479720	1.4836790	-2.5954580
H	-2.0934830	-1.3918230	0.5364340
C	-3.1686070	-1.3214190	0.4244130
C	-2.8649260	3.2767440	-0.2289060
C	-2.1583230	0.7414820	-1.8963670
Cl	-1.1162020	3.3211760	-0.5358480
C	-5.1231030	0.0082610	-0.0339130
H	-5.5614510	0.9641120	-0.2811080
C	-3.9725680	-2.4363220	0.5985770
O	-1.3296690	-0.1151250	-1.7832580
C	-5.9169770	-1.1145820	0.1492280
C	-3.4918300	4.6270460	-0.2055280
H	-3.5180810	-3.3875500	0.8508950
C	-5.3522360	-2.3423020	0.4642730
H	-4.5527170	4.5177030	0.0057700

H	-3.3564600	5.1143680	-1.1719480
H	-3.0228110	5.2510580	0.5558050
H	-6.9909960	-1.0267710	0.0398350
H	-5.9783710	-3.2134620	0.6058970
C	2.6704540	-1.5934670	-3.2560800
C	1.2603720	-2.0790170	-3.0385240
O	1.1550670	-2.6067040	-1.7346260
H	1.0398000	-2.8588340	-3.7795430
H	0.5434410	-1.2603170	-3.1792120
C	-0.1216050	-3.1582920	-1.4745150
C	-0.1445920	-3.6838410	-0.0636490
H	-0.3203740	-3.9845270	-2.1695080
H	-0.8990720	-2.3967060	-1.6019030
H	0.6779790	-4.3931030	0.0932710
H	-1.0946460	-4.2081950	0.1038460
O	-0.0270180	-2.5993150	0.8261860
C	-0.1225290	-2.9674030	2.1832560
C	-0.0871100	-1.7217660	3.0283070
H	0.7055470	-3.6361370	2.4502560
H	-1.0699930	-3.4921010	2.3646100
O	1.1888400	-1.1216560	2.9036220
H	-0.2697080	-1.9955160	4.0759610
H	-0.8639330	-1.0217600	2.7015460
C	1.2828490	0.0852960	3.6303320
C	2.6914080	0.6101510	3.5256300
H	1.0546610	-0.0961960	4.6890950
H	0.5649370	0.8171230	3.2407100
O	2.9257970	1.0697420	2.2115270
H	3.4009830	-0.1887480	3.7738530
H	2.8289460	1.4331230	4.2385270
C	4.2527590	1.4754720	1.9897210
C	4.3875140	1.9585020	0.5682680
H	4.5212040	2.2930850	2.6719120
H	4.9421620	0.6398500	2.1634050
O	4.2451770	0.8669880	-0.3121010
H	5.3718240	2.4256890	0.4354510
H	3.6187830	2.7162600	0.3646500
C	4.3726440	1.2371200	-1.6657540
C	4.2300480	0.0128450	-2.5329930
H	3.6019970	1.9721310	-1.9356160
H	5.3554310	1.6931850	-1.8422110

O	2.9022770	-0.4461160	-2.4678050
H	4.9197480	-0.7662480	-2.1853750
H	4.4926240	0.2724810	-3.5669220
H	2.8140790	-1.3534880	-4.3173700
H	3.3761720	-2.3864030	-2.9793450

3-2 $G = -2111.126620$ a.u.

H	-1.8492140	0.8900370	0.9141420
N	-2.8871860	0.9832250	-0.1323620
F	-1.1567060	0.7841020	1.6561810
C	-3.7439140	-0.1608350	0.0626830
Cs	1.1427070	0.0915850	-0.0304950
N	-3.5964410	2.1657740	0.0224430
O	-2.6193170	1.6296940	-2.4114600
H	-2.0737060	-1.4155980	0.5373520
C	-3.1473030	-1.3699310	0.4090050
C	-2.9957550	3.2631920	-0.0327910
C	-2.1851310	0.8553490	-1.6009370
Cl	-1.2513550	3.4278800	-0.2460510
C	-5.1203720	-0.0903710	-0.1111420
H	-5.5711480	0.8533230	-0.3807690
C	-3.9317200	-2.5003780	0.5786190
O	-1.3350560	-0.0332990	-1.5767240
C	-5.8955740	-1.2274260	0.0678290
C	-3.7000820	4.5700370	0.0906720
H	-3.4633640	-3.4382060	0.8533760
C	-5.3089610	-2.4363780	0.4117720
H	-4.7535810	4.3875790	0.2867940
H	-3.5904280	5.1297600	-0.8389450
H	-3.2627040	5.1609870	0.8953980
H	-6.9678610	-1.1654000	-0.0688690
H	-5.9185960	-3.3197160	0.5512300
C	2.4437050	-1.3250710	-3.4456160
C	1.0434070	-1.7976860	-3.1506810
O	1.0408070	-2.4555770	-1.9006190
H	0.7360980	-2.4943210	-3.9421060
H	0.3378020	-0.9575730	-3.1386330
C	-0.2174980	-3.0276730	-1.5957950
C	-0.1508980	-3.6391450	-0.2213370
H	-0.4555170	-3.8132100	-2.3252250

H	-1.0002780	-2.2615970	-1.6290270
H	0.6907850	-4.3400160	-0.1535750
H	-1.0813300	-4.1907220	-0.0324400
O	0.0005950	-2.6097410	0.7302190
C	-0.0208480	-3.0612200	2.0632240
C	0.0608210	-1.8684770	2.9791680
H	0.8195740	-3.7426340	2.2469950
H	-0.9569590	-3.5993870	2.2642690
O	1.3362300	-1.2715030	2.8414140
H	-0.0864360	-2.1988700	4.0157990
H	-0.7224360	-1.1466440	2.7215700
C	1.4686280	-0.1006240	3.6162120
C	2.8810730	0.4105000	3.4925250
H	1.2629790	-0.3213420	4.6719170
H	0.7538600	0.6611510	3.2793980
O	3.0779000	0.9296720	2.1953610
H	3.5845680	-0.4099320	3.6793100
H	3.0538850	1.1955100	4.2396160
C	4.4116110	1.2898460	1.9327920
C	4.5047640	1.8560770	0.5388680
H	4.7502440	2.0486460	2.6506830
H	5.0667370	0.4141620	2.0194770
O	4.2862730	0.8292520	-0.4010140
H	5.4992210	2.2975190	0.3934630
H	3.7569490	2.6509880	0.4154820
C	4.3673180	1.2850840	-1.7329040
C	4.1243440	0.1331020	-2.6739430
H	3.6198180	2.0691640	-1.9131870
H	5.3610490	1.7092730	-1.9269040
O	2.7835580	-0.2736290	-2.5654540
H	4.7961290	-0.6974010	-2.4237640
H	4.3430840	0.4583340	-3.6997380
H	2.5005160	-0.9740600	-4.4836280
H	3.1465710	-2.1576350	-3.3186770

3-TS₂ **G= -2111.125042 a.u** $\square \nu_{\min}= 26i \text{ cm}^{-1}$

H	-1.7341660	0.9644380	0.8509900
N	-2.6089550	1.1232370	-0.4223130
F	-1.2284870	0.7946330	1.6874660
C	-3.6707130	0.1849340	-0.1546500

Cs	1.0203660	-0.1087290	-0.0141450
N	-3.0738670	2.4192970	-0.4913320
O	-1.5515440	1.6178670	-2.4963330
H	-2.2879940	-1.2728080	0.6309440
C	-3.3315590	-1.0520500	0.4052490
C	-2.2763170	3.3871910	-0.4481660
C	-1.7515790	0.7038480	-1.7359100
Cl	-0.5235670	3.2220830	-0.1560160
C	-5.0069940	0.4804080	-0.4300710
H	-5.2566650	1.4529440	-0.8504190
C	-4.3281070	-1.9878550	0.6683010
O	-1.4281030	-0.4799150	-1.6720320
C	-5.9965680	-0.4625220	-0.1556600
C	-2.7023490	4.8083200	-0.6016390
H	-4.0560090	-2.9508120	1.1056900
C	-5.6648180	-1.7005990	0.3904070
H	-3.7936610	4.8416360	-0.6905240
H	-2.2455060	5.2287330	-1.5086900
H	-2.3693160	5.4043630	0.2587020
H	-7.0389570	-0.2236110	-0.3744540
H	-6.4430630	-2.4351450	0.6026830
C	2.2965680	-1.9975990	-3.1580240
C	0.8957210	-2.4396950	-2.8113360
O	0.8637310	-2.8577990	-1.4664190
H	0.6226820	-3.2810330	-3.4775910
H	0.1724460	-1.6191620	-2.9714540
C	-0.3931620	-3.3718210	-1.0847600
C	-0.3425530	-3.7589140	0.3718100
H	-0.6320890	-4.2733190	-1.6818890
H	-1.1815140	-2.6164160	-1.2484110
H	0.5107110	-4.4406990	0.5509360
H	-1.2729840	-4.2983410	0.6345340
O	-0.2117550	-2.6029880	1.1598820
C	-0.1302250	-2.8606990	2.5366640
C	-0.0526330	-1.5555680	3.2884610
H	0.7604570	-3.4785220	2.7605340
H	-1.0254410	-3.4158150	2.8777550
O	1.1731820	-0.9217800	2.9993480
H	-0.1246160	-1.7641410	4.3735450
H	-0.8948980	-0.9069240	2.9939520
C	1.2877420	0.3428610	3.6039360

C	2.6762380	0.8866670	3.3676490
H	1.1278220	0.2608510	4.6964260
H	0.5275500	1.0334810	3.1946290
O	2.8371930	1.2058180	2.0085030
H	3.4219460	0.1290260	3.6735630
H	2.8246060	1.7884220	3.9916960
C	4.1334170	1.6111830	1.6656010
C	4.1868650	1.9278510	0.1900280
H	4.4216740	2.5149740	2.2359400
H	4.8644640	0.8131580	1.8953170
O	4.0239550	0.7490950	-0.5547330
H	5.1612170	2.3995380	-0.0408990
H	3.3905230	2.6573390	-0.0576290
C	4.1054760	0.9524000	-1.9430500
C	3.9171460	-0.3615120	-2.6630210
H	3.3276350	1.6662870	-2.2773440
H	5.0924840	1.3745790	-2.2123130
O	2.6046130	-0.8075910	-2.4737530
H	4.6421680	-1.1024960	-2.2757730
H	4.1258540	-0.2083270	-3.7392430
H	2.3663030	-1.8365530	-4.2503240
H	3.0132010	-2.7930380	-2.8789280

3-3 $G = -2111.125637$ a.u.

H	-1.9085230	0.7167730	1.0326610
N	-2.7167480	0.9969580	-0.3040940
F	-1.3824250	0.4550890	1.8289770
C	-3.9249960	0.2118510	-0.1597160
Cs	1.0210690	-0.1956620	-0.0226960
N	-3.0286510	2.3320660	-0.5282030
O	-1.1409070	1.2391020	-2.0358540
H	-2.8926410	-1.3435130	0.8864310
C	-3.8459590	-1.0095620	0.5011480
C	-2.1922990	3.2471010	-0.3620500
C	-1.7356430	0.4005090	-1.3850070
Cl	-0.5605560	3.0504470	0.2893040
C	-5.1431590	0.6475690	-0.6656190
H	-5.1973800	1.6007740	-1.1699050
C	-4.9822360	-1.7892450	0.6449380
O	-1.6670000	-0.8247750	-1.3142480

C	-6.2756980	-0.1390520	-0.5118500
C	-2.5143620	4.6703670	-0.6716470
H	-4.9128100	-2.7392260	1.1600940
C	-6.2025770	-1.3597980	0.1413750
H	-3.5534370	4.7405110	-0.9831770
H	-1.8650750	5.0204180	-1.4752460
H	-2.3363940	5.2963070	0.2030090
H	-7.2211630	0.2086620	-0.9091090
H	-7.0888110	-1.9700110	0.2601220
C	2.1912240	-2.0086770	-3.2411430
C	0.9148610	-2.6118420	-2.7103570
O	1.1207810	-3.0074110	-1.3682530
H	0.6520370	-3.4863240	-3.3200960
H	0.0947850	-1.8840870	-2.7681440
C	-0.0237060	-3.6222730	-0.8059630
C	0.2596690	-3.9468070	0.6387020
H	-0.2464210	-4.5523000	-1.3457130
H	-0.8872890	-2.9510910	-0.8796900
H	1.2300450	-4.4536230	0.7218180
H	-0.5175260	-4.6214640	1.0209790
O	0.2701190	-2.7524360	1.3870800
C	0.5985850	-2.9322620	2.7429080
C	0.5444680	-1.5969620	3.4397020
H	1.6027910	-3.3660690	2.8377420
H	-0.1179700	-3.6150880	3.2186730
O	1.6256750	-0.7975840	2.9987970
H	0.6162370	-1.7505350	4.5246660
H	-0.4078660	-1.1044210	3.2136380
C	1.5641300	0.5174050	3.5099420
C	2.8128380	1.2632650	3.1117110
H	1.5019630	0.4901750	4.6059220
H	0.6731940	1.0312910	3.1252500
O	2.7759480	1.5263350	1.7272280
H	3.6944980	0.6586030	3.3582940
H	2.8694060	2.2063320	3.6704620
C	3.9566150	2.1012390	1.2236790
C	3.7970650	2.3314360	-0.2579060
H	4.1517500	3.0626440	1.7172290
H	4.8117010	1.4380880	1.4062290
O	3.7839960	1.0929170	-0.9309820
H	4.6298040	2.9493520	-0.6192470

H	2.8612440	2.8765650	-0.4444140
C	3.6230460	1.2411150	-2.3260340
C	3.5899530	-0.1166430	-2.9819820
H	2.6857690	1.7703060	-2.5458970
H	4.4554900	1.8255600	-2.7396160
O	2.3996480	-0.7635020	-2.6150480
H	4.4619500	-0.7064770	-2.6710110
H	3.6327590	0.0162980	-4.0712970
H	2.1067960	-1.8719240	-4.3268180
H	3.0343720	-2.6812530	-3.0371660

3-TS₃ **$G_{\text{corr}} = -2111.097587$ a.u.** $\square$ **$\nu_{\text{min}} = 437i$ cm⁻¹**

H	1.8514130	0.3113210	-1.4100640
N	2.7272790	1.1685070	-0.1650040
F	1.3813330	-0.3459340	-1.9308850
C	3.9269830	0.3807640	-0.1574340
Cs	-0.9670640	-0.2287410	0.0269620
N	2.9346380	2.5356350	-0.3801570
O	1.1620840	2.1120680	1.1891880
H	2.8570860	-1.4696670	0.0158100
C	3.8288820	-1.0057870	-0.0664810
C	1.8440250	3.1586640	-0.2636030
C	1.8164180	1.0502050	1.0059090
Cl	0.2889020	2.6782230	-1.3557240
C	5.1725420	0.9824660	-0.2896040
H	5.2319100	2.0564830	-0.3811620
C	4.9807780	-1.7755340	-0.0792440
O	1.7252670	-0.0207800	1.5883250
C	6.3169720	0.1973180	-0.3100680
C	1.7115420	4.6071520	0.0313860
H	4.8976600	-2.8525640	-0.0046280
C	6.2300630	-1.1816360	-0.1991970
H	2.6194910	4.9553520	0.5188500
H	0.8591380	4.7467610	0.6936860
H	1.5286590	5.1597270	-0.8888430
H	7.2834450	0.6739490	-0.4151350
H	7.1253460	-1.7894700	-0.2157190
C	-3.9470470	0.9711340	-2.2309570
C	-3.7367810	2.0027750	-1.1515750
O	-3.7190240	1.3649220	0.1077680

H	-4.5505050	2.7387710	-1.1887510
H	-2.7870090	2.5253880	-1.3270740
C	-3.4611290	2.2654930	1.1638340
C	-3.4633560	1.5165970	2.4732710
H	-4.2322520	3.0464880	1.1902680
H	-2.4839830	2.7470120	1.0203030
H	-4.3835030	0.9257990	2.5654170
H	-3.4290230	2.2393180	3.2990270
O	-2.3342430	0.6816230	2.5114820
C	-2.1744680	-0.0376370	3.7118940
C	-0.9081060	-0.8518760	3.6259470
H	-3.0358760	-0.6970150	3.8774360
H	-2.0977990	0.6573390	4.5578820
O	-1.0875400	-1.8911770	2.6834420
H	-0.6919850	-1.2783220	4.6144900
H	-0.0665560	-0.2152840	3.3252780
C	0.0567300	-2.7164950	2.5755180
C	-0.1768920	-3.7506900	1.5039760
H	0.2374210	-3.2261410	3.5311140
H	0.9367100	-2.1127800	2.3261750
O	-0.1560250	-3.1208410	0.2429160
H	-1.1437000	-4.2444300	1.6636030
H	0.6145830	-4.5094960	1.5576560
C	-0.3754090	-3.9973400	-0.8365770
C	-0.3599480	-3.2043800	-2.1184860
H	0.4155640	-4.7578570	-0.8729760
H	-1.3414260	-4.5054930	-0.7239290
O	-1.5219900	-2.4013540	-2.1796130
H	-0.3392890	-3.8949710	-2.9714900
H	0.5380710	-2.5762970	-2.1539680
C	-1.5518480	-1.5822630	-3.3297550
C	-2.8381260	-0.7952000	-3.3445700
H	-0.6944650	-0.8969100	-3.3297260
H	-1.5014280	-2.2028180	-4.2337840
O	-2.7882710	0.1794810	-2.3294260
H	-3.6881290	-1.4700320	-3.1834540
H	-2.9556640	-0.3127870	-4.3232760
H	-4.1381890	1.4821400	-3.1834520
H	-4.8169240	0.3479520	-1.9888390

3-4 **$G = -2111.182388$ a.u.**

C	4.0880730	-0.1885500	-2.4964160
C	3.8242450	-1.5338040	-1.8748610
O	3.7261480	-1.3843070	-0.4714600
H	4.6572070	-2.2068440	-2.1195680
H	2.8958440	-1.9555290	-2.2756290
C	3.4182890	-2.6053000	0.1690790
C	3.3946450	-2.3875720	1.6595220
H	4.1861770	-3.3553030	-0.0646030
H	2.4479270	-2.9789120	-0.1804460
H	4.3242580	-1.9013560	1.9812450
H	3.3163370	-3.3592760	2.1645480
O	2.2888690	-1.5799800	1.9946990
C	2.1843460	-1.3082590	3.3699610
C	1.0205670	-0.3786100	3.5995060
H	3.1072510	-0.8416200	3.7370270
H	2.0200970	-2.2393280	3.9285290
O	1.3270650	0.8883520	3.0608140
H	0.8362200	-0.2951960	4.6788660
H	0.1158730	-0.7816350	3.1250470
C	0.3149410	1.8392290	3.3187990
C	0.6688190	3.1341530	2.6363050
H	0.2344740	2.0141870	4.4000960
H	-0.6487310	1.4760980	2.9461370
O	0.5573280	2.9659520	1.2424070
H	1.6915530	3.4313490	2.9003860
H	-0.0200830	3.9180890	2.9777230
C	0.8088740	4.1437120	0.5168910
C	0.7245080	3.8360850	-0.9557730
H	0.0667370	4.9120600	0.7712500
H	1.8071590	4.5332610	0.7531930
O	1.8200680	3.0265480	-1.3142830
H	0.7430830	4.7737810	-1.5262570
H	-0.2221360	3.3224760	-1.1723590
C	1.8315650	2.6873250	-2.6828700
C	3.0678630	1.8760980	-2.9716950
H	0.9371450	2.1046860	-2.9417960
H	1.8391470	3.5961330	-3.2982680
O	2.9491750	0.6280880	-2.3385880
H	3.9520250	2.4114810	-2.6022210

H	3.1700770	1.7442360	-4.0568670
H	4.3045640	-0.3273890	-3.5635740
H	4.9566970	0.2868620	-2.0231410
H	-0.9495190	-1.2816200	-1.8980140
N	-3.4930550	-1.0836830	0.2679780
F	-1.5191330	-0.5138140	-1.6788690
C	-4.4670610	-0.1550000	-0.1568850
Cs	0.9516880	0.1814830	-0.0581660
N	-3.5212810	-2.3882060	-0.1798820
O	-1.6580900	-2.0149710	0.9271440
H	-3.9270660	1.3409990	1.2828470
C	-4.5866960	1.0815570	0.4691150
C	-2.4259280	-2.8974000	0.2280880
C	-2.3330280	-0.8255910	0.9235340
Cl	0.3454590	-2.6055780	-1.9674160
C	-5.3062000	-0.5034770	-1.2091850
H	-5.1869430	-1.4660680	-1.6836440
C	-5.5569750	1.9685190	0.0259200
O	-1.9039890	0.1789210	1.4363900
C	-6.2719310	0.3938180	-1.6328720
C	-1.9496820	-4.2825710	0.0603100
H	-5.6521740	2.9312480	0.5116570
C	-6.4026870	1.6328660	-1.0209390
H	-2.7033730	-4.8449430	-0.4843000
H	-1.7816310	-4.7392120	1.0364120
H	-1.0149800	-4.2672490	-0.5023590
H	-6.9212820	0.1219510	-2.4548440
H	-7.1568800	2.3311720	-1.3589130

Cartesian coordinates for the structures of the Figure 4 in solution

4-1 $G = -2010.659582$ a.u.

N	1.9305820	-1.1180510	-1.0395980
C	2.9233100	-0.2139330	-0.7694100
Cs	-0.6176570	0.2519030	-0.0448320
N	2.1171630	-2.3009810	-0.4397810
O	1.6286830	-1.5907380	-4.0117030
H	1.9328900	1.2763640	-1.9654100
C	2.7832780	1.0811610	-1.3200550
C	1.2989900	-3.2503370	-0.5269720

C	0.8225660	-0.9059360	-3.5551780
Cl	-0.2211390	-3.0969580	-1.4973740
C	4.0580720	-0.4368970	0.0457290
H	4.2109940	-1.4204240	0.4681950
C	3.6872970	2.0900090	-1.0428520
O	-0.0258770	-0.1906050	-3.2157720
C	4.9562980	0.5828600	0.3094830
C	1.4353920	-4.5790680	0.1265110
H	3.5358480	3.0711400	-1.4799630
C	4.7834100	1.8619360	-0.2144570
H	2.3728550	-4.6003660	0.6802980
H	1.4378710	-5.3841290	-0.6116770
H	0.6082630	-4.7668640	0.8163350
H	5.8135400	0.3748550	0.9409180
H	5.4938900	2.6500290	-0.0024740
C	-4.0813450	1.9476600	-1.0774760
C	-2.9409990	2.8255730	-1.5191370
O	-2.0997790	3.0834800	-0.4175200
H	-3.3448090	3.7650920	-1.9174300
H	-2.3805320	2.3296700	-2.3235690
C	-1.0209370	3.9324670	-0.7431510
C	-0.1812710	4.1647140	0.4849320
H	-1.3940580	4.8950240	-1.1151400
H	-0.4031340	3.4796870	-1.5313750
H	-0.8131710	4.5230010	1.3075270
H	0.5679590	4.9363910	0.2647750
O	0.4501510	2.9585670	0.8381100
C	1.2846370	3.0701710	1.9713260
C	1.9461570	1.7435200	2.2286120
H	0.6949970	3.3776390	2.8443370
H	2.0633160	3.8227330	1.7937250
O	0.9713030	0.8049380	2.6443890
H	2.7079490	1.8663390	3.0092000
H	2.4485380	1.3996130	1.3179850
C	1.5102470	-0.4937760	2.7853130
C	0.4492870	-1.4187110	3.3189470
H	2.3564820	-0.4785080	3.4841510
H	1.8781430	-0.8658870	1.8191700
O	-0.5329290	-1.6150330	2.3252080
H	-0.0043780	-0.9877210	4.2203280
H	0.9102630	-2.3782400	3.5860740

C	-1.6356490	-2.3720210	2.7635550
C	-2.5581150	-2.6125390	1.5988110
H	-1.3020190	-3.3423320	3.1542920
H	-2.1662230	-1.8423500	3.5646390
O	-3.1148110	-1.3847830	1.1759700
H	-3.3548480	-3.3014370	1.9079610
H	-2.0000900	-3.0769390	0.7759260
C	-3.9536000	-1.5371290	0.0525420
C	-4.5800680	-0.2115410	-0.2886200
H	-3.3793030	-1.9126280	-0.8056800
H	-4.7504090	-2.2606760	0.2684380
O	-3.5851300	0.6653570	-0.7670990
H	-5.0600830	0.2115750	0.6025400
H	-5.3501440	-0.3651220	-1.0554170
H	-4.8207730	1.8832390	-1.8860750
H	-4.5681530	2.3895540	-0.1992140

4-TS₁ **$G = -2010.653213$ a.u.** $\square \nu_{\min} = 174.7i \text{ cm}^{-1}$

N	2.0762600	-0.8915100	-0.9798400
C	2.9261850	0.1625660	-0.6923990
Cs	-0.7016000	0.1795220	-0.1043430
N	2.5266490	-2.0714010	-0.5168960
O	2.1718240	-1.7057210	-3.4599570
H	1.7768410	1.5282950	-1.8954880
C	2.6209750	1.4313840	-1.2248960
C	1.8684320	-3.1361430	-0.6049070
C	1.4130100	-0.9546360	-2.9799930
Cl	0.2179130	-3.1791060	-1.3158260
C	4.0486730	0.0759500	0.1566090
H	4.3157010	-0.8858090	0.5710020
C	3.3810920	2.5449720	-0.9099000
O	0.4987760	-0.2059230	-2.9920680
C	4.7983840	1.1997810	0.4621900
C	2.3305680	-4.4693210	-0.1336290
H	3.1121770	3.5038960	-1.3389090
C	4.4743220	2.4496660	-0.0554770
H	3.3205670	-4.3627780	0.3063710
H	2.3817430	-5.1765180	-0.9639630
H	1.6427050	-4.8789730	0.6093580
H	5.6536820	1.0963920	1.1207170

H	5.0665130	3.3218400	0.1889770
C	-4.2460040	1.4540690	-1.3527490
C	-3.1624320	2.4137890	-1.7669910
O	-2.4425990	2.8208020	-0.6243730
H	-3.6219160	3.2817660	-2.2568210
H	-2.4916620	1.9316810	-2.4919630
C	-1.4404890	3.7691580	-0.9191080
C	-0.6989180	4.1189120	0.3437100
H	-1.8895870	4.6781620	-1.3392240
H	-0.7359290	3.3648850	-1.6588960
H	-1.4103410	4.4206060	1.1230560
H	-0.0291950	4.9649480	0.1414010
O	0.0431430	2.9988660	0.7616410
C	0.7976060	3.2295390	1.9315870
C	1.5941290	1.9956570	2.2573810
H	0.1312860	3.4863930	2.7651060
H	1.4936710	4.0633320	1.7731750
O	0.7176980	0.9506240	2.6347660
H	2.2853250	2.2222860	3.0794840
H	2.1865230	1.7011240	1.3853510
C	1.4009780	-0.2709770	2.8253120
C	0.4346750	-1.3015230	3.3436100
H	2.2118370	-0.1434560	3.5539700
H	1.8488410	-0.6137720	1.8816590
O	-0.4890520	-1.6243020	2.3268880
H	-0.0919370	-0.9061540	4.2211790
H	0.9891300	-2.1989740	3.6458730
C	-1.5344800	-2.4569740	2.7706200
C	-2.4136700	-2.8142790	1.6030090
H	-1.1288320	-3.3823880	3.2002580
H	-2.1212960	-1.9463750	3.5443920
O	-3.0606850	-1.6543260	1.1224780
H	-3.1569900	-3.5529170	1.9301110
H	-1.8057250	-3.2650910	0.8090080
C	-3.8882810	-1.9284350	0.0135750
C	-4.5987570	-0.6710190	-0.4095160
H	-3.2910110	-2.3193070	-0.8215340
H	-4.6369980	-2.6867060	0.2776150
O	-3.6596230	0.2450330	-0.9258350
H	-5.1216170	-0.2313960	0.4488660
H	-5.3433600	-0.9234820	-1.1755230

H	-4.9124010	1.2702680	-2.2050700
H	-4.8364740	1.8964700	-0.5410110

4-2 $G = -2010.658810$ a.u.

N	2.8089710	-0.6019840	-0.9690370
C	3.8614810	0.1969650	-0.4521970
Cs	-1.1057760	0.0259240	-0.2438050
N	3.2570200	-1.7871800	-1.5311210
O	1.0194450	-0.6989220	-2.4126960
H	2.5335540	1.3021930	0.8045740
C	3.5642460	1.1700230	0.5044140
C	2.5862210	-2.8355590	-1.4045570
C	1.6701500	0.0414520	-1.6705600
Cl	1.1218270	-2.9640880	-0.4151580
C	5.1890340	-0.0010410	-0.8277800
H	5.4280100	-0.7659650	-1.5524740
C	4.5762100	1.9440570	1.0477440
O	1.4760900	1.2284850	-1.3695100
C	6.1951180	0.7780750	-0.2716910
C	2.9673350	-4.1201400	-2.0519440
H	4.3312480	2.6970630	1.7878950
C	5.8994010	1.7573110	0.6639400
H	3.9174120	-3.9912730	-2.5657370
H	2.2008030	-4.4077460	-2.7733690
H	3.0458570	-4.9133400	-1.3078430
H	7.2207980	0.6135690	-0.5791570
H	6.6873200	2.3610200	1.0957270
C	-2.8176210	3.3479660	-1.4163260
C	-1.3603340	3.5718000	-1.1097390
O	-1.0974020	3.1839590	0.2223730
H	-1.1324620	4.6372040	-1.2455500
H	-0.7296900	2.9978180	-1.8015670
C	0.2397150	3.4627950	0.5986420
C	0.4924150	2.9091360	1.9750790
H	0.4034940	4.5484810	0.6166000
H	0.9345160	3.0077980	-0.1157610
H	-0.2396770	3.3011960	2.6923560
H	1.4939880	3.2206120	2.3009400
O	0.4131180	1.5020450	1.9247440
C	0.7890810	0.8704410	3.1245310

C	0.6456150	-0.6174580	2.9484270
H	0.1553910	1.2128010	3.9525740
H	1.8343560	1.1037120	3.3671360
O	-0.7237450	-0.9313460	2.7947600
H	1.0564760	-1.1264450	3.8293120
H	1.2151580	-0.9452830	2.0662870
C	-0.9640680	-2.3198990	2.7673880
C	-2.4249660	-2.5683760	2.5040380
H	-0.6909830	-2.7712980	3.7300860
H	-0.3584860	-2.8005050	1.9884210
O	-2.7359710	-2.1792450	1.1836400
H	-3.0325920	-1.9981740	3.2176090
H	-2.6378680	-3.6359080	2.6445610
C	-4.0948260	-2.3744490	0.8620650
C	-4.3692660	-1.8327870	-0.5155890
H	-4.3379010	-3.4445800	0.8820480
H	-4.7343810	-1.8624420	1.5915290
O	-4.2700660	-0.4258710	-0.4948640
H	-5.3783100	-2.1374240	-0.8220250
H	-3.6556870	-2.2568470	-1.2351710
C	-4.5976630	0.1584200	-1.7375000
C	-4.4401440	1.6531370	-1.6449960
H	-3.9450670	-0.2340070	-2.5289990
H	-5.6355790	-0.0782110	-2.0045550
O	-3.0767240	1.9615420	-1.4794470
H	-5.0228190	2.0389730	-0.7990290
H	-4.8262510	2.1084380	-2.5662620
H	-3.0615310	3.8184950	-2.3772400
H	-3.4351860	3.8114780	-0.6371750

4-TS₂ **G= -2010.627381 a.u.** $\square \nu_{\min}= 425.2i \text{ cm}^{-1}$

N	-1.4347550	2.2076040	-0.5077110
C	-2.5865950	1.4527870	-0.2392340
Cs	0.4702810	-0.4340450	0.0465470
N	-1.3437040	3.4442130	0.0955630
O	0.1244890	3.1752290	-1.8233780
H	-2.5821350	0.2800590	-2.0496380
C	-3.0889140	0.4659530	-1.1085230
C	-0.1735910	3.9048200	0.0222950
C	-0.6176340	2.1693910	-1.7259260

C1	1.3527420	2.8174290	0.6404000
C	-3.2693030	1.6895650	0.9708630
H	-2.8898250	2.4566860	1.6448720
C	-4.2433840	-0.2387500	-0.7718640
O	-0.6912130	1.1753930	-2.4503970
C	-4.4210670	0.9752680	1.2885710
C	0.2427050	5.3243030	0.1102780
H	-4.6232310	-0.9849380	-1.4737640
C	-4.9216160	0.0023450	0.4220940
H	-0.6229270	5.9645770	-0.0978880
H	1.0219310	5.5038850	-0.6413580
H	0.6604930	5.5409660	1.1023140
H	-4.9357630	1.1896170	2.2274660
H	-5.8283300	-0.5514150	0.6700910
C	2.6083600	-0.7850470	3.3327500
C	3.3966300	0.0588320	2.3636390
O	3.4232230	-0.5643170	1.1041200
H	4.4244160	0.1824010	2.7553240
H	2.9399870	1.0647720	2.2881570
C	4.1411060	0.1756390	0.1455860
C	4.1837100	-0.5835900	-1.1564780
H	5.1780390	0.3484390	0.4910630
H	3.6650250	1.1626650	-0.0139910
H	4.6040250	-1.5933790	-0.9875580
H	4.8533100	-0.0483830	-1.8560100
O	2.8882600	-0.6706020	-1.6856480
C	2.8149220	-1.3316900	-2.9230060
C	1.3822370	-1.3551140	-3.3909470
H	3.2004960	-2.3649930	-2.8321840
H	3.4268100	-0.8033170	-3.6779370
O	0.6214070	-2.1959070	-2.5516170
H	1.3543010	-1.7286180	-4.4324750
H	0.9670160	-0.3296120	-3.3783630
C	-0.7353880	-2.2231220	-2.9233470
C	-1.5171550	-3.0894130	-1.9670100
H	-0.8471170	-2.6308770	-3.9464700
H	-1.1447560	-1.1954830	-2.9145060
O	-1.5267880	-2.4797550	-0.7035620
H	-1.0671550	-4.0987750	-1.9098900
H	-2.5490690	-3.1973750	-2.3530610
C	-2.3295010	-3.1075890	0.2583880

C	-2.3251950	-2.2733140	1.5153100
H	-3.3723100	-3.1953700	-0.1019330
H	-1.9553190	-4.1259890	0.4772390
O	-1.0419060	-2.2840210	2.0946940
H	-3.0719620	-2.6812290	2.2230880
H	-2.6279720	-1.2375700	1.2654610
C	-0.9785160	-1.5347950	3.2813930
C	0.4321560	-1.5397780	3.8133960
H	-1.3017380	-0.4902580	3.0996490
H	-1.6541490	-1.9630140	4.0459080
O	1.2572170	-0.7996800	2.9515980
H	0.7924100	-2.5824100	3.8960090
H	0.4349730	-1.0967570	4.8273100
H	2.7198680	-0.3584810	4.3474530
H	3.0164700	-1.8132810	3.3479300

4-3 $G = -2010.706734$ a.u.

N	-2.9938140	-1.2309410	0.0041160
C	-3.2305670	0.1417690	-0.2118660
Cs	0.6636700	0.0664030	-0.0284990
N	-3.5157870	-2.1866620	-0.8427700
O	-2.2949340	-3.1388500	0.7215640
H	-2.9001230	0.6961070	1.8350330
C	-3.1576940	1.0437910	0.8455390
C	-3.0557990	-3.2879470	-0.3935490
C	-2.2095900	-1.8033790	0.9576710
Cl	-0.2570260	-2.5702410	-1.7826970
C	-3.5556920	0.5746560	-1.4944310
H	-3.5908110	-0.1432950	-2.3019910
C	-3.4404650	2.3822950	0.6133580
O	-1.5712370	-1.3050030	1.8535530
C	-3.8387060	1.9148190	-1.7060670
C	-3.2341590	-4.6386440	-0.9502390
H	-3.3998780	3.0804390	1.4402070
C	-3.7889170	2.8231030	-0.6553610
H	-3.9321370	-4.5918270	-1.7823010
H	-3.6066130	-5.3245240	-0.1890140
H	-2.2655510	-4.9927360	-1.3071440
H	-4.1019530	2.2485620	-2.7016700
H	-4.0183480	3.8671510	-0.8269250

C	3.3705140	0.0981220	-2.8980390
C	3.2599910	-1.2695740	-2.2800570
O	3.4630600	-1.1643080	-0.8832740
H	4.0236470	-1.9240510	-2.7209060
H	2.2707840	-1.6983360	-2.4859400
C	3.3326160	-2.4125790	-0.2328160
C	3.5719710	-2.2265330	1.2415050
H	4.0711350	-3.1220430	-0.6283860
H	2.3306580	-2.8272450	-0.4060420
H	4.5155600	-1.6902700	1.4046050
H	3.6458140	-3.2109040	1.7212580
O	2.4969260	-1.4992710	1.7929310
C	2.6432870	-1.2299020	3.1665240
C	1.3967420	-0.5501250	3.6666370
H	3.5192830	-0.5913470	3.3387940
H	2.7837540	-2.1654040	3.7238840
O	1.2956140	0.7341240	3.0845820
H	1.4481570	-0.4636960	4.7601000
H	0.5178380	-1.1522010	3.4073940
C	0.1009090	1.3879000	3.4496610
C	0.0697220	2.7614440	2.8335450
H	0.0403620	1.4869900	4.5416330
H	-0.7641340	0.8046450	3.1074100
O	-0.0597600	2.6348510	1.4371210
H	0.9889370	3.3059990	3.0830120
H	-0.7831330	3.3187340	3.2447880
C	-0.1071640	3.8667690	0.7579900
C	-0.2022750	3.6079550	-0.7222180
H	-0.9851810	4.4445960	1.0763180
H	0.7904760	4.4585220	0.9775440
O	1.0150410	3.0719530	-1.1911350
H	-0.4267310	4.5515660	-1.2372560
H	-1.0270730	2.9099540	-0.9219020
C	1.0046880	2.8758790	-2.5889620
C	2.2728230	2.1821810	-3.0089940
H	0.1399330	2.2648150	-2.8815150
H	0.9285150	3.8420700	-3.1047140
O	2.2624320	0.8733790	-2.4958190
H	3.1461170	2.7335190	-2.6373700
H	2.3188630	2.1627110	-4.1057860
H	3.3820470	-0.0024410	-3.9908620

H	4.3040270	0.5821120	-2.5835560
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Cartesian coordinates for the structures of the Figure 5 in solution

5-1 $G = -2111.134091$ a.u.

Cs	0.9885970	0.0273980	0.1520650
C	4.3445590	2.1627800	0.3617400
C	3.1586290	3.0729840	0.5351080
O	2.2865120	2.9182550	-0.5575350
H	3.5161090	4.1095840	0.5968920
H	2.6399250	2.8417140	1.4758760
C	1.1641020	3.7813320	-0.4633870
C	0.2244930	3.5209800	-1.6081880
H	1.4939050	4.8279420	-0.5013170
H	0.6332010	3.6051130	0.4768940
H	0.7222610	3.6919830	-2.5718830
H	-0.6195080	4.2121650	-1.5119700
O	-0.2297510	2.1897470	-1.5330770
C	-1.3957780	1.9481990	-2.2788270
C	-1.8303120	0.5321600	-2.0164860
H	-1.2072630	2.0959090	-3.3506870
H	-2.1944540	2.6268580	-1.9560640
O	-0.8374050	-0.3581140	-2.4833400
H	-2.7862340	0.3392640	-2.5215150
H	-1.9809670	0.3979630	-0.9352460
C	-1.1929560	-1.7080290	-2.2986640
C	-0.0260230	-2.5859360	-2.6651870
H	-2.0591980	-1.9648340	-2.9233390
H	-1.4693110	-1.8916450	-1.2519210
O	0.9694850	-2.4494020	-1.6741890
H	0.3694250	-2.2945600	-3.6459100
H	-0.3597210	-3.6301120	-2.7210110
C	2.1330950	-3.1960640	-1.9400850
C	3.0846740	-3.0494070	-0.7828100
H	1.8845850	-4.2585600	-2.0622550
H	2.6084370	-2.8452130	-2.8644370
O	3.5624850	-1.7240200	-0.7331590
H	3.9198440	-3.7499850	-0.9127160
H	2.5684640	-3.3039620	0.1531890
C	4.4322810	-1.5010220	0.3539440

C	4.9750500	-0.0994290	0.2733700
H	3.9014390	-1.6459720	1.3058040
H	5.2698490	-2.2099340	0.3232910
O	3.9299200	0.8188450	0.4933230
H	5.4220760	0.0640760	-0.7147540
H	5.7590320	0.0275570	1.0310390
H	5.0983540	2.3985660	1.1237340
H	4.7910090	2.3219390	-0.6272890
F	-2.8490670	1.9796350	2.0421920
C	-1.7129660	2.5392930	1.3252400
O	-2.0303940	3.4403650	0.5850450
O	-0.6779440	1.9672460	1.6419530
C	-4.4315030	-0.9835770	-0.3213210
N	-3.4876110	-1.5196120	0.3211940
Cl	-4.8977310	0.6860180	-0.0648000
C	-5.2088390	-1.7106340	-1.3617240
N	-2.7824570	-0.8583450	1.2466980
C	-1.7162780	-1.4877540	1.8734040
H	-3.0286360	0.0944770	1.5130950
H	-5.1192680	-1.2069720	-2.3265010
H	-6.2682140	-1.7374130	-1.1009120
H	-4.8300940	-2.7278150	-1.4444440
C	-1.0651930	-0.8213340	2.9174390
C	-1.2485060	-2.7356570	1.4555920
C	0.5415940	-2.6184670	3.0745540
C	-0.1258050	-3.2870240	2.0567820
H	-1.7621330	-3.2610530	0.6631720
H	0.2262530	-4.2549040	1.7205250
C	0.0541120	-1.3863060	3.5031190
H	1.4147910	-3.0566900	3.5402530
H	0.5521450	-0.8553230	4.3052210
H	-1.4192870	0.1536960	3.2243880

5-TS₁ **G= -2111.119051 a.u.** $\square$ **v_{min}= 372i cm⁻¹**

Cs	0.9482120	0.0141240	0.0727830
C	4.2216130	2.2409850	0.3436410
C	3.0324140	3.1483960	0.5267570
O	2.1159050	2.9470400	-0.5177850
H	3.3918690	4.1949010	0.5311400
H	2.5532600	2.9571490	1.5069900

C	1.0696070	3.8885920	-0.5081780
C	0.0775940	3.5610100	-1.5951170
H	1.4665020	4.9066940	-0.6840130
H	0.5632050	3.8860640	0.4729220
H	0.5684160	3.6119000	-2.5857590
H	-0.7274400	4.3188050	-1.5730590
O	-0.4460210	2.2776810	-1.3790450
C	-1.5451820	1.9720360	-2.2005830
C	-1.9191140	0.5293000	-1.9894740
H	-1.2907930	2.1405730	-3.2639870
H	-2.4096340	2.6080070	-1.9370240
O	-0.8793390	-0.2991150	-2.4574540
H	-2.8618800	0.3168520	-2.5283720
H	-2.1040350	0.3526720	-0.9121300
C	-1.2175310	-1.6630740	-2.4455520
C	-0.0069270	-2.4818710	-2.8150380
H	-2.0269570	-1.8672410	-3.1729330
H	-1.5825430	-1.9676980	-1.4457840
O	0.9443200	-2.3868900	-1.7846160
H	0.4166170	-2.1136720	-3.7684300
H	-0.3141230	-3.5347880	-2.9605080
C	2.1181120	-3.1181500	-2.0179470
C	3.0380740	-2.9728830	-0.8324390
H	1.8869130	-4.1908080	-2.1602130
H	2.6288770	-2.7561500	-2.9303000
O	3.4910630	-1.6448160	-0.7472590
H	3.8923220	-3.6656720	-0.9525400
H	2.4969590	-3.2573670	0.0911390
C	4.3488190	-1.4202880	0.3427060
C	4.8786400	-0.0104360	0.2789590
H	3.8150480	-1.5799800	1.3010230
H	5.2031430	-2.1225610	0.3152360
O	3.8288870	0.8987580	0.4890520
H	5.3425160	0.1588820	-0.7105550
H	5.6623370	0.1167520	1.0492830
H	4.9904030	2.5009360	1.0953130
H	4.6571970	2.4048680	-0.6597200
F	-2.8867680	1.3376140	2.3479000
C	-1.6521700	2.5078400	1.2695350
O	-2.4146870	3.1506780	0.6674510
O	-0.6241320	2.1091310	1.6740820

C	-4.2707260	-1.0680290	-0.2211410
N	-3.2890110	-1.5418340	0.4225970
Cl	-4.7726580	0.6197300	-0.0507010
C	-5.0670030	-1.8585200	-1.2048750
N	-2.5737320	-0.8285330	1.2938750
C	-1.5050360	-1.4691720	1.8941440
H	-2.8512060	0.2070070	1.7319690
H	-4.9970740	-1.4170160	-2.2114500
H	-6.1309620	-1.8710280	-0.9254540
H	-4.6873580	-2.8877190	-1.2278770
C	-0.8380720	-0.8014320	2.9466440
C	-1.0132350	-2.7199100	1.4705330
C	0.8193770	-2.5745090	3.0610940
C	0.1362350	-3.2541590	2.0504200
H	-1.5390410	-3.2569780	0.6819320
H	0.4993810	-4.2256100	1.7053940
C	0.3083560	-1.3498190	3.5092020
H	1.7154140	-3.0034160	3.5126950
H	0.8101800	-0.8141470	4.3185180
H	-1.2449030	0.1564310	3.2738420

5-2 $G = -2111.132931$ a.u.

Cs	0.9593950	-0.0093610	0.1395410
C	4.2752650	2.2583300	0.3620710
C	3.0912660	3.1716260	0.5296950
O	2.1780200	2.9490350	-0.5216520
H	3.4462800	4.2100000	0.5133480
H	2.6069420	2.9956240	1.4996380
C	1.1388870	3.9031970	-0.5452870
C	0.1678850	3.5533140	-1.6407460
H	1.5474540	4.9036590	-0.7372450
H	0.6256630	3.9298860	0.4237270
H	0.6878610	3.5153220	-2.6057450
H	-0.6031660	4.3324530	-1.6940260
O	-0.4176540	2.3010010	-1.3627240
C	-1.4481400	1.9628830	-2.2715140
C	-1.8440110	0.5308350	-2.0428730
H	-1.0960410	2.0917080	-3.3020250
H	-2.3169040	2.6120350	-2.1103000
O	-0.7895910	-0.3118540	-2.4678240

H	-2.7576830	0.3136430	-2.6106480
H	-2.0632390	0.3675800	-0.9782010
C	-1.1382800	-1.6794980	-2.4029030
C	0.0623600	-2.5146510	-2.7586080
H	-1.9525300	-1.8947390	-3.1075750
H	-1.4874410	-1.9385710	-1.3954230
O	1.0157510	-2.3966160	-1.7252350
H	0.4899690	-2.1763230	-3.7105900
H	-0.2472180	-3.5617430	-2.8689070
C	2.1896860	-3.1412820	-1.9464050
C	3.0980710	-2.9758910	-0.7576080
H	1.9496870	-4.2056370	-2.0667040
H	2.6959430	-2.7966230	-2.8568290
O	3.5607860	-1.6430320	-0.7060060
H	3.9451560	-3.6674750	-0.8490340
H	2.5511230	-3.2229400	0.1624090
C	4.3925260	-1.4019170	0.4073050
C	4.9241130	0.0036080	0.3305780
H	3.8334980	-1.5448140	1.3431310
H	5.2382130	-2.1014050	0.4098850
O	3.8664840	0.9175330	0.5210260
H	5.3898890	0.1649340	-0.6490410
H	5.6897910	0.1435850	1.1039170
H	5.0345800	2.5139280	1.1122120
H	4.7126820	2.4016120	-0.6334650
F	-3.3178400	1.2224560	2.5256620
C	-1.7050760	2.6330470	1.1313800
O	-2.5448240	3.2031060	0.5854410
O	-0.8061120	2.1292230	1.6609670
C	-4.2564510	-1.0914640	-0.3197050
N	-3.2934470	-1.5254450	0.3673730
Cl	-4.8518320	0.5674790	-0.1757990
C	-4.9727190	-1.9115780	-1.3369230
N	-2.6498980	-0.7835140	1.2865990
C	-1.5774650	-1.4285510	1.8606120
H	-3.1095630	0.3640190	1.9487160
H	-4.9170490	-1.4450380	-2.3237860
H	-6.0303850	-2.0106830	-1.0835750
H	-4.5225930	-2.9025040	-1.3777310
C	-0.9198950	-0.7968580	2.9389730
C	-1.0435440	-2.6507880	1.4042820

C	0.7773470	-2.5208970	2.9959300
C	0.1107710	-3.1748010	1.9650820
H	-1.5425950	-3.1759200	0.6026340
H	0.4939480	-4.1163710	1.5867110
C	0.2324300	-1.3327910	3.4838900
H	1.6744150	-2.9410200	3.4322980
H	0.7121770	-0.8191100	4.3093760
H	-1.3335080	0.1268740	3.3226340

5-TS₂ **G= -2111.117516 a.u. □ v_{min}= 207i cm⁻¹**

Cs	-1.1482310	0.0499500	-0.1754020
C	-3.5896720	3.1627480	-0.5668810
C	-2.1887740	3.6598830	-0.3321740
O	-1.6655240	3.0456590	0.8237300
H	-2.2198690	4.7495810	-0.2043810
H	-1.5561090	3.4417610	-1.2033280
C	-0.3930910	3.5594050	1.1722940
C	0.1377980	2.8179590	2.3694050
H	-0.4742870	4.6254660	1.4213160
H	0.3026480	3.4481910	0.3339620
H	-0.5470760	2.9213610	3.2208180
H	1.1052640	3.2554050	2.6457020
O	0.2938630	1.4567390	2.0410360
C	1.0076970	0.7293570	3.0143440
C	1.0836700	-0.7102220	2.5851810
H	0.5021820	0.8019950	3.9859950
H	2.0233750	1.1289860	3.1103030
O	-0.2210480	-1.2564140	2.5764690
H	1.7226030	-1.2609470	3.2876930
H	1.5448750	-0.7879830	1.5891460
C	-0.2327640	-2.6360340	2.2906850
C	-1.6587470	-3.1092730	2.2155630
H	0.2956610	-3.1925790	3.0750550
H	0.2679100	-2.8313500	1.3338330
O	-2.2621640	-2.5543230	1.0663740
H	-2.2030470	-2.8010490	3.1166950
H	-1.6761570	-4.2051590	2.1594050
C	-3.6220170	-2.8983870	0.9362930
C	-4.1651260	-2.2876890	-0.3269420
H	-3.7359630	-3.9887570	0.8826800

H	-4.1909690	-2.5348840	1.8011440
O	-4.2096800	-0.8848800	-0.1855850
H	-5.1724570	-2.6815980	-0.5120340
H	-3.5281500	-2.5675130	-1.1768430
C	-4.7185660	-0.2386860	-1.3315240
C	-4.8410680	1.2354260	-1.0543520
H	-4.0573110	-0.4080780	-2.1929740
H	-5.7097780	-0.6368330	-1.5832370
O	-3.5543210	1.7931050	-0.9091070
H	-5.4233840	1.3884540	-0.1374140
H	-5.3724100	1.7165120	-1.8851780
H	-4.0494910	3.7418210	-1.3776430
H	-4.1863780	3.3061040	0.3420700
F	4.0469400	0.9603290	-3.0031060
C	2.3254240	1.3906200	-0.2285190
O	3.0029120	1.5504640	0.7245940
O	1.4464140	1.7579710	-0.9388660
C	4.7383000	-0.7127910	0.3632320
N	3.5948320	-1.0218620	-0.0577040
Cl	5.7312720	0.5587760	-0.3386140
C	5.3920760	-1.4225360	1.4989710
N	2.9805530	-0.3040120	-1.0477830
C	1.9077090	-1.0054080	-1.6135040
H	3.7401870	0.4655740	-2.2072700
H	5.5650620	-0.7280790	2.3235450
H	6.3604990	-1.8215480	1.1933780
H	4.7494010	-2.2337530	1.8361160
C	1.2679440	-0.4373390	-2.7280220
C	1.4280880	-2.2348790	-1.1365140
C	-0.3137710	-2.2623350	-2.8129570
C	0.3294780	-2.8447710	-1.7285890
H	1.9372340	-2.7123130	-0.3117600
H	-0.0215930	-3.7939630	-1.3396450
C	0.1774180	-1.0581280	-3.3119110
H	-1.1576460	-2.7511090	-3.2831200
H	-0.2879280	-0.6002480	-4.1769200
H	1.6483950	0.4901550	-3.1308440

5-3 $G_{\text{corr}} = -2111.122122 \text{ a.u.}$

Cs	-1.1361020	0.0894960	-0.1454970
C	-3.2225230	3.3928590	-0.8360590
C	-1.8036830	3.7659150	-0.5007230
O	-1.4354640	3.1708610	0.7213310
H	-1.7342480	4.8594020	-0.4278800
H	-1.1291910	3.4416810	-1.3050260
C	-0.0926520	3.4718890	1.0683610
C	0.2605040	2.7919540	2.3622590
H	0.0281930	4.5563390	1.1901240
H	0.5849090	3.1200780	0.2835500
H	-0.3892330	3.1349640	3.1782890
H	1.2988090	3.0461570	2.6044830
O	0.1303940	1.3992670	2.1973490
C	0.7522760	0.6528630	3.2118010
C	0.6982270	-0.8034250	2.8384610
H	0.2471300	0.8174180	4.1728660
H	1.8038820	0.9474350	3.3059550
O	-0.6517310	-1.2088550	2.7221840
H	1.2106090	-1.3930480	3.6091280
H	1.2280480	-0.9553590	1.8866720
C	-0.7880890	-2.5955230	2.5175630
C	-2.2333150	-2.9172080	2.2462770
H	-0.4575040	-3.1469610	3.4074340
H	-0.1733590	-2.9193010	1.6677780
O	-2.6006770	-2.3869500	0.9904810
H	-2.8639150	-2.4891180	3.0351720
H	-2.3676190	-4.0065590	2.2493190
C	-3.9516220	-2.6275100	0.6684290
C	-4.2724200	-1.9827540	-0.6535130
H	-4.1375840	-3.7070330	0.5955580
H	-4.6077000	-2.2174520	1.4461610
O	-4.2489810	-0.5805410	-0.5075110
H	-5.2666300	-2.3129660	-0.9810470
H	-3.5429510	-2.3019040	-1.4105860
C	-4.5751240	0.0982740	-1.6999690
C	-4.5949840	1.5799260	-1.4352280
H	-3.8414660	-0.1312430	-2.4855160
H	-5.5635050	-0.2165380	-2.0584300
O	-3.2862330	2.0171430	-1.1524890
H	-5.2580080	1.7951160	-0.5883900
H	-4.9867340	2.0981190	-2.3199990

H	-3.5584890	3.9903690	-1.6929680
H	-3.8762270	3.6122220	0.0169220
F	4.0097510	0.2827580	-3.2171220
C	2.3289210	0.9802770	-0.2858030
O	2.8034760	1.3326250	0.7766150
O	1.4540410	1.4254060	-1.0267970
C	4.9439000	-0.4684230	0.2672550
N	3.8261800	-0.9814930	0.0140580
Cl	5.5584250	0.9871110	-0.4899440
C	5.8887800	-1.0808500	1.2425700
N	2.9576450	-0.3498730	-0.8704030
C	1.9470030	-1.2631490	-1.3268480
H	3.6916760	0.1253700	-2.3219330
H	6.0572560	-0.3912070	2.0713570
H	6.8510600	-1.2710160	0.7659060
H	5.4700700	-2.0109510	1.6206440
C	1.2651400	-0.9695820	-2.5086740
C	1.6152930	-2.4174930	-0.6196550
C	-0.0980990	-2.9424460	-2.2354630
C	0.5976080	-3.2471100	-1.0747390
H	2.1660870	-2.6672130	0.2758100
H	0.3527430	-4.1425740	-0.5162780
C	0.2478100	-1.8013560	-2.9513690
H	-0.8829060	-3.5977360	-2.5914930
H	-0.2674310	-1.5621250	-3.8736880
H	1.5357340	-0.0872010	-3.0689000

5-TS₃ G= -2111.090054 a.u. v_{min}= 438i cm⁻¹

Cs	-1.1233280	0.0794010	-0.1656920
C	-4.1001890	-2.3081310	0.9535720
C	-4.4364070	-1.6998770	-0.3818090
O	-4.2860910	-0.2994070	-0.3075090
H	-5.4707260	-1.9567620	-0.6432300
H	-3.7761630	-2.1145780	-1.1562910
C	-4.6442760	0.3516200	-1.5070400
C	-4.4858320	1.8380880	-1.3303370
H	-5.6881640	0.1292980	-1.7619780
H	-4.0121250	0.0044670	-2.3362890
H	-5.0425700	2.1662320	-0.4439630
H	-4.9012990	2.3498100	-2.2080030

O	-3.1180120	2.1440240	-1.1872210
C	-2.8772850	3.5232850	-0.9968430
C	-1.4097120	3.7486080	-0.7494200
H	-3.4564430	3.8897770	-0.1406670
H	-3.1835860	4.0838430	-1.8890250
O	-1.0546260	3.2097960	0.5037460
H	-1.2128000	4.8284990	-0.7688030
H	-0.8131530	3.2834310	-1.5457380
C	0.3005600	3.4778020	0.8259420
C	0.6599800	2.7838850	2.1104970
H	0.4466910	4.5583130	0.9542740
H	0.9543490	3.1215290	0.0245530
O	0.5223350	1.3906160	1.9433610
H	0.0149150	3.1245000	2.9309910
H	1.6996360	3.0331070	2.3554240
C	1.0436890	0.6535720	3.0208000
C	0.8284550	-0.8128570	2.7615040
H	2.1203070	0.8433990	3.1192050
H	0.5491750	0.9456700	3.9567930
O	-0.5603730	-1.0822980	2.7198740
H	1.3040680	-1.3916680	3.5638610
H	1.3069400	-1.0991210	1.8142410
C	-0.8371030	-2.4606650	2.6151900
C	-2.3197620	-2.6617090	2.4519730
H	-0.3094280	-2.8929250	1.7547670
H	-0.5005950	-2.9855460	3.5186730
O	-2.7190750	-2.1620380	1.1938400
H	-2.8577300	-2.1414200	3.2536290
H	-2.5470530	-3.7332630	2.5220390
H	-4.3729990	-3.3711720	0.9432190
H	-4.6781100	-1.8105890	1.7419790
F	4.0702550	-0.5876940	-3.3193000
C	2.4157320	0.7895620	-0.6066290
O	3.1479760	1.3066940	0.2870520
O	1.5093530	1.2944940	-1.2532950
C	4.2767040	-0.1262110	0.6411430
N	3.4641390	-1.0600410	0.3100800
Cl	5.5774290	0.4897550	-0.5881630
C	4.8426180	-0.0075950	2.0122800
N	2.7895400	-0.6211540	-0.8443530
C	1.7761070	-1.4972180	-1.3162490

H	3.8387190	-0.5302150	-2.4054950
H	5.0116840	1.0425320	2.2448630
H	5.8012550	-0.5243080	2.0612710
H	4.1501320	-0.4426020	2.7314330
C	1.1187690	-1.2091500	-2.5144830
C	1.4301920	-2.6423270	-0.6015070
C	-0.2934420	-3.1445480	-2.2133210
C	0.3977840	-3.4556270	-1.0514930
H	1.9810980	-2.8877090	0.2948870
H	0.1386390	-4.3439740	-0.4881560
C	0.0843870	-2.0245590	-2.9468650
H	-1.0944560	-3.7839410	-2.5617800
H	-0.4191170	-1.7905420	-3.8768520
H	1.4198570	-0.3500490	-3.0946240

5-4 $G = -2111.159896$ a.u.

Cs	1.2708920	-0.1165460	-0.2996560
C	4.2433200	2.3854890	0.5409810
C	4.6110340	1.6498630	-0.7192370
O	4.4142230	0.2661450	-0.5229470
H	5.6623460	1.8542120	-0.9571170
H	3.9976350	2.0093880	-1.5566020
C	4.8101990	-0.5055650	-1.6368080
C	4.6394020	-1.9652120	-1.3129020
H	5.8636700	-0.3138240	-1.8754290
H	4.2109730	-0.2425100	-2.5188790
H	5.1801930	-2.2039560	-0.3890820
H	5.0648340	-2.5655840	-2.1269690
O	3.2669900	-2.2518430	-1.1600030
C	3.0251560	-3.5981200	-0.8065750
C	1.5508370	-3.8069840	-0.5909200
H	3.5722250	-3.8495820	0.1100940
H	3.3675130	-4.2647490	-1.6077420
O	1.1379670	-3.1011700	0.5607940
H	1.3641300	-4.8804650	-0.4622060
H	0.9847680	-3.4707830	-1.4698900
C	-0.2248150	-3.3395860	0.8657150
C	-0.5952860	-2.5918230	2.1167240
H	-0.3875170	-4.4103250	1.0417340
H	-0.8581980	-3.0286880	0.0296710

O	-0.5171830	-1.1978960	1.8908140
H	0.0825780	-2.8720330	2.9322330
H	-1.6167040	-2.8701480	2.4050180
C	-0.7583350	-0.4498770	3.0650480
C	-0.5947810	1.0155460	2.7722610
H	-1.7803360	-0.6273320	3.4245260
H	-0.0580210	-0.7548580	3.8520920
O	0.7590720	1.2938530	2.4724960
H	-0.9126870	1.5916340	3.6502110
H	-1.2366340	1.3023940	1.9323060
C	0.9593330	2.6538840	2.1470290
C	2.4272060	2.9107560	1.9402570
H	0.3970740	2.9164870	1.2398890
H	0.5993850	3.2941350	2.9622730
O	2.8573280	2.2557090	0.7656990
H	2.9934760	2.5445220	2.8052860
H	2.5929860	3.9915550	1.8503530
H	4.5130180	3.4435490	0.4312540
H	4.8035420	1.9722450	1.3887430
F	-3.7672700	0.3018290	-2.9011660
C	-2.2425150	-0.7509710	-0.5737870
O	-3.0115180	-1.5657840	0.2000370
O	-1.4286900	-1.1508100	-1.3689460
C	-3.7313500	-0.7598570	1.0189880
N	-3.4752770	0.4804530	0.8611230
Cl	-5.8196700	-0.8996150	-1.3537910
C	-4.6973430	-1.3707170	1.9463570
N	-2.5583540	0.5124780	-0.1704590
C	-2.0739700	1.7352100	-0.6732660
H	-4.4941870	-0.1090990	-2.3911580
H	-4.2078180	-2.0952710	2.5989400
H	-5.4591300	-1.8795800	1.3540710
H	-5.1635100	-0.5880860	2.5399130
C	-1.3565060	1.7735020	-1.8678280
C	-2.3219220	2.9060920	0.0381890
C	-1.0783650	4.1579590	-1.6042340
C	-1.8242580	4.1109740	-0.4348390
H	-2.9181860	2.8665510	0.9386910
H	-2.0304180	5.0199150	0.1162420
C	-0.8557980	2.9865290	-2.3161200
H	-0.6955700	5.1013760	-1.9711410

H	-0.3103510	3.0157800	-3.2509900
H	-1.2378940	0.8714690	-2.4487090

Cartesian coordinates for the structures of the Figure 6 in solution

6-1 $G = -1922.541261$ a.u.

H	1.1232640	-0.4224750	-2.2819170
N	1.7408690	-1.2162120	-1.8283720
F	0.4747650	0.8037660	-2.5530230
Cs	-0.5512000	0.1320720	0.0399480
N	1.3370340	-2.4673360	-1.5847150
C	2.8933050	-0.7978450	-1.1778570
H	2.6383790	1.2002300	-1.8978480
Cl	-0.8712660	-2.0556980	-3.0189300
C	3.2627090	0.5503050	-1.2973850
C	0.2631050	-2.9647970	-2.0174300
C	3.6893500	-1.6502190	-0.4018010
H	3.4189410	-2.6923650	-0.3107760
C	4.3917900	1.0231730	-0.6533850
C	-0.1469210	-4.3710910	-1.7443900
H	-1.1028720	-4.4036890	-1.2177620
C	4.8192400	-1.1567720	0.2351900
H	0.6169870	-4.8525850	-1.1367080
H	4.6612530	2.0675130	-0.7618420
H	-0.2666540	-4.9226500	-2.6787410
C	5.1813590	0.1791150	0.1231200
H	5.4263170	-1.8321440	0.8267550
H	6.0671480	0.5538510	0.6194270
C	-1.7876260	3.0814820	-1.6701660
C	-3.1822390	2.7078840	-1.2452750
O	-3.1802580	1.3832290	-0.7554580
H	-3.8556380	2.7860670	-2.1080360
H	-3.5348280	3.3963630	-0.4669580
C	-4.4263610	0.9663460	-0.2538620
C	-4.3285270	-0.4799510	0.1528980
H	-5.2022080	1.0665410	-1.0240110
H	-4.7161620	1.5788770	0.6089720
H	-3.9574560	-1.0760620	-0.6918400
H	-5.3275330	-0.8489310	0.4183370
O	-3.4572720	-0.5980440	1.2570840

C	-3.3004750	-1.9329790	1.6814940
C	-2.4047330	-1.9755780	2.8909830
H	-2.8661070	-2.5414020	0.8757900
H	-4.2747340	-2.3655710	1.9443000
O	-1.0936960	-1.6259240	2.5119360
H	-2.4214090	-2.9893910	3.3119500
H	-2.7789430	-1.2801480	3.6522650
C	-0.1864560	-1.6199680	3.5926720
C	1.1594240	-1.1472370	3.1106690
H	-0.0877840	-2.6310950	4.0077160
H	-0.5479090	-0.9542330	4.3859040
O	1.0913150	0.2273170	2.8085510
H	1.4632360	-1.7211590	2.2233580
H	1.9041930	-1.3269900	3.8969370
C	2.3295450	0.7362610	2.3502150
C	2.1751750	2.1933880	2.0064140
H	3.0963450	0.6245530	3.1275940
H	2.6623160	0.1851090	1.4617550
O	1.3113930	2.3036580	0.9020120
H	3.1646410	2.6003940	1.7605080
H	1.7738910	2.7496200	2.8637160
C	1.1997050	3.6077820	0.3812770
C	0.3575320	3.5602490	-0.8654980
H	0.7521160	4.2782490	1.1263910
H	2.1934400	3.9955690	0.1199370
O	-0.9719120	3.2141640	-0.5222710
H	0.7597360	2.8173530	-1.5655120
H	0.3754970	4.5479180	-1.3455260
H	-1.8287150	4.0353440	-2.2126730
H	-1.3694010	2.3186750	-2.3401150

6-TS₁ **G= -1922.524824 a.u. □ v_{min}= 216i cm⁻¹**

H	1.0333770	0.0023980	-2.4919720
N	1.8554560	-1.0058870	-1.8041980
F	0.5093980	0.8010550	-2.8329160
Cs	-0.6247780	0.1450620	-0.0058140
N	1.6086160	-2.2922750	-1.8213160
C	3.0287780	-0.6306280	-1.1665220
H	2.7403730	1.4110170	-1.7620460
Cl	-1.3924220	-2.5339180	-1.9792840

C	3.3701010	0.7311160	-1.2017580
C	0.8685530	-3.1985180	-1.9028330
C	3.8517990	-1.5059750	-0.4452100
H	3.6091090	-2.5603950	-0.4084750
C	4.4860120	1.1929610	-0.5304610
C	0.6987150	-4.6423680	-2.0843160
H	0.0168520	-5.0380060	-1.3354000
C	4.9692080	-1.0259990	0.2237870
H	1.6770180	-5.1186390	-2.0038990
H	4.7316080	2.2477060	-0.5770050
H	0.2768840	-4.8321730	-3.0702070
C	5.2961810	0.3227380	0.1956270
H	5.5916290	-1.7207200	0.7754210
H	6.1708460	0.6885250	0.7172150
C	-1.9485580	3.1907090	-1.6517080
C	-3.3128300	2.7391750	-1.2020140
O	-3.2401670	1.3853860	-0.8206440
H	-4.0220240	2.8615510	-2.0306770
H	-3.6538220	3.3552430	-0.3603190
C	-4.4673050	0.8448550	-0.3897830
C	-4.2626440	-0.6046380	-0.0379210
H	-5.2148860	0.9161580	-1.1902260
H	-4.8402440	1.3958850	0.4829890
H	-3.7750460	-1.1263070	-0.8716740
H	-5.2399590	-1.0724280	0.1380920
O	-3.4648100	-0.6949940	1.1262100
C	-3.2212230	-2.0353590	1.5010300
C	-2.3761080	-2.0597050	2.7468250
H	-2.7120050	-2.5692480	0.6878990
H	-4.1707030	-2.5470080	1.7066030
O	-1.0752760	-1.6114380	2.4358960
H	-2.3380240	-3.0862220	3.1339520
H	-2.8241630	-1.4170790	3.5150220
C	-0.2161860	-1.5642790	3.5513030
C	1.1345690	-1.0651810	3.1104150
H	-0.1049540	-2.5654850	3.9872790
H	-0.6254790	-0.8965800	4.3196000
O	1.0398860	0.2966990	2.7604890
H	1.4863420	-1.6568060	2.2532120
H	1.8535160	-1.1983230	3.9293290
C	2.2749100	0.8235930	2.3175390

C	2.0975480	2.2705960	1.9423100
H	3.0263390	0.7499970	3.1145960
H	2.6432020	0.2585430	1.4516540
O	1.2628270	2.3554490	0.8114340
H	3.0843010	2.6978840	1.7213910
H	1.6579750	2.8276040	2.7799250
C	1.1032470	3.6660770	0.3224040
C	0.2275990	3.6306540	-0.9021210
H	0.6549400	4.3084030	1.0912510
H	2.0793070	4.0880050	0.0462240
O	-1.0838700	3.2538060	-0.5354650
H	0.6320670	2.9173070	-1.6315930
H	0.2189820	4.6274530	-1.3624540
H	-2.0330730	4.1802030	-2.1191710
H	-1.5523390	2.4891630	-2.3970150

6-2 $G = -1922.533353$ a.u.

H	-1.2591410	-0.1867910	-2.5602260
N	-2.1367640	0.8510200	-1.9096720
F	-0.6705900	-0.9240920	-2.8768490
Cs	0.6434850	-0.0399640	-0.0869230
N	-1.8814500	2.1113630	-2.0407690
C	-3.1891590	0.5291690	-1.0523000
H	-3.0158580	-1.5369480	-1.5972380
Cl	1.4586400	2.8970810	-1.4887840
C	-3.5500120	-0.8227540	-0.9825900
C	-1.5459520	3.1900910	-2.2188910
C	-3.8724940	1.4551860	-0.2591310
H	-3.6074900	2.5041270	-0.2964450
C	-4.5695870	-1.2290410	-0.1431170
C	-1.1739660	4.5655040	-2.4777930
H	-0.7533100	5.0056010	-1.5757620
C	-4.8922130	1.0302530	0.5831460
H	-2.0415450	5.1259130	-2.8260980
H	-4.8411640	-2.2773900	-0.1096360
H	-0.3961910	4.5562820	-3.2407200
C	-5.2490040	-0.3084480	0.6514880
H	-5.4121450	1.7607510	1.1908710
H	-6.0484430	-0.6309250	1.3052400
C	1.8670870	-3.1310950	-1.8494070

C	3.2535640	-2.6863200	-1.4680480
O	3.2067280	-1.3443760	-1.0456010
H	3.9137260	-2.7875540	-2.3390860
H	3.6430660	-3.3242780	-0.6645510
C	4.4627580	-0.8345020	-0.6581890
C	4.2982220	0.5871720	-0.1930220
H	5.1572320	-0.8562170	-1.5077390
H	4.8845860	-1.4461910	0.1493800
H	3.7688380	1.1792020	-0.9502570
H	5.2930300	1.0274760	-0.0438280
O	3.5774200	0.5975350	1.0227020
C	3.4213790	1.9083280	1.5312930
C	2.6280860	1.8517150	2.8080690
H	2.9078910	2.5388670	0.7953070
H	4.4055930	2.3462400	1.7446420
O	1.3020310	1.4725280	2.5125770
H	2.6401190	2.8427810	3.2796690
H	3.0780440	1.1323920	3.5042310
C	0.4749380	1.4145290	3.6478220
C	-0.9013650	0.9739200	3.2270710
H	0.4075930	2.4023440	4.1221120
H	0.8809150	0.7072200	4.3821090
O	-0.8468580	-0.3663290	2.7964910
H	-1.2689130	1.6211520	2.4181190
H	-1.5888340	1.0730800	4.0772180
C	-2.1082240	-0.8502200	2.3874820
C	-1.9747680	-2.2872010	1.9625710
H	-2.8271610	-0.7852430	3.2146660
H	-2.4962720	-0.2511420	1.5538090
O	-1.2192690	-2.3499110	0.7764580
H	-2.9767060	-2.7043220	1.7989010
H	-1.4846420	-2.8671150	2.7550910
C	-1.0484220	-3.6639470	0.2996390
C	-0.2485240	-3.6306610	-0.9746690
H	-0.5331470	-4.2750210	1.0514890
H	-2.0256650	-4.1224270	0.0951850
O	1.0625250	-3.1919780	-0.6903180
H	-0.7211300	-2.9588690	-1.7009190
H	-0.2240240	-4.6415130	-1.4032300
H	1.9270310	-4.1215420	-2.3190180

H	1.4337130	-2.4319540	-2.5755220
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6-TS₂ **G= -2111.091941 a.u.** **v_{min}= 365i cm⁻¹**

H	-2.0899320	-1.2903370	1.3079470
N	-3.0719660	-1.1804270	-0.0934950
F	-1.3719170	-1.4250120	1.9219760
Cs	0.8753320	-0.0346530	0.0192260
N	-2.2561180	-1.8214570	-0.9423370
C	-3.3296960	0.1876530	-0.4242320
H	-4.2179560	0.5613630	1.4886640
Cl	0.7283230	-2.0322440	-2.6833820
C	-3.9602530	0.9826150	0.5277720
C	-2.1736060	-2.9316390	-1.2916150
C	-2.9713170	0.7134870	-1.6607980
H	-2.4566770	0.0966700	-2.3882680
C	-4.2742330	2.2961770	0.2134670
C	-1.7554930	-4.1777840	-1.8577850
H	-0.8419830	-3.9412260	-2.4212930
C	-3.2814030	2.0350140	-1.9548370
H	-2.5366040	-4.5688820	-2.5078360
H	-4.7807920	2.9086780	0.9485880
H	-1.5310830	-4.8784370	-1.0535190
C	-3.9444680	2.8256460	-1.0278150
H	-3.0065910	2.4390010	-2.9211310
H	-4.1946920	3.8513590	-1.2668600
C	2.0817180	-1.5478240	3.2921710
C	3.3746370	-1.8137010	2.5700290
O	3.1802540	-1.6517150	1.1846150
H	3.7045060	-2.8373420	2.7910900
H	4.1447310	-1.1185600	2.9271180
C	4.3634360	-1.8460820	0.4388310
C	4.0985190	-1.5465560	-1.0113030
H	4.7040540	-2.8848250	0.5370750
H	5.1545240	-1.1856980	0.8156770
H	3.2429000	-2.1264080	-1.3798260
H	4.9840590	-1.8311380	-1.5947480
O	3.8455440	-0.1634750	-1.1566980
C	3.7000660	0.2088610	-2.5138880
C	3.3737510	1.6749460	-2.5888010
H	2.9015840	-0.3779780	-2.9830450

H	4.6384960	0.0258030	-3.0541980
O	2.0930100	1.8875890	-2.0380170
H	3.3897760	1.9889890	-3.6402750
H	4.1218210	2.2614110	-2.0400020
C	1.6489710	3.2177370	-2.1459290
C	0.2951290	3.3222500	-1.4974370
H	1.5667820	3.5079190	-3.2015830
H	2.3532450	3.9009630	-1.6542810
O	0.4349770	3.1606500	-0.1035990
H	-0.3672550	2.5467130	-1.9069610
H	-0.1490840	4.3005750	-1.7231170
C	-0.8054630	3.1915540	0.5674270
C	-0.5732380	3.0710410	2.0487180
H	-1.3275880	4.1345250	0.3587220
H	-1.4487140	2.3702730	0.2223190
O	-0.1459040	1.7613740	2.3444340
H	-1.5078280	3.2933640	2.5803670
H	0.1841470	3.8004430	2.3628000
C	0.2751210	1.6101740	3.6812880
C	0.6196630	0.1681890	3.9335030
H	1.1477750	2.2468110	3.8745070
H	-0.5272310	1.9071680	4.3692460
O	1.7391710	-0.1871190	3.1487480
H	-0.2369650	-0.4662130	3.6845730
H	0.8511870	0.0390650	4.9990800
H	2.2149600	-1.7959620	4.3533950
H	1.2831170	-2.1868960	2.8923950
C	-4.3221170	-2.1906370	0.2463180
O	-4.0583260	-3.3094630	-0.1734680
O	-5.1994710	-1.6360340	0.8522330

6-3 $G = -2111.165754$ a.u.

H	-1.3160650	-1.2016660	1.6201290
N	-3.0811820	-0.9526180	-1.3327990
F	-1.5858930	-1.7501340	0.8679080
Cs	0.8894990	0.0096380	-0.2243160
N	-1.8749570	-0.9926230	-2.0008000
C	-3.5952850	0.2716610	-0.8716560
H	-4.8865620	-0.6127590	0.5988850
Cl	1.6393210	0.0869260	-3.4350630

C	-4.5286840	0.3076380	0.1625160
C	-1.6394970	-2.2359860	-2.1685290
C	-3.1257830	1.4514320	-1.4448720
H	-2.3983500	1.4037460	-2.2443850
C	-4.9898260	1.5363790	0.6127950
C	-0.4677240	-2.8477600	-2.8190680
H	0.1944450	-2.0572450	-3.1772170
C	-3.6006440	2.6685330	-0.9796270
H	-0.7881510	-3.4719970	-3.6545460
H	-5.7184040	1.5634110	1.4136200
H	0.0610610	-3.4842730	-2.1066620
C	-4.5307840	2.7197900	0.0498800
H	-3.2393010	3.5833130	-1.4328520
H	-4.9008270	3.6729310	0.4051740
C	2.2532520	-3.0156360	1.7622610
C	3.6086370	-2.5644900	1.2895370
O	3.4630490	-1.5712010	0.3045680
H	4.1509940	-3.4292040	0.8846300
H	4.1773000	-2.1707120	2.1415080
C	4.7058810	-1.0473430	-0.1207490
C	4.4785010	0.0820620	-1.0867470
H	5.2930220	-1.8310760	-0.6157610
H	5.2706210	-0.6877970	0.7485310
H	3.8463180	-0.2387750	-1.9236710
H	5.4507050	0.3965950	-1.4891620
O	3.8684270	1.1589610	-0.4004980
C	3.6792950	2.2815530	-1.2400760
C	2.9892490	3.3657360	-0.4590000
H	3.0798130	2.0001920	-2.1138610
H	4.6501350	2.6580130	-1.5887550
O	1.6772950	2.9458030	-0.1499090
H	2.9590180	4.2801240	-1.0649370
H	3.5411790	3.5799000	0.4650150
C	0.9347760	3.9056770	0.5607730
C	-0.4416940	3.3559840	0.8199230
H	0.8465120	4.8297850	-0.0251840
H	1.4273750	4.1461680	1.5116620
O	-0.3559880	2.3042310	1.7606290
H	-0.8756410	2.9921390	-0.1203780
H	-1.0907630	4.1524280	1.2060830
C	-1.6138940	1.7411870	2.0520140

C	-1.4604950	0.7578330	3.1794470
H	-2.3219720	2.5191780	2.3642940
H	-2.0374140	1.2490370	1.1651020
O	-0.7160580	-0.3704650	2.7273180
H	-2.4452530	0.4318790	3.5298850
H	-0.9225660	1.2269760	4.0078090
C	-0.1719050	-1.1616290	3.7795800
C	0.5104630	-2.3679380	3.1933150
H	0.5451110	-0.5529220	4.3374510
H	-0.9719250	-1.4840980	4.4544770
O	1.6023200	-1.9421100	2.4125910
H	-0.1943170	-2.9534770	2.5900740
H	0.8538540	-3.0035890	4.0196560
H	2.3901380	-3.8524460	2.4582720
H	1.6466700	-3.3709220	0.9187420
C	-3.5437700	-2.2120440	-1.0804590
O	-2.6089280	-3.0360630	-1.6541970
O	-4.5303750	-2.5989860	-0.5222120

Cartesian coordinates for the structures of the Figure 7 in solution

1_N G= -418.957452 a.u.

N	-1.3758580	-0.4578140	0.0000000
N	-1.7053640	0.7701400	0.0000000
C	0.0000000	-0.6937040	0.0000000
C	-2.1081860	1.8475600	0.0000000
C	0.4001320	-2.0362150	0.0000000
C	0.9853600	0.2994260	0.0000000
H	-0.3674550	-2.8002220	0.0000000
H	0.7054170	1.3457040	0.0000000
C	-2.6313260	3.2030440	0.0000000
C	1.7410580	-2.3694170	0.0000000
C	2.3294440	-0.0492360	0.0000000
H	-1.7965530	3.9043780	0.0000000
H	-3.2355900	3.3779590	0.8903690
C	2.7205680	-1.3795530	0.0000000
H	-3.2355900	3.3779590	-0.8903690
H	2.0281700	-3.4141480	0.0000000
H	3.0779570	0.7344080	0.0000000

H	3.7698920	-1.6437480	0.0000000
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7-TS₁ **G= -837.883494 a.u.** $\square$ **v_{min}= 345i cm⁻¹**

N	1.5103780	0.1402870	-0.5098140
N	0.9534850	1.2426860	-0.1175520
C	2.9014820	0.0633870	-0.2923020
C	0.2438540	2.0929890	0.1684850
C	3.5969540	0.8884190	0.5911770
C	3.5911710	-0.9268540	-0.9939100
H	3.0725670	1.6602130	1.1409770
H	3.0457250	-1.5432300	-1.6976350
C	-0.7078500	3.1268550	0.5081520
C	4.9629240	0.7179740	0.7669170
C	4.9513180	-1.0948870	-0.8019340
H	-0.5304750	3.4996060	1.5160080
H	-1.6921730	2.6534130	0.4532680
C	5.6468090	-0.2744250	0.0792900
H	-0.6571010	3.9427660	-0.2117390
H	5.4943080	1.3656190	1.4532980
H	5.4752680	-1.8656050	-1.3532800
H	6.7111960	-0.4048300	0.2235760
N	-1.6735060	0.0775330	-0.4904730
N	-0.8802050	-0.8340500	0.0230320
C	-3.0166960	-0.1675710	-0.2529850
C	0.2484200	-1.1797110	0.1811700
C	-3.9318090	0.7293170	-0.8318610
C	-3.5345400	-1.2146300	0.5273710
H	-3.5411360	1.5297000	-1.4499230
H	-2.8531050	-1.9194980	0.9867020
C	1.0934690	-2.2536650	0.7226370
C	-5.2935060	0.5855870	-0.6383370
C	-4.9019280	-1.3480920	0.7127290
H	0.4414820	-2.9714400	1.2194600
H	1.8168340	-1.8670580	1.4408810
C	-5.7970610	-0.4542070	0.1379150
H	1.6370080	-2.7667880	-0.0709890
H	-5.9733680	1.2910350	-1.1020140
H	-5.2734500	-2.1656780	1.3200160
H	-6.8627160	-0.5663400	0.2879460

7_N G= -838.014485 a.u.

N	-1.2619140	-0.0226100	-0.0906070
N	-0.6407270	-1.1945860	0.3848310
C	-2.6768780	-0.1054930	-0.1694260
C	0.6305890	-1.1522530	0.3331230
C	-3.3978500	-0.9961280	0.6203610
C	-3.3442320	0.7126390	-1.0764540
H	-2.8715030	-1.6416540	1.3086100
H	-2.7721630	1.3675660	-1.7215280
C	1.4256070	-2.3303910	0.7941800
C	-4.7798700	-1.0467830	0.5103450
C	-4.7266350	0.6659670	-1.1668430
H	0.7431990	-3.0553410	1.2305850
H	2.1679410	-2.0256680	1.5332550
C	-5.4514480	-0.2142150	-0.3740840
H	1.9565870	-2.8010730	-0.0326770
H	-5.3359730	-1.7411190	1.1277550
H	-5.2363240	1.3068170	-1.8752010
H	-6.5299260	-0.2578270	-0.4534840
N	1.2618330	0.0227410	-0.0910480
N	0.6407390	1.1948870	0.3844490
C	2.6768520	0.1055600	-0.1695860
C	-0.6305810	1.1525190	0.3330440
C	3.3441940	-0.7126710	-1.0765830
C	3.3978590	0.9960570	0.6202410
H	2.7720030	-1.3674550	-1.7216980
H	2.8716400	1.6417920	1.3083960
C	-1.4255470	2.3307170	0.7940720
C	4.7265780	-0.6662590	-1.1668170
C	4.7799400	1.0464620	0.5103900
H	-0.7431670	3.0556050	1.2306180
H	-2.1680450	2.0259580	1.5329690
C	5.4514680	0.2137930	-0.3739160
H	-1.9563480	2.8015700	-0.0328010
H	5.2362580	-1.3071540	-1.8751390
H	5.3360650	1.7407210	1.1278690
H	6.5299640	0.2571230	-0.4531840

Cartesian coordinates for the structures of the Figure 8 in solution

8-1 **$G = -1650.279039$ a.u.**

C	-0.6329760	3.3920150	1.0224280
O	-1.4515070	3.9434120	0.4246080
O	0.2240920	2.9105210	1.6341020
C	-0.5569420	2.7372600	-2.3903300
C	-1.6469880	1.7301040	-2.1453540
O	-1.2034190	0.4540450	-2.5501340
H	-2.5381670	2.0216680	-2.7166090
H	-1.9264010	1.7222360	-1.0816440
C	-2.2157590	-0.5230850	-2.4044250
C	-1.6552670	-1.8850520	-2.7131240
H	-3.0512830	-0.3044640	-3.0822670
H	-2.5987590	-0.5194410	-1.3780900
H	-1.1491130	-1.8823570	-3.6873140
H	-2.4827230	-2.6059670	-2.7541430
O	-0.7548900	-2.2334870	-1.6906200
C	-0.2260120	-3.5346250	-1.7993200
C	0.6803210	-3.7859810	-0.6241060
H	0.3290460	-3.6417130	-2.7403490
H	-1.0385630	-4.2730210	-1.7913830
O	1.8372420	-2.9802540	-0.7511770
H	0.9634420	-4.8472140	-0.6127190
H	0.1646740	-3.5447060	0.3147850
C	2.6964850	-3.1225060	0.3637650
C	3.8960820	-2.2342170	0.1760990
H	3.0412960	-4.1628980	0.4395300
H	2.1540140	-2.8607830	1.2808950
O	3.5094270	-0.8816000	0.3103930
H	4.3343350	-2.3997150	-0.8163170
H	4.6522630	-2.4816270	0.9323150
C	4.5617010	0.0169380	0.0625390
C	4.0631560	1.4261070	0.2359630
H	5.3863120	-0.1559870	0.7672620
H	4.9472130	-0.1176840	-0.9559990
O	3.1089160	1.7156100	-0.7603140
H	4.9140050	2.1158530	0.1598800
H	3.6184170	1.5461590	1.2334730
C	2.6983330	3.0629950	-0.7297050
C	1.6395950	3.2895160	-1.7742200
H	2.3109510	3.3210850	0.2629230

H	3.5486480	3.7243140	-0.9443110
O	0.4862380	2.5425770	-1.4555060
H	2.0184040	2.9872640	-2.7580530
H	1.4013760	4.3610640	-1.8108620
H	-0.9638910	3.7505970	-2.2912380
H	-0.1722720	2.6152210	-3.4098690
F	0.2253170	-2.0885390	2.1321940
Cs	0.5283560	-0.2031350	0.1040720
N	-2.1732310	1.2488670	1.9017060
N	-1.3451200	0.7159700	2.7313470
C	-3.0079450	0.3086440	1.2835210
C	-0.5856680	0.3078270	3.4884400
C	-4.1019180	0.8142380	0.5670430
C	-2.8020240	-1.0778040	1.3206540
H	-4.2548390	1.8867010	0.5457020
H	-1.9357660	-1.4972940	1.8291000
C	0.4209000	-0.2627370	4.3603520
C	-4.9782100	-0.0430500	-0.0738310
C	-3.6920740	-1.9226260	0.6693050
H	0.6234590	-1.2539070	3.9379230
H	0.0626330	-0.3213600	5.3873070
C	-4.7842150	-1.4215070	-0.0266990
H	1.3247400	0.3463240	4.3201010
H	-5.8255610	0.3675580	-0.6102560
H	-3.5145420	-2.9911570	0.7042750
H	-5.4745930	-2.0906170	-0.5239240

8-TS₁ **$G = -1650.247814$ a.u.** $\square \nu_{\min} = 359.8i \text{ cm}^{-1}$

C	1.2897590	-2.0502540	1.8647790
O	1.8186240	-2.8043440	1.0727060
O	0.1803000	-2.0168720	2.4269620
C	0.0025700	-3.0976900	-2.3879460
C	1.2773410	-2.3047120	-2.2732330
O	1.0351870	-0.9596780	-2.6116540
H	2.0298680	-2.7417160	-2.9578050
H	1.6661440	-2.3834180	-1.2399870
C	2.1916580	-0.1717460	-2.4931180
C	1.8681550	1.2643320	-2.8165490
H	2.9791970	-0.5300260	-3.1846480
H	2.5962700	-0.2361340	-1.4650480

H	1.3966470	1.3284590	-3.8161750
H	2.8109560	1.8445640	-2.8465530
O	1.0097110	1.7701460	-1.8323070
C	0.6792040	3.1260860	-1.9880090
C	-0.2228430	3.5563310	-0.8599830
H	0.1758260	3.2905600	-2.9601010
H	1.5948660	3.7484670	-1.9721950
O	-1.4850560	2.9398580	-0.9981780
H	-0.3313640	4.6582400	-0.8986180
H	0.2080370	3.2724940	0.1189960
C	-2.3378310	3.2715820	0.0765380
C	-3.6383280	2.5235210	-0.0549090
H	-2.5563180	4.3576050	0.0656560
H	-1.8350750	3.0119840	1.0270470
O	-3.4356500	1.1596650	0.2299460
H	-4.0418800	2.6441880	-1.0781970
H	-4.3725440	2.9526400	0.6532770
C	-4.5846640	0.3744920	0.0692710
C	-4.2576060	-1.0560490	0.4135670
H	-5.3962760	0.7278840	0.7339300
H	-4.9520570	0.4279650	-0.9730800
O	-3.3544750	-1.5656030	-0.5300180
H	-5.1911700	-1.6505420	0.4204590
H	-3.8256680	-1.1012890	1.4332650
C	-2.9813750	-2.8972230	-0.2796190
C	-2.1043710	-3.3931040	-1.3999410
H	-2.4347960	-2.9756100	0.6800410
H	-3.8769220	-3.5442430	-0.2153350
O	-0.8997940	-2.6797990	-1.3977960
H	-2.6307570	-3.2676110	-2.3656670
H	-1.9178980	-4.4738130	-1.2510260
H	0.2419470	-4.1706160	-2.2624300
H	-0.4374510	-2.9607740	-3.3946110
F	-0.1396600	2.0759990	1.8726180
Cs	-0.6110490	0.0532010	-0.0120860
N	2.1449000	-0.8428040	2.2687610
N	1.4451330	-0.0321010	3.0393800
C	3.0550560	-0.2104420	1.3721290
C	0.3591570	-0.0817490	3.4884790
C	4.1310600	-0.9341820	0.8538510
C	2.8383500	1.1256970	1.0124150

H	4.2608510	-1.9764470	1.1408060
H	1.9459290	1.6467550	1.3905610
C	-0.9165960	0.3248030	4.0206640
C	5.0099160	-0.3010960	-0.0228640
C	3.7414160	1.7469490	0.1510810
H	-1.1062920	1.2671060	3.4677030
H	-0.8896170	0.4429830	5.1107640
C	4.8271730	1.0400510	-0.3673280
H	-1.6549890	-0.4378090	3.7379330
H	5.8542160	-0.8597420	-0.4305820
H	3.5801620	2.7910480	-0.1246530
H	5.5306130	1.5305840	-1.0424870

8-2 $G = -1650.324677$ a.u.

C	1.9350850	-1.0245860	-2.1738070
O	1.2782810	-0.1342880	-2.6559270
O	1.7891950	-2.3420360	-2.4739710
C	-1.4969450	3.8899420	-0.7056600
C	-0.0938140	3.6448880	-0.2188900
O	-0.1360570	2.8999940	0.9760230
H	0.4001450	4.6105450	-0.0468820
H	0.4761470	3.1058150	-0.9889850
C	1.1538620	2.6461270	1.4915710
C	1.0399780	1.8268690	2.7485880
H	1.6667330	3.5918060	1.7121860
H	1.7552020	2.0952170	0.7567060
H	0.3412390	2.3004220	3.4507690
H	2.0269820	1.7716670	3.2276400
O	0.5929690	0.5423230	2.3988810
C	0.5107820	-0.3527850	3.4850030
C	0.0287710	-1.6860430	2.9811520
H	-0.1759810	0.0402070	4.2459370
H	1.5008820	-0.4775680	3.9434150
O	-1.3288820	-1.5704330	2.5943290
H	0.1236970	-2.4255870	3.7885330
H	0.6260540	-2.0108020	2.1194150
C	-1.8126110	-2.7815910	2.0458780
C	-3.2422550	-2.5947610	1.6146950

H	-1.7775880	-3.5741620	2.8065270
H	-1.1830840	-3.0758850	1.1963640
O	-3.2827270	-1.7723380	0.4675960
H	-3.8231230	-2.1363220	2.4254120
H	-3.6810590	-3.5748540	1.3864980
C	-4.5859010	-1.5086880	0.0131300
C	-4.5055400	-0.6682950	-1.2336480
H	-5.1075750	-2.4461270	-0.2223880
H	-5.1614690	-0.9797570	0.7835420
O	-4.0051420	0.6078020	-0.9032760
H	-5.5057660	-0.5804730	-1.6776420
H	-3.8491270	-1.1579360	-1.9658690
C	-3.8917960	1.4534330	-2.0242640
C	-3.3845680	2.8004200	-1.5832870
H	-3.2028600	1.0217040	-2.7628620
H	-4.8702930	1.5797390	-2.5060970
O	-2.0449450	2.6776430	-1.1682540
H	-4.0052900	3.1771820	-0.7606090
H	-3.4598030	3.5046480	-2.4225400
H	-1.4741260	4.6295740	-1.5169530
H	-2.1058640	4.2946670	0.1124990
F	0.5764480	-2.3836810	-0.0267520
Cs	-0.8523320	-0.0646160	-0.2005100
N	2.9590120	-0.9841490	-1.2787660
N	3.3693330	-2.2577370	-0.9422730
C	3.4780430	0.1467370	-0.6229050
C	2.6277840	-3.0166800	-1.6487830
C	3.5608820	1.3661050	-1.2892910
C	3.9305060	0.0206220	0.6864030
H	3.2056720	1.4467390	-2.3068630
H	3.8432050	-0.9361540	1.1831450
C	2.5874800	-4.4880840	-1.6524940
C	4.1142100	2.4587380	-0.6373670
C	4.4866000	1.1207430	1.3211110
H	1.6042450	-4.8043020	-1.3013830
H	3.3532510	-4.8682230	-0.9810010
C	4.5831190	2.3414810	0.6645880
H	2.7473080	-4.8794000	-2.6576320
H	4.1878180	3.4052890	-1.1582560
H	4.8483750	1.0205220	2.3368410

H	5.0242710	3.1951330	1.1631100
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Cartesian coordinates for the structures of the Figure 9 in solution

9-1 $G = -2434.085516$ a.u.

N	-1.9028610	0.3185290	-1.7270080
H	-0.8940470	0.0674980	-2.2703780
N	-2.9726410	-0.4915950	-1.7035860
Cs	0.7728160	-0.0473620	0.1079600
C	-2.1319140	1.6466370	-1.4265500
O	-2.2997920	-0.3229440	1.3144340
F	0.2776550	-0.0062110	-2.7193850
C	-2.8664900	-1.7465180	-1.7098260
C	-1.0832890	2.5632180	-1.6237450
H	-0.1642260	2.2109410	-2.0797080
C	-3.4376980	-0.4854880	1.2958760
Cl	-1.2943440	-2.5628170	-1.6576650
C	-3.3372160	2.1189480	-0.8858100
H	-4.1571500	1.4275300	-0.7502120
S	-4.9800060	-0.7154540	1.3151910
C	-4.0361330	-2.6687900	-1.7445680
C	-1.2480940	3.8960860	-1.2857820
H	-4.9482840	-2.0757210	-1.7338090
H	-4.0241960	-3.3421260	-0.8851770
C	-3.4793960	3.4563890	-0.5532480
C	-2.4405110	4.3595660	-0.7409200
H	-4.0142370	-3.2821010	-2.6471130
H	-0.4346170	4.5895630	-1.4684460
H	-4.4223900	3.7986390	-0.1433390
H	-2.5630370	5.4032520	-0.4846550
C	3.7435740	1.6929640	-1.7959170
C	3.2986640	0.4901690	-2.5853300
O	3.2853200	-0.6388770	-1.7317000
H	4.0120260	0.3253020	-3.4045380
H	2.2987550	0.6517910	-3.0035050
C	2.7893930	-1.7905120	-2.3872930
C	2.8744850	-2.9613540	-1.4440460
H	3.4028440	-2.0097910	-3.2718470
H	1.7540270	-1.6185760	-2.7070210
H	3.8865690	-3.0373940	-1.0268910

H	2.6514640	-3.8856050	-1.9926440
O	1.9388870	-2.7872900	-0.4015610
C	1.9692370	-3.8090860	0.5605500
C	0.9018580	-3.5432460	1.5907940
H	2.9530910	-3.8501090	1.0454750
H	1.7746380	-4.7820290	0.0896140
O	1.2423060	-2.3921220	2.3327430
H	0.8192190	-4.4108850	2.2585700
H	-0.0644130	-3.3998330	1.0883690
C	0.2933920	-2.0957850	3.3298460
C	0.6999630	-0.8383740	4.0536120
H	0.2293450	-2.9225740	4.0497430
H	-0.6979780	-1.9524950	2.8812930
O	0.5626970	0.2564890	3.1810540
H	1.7386380	-0.9249080	4.3959230
H	0.0544500	-0.7064180	4.9322470
C	0.8759070	1.4923010	3.7781930
C	0.8061800	2.5766570	2.7336570
H	0.1629090	1.7134360	4.5831300
H	1.8859430	1.4628590	4.2054950
O	1.8825260	2.4188560	1.8387200
H	0.8638960	3.5557170	3.2270610
H	-0.1521830	2.5228480	2.1973280
C	1.9354760	3.4432810	0.8681450
C	3.0681040	3.1637640	-0.0852580
H	0.9895630	3.4908790	0.3131820
H	2.0984260	4.4133190	1.3556610
O	2.7343970	2.0507490	-0.8755900
H	3.9893410	2.9699170	0.4791640
H	3.2307860	4.0452750	-0.7199340
H	3.9316000	2.5267080	-2.4849060
H	4.6742300	1.4686990	-1.2591660

9-TS₁ **G= -2434.066465 a.u.** **v_{min}= 319i cm⁻¹**

H	1.8205520	0.7256920	-1.0254750
N	2.8912960	0.8101980	-0.2674080
F	0.9597990	0.5953650	-1.7136510
C	3.6383900	-0.3922980	-0.3601080
Cs	-1.2598010	0.1088300	0.0067100
N	3.6450750	1.9160660	-0.5624020

S	3.3093760	1.6722020	2.5055010
H	1.8405950	-1.5407010	-0.5648570
C	2.9201050	-1.5821930	-0.4892310
C	3.1265400	3.0576290	-0.5212100
C	2.2869030	0.8093060	1.6060220
Cl	1.4256140	3.3427690	-0.1249900
C	5.0274650	-0.4347240	-0.2659120
H	5.5749310	0.4905990	-0.1601610
C	3.5882620	-2.7956280	-0.5258500
O	1.3190200	0.1276300	1.5821120
C	5.6839170	-1.6557040	-0.3105870
C	3.8860930	4.3064940	-0.8048170
H	3.0235210	-3.7146060	-0.6341680
C	4.9740580	-2.8417710	-0.4395660
H	4.9088960	4.0459550	-1.0658060
H	3.8823020	4.9471170	0.0782590
H	3.4196420	4.8565260	-1.6226970
H	6.7641970	-1.6792890	-0.2383820
H	5.4946880	-3.7898040	-0.4748370
C	-2.5748040	-1.0208060	3.5517420
C	-1.1985220	-1.5722770	3.2808500
O	-1.2326470	-2.3046550	2.0755610
H	-0.9094230	-2.2266930	4.1135260
H	-0.4638600	-0.7601110	3.2136140
C	-0.0019630	-2.9395580	1.7865280
C	-0.1171100	-3.6444640	0.4599860
H	0.2321750	-3.6744940	2.5674780
H	0.8088140	-2.2026610	1.7440140
H	-0.9849510	-4.3157930	0.4587910
H	0.7890240	-4.2424390	0.2974840
O	-0.2482060	-2.6783930	-0.5562960
C	-0.2329520	-3.2122900	-1.8607560
C	-0.2731670	-2.0786390	-2.8518980
H	-1.0919810	-3.8797920	-2.0049050
H	0.6892070	-3.7868950	-2.0199060
O	-1.5261420	-1.4264550	-2.7547890
H	-0.1421540	-2.4850320	-3.8633740
H	0.5349290	-1.3682900	-2.6451300
C	-1.6010630	-0.2855210	-3.5829080
C	-2.9921720	0.2878290	-3.4945130
H	-1.3996850	-0.5632400	-4.6259390

H	-0.8535220	0.4556160	-3.2721480
O	-3.1763370	0.8785010	-2.2247160
H	-3.7277820	-0.5114600	-3.6452500
H	-3.1301190	1.0428030	-4.2784470
C	-4.4992220	1.2870920	-1.9821440
C	-4.5704190	1.9516840	-0.6310720
H	-4.8250170	2.0030520	-2.7483970
H	-5.1751060	0.4233830	-2.0060600
O	-4.3516500	0.9922820	0.3789970
H	-5.5587290	2.4125130	-0.5059770
H	-3.8134850	2.7452710	-0.5715960
C	-4.3975210	1.5486850	1.6733230
C	-4.1913150	0.4626910	2.6980220
H	-3.6185110	2.3143960	1.7876200
H	-5.3713590	2.0251650	1.8453780
O	-2.8701040	-0.0108650	2.6104880
H	-4.9013790	-0.3540620	2.5191400
H	-4.3823980	0.8757760	3.6973060
H	-2.6111760	-0.6072580	4.5674980
H	-3.3125130	-1.8289000	3.4764650

9-2 $G = -2434.071077$ a.u.

H	1.7415220	0.4710760	-1.2677070
N	2.8936200	0.7694150	-0.3409700
F	0.9972860	0.2171300	-1.9021120
C	3.6575530	-0.4570860	-0.2493760
Cs	-1.2809510	0.1201160	-0.0315810
N	3.6715270	1.7882570	-0.8834310
S	3.1539270	2.0941100	2.0756810
H	1.8856140	-1.6534120	-0.3832240
C	2.9625570	-1.6605640	-0.2730920
C	3.1510270	2.9024220	-1.1237310
C	2.3058460	1.0539500	1.0977680
Cl	1.4512670	3.2792700	-0.8593240
C	5.0370660	-0.4444000	-0.0930030
H	5.5554850	0.5028230	-0.0603180
C	3.6581530	-2.8544920	-0.1465990
O	1.2982670	0.3888720	1.2764860
C	5.7217530	-1.6450120	0.0241680
C	3.9386610	4.0476730	-1.6565480

H	3.1177420	-3.7933870	-0.1727030
C	5.0388740	-2.8531020	-0.0019600
H	4.9518290	3.7148210	-1.8666990
H	3.9617800	4.8411970	-0.9079190
H	3.4729800	4.4440730	-2.5585340
H	6.7973240	-1.6337440	0.1461740
H	5.5787670	-3.7866730	0.0895240
C	-2.3140420	-0.1546250	3.7377570
C	-0.9422360	-0.7325660	3.5027570
O	-1.0366830	-1.7274170	2.5029880
H	-0.5861730	-1.1763350	4.4417190
H	-0.2300620	0.0450200	3.1997680
C	0.1819230	-2.4209480	2.3133840
C	0.0059080	-3.4119110	1.1930050
H	0.4499040	-2.9633490	3.2295150
H	0.9855140	-1.7172830	2.0703580
H	-0.8478760	-4.0709570	1.3951450
H	0.9130950	-4.0257840	1.1183510
O	-0.2026950	-2.7091140	-0.0117000
C	-0.2825730	-3.5372020	-1.1468780
C	-0.4167640	-2.6695840	-2.3711150
H	-1.1421170	-4.2143580	-1.0640290
H	0.6301410	-4.1414920	-1.2378410
O	-1.6718170	-2.0166790	-2.3343770
H	-0.3507560	-3.2984780	-3.2683820
H	0.3930600	-1.9310690	-2.3960550
C	-1.8465350	-1.1234770	-3.4115280
C	-3.2450960	-0.5627120	-3.3604320
H	-1.7118290	-1.6501020	-4.3654450
H	-1.1051830	-0.3151200	-3.3608530
O	-3.3574080	0.3227910	-2.2672100
H	-3.9623530	-1.3851720	-3.2521650
H	-3.4622660	-0.0311420	-4.2955400
C	-4.6757440	0.7529160	-2.0299580
C	-4.6823480	1.7109870	-0.8663910
H	-5.0754830	1.2635120	-2.9160890
H	-5.3199660	-0.1056970	-1.8045030
O	-4.3675340	1.0152270	0.3179880
H	-5.6763140	2.1693080	-0.7826030
H	-3.9518760	2.5116500	-1.0443930
C	-4.3667350	1.8513580	1.4541760

C	-4.0485420	1.0345690	2.6802940
H	-3.6206570	2.6488360	1.3390540
H	-5.3514610	2.3199540	1.5784550
O	-2.7170320	0.5918240	2.6073360
H	-4.7319310	0.1784010	2.7415520
H	-4.1958890	1.6590240	3.5715340
H	-2.2915880	0.4931710	4.6227650
H	-3.0276560	-0.9681110	3.9172090

9-TS₂ **$G = -2434.067279$ a.u. □ $v_{\min} = 26i$ cm⁻¹**

F	-1.1035040	-0.0389210	-1.9468610
CS	1.1726380	0.0103780	-0.0229720
C	-2.0914690	-0.9331250	1.1201280
O	-1.4349600	0.0835920	1.2791190
S	-2.3373950	-2.2521950	2.1072900
C	-2.6795590	-3.0592990	-0.9874420
N	-3.3956040	-2.0754620	-0.6940140
Cl	-0.9136370	-3.0550560	-0.9824760
C	-3.2594730	-4.3753130	-1.3712860
N	-2.8105950	-0.8868740	-0.2698370
C	-3.8006860	0.1748620	-0.2278940
H	-1.7646010	-0.4004540	-1.2890480
H	-3.0204420	-5.1034330	-0.5942900
H	-2.8313350	-4.7241770	-2.3105490
H	-4.3385080	-4.2758150	-1.4569690
C	-3.3710810	1.4871540	-0.3896190
C	-5.1408850	-0.1015120	0.0054660
C	-5.6371540	2.2536370	-0.0995990
C	-6.0548240	0.9405240	0.0636570
H	-5.4524940	-1.1272130	0.1385230
H	-7.0993580	0.7221500	0.2459080
C	-4.2933030	2.5209510	-0.3218440
H	-6.3540680	3.0632080	-0.0531990
H	-3.9575680	3.5425420	-0.4506250
H	-2.3211020	1.6894450	-0.5556190
C	2.1802100	0.3676230	3.7367050
C	0.8457050	1.0146800	3.4683470
O	1.0005900	1.9535590	2.4219370
H	0.5188690	1.5245840	4.3841370
H	0.0893640	0.2664250	3.2007990

C	-0.1511890	2.7529250	2.2330460
C	0.0772770	3.6554490	1.0496200
H	-0.3232910	3.3725900	3.1234000
H	-1.0282940	2.1219890	2.0620090
H	1.0109170	4.2179900	1.1790160
H	-0.7526670	4.3706950	0.9778280
O	0.1467060	2.8772910	-0.1251960
C	0.3483540	3.6468960	-1.2863160
C	0.4538490	2.7293510	-2.4761480
H	1.2663280	4.2416060	-1.1929780
H	-0.4949700	4.3344780	-1.4356290
O	1.6675500	2.0058720	-2.3884550
H	0.4464270	3.3299190	-3.3949120
H	-0.3978290	2.0404220	-2.4960180
C	1.8235250	1.0794490	-3.4405320
C	3.1942460	0.4583250	-3.3459140
H	1.7327420	1.5889500	-4.4087730
H	1.0460410	0.3061470	-3.3870260
O	3.2442810	-0.4005240	-2.2276060
H	3.9456610	1.2505600	-3.2441780
H	3.4055710	-0.1074720	-4.2621290
C	4.5330170	-0.8977770	-1.9605910
C	4.4734970	-1.8135750	-0.7647190
H	4.9098490	-1.4616030	-2.8241850
H	5.2247210	-0.0707510	-1.7581820
O	4.1871630	-1.0602910	0.3911060
H	5.4397300	-2.3229720	-0.6541630
H	3.7017680	-2.5787390	-0.9238520
C	4.1130650	-1.8571930	1.5532530
C	3.8379550	-0.9816510	2.7488430
H	3.3149760	-2.6045350	1.4515680
H	5.0615170	-2.3880330	1.7071980
O	2.5476100	-0.4383620	2.6361380
H	4.5859300	-0.1804140	2.8021390
H	3.9178000	-1.5902660	3.6593320
H	2.1112690	-0.2478180	4.6422460
H	2.9390420	1.1435350	3.8965400

9-3 **$G = -2434.070889$ a.u.**

F	1.2805350	0.2608950	1.9951760
Cs	-1.0787490	0.2501190	-0.0071290
C	1.9081650	-0.3745530	-1.0711030
O	1.7305810	0.8299200	-1.0710470
S	1.2757580	-1.5479130	-2.1028600
C	2.2775990	-3.0287460	0.5380760
N	3.1049530	-2.1725710	0.1579480
Cl	0.6623220	-2.6771690	1.1633920
C	2.5773080	-4.4869100	0.4994660
N	2.7832470	-0.8157820	0.1154620
C	4.0073170	-0.0283650	0.1556700
H	1.8465270	-0.2013190	1.3501430
H	1.9230420	-4.9578400	-0.2362000
H	2.3851320	-4.9427920	1.4702880
H	3.6144860	-4.6297790	0.2081040
C	3.9675580	1.2432560	0.7109930
C	5.1930780	-0.5231380	-0.3729500
C	6.3091460	1.5272970	0.2208030
C	6.3397630	0.2564240	-0.3349950
H	5.2098820	-1.5135930	-0.8032390
H	7.2614260	-0.1340580	-0.7475700
C	5.1191640	2.0164640	0.7395290
H	7.2066830	2.1315750	0.2490880
H	5.0824020	3.0070880	1.1744910
H	3.0380950	1.6238930	1.1087380
C	-3.4083940	-2.6825590	0.4161430
C	-3.7930210	-2.0138270	1.7120190
O	-2.7741090	-1.1150190	2.0812630
H	-3.9217310	-2.7792150	2.4881890
H	-4.7440780	-1.4815520	1.5873110
C	-3.0195990	-0.4350160	3.2912450
C	-1.9138990	0.5628830	3.5305110
H	-3.0502990	-1.1502240	4.1232080
H	-3.9831990	0.0870190	3.2444430
H	-0.9373660	0.0793730	3.3929990
H	-1.9765840	0.9256740	4.5647750
O	-2.0556010	1.6424030	2.6316950
C	-1.0594810	2.6296570	2.8156700
C	-1.2221270	3.7032990	1.7685800
H	-0.0628400	2.1802920	2.7258230
H	-1.1576570	3.0754930	3.8137930

O	-0.8418030	3.1733230	0.5234040
H	-0.5831000	4.5572890	2.0284770
H	-2.2642630	4.0459450	1.7389910
C	-0.8923730	4.0891670	-0.5465840
C	-0.4316040	3.3915680	-1.8019610
H	-0.2295970	4.9399790	-0.3425700
H	-1.9145600	4.4662140	-0.6768600
O	-1.4178610	2.4625250	-2.2062590
H	0.5177550	2.8765720	-1.6113460
H	-0.2754900	4.1375570	-2.5921390
C	-0.9913360	1.6776030	-3.3047200
C	-2.0998750	0.7353630	-3.7021960
H	-0.7500240	2.3258450	-4.1572690
H	-0.0955110	1.1003380	-3.0390810
O	-2.2841120	-0.1994720	-2.6658700
H	-1.8090330	0.2188680	-4.6254660
H	-3.0288090	1.2902680	-3.8853810
C	-3.1768440	-1.2431260	-2.9494010
C	-3.0424150	-2.2851650	-1.8667730
H	-4.2081170	-0.8705470	-2.9961870
H	-2.9287930	-1.7071410	-3.9128700
O	-3.4858100	-1.7488020	-0.6364770
H	-1.9886540	-2.5876440	-1.7893500
H	-3.6413010	-3.1661240	-2.1313940
H	-4.0883560	-3.5233630	0.2259440
H	-2.3877320	-3.0802140	0.5000590

9-TS₃ **G= -2434.054389 a.u.** **$\nu_{\min}$ = 353i cm⁻¹**

F	-1.3039550	0.5944030	-1.8974760
Cs	1.0299220	0.2686340	0.0127770
C	-1.9099970	-0.8333070	1.0044000
O	-1.7926870	0.2657760	1.5070590
S	-1.1199550	-2.2834460	1.4793430
C	-1.9996690	-3.0149790	-0.5591700
N	-3.0267490	-2.2735710	-0.5356600
Cl	-0.4588100	-2.5070560	-1.5840930
C	-2.0892930	-4.5029490	-0.5948660
N	-2.7511170	-0.9453520	-0.2175990
C	-3.9332550	-0.1125170	-0.2214640
H	-1.8075160	-0.0603630	-1.4070800

H	-2.2426920	-4.8257620	-1.6255520
H	-2.9234090	-4.8204520	0.0269620
H	-1.1640220	-4.9404320	-0.2291280
C	-3.7971580	1.2723120	-0.2034350
C	-5.1984880	-0.6853690	-0.2746720
C	-6.1956000	1.5082980	-0.2601160
C	-6.3221360	0.1279470	-0.2946590
H	-5.2894010	-1.7602090	-0.3085860
H	-7.3037050	-0.3266910	-0.3386010
C	-4.9290120	2.0730870	-0.2155060
H	-7.0751860	2.1387390	-0.2769190
H	-4.8148140	3.1495230	-0.2001600
H	-2.8131940	1.7156430	-0.1837560
C	3.5918850	-2.2214640	-1.0992150
C	3.9319840	-1.2141180	-2.1682590
O	2.8589300	-0.3119280	-2.2953680
H	4.0985510	-1.7389210	-3.1177610
H	4.8512100	-0.6788370	-1.8998020
C	3.0375160	0.6621070	-3.2967070
C	1.8301460	1.5659880	-3.3168240
H	3.1445180	0.1790860	-4.2762620
H	3.9407630	1.2519810	-3.0973150
H	0.9145670	0.9605510	-3.3449630
H	1.8610790	2.1894250	-4.2195890
O	1.8403030	2.3831390	-2.1650870
C	0.7407930	3.2712330	-2.1258010
C	0.7857370	4.0627690	-0.8432580
H	-0.2001250	2.7102850	-2.1802260
H	0.7880630	3.9608370	-2.9785260
O	0.4684780	3.2087330	0.2295900
H	0.0578950	4.8825800	-0.9012240
H	1.7848480	4.4947080	-0.7052190
C	0.4935350	3.8365110	1.4916000
C	0.1383850	2.8242020	2.5508620
H	-0.2363220	4.6560740	1.5176300
H	1.4900470	4.2520000	1.6874070
O	1.2022510	1.9029730	2.6896320
H	-0.7826810	2.2990180	2.2719440
H	-0.0294730	3.3448420	3.5027960
C	0.8990940	0.8730020	3.6107950
C	2.0861790	-0.0486090	3.7341700

H	0.6782950	1.3050400	4.5957510
H	0.0210970	0.3083310	3.2708920
O	2.2524480	-0.7307900	2.5144860
H	1.8962670	-0.7657290	4.5428660
H	2.9899920	0.5240020	3.9773780
C	3.2506700	-1.7184170	2.5182620
C	3.1988300	-2.4530710	1.2017690
H	4.2404820	-1.2669110	2.6612740
H	3.0726030	-2.4356210	3.3300110
O	3.6059670	-1.5882840	0.1618210
H	2.1721840	-2.8028430	1.0231630
H	3.8612860	-3.3272330	1.2459190
H	4.3271710	-3.0364620	-1.1197490
H	2.5991990	-2.6460590	-1.3006510

9-4 $G = -2434.137243$ a.u.

F	0.2887150	0.4755820	-2.7541790
Cs	-0.6655160	-0.2501180	0.0702740
C	1.7183170	2.1209690	1.0295700
O	1.6317990	1.4560910	2.0422820
S	0.9407070	3.6760040	0.7326450
C	1.5781540	3.6645910	-0.8901380
N	2.3017230	2.6506980	-1.1746860
Cl	-1.4138550	2.5000450	-1.7525150
C	1.2802840	4.7495060	-1.8594320
N	2.3933220	1.7861640	-0.1182400
C	3.1231390	0.5780040	-0.2913790
H	-0.2947330	1.2325600	-2.5264830
H	1.8083740	4.5408940	-2.7873310
H	1.5935530	5.7179210	-1.4676380
H	0.2066570	4.7631940	-2.0520380
C	3.8168150	0.0188160	0.7761510
C	3.1452060	-0.0178060	-1.5468170
C	4.5526660	-1.7657560	-0.6643050
C	3.8690380	-1.1869730	-1.7250200
H	2.5898510	0.4353010	-2.3569010
H	3.8929240	-1.6498770	-2.7038860
C	4.5224480	-1.1589580	0.5833400
H	5.1160870	-2.6783690	-0.8124830
H	5.0671580	-1.5926280	1.4127590

H	3.8039930	0.5042820	1.7407220
C	0.8290360	-3.0072400	-1.8099330
C	1.3983220	-3.5222740	-0.5134200
O	1.2634720	-2.5322060	0.4792850
H	2.4584800	-3.7700850	-0.6519410
H	0.8599390	-4.4308540	-0.2155570
C	1.6297740	-2.9802750	1.7626530
C	1.4205470	-1.8748260	2.7648460
H	2.6893480	-3.2697840	1.7689190
H	1.0272080	-3.8541570	2.0405140
H	1.9465570	-0.9691370	2.4424400
H	1.8364440	-2.1951890	3.7300970
O	0.0404620	-1.6069800	2.9000580
C	-0.2094050	-0.6112890	3.8718600
C	-1.6822650	-0.2977640	3.9045930
H	0.3569930	0.2954220	3.6352840
H	0.0997840	-0.9724390	4.8620850
O	-2.0496820	0.3419800	2.7046880
H	-1.8847820	0.3594070	4.7606700
H	-2.2632560	-1.2199750	4.0311210
C	-3.3901360	0.7779950	2.6919260
C	-3.7583240	1.2200130	1.2989220
H	-3.5198570	1.6116940	3.3937680
H	-4.0546110	-0.0402800	2.9961200
O	-3.8059120	0.0819080	0.4689350
H	-3.0300370	1.9456130	0.9112120
H	-4.7411690	1.7089010	1.3299200
C	-4.2767760	0.3763180	-0.8332380
C	-4.1948020	-0.8743250	-1.6664420
H	-5.3221430	0.7090600	-0.7837260
H	-3.6701530	1.1667820	-1.2898110
O	-2.8396210	-1.2011660	-1.8662020
H	-4.6843700	-0.6939820	-2.6320750
H	-4.7117590	-1.7009730	-1.1619930
C	-2.6530880	-2.3258730	-2.6887110
C	-1.1777530	-2.5209820	-2.9146230
H	-3.0864010	-3.2189700	-2.2196850
H	-3.1435990	-2.1709110	-3.6586060
O	-0.5734040	-2.9189090	-1.6998870
H	-0.7353770	-1.5828660	-3.2694080
H	-1.0261910	-3.2964580	-3.6769880

H	1.1028960	-3.6978240	-2.6192750
H	1.2519900	-2.0218520	-2.0420390

Cartesian coordinates for the structures of the Figure 1-SI in solution

10-1 $G = -999.862156$ a.u.

C	-1.3942190	2.4717120	-0.1151640
N	-0.1742670	2.1682270	-0.1466730
Cl	-2.6070130	1.3949960	0.5863130
C	-1.9370490	3.7462080	-0.6586180
N	0.3051550	1.0225560	0.3637280
C	1.6660020	0.7698030	0.2165600
H	-0.2066650	0.4573500	1.0957750
H	-2.4156820	4.3253470	0.1329340
H	-2.6871250	3.5506830	-1.4270100
H	-1.1202900	4.3256650	-1.0847240
C	2.2287530	-0.2877460	0.9435110
C	2.4723670	1.5028980	-0.6586300
C	4.3739570	0.1257280	-0.0867090
C	3.8131600	1.1780580	-0.7982400
H	2.0421670	2.3230820	-1.2155220
H	4.4270750	1.7601300	-1.4750910
C	3.5692800	-0.5997080	0.7843510
H	5.4216820	-0.1189340	-0.2014290
H	3.9931120	-1.4127700	1.3617680
H	1.5979610	-0.8258750	1.6420810
F	-0.6209330	-0.8284980	1.9137800
Cs	-0.9238970	-1.9349150	-0.4600340

10-TS₁ $G = -999.847117$ a.u. $\square \nu_{\min} = 230.5i$ cm⁻¹

H	0.1148750	-0.1832950	1.4549060
N	0.7965140	0.4955900	0.4090650
F	-0.3970160	-0.8025730	2.1082950
Cs	-1.8195600	-1.4124090	-0.3516640
N	0.5272670	1.7675200	0.2030490
C	2.1178390	0.1269920	0.1506800
H	1.7974930	-1.8065120	1.0286220
Cl	-2.4472030	1.7924400	-0.0033300

C	2.5071960	-1.1694170	0.5135660
C	-0.2681010	2.6179710	0.0565520
C	3.0510980	0.9551200	-0.4800130
H	2.7673940	1.9595430	-0.7667160
C	3.7888080	-1.6172650	0.2472460
C	-0.5333430	4.0544810	-0.0492970
H	-1.1079480	4.2663580	-0.9481980
C	4.3330790	0.4935830	-0.7384480
H	0.4235230	4.5775320	-0.0762710
H	4.0710690	-2.6205040	0.5429780
H	-1.1070270	4.3811900	0.8163180
C	4.7146250	-0.7928370	-0.3833880
H	5.0418000	1.1522800	-1.2260540
H	5.7165250	-1.1459850	-0.5883010

10-2 $G = -999.857104$ a.u.

H	0.2330920	-0.4930190	1.7120190
N	0.9341960	0.3582510	0.7362600
F	-0.3281950	-1.1289680	2.2556090
Cs	-1.8891100	-1.3047140	-0.2620600
N	0.5622190	1.5948090	0.6426390
C	2.2031580	0.0636380	0.2209460
H	2.0420310	-1.9505840	0.9398270
Cl	-2.5728870	1.7726460	-0.7732410
C	2.6616020	-1.2460270	0.3973340
C	0.1103420	2.6430380	0.5854450
C	3.0067960	0.9808420	-0.4566150
H	2.6679920	1.9980770	-0.6055510
C	3.8968220	-1.6235960	-0.0963660
C	-0.4516520	3.9750820	0.5092520
H	-0.6834490	4.2095210	-0.5284430
C	4.2454880	0.5875510	-0.9451340
H	0.2434060	4.6996720	0.9327670
H	4.2391110	-2.6402730	0.0526670
H	-1.3848740	3.9728050	1.0720540
C	4.7000350	-0.7110500	-0.7726970
H	4.8592110	1.3107400	-1.4680160
H	5.6668800	-1.0102410	-1.1547070

10-TS₂ ***G* = -1188.414855 a.u.** $\square \nu_{\min} = 377.1i \text{ cm}^{-1}$

H	-0.8524240	0.1823140	-1.7891090
N	-1.6109740	0.4876420	-0.2285910
F	-0.1896980	-0.0584000	-2.4295620
Cs	2.1409360	-0.7158410	-0.5508440
N	-0.7505810	1.3717360	0.2863220
C	-1.5514490	-0.8186260	0.3516650
H	-2.7156310	-1.6671770	-1.2361350
Cl	2.4493890	1.9199770	1.2297510
C	-2.1772760	-1.8639940	-0.3198180
C	-0.7526720	2.5343030	0.3810890
C	-0.8384110	-1.0534620	1.5227220
H	-0.3462230	-0.2347620	2.0354690
C	-2.1013160	-3.1453720	0.2035300
C	-0.4098990	3.8986630	0.6495510
H	0.6337010	3.8688210	0.9879180
C	-0.7592250	-2.3454560	2.0253220
H	-1.0642230	4.2998500	1.4223080
H	-2.5931620	-3.9581190	-0.3152340
H	-0.4899850	4.4806270	-0.2686660
C	-1.3926040	-3.3930580	1.3724740
H	-0.2074550	-2.5241080	2.9395210
H	-1.3335210	-4.3972530	1.7712980
C	-3.0275490	1.2611290	-0.4805890
O	-2.8444290	2.4679350	-0.3765120
O	-3.9207730	0.5003960	-0.7397930

10-3 ***G* = -1188.481794 a.u.**

H	-1.0940080	0.1846990	-2.0672670
N	-1.5094540	0.9904130	0.0408190
F	-0.3606230	-0.2212500	-2.4674610
Cs	1.8622270	-1.1610990	-0.5566090
N	-0.1677950	1.2523990	0.2704190
C	-2.0512810	-0.2770940	0.3753760
H	-3.7421000	-0.0740120	-0.9332160
Cl	3.4411020	0.6963170	1.4459480
C	-3.2255640	-0.7113170	-0.2286620

C	-0.0582200	2.5209810	0.1646220
C	-1.3808370	-1.0729370	1.2985010
H	-0.4897310	-0.6967710	1.7855250
C	-3.7265320	-1.9625060	0.0998660
C	1.1597180	3.3365520	0.2957880
H	1.9908630	2.6908510	0.5837840
C	-1.8906800	-2.3254490	1.6045900
H	1.0055310	4.1006970	1.0588700
H	-4.6432760	-2.3034450	-0.3635670
H	1.3746900	3.8392370	-0.6486490
C	-3.0613940	-2.7743400	1.0079130
H	-1.3766100	-2.9440800	2.3290750
H	-3.4579890	-3.7499770	1.2562880
C	-2.2048960	2.1588160	-0.1593580
O	-1.2418000	3.1343020	-0.1072610
O	-3.3662150	2.3545960	-0.3542130

Cartesian coordinates for the structures of the Figure 2-SI in solution

11-1 $G = -2111.134619$ a.u.

H	-0.1918440	2.7380720	0.9832660
N	-2.1377090	1.2441050	-1.4414000
F	-0.8628930	2.4411840	1.6229340
C	-3.0768440	0.3858670	-0.8765730
Cs	0.5419560	-0.2009170	0.0274780
N	-2.2174320	2.4593240	-1.0330120
O	-0.5795990	2.9640420	-3.4432950
H	-2.4727640	-1.1696480	-2.2163750
C	-3.1396670	-0.9126510	-1.4022160
C	-2.1800370	3.5739100	-0.7701340
C	-0.0166330	1.9827830	-3.2176150
Cl	1.0495440	3.1828440	-0.3669410
C	-3.9405050	0.7217740	0.1757130
H	-3.8928800	1.7094280	0.6170190
C	-4.0478150	-1.8310640	-0.9082950
O	0.5673980	0.9945920	-3.0712290
C	-4.8467110	-0.2099860	0.6621120
C	-1.9792290	4.9428940	-0.3372790
H	-4.0877810	-2.8238560	-1.3416380
C	-4.9134980	-1.4899130	0.1275850

H	-2.8351360	5.5652950	-0.5944470
H	-1.0837260	5.3139000	-0.8375750
H	-1.8073950	4.9600670	0.7394930
H	-5.5063930	0.0719780	1.4741300
H	-5.6276500	-2.2083620	0.5086330
C	2.3727570	0.8171180	3.4565590
C	3.1345700	1.4321130	2.3150750
O	3.4500220	0.4247070	1.3766690
H	4.0551420	1.8892460	2.7021720
H	2.5307770	2.2151140	1.8397630
C	4.1314330	0.9398290	0.2528220
C	4.5048200	-0.1984290	-0.6557150
H	5.0492900	1.4536040	0.5692640
H	3.4981970	1.6635650	-0.2761120
H	5.0553850	-0.9606580	-0.0898650
H	5.1572920	0.1771680	-1.4545570
O	3.3355480	-0.7609270	-1.2093230
C	3.6047820	-1.8766190	-2.0232630
C	2.3139420	-2.4032510	-2.5869920
H	4.1032350	-2.6613660	-1.4401490
H	4.2649610	-1.5931730	-2.8536700
O	1.5256660	-2.9245670	-1.5401120
H	2.5386700	-3.1889980	-3.3199830
H	1.7787190	-1.5966240	-3.1042170
C	0.3136720	-3.4717290	-2.0039180
C	-0.4653710	-4.0192370	-0.8386840
H	0.5090810	-4.2815570	-2.7191880
H	-0.2784200	-2.7013680	-2.5171420
O	-0.8366840	-2.9536970	-0.0004760
H	0.1439960	-4.7458030	-0.2864190
H	-1.3568680	-4.5367400	-1.2184550
C	-1.6350740	-3.3516160	1.0909410
C	-1.9592740	-2.1432870	1.9267110
H	-2.5701900	-3.7997070	0.7318890
H	-1.1031360	-4.0959920	1.6972340
O	-0.7885100	-1.6975380	2.5761210
H	-2.7269170	-2.4100740	2.6652960
H	-2.3685890	-1.3502900	1.2873570
C	-1.0221550	-0.5450910	3.3570380
C	0.2701750	-0.0991160	3.9851170
H	-1.4249830	0.2655740	2.7353510

H	-1.7516810	-0.7644150	4.1479010
O	1.1419980	0.3370840	2.9713070
H	0.7222770	-0.9261570	4.5480820
H	0.0590730	0.7214520	4.6830910
H	2.2066850	1.5844410	4.2236690
H	2.9490100	-0.0020200	3.9061130

11-TS₁ **G= -2111.101525 a.u.** $\square \nu_{\min} = 249.8i \text{ cm}^{-1}$

H	-0.1738290	2.3822830	1.5756840
N	-2.1508590	1.6537620	-0.9263830
F	-0.9013350	1.8725510	1.9883830
C	-3.0432100	0.7207570	-0.3437460
Cs	0.6298970	-0.2087530	0.0071530
N	-2.1579020	2.8883160	-0.4668000
O	-0.9317870	2.6666280	-2.5869320
H	-2.9295360	-0.6943890	-1.9515100
C	-3.3719640	-0.4667000	-0.9959950
C	-1.6547720	3.8920100	-0.7680190
C	-1.3189780	1.5642130	-2.2180000
Cl	1.1626970	3.2162570	0.6101650
C	-3.6117850	1.0081440	0.8988770
H	-3.3335470	1.9143770	1.4182280
C	-4.2746750	-1.3402120	-0.4054650
O	-1.1626450	0.4188040	-2.6205500
C	-4.5143220	0.1255440	1.4688950
C	-1.1195340	5.2176110	-0.8920020
H	-4.5315810	-2.2532190	-0.9286380
C	-4.8538840	-1.0559450	0.8222670
H	-1.6550650	5.7809600	-1.6541050
H	-0.0617480	5.1087440	-1.1362500
H	-1.1952930	5.7033210	0.0834760
H	-4.9493700	0.3662300	2.4305240
H	-5.5610610	-1.7426070	1.2690380
C	3.1353120	-0.0565870	3.1074310
C	3.7148460	0.7796410	1.9991680
O	3.7329940	0.0233600	0.8046030
H	4.7366780	1.0759290	2.2704840
H	3.1115600	1.6850920	1.8631570
C	4.2049730	0.7779660	-0.2915590
C	4.2815220	-0.1077430	-1.5059070

H	5.2075470	1.1707360	-0.0769840
H	3.5379960	1.6291640	-0.4809000
H	4.8762570	-1.0016000	-1.2791920
H	4.7762910	0.4391910	-2.3187530
O	2.9781920	-0.4776860	-1.8921490
C	2.9508200	-1.3466280	-3.0004040
C	1.5214790	-1.6747880	-3.3381310
H	3.5037380	-2.2665720	-2.7722300
H	3.4215440	-0.8675440	-3.8685200
O	0.9631050	-2.4591440	-2.3032750
H	1.5008380	-2.2308620	-4.2846530
H	0.9399010	-0.7535180	-3.4662840
C	-0.3684450	-2.8323130	-2.5889020
C	-0.9359980	-3.5981250	-1.4241750
H	-0.3982160	-3.4687500	-3.4833830
H	-0.9735430	-1.9380750	-2.7763470
O	-1.0419820	-2.7335250	-0.3184910
H	-0.2934630	-4.4528400	-1.1778320
H	-1.9270020	-3.9817720	-1.7024790
C	-1.6623640	-3.3188440	0.8008970
C	-1.6892390	-2.3112720	1.9187820
H	-2.6906580	-3.6132080	0.5550120
H	-1.1126110	-4.2141130	1.1182940
O	-0.3761880	-2.1133570	2.3945690
H	-2.3363490	-2.6793920	2.7258300
H	-2.1111820	-1.3648480	1.5532490
C	-0.3268150	-1.1921850	3.4647710
C	1.1081790	-0.9832770	3.8680250
H	-0.7670560	-0.2329810	3.1640090
H	-0.8913820	-1.5806310	4.3223440
O	1.7711900	-0.2857130	2.8410200
H	1.5921270	-1.9521770	4.0461790
H	1.1390550	-0.4048560	4.8002550
H	3.2507400	0.4841060	4.0557200
H	3.6714790	-1.0111400	3.1860000

11-2 $G = -2111.181552$ a.u.

H	0.4914720	1.8217260	-1.9839980
N	2.5146990	1.6962290	0.3842520
F	1.0707810	1.0885820	-2.2693150

C	3.1789540	0.4858990	0.0819600
Cs	-0.7057940	-0.1936180	0.0006840
N	2.7752590	2.8464640	-0.3348260
O	1.4103200	3.2886490	1.3329210
H	2.8405260	-0.3919730	2.0119790
C	3.2904240	-0.5180030	1.0388060
C	2.0909710	3.7494120	0.2516980
C	1.6563910	1.9525430	1.4091960
Cl	-0.7109030	3.0165280	-1.2088910
C	3.7534300	0.3342140	-1.1775270
H	3.6359900	1.1183920	-1.9103120
C	4.0000240	-1.6706880	0.7298600
O	1.1711270	1.2184770	2.2360840
C	4.4582440	-0.8223620	-1.4659170
C	1.9640840	5.1709220	-0.1092340
H	4.1002160	-2.4437060	1.4818260
C	4.5898360	-1.8286120	-0.5153300
H	2.5992460	5.3788620	-0.9666040
H	2.2544660	5.8027130	0.7309760
H	0.9238410	5.3751860	-0.3659430
H	4.9080210	-0.9364420	-2.4440830
H	5.1487130	-2.7266160	-0.7462700
C	-3.2537980	-0.5295870	-3.0015650
C	-3.6444290	0.6588470	-2.1647690
O	-3.7530500	0.2600570	-0.8120890
H	-4.6083380	1.0459380	-2.5202290
H	-2.8919000	1.4507820	-2.2668660
C	-4.0589760	1.3458090	0.0390570
C	-4.2174610	0.8397160	1.4474750
H	-4.9975210	1.8198050	-0.2766640
H	-3.2608830	2.0982770	-0.0072470
H	-4.9353890	0.0099270	1.4684860
H	-4.6044830	1.6491230	2.0797560
O	-2.9626480	0.4100430	1.9256770
C	-3.0123920	-0.1314820	3.2245780
C	-1.6212030	-0.5142070	3.6526980
H	-3.6669980	-1.0119210	3.2447190
H	-3.4098800	0.6097590	3.9299940
O	-1.1728350	-1.6070310	2.8767310
H	-1.6381700	-0.7889560	4.7154590
H	-0.9424010	0.3385080	3.5267330

C	0.1216240	-2.0255100	3.2500180
C	0.5618830	-3.1527010	2.3542450
H	0.1215870	-2.3753950	4.2909550
H	0.8261690	-1.1876880	3.1695130
O	0.7211720	-2.6588250	1.0459150
H	-0.1816110	-3.9596350	2.3687090
H	1.5128790	-3.5543610	2.7292380
C	1.2185560	-3.6082270	0.1323940
C	1.2959170	-2.9743970	-1.2315530
H	2.2200540	-3.9386970	0.4362470
H	0.5613460	-4.4863950	0.0977600
O	-0.0106370	-2.7871290	-1.7299540
H	1.8713550	-3.6266220	-1.9018370
H	1.8227950	-2.0112030	-1.1655250
C	-0.0145850	-2.2403450	-3.0336050
C	-1.4342020	-1.9636280	-3.4512080
H	0.5624170	-1.3070630	-3.0584590
H	0.4396690	-2.9480110	-3.7390450
O	-1.9347010	-0.9019580	-2.6748780
H	-2.0499160	-2.8618470	-3.3136390
H	-1.4468540	-1.6946160	-4.5151880
H	-3.3175050	-0.2545230	-4.0621820
H	-3.9413580	-1.3653470	-2.8177910

Cartesian coordinates for the structures of the Figure 3-SI in solution

12-1 $G = -2111.131518$ a.u.

H	1.8795370	1.5607210	-0.7483200
N	2.5537100	0.3056240	-1.1045000
F	1.3923730	2.4158350	-0.5347760
Cs	-0.8426610	0.0900980	-0.0390190
N	2.3082790	-0.1349500	-2.2967980
C	2.9932360	-0.6600250	-0.1848880
H	3.4203360	0.8789380	1.2436830
Cl	-0.3597770	-2.2345510	-2.4602260
C	3.4395920	-0.1870810	1.0528240
C	2.0731180	-0.4555980	-3.3676300
C	3.0010070	-2.0329430	-0.4389850
H	2.5991800	-2.4160010	-1.3689570
C	3.9205280	-1.0726670	2.0014880

C	1.7188450	-0.8803220	-4.7048180
H	1.4743490	-1.9414240	-4.6554020
C	3.4889920	-2.9081880	0.5225980
H	2.5344090	-0.6899650	-5.4010440
H	4.2813550	-0.6903390	2.9488500
H	0.8208810	-0.3445010	-5.0119990
C	3.9581180	-2.4393080	1.7418750
H	3.4917300	-3.9706860	0.3121950
H	4.3428710	-3.1281820	2.4825160
C	-3.9588680	-1.2416870	-1.5020660
C	-3.9051760	-2.3746430	-0.5123600
O	-2.7240620	-2.2556370	0.2402860
H	-3.9048750	-3.3153320	-1.0764440
H	-4.7842030	-2.3611830	0.1448650
C	-2.3194740	-3.4336600	0.8932220
C	-0.8779420	-3.2819660	1.2986980
H	-2.3939890	-4.2903850	0.2123340
H	-2.9519810	-3.6253740	1.7698770
H	-0.2731440	-3.0911830	0.4011060
H	-0.5288030	-4.2162510	1.7584240
O	-0.7584470	-2.2120880	2.2144800
C	0.5783170	-2.0069130	2.6134000
C	0.6491850	-0.7999820	3.5082700
H	1.2202090	-1.8519610	1.7363290
H	0.9543130	-2.8858390	3.1537560
O	0.4203080	0.3564310	2.7352600
H	1.6417600	-0.7515940	3.9740160
H	-0.1034710	-0.8807480	4.3028230
C	0.4048850	1.5386320	3.5002160
C	0.2364730	2.7195970	2.5839530
H	1.3509540	1.6486090	4.0475600
H	-0.4133630	1.5053030	4.2307700
O	-1.0376380	2.6645840	1.9789500
H	1.0186740	2.7150150	1.8157060
H	0.3348800	3.6417670	3.1727240
C	-1.2441400	3.7326730	1.0793430
C	-2.6369430	3.6480230	0.5170880
H	-1.1338860	4.6926400	1.6013810
H	-0.5047480	3.6938280	0.2702690
O	-2.7405230	2.5160020	-0.3174550
H	-2.8473660	4.5599000	-0.0571030

H	-3.3662910	3.5804940	1.3340050
C	-4.0276970	2.3629340	-0.8718950
C	-4.0720990	1.0928130	-1.6780830
H	-4.7810790	2.3185440	-0.0754950
H	-4.2633050	3.2156460	-1.5217800
O	-4.0009090	-0.0104000	-0.8068890
H	-3.2364960	1.0746040	-2.3920610
H	-5.0058360	1.0644410	-2.2549950
H	-4.8527290	-1.3519870	-2.1303190
H	-3.0684530	-1.2888340	-2.1422420
C	4.0388690	2.7459280	-1.6368080
O	3.6177160	2.7125500	-2.7124570
O	4.4976680	2.8088550	-0.5793890

12-TS₁ **G= -2111.081946 a.u.** $\square \nu_{\min}= 383.8i \text{ cm}^{-1}$

H	-1.7559880	-1.9993920	0.9415170
N	-2.8504840	-0.7931190	1.3430820
F	-1.0023930	-2.5266440	0.6650940
Cs	1.0538090	-0.1441690	0.0792660
N	-3.4022520	-0.3817660	0.1924330
C	-1.9657110	0.1740570	1.9281720
H	-1.2072240	-1.2534220	3.3362430
Cl	-3.6285340	2.2063860	-1.8932840
C	-1.1413110	-0.2385370	2.9706880
C	-4.4663310	-0.5044690	-0.2694530
C	-1.9005770	1.4711350	1.4301850
H	-2.5252890	1.7758080	0.5933140
C	-0.2520390	0.6690690	3.5274630
C	-5.5924890	-0.4644370	-1.1532440
H	-5.3327890	0.3048450	-1.8942410
C	-1.0038410	2.3644700	2.0016660
H	-6.4731190	-0.1537200	-0.5916220
H	0.3847760	0.3539130	4.3443320
H	-5.7481690	-1.4393850	-1.6132230
C	-0.1768150	1.9707780	3.0452600
H	-0.9646040	3.3791260	1.6257150
H	0.5200510	2.6741380	3.4832740
C	-0.8985260	-1.3942160	-2.7244930
C	-0.9203400	0.0060110	-3.2749400
O	-0.3300360	0.8707600	-2.3332620

H	-1.9565000	0.3135090	-3.4602570
H	-0.3601050	0.0386700	-4.2187770
C	-0.2608790	2.2063660	-2.7878100
C	0.1515390	3.0840030	-1.6415550
H	-1.2461820	2.5328080	-3.1338550
H	0.4675780	2.2819140	-3.6057870
H	-0.5739410	2.9764130	-0.8257640
H	0.1452850	4.1307510	-1.9694300
O	1.4513250	2.7177450	-1.2055050
C	1.9287750	3.5484680	-0.1748610
C	3.3230900	3.1272390	0.2031260
H	1.2713850	3.4867900	0.7026140
H	1.9524220	4.5946480	-0.5065950
O	3.2817460	1.8410200	0.7856060
H	3.7366560	3.8515210	0.9163640
H	3.9623950	3.1149400	-0.6876480
C	4.5534120	1.3752650	1.1769200
C	4.4353170	-0.0508050	1.6431750
H	4.9499410	1.9926190	1.9930930
H	5.2527530	1.4268840	0.3336740
O	4.1031910	-0.8676870	0.5425930
H	3.6667820	-0.1304180	2.4252580
H	5.3921260	-0.3671640	2.0769140
C	4.0918840	-2.2422410	0.8629330
C	3.7445850	-3.0340750	-0.3689300
H	5.0796010	-2.5548580	1.2243110
H	3.3600190	-2.4455770	1.6565090
O	2.4016210	-2.7876410	-0.7165580
H	3.8947610	-4.1014220	-0.1624160
H	4.4100580	-2.7458070	-1.1921770
C	2.0047210	-3.4683750	-1.8894900
C	0.5610900	-3.1595130	-2.1803610
H	2.6328030	-3.1592580	-2.7338860
H	2.1187030	-4.5510680	-1.7520770
O	0.4429620	-1.7979380	-2.5324800
H	-0.0514010	-3.3823540	-1.2996180
H	0.2221320	-3.7946920	-3.0090550
H	-1.4011280	-2.0660850	-3.4316290
H	-1.4440660	-1.4363490	-1.7710740
C	-4.0352400	-1.4425950	2.2501030
O	-5.0625350	-1.5262460	1.5854840

O	-3.6564430	-1.7311610	3.3554250
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12-2 $G = -2111.173721$ a.u.

H	1.5635260	0.0680840	-2.3161000
N	3.4891650	-0.7325110	-0.7785850
F	0.7953950	0.6389370	-2.4867850
Cs	-1.1634360	-0.0942250	-0.1866320
N	2.7982270	-0.8716860	-1.9620940
C	3.6913920	0.5284230	-0.1850800
H	3.4275090	1.5873590	-2.0356850
Cl	0.6698030	-2.8551280	-0.3111290
C	3.6397360	1.6712110	-0.9785310
C	2.9271920	-2.1046420	-2.2832020
C	3.9619230	0.6193430	1.1766750
H	3.9815030	-0.2759830	1.7807300
C	3.8787380	2.9095200	-0.4028650
C	2.3096300	-2.8040530	-3.4194070
H	1.6447160	-3.5713060	-3.0210350
C	4.2132360	1.8656960	1.7316150
H	3.0753730	-3.2740730	-4.0373530
H	3.8444970	3.7966650	-1.0225470
H	1.7355840	-2.0952250	-4.0118300
C	4.1768610	3.0125490	0.9491140
H	4.4392400	1.9360000	2.7882280
H	4.3752690	3.9804350	1.3913550
C	-4.7492500	-0.7763870	-1.3407090
C	-4.8836900	-1.5698580	-0.0684970
O	-3.6019310	-1.8224330	0.4527320
H	-5.3992080	-2.5137130	-0.2901900
H	-5.4878770	-1.0106990	0.6572530
C	-3.6251100	-2.5943090	1.6348670
C	-2.2194580	-2.7792920	2.1383450
H	-4.0659950	-3.5784760	1.4313950
H	-4.2338570	-2.0929530	2.3981300
H	-1.5727830	-3.1618170	1.3386140
H	-2.2309890	-3.5134290	2.9550380
O	-1.7281440	-1.5398150	2.6096100
C	-0.4076940	-1.6492230	3.1054840
C	0.0586280	-0.2951510	3.5660430
H	0.2580620	-2.0352640	2.3235160

H	-0.3824650	-2.3418400	3.9573460
O	0.2092320	0.5475210	2.4447810
H	1.0196100	-0.4048440	4.0852480
H	-0.6669230	0.1364210	4.2671850
C	0.6082070	1.8555350	2.7741790
C	0.7815700	2.6420960	1.5034370
H	1.5632360	1.8376650	3.3154830
H	-0.1429210	2.3344560	3.4156570
O	-0.4801320	2.8591290	0.9075030
H	1.4375710	2.0898820	0.8167890
H	1.2612810	3.6031020	1.7302920
C	-0.3746360	3.5552000	-0.3146410
C	-1.7515240	3.7926010	-0.8740390
H	0.1198350	4.5230450	-0.1574870
H	0.2244990	2.9781090	-1.0323630
O	-2.2991060	2.5632660	-1.2917870
H	-1.6821020	4.4842050	-1.7237000
H	-2.3892140	4.2503740	-0.1074290
C	-3.6180590	2.6802820	-1.7702010
C	-4.1162680	1.3210740	-2.1822020
H	-4.2706810	3.0943640	-0.9913440
H	-3.6502250	3.3510390	-2.6388230
O	-4.2514350	0.5084670	-1.0386100
H	-3.4137950	0.8679610	-2.8947440
H	-5.0853080	1.4335600	-2.6857180
H	-5.7324330	-0.6980410	-1.8224220
H	-4.0717130	-1.2961950	-2.0315120
C	4.0625620	-1.9214520	-0.4204590
O	3.7129030	-2.7842740	-1.4336130
O	4.7580260	-2.2125280	0.5054140