

Supporting Information
**Hyperconjugative Aromaticity and Antiaromaticity Control the
Reactivities and π -Facial Stereoselectivities of 5-Substituted
Cyclopentadiene Diels-Alder Cycloadditions**

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Table of Contents

Figure S1.....	S2
Table S1 Optimized Cartesian Coordinates.....	S3
Table S2 Energetic Data.....	S60

Figure S1 shows the results from the distortion/interaction-activation strain analysis performed along the intrinsic reaction coordinate (IRC) for the *syn* (red) and *anti* (blue) Diels-Alder reactions of C₅-F, C₅-Br, and C₅-SiH₃ with ethylene. There is a modest preference in the interaction energies for the *syn* addition of ethylene to C₅-F, but it is the differences in the distortion energies, which strongly favor the *anti* cycloaddition that control the π -facial stereoselectivity. In the reaction of C₅-SiH₃ with ethylene the interaction and distortion energies both favor the *anti* cycloaddition. The preference for *anti* reaction in the distortion energies is larger than in the interaction energies for C₅-SiH₃. In the Diels-Alder reaction of C₅-Br the *syn* preference of the interaction energies is countered by the *anti* preference in the distortion energies and poor stereoselectivity is predicted. The *syn* preference in the interaction energies suggests there are stabilizing dispersive interactions between the substituent and ethylene in the *syn* transition state. The differences in the distortion energies of the *syn* and *anti* reactions appear early on in the course of the intrinsic reaction coordinate. This suggests that the ground state geometries of the dienes are pre-distorted towards either the *syn* or *anti* transition states.

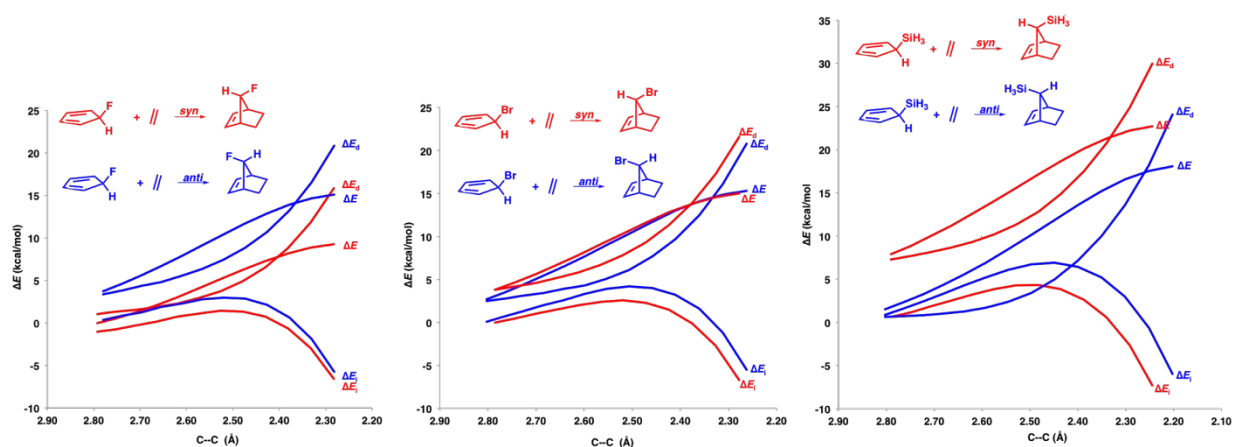


Figure S1. Distortion/Interaction analysis performed along the reaction coordinate defined by the average C-C bond forming distances for the *syn* (red) and *anti* (blue) Diels-Alder reactions of C₅-F (left), C₅-Br (center), and C₅-SiH₃ (right) with ethylene. Electronic energies (ΔE), distortion energies (ΔE_d) and interaction energies (ΔE_i) are reported in kcal/mol and forming C-C bond length in Å.

Table S1 M06-2X/6-31G(d) Optimized Cartesian Coordinates

C₅-Br

C	-0.32813400	0.00000300	0.71261100
H	-0.11863200	0.00000700	1.78501300
C	-1.13486700	1.18235500	0.26383700
H	-0.81517700	2.20516500	0.41255000
C	-2.26145800	0.73902500	-0.31203700
H	-3.05359500	1.35206700	-0.72548900
C	-1.13486600	-1.18235300	0.26384700
H	-0.81517200	-2.20516100	0.41257000
C	-2.26144900	-0.73903100	-0.31204800
H	-3.05358100	-1.35207500	-0.72550500
Br	1.44516600	0.00000000	-0.13875400

C₅-Cl

C	0.26870800	0.00000000	0.58274800
H	0.49877300	0.00000000	1.65377400
C	-0.58134900	1.18412200	0.20853500
H	-0.24899300	2.20750100	0.32308100
C	-1.76308900	0.73975800	-0.23812400
H	-2.59936400	1.35118900	-0.55605800
C	-0.58134900	-1.18412300	0.20853500
H	-0.24899400	-2.20750100	0.32308300
C	-1.76308900	-0.73975800	-0.23812600
H	-2.59936300	-1.35118900	-0.55606000
Cl	1.86582000	0.00000000	-0.25466000

C₅-H

C	0.00045200	-1.21457800	-0.00018000
H	0.00070300	-1.87403700	0.87890700
C	1.17770600	-0.28016700	0.00016800
H	2.20981600	-0.60898500	0.00025100
C	0.73518200	0.98846000	-0.00004400
H	1.34836400	1.88243100	-0.00009900
C	-1.17749200	-0.28103900	0.00019200
H	-2.20935600	-0.61061500	0.00029300
C	-0.73592100	0.98790600	-0.00008200
H	-1.34977500	1.88141500	-0.00015900
H	0.00068900	-1.87370800	-0.87951800

C₅-F

C	0.74397300	0.00000100	0.36930200
H	1.02442900	0.00000000	1.43527200
C	-0.15115500	1.18607700	0.10462500
H	0.19110800	2.21162000	0.15776000
C	-1.39390300	0.74183600	-0.11751800

H	-2.27659100	1.34988500	-0.27918600
C	-0.15115500	-1.18607700	0.10462700
H	0.19111000	-2.21161900	0.15776400
C	-1.39390200	-0.74183700	-0.11752100
H	-2.27659100	-1.34988600	-0.27919100
F	1.91371000	0.00000000	-0.36150100

C₅-Me

C	0.69635500	0.00000000	0.46696600
H	0.99056200	-0.00000100	1.52834500
C	-0.20618600	1.17448800	0.19468800
H	0.11575000	2.20599400	0.28368100
C	-1.41954300	0.73608300	-0.17864000
H	-2.27310900	1.34979900	-0.44385500
C	-0.20618600	-1.17448800	0.19468600
H	0.11575100	-2.20599400	0.28367800
C	-1.41954400	-0.73608300	-0.17863800
H	-2.27311100	-1.34979800	-0.44385100
C	1.96722400	0.00000000	-0.39446200
H	2.57574100	0.88592100	-0.19034900
H	2.57574000	-0.88592200	-0.19035000
H	1.69995800	0.00000100	-1.45490100

C₅-NH₂

C	-0.72431000	-0.00974500	0.42038400
H	-0.98743500	-0.01045000	1.49035400
C	0.19857500	-1.17656400	0.16419400
H	-0.13202300	-2.20517100	0.23919000
C	1.42152400	-0.72476700	-0.14686600
H	2.29614000	-1.32726700	-0.36455500
C	0.17360500	1.18201900	0.15090600
H	-0.16334500	2.21046500	0.22264700
C	1.40633200	0.75373000	-0.15617100
H	2.26849700	1.37116500	-0.38329000
N	-1.97564600	-0.11556800	-0.33309600
H	-2.55454300	0.69968900	-0.14097100
H	-1.75211700	-0.07749300	-1.32638900

C₅-OH

C	0.74263000	0.00000000	0.40032100
H	1.01494300	-0.00000100	1.46611300
C	-0.16561000	1.18368700	0.13811500
H	0.17217900	2.21065000	0.20593400
C	-1.39951600	0.74132800	-0.13674300
H	-2.27570100	1.34902600	-0.33335100
C	-0.16561000	-1.18368700	0.13811400

H	0.17217900	-2.21065000	0.20593300
C	-1.39951700	-0.74132800	-0.13674200
H	-2.27570300	-1.34902500	-0.33334900
O	1.97066700	0.00000000	-0.29845400
H	1.75250200	0.00000000	-1.24203300

C₅-SH

C	0.26163400	-0.00000100	0.61307700
H	0.50076200	-0.00000100	1.68438400
C	-0.59492700	1.18067900	0.24442000
H	-0.26965900	2.20554200	0.37066500
C	-1.75915200	0.73814600	-0.25411500
H	-2.58011500	1.35093700	-0.60798200
C	-0.59492700	-1.18067900	0.24442000
H	-0.26966000	-2.20554300	0.37066400
C	-1.75915300	-0.73814600	-0.25411500
H	-2.58011600	-1.35093500	-0.60798100
S	1.90447800	0.00000000	-0.20725600
H	1.40629600	0.00000100	-1.45578300

C₅-SiH₃

C	0.20109000	0.00001300	0.80181400
H	0.53285200	0.00002800	1.84544500
C	-0.60329800	1.17053900	0.35821500
H	-0.32624500	2.20170500	0.54351600
C	-1.66938300	0.72699900	-0.34965800
H	-2.40757300	1.34557700	-0.84653900
C	-0.60329200	-1.17053100	0.35825100
H	-0.32623000	-2.20169000	0.54357900
C	-1.66934500	-0.72702000	-0.34968800
H	-2.40750800	-1.34561700	-0.84658400
Si	1.75167800	0.00000100	-0.31185700
H	2.57788100	1.20140900	-0.03006400
H	2.57788200	-1.20139900	-0.03003100
H	1.32082400	-0.00001800	-1.72693300

Ethylene

C	0.00000000	0.66351800	0.00000000
H	0.92385000	1.23453000	0.00000000
H	-0.92381200	1.23456900	0.00000000
C	0.00000000	-0.66351800	0.00000000
H	-0.92385000	-1.23453000	0.00000000
H	0.92381200	-1.23456900	0.00000000

C₅-Br-Syn-Ethylene

C	0.08619800	-0.82254500	0.00004900
C	0.97801100	-0.49278500	1.16330700

H	0.64393500	-0.55367100	2.19239900
C	2.26606900	-0.72313800	0.70601600
H	3.15001100	-0.77503800	1.33105300
C	0.97806800	-0.49273200	-1.16318800
H	0.64389000	-0.55362200	-2.19224900
C	2.26605000	-0.72312400	-0.70608300
H	3.14995100	-0.77500100	-1.33118200
C	0.84102200	1.73054600	0.68682800
H	1.73862900	1.98157600	1.24020700
H	-0.09364300	1.80806000	1.23293400
C	0.84112300	1.73045400	-0.68682300
H	-0.09352100	1.80782600	-1.23297500
H	1.73876500	1.98141300	-1.24016500
H	-0.06145300	-1.90921200	0.00007900
Br	-1.72445100	-0.12149700	-0.00002100

C₅-Cl-Syn-Ethylene

C	-0.35928600	-0.86179500	-0.00026800
C	0.51728900	-0.48698100	1.16342100
H	0.18853400	-0.56564600	2.19308800
C	1.81495200	-0.64379000	0.70631500
H	2.70073400	-0.64782200	1.33078900
C	0.51727600	-0.48565900	-1.16359700
H	0.18832400	-0.56343500	-2.19327300
C	1.81498000	-0.64310600	-0.70669300
H	2.70078400	-0.64632900	-1.33113700
C	0.24533900	1.73148300	0.68666200
H	1.12875200	2.02839900	1.24013800
H	-0.69028900	1.75477200	1.23605600
C	0.24563100	1.73168300	-0.68563800
H	-0.68979000	1.75519700	-1.23539900
H	1.12922300	2.02902700	-1.23860400
H	-0.42842700	-1.95770500	-0.00098700
Cl	-2.05911400	-0.30808600	-0.00011100

C₅-F-Syn-Ethylene

C	0.16873200	1.09537100	-0.00015900
C	-0.44049200	0.36097300	1.16365600
H	-0.19309400	0.58471300	2.19513700
C	-1.64962000	-0.12800000	0.70826800
H	-2.43304900	-0.54421100	1.33088700
C	-0.44033900	0.36065000	-1.16385400
H	-0.19303400	0.58403600	-2.19543400
C	-1.64956900	-0.12821700	-0.70822200
H	-2.43296100	-0.54466900	-1.33072800
C	0.95642500	-1.37959100	0.68591200

H	0.37641700	-2.10590500	1.24358000
H	1.75003300	-0.87705600	1.22862200
C	0.95645900	-1.37966900	-0.68562300
H	1.75014200	-0.87722000	-1.22829800
H	0.37656900	-2.10612900	-1.24322000
H	-0.24188900	2.11874900	-0.00039400
F	1.53681100	1.21762100	-0.00000300

C₅-Me-Syn-Ethylene

C	0.58466200	0.94677800	-0.00000100
C	-0.27380600	0.49059000	1.15281400
H	0.02686100	0.60262700	2.19026200
C	-1.58897400	0.48894800	0.70288500
H	-2.46647200	0.37928600	1.33038500
C	-0.27381200	0.49059200	-1.15281700
H	0.02687300	0.60262300	-2.19026000
C	-1.58898200	0.48893900	-0.70288000
H	-2.46648000	0.37922600	-1.33037200
C	0.19949800	-1.67450000	0.68797600
H	-0.65073100	-2.06115500	1.23707700
H	1.12994900	-1.63675700	1.24653700
C	0.19945600	-1.67451600	-0.68796700
H	1.12987300	-1.63677300	-1.24658600
H	-0.65081900	-2.06118000	-1.23699100
H	0.45103300	2.04507500	0.00001300
C	2.08312600	0.68870100	-0.00001300
H	2.54382100	1.14333100	-0.88310600
H	2.54384400	1.14344200	0.88301200
H	2.33523800	-0.37293300	0.00005000

C₅-NH₂-Syn-Ethylene

C	-0.46783600	1.01686300	-0.01832800
C	0.33324700	0.44568800	-1.16025000
H	0.03719300	0.58162200	-2.19486800
C	1.63075800	0.28100700	-0.70078200
H	2.49297800	0.05768100	-1.31894400
C	0.32318300	0.46506500	1.15419600
H	0.03604400	0.62826800	2.18916600
C	1.62641300	0.30047900	0.70878900
H	2.48667000	0.09961000	1.33787700
C	-0.46092200	-1.62554400	-0.67167900
H	0.32202500	-2.13462000	-1.22039300
H	-1.37142100	-1.43916000	-1.23480900
C	-0.45431000	-1.61612900	0.70360700
H	-1.36418000	-1.43636500	1.27035300
H	0.33269100	-2.11754800	1.25398500

H	-0.21877500	2.09261600	-0.03156100
N	-1.91049700	0.93814600	-0.11372600
H	-2.22872500	-0.01365200	0.03967600
H	-2.33422600	1.50994800	0.61228000

C₅-OH-Syn-Ethylene

C	0.32018200	1.08242200	0.00014900
C	-0.38027000	0.41245600	1.16107800
H	-0.11293600	0.60469200	2.19487700
C	-1.64213800	0.06673200	0.70585700
H	-2.47008000	-0.25431200	1.32789800
C	-0.38022800	0.41283300	-1.16101800
H	-0.11280200	0.60527700	-2.19475400
C	-1.64211300	0.06692600	-0.70593400
H	-2.47004000	-0.25389400	-1.32811000
C	0.71512000	-1.52432400	0.68751000
H	0.00879600	-2.13279700	1.23843700
H	1.59126600	-1.22101800	1.25619200
C	0.71521100	-1.52425500	-0.68772700
H	1.59141300	-1.22078700	-1.25624000
H	0.00888600	-2.13255100	-1.23884500
H	-0.04963000	2.12073500	0.00034500
O	1.71189800	1.20209600	0.00015300
H	2.08535500	0.31113500	-0.00051500

C₅-SH-Syn-Ethylene

C	-0.38060700	-0.84396800	0.01212900
C	0.53670200	-0.48847800	1.15633700
H	0.23062200	-0.55811300	2.19476200
C	1.82813200	-0.67856000	0.68291700
H	2.72297900	-0.69336900	1.29475800
C	0.50087500	-0.50396000	-1.16039300
H	0.15760500	-0.57684500	-2.18625400
C	1.80632300	-0.67756400	-0.72571500
H	2.68152100	-0.68797000	-1.36506300
C	0.33812300	1.70569700	0.70679800
H	1.25012100	1.97580100	1.22650800
H	-0.57763700	1.77035500	1.28599900
C	0.28751400	1.72211600	-0.66760500
H	-0.66580100	1.80593900	-1.18286000
H	1.15697100	1.99818700	-1.25245700
H	-0.45522900	-1.94157700	0.01258000
S	-2.08637200	-0.20794500	-0.04787700
H	-2.62157000	-1.17699100	0.71125600

C₅-SiH₃-Syn-Ethylene

C	-0.39187800	-0.81623100	-0.00002200
C	0.53214100	-0.51073800	1.15222000
H	0.22181700	-0.57953000	2.19020400
C	1.83287800	-0.72871100	0.70046600
H	2.71596400	-0.75103300	1.32917100
C	0.53215100	-0.51068600	-1.15223700
H	0.22185500	-0.57946800	-2.19022900
C	1.83288700	-0.72868400	-0.70047100
H	2.71598000	-0.75100400	-1.32916600
C	0.45111700	1.68380300	0.69015200
H	1.35455200	1.92213200	1.23851900
H	-0.47286900	1.84101600	1.23960600
C	0.45113500	1.68384700	-0.69010800
H	-0.47285100	1.84104500	-1.23956800
H	1.35458700	1.92220100	-1.23843500
H	-0.48322000	-1.92019100	-0.00004200
Si	-2.18129200	-0.22074800	-0.00000500
H	-2.35259000	1.25046500	-0.00018800
H	-2.85391800	-0.77053000	-1.20439300
H	-2.85380000	-0.77022900	1.20459100

C₅-Br-Anti-Ethylene

C	0.05946600	-0.48902600	-0.00012600
H	0.14352100	-1.57074300	-0.00032500
C	0.67754600	0.24347500	-1.16109700
H	0.46722400	-0.02125300	-2.19041000
C	1.04375600	1.49737000	-0.70546100
H	1.37996300	2.31512800	-1.33167600
C	0.67757500	0.24307300	1.16110900
H	0.46716700	-0.02183700	2.19036600
C	1.04370300	1.49717900	0.70575200
H	1.38007400	2.31471200	1.33217200
C	2.55952300	-0.92047700	-0.68951900
H	3.20715800	-0.25118100	-1.24252600
H	2.20870900	-1.78850800	-1.23981900
C	2.55950600	-0.92049200	0.68938900
H	2.20888700	-1.78865800	1.23960800
H	3.20719600	-0.25127100	1.24241700
Br	-1.89703900	-0.16694300	-0.00000300

C₅-Cl-Anti-Ethylene

C	-0.45873700	-0.54487700	0.00009300
H	-0.28495700	-1.61688600	0.00041600
C	0.12776000	0.22187900	-1.16247300
H	-0.06426000	-0.05472300	-2.19237600
C	0.42086100	1.49237700	-0.70763700

H	0.71256700	2.32832600	-1.33232400
C	0.12790000	0.22250500	1.16215600
H	-0.06413500	-0.05352300	2.19220900
C	0.42080000	1.49277000	0.70676400
H	0.71219900	2.32916500	1.33098700
C	2.07479600	-0.84176200	-0.68840000
H	2.68238400	-0.13635400	-1.24199800
H	1.76839700	-1.72577100	-1.23977700
C	2.07522700	-0.84053700	0.68890700
H	1.76966900	-1.72376400	1.24203600
H	2.68338400	-0.13422500	1.24073100
Cl	-2.27334700	-0.37802200	0.00021400

C₅-F-Anti-Ethylene

C	0.67684800	0.76276000	0.00048800
H	0.24178600	1.76285800	0.00109800
C	0.26880600	-0.12418100	-1.16565800
H	0.38440500	0.18422100	-2.19835500
C	0.28542100	-1.42235200	-0.71192900
H	0.20392200	-2.30739800	-1.33270900
C	0.26851100	-0.12554000	1.16538900
H	0.38292200	0.18158400	2.19861500
C	0.28504100	-1.42318300	0.71029700
H	0.20326200	-2.30890900	1.33007100
C	-1.87412200	0.49620100	-0.68705000
H	-2.30714600	-0.32703100	-1.24209400
H	-1.75837200	1.42381700	-1.23975700
C	-1.87490600	0.49434100	0.68730800
H	-1.75932500	1.42038200	1.24270500
H	-2.30777500	-0.33095700	1.23940800
F	2.05585900	0.92812800	0.00088200

C₅-Me-Anti-Ethylene

C	-0.74357600	0.70133900	-0.00001600
H	-0.38725400	1.73412800	-0.00000400
C	-0.20620700	-0.11895500	1.15164200
H	-0.35265100	0.16394200	2.18974200
C	-0.07650400	-1.42643100	0.70421300
H	0.12311000	-2.28849700	1.33099500
C	-0.20608200	-0.11898500	-1.15158200
H	-0.35246400	0.16373100	-2.18974000
C	-0.07644600	-1.42646800	-0.70404500
H	0.12322400	-2.28860000	-1.33071900
C	1.85785400	0.62942200	0.68939100
H	2.37780600	-0.14529900	1.24038400
H	1.67830100	1.54851100	1.23891000

C	1.85796700	0.62905100	-0.68943600
H	1.67859400	1.54789300	-1.23942200
H	2.37802100	-0.14599700	-1.23987200
C	-2.28404100	0.71887400	-0.00012700
H	-2.66185000	1.24093000	0.88443100
H	-2.66167400	1.24143700	-0.88447000
H	-2.68095200	-0.29926000	-0.00047300

C₅-NH₂-Anti-Ethylene

C	-0.73334100	-0.72575500	-0.04191600
H	-0.33098200	-1.73953800	-0.08374300
C	-0.22192100	0.17482400	-1.15247100
H	-0.35865700	-0.07443400	-2.19911700
C	-0.14521800	1.45721800	-0.64389100
H	0.02260500	2.35600700	-1.22697200
C	-0.23669000	0.07260900	1.16030900
H	-0.37239800	-0.26539700	2.18361800
C	-0.15412700	1.39578600	0.77202400
H	-0.00226000	2.24114400	1.43404900
C	1.87033400	-0.54920600	-0.70407600
H	2.36464900	0.27038500	-1.21182000
H	1.70877400	-1.43987400	-1.30363100
C	1.86077200	-0.61899800	0.67021400
H	1.69090100	-1.56632800	1.17299700
H	2.34758000	0.14366200	1.26614200
N	-2.19595200	-0.84440000	-0.13988000
H	-2.54064000	-1.34527300	0.67740400
H	-2.59676200	0.09157500	-0.09091700

C₅-OH-Anti-Ethylene

C	0.69962800	0.76412400	0.00070300
H	0.26883000	1.76476000	0.00173700
C	0.24948400	-0.11426500	-1.16297900
H	0.36814600	0.19100900	-2.19698200
C	0.24432300	-1.41661000	-0.71282400
H	0.14183200	-2.29982500	-1.33361600
C	0.25004800	-0.11628400	1.16307800
H	0.36829000	0.18736000	2.19761500
C	0.24450900	-1.41785200	0.71059900
H	0.14196400	-2.30213800	1.32986500
C	-1.88240100	0.51345200	-0.68668400
H	-2.33074900	-0.30200000	-1.24143000
H	-1.75025200	1.43899500	-1.23886200
C	-1.88282300	0.51194200	0.68742500
H	-1.75110700	1.43615600	1.24192500
H	-2.33088600	-0.30511700	1.24004400

O	2.10341800	0.96937500	0.00039500
H	2.50997600	0.08875500	0.00064000

C₅-SH-Anti-Ethylene

C	-0.47402900	-0.54339400	-0.00041300
H	-0.29280300	-1.61777900	-0.00119700
C	0.14443600	0.20436100	-1.15786600
H	-0.04931100	-0.06556700	-2.18980600
C	0.45106500	1.47761500	-0.70485000
H	0.75977100	2.30739600	-1.33006300
C	0.14465500	0.20266100	1.15804900
H	-0.04895300	-0.06875900	2.18963100
C	0.45119000	1.47659300	0.70687000
H	0.76012300	2.30540400	1.33325200
C	2.08625800	-0.83455000	-0.68995300
H	2.70367100	-0.13489400	-1.24029000
C	2.08551500	-0.83660800	0.68891000
H	1.78129900	-1.72270300	1.23806600
H	2.70280500	-0.13916100	1.24217200
H	-2.36922300	0.90976600	0.00104200
S	-2.31657100	-0.43342000	-0.00031200
H	1.78320200	-1.71905300	-1.24228600

C₅-SiH₃-Anti-Ethylene

C	-0.43191500	-0.61416100	0.00025100
H	-0.26325700	-1.69401200	0.00068000
C	0.17903900	0.13058500	-1.14643400
H	0.00562300	-0.13586600	-2.18457100
C	0.42931900	1.43626300	-0.69782200
H	0.71129100	2.27006100	-1.33022200
C	0.17901400	0.13151400	1.14633500
H	0.00564200	-0.13411100	2.18469100
C	0.42933900	1.43681800	0.69668000
H	0.71134800	2.27111100	1.32841100
C	2.14388000	-0.75422300	-0.69221600
H	2.73810600	-0.03238300	-1.24035300
H	1.91461000	-1.66618600	-1.23529100
C	2.14412900	-0.75323200	0.69277000
H	1.91524500	-1.66441800	1.23730300
H	2.73834300	-0.03038000	1.23958600
Si	-2.31719300	-0.31946500	0.00014600
H	-2.91798100	-0.95840200	-1.19894900
H	-2.91814800	-0.95865200	1.19904000
H	-2.63695500	1.12435600	0.00024700

C₅-H Ethylene

C	-0.36904600	0.00109400	-1.32274000
H	0.49489400	0.00229000	-1.98854500
C	-0.46357500	1.15429200	-0.35970200
H	-0.39767900	2.19226100	-0.66797700
C	-1.17834700	0.70194400	0.74319800
H	-1.55653600	1.32763400	1.54392500
C	-0.46176700	-1.15376400	-0.36148200
H	-0.39494300	-2.19112100	-0.67163600
C	-1.17739300	-0.70441400	0.74202800
H	-1.55500400	-1.33195800	1.54157300
C	1.61665200	0.68971100	0.33376300
H	1.54402100	1.24035100	1.26418600
H	2.05005200	1.23911900	-0.49663500
C	1.61711500	-0.68914600	0.33303400
H	2.05094300	-1.23700700	-0.49816600
H	1.54526700	-1.24071800	1.26296200
H	-1.28285100	0.00084100	-1.93828700

C₅-Br-Syn-Ethylene-Adduct

C	0.07599800	-0.74250500	-0.00010400
C	0.94657000	-0.16878700	1.13016100
H	0.63816700	-0.40421800	2.14909900
C	2.27845900	-0.73248900	0.66910000
H	3.09693000	-1.00061100	1.32796600
C	0.94654900	-0.16846900	-1.13022400
H	0.63812500	-0.40361200	-2.14922200
C	2.27844700	-0.73230100	-0.66934600
H	3.09690500	-1.00023800	-1.32830300
C	0.96302400	1.34824700	0.77651200
H	1.83961300	1.83941200	1.20416400
H	0.06725200	1.83668200	1.16805100
C	0.96301400	1.34846900	-0.77614400
H	0.06724100	1.83702300	-1.16753300
H	1.83960000	1.83975200	-1.20366800
H	0.01884800	-1.82936600	-0.00025700
Br	-1.77185800	-0.10365200	-0.00000100

C₅-Cl-Syn-Ethylene-Adduct

C	-0.86387500	0.10397000	0.00000000
C	0.00434900	-0.47902200	1.12985400
H	-0.33273300	-0.28676800	2.14888000
C	0.00434900	-1.92401200	0.66915200
H	0.07544100	-2.78219200	1.32814100
C	0.00434900	-0.47902200	-1.12985400
H	-0.33273300	-0.28676800	-2.14888000
C	0.00434900	-1.92401200	-0.66915200

H	0.07544100	-2.78219200	-1.32814100
C	1.40804500	0.09776400	0.77639600
H	2.20134000	-0.52098100	1.20160600
H	1.51565100	1.11115400	1.17096500
C	1.40804500	0.09776400	-0.77639600
H	1.51565100	1.11115400	-1.17096500
H	2.20134000	-0.52098100	-1.20160600
H	-1.88345200	-0.27952200	0.00000000
Cl	-0.99138800	1.89861900	0.00000000

C₅-F-Syn-Ethylene-Adduct

C	1.00088900	0.42632000	0.00000000
C	0.15387300	-0.18013800	-1.13008200
H	0.49028700	0.01084900	-2.15012800
C	0.15387300	-1.62036000	-0.66942300
H	0.08940200	-2.48164600	-1.32507400
C	0.15387300	-0.18013800	1.13008200
H	0.49028700	0.01084900	2.15012800
C	0.15387300	-1.62036000	0.66942300
H	0.08940200	-2.48164600	1.32507400
C	-1.23862400	0.42430100	-0.77665900
H	-2.04970000	-0.16835200	-1.20508300
H	-1.31096900	1.44309600	-1.16532200
C	-1.23862400	0.42430100	0.77665900
H	-1.31096900	1.44309600	1.16532200
H	-2.04970000	-0.16835200	1.20508300
F	0.96467800	1.80523900	0.00000000
H	2.04505400	0.10140900	0.00000000

C₅-Me-Syn-Ethylene-Adduct

C	-0.70530200	-0.81880300	-0.00010000
C	0.15784200	-0.19390500	1.12299800
H	-0.11657800	-0.44217700	2.15083000
C	1.53896800	-0.62554600	0.66849800
H	2.38615600	-0.78677400	1.32678400
C	0.15779800	-0.19359400	-1.12305900
H	-0.11666100	-0.44158200	-2.15094900
C	1.53894200	-0.62536100	-0.66873200
H	2.38610400	-0.78640400	-1.32709600
C	0.05924100	1.32526400	0.77688100
H	0.89757300	1.88410500	1.19956800
H	-0.86237800	1.75804100	1.17839000
C	0.05921100	1.32548200	-0.77651300
H	-0.86242400	1.75836800	-1.17786800
H	0.89752700	1.88444100	-1.19907600
H	-0.57989000	-1.90720700	-0.00025400

C	-2.18918800	-0.47928600	-0.00002500
H	-2.67812600	-0.90186400	-0.88423400
H	-2.67810500	-0.90215400	0.88405700
H	-2.37826200	0.59770400	0.00015400

C₅-NH₂-Syn-Ethylene-Adduct

C	0.68070600	-0.84842100	-0.05447600
C	-0.16203900	-0.13091900	-1.13384700
H	0.10631300	-0.34499200	-2.16936000
C	-1.55083500	-0.52833100	-0.68594300
H	-2.40499500	-0.64494100	-1.34437900
C	-0.14989700	-0.24280600	1.11787900
H	0.12252600	-0.55658200	2.12847500
C	-1.54370300	-0.59649900	0.65095100
H	-2.38986400	-0.78705900	1.30269800
C	0.02604400	1.35882100	-0.71008400
H	-0.77902200	1.98864600	-1.09515200
H	0.96899000	1.75430800	-1.10278600
C	0.03439800	1.28024500	0.84321700
H	0.98303000	1.63765200	1.25951900
H	-0.76308600	1.86903500	1.30173100
H	0.53552000	-1.93135100	-0.11152600
N	2.10227600	-0.57715300	-0.13592300
H	2.29911300	0.40566300	0.03599500
H	2.59749800	-1.10284700	0.58006600

C₅-OH-Syn-Ethylene-Adduct

C	0.63924000	-0.89142900	0.00002600
C	-0.15220900	-0.18369300	-1.12998700
H	0.10487800	-0.46480600	-2.15243600
C	-1.55930600	-0.48643600	-0.66954500
H	-2.41484300	-0.60710500	-1.32528200
C	-0.15209000	-0.18354300	1.13002800
H	0.10510300	-0.46452100	2.15248800
C	-1.55923500	-0.48634600	0.66977500
H	-2.41470200	-0.60692500	1.32561900
C	0.12449700	1.30931200	-0.77820400
H	-0.63638700	1.96899300	-1.19997500
H	1.09021500	1.63140100	-1.18584500
C	0.12457900	1.30941600	0.77801700
H	1.09034000	1.63156000	1.18551300
H	-0.63626100	1.96915200	1.19977900
H	0.47126700	-1.97071000	0.00010600
O	2.02869800	-0.70661800	-0.00006100
H	2.21794500	0.24221300	-0.00014200

C₅-SH-Syn-Ethylene-Adduct

C	-0.42845600	-0.74824000	-0.08668900
C	0.46504400	-0.31647000	1.09965900
H	0.17150100	-0.67540200	2.08796200
C	1.80414200	-0.79665600	0.57146200
H	2.63610800	-1.11519500	1.19009300
C	0.45219500	-0.03694900	-1.13628200
H	0.14808700	-0.14322100	-2.17877800
C	1.79633100	-0.63023500	-0.75546500
H	2.62017200	-0.78020800	-1.44458800
C	0.46917800	1.23387000	0.94199400
H	1.34526300	1.67516400	1.42260600
H	-0.42756500	1.66611600	1.39292100
C	0.46344400	1.42788600	-0.59854600
H	-0.42871300	1.97047000	-0.92492100
H	1.33880400	1.97086300	-0.96240600
H	-0.41933400	-1.83009300	-0.23172800
S	-2.15829900	-0.15995000	-0.09087400
H	-2.58280800	-0.97853400	0.88603200

C₅-SiH₃-Syn-Ethylene-Adduct

C	-0.42527400	-0.72688900	-0.00000400
C	0.49777300	-0.18987800	1.12407400
H	0.20599800	-0.40961200	2.15296200
C	1.83644800	-0.74964600	0.66790000
H	2.66842200	-0.97359900	1.32692200
C	0.49777400	-0.18986800	-1.12407400
H	0.20600600	-0.40959500	-2.15296500
C	1.83644700	-0.74964100	-0.66790500
H	2.66842200	-0.97358700	-1.32692700
C	0.54929900	1.33178300	0.77664400
H	1.43740000	1.80683100	1.19988800
H	-0.32722800	1.85320000	1.17451500
C	0.54930000	1.33178800	-0.77663400
H	-0.32722800	1.85320800	-1.17450100
H	1.43739900	1.80684400	-1.19987600
H	-0.40970500	-1.82423900	-0.00000800
Si	-2.23965500	-0.20258700	-0.00000100
H	-2.43211300	1.26950300	0.00004000
H	-2.91139000	-0.75428300	-1.20463500
H	-2.91140900	-0.75434300	1.20459400

C₅-Br-Anti-Ethylene-Adduct

C	0.55217600	-0.31566100	0.00000000
H	1.53594500	-0.78832200	0.00000000
C	-0.36530700	-0.80384200	1.12936200

H	-0.05856100	-0.56072400	2.14672100
C	-1.71068800	-0.27395600	0.66741200
H	-2.53926600	-0.04593400	1.32773800
C	-0.36530700	-0.80384200	-1.12936200
H	-0.05856100	-0.56072400	-2.14672100
C	-1.71068800	-0.27395600	-0.66741200
H	-2.53926600	-0.04593400	-1.32773800
C	-0.36530700	-2.32666000	0.77941500
H	-1.23554700	-2.83102000	1.20433000
H	0.53238200	-2.81176500	1.17425000
C	-0.36530700	-2.32666000	-0.77941500
H	0.53238200	-2.81176500	-1.17425000
H	-1.23554700	-2.83102000	-1.20433000
Br	0.88710300	1.60099000	0.00000000

C₅-Cl-Anti-Ethylene-Adduct

C	-0.79158800	0.14858100	0.00000000
H	-1.77011400	-0.33739800	0.00000000
C	0.12736400	-0.34420200	-1.12921100
H	-0.17991200	-0.10255600	-2.14690800
C	1.47129700	0.18944800	-0.66742700
H	2.29892100	0.42187700	-1.32744900
C	0.12736400	-0.34420200	1.12921100
H	-0.17991200	-0.10255600	2.14690800
C	1.47129700	0.18944800	0.66742700
H	2.29892100	0.42187700	1.32744900
C	0.12736400	-1.86554700	-0.77932200
H	0.99828500	-2.36909000	-1.20369600
H	-0.76952400	-2.35206700	-1.17433600
C	0.12736400	-1.86554700	0.77932200
H	-0.76952400	-2.35206700	1.17433600
H	0.99828500	-2.36909000	1.20369600
Cl	-1.11107000	1.91136400	0.00000000

C₅-F-Anti-Ethylene-Adduct

C₅-Me-Anti-Ethylene-Adduct

C	0.94664400	0.46012100	0.00000000
H	1.90086000	-0.08465100	0.00000000
C	0.02594900	-0.07471600	1.12311700
H	0.31571700	0.15835400	2.15027700
C	-1.32570600	0.44665500	0.66815200

H	-2.16152800	0.65996300	1.32595500
C	0.02594900	-0.07471600	-1.12311700
H	0.31571700	0.15835400	-2.15027700
C	-1.32570600	0.44665500	-0.66815200
H	-2.16152800	0.65996300	-1.32595500
C	0.02594900	-1.59609200	0.77788200
H	-0.84076000	-2.10885700	1.20197000
H	0.92691200	-2.07606400	1.17290600
C	0.02594900	-1.59609200	-0.77788200
H	0.92691200	-2.07606400	-1.17290600
H	-0.84076000	-2.10885700	-1.20197000
C	1.22191600	1.95552800	0.00000000
H	1.80066200	2.24254100	0.88406900
H	1.80066200	2.24254100	-0.88406900
H	0.29146000	2.52873200	0.00000000

C₅-NH₂-Anti-Ethylene-Adduct

C	-0.75241100	-0.75425000	-0.05053800
H	-0.56199300	-1.83339000	-0.11120600
C	0.04886000	0.01061400	-1.12564700
H	-0.27534100	-0.13841500	-2.15654800
C	-0.03070300	1.42754700	-0.58428000
H	0.02199700	2.32620300	-1.18963700
C	0.04742800	-0.11792800	1.12378900
H	-0.27001800	-0.38269200	2.13528800
C	-0.02910600	1.35059600	0.75152800
H	0.02177900	2.17496700	1.45497700
C	1.48986100	-0.48581200	-0.80442500
H	2.24884100	0.20393500	-1.18069700
H	1.66709800	-1.46377200	-1.26242200
C	1.48544200	-0.58442000	0.74992900
H	1.64922400	-1.61547500	1.07935300
H	2.25071300	0.04055900	1.21623400
N	-2.18405800	-0.54839000	-0.13524600
H	-2.64282200	-0.99985100	0.65293900
H	-2.37730100	0.44857700	-0.05369200

C₅-OH-Anti-Ethylene-Adduct

C	0.96249700	0.48265600	0.00000000
H	1.94798700	0.00432900	0.00000000
C	0.04944800	-0.05452800	1.12947300
H	0.35066400	0.18579100	2.15014800
C	-1.29173800	0.48918600	0.66998500
H	-2.12512800	0.72431700	1.32344800
C	0.04944800	-0.05452800	-1.12947300
H	0.35066400	0.18579100	-2.15014800

C	-1.29173800	0.48918600	-0.66998500
H	-2.12512800	0.72431700	-1.32344800
C	0.04944800	-1.57026900	0.77870400
H	-0.81650600	-2.08423400	1.20172400
H	0.95007300	-2.05102800	1.17296700
C	0.04944800	-1.57026900	-0.77870400
H	0.95007300	-2.05102800	-1.17296700
H	-0.81650600	-2.08423400	-1.20172400
O	1.19417100	1.86179100	0.00000000
H	0.31955700	2.28304200	0.00000000

C₅-SH-Anti-Ethylene-Adduct

C	-0.78513900	0.15983800	0.00000000
H	-1.75401000	-0.35161000	0.00000000
C	0.13310600	-0.35829400	-1.12862100
H	-0.16684100	-0.11738500	-2.14898600
C	1.48168200	0.16657800	-0.66859800
H	2.31617200	0.38409500	-1.32612800
C	0.13310600	-0.35829400	1.12862100
H	-0.16684100	-0.11738500	2.14898600
C	1.48168200	0.16657800	0.66859800
H	2.31617200	0.38409500	1.32612800
C	0.13310600	-1.87884400	-0.77865100
H	1.00021600	-2.38995700	-1.20295000
C	0.13310600	-1.87884400	0.77865100
H	-0.76733600	-2.35904400	1.17379000
H	1.00021600	-2.38995700	1.20295000
H	0.05989400	2.37205700	0.00000000
S	-1.20838700	1.92698900	0.00000000
H	-0.76733600	-2.35904400	-1.17379000

C₅-SiH₃-Anti-Ethylene-Adduct

C	0.45775300	-0.64202300	0.00000000
H	0.38586900	-1.73985100	-0.00000100
C	-0.42280200	-0.03943900	1.12423500
H	-0.09637600	-0.20052500	2.15361100
C	-0.53018900	1.40552700	0.66792500
H	-0.70232200	2.24983300	1.32645000
C	-0.42280300	-0.03943800	-1.12423500
H	-0.09637600	-0.20052400	-2.15361100
C	-0.53018900	1.40552700	-0.66792400
H	-0.70232200	2.24983300	-1.32644800
C	-1.80186500	-0.68808700	0.77695700
H	-2.63372300	-0.12060200	1.20142500
H	-1.85162200	-1.70664500	1.17375000
C	-1.80186600	-0.68808700	-0.77695700

H	-1.85162200	-1.70664400	-1.17375100
H	-2.63372300	-0.12060100	-1.20142400
Si	2.29090000	-0.19220800	0.00000000
H	2.93793200	-0.78206300	1.20136100
H	2.93792100	-0.78201300	-1.20139100
H	2.54552300	1.26683200	0.00003000

C₅-H-Ethylene-Adduct

C	-1.12749700	0.78977100	0.00000000
H	-2.12870300	0.34359800	0.00000000
C	-0.22227600	0.25035700	-1.12452000
H	-0.51066400	0.47793300	-2.15212700
C	1.12433700	0.78370800	-0.66816800
H	1.95970800	0.99963900	-1.32570000
C	-0.22227600	0.25035700	1.12452000
H	-0.51066400	0.47793300	2.15212700
C	1.12433700	0.78370800	0.66816800
H	1.95970800	0.99963900	1.32570000
C	-0.22227600	-1.27146700	-0.77687700
H	0.64338100	-1.78459400	-1.20256700
H	-1.12428100	-1.74982200	-1.17169600
C	-0.22227600	-1.27146700	0.77687700
H	-1.12428100	-1.74982200	1.17169600
H	0.64338100	-1.78459400	1.20256700
H	-1.20001700	1.88029600	0.00000000

Br-Cyclopentane

C	-0.78993052	0.86805554	0.00000000
H	-1.15109352	1.92623154	0.00000000
C	-1.33699252	0.10241654	-1.17992100
H	-1.94728764	0.75052022	-1.77355513
C	-2.08446052	-0.94253346	-0.73586700
H	-1.66593160	-1.85988456	-1.09391796
C	-1.33707152	0.10243954	1.17988900
H	-1.94737372	0.75057583	1.77348025
C	-2.08454052	-0.94252146	0.73590900
H	-1.66605722	-1.85986167	1.09404120
Br	1.12006948	0.86805554	0.00000000
H	-0.52619496	-0.26580005	1.77299845
H	-3.08791022	-0.84276243	1.09395562
H	-0.52608610	-0.26584096	-1.77297849
H	-3.08780412	-0.84283474	-1.09400354

Cl-Cyclopentane

C	-0.78993052	0.86805554	0.00000000
H	-1.15109352	1.92623154	0.00000000
C	-1.33699252	0.10241654	-1.17992100
H	-1.94728764	0.75052022	-1.77355513
C	-2.08446052	-0.94253346	-0.73586700
H	-1.66593160	-1.85988456	-1.09391796
C	-1.33707152	0.10243954	1.17988900
H	-1.94737372	0.75057583	1.77348025
C	-2.08454052	-0.94252146	0.73590900
H	-1.66605722	-1.85986167	1.09404120
Cl	0.97006948	0.86805554	0.00000000
H	-0.52619496	-0.26580005	1.77299845
H	-3.08791022	-0.84276243	1.09395562
H	-3.08780412	-0.84283474	-1.09400354
H	-0.52608610	-0.26584096	-1.77297849

Br-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08920446
C	1.38068604	0.00000000	-0.64471874
H	1.96798020	0.78940141	-0.15731516
C	1.10774678	0.36246317	-2.11737614
H	1.01253730	-0.55021281	-2.71122535
C	-0.68712645	1.19757340	-0.64470487
H	-0.29487862	2.09981649	-0.15713222
C	-0.23670129	1.14147708	-2.11733546
H	-0.98108603	0.60527411	-2.71153723
Br	-0.95475025	-1.64853703	-0.51382569
H	-1.77130291	1.19031287	-0.51583519
H	-0.13976977	2.14308484	-2.54296689
H	1.91404929	-0.94391660	-0.51569984
H	1.92843380	0.94448087	-2.54340457

Cl-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09040961
C	1.38954341	0.00000000	-0.62766698
H	1.97997422	0.76645028	-0.10985952
C	1.14569936	0.40609289	-2.09457131
H	1.05408880	-0.48607000	-2.71892775
C	-0.66289452	1.22124809	-0.62764631
H	-0.27117803	2.10578450	-0.10964461
C	-0.18942697	1.20096348	-2.09450882
H	-0.92997675	0.69552298	-2.71923349
Cl	-0.89489452	-1.50395805	-0.48522353
H	-1.74915350	1.22066865	-0.51552880

H	-0.07054610	2.21359687	-2.48737643
H	1.97916108	0.99306527	-2.48790547
H	1.90737274	-0.95486828	-0.51536607

H-Cyclopentane

C	-1.29424400	-0.14014200	0.00577400
H	-1.94065800	-0.11167600	0.88761200
C	-0.23228500	-1.26213800	0.13883800
H	-0.17303800	-1.59874300	1.17984100
C	1.09781900	-0.60404400	-0.25553000
H	1.20263700	-0.58811400	-1.34778700
C	-0.49840600	1.18013800	-0.15021800
H	-0.92078900	2.00027100	0.43684900
C	0.93836700	0.82811500	0.26091500
H	1.68146500	1.52382300	-0.13947800
H	-1.94605400	-0.30730700	-0.85631300
H	-0.50386700	1.49806600	-1.19891000
H	1.02997900	0.83487600	1.35455200
H	-0.46699400	-2.14032700	-0.46887300
H	1.96981300	-1.12244400	0.15382900

F-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09444844
C	1.39821335	0.00000000	-0.62262699
H	2.10540578	0.50743829	0.04014934
C	1.25495865	0.75164417	-1.97301774
H	1.60835292	0.15730684	-2.81881809
C	-0.70704311	1.18762444	-0.63451968
H	-0.34397001	2.11422039	-0.17279727
C	-0.24351647	1.09599499	-2.09281391
H	-0.78024651	0.27777893	-2.58253602
F	-0.66471834	-1.15377496	-0.41052979
H	-1.79073939	1.13385716	-0.50248527
H	-0.42619871	2.00985563	-2.66347822
H	1.73748429	-1.03224866	-0.73827038
H	1.84970982	1.67039106	-1.95487375

Me-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.10063221
C	1.45611301	0.00000000	-0.47881195
H	2.06441819	-0.77548373	-0.00257738
C	1.95801844	1.42645541	-0.18617068
H	2.69796046	1.75722979	-0.91991429
C	-0.48817799	1.37184452	-0.47877475

H	-1.42284274	1.68486506	-0.00271612
C	0.68734702	2.32288898	-0.18571689
H	0.75064659	3.13150954	-0.91881356
C	-0.82821601	-1.17383273	-0.50248684
H	-0.41831849	-2.12874792	-0.15762253
H	-1.86528040	-1.10783455	-0.15759740
H	-0.83918136	-1.18935259	-1.59889961
H	-0.67379874	1.31786519	-1.56031814
H	0.55700243	2.79367109	0.79365401
H	1.46746498	-0.19327363	-1.56029998
H	2.44606640	1.46166393	0.79278450

NH₂-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09935433
C	1.45121793	0.00000000	-0.48491429
H	2.05510358	-0.76780769	0.00468161
C	1.94500391	1.43553334	-0.22999605
H	2.64999155	1.76400929	-0.99800555
C	-0.50179643	1.36821343	-0.48851660
H	-1.44269527	1.67483645	-0.01981201
C	0.66573781	2.32285812	-0.19251871
H	0.71271753	3.14972871	-0.90586377
N	-0.72508087	-1.18681148	-0.43350096
H	-1.68644521	-1.14260099	-0.10118782
H	-0.77892703	-1.18481073	-1.45192454
H	-0.67811582	1.30053226	-1.57138485
H	0.54524437	2.76876019	0.79974714
H	1.45181811	-0.22004069	-1.56179839
H	2.47268088	1.49195212	0.72680067

OH-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09307422
C	1.40952334	0.00000000	-0.59885286
H	2.02719257	0.73678731	-0.07301052
C	1.19093110	0.43418110	-2.06438690
H	1.09869358	-0.44132428	-2.71598892
C	-0.61397030	1.26879182	-0.59883909
H	-0.22009790	2.14569380	-0.07273779
C	-0.12759691	1.26152819	-2.06430459
H	-0.87564694	0.79805254	-2.71637606
O	-0.72804265	-1.16110510	-0.37212118
H	-0.75100967	-1.19746647	-1.33962880
H	-1.70256496	1.27574333	-0.50039551
H	0.02464799	2.27443359	-2.44406290

H	1.89012096	-0.97676177	-0.50016234
H	2.03663430	1.01164456	-2.44477800

SH-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09749253
C	1.44448488	0.00000000	-0.50523776
H	2.06301994	-0.75745139	-0.01762485
C	1.91590814	1.44435463	-0.25167998
H	2.63659921	1.77183055	-1.00519467
C	-0.53843513	1.34038112	-0.50523470
H	-1.47185686	1.63199631	-0.01761910
C	0.62610205	2.31621570	-0.25166880
H	0.66133078	3.10704433	-1.00517143
S	-0.99022403	-1.46491429	-0.43733010
H	-0.88317625	-1.30657002	-1.77004376
H	-0.73907829	1.25451848	-1.58085972
H	0.50169384	2.80712505	0.71811371
H	1.43959825	-0.21819508	-1.58086121
H	2.41782972	1.51190790	0.71809184

C₅-SiH₃-Cyclopentane

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.10035568
C	1.45920633	0.00000000	-0.48710544
H	2.07334037	-0.76564820	-0.00372117
C	1.95479981	1.43370843	-0.20282709
H	2.69255291	1.76124404	-0.94038301
C	-0.49543580	1.37252816	-0.48708011
H	-1.42420325	1.69016464	-0.00382029
C	0.68476495	2.32542751	-0.20250373
H	0.74217438	3.13099706	-0.93959841
Si	-1.02345137	-1.45753376	-0.60747360
H	-0.45663476	-2.74552405	-0.13217603
H	-2.42735700	-1.36176464	-0.13209624
H	-1.02768695	-1.46348140	-2.09444664
H	-0.68736937	1.32924698	-1.56758074
H	0.55379372	2.79770484	0.77594443
H	1.48365440	-0.19543714	-1.56756658
H	2.44406930	1.47099329	0.77532368

Br-Cyclopentene

C	-0.26914200	0.05987800	0.88287300
H	0.07613200	0.10231500	1.91432000
C	-1.08287600	1.22522800	0.41321300

H	-0.84281700	2.24863700	0.67765700
C	-2.05079500	0.82360800	-0.41215000
H	-2.74634700	1.48177500	-0.92257200
C	-1.14268100	-1.15051900	0.54447800
H	-1.78147600	-1.34800600	1.41344100
C	-2.01815000	-0.66989000	-0.62525700
H	-1.54831100	-0.89486400	-1.59219700
Br	1.42271000	-0.00395300	-0.17182700
H	-0.56107200	-2.04827000	0.33165100
H	-3.00908500	-1.13305500	-0.62728100

Cl-Cyclopentene

C	0.34130500	0.03719000	0.74115900
H	0.76428300	0.05998600	1.74554900
C	-0.51281300	1.22012300	0.38844600
H	-0.22426300	2.23728200	0.62789400
C	-1.58548200	0.84394200	-0.30735500
H	-2.32910600	1.52118800	-0.71499800
C	-0.58331500	-1.16008600	0.48874400
H	-1.08432500	-1.39347200	1.43456100
C	-1.62554600	-0.64897600	-0.52322100
H	-1.33997400	-0.88633400	-1.55605000
Cl	1.80375000	-0.00956300	-0.35710500
H	-0.03896000	-2.04745100	0.16241500
H	-2.61630900	-1.08177400	-0.35523600

H-Cyclopentene

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09507581
C	1.38945751	0.00000000	-0.59351751
H	2.17624873	-0.66661946	-0.25399523
C	1.49855078	0.86422379	-1.60081395
H	2.38773328	1.00877196	-2.20675087
C	-0.62270334	1.28505648	-0.58920562
H	-0.49480393	2.10318234	0.12655508
C	0.20128556	1.59462055	-1.85865266
H	-0.28211343	1.20191417	-2.76380949
H	-0.54733491	-0.89917161	-0.31482624
H	-1.69227253	1.18617785	-0.78986527
H	0.33698970	2.66970508	-2.01667313

F-Cyclopentene

C	0.79316900	-0.00333000	0.40685000
H	1.07038200	-0.03293700	1.46866900
C	-0.04061300	1.20806400	0.08736700
H	0.37147500	2.21140500	0.09993200

C	-1.30913500	0.87624900	-0.14149900
H	-2.11005200	1.57859700	-0.35119200
C	-0.10314400	-1.17852100	-0.00789000
H	0.00960700	-2.05469000	0.63398000
C	-1.53830500	-0.61264800	-0.03198900
H	-2.13867100	-1.01077300	-0.85635100
F	1.98417300	-0.01417300	-0.30500300
H	0.20603600	-1.45391700	-1.02076900
H	-2.07817100	-0.84901000	0.89372200

Me-Cyclopentene

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.10114693
C	1.43350635	0.00000000	-0.48608045
H	2.05483044	-0.89153926	-0.46475748
C	1.82944762	1.20595998	-0.88831869
H	2.82520057	1.45274719	-1.24407497
C	-0.51932136	1.35794570	-0.52494399
H	-1.26135481	1.81312670	0.13679885
C	0.73327072	2.23459234	-0.73120804
H	0.64232134	2.90315609	-1.59374696
C	-0.82281589	-1.19313774	-0.47991373
H	-0.41727108	-2.13692991	-0.10094546
H	-1.86217357	-1.11437766	-0.14446648
H	-0.82115317	-1.23913209	-1.57448201
H	-1.00071592	1.18976780	-1.49607637
H	0.93216339	2.87132862	0.14188485

NH₂-Cyclopentene

C	0.77088700	0.00045400	0.41068300
H	0.93463100	-0.04351300	1.49750800
C	-0.08748300	1.20305100	0.09113900
H	0.32137200	2.20844600	0.10352000
C	-1.35297300	0.86647700	-0.14843500
H	-2.15715000	1.56369200	-0.36284200
C	-0.13269600	-1.17546200	-0.04103800
H	-0.00275900	-2.07509900	0.56748500
C	-1.57265400	-0.62423100	-0.02246400
H	-2.19810200	-1.03686800	-0.82108700
N	2.09378800	0.09718500	-0.19992000
H	2.64291300	-0.72657900	0.03737000
H	1.98879300	0.09011100	-1.21374800
H	0.14211700	-1.42787400	-1.07284400
H	-2.07881600	-0.85434400	0.92477200

OH-Cyclopentene

C	0.84745800	-0.01751000	0.47007400
H	1.40330400	-0.04939400	1.41129700
C	-0.03582800	1.20322900	0.33656900
H	0.33264200	2.20731400	0.52089100
C	-1.24060300	0.88749900	-0.13802300
H	-2.02012100	1.60188800	-0.38700900
C	-0.16051000	-1.18314500	0.36222200
H	-0.42928800	-1.52041200	1.36784000
C	-1.41136400	-0.60121400	-0.33083300
H	-1.45851400	-0.84919400	-1.39936500
O	1.85250800	-0.03431100	-0.53539000
H	1.41049700	0.15295500	-1.37692000
H	0.28727700	-2.02841600	-0.16601100
H	-2.34077900	-0.97341100	0.11234300

SH-Cyclopentene

C	0.34326100	-0.01266900	0.72743800
H	0.72685400	-0.03165800	1.75143700
C	-0.49715600	1.20054100	0.42645600
H	-0.18057400	2.20315700	0.69331400
C	-1.58647100	0.87770500	-0.27069100
H	-2.31312200	1.58735200	-0.65330000
C	-0.62375700	-1.18141300	0.44599900
H	-1.11786600	-1.44852100	1.38642600
C	-1.67583100	-0.60877900	-0.52530100
H	-1.43702800	-0.83312900	-1.57372000
S	1.88006400	-0.01910300	-0.29380300
H	1.26589200	0.25853200	-1.45742400
H	-0.11057100	-2.06774900	0.06878900
H	-2.67488800	-1.01463800	-0.33807000

C₅-SiH₃-Cyclopentane

C	0.29496100	0.03000900	0.78540100
H	0.61141300	0.05967300	1.83476500
C	-0.56422400	1.21399400	0.40810800
H	-0.29986300	2.23465900	0.66920000
C	-1.61785800	0.85497300	-0.32615000
H	-2.34306600	1.53889900	-0.75489100
C	-0.65348500	-1.16494100	0.50150100
H	-1.19634000	-1.40967000	1.42087600
C	-1.65333300	-0.63891000	-0.55126500
H	-1.32695200	-0.87811500	-1.57299600
Si	1.83938800	-0.00775500	-0.31327600
H	2.58465600	1.27331800	-0.22484400
H	2.74777900	-1.11538500	0.08410700
H	1.42233100	-0.22026400	-1.72232600

H	-0.13643100	-2.07339100	0.17527100
H	-2.65131900	-1.07190600	-0.42887000

Acetylene

C	0.00000000	0.00000000	0.60101500
H	0.00000000	0.00000000	1.66778000
C	0.00000000	0.00000000	-0.60101500
H	0.00000000	0.00000000	-1.66778000

C₅-Br-Syn-Acetylene

C	0.10745000	-0.77179000	-0.00017100
C	0.99913900	-0.42671400	1.15888000
H	0.66477900	-0.48186600	2.18856500
C	2.29038000	-0.64726600	0.70562700
H	3.17448300	-0.68864700	1.33079900
C	0.99930700	-0.42619800	-1.15899400
H	0.66511300	-0.48117800	-2.18874300
C	2.29050400	-0.64698800	-0.70561100
H	3.17470200	-0.68820600	-1.33065800
C	0.87222500	1.76158900	0.61616500
C	0.87250700	1.76163800	-0.61574100
H	-0.01731000	-1.86121200	-0.00042000
Br	-1.71189400	-0.10617600	-0.00002800
H	0.83282300	2.14595100	-1.61319800
H	0.83261800	2.14568600	1.61370700

C₅-Cl-Syn-Acetylene

C	-0.36073500	-0.80477100	-0.00016800
C	0.51915700	-0.42227700	1.15934400
H	0.18958900	-0.49238500	2.18979300
C	1.81784400	-0.58196600	0.70600500
H	2.70330300	-0.58312500	1.33053400
C	0.51923800	-0.42181200	-1.15946500
H	0.18984100	-0.49169100	-2.18998100
C	1.81792700	-0.58169200	-0.70599400
H	2.70347800	-0.58250500	-1.33039400
C	0.27969000	1.76187300	0.61584300
C	0.27983900	1.76199700	-0.61539800
H	-0.41994200	-1.90113000	-0.00038400
Cl	-2.06144500	-0.26430700	-0.00006400
H	0.22072500	2.13819500	-1.61481500
H	0.21981100	2.13775400	1.61533300

C₅-F-Syn-Acetylene

C	0.33443200	1.02531400	-0.00032500
C	-0.34915300	0.35242900	1.16054100

H	-0.07393400	0.53969400	2.19264600
C	-1.60715100	0.00504000	0.70824100
H	-2.43240500	-0.32119300	1.33015500
C	-0.34924800	0.35183600	-1.16075000
H	-0.07440700	0.53836600	-2.19308400
C	-1.60722900	0.00464000	-0.70790800
H	-2.43260400	-0.32189200	-1.32951000
C	0.76817600	-1.54568700	0.61547200
C	0.76795700	-1.54608100	-0.61487100
H	0.00870400	2.07915300	-0.00058100
F	1.70217600	1.03515600	-0.00029500
H	0.96825500	-1.85849900	-1.61765600
H	0.97011000	-1.85697500	1.61829200

C₅-Me-Syn-Acetylene

C	0.63489600	0.86761400	0.00009300
C	-0.24266600	0.43593600	1.14973500
H	0.06361200	0.52469900	2.18817300
C	-1.55705200	0.48765000	0.70316900
H	-2.43804800	0.41119700	1.33012500
C	-0.24257000	0.43614900	-1.14967900
H	0.06375400	0.52508400	-2.18808800
C	-1.55698500	0.48778700	-0.70321200
H	-2.43792600	0.41146300	-1.33026000
C	0.11428900	-1.72666600	0.61678000
C	0.11444500	-1.72658400	-0.61698700
H	0.53534100	1.96922700	0.00019300
C	2.12359000	0.55837300	0.00008800
H	2.59896300	0.99823100	-0.88297000
H	2.59919800	0.99900500	0.88263100
H	2.31865300	-0.51374600	0.00052100
H	0.18457200	-2.12324500	-1.60837500
H	0.18420400	-2.12346900	1.60812800

C₅-NH₂-Syn-Acetylene

C	-0.53931800	0.94147400	-0.01141800
C	0.28949400	0.41300000	-1.15498800
H	-0.01719000	0.53155900	-2.18897800
C	1.59368500	0.30514800	-0.70126900
H	2.46420700	0.12649700	-1.32195100
C	0.28102600	0.41174500	1.15314500
H	-0.01481200	0.54359500	2.19054900
C	1.59034400	0.31262200	0.70876900
H	2.45946900	0.14607700	1.33534700
C	-0.36907300	-1.68808800	-0.60608000
C	-0.36529500	-1.67755200	0.62811100

H	-0.33969700	2.02742700	-0.01398600
N	-1.97403000	0.78901100	-0.10989000
H	-2.21573400	-0.19044500	0.01150700
H	-2.42737100	1.30980700	0.63642900
H	-0.47916000	-2.06032200	1.62125200
H	-0.49668100	-2.06737400	-1.59855800

C₅-OH-Syn-Acetylene

C	0.40466900	1.01638400	0.00022100
C	-0.33449700	0.37871400	1.15790900
H	-0.05359300	0.54734700	2.19260900
C	-1.61053900	0.09183900	0.70624200
H	-2.45180500	-0.19341800	1.32747700
C	-0.33423400	0.37925000	-1.15790700
H	-0.05325700	0.54828000	-2.19252700
C	-1.61043200	0.09221700	-0.70635900
H	-2.45163800	-0.19273000	-1.32782200
C	0.64249400	-1.58962000	0.61710300
C	0.64269100	-1.58916400	-0.61767200
H	0.09636700	2.07420300	0.00043900
O	1.79873100	1.03969700	0.00039900
H	2.08108700	0.11176800	0.00024300
H	0.82164300	-1.94452700	-1.61147400
H	0.82043900	-1.94621000	1.61064500

C₅-SH-Syn-Acetylene

C	-0.39588200	-0.77271700	-0.00005100
C	0.51272000	-0.43542600	1.15615800
H	0.18455100	-0.49169600	2.18857100
C	1.80889600	-0.63870000	0.70426500
H	2.69411200	-0.66289800	1.32916700
C	0.51280200	-0.43533800	-1.15615100
H	0.18479300	-0.49159600	-2.18861400
C	1.80897100	-0.63863400	-0.70413100
H	2.69425000	-0.66290700	-1.32893800
C	0.39201300	1.74708100	0.61730700
C	0.39210400	1.74706200	-0.61735800
H	-0.46264900	-1.87303400	-0.00009600
S	-2.14165700	-0.28710300	-0.00009900
H	0.36269800	2.14801100	-1.60938500
H	0.36212600	2.14811300	1.60928500
H	-1.94312500	1.03967600	0.00135000

C₅-SiH₃-Syn-Acetylene

C	-0.29582600	-0.85161400	-0.00003100
C	0.59500500	-0.43951000	1.14772100

H	0.29174000	-0.52413500	2.18702600
C	1.91204600	-0.50583700	0.70107700
H	2.79175700	-0.42466200	1.32933200
C	0.59499700	-0.43942000	-1.14775400
H	0.29162300	-0.52386200	-2.18704300
C	1.91205200	-0.50578900	-0.70113900
H	2.79176500	-0.42446100	-1.32937300
C	0.23067200	1.69793200	0.61873500
C	0.23070500	1.69804800	-0.61858200
H	-0.29022900	-1.95588400	-0.00006700
Si	-2.10155000	-0.27599800	-0.00002300
H	-2.41784100	0.51663100	-1.21269700
H	-2.98886600	-1.47177300	-0.00033800
H	-2.41778100	0.51594900	1.21311100
H	0.14590000	2.11679700	-1.60059700
H	0.14573100	2.11651600	1.60080700

C₅-Br-Anti-Acetylene

C	-0.10715000	-0.53006700	-0.00021000
H	-0.16470000	-1.61137300	-0.00044700
C	-0.74464600	0.19186300	1.15860200
H	-0.53942800	-0.07405700	2.18894200
C	-1.13001300	1.43970100	0.70626300
H	-1.48201900	2.25043100	1.33241900
C	-0.74461300	0.19230800	-1.15871800
H	-0.53945500	-0.07332700	-2.18914500
C	-1.12997500	1.43997400	-0.70586100
H	-1.48206200	2.25090800	-1.33170700
C	-2.60280400	-0.96050300	0.61728000
C	-2.60294900	-0.96041500	-0.61738700
Br	1.84150200	-0.15037800	0.00000800
H	-2.93602000	-1.17816900	-1.61083900
H	-2.93600200	-1.17834900	1.61067600

C₅-Cl-Anti-Acetylene

C	0.41567500	-0.57492300	-0.00029900
H	0.27702700	-1.64994000	-0.00069500
C	-0.19834200	0.17690600	1.15969600
H	-0.00845600	-0.09862200	2.19058600
C	-0.52268700	1.43934300	0.70804900
H	-0.83742100	2.26666700	1.33255200
C	-0.19809500	0.17765000	-1.15984600
H	-0.00863100	-0.09731500	-2.19096500
C	-0.52263400	1.43977900	-0.70722900
H	-0.83733300	2.26752200	-1.33119800

C	-2.11055100	-0.89233400	0.61667500
C	-2.11077800	-0.89197200	-0.61699000
Cl	2.22329400	-0.33855700	-0.00001000
H	-2.44854500	-1.08913100	-1.61297700
H	-2.44816400	-1.09040900	1.61253800

C₅-F-Anti-Acetylene

C	0.65480000	-0.76600600	-0.00088800
H	0.28377700	-1.78892100	-0.00220700
C	0.19576700	0.10038000	1.16366000
H	0.31445300	-0.20396700	2.19750000
C	0.14822900	1.39673000	0.71344700
H	0.01875800	2.27604900	1.33382300
C	0.19607700	0.10308600	-1.16359900
H	0.31479300	-0.19920100	-2.19804700
C	0.14839800	1.39834200	-0.71052400
H	0.01850200	2.27898600	-1.32893400
C	-1.90633800	-0.57256800	0.61508000
C	-1.90664500	-0.57068700	-0.61622100
F	2.04307100	-0.83546500	-0.00073600
H	-2.26024200	-0.68754600	-1.61885900
H	-2.25941200	-0.69187800	1.61761700

C₅-Me-Anti-Acetylene

C	-0.70900400	0.71262900	0.00095300
H	-0.39387800	1.75606600	0.00244800
C	-0.13718600	-0.09079400	1.14923600
H	-0.28101300	0.18951000	2.18868300
C	0.03360000	-1.39253100	0.70333300
H	0.26220700	-2.24835200	1.32822700
C	-0.13630900	-0.08781500	-1.14903500
H	-0.28007400	0.19487800	-2.18785300
C	0.03403800	-1.39085100	-0.70615200
H	0.26292900	-2.24521300	-1.33292700
C	1.89684000	0.68834400	0.61804000
C	1.89627000	0.68927200	-0.61665700
C	-2.24895300	0.65863200	0.00019500
H	-2.65061900	1.16173600	0.88524800
H	-2.64987900	1.16517200	-0.88324100
H	-2.59883400	-0.37662400	-0.00195000
H	2.27683900	0.84188800	-1.60520900
H	2.27654300	0.83963000	1.60710000

C₅-NH₂-Anti-Acetylene

C	-0.70497000	-0.73136300	-0.05081500
H	-0.35269400	-1.76021400	-0.10629100

C	-0.15368000	0.16068300	-1.15067800
H	-0.29146900	-0.07445700	-2.20070900
C	-0.02373500	1.43229800	-0.63138200
H	0.18086300	2.32967400	-1.20416900
C	-0.16439900	0.03315900	1.15696400
H	-0.29926800	-0.31329000	2.17781900
C	-0.03032600	1.35513900	0.78564800
H	0.16060600	2.18600100	1.45544100
C	1.90430900	-0.61808000	-0.64125400
C	1.89671300	-0.68428200	0.58957300
N	-2.17188700	-0.76764300	-0.14337300
H	-2.53962600	-1.28200000	0.65515200
H	-2.52283100	0.18551600	-0.05721500
H	2.25548400	-0.87823600	1.57853600
H	2.26866400	-0.70481800	-1.64328800

C₅-OH-Anti-Acetylene

C	-0.67663100	-0.76634600	-0.00065000
H	-0.30155600	-1.78647000	-0.00160100
C	-0.17833100	0.09314100	-1.16095200
H	-0.29996600	-0.20652200	-2.19654100
C	-0.10914400	1.39183800	-0.71140100
H	0.04137200	2.26954900	-1.32977600
C	-0.17814500	0.09109400	1.16101200
H	-0.29967400	-0.21004500	2.19619000
C	-0.10910400	1.39054800	0.71364400
H	0.04154000	2.26714200	1.33357500
C	1.91335200	-0.58648100	-0.61608100
C	1.91267900	-0.58809100	0.61525200
O	-2.08999900	-0.88545000	-0.00086400
H	-2.44396100	0.01769900	0.00116800
H	2.26665000	-0.71297500	1.61676500
H	2.26753100	-0.70899300	-1.61780300

C₅-SH-Anti-Acetylene

C	-0.42999600	-0.57169300	0.00039100
H	-0.27823800	-1.64864100	0.00089000
C	0.21411900	0.15969000	-1.15516100
H	0.02421500	-0.11116200	-2.18789100
C	0.55001700	1.42582400	-0.70673600
H	0.88055200	2.24622600	-1.33265900
C	0.21392900	0.16073700	1.15537800
H	0.02417200	-0.10941400	2.18831200
C	0.54990700	1.42647000	0.70583400
H	0.88040500	2.24742600	1.33105300
C	2.12396300	-0.88631600	-0.61722100

C	2.12405200	-0.88630900	0.61759000
H	-2.27483000	0.94657400	0.00034600
S	-2.26737900	-0.39762400	-0.00006200
H	2.47284500	-1.08963000	1.60872100
H	2.47300300	-1.08981900	-1.60823700

C₅-SiH₃-Anti-Acetylene

C	-0.38458500	0.63472300	-0.00015700
H	-0.23520700	1.71538700	-0.00035700
C	0.24991300	-0.09685200	1.14314800
H	0.08211900	0.17044100	2.18225600
C	0.52417100	-1.39786400	0.69777200
H	0.82240000	-2.22590700	1.32973500
C	0.24978900	-0.09732000	-1.14328600
H	0.08191000	0.16979600	-2.18242600
C	0.52411700	-1.39815500	-0.69736400
H	0.82241000	-2.22641900	-1.32900700
C	2.18738700	0.80673500	0.61930800
C	2.18738500	0.80668500	-0.61948700
Si	-2.26238300	0.29688500	0.00002200
H	-2.87657500	0.92336400	1.19893200
H	-2.87665500	0.92194400	-1.19959300
H	-2.55171900	-1.15378900	0.00082400
H	2.58774800	1.00041200	-1.59383700
H	2.58787700	1.00066400	1.59357000

Maleic Anhydride (MA)

C	-0.00109300	1.25976300	-0.66485900
H	-0.00206600	2.08670600	-1.36184400
C	-0.00109300	1.25976300	0.66485900
H	-0.00206600	2.08670600	1.36184400
C	0.00023300	-0.16277200	1.12414800
C	0.00023300	-0.16277200	-1.12414800
O	0.00023300	-0.60099200	-2.23100700
O	0.00023300	-0.60099200	2.23100700
O	0.00133900	-0.96517800	0.00000000

C₅-Br-Syn-MA

C	1.25388600	0.00212500	0.98152800
C	0.30630200	-1.15855200	1.10977000
C	-0.73416500	-0.69931000	1.91126500
C	0.30651800	1.16366200	1.10407200
C	-0.73394900	0.70863100	1.90794500
C	-0.56706500	-0.69246900	-0.90730600
H	0.13932000	-1.34989200	-1.39500600
C	-0.56711900	0.68861200	-0.91025400

H	0.13887200	1.34391700	-1.40140600
C	-1.95469100	1.13169700	-0.62737300
C	-1.95461900	-1.13457900	-0.62306700
O	-2.42487200	-2.23098400	-0.58042900
O	-2.42499300	2.22812900	-0.58807600
O	-2.70949300	-0.00110800	-0.36056900
Br	2.51265300	-0.00119300	-0.49221600
H	0.61297800	2.19700700	0.99041600
H	1.89137700	0.00426900	1.87310400
H	0.61192100	-2.19261900	1.00060500
H	-1.49682400	-1.32536700	2.35959000
H	-1.49621400	1.33723400	2.35336200

C₅-Cl-Syn-MA

C	1.82916800	-0.00080200	0.59104100
C	0.91241500	-1.16316200	0.86958300
C	0.01416200	-0.70644300	1.82603300
C	0.91281700	1.16127500	0.87209400
C	0.01436300	0.70293600	1.82746300
C	-0.26723200	-0.68897500	-0.99560400
H	0.35035400	-1.34730900	-1.59080200
C	-0.26673600	0.69025600	-0.99467600
H	0.35144600	1.34857100	-1.58927200
C	-1.58818900	1.13377600	-0.48554900
C	-1.58897200	-1.13231200	-0.48682000
O	-2.04759300	-2.22866900	-0.37301800
O	-2.04659600	2.23002300	-0.37055100
O	-2.28633400	0.00043500	-0.09478300
Cl	2.75682500	0.00077300	-0.93201500
H	1.19467600	2.19571000	0.71303800
H	2.58889700	-0.00187500	1.38327100
H	1.19379800	-2.19739600	0.70833800
H	-0.66612100	-1.33268800	2.39117500
H	-0.66567500	1.32824000	2.39393300

C₅-F-Syn-MA

C	2.11607200	-0.00010600	-0.02652000
C	1.31817000	-1.16373200	0.50187800
C	0.68518100	-0.70644800	1.64566100
C	1.31849900	1.16408200	0.50115200
C	0.68539800	0.70780300	1.64520400
C	-0.23506100	-0.68864300	-1.07459100
H	0.25449700	-1.34794400	-1.77729200
C	-0.23515300	0.68832700	-1.07482200
H	0.25421900	1.34747000	-1.77780500
C	-1.40906400	1.13322400	-0.28458600

C	-1.40889900	-1.13346700	-0.28418700
O	-1.83017800	-2.22984900	-0.07036000
O	-1.83054800	2.22960400	-0.07113200
O	-2.00387100	-0.00010500	0.25062200
F	2.36396600	-0.00056000	-1.37571900
H	0.16993600	1.33102800	2.36636000
H	0.16936300	-1.32897200	2.36716500
H	1.54478100	-2.19933700	0.27616900
H	3.09193900	-0.00009900	0.48398900
H	1.54549300	2.19944600	0.27470100

C₅-Me-Syn-MA

C	2.13375200	0.00007000	0.13085300
C	1.27071000	-1.15195200	0.58427400
C	0.51488800	-0.70106300	1.66533300
C	1.27076800	1.15234500	0.58377700
C	0.51493300	0.70194600	1.66504200
C	-0.20440100	-0.69130200	-1.04902900
H	0.29014800	-1.35938000	-1.74082300
C	-0.20448300	0.69116900	-1.04914400
H	0.28981100	1.35918000	-1.74119000
C	-1.43234700	1.13239600	-0.34606100
C	-1.43217500	-1.13262700	-0.34579400
O	-1.87027900	-2.22934000	-0.16578300
O	-1.87079600	2.22900700	-0.16630200
O	-2.06603900	-0.00021400	0.14272300
H	-0.08233400	1.33042100	2.31541200
H	-0.08242200	-1.32924200	2.31594800
H	1.51046800	-2.19312200	0.39254200
H	2.96350300	0.00023700	0.86143500
H	1.51075600	2.19342700	0.39182100
C	2.76938700	-0.00030000	-1.25158900
H	3.40430000	-0.88346200	-1.37102300
H	2.04107200	0.00017100	-2.06416500
H	3.40541800	0.88205100	-1.37103200

C₅-NH₂-Syn-MA

C	2.12899700	-0.00030200	0.06992000
C	1.28835100	-1.15467200	0.55880400
C	0.57955400	-0.70326000	1.66488400
C	1.28895900	1.15487700	0.55800300
C	0.57986200	0.70467200	1.66434500
C	-0.21724400	-0.68875800	-1.06517800
H	0.30099900	-1.33869800	-1.75462200
C	-0.21694400	0.68791600	-1.06572300
H	0.30154100	1.33728600	-1.75550900

C	-1.42319700	1.13304100	-0.32865300
C	-1.42392800	-1.13277100	-0.32795300
O	-1.85644600	-2.22923300	-0.13133800
O	-1.85529700	2.22967800	-0.13239400
O	-2.04541000	0.00021000	0.17770700
N	2.52250400	-0.00088500	-1.32865700
H	3.11020800	0.81068100	-1.50996400
H	3.10724500	-0.81457300	-1.51005900
H	0.01450000	1.33271700	2.34274200
H	0.01410300	-1.33052900	2.34392200
H	3.00249800	-0.00030000	0.75379700
H	1.52063100	-2.19512700	0.35490800
H	1.52150400	2.19503300	0.35289000

C₅-OH-Syn-MA

C	2.12151700	0.00263500	0.01742000
C	1.29682600	-1.16043300	0.53226200
C	0.63031800	-0.70327000	1.65884400
C	1.30623700	1.15974400	0.53134200
C	0.63094800	0.70862700	1.65427800
C	-0.22587200	-0.69071800	-1.06866900
H	0.28050700	-1.34678000	-1.76158100
C	-0.22622900	0.68603000	-1.07325700
H	0.28600900	1.33992500	-1.76458600
C	-1.41590500	1.13188400	-0.30942000
C	-1.41754900	-1.13467500	-0.30668600
O	-1.84450600	-2.23145100	-0.10156700
O	-1.84354400	2.22795000	-0.10425400
O	-2.02617500	-0.00153300	0.21157500
O	2.43800900	0.07324600	-1.34710900
H	3.15758200	-0.54669700	-1.52751600
H	3.04518600	0.00548500	0.62492400
H	1.52130300	-2.20134500	0.32279700
H	0.09031800	-1.32459700	2.36379600
H	0.08813400	1.33545800	2.35186500
H	1.53894100	2.19390500	0.30446300

C₅-SH-Syn-MA

C	1.81708600	0.05626400	0.60115700
C	0.90506200	-1.08987000	0.95780900
C	-0.02143500	-0.58960100	1.86709600
C	0.87846900	1.22048200	0.81493800
C	-0.03184700	0.81383700	1.78764500
C	-0.25082100	-0.72692100	-0.95149800
H	0.37228100	-1.40414600	-1.52165400
C	-0.27085500	0.65429000	-1.00707600

H	0.33777800	1.29272200	-1.63282300
C	-1.61151300	1.09327500	-0.54502600
C	-1.57246700	-1.17103600	-0.44710200
O	-2.01641000	-2.26890700	-0.29440000
O	-2.09155800	2.18507100	-0.48748300
O	-2.29796100	-0.03418600	-0.12058900
S	2.76026800	-0.09494800	-0.95118900
H	3.86928800	0.50868700	-0.49958200
H	-0.73074900	1.46528600	2.29960400
H	-0.71236800	-1.19023500	2.44695400
H	1.14776900	2.24958300	0.60340600
H	2.55405800	0.10719000	1.41504200
H	1.19500900	-2.13006000	0.86019900

C₅-SiH₃-Syn-MA

C	1.78552900	0.02958000	0.65062100
C	0.84853100	-1.11497100	0.94892600
C	-0.11626200	-0.64086300	1.84428400
C	0.84471300	1.18536300	0.88664100
C	-0.11832200	0.75624800	1.80668900
C	-0.25617600	-0.71018000	-0.93698600
H	0.36043400	-1.37648000	-1.52558800
C	-0.27088300	0.67657300	-0.96754000
H	0.33000100	1.32874800	-1.58657600
C	-1.62508100	1.10998500	-0.54706300
C	-1.60036200	-1.15524600	-0.49842900
O	-2.05587500	-2.25416500	-0.39066100
O	-2.10432800	2.20232200	-0.48619300
O	-2.33182900	-0.02288800	-0.17244700
Si	2.95594100	-0.02239700	-0.83804200
H	3.89070400	1.12210700	-0.72726100
H	3.72023900	-1.29081500	-0.76812800
H	2.26339100	0.04899100	-2.14431100
H	1.11749500	2.22430500	0.73134700
H	-0.84237400	1.39912600	2.29404900
H	-0.83838000	-1.25825200	2.36607600
H	1.12628200	-2.15937200	0.84865500
H	2.47517100	0.05409900	1.51587100

C₅-Br-Anti-MA

C	-1.07210100	-0.00004200	0.53499500
C	-0.39433600	-1.15947100	-0.14825100
C	0.06942500	-0.70384000	-1.37539900
C	-0.39464200	1.15947300	-0.14834600
C	0.06935300	0.70378700	-1.37540400
C	1.37750700	-0.69259600	1.14414400

H	1.04106000	-1.35531900	1.92998900
C	1.37754600	0.69231800	1.14449200
H	1.04068100	1.35479200	1.93036500
Br	-2.98548400	-0.00008200	0.06799000
C	2.42360100	1.13452700	0.19020500
C	2.42398000	-1.13432500	0.19002800
O	2.92508600	0.00020500	-0.43069200
O	2.81503200	-2.22949000	-0.07761900
O	2.81415400	2.22983800	-0.07754800
H	-1.05961800	-0.00003300	1.62089300
H	-0.60122000	2.19336400	0.10139100
H	-0.60109800	-2.19332700	0.10147800
H	0.47806100	-1.33189400	-2.15782000
H	0.47788400	1.33185300	-2.15786900

C₅-Cl-Anti-MA

C	-1.62903900	-0.00010800	0.53690900
C	-0.94367500	-1.16085000	-0.14970600
C	-0.48511000	-0.70529600	-1.37544400
C	-0.94383700	1.16100000	-0.14925300
C	-0.48519000	0.70599900	-1.37515900
C	0.83307300	-0.69182200	1.14728400
H	0.49385300	-1.35608000	1.93062600
C	0.83313800	0.69158700	1.14744700
H	0.49393500	1.35569200	1.93092600
C	1.87453000	1.13429400	0.18810600
C	1.87454200	-1.13439000	0.18796500
O	2.37123300	0.00000000	-0.43670800
O	2.26454000	-2.22951700	-0.08082000
O	2.26440600	2.22948000	-0.08065900
Cl	-3.39590800	-0.00015300	0.14522900
H	-1.58162300	-0.00031700	1.62297100
H	-1.14678600	2.19543500	0.10160200
H	-0.07728400	1.33262200	-2.15929300
H	-0.07713700	-1.33154900	-2.15983800
H	-1.14655900	-2.19540200	0.10071700

C₅-F-Anti-MA

C	-1.95122300	0.00004900	0.57426600
C	-1.26994100	-1.16564400	-0.12944200
C	-0.84552600	-0.71073100	-1.35925500
C	-1.26959000	1.16555100	-0.12939500
C	-0.84538800	0.71055900	-1.35925500
C	0.53922800	-0.68930400	1.16365400
H	0.20181700	-1.35744700	1.94437500
C	0.53920700	0.68949600	1.16352500

H	0.20194200	1.35754900	1.94439000
C	1.54715200	1.13418800	0.17039100
C	1.54695800	-1.13425200	0.17046600
O	2.02283700	-0.00009500	-0.47090400
O	1.92900300	-2.22953700	-0.10886000
O	1.92927400	2.22940000	-0.10908700
F	-3.29996200	0.00028300	0.27129600
H	-0.46019400	1.33153100	-2.15973500
H	-0.46046200	-1.33178300	-2.15973800
H	-1.45559100	-2.20290400	0.12391800
H	-1.86699900	0.00001300	1.66233600
H	-1.45503300	2.20288000	0.12386000

C₅-Me-Anti-MA

C	1.96761200	-0.00026800	-0.57162000
C	1.24982600	-1.15100500	0.09790600
C	0.79940600	-0.70249100	1.33651000
C	1.24973900	1.15088200	0.09707800
C	0.79939300	0.70309300	1.33605800
C	-0.54891400	-0.69230200	-1.13652200
H	-0.22594200	-1.35340000	-1.92883900
C	-0.54879900	0.69249600	-1.13632200
H	-0.22610600	1.35362500	-1.92873400
C	-1.58418700	1.13355900	-0.17304900
C	-1.58401100	-1.13373300	-0.17320300
O	-2.07950300	-0.00014400	0.45515900
O	-1.97342200	-2.22908700	0.10074600
O	-1.97387500	2.22884200	0.10089800
C	3.46933200	0.00011500	-0.22124600
H	3.95658200	-0.88410600	-0.64147600
H	3.95579500	0.88550800	-0.63991400
H	3.61484700	-0.00075500	0.86136700
H	1.43607800	2.19240600	-0.14473700
H	0.39046600	1.33185700	2.11856000
H	0.39053800	-1.33076200	2.11943600
H	1.43588100	-2.19264300	-0.14359500
H	1.86987800	-0.00068900	-1.66003600

C₅-NH₂-Anti-MA

C	-1.97613000	-0.00020700	0.56910900
C	-1.25928800	-1.16215000	-0.09815800
C	-0.81321100	-0.72703500	-1.33534600
C	-1.25774200	1.15281400	-0.12936100
C	-0.81223500	0.68792000	-1.35571300
C	0.54670000	-0.68339400	1.15060700
H	0.21442100	-1.34527400	1.93846900

C	0.54388900	0.69807600	1.14367200
H	0.20616200	1.36602800	1.92404600
C	1.56743600	1.13972900	0.16784900
C	1.57393100	-1.12799500	0.17856700
O	2.05892400	0.00421500	-0.46020000
O	1.96490300	-2.22328000	-0.09148900
O	1.95250300	2.23486200	-0.11185600
N	-3.41388700	-0.08935700	0.29723700
H	-3.87939800	0.73333000	0.67487000
H	-3.56538900	-0.07580400	-0.71002500
H	-1.43552900	2.19799600	0.10428200
H	-0.41074200	1.30022400	-2.15510500
H	-0.40632400	-1.36275700	-2.11345300
H	-1.45633300	-2.19600400	0.16249600
H	-1.86040000	0.01482700	1.65477400

C₅-OH-Anti-MA

C	-1.96888300	-0.00082200	-0.56347700
C	-1.26528400	1.15545800	0.14557400
C	-0.82470800	0.68870100	1.36753700
C	-1.26576500	-1.16620900	0.11588200
C	-0.82408700	-0.72840400	1.34821500
C	0.54023800	0.69587800	-1.15604000
H	0.19763700	1.36520600	-1.93316500
C	0.54312900	-0.68358900	-1.16092500
H	0.20676300	-1.34919300	-1.94397900
C	1.56150800	-1.12778200	-0.17920500
C	1.55411100	1.14008200	-0.17118200
O	2.04100900	0.00566800	0.46157000
O	1.93514000	2.23609200	0.11012800
O	1.95056000	-2.22259000	0.09418300
O	-3.34135700	-0.08302400	-0.22128400
H	-1.44027300	2.20051900	-0.08976800
H	-1.85039800	0.01290100	-1.65239400
H	-1.45999700	-2.20015700	-0.14516900
H	-0.42575700	-1.36227700	2.13199600
H	-0.42914100	1.30101800	2.16978200
H	-3.78320400	0.70293000	-0.57234800

C₅-SH-Anti-MA

C	1.64477300	0.00041300	-0.53310800
C	0.93701000	-1.15628900	0.13181400
C	0.46865700	-0.70433800	1.36154800
C	0.93718500	1.15652800	0.13298300
C	0.46865800	0.70336600	1.36220900
C	-0.83750200	-0.69271400	-1.13518200

H	-0.50395800	-1.35387300	-1.92345500
C	-0.83775200	0.69309200	-1.13507700
H	-0.50378800	1.35464800	-1.92282400
C	-1.88894900	1.13419100	-0.18714300
C	-1.88867900	-1.13420300	-0.18726500
O	-2.39204300	-0.00014100	0.43314500
O	-2.28175200	-2.22937900	0.07931800
O	-2.28252200	2.22917400	0.07944400
S	3.45716200	0.00018500	-0.20715300
H	3.35320500	-0.00091300	1.13312900
H	1.14035000	2.19248300	-0.11315800
H	0.04901600	1.33081000	2.13971400
H	0.04904900	-1.33256500	2.13843600
H	1.14077200	-2.19200800	-0.11488500
H	1.59088900	0.00096600	-1.62244100

C₅-SiH₃-Anti-MA

C	-1.62540800	0.00002400	-0.60395200
C	-0.91554700	1.14454500	0.04874600
C	-0.47860500	0.69520500	1.31074700
C	-0.91554800	-1.14452300	0.04870600
C	-0.47861200	-0.69522700	1.31072600
C	0.86677300	0.69655600	-1.11502100
H	0.57983400	1.34709200	-1.93002200
C	0.86676200	-0.69651900	-1.11504200
H	0.57980300	-1.34701400	-1.93006800
C	1.91631600	-1.13352700	-0.16415500
C	1.91635900	1.13350500	-0.16414200
O	2.42105600	-0.00002400	0.45604500
O	2.30642600	2.22890000	0.10943400
O	2.30632400	-2.22894200	0.10942400
Si	-3.46814300	0.00001100	-0.07728900
H	-4.11723200	1.20442400	-0.64766600
H	-4.11715700	-1.20464500	-0.64724600
H	-3.58713800	0.00026000	1.39520300
H	-1.10399000	2.18625900	-0.19078300
H	-0.07623000	1.33035000	2.09096600
H	-0.07625100	-1.33040700	2.09092200
H	-1.10399800	-2.18623200	-0.19084300
H	-1.60903200	0.00004200	-1.69732000

Tetracyanoethylene (TCNE)

C	0.00003200	0.67880600	0.00000000
C	-0.00003200	-0.67880600	0.00000000
C	1.22612000	-1.42366000	0.00000000
C	-1.22615200	-1.42369300	0.00000000

C	-1.22612000	1.42366000	0.00000000
C	1.22615200	1.42369300	0.00000000
N	2.20898900	-2.03234700	0.00000000
N	-2.20898900	-2.03243300	0.00000000
N	-2.20898900	2.03234700	0.00000000
N	2.20898900	2.03243300	0.00000000

C₅-Br-Syn-TCNE

C	-0.82976100	1.41367000	-0.01222700
C	0.12654200	1.39444000	-1.17009100
H	-0.19041400	1.30445300	-2.20369400
C	1.27471400	2.05200600	-0.71780600
H	2.09012500	2.38628300	-1.34782900
C	0.12550100	1.41566800	1.14646500
H	-0.19139300	1.34151700	2.18133500
C	1.27427300	2.06436700	0.68349700
H	2.08936100	2.40958600	1.30800000
C	0.86529800	-0.69902000	-0.70559800
C	0.86479900	-0.68787900	0.71706800
H	-1.28551400	2.41197400	-0.02179400
Br	-2.33149900	0.21961300	-0.00195400
C	2.13424100	-0.55156100	1.39167600
C	2.13577600	-0.57493900	-1.38121800
C	-0.10463800	-1.44134700	1.47285600
C	-0.10364900	-1.46504700	-1.44949000
N	-0.82689300	-2.05181900	2.13855800
N	-0.82578100	-2.08665600	-2.10491700
N	3.14751500	-0.41880800	1.93322900
N	3.14968800	-0.45163700	-1.92378400

C₅-Cl-Syn-TCNE

C	-1.09214500	-1.48453100	-0.31940000
C	-0.13661900	-1.65232400	0.83058200
H	-0.45764600	-1.81010400	1.85480900
C	1.05433700	-2.11136400	0.26372700
H	1.89221800	-2.51797300	0.81722600
C	-0.13624200	-1.16598900	-1.43660400
H	-0.45616000	-0.88884300	-2.43544400
C	1.05462800	-1.81680600	-1.10768800
H	1.89265500	-1.95943100	-1.77925400
C	0.43796400	0.54675300	0.84445800
C	0.43727600	0.84706500	-0.54419600
H	-1.45978100	-2.49719200	-0.53676600
Cl	-2.54630200	-0.50250800	-0.10878700
C	1.71018500	0.96027000	-1.21611500
C	1.71213900	0.37124700	1.50051300

C	-0.59736400	1.04487400	1.71464600
C	-0.59983700	1.65824500	-1.13027800
N	-1.38862500	2.32661700	-1.64846800
N	-1.38341000	1.44120400	2.46463900
N	2.72757400	1.02937100	-1.76177800
N	2.73159100	0.20731400	2.02145500

C₅-F-Syn-TCNE

C	0.79146100	-0.00165500	1.77916800
C	-0.12368100	-1.16428600	1.49866400
H	0.20026800	-2.19937500	1.51449500
C	-1.41336200	-0.70605800	1.74174100
H	-2.29706800	-1.32920700	1.80829700
C	-0.12360500	1.16147400	1.50039800
H	0.20029400	2.19655100	1.51823000
C	-1.41331300	0.70290000	1.74285300
H	-2.29698000	1.32599100	1.81051600
C	-0.00654400	-0.70728000	-0.72681900
C	-0.00637800	0.70862700	-0.72534500
H	1.00164100	-0.00241900	2.86052200
F	1.98338600	-0.00124700	1.12158800
C	-1.21899300	1.39874500	-1.09107100
C	-1.21945800	-1.39634100	-1.09355300
C	1.20570300	1.44701000	-0.97488600
C	1.20522000	-1.44550100	-0.97764500
N	2.14645700	2.08590400	-1.18384500
N	2.14578600	-2.08430900	-1.18772200
N	-2.19725100	1.95447400	-1.35882700
N	-2.19798300	-1.95123000	-1.36209100

C₅-Me-Syn-TCNE

C	-1.18346300	0.00084200	1.60481400
C	-0.21808500	1.15130500	1.48833100
H	-0.52560200	2.19227300	1.45152500
C	1.02715600	0.70001600	1.94190900
H	1.88587200	1.32949000	2.14220300
C	-0.21786700	-1.14954000	1.48922100
H	-0.52489600	-2.19067600	1.45316100
C	1.02726700	-0.69756000	1.94255400
H	1.88595500	-1.32670300	2.14396000
C	0.21483800	0.71000800	-0.70670900
C	0.21487600	-0.71072600	-0.70575900
H	-1.40117400	0.00109800	2.68995900
C	-2.54011100	0.00041400	0.91370200
H	-3.10340400	-0.88510400	1.22136300
H	-3.10351600	0.88619800	1.22032100

H	-2.49743000	-0.00040500	-0.17179100
C	1.48133100	-1.39581900	-0.79004900
C	1.48126600	1.39498400	-0.79165800
C	-0.88803900	-1.45495700	-1.25672400
C	-0.88813100	1.45354600	-1.25858900
N	-1.75802900	-2.08673400	-1.68441300
N	-1.75809700	2.08478000	-1.68714800
N	2.49502900	-1.95062600	-0.84022500
N	2.49509200	1.94954500	-0.84206400

C₅-NH₂-Syn-TCNE

C	0.96284500	0.00070000	1.71975100
C	0.01258300	-1.15235400	1.51286900
H	0.32426400	-2.19265300	1.50923300
C	-1.26550100	-0.69957600	1.83993500
H	-2.14000500	-1.32770600	1.96024100
C	0.01326400	1.15406600	1.51208900
H	0.32552100	2.19418200	1.50699600
C	-1.26510900	0.70227400	1.83936700
H	-2.13933800	1.33097700	1.95865200
C	-0.07673500	-0.70873200	-0.71675500
C	-0.07658600	0.70781100	-0.71776200
H	1.13839500	0.00084800	2.81639500
N	2.17001200	0.00013000	0.93862500
H	2.73542900	0.82552700	1.12031600
H	2.73659800	-0.82379300	1.12330700
C	-1.32429500	-1.38791800	-0.97496500
C	-1.32390900	1.38706300	-0.97670600
C	1.08741000	1.47396500	-1.08772500
C	1.08697600	-1.47553400	-1.08607400
N	-2.32530000	-1.93754500	-1.15877400
N	-2.32466100	1.93695900	-1.16110900
N	1.95625400	-2.17472600	-1.39266400
N	1.95704900	2.17261700	-1.39454800

C₅-OH-Syn-TCNE

C	0.92224900	-0.24132200	1.70817600
C	-0.00367900	-1.36891100	1.30067900
H	0.32227900	-2.39263200	1.14046300
C	-1.28660000	-0.98999000	1.68650400
H	-2.15280700	-1.64041600	1.70609500
C	-0.03763500	0.91625000	1.67822200
H	0.27279000	1.94431400	1.83259300
C	-1.30835400	0.39841600	1.90785000
H	-2.19525700	0.98354600	2.11880500
C	-0.03752000	-0.58501500	-0.82482500

C	-0.08996500	0.81428200	-0.61840100
H	1.12510600	-0.41753600	2.78268700
O	2.09949400	-0.00430900	1.00994100
H	2.62681600	-0.81575800	0.94786000
C	-1.36033500	1.47559700	-0.79104500
C	-1.23745700	-1.27552000	-1.22939100
C	1.18596000	-1.23800500	-1.21552200
C	1.05641000	1.65362800	-0.85689000
N	-2.38458600	2.00039500	-0.90662400
N	-2.19973200	-1.84075500	-1.53311000
N	1.92803000	2.38321500	-1.06914000
N	2.14009900	-1.82621200	-1.50258000

C₅-SH-Syn-TCNE

C	-1.12687600	-0.40348000	1.42692800
C	-0.12886700	0.70085800	1.68276200
H	-0.41407500	1.72147200	1.91938400
C	1.04347800	0.07346300	2.12378400
H	1.89074000	0.57833200	2.57215900
C	-0.19223700	-1.52502100	1.07425900
H	-0.52806600	-2.49490800	0.72197300
C	1.01041800	-1.27115800	1.73899100
H	1.83032000	-1.97287500	1.83138600
C	0.47184000	0.87716900	-0.45516200
C	0.45312400	-0.47894000	-0.88310000
H	-1.48994800	-0.67470400	2.43068300
S	-2.59777700	-0.17775000	0.38766100
C	1.71358400	-1.16569600	-1.02381700
C	1.76000400	1.49371500	-0.22961900
C	-0.58134000	-0.98629100	-1.74617900
C	-0.52950600	1.81959100	-0.89515800
N	-1.37182100	-1.45435000	-2.44983200
N	-1.26561900	2.64553700	-1.23184900
N	2.72211800	-1.72462200	-1.11702700
N	2.78582500	1.98758600	-0.02697900
H	-3.17978700	0.70236200	1.21951600

C₅-SiH₃-Syn-TCNE

C	1.17845200	0.00054100	-1.30828100
C	0.20976900	1.14713000	-1.38113300
H	0.50545600	2.18921400	-1.30153100
C	-0.94233800	0.69675200	-2.04943500
H	-1.75703000	1.33001600	-2.37950600
C	0.20962500	-1.14584900	-1.38222300
H	0.50513100	-2.18806000	-1.30364200
C	-0.94242200	-0.69463700	-2.05011700

H	-1.75719400	-1.32745400	-2.38084600
C	-0.58992500	0.71273400	0.66702800
C	-0.59020200	-0.71332400	0.66624500
H	1.61302900	0.00099200	-2.32929700
Si	2.84929700	0.00011000	-0.35871400
H	2.82107100	-0.00178000	1.10691300
H	3.53444700	-1.20971800	-0.87021800
H	3.53354100	1.21172500	-0.86718800
C	0.42358200	-1.45405800	1.36988600
C	0.42438400	1.45219000	1.37129200
C	-1.85635200	1.39625900	0.57085400
C	-1.85692400	-1.39617900	0.56920300
N	1.23220400	-2.09328700	1.89630400
N	1.23350900	2.09036200	1.89822400
N	-2.86858900	-1.94716200	0.46497600
N	-2.86776600	1.94782400	0.46726700

C₅-Br-Anti-TCNE

C	-1.01792700	0.18705500	-0.00011600
H	-0.86346800	1.26413500	-0.00035500
C	-0.44133800	-0.58138500	1.15559900
H	-0.60230200	-0.29581200	2.18938000
C	-0.13427200	-1.86429100	0.70053600
H	0.17420500	-2.69054200	1.32918800
C	-0.44177200	-0.58151600	-1.15592000
H	-0.60212400	-0.29530100	-2.18961200
C	-0.13453400	-1.86439600	-0.70082100
H	0.17457100	-2.69046800	-1.32940200
C	1.54702800	0.37584000	0.71284300
C	1.54768000	0.37513500	-0.71285400
Br	-2.96644300	-0.03541400	0.00018400
C	2.38882800	-0.56430400	-1.40820400
C	2.38818100	-0.56254700	1.40986700
C	1.25509800	1.59981900	1.41293200
C	1.25603100	1.59829800	-1.41457500
N	0.97743700	2.56908800	-1.97893300
N	0.97638000	2.57142600	1.97581000
N	3.04242000	-1.34010800	-1.96386700
N	3.04185000	-1.33737300	1.96679500

C₅-Cl-Anti-TCNE

C	-1.51385500	0.12926400	0.00011800
H	-1.35871600	1.20731600	0.00005400
C	-0.90533800	-0.62463000	1.15769100
H	-1.07131500	-0.34391900	2.19209400
C	-0.56402400	-1.89500000	0.70249300

H	-0.23119100	-2.71325900	1.32947100
C	-0.90571800	-0.62453700	-1.15769500
H	-1.07199800	-0.34361400	-2.19199400
C	-0.56428300	-1.89494600	-0.70279100
H	-0.23144900	-2.71305600	-1.32996500
C	1.05834100	0.39798300	0.71188000
C	1.05845200	0.39769400	-0.71208400
Cl	-3.30185900	-0.09485100	0.00039400
C	1.92358300	-0.51975400	-1.40760200
C	1.92363900	-0.51877600	1.40815100
C	0.72871400	1.61024400	1.41534500
C	0.72901000	1.60959500	-1.41624300
N	0.42227000	2.57050300	-1.98289900
N	0.42177300	2.57163700	1.98106600
N	2.59827000	-1.27795200	-1.96228700
N	2.59842100	-1.27616100	1.96384300

C₅-F-Anti-TCNE

C	1.80404300	-0.00846400	0.00031800
H	1.69555600	-1.09479800	0.00003600
C	1.14356500	0.71481700	1.16415400
H	1.31590900	0.44733600	2.20103400
C	0.74046400	1.95694400	0.70850400
H	0.36797700	2.76292000	1.32987800
C	1.14418900	0.71521300	-1.16362600
H	1.31648800	0.44765200	-2.20049100
C	0.74075700	1.95714600	-0.70786500
H	0.36862000	2.76329700	-1.32921600
C	-0.77072700	-0.45079900	0.70856300
C	-0.77054200	-0.45042000	-0.70903100
F	3.15364800	0.27227300	0.00082500
C	-1.67690400	0.42348900	-1.40744600
C	-1.67710100	0.42290400	1.40726000
C	-0.35375200	-1.63032400	-1.42054300
C	-0.35449000	-1.63123900	1.41957400
N	0.01407200	-2.56513200	-1.99438700
N	0.01272800	-2.56650000	1.99306500
N	-2.38949000	1.14451900	1.96366600
N	-2.38936600	1.14533300	-1.96346400

C₅-Me-Anti-TCNE

C	1.80462200	-0.01028100	0.00005900
H	1.67801400	-1.09625800	0.00015700
C	1.12129700	0.68595000	1.14789100
H	1.28981100	0.42597300	2.18869500
C	0.69272700	1.93918700	0.69984100

H	0.30090400	2.72888400	1.32982900
C	1.12121700	0.68581400	-1.14781200
H	1.28988600	0.42591900	-2.18861300
C	0.69266600	1.93910300	-0.69983900
H	0.30078400	2.72872700	-1.32988100
C	-0.77735100	-0.42737000	0.71250100
C	-0.77742500	-0.42741900	-0.71238700
C	3.32258000	0.28238000	-0.00007200
H	3.78564200	-0.16004500	0.88509100
H	3.78563500	-0.16086600	-0.88482300
H	3.51357900	1.35789400	-0.00057400
C	-1.70228900	0.42779600	-1.41079100
C	-1.70231800	0.42781900	1.41077800
C	-0.37860000	-1.61973500	-1.41417200
C	-0.37864400	-1.61974100	1.41424000
N	-2.42334400	1.13663000	-1.97274900
N	-2.42341300	1.13675700	1.97255500
N	-0.01765300	-2.56175000	-1.98098900
N	-0.01775200	-2.56181300	1.98099700

C₅-NH₂-Anti-TCNE

C	-1.82014200	0.01520900	-0.02611300
H	-1.68419900	-1.06877700	-0.03962900
C	-1.11319300	0.72671500	-1.16288800
H	-1.28632800	0.47434900	-2.20376100
C	-0.67590100	1.96008700	-0.69335200
H	-0.26588000	2.75452300	-1.30600700
C	-1.13476300	0.70191600	1.14815800
H	-1.31238400	0.43040600	2.18468900
C	-0.69060000	1.94676000	0.71618100
H	-0.29963000	2.73200600	1.35261600
C	0.78133500	-0.43464200	-0.70929600
C	0.76388900	-0.45507300	0.71131000
N	-3.26089500	0.25495800	-0.11945800
H	-3.73590600	-0.23228000	0.63657900
H	-3.45723000	1.24832500	-0.01296000
C	1.68116300	0.38499600	1.43660400
C	1.71707300	0.42928500	-1.38166400
C	0.32483200	-1.64232600	1.39672400
C	0.37450800	-1.60842400	-1.43670800
N	2.39968500	1.07912600	2.01983100
N	2.45089400	1.14498300	-1.91767500
N	-0.06617800	-2.57890500	1.95243200
N	0.01825600	-2.54095900	-2.02159500

C₅-OH-Anti-TCNE

C	1.82228500	-0.03467600	-0.00006000
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H	1.67859600	-1.11621600	0.00001600
C	1.14844700	0.68821300	1.16069700
H	1.31649200	0.41908700	2.19840800
C	0.75003900	1.93691300	0.70743200
H	0.37763200	2.74315100	1.32879100
C	1.14856800	0.68802000	-1.16101300
H	1.31674500	0.41873200	-2.19865600
C	0.75008800	1.93680100	-0.70795500
H	0.37765500	2.74292300	-1.32944900
C	-0.77776200	-0.43415500	0.70936600
C	-0.77785900	-0.43434000	-0.70930600
O	3.22090400	0.14609300	-0.00003500
H	3.40396400	1.09873300	-0.00015800
C	-0.38376100	-1.62302600	-1.41932200
C	-0.38357500	-1.62266800	1.41961200
C	-1.67739700	0.44750200	-1.40738300
C	-1.67720600	0.44779600	1.40739000
N	-0.03802800	-2.56543600	-1.99442500
N	-0.03771700	-2.56488300	1.99496100
N	-2.38295200	1.17547600	-1.96431200
N	-2.38266200	1.17577900	1.96443100

C₅-SH-Anti-TCNE

C	-1.52393700	0.11724900	-0.00011400
H	-1.36905700	1.19880700	-0.00046800
C	-0.89382800	-0.61545700	1.15296900
H	-1.06181100	-0.33828200	2.18833300
C	-0.53516400	-1.88938700	0.70090400
H	-0.18534400	-2.69894300	1.33012100
C	-0.89390700	-0.61613600	-1.15276700
H	-1.06089800	-0.33926200	-2.18836700
C	-0.53517400	-1.88977900	-0.69998800
H	-0.18490300	-2.69951100	-1.32872700
C	1.05794300	0.39069700	0.71352300
C	1.05792800	0.39044500	-0.71373200
H	-3.38340500	-1.37559700	-0.00012900
S	-3.35867400	-0.03130500	0.00014000
C	1.93658900	-0.51423300	-1.40908600
C	1.93705300	-0.51339400	1.40924100
C	0.73002000	1.60634500	-1.41205200
C	0.72986200	1.60675700	1.41138500
N	2.62023000	-1.26307400	-1.96574800
N	2.62095800	-1.26174200	1.96624600
N	0.42098200	2.57029800	-1.97243600
N	0.42067300	2.57095000	1.97126800

C₅-SiH₃-Anti-TCNE

C	-1.49615800	0.20219000	0.00008500
H	-1.35965000	1.28865100	0.00011600
C	-0.88275700	-0.53346500	1.13963600
H	-1.02877100	-0.26062800	2.18078200
C	-0.58596800	-1.84512400	0.69157400
H	-0.27488600	-2.66397000	1.32856900
C	-0.88271800	-0.53333700	-1.13954800
H	-1.02875400	-0.26038000	-2.18066200
C	-0.58596600	-1.84505700	-0.69161300
H	-0.27487900	-2.66384100	-1.32868600
C	1.06434800	0.34347000	0.71847900
C	1.06419300	0.34357700	-0.71844800
Si	-3.40291400	-0.08004800	-0.00005900
H	-3.95676200	0.55972800	1.21226500
H	-3.95650600	0.55992100	-1.21240500
H	-3.67461500	-1.53236400	-0.00026000
C	0.81507600	1.58700600	-1.40347200
C	0.81524600	1.58673000	1.40379900
C	1.92833800	-0.57919100	1.41109300
C	1.92820600	-0.57884700	-1.41137100
N	2.59125800	-1.34234800	-1.97293900
N	2.59141900	-1.34290400	1.97234100
N	0.55907100	2.57140800	1.95483600
N	0.55890700	2.57182100	-1.95426400

1,2,4-triazoline-3,5-dione (TAD)

N	-0.00967900	-0.94432900	0.00000000
N	0.00860500	1.25738700	-0.61640800
N	0.00860500	1.25738700	0.61640800
C	-0.00152900	-0.15232900	-1.12830600
C	-0.00152900	-0.15232900	1.12830600
O	-0.00152900	-0.45070200	2.27966800
O	-0.00152900	-0.45070200	-2.27966800
H	-0.00991400	-1.95393300	0.00000000

C₅-Br-Syn-TAD

C	-1.27369000	0.00050100	-0.97371800
C	-0.32753900	-1.15823600	-1.12732300
H	-0.60766600	-2.18831500	-0.94774300
C	0.73055900	-0.70789800	-1.89988500
H	1.49836400	-1.33855800	-2.33227300
C	-0.32741900	1.15925300	-1.12600500
H	-0.60727700	2.18926600	-0.94565000
C	0.73069000	0.70930900	-1.89914600
H	1.49862400	1.34027900	-2.33084200

N	2.70055100	-0.00049200	0.51448300
N	0.54566600	0.64387900	0.78397600
N	0.54541500	-0.64411300	0.78379200
C	1.91327400	1.13373700	0.60706300
C	1.91277200	-1.13444900	0.60653800
O	2.24962700	-2.28323200	0.60059000
O	2.25057900	2.28239100	0.60180500
H	3.70808900	-0.00069000	0.45653400
H	-1.92497400	0.00115200	-1.85602800
Br	-2.46457500	-0.00013200	0.53245500

C₅-Cl-Syn-TAD

C	1.84364300	-0.00067100	0.54883300
C	0.93754200	-1.16176000	0.86530500
H	1.18120000	-2.19188500	0.63899000
C	0.03143600	-0.71155900	1.80867700
H	-0.64796000	-1.34131900	2.37072200
C	0.93755100	1.15969600	0.86806400
H	1.18107400	2.19031900	0.64386500
C	0.03144800	0.70745000	1.81029600
H	-0.64789000	1.33598400	2.37377800
N	-2.32383800	0.00053700	-0.22512300
N	-0.25075500	0.64342900	-0.87738900
N	-0.25098000	-0.64201500	-0.87829800
C	-1.56628900	1.13449700	-0.46009400
C	-1.56663300	-1.13329500	-0.46156200
O	-1.89712400	-2.28195800	-0.39942900
O	-1.89651500	2.28314800	-0.39648500
H	-3.30510800	0.00052000	0.01103700
H	2.62378700	-0.00163500	1.32221400
Cl	2.69710700	0.00109900	-1.00027900

C₅-F-Syn-TAD

C	-2.12131300	-0.00004300	-0.07104500
C	-1.33377900	1.16337100	0.47578200
H	-1.51090900	2.19423300	0.19704700
C	-0.68707200	0.71147800	1.60724700
H	-0.16777800	1.33636500	2.32419900
C	-1.33394700	-1.16376800	0.47521700
H	-1.51120100	-2.19448000	0.19603800
C	-0.68715500	-0.71246400	1.60690800
H	-0.16786900	-1.33774800	2.32352100
N	2.07581300	0.00022000	0.14692300
N	0.21518300	-0.64164900	-0.97862300
N	0.21497400	0.64173100	-0.97846400
C	1.39849400	-1.13331400	-0.26590700

C	1.39813200	1.13363400	-0.26568400
O	1.70705100	2.28204700	-0.13231000
O	1.70777800	-2.28165500	-0.13275900
H	2.97829200	0.00031000	0.59863000
H	-3.09597000	-0.00008500	0.44521900
F	-2.35390500	0.00031000	-1.40756200

C₅-Me-Syn-TAD

C	2.13209700	0.00000100	0.08205400
C	1.29367900	-1.15064600	0.57504800
H	1.48713600	-2.18779100	0.32672700
C	0.52676000	-0.70632300	1.64268300
H	-0.06815200	-1.33836400	2.29151900
C	1.29363900	1.15060900	0.57507400
H	1.48707800	2.18776800	0.32679700
C	0.52674100	0.70623700	1.64270200
H	-0.06818700	1.33824400	2.29155700
N	-2.11522400	0.00001700	0.02546600
N	-0.18112400	0.64482100	-0.95406400
N	-0.18114200	-0.64480900	-0.95408600
C	-1.40321600	1.13443500	-0.32454300
C	-1.40324300	-1.13441200	-0.32457200
O	-1.72185100	-2.28321700	-0.20523700
O	-1.72179500	2.28324600	-0.20518200
H	-3.03747300	0.00002300	0.43480700
H	3.00360400	0.00001800	0.76222300
C	2.65146000	0.00002500	-1.34663800
H	1.83537300	-0.00022500	-2.06731500
H	3.27213800	0.88456500	-1.51757500
H	3.27257300	-0.88423300	-1.51744900

C₅-NH₂-Syn-TAD

C	2.14080000	0.01136900	0.00657200
C	1.34999000	-1.14521100	0.55854300
H	1.55263300	-2.17599200	0.29503500
C	0.60986200	-0.69676100	1.63495800
H	0.05241800	-1.32648900	2.31848300
C	1.29928700	1.16868600	0.52328600
H	1.47016200	2.20643900	0.26005200
C	0.59042400	0.72197600	1.62314500
H	0.02377000	1.34722100	2.30377600
N	-2.09583100	-0.00881600	0.09126800
N	-0.20873500	0.64091100	-0.97280200
N	-0.20435900	-0.64497400	-0.97423700
C	-1.41226800	1.12820900	-0.29770800
C	-1.39794900	-1.14139400	-0.29538000

O	-1.70921600	-2.29022000	-0.16784900
O	-1.73189200	2.27578400	-0.17692500
H	-3.00390700	-0.01436500	0.53126800
H	3.04732700	0.04150300	0.63730400
N	2.56845400	-0.10423600	-1.36083300
H	1.75571700	-0.12367700	-1.97081600
H	3.13316200	0.69941400	-1.62117500

C₅-OH-Syn-TAD

C	2.13803700	0.01294900	-0.06056900
C	1.36017500	-1.10850000	0.59403400
H	1.54043500	-2.15757400	0.39287100
C	0.67327000	-0.58252500	1.66616100
H	0.14648900	-1.15565900	2.42042500
C	1.33660700	1.20908700	0.41536100
H	1.51147600	2.22048200	0.06965600
C	0.66371300	0.83654700	1.56180300
H	0.13071300	1.50834900	2.22488300
N	-2.07714900	-0.03533000	0.14439000
N	-0.23616400	0.61079000	-1.00074200
N	-0.21188300	-0.67257900	-0.96194500
C	-1.42746900	1.10106000	-0.30172300
C	-1.37950500	-1.16878400	-0.23694500
O	-1.66864500	-2.31816200	-0.07372100
O	-1.76172400	2.24570600	-0.20579800
H	-2.97505400	-0.04147500	0.60509900
H	3.08934200	0.07094200	0.49464700
H	1.65764600	-0.24728000	-1.89230000
O	2.47866300	-0.09216400	-1.39747100

C₅-SH-Syn-TAD

C	1.82880600	0.14214600	0.55856300
C	0.95123200	-0.95954900	1.09126900
H	1.21487100	-2.00848700	1.03582200
C	0.00403300	-0.38735600	1.92006800
H	-0.67944600	-0.93478300	2.55848700
C	0.88549300	1.31509100	0.68509400
H	1.10961100	2.30453400	0.30612700
C	-0.02862600	1.00803300	1.68463000
H	-0.73694400	1.70506000	2.11667500
N	-2.31738300	-0.12937300	-0.25107000
N	-0.26816700	0.55559700	-0.92183300
N	-0.20039800	-0.72457800	-0.78622300
C	-1.61815400	1.01501100	-0.58475700
C	-1.49215200	-1.23933300	-0.34793900
O	-1.76771300	-2.39053600	-0.16864300

O	-2.01035900	2.14455500	-0.64954200
H	-3.30159100	-0.16129600	-0.03037100
H	2.60817000	0.29934100	1.31663800
S	2.65460800	-0.17493100	-1.02810000
H	3.85400800	0.28658700	-0.63599600

C₅-SiH₃-Syn-TAD

C	-1.79208200	-0.29885900	-0.62515800
C	-0.80171000	-1.43248500	-0.56616000
H	-1.00468800	-2.38903200	-0.09909100
C	0.16550200	-1.22283500	-1.55710200
H	0.92697700	-1.93995300	-1.84026500
C	-0.92666900	0.74481600	-1.27531900
H	-1.21274000	1.78522300	-1.38037400
C	0.09542100	0.11660300	-1.97520300
H	0.80020300	0.61120800	-2.63340700
N	2.29651500	0.26377400	0.30721100
N	0.12792300	0.77971000	0.67525100
N	0.26159400	-0.48492600	0.93131900
C	1.40456900	1.32668700	0.26134800
C	1.64630400	-0.88944100	0.69975200
O	2.09731200	-1.98519300	0.88018800
O	1.63163700	2.47239000	-0.00663200
H	3.28603600	0.33544000	0.12257500
Si	-2.75042800	0.23041200	0.93744100
H	-4.04831300	-0.49438200	0.91250800
H	-2.05005600	-0.09202000	2.19219300
H	-3.02894000	1.68015000	0.81907800
H	-2.54432300	-0.59680300	-1.37524600

C₅-Br-Anti-TAD

C	-1.07010900	0.00011700	0.54102700
H	-1.01701900	0.00029700	1.62477000
C	-0.39604100	-1.15701100	-0.14734200
H	-0.54891600	-2.18847100	0.14215500
C	0.09596000	-0.70703400	-1.36257500
H	0.52316200	-1.33894600	-2.13173300
C	-0.39609700	1.15703600	-0.14773000
H	-0.54894600	2.18858100	0.14146900
C	0.09594200	0.70669700	-1.36279000
H	0.52315200	1.33836200	-2.13214800
N	3.02163100	-0.00000300	-0.28826500
N	1.31310900	0.64815600	1.04413300
N	1.31308000	-0.64805800	1.04413200
C	2.39788200	1.13590700	0.19766500
C	2.39783700	-1.13588400	0.19765700

O	2.68977900	-2.28390500	0.02361600
O	2.68990300	2.28390700	0.02361300
H	3.85895900	-0.00001700	-0.85196000
Br	-2.97470900	0.00001600	0.07811800

C₅-Cl-Anti-TAD

C	-1.62384600	-0.00019000	0.54472200
H	-1.53358800	-0.00047500	1.62696300
C	-0.94551300	-1.15905900	-0.14940200
H	-1.09472600	-2.19103500	0.14052100
C	-0.45909300	-0.70855700	-1.36298100
H	-0.03265800	-1.33812100	-2.13472800
C	-0.94553600	1.15904500	-0.14878200
H	-1.09485400	2.19081800	0.14172700
C	-0.45912600	0.70915800	-1.36263500
H	-0.03268400	1.33913100	-2.13403900
N	2.47081200	0.00000100	-0.29886300
N	0.77058300	0.64701100	1.04594300
N	0.77056600	-0.64713800	1.04593100
C	1.85292500	1.13565700	0.19480000
C	1.85293700	-1.13573500	0.19481800
O	2.14577200	-2.28354700	0.02301700
O	2.14570700	2.28349200	0.02303900
H	3.30870500	0.00000700	-0.86180700
Cl	-3.38660300	-0.00005300	0.16697600

C₅-F-Anti-TAD

C	-1.94703100	0.00007700	-0.58979400
H	-1.81811200	0.00017100	-1.67107200
C	-1.28017300	1.16518100	0.12706500
H	-1.41334300	2.19946300	-0.16294600
C	-0.82616400	0.71433100	1.34369300
H	-0.42175000	1.33768900	2.13283100
C	-1.28012700	-1.16512300	0.12684700
H	-1.41327800	-2.19933200	-0.16342500
C	-0.82613400	-0.71448700	1.34357200
H	-0.42169000	-1.33799700	2.13257100
N	2.12548700	-0.00002700	0.35128800
N	0.47888400	-0.64381600	-1.06305700
N	0.47891400	0.64388200	-1.06306700
C	1.53343500	-1.13507300	-0.17453100
C	1.53349400	1.13506200	-0.17454100
O	1.82523600	2.28251600	-0.00212600
O	1.82509000	-2.28254700	-0.00211500
H	2.94970100	-0.00005100	0.93410500
F	-3.29899300	0.00002500	-0.30646200

C₅-Me-Anti-TAD

C	1.95407600	-0.00002900	-0.57936600
H	1.81046000	-0.00006500	-1.66046500
C	1.25123900	-1.14903500	0.10012800
H	1.38158100	-2.18679600	-0.18338600
C	0.76764200	-0.70679200	1.32349500
H	0.34059100	-1.33864600	2.09358200
C	1.25125900	1.14904000	0.10003900
H	1.38159500	2.18677600	-0.18356400
C	0.76765300	0.70690200	1.32344000
H	0.34060900	1.33882200	2.09347800
N	-2.17417500	-0.00000100	0.32168800
N	-0.49886800	0.64712700	-1.05249300
N	-0.49886900	-0.64715500	-1.05248100
C	-1.55935700	1.13469700	-0.17923600
C	-1.55936700	-1.13470600	-0.17922500
O	-1.84854000	-2.28334300	0.00342200
O	-1.84851500	2.28333800	0.00340800
H	-2.99110000	0.00000600	0.91389100
C	3.46143200	-0.00003500	-0.25785800
H	3.93864100	0.88462100	-0.68771000
H	3.63135100	-0.00004600	0.82176300
H	3.93863800	-0.88468500	-0.68772700

C₅-NH₂-Anti-TAD

C	-1.96785700	-0.00347400	-0.57699800
H	-1.80794900	-0.02481900	-1.65480400
C	-1.26451600	1.16349900	0.08891100
H	-1.40877700	2.19086700	-0.22063500
C	-0.78395500	0.74375100	1.31436900
H	-0.35614400	1.38822700	2.07367900
C	-1.26628300	-1.14951000	0.14143400
H	-1.39233500	-2.19321300	-0.12263100
C	-0.78554900	-0.67909600	1.34734600
H	-0.36360400	-1.28752700	2.13919800
N	-3.40900900	0.08478600	-0.32933800
H	-3.87370500	-0.71093100	-0.76070800
H	-3.58746100	0.02567200	0.67180600
N	2.15552100	-0.00783200	0.33467100
N	0.48986400	-0.65492100	-1.05335600
N	0.49357300	0.63550200	-1.05967000
C	1.54711800	-1.14301500	-0.17329000
C	1.55511100	1.12650000	-0.18340600
O	1.85091300	2.27435500	-0.01314300
O	1.83632900	-2.29122000	0.00793700

H	2.97798100	-0.00803200	0.91940000
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C₅-OH-Anti-TAD

C	1.96589800	0.00002300	-0.59430800
H	1.82121000	0.00005500	-1.67268000
C	1.27465400	-1.16235500	0.10999100
H	1.40777500	-2.19706800	-0.18024700
C	0.81237600	-0.71454600	1.32835900
H	0.39971000	-1.33786500	2.11350900
C	1.27471300	1.16239500	0.11003900
H	1.40774500	2.19710900	-0.18022900
C	0.81239200	0.71455500	1.32837900
H	0.39971500	1.33785400	2.11353800
H	3.51137400	0.00004300	0.58154900
N	-2.13917600	-0.00001000	0.35129400
N	-0.48983500	0.64388700	-1.05991700
N	-0.48980000	-0.64387700	-1.05990200
C	-1.54398300	1.13479000	-0.17157600
C	-1.54394100	-1.13481700	-0.17156600
O	-1.83517500	-2.28250000	0.00281500
O	-1.83524300	2.28247200	0.00280100
H	-2.96139700	-0.00001800	0.93667600
O	3.36203000	-0.00001800	-0.37666000

C₅-SH-Anti-TAD

C	-1.63566900	-0.00010900	-0.53849600
H	-1.53877300	-0.00036800	-1.62364600
C	-0.93773000	1.15442300	0.13304900
H	-1.08688500	2.18700700	-0.15577100
C	-0.43959600	0.70776300	1.34949300
H	-0.00199200	1.33924700	2.11351800
C	-0.93737500	-1.15416800	0.13349900
H	-1.08660100	-2.18684400	-0.15492500
C	-0.43946600	-0.70695400	1.34981600
H	-0.00153600	-1.33806100	2.11396000
N	2.48871700	-0.00000500	0.29163100
N	0.78006600	-0.64830700	-1.03988500
N	0.78011900	0.64804700	-1.04011500
C	1.86379800	-1.13562700	-0.19401900
C	1.86375500	1.13552000	-0.19421800
O	2.15645200	2.28375400	-0.01912500
O	2.15660200	-2.28382200	-0.01887600
H	3.32462900	0.00004700	0.85716800
S	-3.44544000	-0.00026800	-0.22965100
H	-3.35484800	0.00056900	1.11195300

C₅-SiH₃-Anti-TAD

C	1.60780600	0.00009000	-0.59783200
H	1.54780000	0.00018100	-1.68812400
C	0.90360800	-1.14042500	0.05865300
H	1.03289100	-2.17823000	-0.22492900
C	0.43424400	-0.69887200	1.30711700
H	0.01320200	-1.33867900	2.07318200
C	0.90359100	1.14048300	0.05883500
H	1.03279900	2.17834600	-0.22457700
C	0.43422800	0.69871000	1.30722400
H	0.01314400	1.33837700	2.07338400
N	-2.51871500	-0.00003000	0.29337600
N	-0.81228200	0.65238900	-1.03492000
N	-0.81226200	-0.65232400	-1.03493700
C	-1.88135600	1.13532600	-0.17771200
C	-1.88130600	-1.13533800	-0.17771900
O	-2.16307600	-2.28451400	0.01866400
O	-2.16320600	2.28447900	0.01867700
H	-3.33071900	-0.00005100	0.89234100
Si	3.45716000	0.00001900	-0.10365500
H	4.09531200	1.20735900	-0.67685700
H	3.58830400	-0.00005700	1.36898000
H	4.09521200	-1.20730600	-0.67699500

Table S2 Energetic Data

E- Electronic Energy

ZPE- Zero Point Energy

H- Enthalpy

qG- Corrected Gibbs Free Energy

C ₅ -X	E	ZPE	H	qG
Cyclopentadiene.out	-194.004692	-193.910661	-193.905603	-193.9916
Br.out	-2765.184849	-2765.100437	-2765.094186	-2767.5761
Cl.out	-653.569647	-653.484463	-653.478395	-653.5994
F.out	-293.197241	-293.110798	-293.105029	-293.2317
Me.out	-233.298065	-233.17513	-233.168749	-233.2687
NH ₂ .out	-249.322657	-249.210834	-249.204573	-249.3173
OH.out	-269.183262	-269.084431	-269.078293	-269.2003
SH.out	-592.154788	-592.061163	-592.054479	-592.1783
SiH ₃ .out	-484.658123	-484.549202	-484.54177	-484.6615
Ethylene.out	-78.536835	-78.485078	-78.481103	-78.5334
TS-Syn-Ethylene				
Br.out	-2843.702952	-2843.563276	-2843.555104	-2846.062532
Cl.out	-732.088013	-731.947638	-731.939658	-732.089086
F.out	-371.723774	-371.581965	-371.574277	-371.727502

Me.out	-311.811424	-311.63392	-311.625536	-311.754243
NH2.out	-327.841331	-327.674244	-327.66614	-327.806961
OH.out	-347.704943	-347.550745	-347.542724	-347.692118
SH.out	-670.668272	-670.518862	-670.5105	-670.6623499
SiH3.out	-563.160827	-562.99624	-562.987063	-563.135228
H.out	-272.518792	-272.369459	-272.362497	-272.4771

TS-Anti-Ethylene

Br.out	-2843.701045	-2843.561267	-2843.552901	-2846.062348
Cl.out	-732.085421	-731.944923	-731.936773	-732.085786
F.out	-371.713266	-371.571633	-371.563779	-371.718677
Me.out	-311.811426	-311.633416	-311.625035	-311.7527
NH2.out	-327.837147	-327.67018	-327.66192	-327.802491
OH.out	-347.699392	-347.545293	-347.537203	-347.686909
SH.out	-670.668986	-670.519491	-670.510976	-670.662211
SiH3.out	-563.169749	-563.004526	-562.995386	-563.141871

Syn-Adducts

Br-Syn.out	-2843.787983	-2843.642995	-2843.635593	-2846.137347
Cl-Syn.out	-732.173626	-732.027855	-732.020675	-732.163489

F-Syn.out	-371.807673	-371.660327	-371.65344	-371.800865
Me-Syn.out	-311.892262	-311.70905	-311.701483	-311.823229
NH2-syn.out	-327.923201	-327.75092	-327.743479	-327.878292
OH-syn.out	-347.787044	-347.627659	-347.620376	-347.763977
SH-syn.out	-670.751012	-670.596496	-670.588858	-670.73407
SiH3-Syn.out	-563.239758	-563.069507	-563.061008	-563.202528

H-anti.out	-272.597907	-272.443039	-272.436915	-272.544593
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Anti-Adducts

Br-anti.out	-2843.782811	-2843.63791	-2843.630459	-2846.133423
Cl-anti.out	-732.169293	-732.023736	-732.016493	-732.159173
F-Anti.out	-371.8018	-371.654706	-371.64778	-371.795863
Me-anti.out	-311.892054	-311.708834	-311.701278	-311.822517
NH2-anti.out	-327.922572	-327.750084	-327.742748	-327.876861
OH-anti.out	-347.787421	-347.627684	-347.620582	-347.763496
SH-anti.out	-670.75056	-670.596369	-670.588632	-670.733565
SiH3-Anti.out	-563.240425	-563.070392	-563.061752	-563.203134

Cyclopentanes

H.out	-196.447889	-196.305257	-196.29915	-196.3874
Br.out	-2767.637808	-2767.504747	-2767.497652	-2769.9808
Cl.out	-656.0233	-655.889462	-655.882631	-656.0066
F.out	-295.65584	-295.520683	-295.514081	-295.6435
Me.out	-235.743271	-235.572508	-235.565018	-235.6674
NH2.out	-251.771502	-251.611496	-251.604229	-251.7197
OH.out	-271.634355	-271.487219	-271.480112	-271.6051
SH.out	-594.601079	-594.45881	-594.45127	-594.5773
SiH3.out	-487.092042	-486.934788	-486.92633	-487.0488

Cyclopentenes

H.out	-195.224083	-195.105593	-195.100052	-195.187265
Br.out	-2766.412438	-2766.303525	-2766.296928	-2768.779942
Cl.out	-654.797927	-654.688335	-654.68189	-654.804778
F.out	-294.428892	-294.318024	-294.311817	-294.440509
Me.out	-234.518775	-234.372008	-234.365121	-234.46648
NH2.out	-250.547658	-250.411719	-250.405036	-250.519211
OH.out	-270.410813	-270.287572	-270.281035	-270.404831
SH.out	-593.377729	-593.259283	-593.252392	-593.377336
SiH3.out	-485.869208	-485.73546	-485.727782	-485.848613

Acetylene	-77.28777146			-78.5334
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TS-Syn-Actylene

Br.out	-2765.184849	-2765.100437	-2765.094186	-2767.576083
Cl.out	-653.569647	-653.484463	-653.478395	-653.599363
F.out	-293.197241	-293.110798	-293.105029	-293.231691
Me.out	-233.298065	-233.17513	-233.168749	-233.26869
NH2.out	-249.322657	-249.210834	-249.204573	-249.317346
OH.out	-269.183262	-269.084431	-269.078293	-269.200273
SH.out	-592.154788	-592.061163	-592.054479	-592.178282
SiH3.out	-484.658123	-484.549202	-484.54177	-484.661515

TS-Anti-Actylene

Br.out	-2842.447199	-2842.332885	-2842.324577	-2844.916825
Cl.out	-730.831669	-730.716704	-730.708592	-730.942168
F.out	-370.459932	-370.343673	-370.335873	-370.577647
Me.out	-310.557173	-310.404394	-310.39607	-310.646876
NH2.out	-326.58334	-326.441667	-326.433463	-326.686231
OH.out	-346.445894	-346.317267	-346.309187	-346.558153

SH.out	-669.415058	-669.291292	-669.282744	-669.527327
SiH3.out	-561.914981	-561.775077	-561.766022	-562.021361
MA.out	-379.143394	-379.086564	-379.080471	-379.2301

TS-Syn-MA

Br.out	-3144.324166	-3144.180562	-3144.169371	-3146.879714
Cl.out	-1032.70885	-1032.564512	-1032.553504	-1032.907952
F.out	-672.345568	-672.199547	-672.188903	-672.549056
Me.out	-612.435487	-612.253334	-612.241944	-612.613678
NH-1.out	-628.465548	-628.294579	-628.28339	-628.656338
OH-1.out	-648.328058	-648.169933	-648.158899	-648.528132
SH-1.out	-971.290206	-971.136792	-971.125366	-971.491268
SiH3.out	-863.783702	-863.615256	-863.602835	-863.979395

TS-Anti-MA

Br.out	-3144.320234	-3144.176222	-3144.164914	-3146.770661
Cl.out	-1032.704442	-1032.559767	-1032.548674	-1032.794369
F.out	-672.333122	-672.186969	-672.176199	-672.427049
Me.out	-612.435461	-612.253049	-612.241693	-612.466246

NH.out	-628.459906	-628.288499	-628.277296	-628.514363
OH.out	-648.320341	-648.161764	-648.150727	-648.39672
SH.out	-971.289969	-971.136258	-971.124785	-971.372726
SiH3.out	-863.792946	-863.623727	-863.611517	-863.855344

TCNE.out	-447.355429	-447.307642	-447.29757	-447.4603
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TS-Syn-TCNE

Br.out	-3212.532606	-3212.398867	-3212.383475	-3214.998944
Cl.out	-1100.916095	-1100.781629	-1100.766496	-1101.026455
F.out	-740.557634	-740.421139	-740.406392	-740.667909
Me.out	-680.650934	-680.478286	-680.46285	-680.70187
NH2.out	-696.684245	-696.522815	-696.507641	-696.757346
OH.out	-716.54476	-716.396171	-716.381141	-716.639397
SH.out	-1039.499155	-1039.35582	-1039.340153	-1039.603099
SiH3.out	-931.99878	-931.839638	-931.823306	-932.081486

TS-Anti-TCNE

Br.out	-3212.536073	-3212.401791	-3212.386245	-3215.006263
Cl.out	-1100.91949	-1100.784554	-1100.769247	-1101.029698

F.out	-740.547335	-740.410902	-740.39593	-740.661036
Me.out	-680.655861	-680.483041	-680.467515	-680.706681
NH2.out	-696.677746	-696.515987	-696.500585	-696.752158
OH.out	-716.535088	-716.386302	-716.371042	-716.631388
SH.out	-1039.507181	-1039.363335	-1039.347614	-1039.610416
SiH3.out	-932.014688	-931.855018	-931.838623	-932.097151
TAD.out	-391.325496	-391.280531	-391.274385	-391.4283

TS-Syn-TAD

Br.out	-3156.512587	-3156.380714	-3156.369486	-3158.977822
Cl.out	-1044.89797	-1044.765276	-1044.754236	-1045.003778
F.out	-684.532799	-684.39862	-684.387937	-684.641122
CH3.out	-624.632388	-624.461926	-624.45047	-624.679684
NH.out	-640.663072	-640.503621	-640.492363	-640.733298
OH.out	-660.527101	-660.380429	-660.369383	-660.618192
SH.out	-983.486825	-983.345158	-983.333627	-983.585562
SiH3.out	-875.98234	-875.825324	-875.813084	-876.061125

TS-Anti-TAD

Br.out	-3156.514175	-3156.382047	-3156.370654	-3158.980556
Cl.out	-1044.898415	-1044.765646	-1044.75446	-1045.0044
F.out	-684.526847	-684.392528	-684.381677	-684.636481
CH3.out	-624.630368	-624.459874	-624.448404	-624.677297
NH2.out	-640.654034	-640.494488	-640.483189	-640.724564
OH.out	-660.513417	-660.3668	-660.355648	-660.605837
SH.out	-983.484448	-983.342659	-983.33108	-983.58338
SiH3.out	-875.987845	-875.830388	-875.818131	-876.066299