Supplementary Data

Substituent effects on stereoselectivity of dihalocarbene reactions with cyclohexadiene and on the reactivity of bis-dihalocyclopropanes in electrophilic nitrations on route to pyrimidine N-oxides

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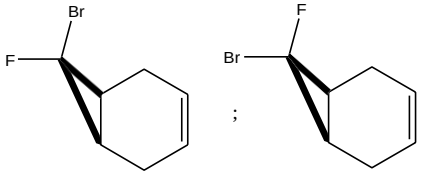
Experimental

General experimental details. NMR spectra were recorded on an Agilent 400-MR spectrometer (400.0 MHz for ^{1}H; 100.6 MHz for ^{13}C; 376.3 MHz for ^{19}F) at room temperature; chemical shifts were measured with reference to the solvent ($CDCl_3$, δ_H 7.24 ppm, δ_C 77.13 ppm) or to $CFCl_3$ as external standard for ^{19}F. Chemical shifts (δ) are given in ppm; *J* values are given in Hz. When necessary, assignments of signals in NMR spectra were made using 2D techniques. Accurate mass measurements (HRMS) were done on Jeol GCMate II mass spectrometer (70 eV). Elemental analysis was performed on Carlo Erba 1106 instrument. Analytical thin layer chromatography was carried out with silica or aluminum oxide plates (supported on aluminum); the detection was done by UV lamp (254 nm).
Column chromatography was performed on silica gel (Macherey-Nagel, 40/60) or aluminum oxide (neutral, 50/200). All the starting materials were commercially available. All reagents except commercial products of satisfactory quality were purified by literature procedures prior to use.

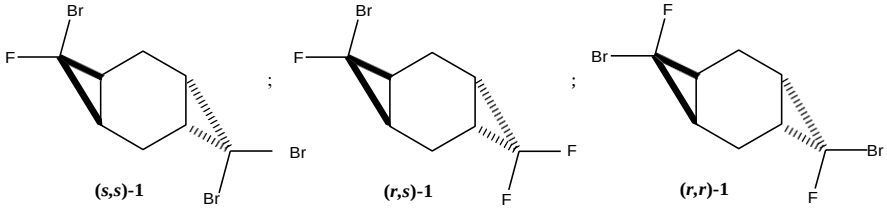
7-Bromo-7-fluorobicyclo[4.1.0]hept-3-ene (4).



***(s)*-4** ***(r)*-4**

A 50% aqueous solution of NaOH (32 mL) was added dropwise to a stirred mixture of hexa-1,4-diene (3.2 g, 40.0 mmol), $CHBr_2F$ (30.8 g, 160.0 mmol) and TEBAC (0.24 g, 0.08 mmol) in dichloromethane (40 mL) at 0^{o}C. A drop of ethanol was added and the reaction mixture was warmed up to room temperature and stirred for 48 h. Then it was treated with equal amount of icy water. The organic phase was separated and the water phase extracted with dichloromethane (3×30 mL). The combined organic layers were washed with water (3×30 mL) and dried over $MgSO_4$. The solvent and unreacted diene were evaporated *in vacuo* (20 torr); the residue was condensed at 1 torr into the cooled trap (-78^{o}C) to afford mono-adduct **4** as mixture of isomers ***(r)*-4:*(s)*-4** = 0.6:1.
Obtained as colorless liquid (4.73 g, 62%); R_f 0.3 (petroleum ether); ***(r)*-4** δ_H (400 MHz, $CDCl_3$): 1.67–1.73 (2H, m, 2CH), 2.27 (2H, br.d, $^{2}J_{HH}$ 17.0, $2CH_2$), 2.32–2.42 (2H, m, $2CH_2$), 5.55 (2H, br.s, 2CH=); δ_C (101 MHz, $CDCl_3$): 17.2 (d, $^{3}J_{CF}$ 5, $2CH_2$), 22.1 (d, $^{2}J_{CF}$ 10, 2CH), 83.4 (d, $^{1}J_{CF}$ 307, CBrF), 122.5 (s, 2CH=); δ_F (376 MHz, $CDCl_3$): -159.20 (br.t, $^{3}J_{HF}$ 4.4); ***(s)*-4** δ_H (400 MHz, $CDCl_3$): 1.74 (2H, ddd, $^{3}J_{HF}$ 19.5, $^{3}J_{HH}$ 5.1, $^{3}J_{HH}$ 2.4, 2CH), 2.05 (2H, br.d, $^{2}J_{HH}$ 17.0, $2CH_2$), 2.38–2.48 (2H, m, $2CH_2$), 5.49 (2H, br.s, 2CH=); δ_C (101 MHz, $CDCl_3$): 19.5 (s, $2CH_2$), 19.9 (d, $^{2}J_{CF}$ 11, 2CH), 95.6 (d, $^{1}J_{CF}$ 296, CBrF), 122.3 (d, $^{4}J_{CF}$ 3, 2CH=); δ_F (376 MHz, $CDCl_3$) for: -124.00 (t, $^{3}J_{HF}$ 19.5).[1]

4,8-Dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane (1).



(*s*,*s*)-1 **(*r*,*s*)-1** **(*r*,*r*)-1**

A 50% aqueous solution of NaOH (10 mL) was added dropwise to a stirred mixture of alkene **4** (1.91 g, 10.0 mmol), $CHBr_2F$ (7.7 g, 40.0 mmol) and TEBAC (0.06 g, 0.02 mmol) in dichloromethane (10 mL) at 0^{o}C. A drop of ethanol was added and the reaction mixture was warmed up to room temperature and stirred for 20 days. Then it was treated with equal amount of icy water. The organic

[1] No elemental analysis could be obtained for compound **4** due to its high volatility in analysis conditions. Nevertheless, the structure and purity of **4** are proved with unambiguously resolved structures of its' adducts with dihalocarbenes, as well as ^{1}H, ^{19}F, ^{13}C NMR spectra.

phase was separated and the water phase extracted with dichloromethane (3×10 mL). The combined organic layers were washed with water (30 mL) and dried over $MgSO_4$. The solvent and unreacted alkene were evaporated *in vacuo* (1 torr); the residue was purified by column chromatography (silica gel, petroleum ether).

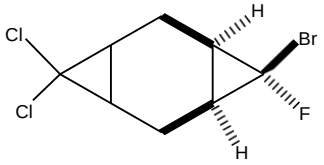
(*s,s*)-4,8-Dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*s,s*)-1).

Obtained as colorless crystals (1.96 g, 65%); m.p. 136–138°C (from petroleum ether); R_f 0.25 (petroleum ether); δ_H (400 MHz, $CDCl_3$): 1.53–1.63 (4H, m, $^3J_{HF}$ 18.8, 4CH), 1.90–2.01 (4H, m, $2CH_2$); δ_C (101 MHz, $CDCl_3$): 13.1 (s, $^1J_{CH}$ 132, $2CH_2$), 18.7 (dd, $^2J_{CF}$ 10, $^4J_{CF}$ 4, $^1J_{CH}$ 165, 4CH), 93.2 (d, $^1J_{CF}$ 300, 2CBrF); δ_F (376 MHz, $CDCl_3$): -123.73 (t, $^3J_{HF}$ 18.8).

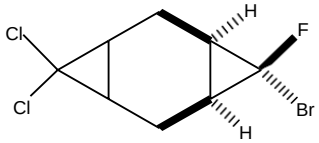
(*r,s*)- and (*r,r*)-4,8-Dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*r,s*)-1 and (*r,r*)-1). Mixture of isomers (*r,s*)-**1**/(*r,r*)-**1** = 1:0.13.

Obtained as white solid (0.24 g, 8%); R_f 0.3 (petroleum ether); (*r,s*)-**1** δ_H (400 MHz, $CDCl_3$): 1.46– 1.53 (2H, m, 2CH), 1.54–1.63 (2H, m, $^3J_{HF}$ 18.7, 2CH), 1.86–1.94 (2H, m, $^2J_{HH}$ 15.6, $2CH_2$), 2.06–2.14 (2H, m, $^2J_{HH}$ 15.6, $2CH_2$); δ_C (101 MHz, $CDCl_3$): 10.3 (d, $^3J_{CF}$ 4, $^1J_{CH}$ 132, $2CH_2$), 18.8 (dd, $^2J_{CF}$ 11, $^4J_{CF}$ 2, $^1J_{CH}$ 160, 2CH), 20.4 (dd, $^2J_{CF}$ 10, $^4J_{CF}$ 3, $^1J_{CH}$ 160, 2CH), 81.1 (d, $^1J_{CF}$ 301, ***(r)***-CBrF), 93.2 (dd, $^1J_{CF}$ 299, $^5J_{CF}$ 2, ***(s)***-CBrF); δ_F (376 MHz, $CDCl_3$): -157.29 (1F, tt, $^3J_{HF}$ 5.7, $^4J_{HF}$ 2.2, ***(r)***-CBrF), -124.07 (1F, t, $^3J_{HF}$ 18.7, ***(s)***-CBrF); (*r,r*)-**1** δ_H (400 MHz, $CDCl_3$): 1.47–1.54 (4H, m, 4CH), 2.02–2.06 (4H, m, $2CH_2$); δ_C (101 MHz, $CDCl_3$): 7.7 (t, $^3J_{CF}$ 4, $2CH_2$), 20.7 (dd, $^2J_{CF}$ 10, $^4J_{CF}$ 2, 4CH), 81.3 (dd, $^1J_{CF}$ 302, $^5J_{CF}$ 3, 2CBrF); δ_F (376 MHz, $CDCl_3$): -158.19-(-158.14) (2F, m, $^3J_{HF}$ 6, 2CBrF); anal. calcd for $C_8H_8Br_2F_2$: C 31.82, H 2.67; found: C 31.66, H 2.55.

4-Bromo-8,8-dichloro-4-fluorotricyclo[5.1.0.0]octane (2)



***(s)*-2**



***(r)*-2**

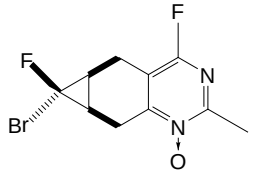
A 50% aqueous solution of NaOH (5 mL) was added dropwise to the stirred mixture of alkene **4** (1.04 g, 5.4 mmol), chloroform (2.83 g, 23.7 mmol) and TEBAC (19 mg, 0.08 mmol) in benzene (5 mL) at -10°C. The reaction mixture was warmed up to room temperature, stirred for 24 h and worked up as described for the first stage. The solvent and residue of **4** were evaporated *in vacuo* (1 torr) to give analytically pure tetrahalogenide **2** as mixture of isomers ***(s)*-2**/***(r)*-2** = 1:0.6. Obtained as yellowish crystals (0.98 g, 65%); m.p. 95–100°C (from CH_2Cl_2);); δ_H (400 MHz, $CDCl_3$) for the mixture of isomers: 1.44–1.66 (4H, m), 1.93–2.18 (4H, m); ***(s)*-2** δ_C (101 MHz, $CDCl_3$): 12.6 (s, $^1J_{CH}$ 132, $2CH_2$), 18.9 (d, $^2J_{CF}$ 10, $^1J_{CH}$ 66, 2CH), 22.9 (d, $^4J_{CF}$ 3, $^1J_{CH}$ 168, 2CH), 63.8 (s, CCl_2), 92.9 (d, $^1J_{CF}$ 300, CBrF); δ_F (376 MHz, $CDCl_3$): -124.04 (t, $^3J_{HF}$ 19); ***(r)*-2** δ_C (101 MHz, $CDCl_3$): 9.9 (d, $^3J_{CF}$ 4, $^1J_{CH}$ 132, $2CH_2$), 20.6 (d, $^2J_{CF}$ 10, $^1J_{CH}$ 166, 2CH), 23.0 (d, $^4J_{CF}$ 2, $^1J_{CH}$ 168, 2CH), 63.9 (d, $^5J_{CF}$ 3, CCl_2), 81.0 (d, $^1J_{CF}$ 300, CBrF); δ_F (376 MHz, $CDCl_3$): -157.37 (s); anal. calcd. for $C_8H_8BrCl_2F$: C 35.07, H 2.94; found: C 35.08, H 2.99.

General procedures for heterocyclization of compounds 1,2

(*Method A*): to the mixture of fuming HNO_3 (4.0 mmol, 0.16 mL) and HSO_3CF_3 (4.0 mmol, 0.36 mL) the solution of corresponding tetrahalogenide (1.0 mmol) in acetonitrile (1 mL) was added at 10°C; *OR* (*Method B*): to the solution of corresponding tetrahalogenide (1.0 mmol) in acetonitrile (1 mL) NO_2OTf (4 mmol, 0.78 mg) was added at 10°C.

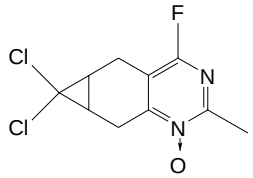
Then *(for both Methods)* the reaction mixture was stirred for 14 days at r.t. and treated with an equal amount of saturated aqueous $NaHCO_3$. The organic phase was separated and the water phase extracted with DCM (3×5 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (5×5 mL) and dried over $MgSO_4$. The solvent was evaporated in vacuo to give corresponding pyrimidine *N*-oxide. The product was isolated *via* preparative column chromatography on alumina.

(*r*)-(5a*S*,6*R*,6a*R*)-6-bromo-4,6-difluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (5)



Obtained as colorless oil (134 mg, 46% (method A), 101 mg, 35% (method B)); R_f 0.3 ($CHCl_3$); δ_H (400 MHz, $CDCl_3$): 2.13–2.33 (2H, m, 2CH), 2.69 (3H, s, CH_3), 3.15–3.29 (2H, m, $2CH_2$), 3.34 (1H, br.d, $^2J_{HH}$ 20.9, CH_2), 3.35 (1H, br.d, $^2J_{HH}$ 18.1, CH_2); δ_C (101 MHz, $CDCl_3$): 16.6 (dd, J_{CF} 4, J_{CF} 2, CH_2), 18.9 (d, J_{CF} 2, CH_2), 19.5 (s, CH_3), 22.1 (d, $^3J_{CF}$ 10, CH), 23.5 (d, $^3J_{CF}$ 9, CH), 79.6 (d, $^1J_{CF}$ 301, CBrF), 112.4 (dd, $^2J_{CF}$ 36, $^4J_{CF}$ 4, C4a), 153.6 (d, $^1J_{CF}$ 249, C4), 155.8 (d, $^3J_{CF}$ 17, C2), 156.1 (dd, $^3J_{CF}$ 7, $^4J_{CF}$ 4, C8a); δ_F (376 MHz, $CDCl_3$): -158.51 (1F, t, $^3J_{HF}$ 4.6, CBrF), -72.64 (1F, s, CF); HRMS (ESI$^+$, *m/z*): calc. for $C_{10}H_9BrF_2N_2O$ [M+H] 290.9939, found 290.9943.

6,6-Dichloro-4-fluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (6).



Obtained as yellowish oil (195 mg, 74% (method A), 184 mg, 70% (method B)); R_f 0.2 (CH_2Cl_2); δ_H (400 MHz, $CDCl_3$): 2.13 (1H, ddd, $^3J_{HH}$ 11.0, $^3J_{HH}$ 7.8, $^3J_{HH}$ 1.1, CH), 2.26 (1H, ddd, $^3J_{HH}$ 11.0, $^3J_{HH}$ 7.7, $^3J_{HH}$ 1.1, CH), 2.66 (3H, s, CH_3), 3.02 (1H, br.d, $^2J_{HH}$ 19.1, CH_2), 3.19 (1H, br.d, $^2J_{HH}$ 21.2, CH_2), 3.21 (1H, br.dd, $^2J_{HH}$ 19.1, $^3J_{HH}$ 7.8, CH_2), 3.33 (1H, br.dd, $^2J_{HH}$ 21.2, $^3J_{HH}$ 7.7, CH_2); δ_C (101 MHz, $CDCl_3$): 17.3 (d, J_{CF} 2, CH_2), 19.4 (s, CH_3), 20.8 (d, J_{CF} 2, CH_2), 22.9 (s, CH), 24.2 (s, CH), 63.3 (s, CCl_2), 112.3 (d, $^2J_{CF}$ 35, C4a), 154.2 (d, $^1J_{CF}$ 246, C4), 155.5 (d, $^3J_{CF}$ 17, C2), 155.9 (d, $^3J_{CF}$ 7, C8a); δ_F (376 MHz, $CDCl_3$): -73.03 (s, CF); HRMS (ESI$^+$, *m/z*): calc. for $C_{10}H_9Cl_2FN_2O$ [M+H] 263.0149, found 263.0145.

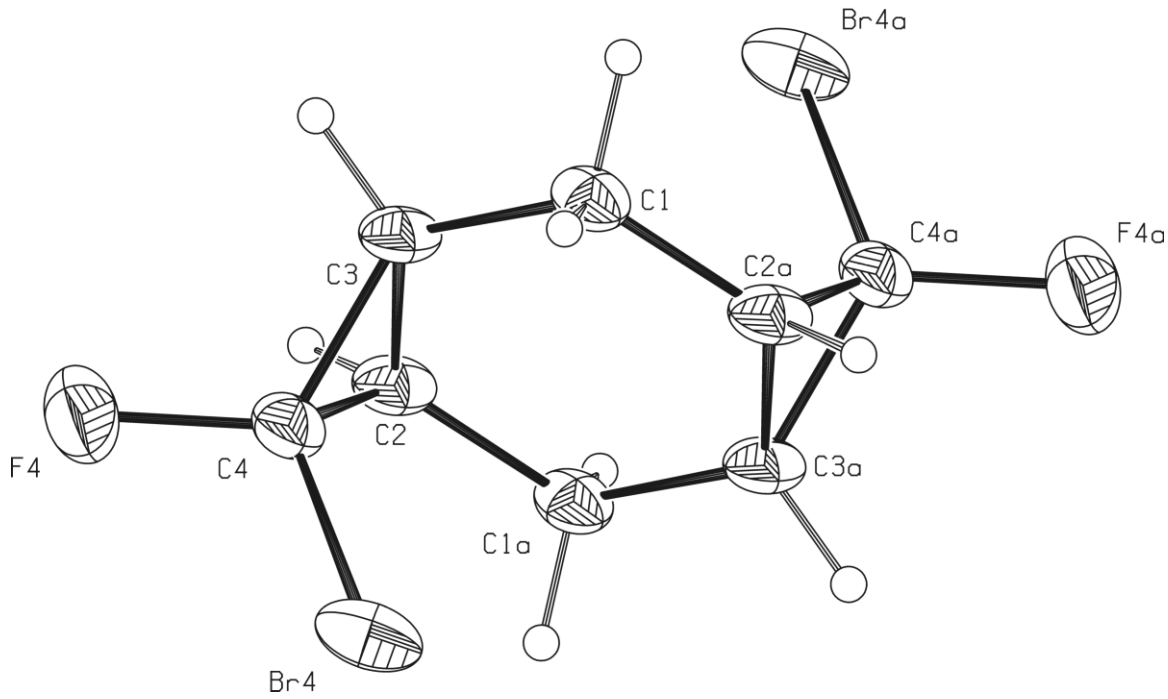


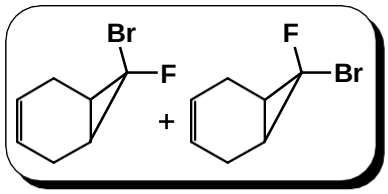
Figure S1. The molecular structure of compound **(*s*,*s*)-1**. Displacement ellipsoids are drawn at 25% probability level. Hydrogen atoms are presented as small circles of arbitrary radius.

Table S1. Crystal data and structure refinement for compound **(*s*,*s*)-1**

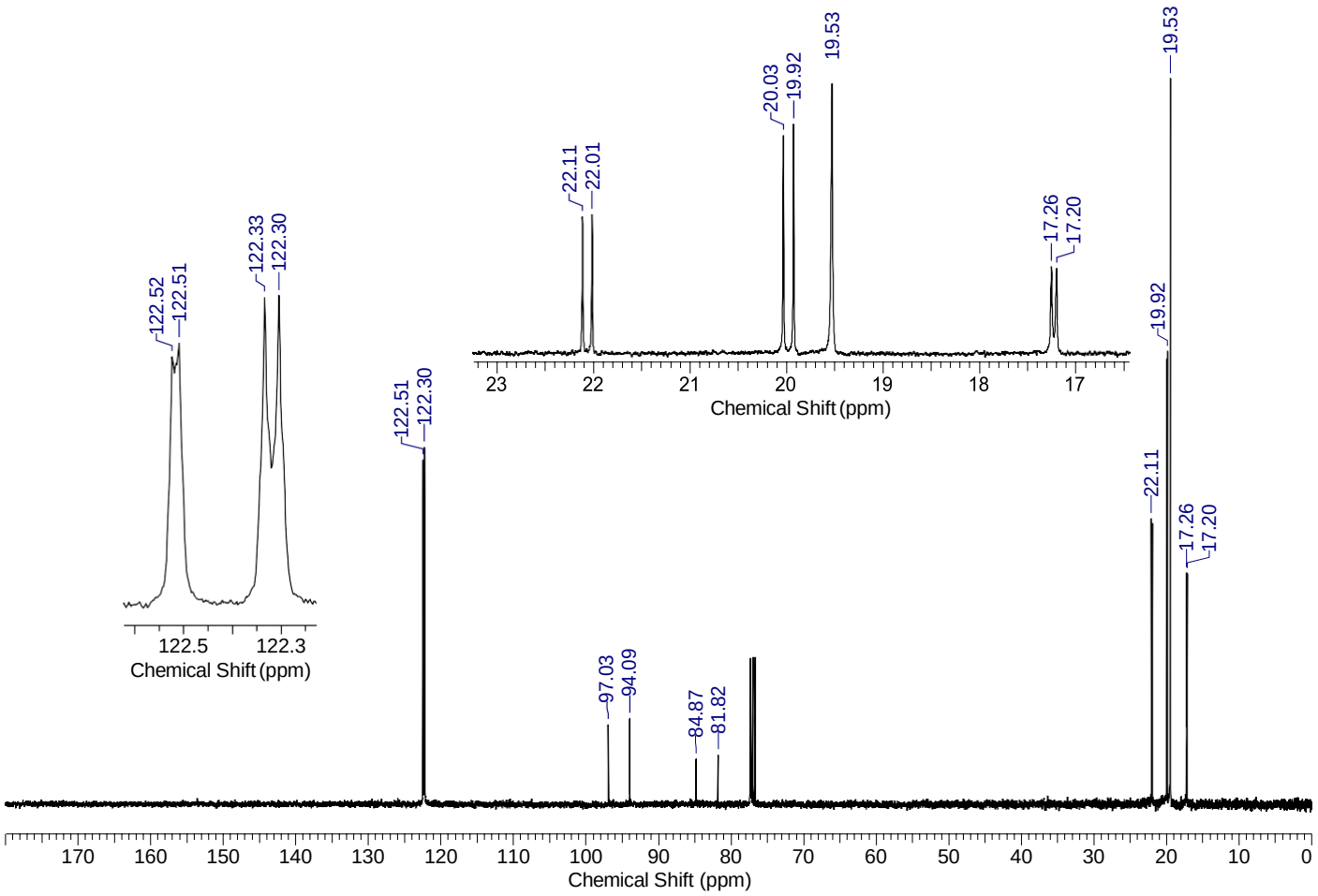
Empirical formula	$C_8H_8Br_2F_2$	Absorption coefficient, mm^{-1}	8.697
Formula weight	301.94	*F*(000)	288
Temperature, K	295(2)	Crystal size, mm	0.20 × 0.20 × 0.20
Wavelength, Å	0.71073	Theta range for data collection, deg.	3.45 - 26.70
Crystal system	Monoclinic	Index ranges	$-7\leq h\leq 7$, $-7\leq k\leq 8$, $-14\leq l\leq 14$
Space group	$P2_1/n$	Reflections collected	3642
a, Å	6.2656(6	Independent reflections [R_{int}]	969 [0.0417]
b, Å	6.3728(4)	Max. and min. transmission	0.1706, 0.0640
c, Å	11.8196(12)	Data / restraints / parameters	671 / 0 / 56
α, deg.	90	Goodness-of-fit on F^2	0.938
β, deg.	100.172(7)	R_1 / wR_2, $I>2\sigma(I)$	0.0615 / 0.1400
γ, deg.	90	R_1 / wR_2, all data	0.0778 / 0.1463
Volume, $Å^3$	464.53(7)	$\Delta\rho_{max}$ / $\Delta\rho_{min}$, ·e/ $Å^3$	0.936 / -1.089
Z	2	Extinction coefficient	0.029(6)
Density (calculated), Mg/m^3	2.159	Diffractometer model	STADI-VARY Pilatus-100K

7-bromo-7-fluorobicyclo[4.1.0]hept-3-ene (4)

^{1}H NMR (100.6 MHz, $CDCl_3$)

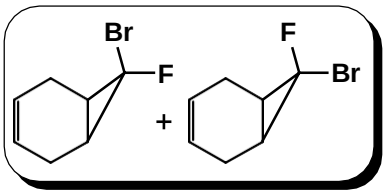


^{13}C NMR (400.0 MHz, $CDCl_3$)

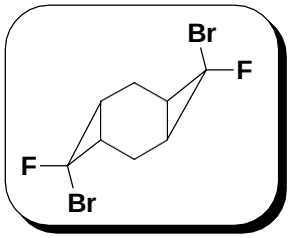


7-bromo-7-fluorobicyclo[4.1.0]hept-3-ene (4)

^{19}F NMR (376.3 MHz, $CDCl_3$)

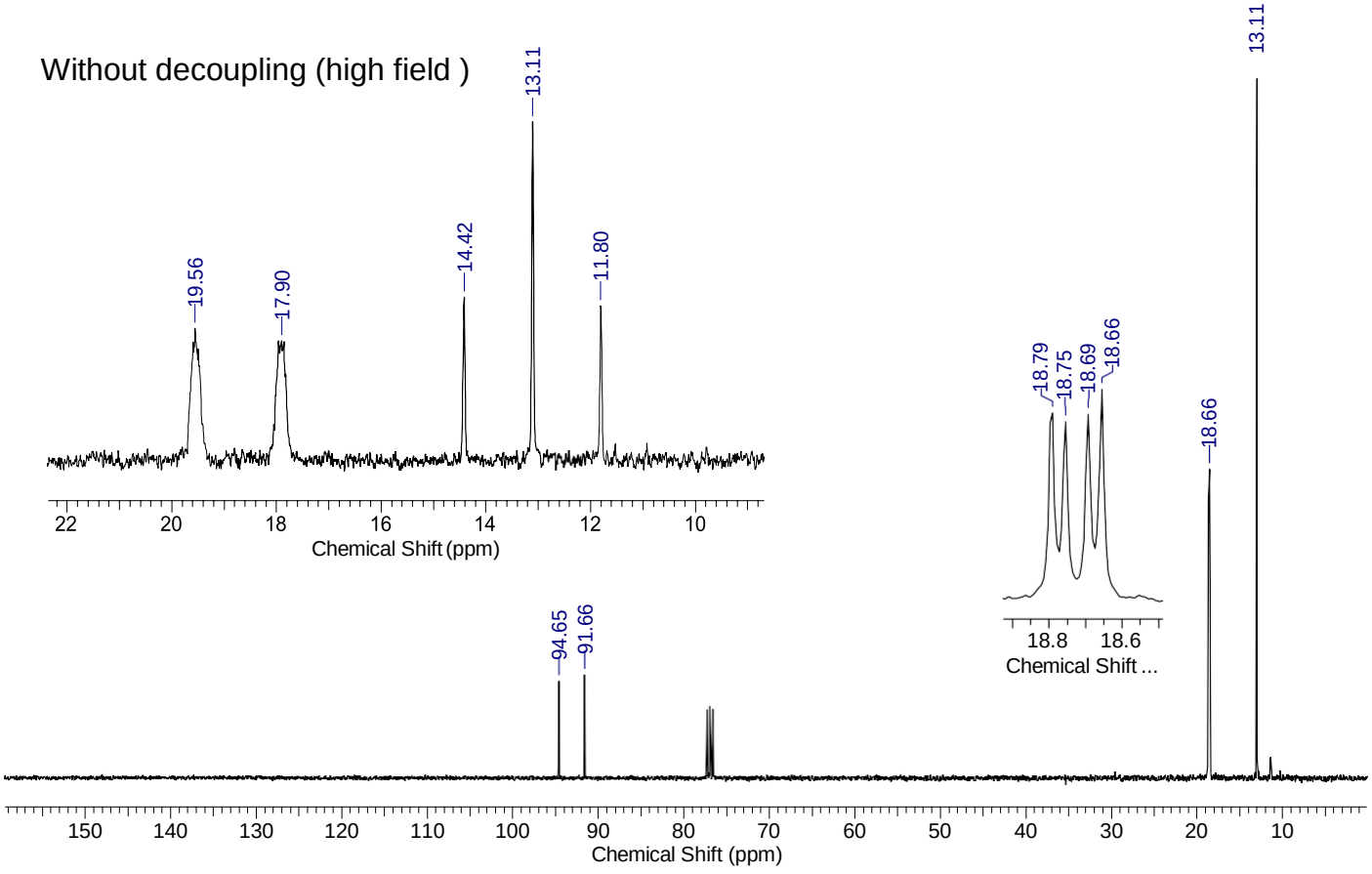


(*s*,*s*)-4,8-dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*s*,*s*)-1)

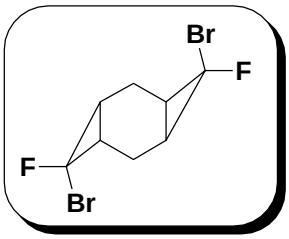


^{1}H NMR (100.6 MHz, $CDCl_3$)

^{13}C NMR (400.0 MHz, $CDCl_3$)



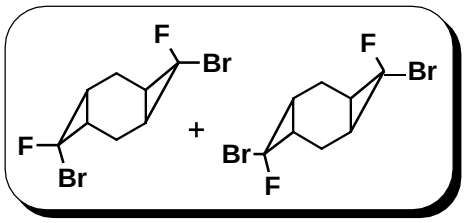
(*s*,*s*)-4,8-dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*s*,*s*)-1)



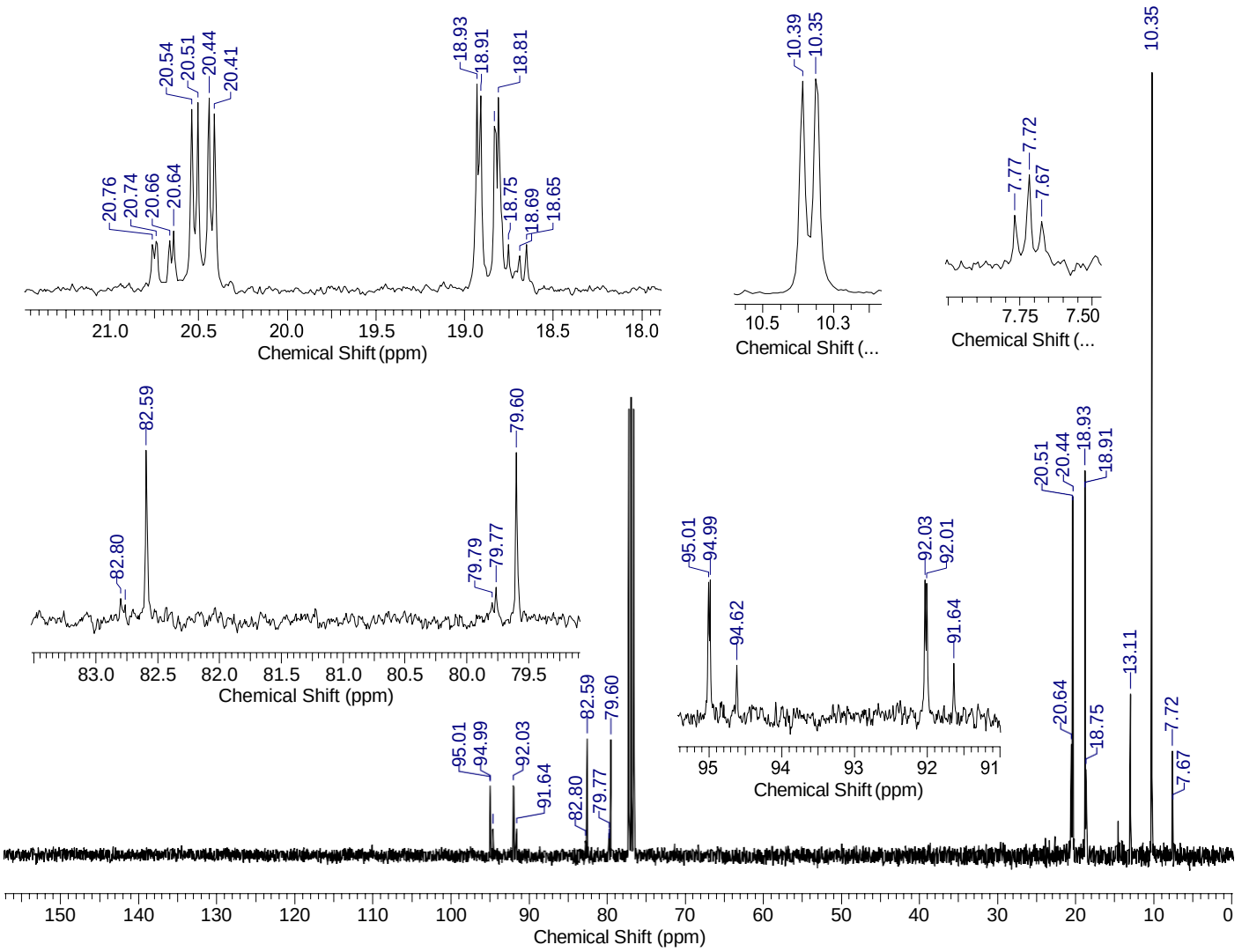
^{19}F NMR (376.3 MHz, $CDCl_3$)

(*r*,*s*)- and (*r*,*r*)-4,8-dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*r*,*s*)-1 and (*r*,*r*)-1)

^{1}H NMR (100.6 MHz, $CDCl_3$)

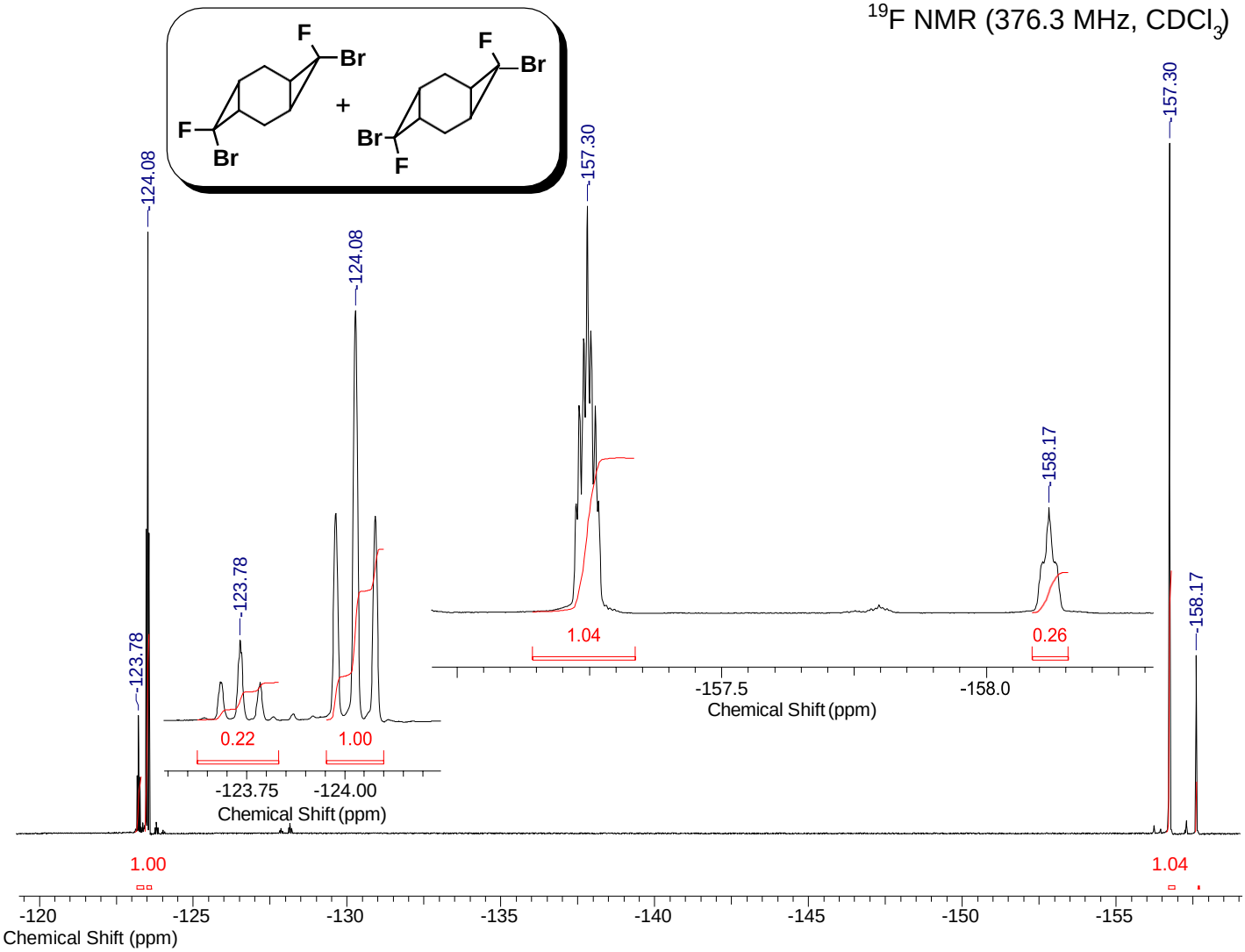


^{13}C NMR (400.0 MHz, $CDCl_3$)

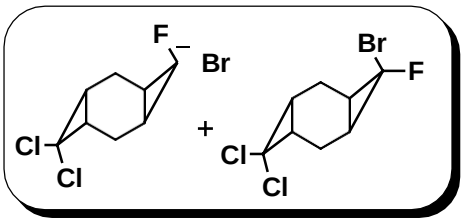


(*r*,*s*)- and (*r*,*r*)-4,8-dibromo-4,8-difluorotricyclo[5.1.0.0^{3,5}]octane ((*r*,*s*)-1 and (*r*,*r*)-1)

^{19}F NMR (376.3 MHz, $CDCl_3$)

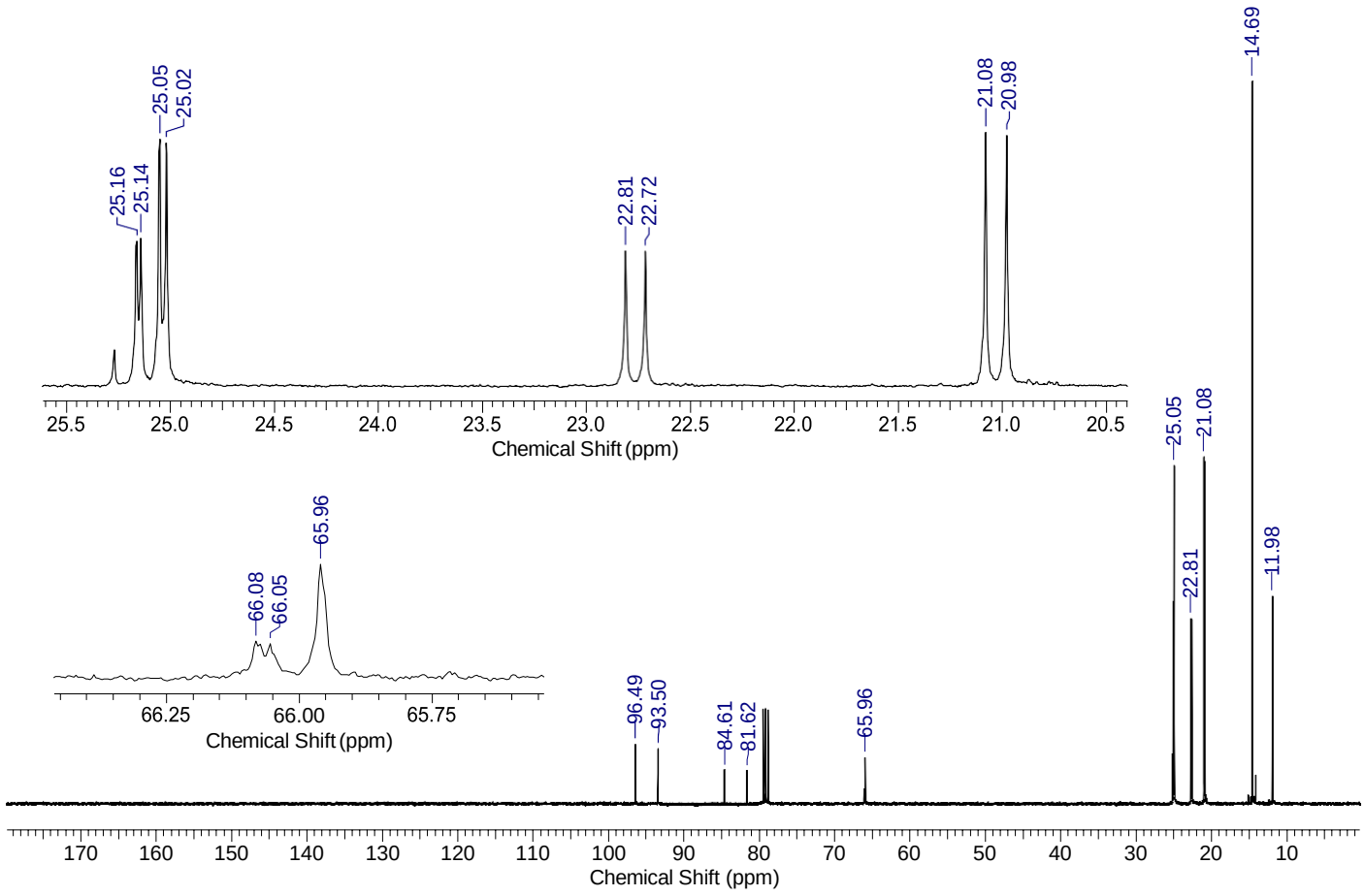


4-bromo-8,8-dichloro-4-fluorotricyclo[5.1.0.0^{3,5}]octane (2)

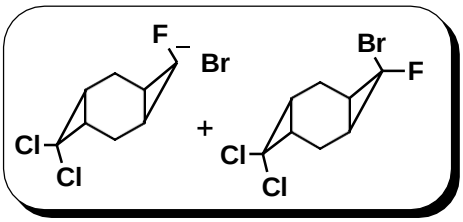


^{1}H NMR (100.6 MHz, $CDCl_3$)

^{13}C NMR (400.0 MHz, $CDCl_3$)

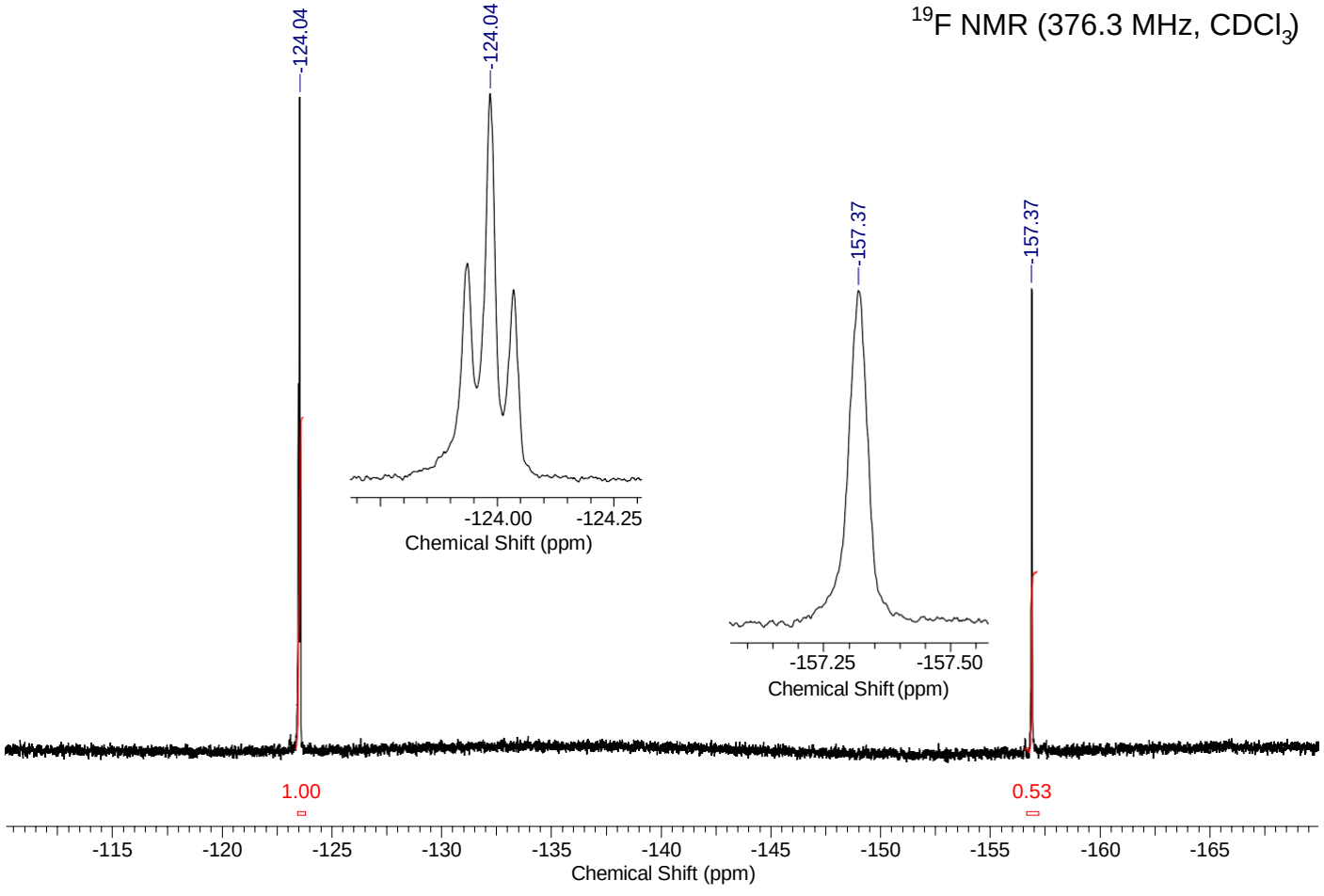


4-bromo-8,8-dichloro-4-fluorotricyclo[5.1.0.0^{3,5}]octane (2)



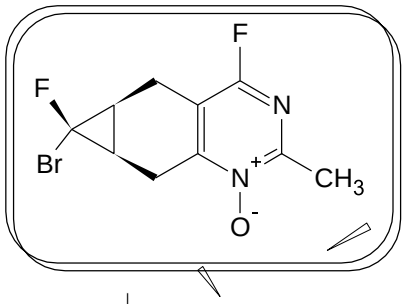
^{13}C NMR without decoupling (400.0 MHz, $CDCl_3$)

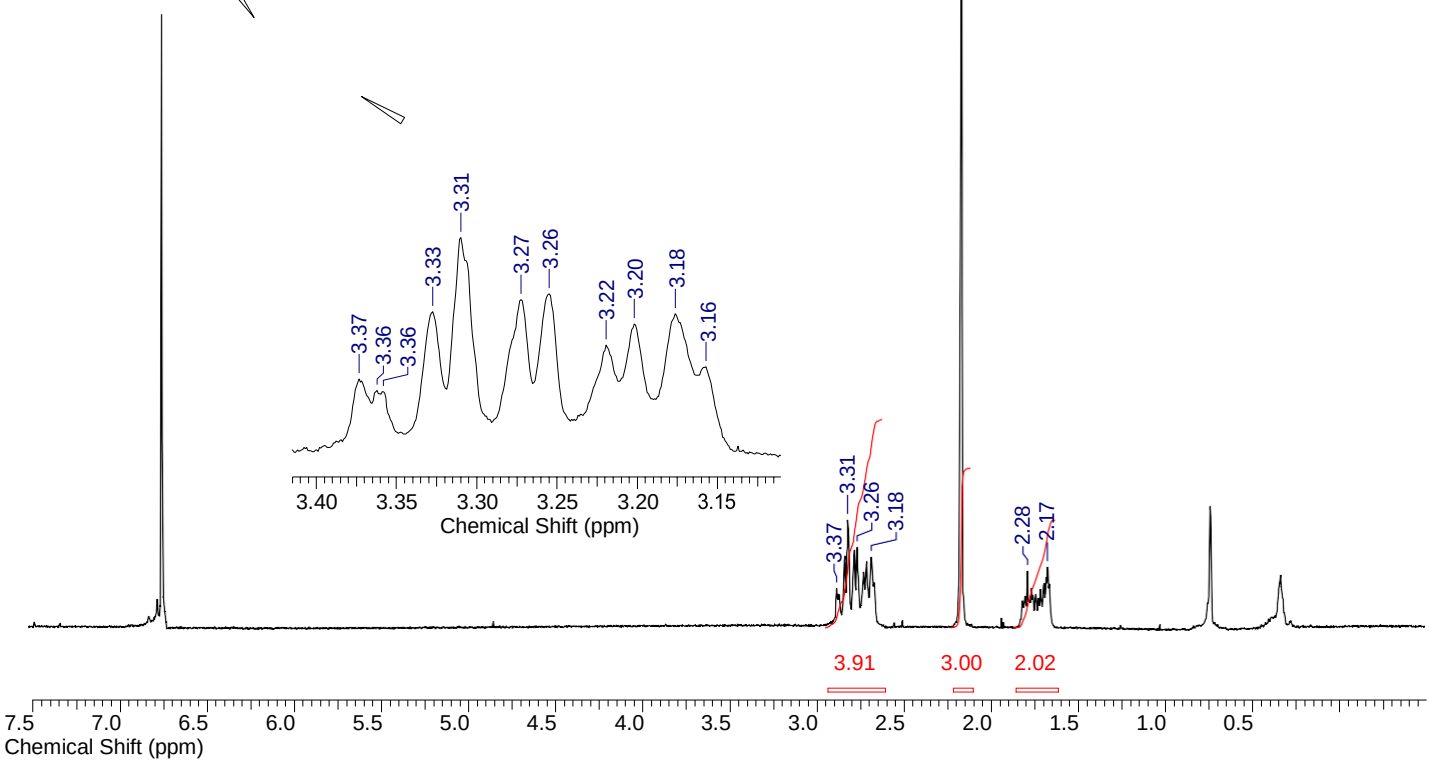
^{19}F NMR (376.3 MHz, $CDCl_3$)



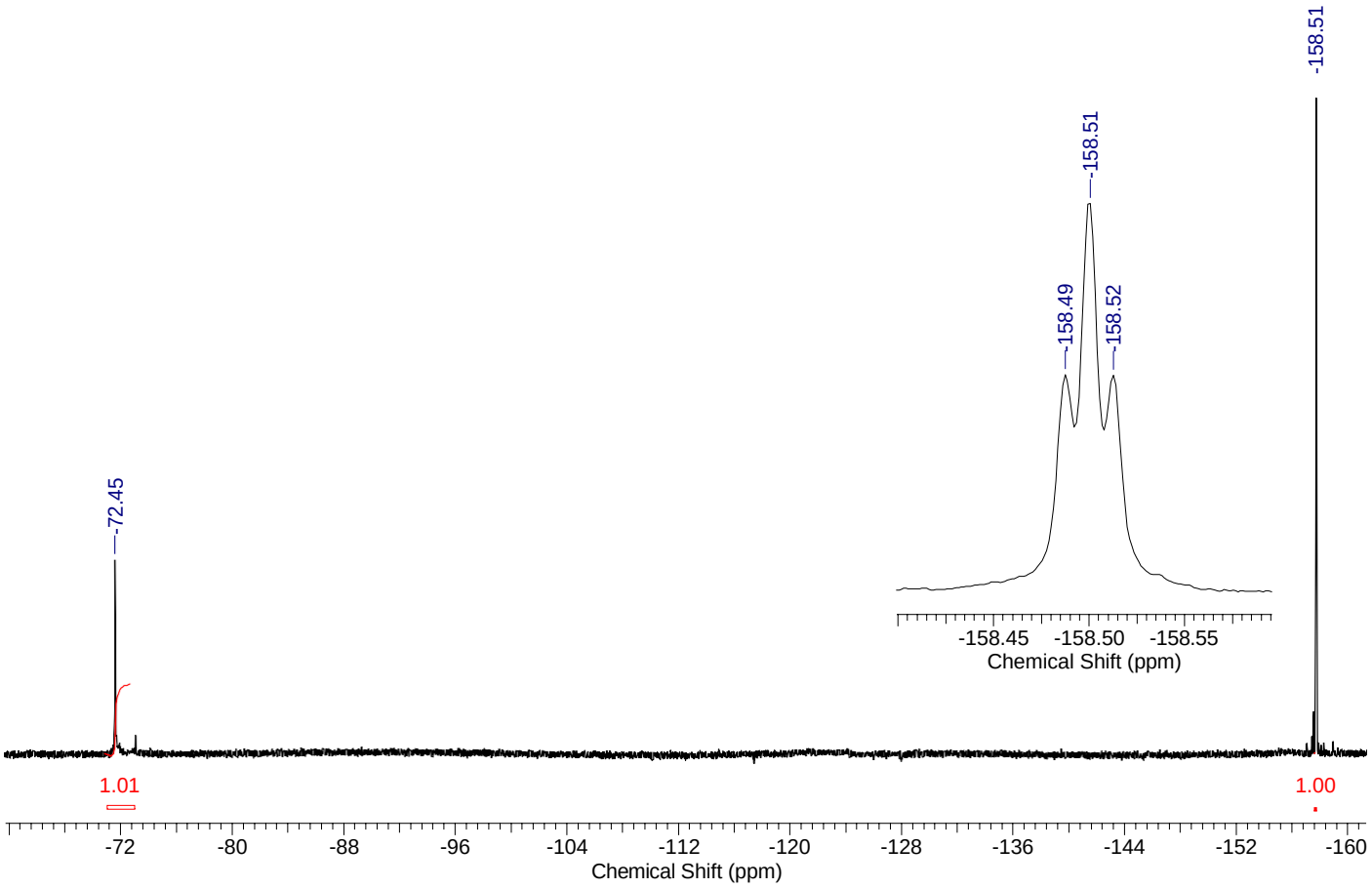
6-bromo-4,6-вшfluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (5)

^{1}H NMR (100.6 MHz, $CDCl_3$)



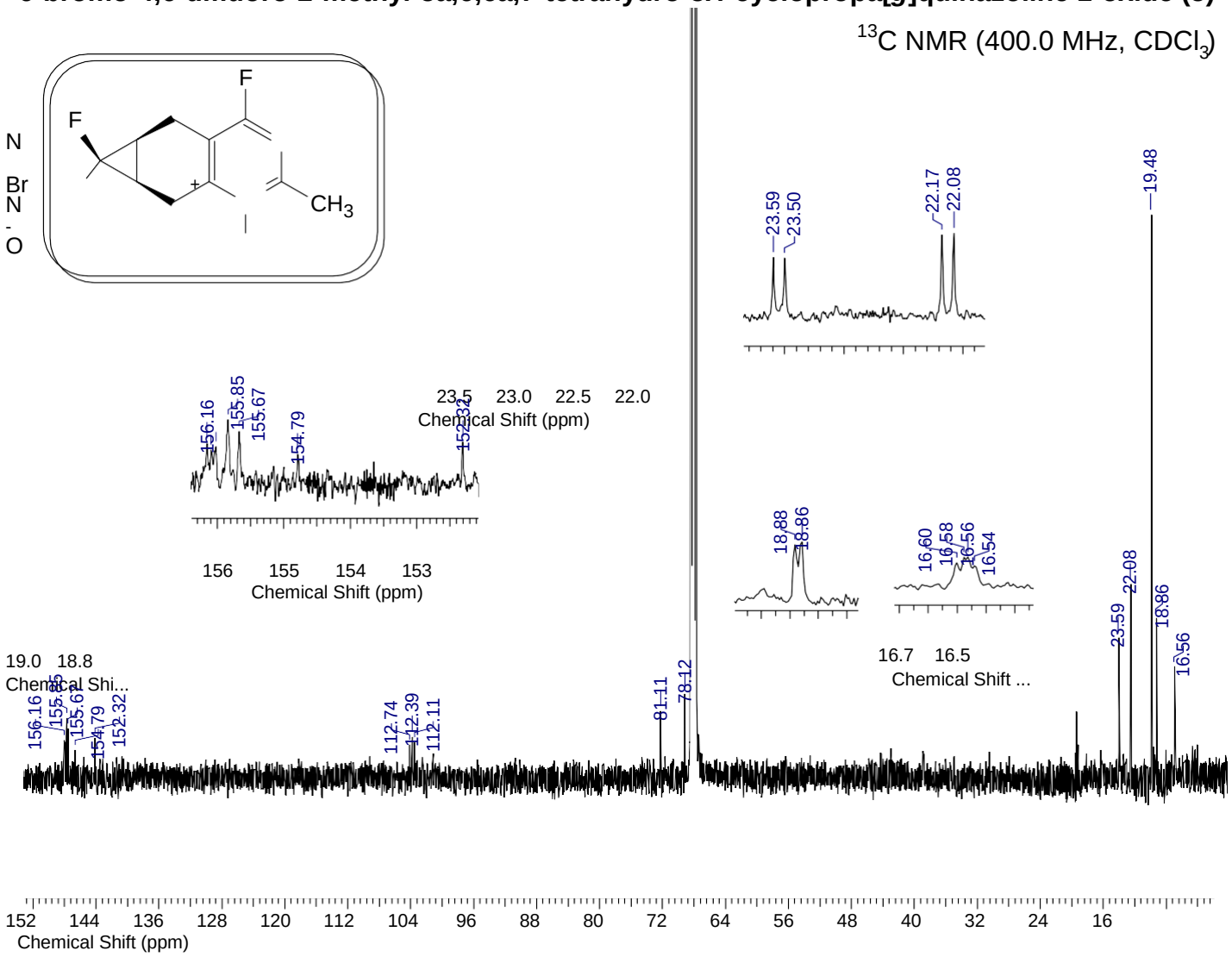


^{19}F NMR (376.3 MHz, $CDCl_3$)

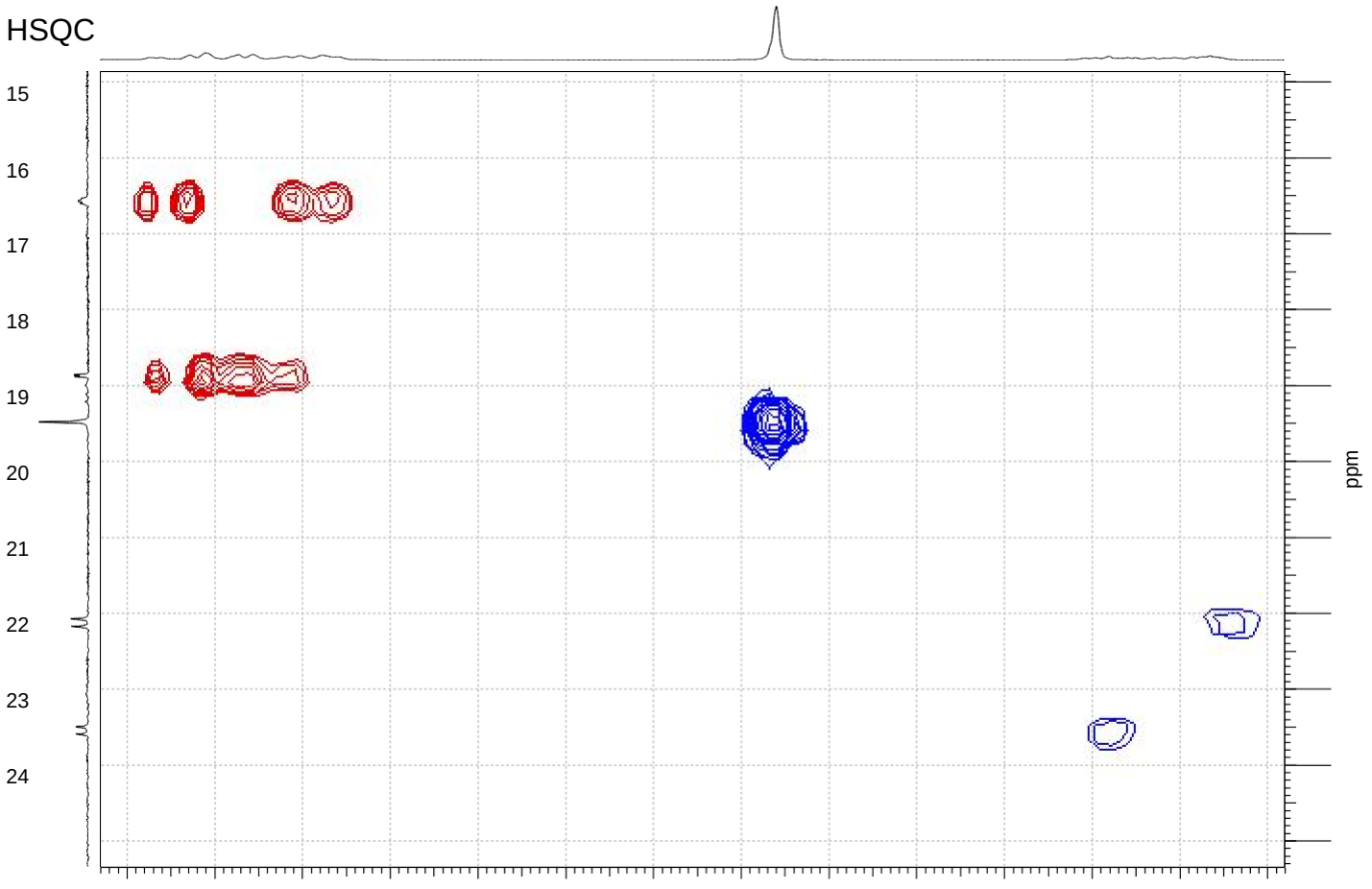


6-bromo-4,6-difluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (5)

^{13}C NMR (400.0 MHz, $CDCl_3$)

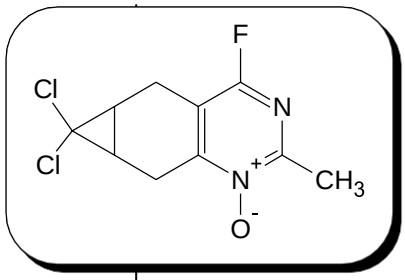


HSQC



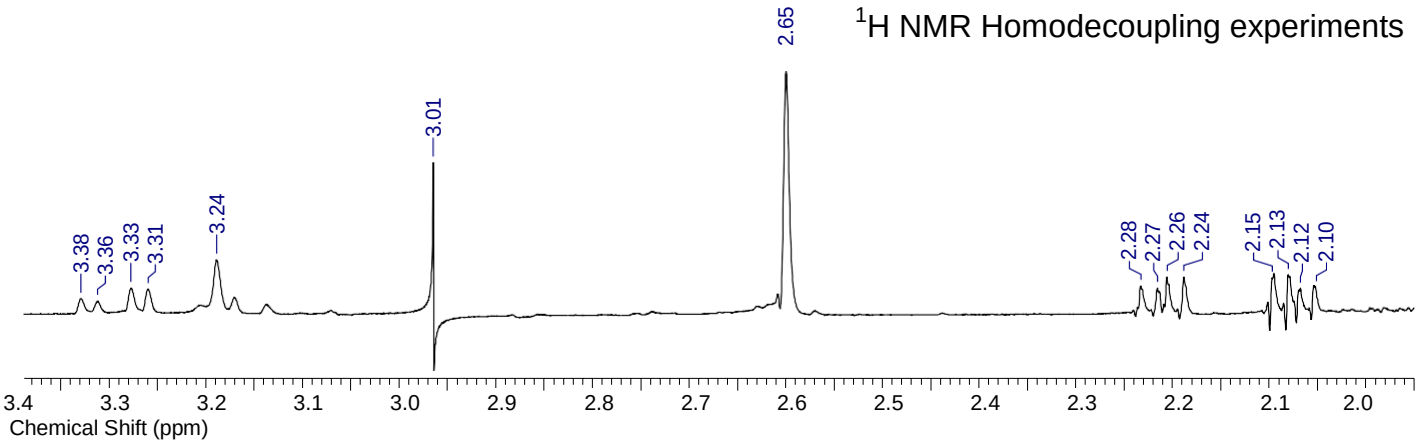

25
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
ppm

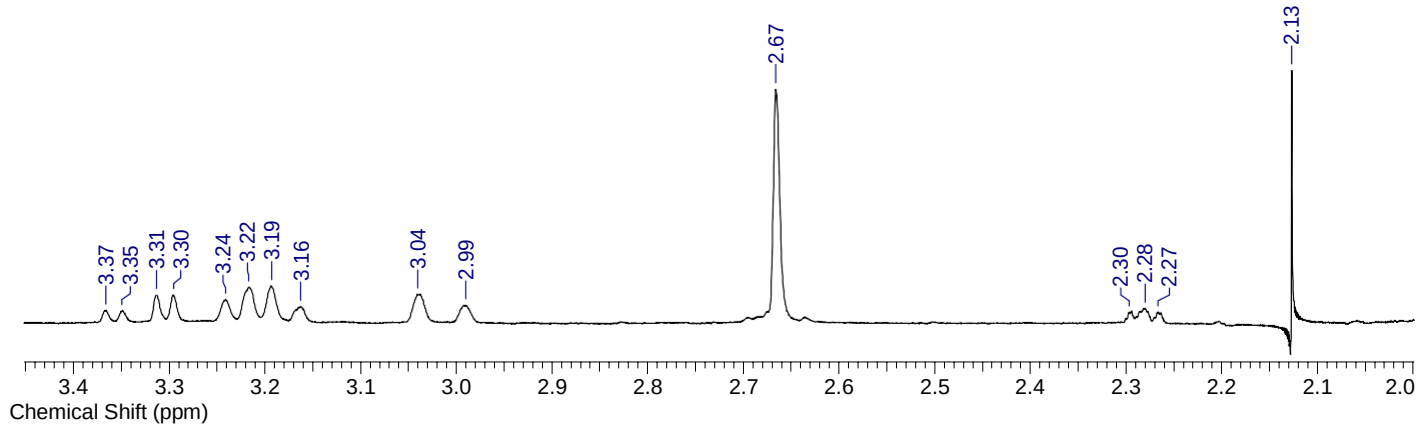
6,6-dichloro-4-fluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (6)



^{1}H NMR (100.6 MHz, $CDCl_3$)

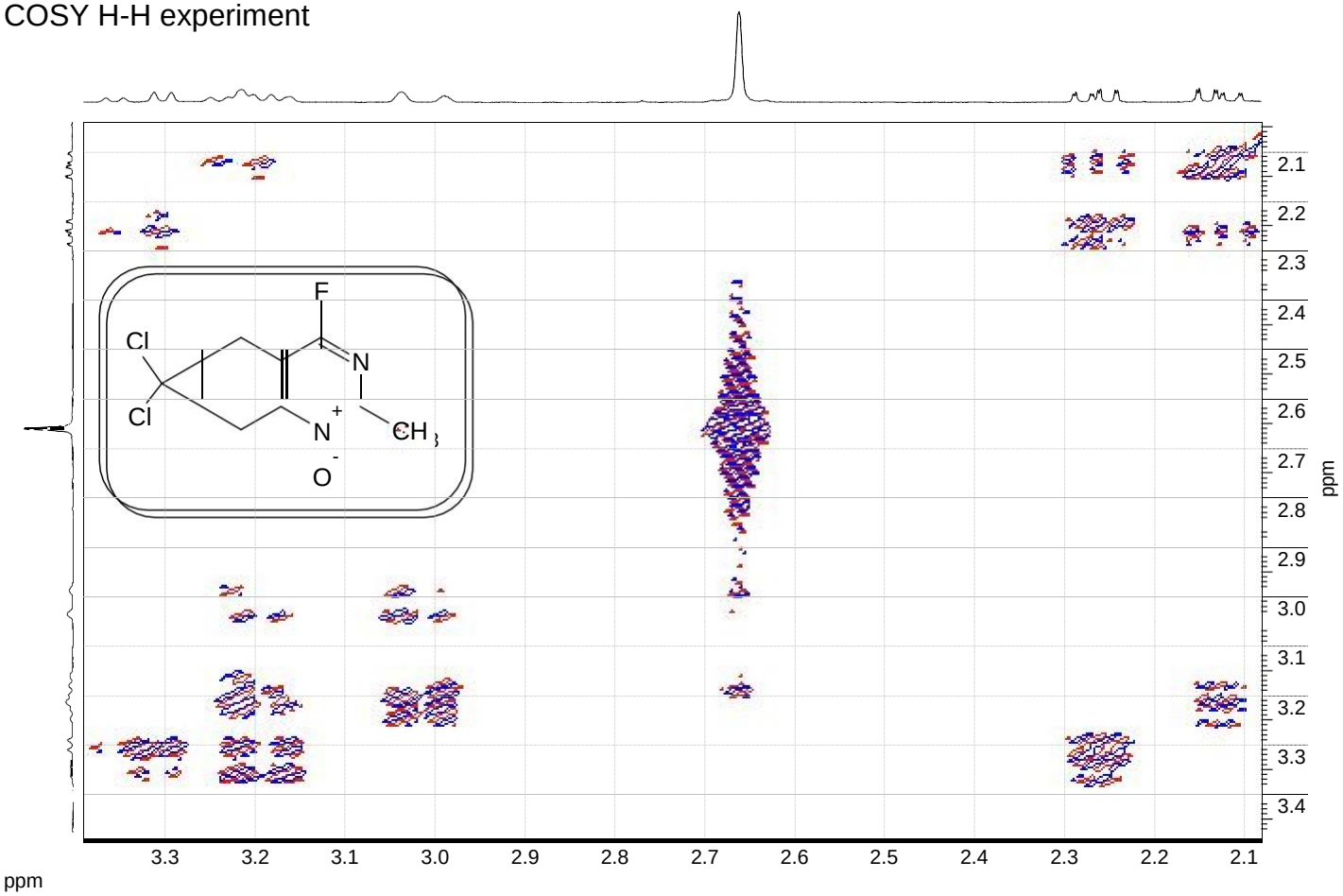
^{1}H NMR Homodecoupling experiments



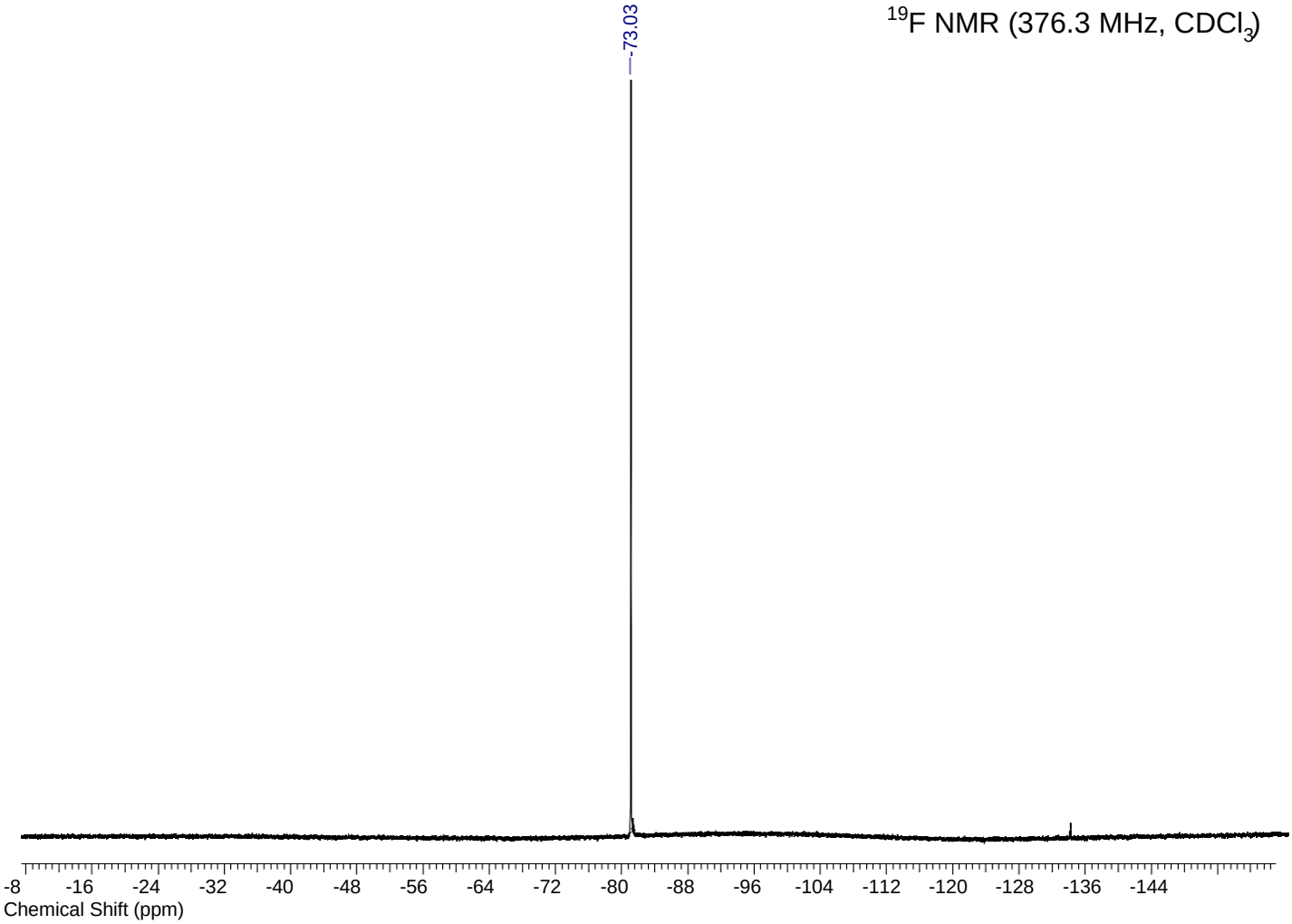


6,6-dichloro-4-fluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (6)

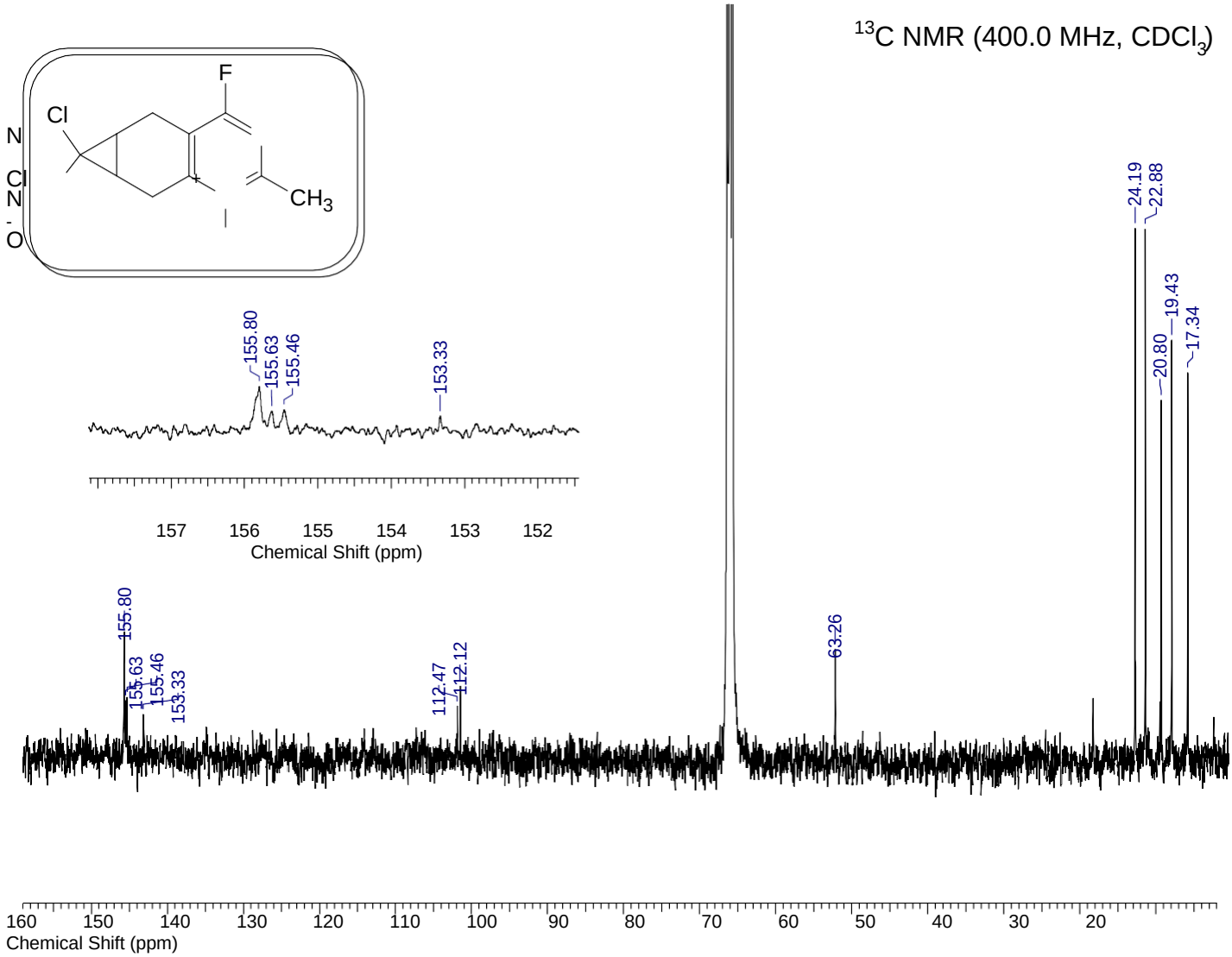
COSY H-H experiment



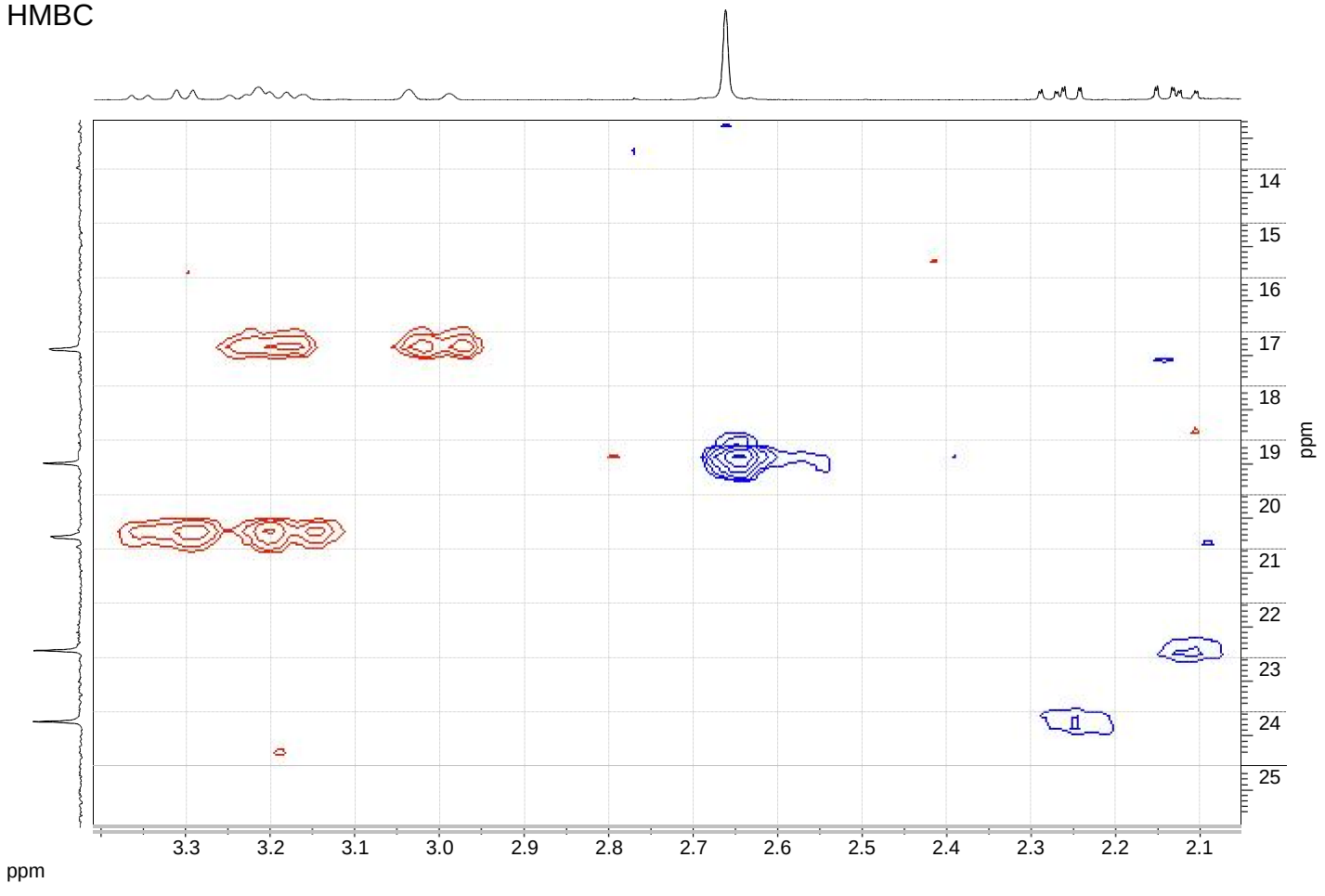
^{19}F NMR (376.3 MHz, $CDCl_3$)



6,6-dichloro-4-fluoro-2-methyl-5a,6,6a,7-tetrahydro-5*H*-cyclopropa[*g*]quinazoline 1-oxide (6)



HMBC

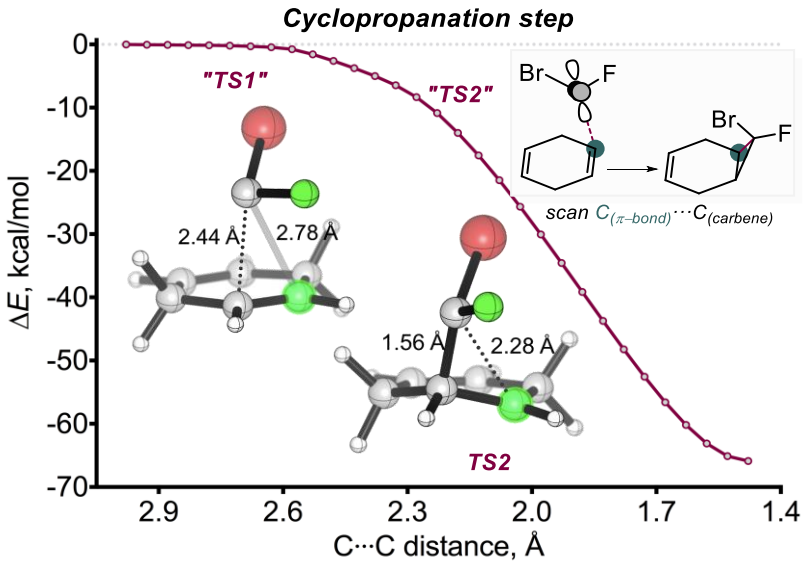


Computational Details

Calculations were carried using the meta-hybrid (U)M06-2X functional[1] and the 6-31+G(d,p) basis set for all atoms, with an ultrafine integration grid (99,590 points). A broken-spin approach was applied when necessary. The implicit SMD[2] solvation model was used to simulate the effects of acetonitrile (MeCN) throughout the calculated structures when necessary. Grimme's D3 version (zero damping) for empirical dispersion[3] was also included. Frequency calculations were carried for all structures to confirm them as either a minimum or a TS. All calculations were performed with the *Gaussian 09* software package.[4] Three-dimensional structures and orbital plots were produced with CYLView 1.0.1[5] and Chemcraft 1.8.[6]

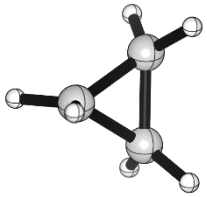
Carbene addition: cyclopropanation step.

Scheme 7 in the main manuscript details the cyclopropanation step. Although the process is barrierless at the potential energy surface, inclusion of entropy creates small barriers at the Gibbs Free Energy surface. Similar behaviour was observed for the 2nd regiosomer herein described. Further analysis was done on Scheme 8, showing the selectivity of the carbene addition stems from electrostatic interactions that are favoured in the regiosomer where F points out of the ring.



Calculated geometries.

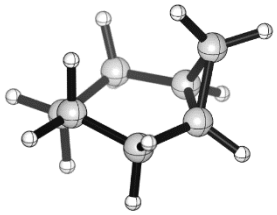
cprop
E = -117.8414182



0 1

C	0.00000000	-0.86767200	0.00000000
H	0.00016400	-1.45391000	0.91208300
C	-0.75154900	0.43362600	0.00000000
C	0.75153300	0.43402800	0.00000000
H	-1.25916500	0.72683700	0.91209500
H	1.25905000	0.72712400	0.91217000
H	1.25905000	0.72712400	-0.91217000
H	0.00016400	-1.45391000	-0.91208300
H	-1.25916500	0.72683700	-0.91209500

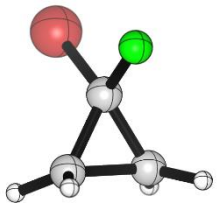
chex_cprop
E = -273.8303065



0 1

C	0.97031100	0.83188900	-0.35256700
C	-0.21321700	-1.51086600	-0.27316400
H	1.60860500	1.38644600	-1.03428000
H	-0.60175700	-1.79191900	-1.26081200
H	0.04121800	-2.44334000	0.24495000
C	1.03793500	-0.67415200	-0.47186400
C	1.69422200	0.01618400	0.68867700
H	1.71648800	-1.05685900	-1.22993100
C	-1.56567500	0.60161200	-0.16542700
H	-2.45130400	1.08130800	0.26486600
H	-1.76722800	0.45504100	-1.23536400
C	-1.32152100	-0.76406900	0.47647300
H	-2.23582800	-1.36648100	0.46435700
H	-1.05048600	-0.63025200	1.53267000
C	-0.34800600	1.51627200	0.00494900
H	-0.30859000	1.86768500	1.04431600
H	-0.47072300	2.40860600	-0.61704500
H	2.77782900	0.05438900	0.72128900
H	1.21747700	-0.06583500	1.66252200

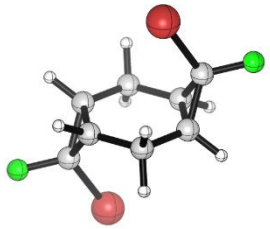
cprop_Br_F
E = -2788.2440812



0 1

C	1.61832300	-0.70097800	0.76725700
H	1.17691100	-1.54704000	1.27966700
C	1.61857600	-0.70149200	-0.76710900
C	0.73374100	0.19715200	0.00003100
H	1.17700800	-1.54780400	-1.27893900
H	2.46054300	-0.22882300	1.26146900
H	2.46089500	-0.22949600	-1.26126000
F	1.03285700	1.52257500	-0.00018000
Br	-1.15414000	-0.08337400	-0.00001100

A_2
E = -5652.7155358

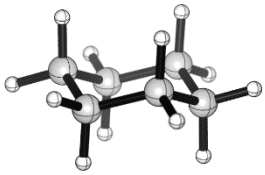


0 1

C	-0.94869200	-1.13266600	-0.56509100
C	0.53425500	-1.08284700	-0.87963900
C	0.94869200	1.13266600	0.56509100
C	-0.53425500	1.08284700	0.87963900
H	1.01534500	-2.05042200	-0.99235300
H	-1.50590900	-1.10330300	-1.50665600
H	-1.16997200	-2.09198900	-0.08701100
H	1.50590900	1.10330300	1.50665600
H	1.16997200	2.09198900	0.08701100
H	-1.01534500	2.05042200	0.99235300
C	1.45703100	0.01855300	-0.32982600
C	1.10569300	-0.04445600	-1.76648600
C	-1.45703100	-0.01855300	0.32982600
C	-1.10569300	0.04445600	1.76648600
H	2.47122300	-0.31251200	-0.12457400
H	-2.47122300	0.31251200	0.12457400
F	2.08062300	-0.42806700	-2.63501600
F	-2.08062300	0.42806700	2.63501600
Br	0.01531000	-1.28826900	2.55258900
Br	-0.01531000	1.28826900	-2.55258900

chex

E = -235.7692965



0 1

C	1.26344400	0.72945000	0.23321400
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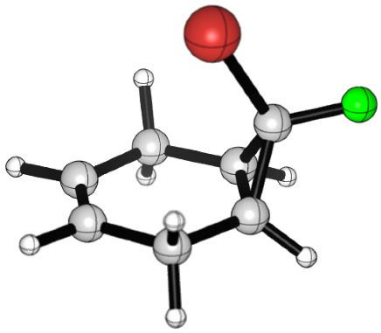
H	1.30763500	0.75496300	1.33142300
H	-1.30763500	0.75496300	1.33142300
H	-2.15828700	1.24608800	-0.13122700
C	0.00000000	1.45889900	-0.23321400
H	0.00000000	2.49217600	0.13122700
C	0.00000000	-1.45889900	0.23321400
H	0.00000000	-2.49217600	-0.13122700
H	0.00000000	-1.50992700	1.33142300
C	-1.26344400	-0.72945000	-0.23321400
H	-2.15828700	-1.24608800	0.13122700
H	-1.30763500	-0.75496300	-1.33142300
C	1.26344400	-0.72945000	-0.23321400
H	1.30763500	-0.75496300	-1.33142300
H	2.15828700	-1.24608800	0.13122700
H	2.15828700	1.24608800	-0.13122700
H	0.00000000	1.50992700	-1.33142300

B2

E = -2943.0281223

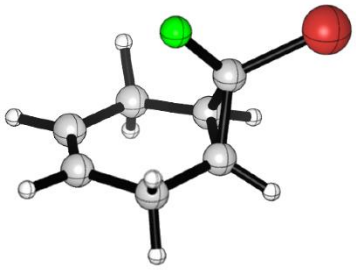


0 1

C	-0.65130300	1.22084300	0.77078000
C	-1.44181400	0.17666700	1.53213600
C	-2.18059300	-0.80606600	0.66721800
C	-2.18098300	-0.80551400	-0.66718400
C	-1.44206100	0.17720600	-1.53207500
C	-0.65137900	1.22094800	-0.77053400
H	-0.58948400	2.20023200	1.23743700
H	-0.77692300	-0.36542200	2.21866400
H	-2.75580000	-1.56246900	1.19742600
H	-2.75641600	-1.56159700	-1.19760400
H	-0.77727300	-0.36518900	-2.21848500
H	-0.58924900	2.20046400	-1.23692400
H	-2.16733700	0.69561300	-2.16916500
H	-2.16727600	0.69492100	2.16913400
C	0.56252600	0.87563100	0.00015700
Br	1.32546300	-0.87446200	-0.00014300
F	1.56691100	1.81237000	0.00017000

B1

E = -2943.0284197



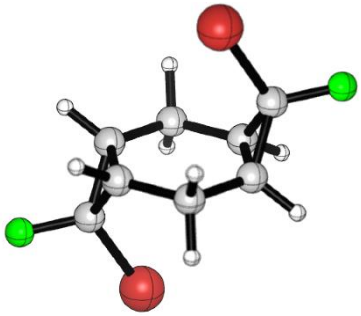
0 1

C	0.56237800	-0.76966700	-0.83402500
C	1.77200700	-1.52910100	-0.32370500
C	2.83869000	-0.66728700	0.29282200
C	2.83891400	0.66722400	0.29263100
C	1.77223400	1.52891600	-0.32383100
C	0.56242400	0.76959300	-0.83416500
H	0.02317000	-1.24175400	-1.64912600
H	1.45491100	-2.29328200	0.39738900
H	3.66860200	-1.19797900	0.75506500
H	3.66896900	1.19777900	0.75477600
H	1.45510600	2.29305700	0.39729600
H	0.02341200	1.24178000	-1.64933200
H	2.20669500	2.07810700	-1.16728500
H	2.20647700	-2.07831400	-1.16715400
Br	-2.17658000	0.00000200	0.00212400

C	-0.26712900	0.00005400	0.12012500
F	0.11065100	0.00023600	1.43499100

cyhex_FBr_BrF

E = -5652.7155358

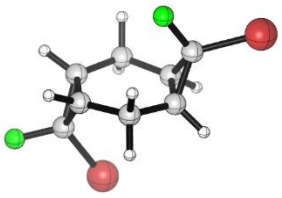


0 1

C	-0.94869200	-1.13266600	-0.56509100
C	0.53425500	-1.08284700	-0.87963900
C	0.94869200	1.13266600	0.56509100
C	-0.53425500	1.08284700	0.87963900
H	1.01534500	-2.05042200	-0.99235300
H	-1.50590900	-1.10330300	-1.50665600
H	-1.16997200	-2.09198900	-0.08701100
H	1.50590900	1.10330300	1.50665600
H	1.16997200	2.09198900	0.08701100
H	-1.01534500	2.05042200	0.99235300
C	1.45703100	0.01855300	-0.32982600
C	1.10569300	-0.04445600	-1.76648600
C	-1.45703100	-0.01855300	0.32982600
C	-1.10569300	0.04445600	1.76648600
H	2.47122300	-0.31251200	-0.12457400
H	-2.47122300	0.31251200	0.12457400
F	2.08062300	-0.42806700	-2.63501600
F	-2.08062300	0.42806700	2.63501600
Br	0.01531000	-1.28826900	2.55258900
Br	-0.01531000	1.28826900	-2.55258900

cyhex_FBr_FBr

E = -5652.7148922



0 1

C	-0.28130700	0.63604500	-1.57267100
C	0.62568900	-0.28019600	-0.76856600
C	-0.28131700	0.63603000	1.57267500
C	-1.32562500	1.38440900	0.76751600
H	0.82344800	-1.25023400	-1.21186600
H	0.33248700	1.37010500	-2.10275600
H	-0.79507400	0.03523100	-2.32952700
H	-0.79508800	0.03520900	2.32952300
H	0.33247400	1.37008500	2.10277000
H	-1.68170800	2.30405300	1.22403700
C	0.62568400	-0.28020400	0.76856700

C	1.74073100	0.31806200	0.00000700
C	-1.32562000	1.38441600	-0.76751100
C	-2.37785100	0.67943500	-0.00000400
H	0.82343900	-1.25024600	1.21185900
H	-1.68170100	2.30406500	-1.22402600
F	-3.62067100	1.23667200	-0.00000500
Br	-2.49936500	-1.22743200	-0.00001400
F	1.79602200	1.68138600	0.00001500
Br	3.48968700	-0.43110400	0.00000900

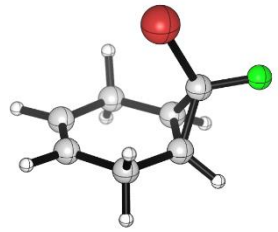
cyhex_BrF_FBr_2
E = -5652.7134328

0 1

C	0.00099600	-1.57715900	-0.11109300
C	1.06769400	-0.76842800	0.60634500
C	0.00099600	1.57716800	-0.11105200
C	-1.12733800	0.76733300	-0.72293700
H	1.46619800	-1.21835800	1.50937900
H	0.47434600	-2.15962000	-0.90690800
H	-0.42688300	-2.29015700	0.59936000
H	-0.42687900	2.29014800	0.59941900
H	0.47434600	2.15964700	-0.90685400
H	-1.60830000	1.22370800	-1.58190200
C	1.06769500	0.76841700	0.60636300
C	2.03652000	0.00000300	-0.20776800
C	-1.12733700	-0.76730800	-0.72296100
C	-2.02038900	-0.00000200	0.17577700
H	1.46620100	1.21832400	1.50940800
H	-1.60829700	-1.22365900	-1.58194000
Br	-3.91179100	0.00000000	-0.03974900
F	-1.69163400	-0.00002500	1.49986300
F	1.81205800	0.00001700	-1.55413400
Br	3.90357400	-0.00000300	0.15896100

SMD=MeCN

cyhexeneBrF_s
E = -2943.0281223



0 1

C	-0.65130300	1.22084300	0.77078000
C	-1.44181400	0.17666700	1.53213600
C	-2.18059300	-0.80606600	0.66721800

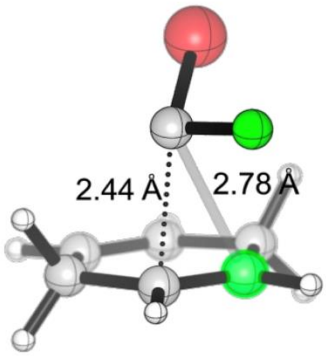
C	-2.18098300	-0.80551400	-0.66718400
C	-1.44206100	0.17720600	-1.53207500
C	-0.65137900	1.22094800	-0.77053400
H	-0.58948400	2.20023200	1.23743700
H	-0.77692300	-0.36542200	2.21866400
H	-2.75580000	-1.56246900	1.19742600
H	-2.75641600	-1.56159700	-1.19760400
H	-0.77727300	-0.36518900	-2.21848500
H	-0.58924900	2.20046400	-1.23692400
H	-2.16733700	0.69561300	-2.16916500
H	-2.16727600	0.69492100	2.16913400
C	0.56252600	0.87563100	0.00015700
Br	1.32546300	-0.87446200	-0.00014300
F	1.56691100	1.81237000	0.00017000

cyhexeneFBr_s
E = -2943.0284197

0 1

C	0.56237800	-0.76966700	-0.83402500
C	1.77200700	-1.52910100	-0.32370500
C	2.83869000	-0.66728700	0.29282200
C	2.83891400	0.66722400	0.29263100
C	1.77223400	1.52891600	-0.32383100
C	0.56242400	0.76959300	-0.83416500
H	0.02317000	-1.24175400	-1.64912600
H	1.45491100	-2.29328200	0.39738900
H	3.66860200	-1.19797900	0.75506500
H	3.66896900	1.19777900	0.75477600
H	1.45510600	2.29305700	0.39729600
H	0.02341200	1.24178000	-1.64933200
H	2.20669500	2.07810700	-1.16728500
H	2.20647700	-2.07831400	-1.16715400
Br	-2.17658000	0.00000200	0.00212400
C	-0.26712900	0.00005400	0.12012500
F	0.11065100	0.00023600	1.43499100

B2_scan_TS1

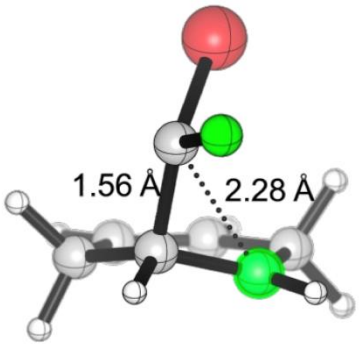


0 1

C	-1.16521300	0.98224400	1.07843800
C	-1.48751600	-0.42065800	1.48428500

C	-2.13789000	-1.21779300	0.38770300
C	-2.29665400	-0.76084400	-0.85658100
C	-1.86312800	0.60853900	-1.30404800
C	-1.30814200	1.44014600	-0.18148500
H	-0.78107600	1.64845300	1.84875300
H	-0.56619500	-0.92523700	1.81980700
H	-2.47703000	-2.21946000	0.64346100
H	-2.77040100	-1.39260100	-1.60547800
H	-1.10673300	0.52596600	-2.09893000
H	-1.10031400	2.48613600	-0.39583800
H	-2.70813600	1.13728800	-1.76452100
H	-2.12992000	-0.40059400	2.37525900
C	1.07746100	1.08262500	-0.55901200
Br	1.53463200	-0.78272100	-0.12328100
F	1.66824200	1.80552700	0.35516800

B2_scan_TS2

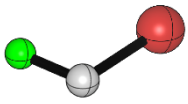


0 1

C	-0.99697200	1.00398200	1.13209500
C	-1.46564800	-0.35599900	1.48456600
C	-2.12402000	-1.08688300	0.34856500
C	-2.16412300	-0.61517500	-0.89984300
C	-1.58415700	0.70473500	-1.33213400
C	-0.72537300	1.38324900	-0.26768600
H	-0.64321500	1.66149500	1.92132300
H	-0.63010200	-0.97114300	1.87779200
H	-2.56731000	-2.05307300	0.57883100
H	-2.65963700	-1.19687000	-1.67488500
H	-0.98674300	0.57552200	-2.24334700
H	-0.67519900	2.46289700	-0.42004300
H	-2.40557100	1.38272300	-1.59554300
H	-2.15582200	-0.26877400	2.33573300
C	0.77072700	0.93625300	-0.30418800
Br	1.36065300	-0.84517800	-0.11877500
F	1.64868000	1.79638700	0.26767000

CBrF

E = -2709.5820423

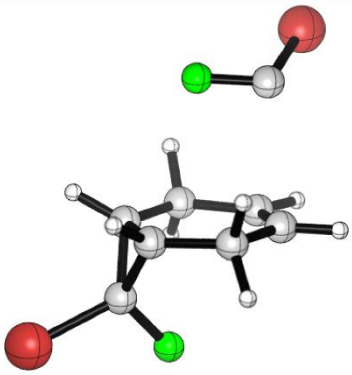


0 1

Br	0.00000000	0.68182200	0.00000000
C	0.62954700	-1.14375600	0.00000000
F	-0.41969800	-1.88902600	0.00000000

B1_complex1

E = -5652.6273843

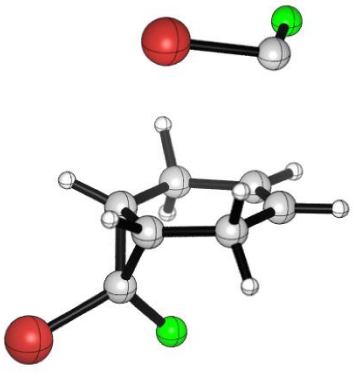


0 1

C	-0.90024400	0.58511600	-0.42030100
C	0.16574700	0.01467200	-1.33562500
C	0.88116900	-1.18558900	-0.79230900
C	0.70827800	-1.69256800	0.43741900
C	-0.26740500	-1.17673700	1.45593600
C	-1.11595400	-0.01203800	0.98186900
H	-1.06768800	1.65408100	-0.50594900
H	-0.26449000	-0.22885600	-2.31511500
H	1.60710300	-1.64905900	-1.45675000
H	1.29262200	-2.56033900	0.73604600
H	-0.91107700	-2.00209000	1.78544600
H	-1.41570600	0.69324000	1.75045500
H	0.28947300	-0.85785900	2.34536600
H	0.90667600	0.80283700	-1.53023600
Br	-3.84833500	0.52321000	-0.04915300
C	-2.09343300	-0.23136900	-0.10707100
F	-2.15117400	-1.48718500	-0.64910000
Br	3.94615400	0.27545200	-0.26040300
C	2.52567800	0.15424300	1.08102900
F	1.78632900	1.20501800	0.89571100

B1_cp2

E = -5652.6303681

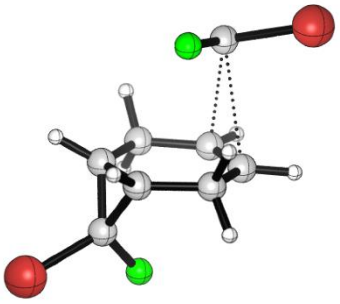


0 1

C	0.58799100	-0.05758100	-0.74956500
C	-0.23184500	0.99546200	-1.46940800
C	-0.90256600	1.98763900	-0.56543800
C	-0.87802200	1.95025900	0.77299400
C	-0.16292100	0.91646600	1.59545100
C	0.62055800	-0.09938700	0.78634800
H	0.64748500	-1.02272400	-1.24331400
H	0.39221000	1.52814100	-2.19837200

H	-1.46021500	2.77988000	-1.06118900
H	-1.40804600	2.71835100	1.33228300
H	0.49834800	1.41711000	2.31387500
H	0.69732400	-1.08961000	1.22440200
H	-0.90486800	0.37974300	2.20060600
H	-1.00319600	0.48555900	-2.06256100
Br	3.41076600	-0.66036200	-0.06162600
C	1.79220500	0.35542200	0.00486300
F	2.08557700	1.69152200	0.03671200
C	-3.23705200	0.42365700	0.50931100
F	-3.81865800	0.85734900	-0.56197400
Br	-2.47909200	-1.31015000	0.03060500

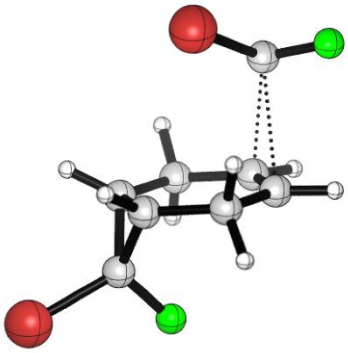
B1_TS3
E = -5652.627369



0 1

C	-1.12868300	0.01553400	0.99146400
C	-0.24077800	1.16990100	1.41706200
C	0.77197000	1.58813600	0.39105900
C	0.91543100	1.03154500	-0.82639000
C	0.16264700	-0.16611500	-1.31349700
C	-0.92931500	-0.65291500	-0.38065700
H	-1.45850800	-0.64117000	1.78992900
H	-0.85403300	2.04126200	1.67897700
H	1.37964400	2.45307400	0.64706800
H	1.64687800	1.44963500	-1.51348000
H	-0.24857300	0.04319300	-2.30870300
H	-1.13700700	-1.71735100	-0.41919000
H	0.87978000	-0.98654500	-1.46073200
H	0.28516500	0.88510100	2.33581400
Br	-3.87413000	-0.46113900	-0.03353300
C	-2.09167600	0.22227700	-0.11317500
F	-2.09638600	1.45357000	-0.71163200
Br	3.95517100	-0.23314200	-0.23872700
C	2.45710600	-0.10746400	1.04440800
F	1.78193900	-1.21276600	0.88027300

B1_TS4
E = -5652.6292597

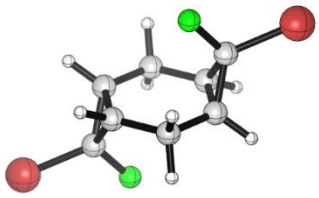


0 1

C	0.67671500	-0.08746900	-0.83328300
C	-0.17513000	0.98925100	-1.48070200
C	-1.04236900	1.76016700	-0.52474900
C	-1.03668500	1.59181300	0.82118500
C	-0.26707700	0.54808700	1.55527400
C	0.63658700	-0.30340400	0.68695100
H	0.83196900	-0.98345800	-1.42531700
H	0.46083800	1.69991100	-2.02186300
H	-1.56190300	2.62088400	-0.93827900
H	-1.65400400	2.24819000	1.43106500
H	0.30480600	1.03535800	2.35576100
H	0.76695700	-1.32988400	1.01377700
H	-0.98208500	-0.11111400	2.06773200
H	-0.82191200	0.52392900	-2.23260300
Br	3.50740300	-0.53742400	-0.03903400
C	1.80484700	0.32571300	0.03211300
F	1.97244300	1.67094300	0.22565900
C	-2.91312900	0.58968900	-0.66392600
Br	-2.56703000	-1.26453700	-0.00314300
F	-3.79025100	1.09369600	0.18198300

A_GS_dual_rr

E = -5652.7308263

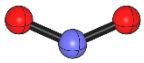


0 1

C	-0.00002900	-1.58047600	-0.00072500
C	1.09505200	-0.76931000	0.66968200
C	0.00001600	1.58043200	-0.00178500
C	-1.09570600	0.76925500	-0.67110500
H	1.53062600	-1.22380500	1.55369700
H	0.45131300	-2.23207100	-0.75422700
H	-0.45095100	-2.23279500	0.75239600
H	-0.45088800	2.23329300	0.75087900
H	0.45140300	2.23150500	-0.75571300
H	-1.53213500	1.22374800	-1.55470600
C	1.09505300	0.76966200	0.66917700
C	2.02719400	-0.00010100	-0.18258700
C	-1.09572800	-0.76969500	-0.67055200
C	-2.02701800	0.00009800	0.18213700

H	1.53063500	1.22474600	1.55288500
H	-1.53219900	-1.22480500	-1.55381400
F	1.76197800	-0.00056000	-1.52663700
Br	3.91629000	0.00005200	0.09937200
F	-1.76060900	0.00061300	1.52594600
Br	-3.91637900	-0.00003700	-0.09796100

NO2_r
E = -204.99165



0 2

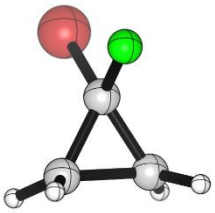
N	0.00000000	-0.32703600	0.00000000
O	1.09026900	0.14310600	0.00000000
O	-1.09026900	0.14305100	0.00000000

NO2+_SMD
E = -204.7331183

1 1

N	0.00000000	0.00000000	-0.00005500
O	0.00000000	0.00000000	1.11624200
O	0.00000000	0.00000000	-1.11619400

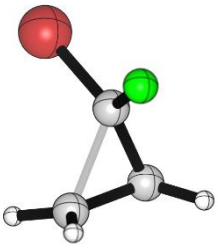
cpropBrF
E = -2788.2534033



0 1

C	-1.62918200	-0.69594700	0.76723800
C	-1.62918500	-0.69594600	-0.76723700
C	-0.73821800	0.19135200	0.00000000
H	-2.46744600	-0.21385900	1.26018700
H	-1.19735500	-1.54824200	1.27914700
H	-2.46745000	-0.21385800	-1.26018300
H	-1.19736000	-1.54824100	-1.27914900
Br	1.15634000	-0.08672000	0.00000000
F	-1.01808800	1.52918300	0.00000000

cpropBrF_rc
E = -2787.9806219

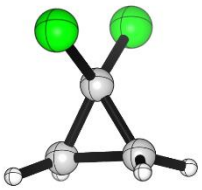


1 2

C	-1.67814800	-0.57516900	0.74407300

C	-1.74715800	-0.81968100	-0.70303800
C	-0.63115100	0.29421100	0.14423200
H	-2.48187200	0.03030700	1.16423500
H	-1.28559500	-1.38970800	1.35013100
H	-2.38360200	-0.20443600	-1.33311700
H	-1.23078700	-1.66650500	-1.14387100
Br	1.14555400	-0.11519100	-0.00496900
F	-0.93042200	1.54065100	-0.10834100

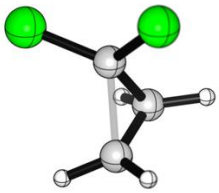
cpropCl2
E = -1036.9818771



0 1

C	-0.75860400	1.49470500	0.00000000
C	0.75860400	1.49470500	0.00000000
C	0.00000000	0.21599400	0.00000000
H	-1.26738000	1.76419300	0.91948900
H	-1.26738000	1.76419300	-0.91948900
H	1.26738000	1.76419400	0.91948900
H	1.26738000	1.76419400	-0.91948900
Cl	0.00000000	-0.77321200	-1.46693000
Cl	0.00000000	-0.77321200	1.46693000

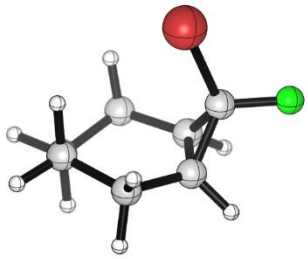
cpropCl2_rc_ubs
E = -1036.7122803



1 2

C	-0.25325900	1.77925400	0.00000000
C	1.20814400	1.33376000	0.00000000
C	0.11215600	0.36020800	0.00000000
H	-0.66899700	2.17349200	0.92256500
H	-0.66899700	2.17349200	-0.92256500
H	1.77328400	1.42949700	0.92272600
H	1.77328400	1.42949700	-0.92272600
Cl	-0.25325900	-0.82486200	-1.27563600
Cl	-0.25325900	-0.82486200	1.27563600

A
E = -2944.2499849

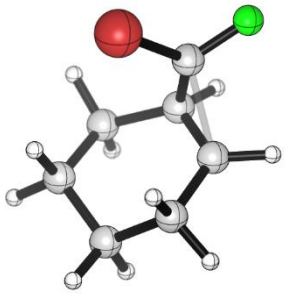


0 1

C	-0.63958900	1.24411400	0.65657700
C	-1.37865900	-0.02286100	-1.55697200
H	-0.61446400	2.26697300	1.02330400
H	-2.19413100	0.45709600	-2.10872500
H	-0.73913800	-0.51354500	-2.30079300
C	-0.60087500	1.09408600	-0.88041900
C	0.60504700	0.87634400	-0.05911400
H	-0.55677900	2.02766800	-1.43663800
F	1.56693700	1.85540900	-0.12948900
Br	1.46290100	-0.82583800	0.09936500
C	-2.56283200	-0.39999800	0.65167900
H	-3.08684000	-1.14027200	1.26481100
H	-3.29706300	0.36436100	0.36272100
C	-1.99328600	-1.05975100	-0.60297200
H	-2.77898100	-1.59989600	-1.14096000
H	-1.24621600	-1.80437100	-0.30543700
C	-1.45023100	0.25118400	1.47713700
H	-0.79251100	-0.52998400	1.87892500
H	-1.87528700	0.77892600	2.33491800

A_cat_rad

E = -2943.9933855

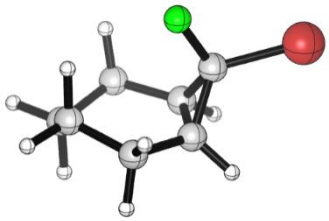


1 2

C	-1.33979700	0.00434900	-1.54783600
H	-2.16039300	0.52073200	-2.05619500
H	-0.68706100	-0.40491000	-2.32435000
C	0.73174300	0.82800700	-0.19825600
F	1.57884600	1.82666900	-0.10124200
Br	1.48305000	-0.80927800	0.13407200
C	-2.59211900	-0.50770100	0.58794800
H	-3.02094400	-1.30068900	1.20471700
H	-3.41065600	0.15595200	0.28651900
C	-1.92322400	-1.09343900	-0.65191700
H	-2.65542600	-1.65226600	-1.24117500
H	-1.15578200	-1.81496800	-0.35371800
C	-1.59949700	0.29643900	1.43927900
H	-0.89423400	-0.37873600	1.95064100
H	-2.09481300	0.84378600	2.24725600
C	-0.59208600	1.11280600	-0.81108100

H	-0.49418400	2.06298900	-1.34495900
C	-0.84822100	1.29456200	0.64129700
H	-0.56366500	2.24267800	1.09331600

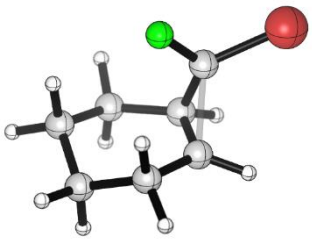
A_regio
E = -2944.25167



0 1

C	1.71583800	1.49107800	-0.43894300
H	2.21912600	1.80128200	-1.36167500
H	1.37423200	2.40532700	0.05917800
C	-0.35237200	0.01088900	0.14550800
C	2.99076300	-0.66466300	-0.10003500
H	3.80490400	-1.14091300	0.45589900
H	3.30599700	-0.60168200	-1.15048300
C	2.73234800	0.74343700	0.43526200
H	3.66261000	1.32028000	0.45508100
H	2.37776500	0.67584300	1.47037000
C	1.73184100	-1.52912000	0.00353100
H	1.51438000	-1.72450600	1.06049400
H	1.89780000	-2.49971500	-0.47056600
C	0.51485400	0.65845000	-0.85837200
H	0.00185600	1.00562500	-1.75044000
C	0.52524100	-0.87201300	-0.66033200
H	0.02585000	-1.44590100	-1.43449900
Br	-2.25767400	-0.01326600	-0.04834900
F	-0.03522400	0.18225900	1.46657000

A_cat_rad_regio
E = -2943.9952724

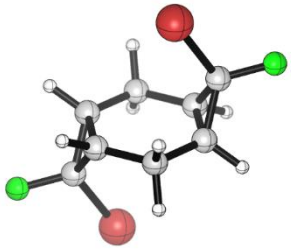


1 2

C	1.69516600	1.39944800	-0.61275500
H	2.20027000	1.55330900	-1.57199200
H	1.30198300	2.36518700	-0.28565500
C	-0.44287900	0.20982300	0.15307100
C	3.01509600	-0.64104000	0.07771900
H	3.74467700	-1.03691700	0.78796600
H	3.45440800	-0.71124900	-0.92405700
C	2.68559600	0.81451300	0.39734300
H	3.59716700	1.41782000	0.36189200
H	2.29604000	0.89331900	1.41747000
C	1.75730800	-1.52569300	0.12648000
H	1.40603800	-1.61439100	1.16757300

H	1.94912000	-2.54883200	-0.20745900
C	0.51500600	0.48234300	-0.94650300
H	-0.01832700	0.70868600	-1.87136200
C	0.66562400	-0.97952400	-0.71434600
H	0.02350400	-1.65493400	-1.27436300
Br	-2.25108100	-0.04431400	-0.02870500
F	-0.05694900	0.40219700	1.39095700

A_GS_dual_ss
E = -5652.7318807



0 1

C	-0.94866200	-1.13255000	-0.56489300
C	0.53437900	-1.08410100	-0.88044700
C	0.94866200	1.13255000	0.56489300
C	-0.53437900	1.08410100	0.88044700
H	1.01528500	-2.05152500	-0.99697400
H	-1.51087500	-1.10681700	-1.50338600
H	-1.16965900	-2.09482900	-0.09291000
H	1.51087500	1.10681700	1.50338600
H	1.16965900	2.09482900	0.09291000
H	-1.01528500	2.05152500	0.99697400
C	1.45884600	0.01864200	-0.32986800
C	1.10446700	-0.04479000	-1.76350200
C	-1.45884600	-0.01864200	0.32986800
C	-1.10446700	0.04479000	1.76350200
H	2.47439900	-0.31035100	-0.12683800
H	-2.47439900	0.31035100	0.12683800
F	2.08347100	-0.42755200	-2.64163400
F	-2.08347100	0.42755200	2.64163400
Br	0.00743800	-1.28942100	2.56693700
Br	-0.00743800	1.28942100	-2.56693700

A_cat_rad_dual_ss
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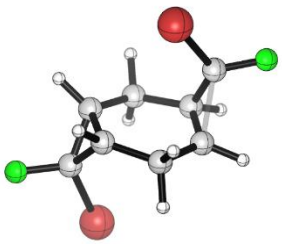
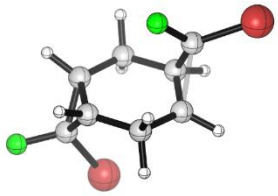


1 2

C	-0.06669900	-0.20303300	-1.57107600
C	0.53347400	-1.30106900	-0.78401900
C	-0.01676400	-0.23065100	1.52371700
C	-0.52204300	0.97697800	0.75884600
H	0.79059000	-2.21939100	-1.30908500
H	0.64650700	0.10707300	-2.34704200

H	-0.87840700	-0.67151400	-2.14956600
H	-0.84465300	-0.75920300	2.00677600
H	0.65169200	0.09359800	2.32429500
H	-0.31636000	1.94067700	1.21574800
C	0.71219300	-1.27165400	0.68409100
C	2.05780300	-0.91001200	0.14251400
C	-0.55068000	0.99090400	-0.78110800
C	-1.80077300	0.94143300	0.01078500
H	0.79123100	-2.26846500	1.12506000
H	-0.35883500	1.95935300	-1.23428900
F	2.94146000	-1.86655600	0.00171500
F	-2.56513200	2.06721100	0.03095300
Br	-2.90712400	-0.61405000	0.01336700
Br	2.73718700	0.78703800	-0.00846500

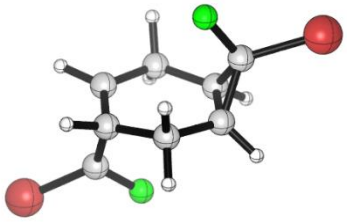
rs_dual_cat_rad
E = -5652.4695478



1 2

C	-0.26520300	0.44609400	-1.55098100
C	0.68586600	-0.43419500	-0.74086200
C	-0.27393200	0.34778900	1.56236000
C	-1.18184700	1.28893600	0.80592100
H	0.99568900	-1.36049500	-1.22573700
H	0.32844300	1.06461500	-2.22708000
H	-0.84982700	-0.23631600	-2.17604400
H	-0.83013600	-0.26754000	2.28227800
H	0.41854200	0.92669600	2.19228100
H	-1.37997800	2.23632900	1.29789300
C	0.51207800	-0.58599500	0.72479300
C	1.85527300	0.28613400	-0.16030100
C	-1.17742200	1.33231300	-0.72843200
C	-2.32453000	0.76520000	0.02148200
H	0.93094200	-1.47106900	1.19805200
H	-1.37748900	2.31004800	-1.15633000
F	-3.48332800	1.47758400	0.04371200
Br	-2.69027200	-1.11185500	-0.02722000
Br	3.55926100	-0.35717000	0.01890900
F	1.74638400	1.58196600	0.01203100

A_cat_rad_dual_rr
E = -5652.4702871



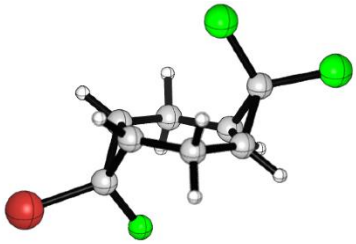
1 2

C	0.00487300	0.82140200	-1.35509800
C	1.01799200	-0.20430600	-0.89462500

C	-0.00708900	-0.20841300	1.55733000
C	-1.17734500	0.56232600	0.95297700
H	1.31624600	-0.93003600	-1.64300000
H	0.47845100	1.77929300	-1.62212400
H	-0.47240100	0.49278700	-2.28881300
H	-0.40921900	-1.04719600	2.12791900
H	0.45856400	0.47976200	2.26894400
H	-1.75221800	1.16911200	1.65315500
C	1.00976200	-0.71739700	0.55301500
C	2.05454400	0.22001700	0.07561100
C	-1.04788000	1.18007700	-0.38309500
C	-2.08477400	-0.24479400	0.08021500
H	1.30568300	-1.75377300	0.67185800
H	-1.70169800	2.01239800	-0.63288400
Br	3.88154800	-0.27187100	-0.09340600
F	1.94542600	1.50513800	0.53094200
Br	-3.90423000	-0.07150600	-0.04548400
F	-1.61765400	-1.35376400	-0.44115300

Cl_rs

E = -3901.4557365



0 1

C	0.40959800	-0.13798400	-1.57529300
C	-0.65775200	0.58203200	-0.76900900
C	0.40962300	-0.13789300	1.57533100
C	1.47402100	-0.85202200	0.76179300
H	-1.05144200	1.48571500	-1.22325400
H	-0.07188100	-0.87623800	-2.22295900
H	0.89350100	0.59045400	-2.23260600
H	0.89353300	0.59061500	2.23256300
H	-0.07182400	-0.87609500	2.22307900
H	1.86310900	-1.75512900	1.22276100
C	-0.65775800	0.58204100	0.76901600
C	-1.62711800	-0.22841900	0.00000100
C	1.47401000	-0.85206400	-0.76172800
C	2.49854200	-0.07635200	0.00000300
H	-1.05147600	1.48572500	1.22323200
H	1.86309200	-1.75519500	-1.22265200
F	-1.41651100	-1.58259600	-0.00001700
Br	-3.50394900	0.12793000	0.00000000
Cl	4.17338600	-0.65405200	0.00000600
Cl	2.42550700	1.68934100	-0.00004700

Cl_rs_cat_rad_ubs

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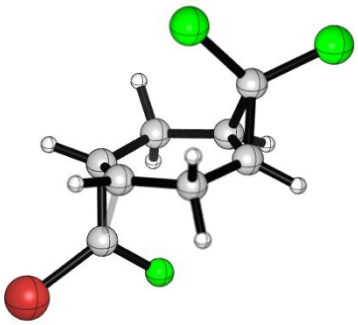

1 2

C	0.40483200	-0.12542000	-1.55043600
C	-0.67228600	0.60898700	-0.75492100
C	0.40987500	0.02838800	1.54913300
C	1.43631100	-0.79318300	0.80191100
H	-1.13214100	1.46325700	-1.25329200
H	-0.08267600	-0.83104000	-2.22561700
H	0.88680800	0.63378100	-2.17391400
H	0.88218300	0.75892700	2.22051600
H	-0.16417100	-0.62258600	2.22545500
H	1.76187900	-1.69011100	1.31840800
C	-0.53338100	0.79681300	0.70699800
C	-1.71268800	-0.28019600	-0.15212800
C	1.43358900	-0.86222800	-0.71617500
C	2.50049300	-0.10061800	0.00863900
H	-1.09406200	1.60267900	1.17482400
H	1.76362700	-1.80525200	-1.13952000
Br	-3.49764700	0.08985500	0.02361700
F	-1.40340300	-1.54274800	0.02684600
Cl	4.13872200	-0.74644100	0.03877200
Cl	2.48635800	1.66378600	-0.07248800

Cl_rs_cat_rad

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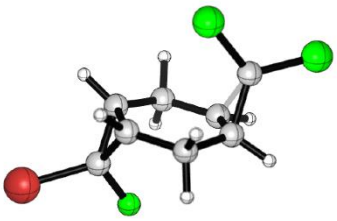


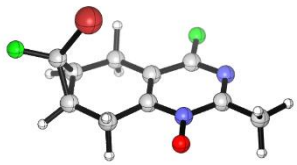
1 2

C	0.38271300	-0.41579000	-1.54810400
C	-0.63223900	0.44018100	-0.82171700
C	0.42328500	-0.19278300	1.53817200
C	1.53245700	-0.86956600	0.74359800
H	-0.95450200	1.33152500	-1.34886000
H	-0.10007300	-1.23588400	-2.10117500
H	0.89167700	0.16517900	-2.32910000
H	0.87651900	0.48968100	2.25965500
H	-0.05491800	-0.99235900	2.11191200
H	2.03008500	-1.69176100	1.25981500
C	-0.60996500	0.54920800	0.70953900
C	-1.64374000	-0.25237400	0.01161500
C	1.39577000	-1.07922300	-0.70147800
C	2.59657000	0.03385400	0.13539000
H	-0.92315500	1.51015800	1.10307700

H	2.01038700	-1.84424400	-1.16970900
Br	-3.48838800	0.20449400	0.00256100
F	-1.49150200	-1.60931600	0.10719400
Cl	4.20145700	-0.49770500	0.01088400
Cl	2.33219000	1.69259900	-0.08394900

P2

E = -3342.3833493

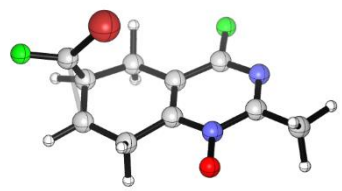


0 1

C	0.81383800	-0.43886000	-0.66784500
C	3.00501900	-0.30411300	0.22647600
C	1.77529400	1.57814200	0.02080200
C	0.67397200	0.93312300	-0.52622200
C	-0.21656500	-1.34931900	-1.24422100
H	0.19359200	-1.76836000	-2.17003300
H	-0.34142600	-2.20232700	-0.56638400
C	-1.71221700	0.83321200	-1.37417600
H	-2.40052900	1.30197500	-2.07155300
C	-0.55016100	1.70052800	-0.94675400
H	-0.27436500	2.34677600	-1.78647000
H	-0.85481900	2.36484200	-0.12958400
C	4.24523300	-1.03107400	0.59898300
H	4.02236800	-1.81013700	1.33372500
H	4.66466000	-1.53090200	-0.27955400
H	4.96463400	-0.32219500	1.00741300
N	1.98359500	-1.04273400	-0.29225000
O	2.12650900	-2.32260900	-0.44398800
N	2.89394400	1.00858200	0.38460200
F	1.71482000	2.90761200	0.18956800
C	-1.54105400	-0.68265600	-1.53260300
H	-2.11995100	-1.14267900	-2.32798900
C	-2.37358000	-0.11406900	-0.44716500
Br	-1.87447800	-0.25901100	1.39220900
F	-3.72825900	-0.25218500	-0.57568800

P2_rc

E = -3342.1152612

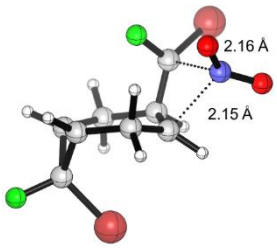


1 2

C	-0.81798400	-0.44867600	0.75447500
C	-2.93914800	-0.25819400	-0.26647800
C	-1.67982300	1.60005000	0.03486700
C	-0.63208600	0.91895300	0.63902000
C	0.17925000	-1.37344200	1.36379000
H	-0.19882800	-1.75113000	2.32999800
H	0.29469700	-2.28732400	0.76412200

C	1.77015800	0.67839900	1.40586700
H	2.55866700	1.08400000	2.04479200
C	0.60712400	1.61683500	1.12900700
H	0.38767400	2.11987500	2.07671600
H	0.92159100	2.38905100	0.42141900
C	-4.15959700	-0.95757800	-0.73679400
H	-3.89245300	-1.72403000	-1.47055000
H	-4.64463400	-1.46903200	0.09999600
H	-4.83892500	-0.23071000	-1.17979600
N	-1.96968700	-1.02955900	0.31518900
O	-2.14483300	-2.30244400	0.44945000
N	-2.78392200	1.05032400	-0.40127700
F	-1.58307400	2.92458900	-0.11427900
C	1.48243400	-0.74933800	1.66267900
H	2.22854900	-1.34953800	2.17914800
C	2.42667200	-0.01652600	0.25920200
F	3.69650700	-0.30777100	0.37319900
Br	1.74784900	-0.23203500	-1.43036900

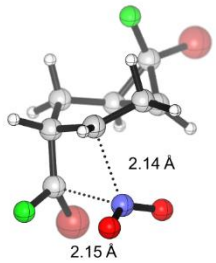
Rs1_5_NO2_TS_attN4
E = -5857.4687573



1 1

C	0.57129600	-1.66954900	-0.10795300
C	-0.34558700	-0.51044200	-0.57627200
C	0.75213700	1.23273100	1.02531000
C	1.64813900	0.12718500	1.54159500
H	-0.58598100	-0.58249100	-1.63722700
H	-0.05422800	-2.49064700	0.25098200
H	1.08951400	-2.03837700	-0.99601800
H	1.29202500	2.17648700	0.89408900
H	-0.00451600	1.43899600	1.80103000
H	1.90534300	0.20158300	2.59346700
C	0.05361700	0.91088400	-0.23225700
C	-1.58934100	-0.42362400	0.21305700
C	1.56206800	-1.29416000	0.97204800
C	2.71673500	-0.41408800	0.67123200
H	-0.00228400	1.63086900	-1.04587600
H	1.78415500	-2.08217400	1.68530900
F	3.91920000	-0.70291600	1.22663200
Br	2.92979700	0.29020200	-1.10063100
F	-1.47765300	-0.47998300	1.50330400
Br	-3.23487100	-0.89703500	-0.43275400
N	-1.90027900	1.71746500	0.16427800
O	-2.38238900	2.11760100	-0.86206900
O	-2.07170900	2.11429000	1.28241700

rS2_O_NO2_TS_attN4
E = -5857.4761135

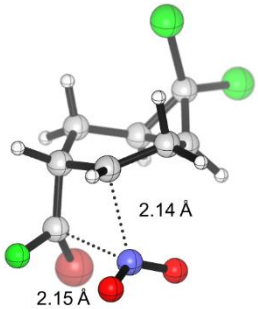


1 1

C	1.13925500	0.54079300	1.51830100
C	-0.24416500	1.91996000	-0.15500800
H	1.60991700	0.87169000	2.45051000
H	-0.76608200	2.52139100	0.62578300
H	-0.11806600	2.59872200	-0.99967900
C	1.00899400	1.70142100	0.56908200
C	2.20578500	-0.06862900	0.68400000
H	1.70399400	2.52854900	0.71173900
C	-0.14499200	-0.25690100	1.76642100
H	0.11573400	-1.21035200	2.23107400
H	-0.70363400	0.31293800	2.51335600
N	2.24181400	1.14592200	-1.09328900
O	1.58277500	0.75573500	-2.01975800
O	3.27388600	1.75845200	-1.11627200
C	-2.20990400	0.32487500	0.31586200
C	-1.02616400	0.67299000	-0.50298400
H	-1.04290000	0.40833100	-1.55436700
C	-0.98304200	-0.48021500	0.52094900
H	-1.00700400	-1.48407900	0.11095500
F	3.41998700	0.27210900	0.98351700
Br	2.03856400	-1.68518400	-0.16881600
Br	-3.76948700	-0.43019300	-0.46655300
F	-2.55668100	1.19792600	1.30426900

Scl2_O_NO2_TS_attN4

E = -4106.1963974

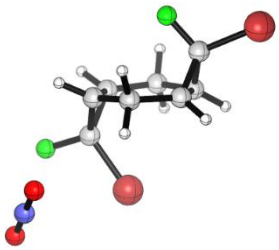


1 1

C	0.62143400	0.64702200	1.40350600
C	-0.71853800	1.68582800	-0.53237900
H	0.92233500	1.12015400	2.34469700
H	-1.38298500	2.30248400	0.11800900
H	-0.57302400	2.28696400	-1.43115100
C	0.46229400	1.69245600	0.33325000
C	1.85430100	0.12194100	0.76252700
H	1.03050200	2.61305400	0.46484200
C	-0.56241100	-0.30702100	1.59174800
H	-0.22224800	-1.18749900	2.14122100
H	-1.25959700	0.21580900	2.25149700

N	1.93283400	1.15480400	-1.12333900
O	1.44038800	0.58658100	-2.06131700
O	2.87114600	1.90325300	-1.11109500
C	-2.55301500	-0.13854900	-0.11971400
C	-1.31281800	0.32513000	-0.81638600
H	-1.19071200	-0.02161800	-1.83704200
C	-1.23559900	-0.71660000	0.29557900
H	-1.09420300	-1.74521000	-0.01902900
Cl	-3.63456300	-1.18939600	-1.03421200
Cl	-3.44572600	0.94011000	0.94890700
F	2.96729500	0.66054200	1.15032300
Br	2.00209100	-1.57584900	0.07994600

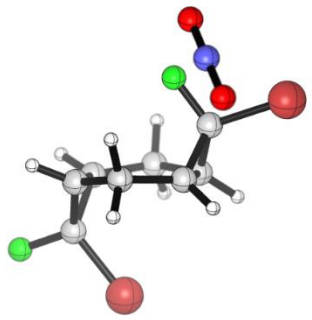
rS2_c_NO2_4
E = -5857.478723



1 1

C	-0.63833300	-0.14021500	1.85437800
C	0.47901800	0.82978600	1.52087300
C	-0.17738400	0.95441400	-1.07333000
C	-1.22125700	-0.10411200	-0.76026700
H	0.74363200	1.52297000	2.31474600
H	-0.20893100	-1.00344900	2.37203300
H	-1.30860600	0.35113300	2.56480900
H	-0.67222200	1.84823900	-1.46221600
H	0.46396600	0.57441100	-1.87569000
H	-1.39339600	-0.83312900	-1.54529700
C	0.69546000	1.37158300	0.09675300
C	1.64159900	0.41703200	0.71701600
C	-1.44505000	-0.63885500	0.66737700
C	-2.40609400	0.28858500	0.03222000
H	1.08048600	2.38758200	0.05061700
H	-1.74656200	-1.68002300	0.71434200
N	4.26973800	0.53189800	-0.95692300
O	3.48590700	1.03070600	-1.57742900
O	5.05366100	0.03016800	-0.34107300
Br	-4.18435500	-0.22628600	-0.42928600
F	-2.40325600	1.57130000	0.51261800
Br	1.86801800	-1.35960300	0.03556800
F	2.88558800	0.90190000	1.08328700

Rs1_c_NO2
E = -5857.4729919



1 1

C	1.05351100	-0.79437400	1.68451300
C	0.11895900	-1.10025200	0.52453200
C	0.45706900	1.32024300	-0.55990100
C	1.57361100	1.51205600	0.44711600
H	0.12413100	-2.12671200	0.17327400
H	0.47391100	-0.72480100	2.60904800
H	1.73717100	-1.64040100	1.80086000
H	0.84505500	1.51991400	-1.56277600
H	-0.30559200	2.08039600	-0.36133100
H	1.76007800	2.54524600	0.72776900
C	-0.18286400	-0.06024900	-0.56821400
C	-1.18148900	-0.40394300	0.47136400
C	1.87020500	0.47489500	1.54127100
C	2.80236000	0.68910200	0.41321000
H	-0.35552600	-0.48791600	-1.55121900
H	2.23495200	0.88749900	2.47818100
F	3.98237400	1.32506800	0.69507800
Br	3.09390700	-0.64565100	-0.92717500
F	-1.42713100	0.54214200	1.42992500
Br	-2.82159400	-1.31223600	0.04541000
N	-3.39743600	1.73646800	-0.70951900
O	-3.23286400	1.47805800	-1.78389000
O	-3.55818900	1.98291200	0.36717000

ss1_c_NO2
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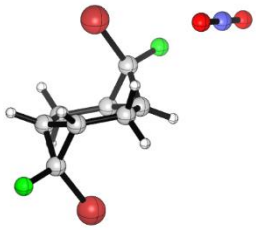
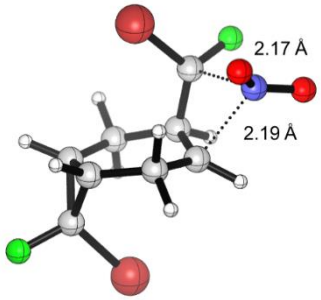


1 1

C	-0.93475300	-0.86537100	1.53366700
C	0.06324300	0.25972000	1.33189300
C	-0.30301500	0.34004800	-1.32342800
C	-1.30582900	-0.77923300	-1.11821800
H	0.12842400	0.97869600	2.14391800
H	-0.42345400	-1.70725700	2.01050200
H	-1.69804100	-0.52306800	2.23864300
H	-0.80119800	1.18257500	-1.81163400
H	0.46896400	-0.01210900	-2.01585500
H	-1.37030800	-1.49681100	-1.93163400
C	0.36341300	0.84829700	-0.05764500

C	1.35663000	0.01964500	0.66588400
C	-1.61512500	-1.36480500	0.27288200
C	-2.60332400	-0.53725700	-0.45177600
H	0.59722200	1.91080300	-0.04834000
H	-1.85826400	-2.42376200	0.26836300
F	-3.70314600	-1.17021000	-0.96404000
Br	-3.08308000	1.20451500	0.17777100
N	3.82911800	1.58205000	-0.65642700
O	4.36343300	2.26984400	0.04159200
O	3.30074800	0.89236200	-1.35913400
F	2.46787100	0.67550300	1.17611300
Br	1.87820600	-1.70037100	0.02946200

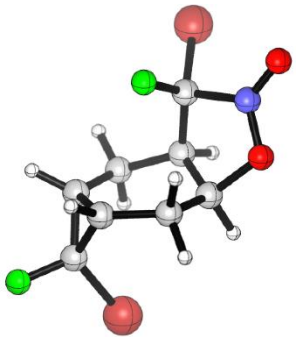
ss1_5_NO2_TS_attN4
E = -5857.4710252



1 1

C	-0.55076800	-0.80050900	1.50441400
C	0.34036700	0.41251100	1.16755200
C	-0.30392300	0.39048000	-1.36565100
C	-1.08074200	-0.88254700	-1.10806000
H	0.35670900	1.14249400	1.98035500
H	0.05250300	-1.52830600	2.05137500
H	-1.30828500	-0.44406500	2.20666200
H	-0.84373600	1.08965200	-2.01498900
H	0.59977000	0.13374000	-1.94599100
H	-1.05445200	-1.60903300	-1.91483800
C	0.11739700	1.11277400	-0.15512500
C	1.74967200	0.10071700	0.83774900
C	-1.20526600	-1.46253100	0.30905300
C	-2.36066700	-0.82384200	-0.36732800
H	0.06798600	2.19983300	-0.11670400
H	-1.26402700	-2.54643400	0.34904000
F	-3.38098400	-1.61097200	-0.78960400
Br	-3.01257700	0.86326000	0.26263700
N	2.19315300	1.59754300	-0.67294100
O	2.54218800	2.60099100	-0.11596200
O	2.52743500	1.17028400	-1.74118400
F	2.66219500	0.61895000	1.59763400
Br	2.26163900	-1.41026100	-0.06935200

Rs1_5_NO2_i
E = -5857.5554058

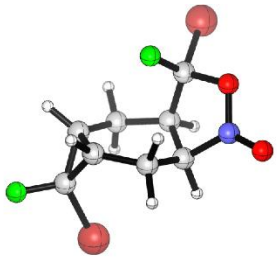


1 1

C	0.35760100	-1.27789100	-0.47764900
C	-0.54194300	-0.05207900	-0.68522800
C	0.86109800	1.41728200	0.97743100
C	1.50575400	0.12943500	1.45579700
H	-0.87146700	-0.01264700	-1.72799100
H	-0.27193900	-2.17025800	-0.42252900
H	0.95929000	-1.39155100	-1.38294300
H	1.60423400	2.21472600	0.89207100
H	0.15529800	1.72348200	1.75594000
H	1.61939000	0.07190900	2.53465100
C	0.10101100	1.30185300	-0.34624100
C	-1.77620700	-0.05226100	0.17640600
C	1.23697700	-1.21001300	0.75666800
C	2.57512700	-0.56611700	0.71334000
H	0.61946000	1.72667100	-1.20415100
H	1.19047700	-2.07149700	1.41585200
F	3.56445200	-1.14552900	1.44957700
Br	3.29011100	0.15812500	-0.90319000
F	-1.54672400	-0.27267700	1.47440000
Br	-3.29249600	-1.00417500	-0.40608800
N	-2.12782300	1.50745500	0.13156200
O	-3.15944000	1.99422300	0.38702600
O	-1.10337900	2.20469300	-0.22403400

Rs1_5_NO2

E = -5857.5720231

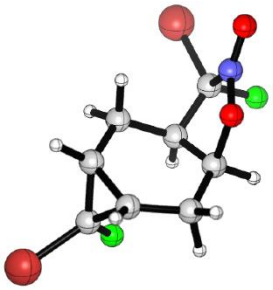


1 1

C	-0.22441500	1.28883400	-0.55588000
C	0.62686100	0.02203500	-0.66461500
C	-0.84247100	-1.27187000	1.11255900
C	-1.44265600	0.07298800	1.46451800
H	0.96879100	-0.10631700	-1.69542500
H	0.44536700	2.15318400	-0.53691900
H	-0.80323800	1.37870100	-1.47835400
H	-1.60801900	-2.04903000	1.04662600
H	-0.18105000	-1.54337200	1.94073000
H	-1.56321500	0.22486000	2.53342700
C	-0.04814900	-1.28267100	-0.22588900
C	1.85867200	0.03547500	0.22857700

C	-1.12925500	1.34191700	0.65931800
C	-2.48201700	0.73096800	0.64641700
H	-0.55877100	-1.80795000	-1.03469900
H	-1.06953800	2.25008700	1.25116100
F	-3.46937800	1.39154300	1.31245300
Br	-3.18452900	-0.11797400	-0.91376100
F	1.59253600	0.44945800	1.47741600
Br	3.38231600	0.95385200	-0.42788700
N	1.17836500	-2.11486000	0.05597500
O	1.28116500	-3.27426000	0.07607400
O	2.24267200	-1.36911000	0.35398000

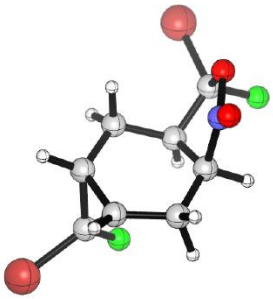
rS2_5_NO2_i
E = -5857.5602461



1 1

C	0.69905600	0.09062800	0.63594100
C	-0.96402200	2.09215000	0.34659600
H	0.42520100	-0.31889600	1.61228000
H	-1.42228800	2.23146600	1.33103500
H	-0.89121600	3.08835900	-0.09766900
C	0.43484800	1.60077500	0.61859000
C	2.20152200	0.08421500	0.50932300
H	0.86154600	2.10758800	1.48544800
C	0.05400800	-0.66486000	-0.54317600
H	0.66324300	-0.55308300	-1.44867200
H	0.03767500	-1.73154500	-0.30313100
C	-2.38036300	-0.03207400	0.11243000
C	-1.82612300	1.19442300	-0.51899000
H	-2.45753300	1.70202400	-1.23947000
C	-1.33560300	-0.19987100	-0.91838600
H	-1.66578000	-0.55435300	-1.88918100
F	2.82486500	0.61204200	1.56705600
Br	3.12461200	-1.43729900	-0.09760100
Br	-4.18509900	-0.57483100	-0.14263600
F	-2.00070300	-0.26027500	1.40796700
O	3.22197500	1.39807200	-1.35257400
O	1.33480200	2.04718700	-0.53366300
N	2.34208100	1.24753000	-0.59737200

rS2_5_NO2
E = -5857.5766457

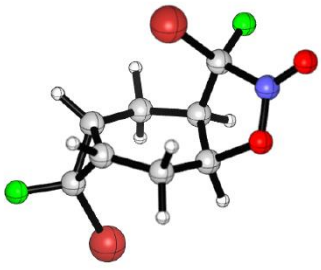


1 1

C	0.77477500	-0.01052100	0.58246700
C	-0.90244400	2.03106200	0.37909100
H	0.51620000	-0.47790000	1.53407700
H	-1.35745600	2.17421900	1.36282500
H	-0.82166400	3.02692900	-0.06436700
C	0.49065100	1.49534400	0.64772100
C	2.29115700	0.02796300	0.45758000
H	0.90178500	1.93511400	1.56772100
C	0.11646300	-0.70334400	-0.62289500
H	0.70421000	-0.51421800	-1.52895100
H	0.11996400	-1.78269900	-0.45089000
N	1.51404600	1.97533200	-0.37844400
O	2.55299800	1.14706600	-0.45872000
O	1.50270600	2.93600900	-1.03465700
C	-2.30672300	-0.10171800	0.12756800
C	-1.77567100	1.14370600	-0.48705200
H	-2.42892600	1.66895000	-1.17483200
C	-1.28957300	-0.23664400	-0.93561900
H	-1.64933000	-0.56349000	-1.90581500
F	2.87681900	0.37003000	1.61585800
Br	3.19443700	-1.47100800	-0.27068900
Br	-4.11619100	-0.64194000	-0.09645300
F	-1.89450300	-0.35678300	1.40782700

ss1_5_NO2_i

E = -5857.5607416

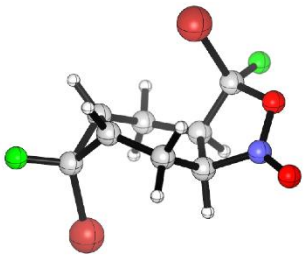


1 1

C	-0.38762500	-0.34008000	1.51252300
C	0.52985500	0.73609800	0.91974400
C	-0.40436700	0.37625100	-1.52151100
C	-1.05998600	-0.89035100	-0.99991400
H	0.61825700	1.56385200	1.63458300
H	0.19905300	-0.93269000	2.22027300
H	-1.14870200	0.17083100	2.10763100
H	-1.09245100	0.92299100	-2.17202500
H	0.43882900	0.07396100	-2.14967900
H	-0.99451800	-1.73309400	-1.68330900
C	0.10261900	1.32683700	-0.43318600
C	1.95205800	0.30296200	0.67714200

C	-1.03237900	-1.25852400	0.49116100
C	-2.29615800	-0.88405500	-0.19173400
H	-0.51841400	2.21085700	-0.29971900
H	-0.95357600	-2.32226300	0.69725000
F	-3.19439700	-1.88172100	-0.42293200
Br	-3.20715800	0.74497700	0.21139400
N	2.40010900	1.38660800	-0.36181100
O	3.50664400	1.68410200	-0.59661700
O	1.39158500	1.92973100	-0.95122000
F	2.78129800	0.43177900	1.70143000
Br	2.25740700	-1.36602600	-0.20200700

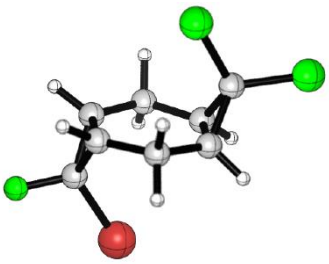
ss1_5_NO2
E = -5857.5607416



1 1

C	0.27548700	-0.65851200	-1.44741000
C	-0.59561100	0.53972100	-1.06725800
C	0.34351500	0.62524600	1.40042400
C	0.94052200	-0.74011400	1.12389900
H	-0.68723400	1.20573500	-1.93342600
H	-0.33995000	-1.35261200	-2.02640800
H	1.04892900	-0.30000300	-2.13119400
H	1.05350000	1.27229400	1.92217100
H	-0.50082000	0.47488600	2.08075100
H	0.83601600	-1.43317300	1.95448400
C	-0.12147100	1.37722500	0.12029800
C	-2.03809500	0.21628400	-0.69703700
C	0.89622300	-1.38579800	-0.26986600
C	2.17436100	-0.93667600	0.33484200
H	0.53806600	2.20022000	-0.15861300
H	0.77513100	-2.46518300	-0.26079600
F	3.03472100	-1.90209300	0.76007700
Br	3.14123000	0.55375000	-0.36391200
N	-1.42227200	2.04928000	0.49140700
O	-1.57516300	3.03274900	1.09800100
O	-2.48574200	1.35695400	0.10728100
F	-2.84428900	0.20444500	-1.75692700
Br	-2.37677100	-1.35404000	0.34834700

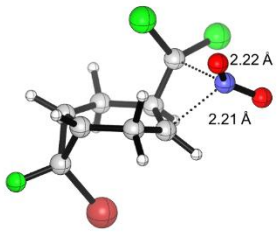
sCl
E = -3901.4562572



0 1

C	0.12768800	0.40382500	-1.57320800
C	0.91909900	-0.60759800	-0.76226700
C	0.12769100	0.40383100	1.57320200
C	-0.77571000	1.31916500	0.76883000
H	0.99324000	-1.59254600	-1.21333800
H	0.81977400	1.02394800	-2.15058900
H	-0.48285100	-0.14416300	-2.29748800
H	-0.48284500	-0.14415200	2.29748700
H	0.81978200	1.02395500	2.15057600
H	-0.97751900	2.28450000	1.22567800
C	0.91909800	-0.60759800	0.76226300
C	2.13717600	-0.19898200	-0.00000100
C	-0.77571200	1.31916300	-0.76883800
C	-1.92364200	0.79083100	-0.00000100
H	0.99323600	-1.59254600	1.21333600
H	-0.97752200	2.28449500	-1.22568800
F	-3.07481700	1.53376600	-0.00000100
Br	-2.35204900	-1.07509600	0.00000300
Cl	2.62063400	1.49926400	0.00000400
Cl	3.54146200	-1.27896000	-0.00000100

sCl1_5_NO2_TS_attN4
E = -4106.1872553

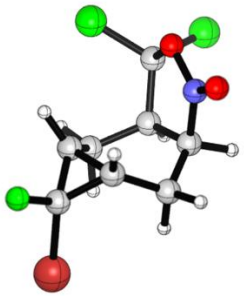


1 1

C	-0.44830800	1.12881400	-1.31999100
C	0.51174600	-0.03276200	-0.96774300
C	-0.32064200	-0.17948100	1.49976800
C	-1.28212000	0.95191900	1.20581400
H	0.60971900	-0.72727000	-1.80305000
H	0.14152500	1.97483200	-1.67824000
H	-1.05168000	0.79169600	-2.16665400
H	-0.77021100	-0.95652500	2.12729400
H	0.50880000	0.22898900	2.10381300
H	-1.48034100	1.61499300	2.04200200
C	0.25024200	-0.80856900	0.29892800
C	1.88783200	0.39989900	-0.55792600
C	-1.34929500	1.58205000	-0.19006600
C	-2.43462100	0.70406100	0.30878500
H	0.33865400	-1.89026300	0.22497800
H	-1.60758400	2.63696100	-0.20065400
N	2.32924800	-1.14085800	0.97590800
O	2.73652200	-2.16037000	0.48874600
O	2.56995600	-0.67400800	2.05290700
Cl	3.19422000	-0.00891600	-1.54811100
Cl	2.07083700	1.75168900	0.43443900
F	-3.63241900	1.25468300	0.62272300
Br	-2.66139000	-1.04020700	-0.46147300

sCl1_5_NO2

E = -4106.2882318

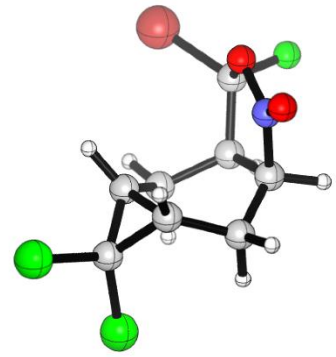


1 1

C	0.13716200	-1.12102500	-0.42027900
C	0.79072700	-0.51193200	0.80023300
C	0.64729400	1.61673900	-0.64152500
C	-0.80247200	1.19692600	-0.90020500
H	0.47647300	-0.86303300	1.77974300
H	0.83751200	-1.13680300	-1.25989500
H	-0.14599000	-2.15950500	-0.24425000
H	0.71829000	2.70561100	-0.62178400
H	1.21623300	1.27012300	-1.50944500
H	-1.26117800	1.73277600	-1.74003800
C	1.10999500	0.99892400	0.66151900
C	2.18351100	-0.01122500	0.75529900
C	-1.07682700	-0.31606000	-0.91461600
C	-2.37301300	-0.44656300	-0.07821600
H	1.01289100	1.60917900	1.55639900
H	-1.31173600	-0.62808600	-1.93282300
O	-2.40191600	0.73446300	0.79537400
N	-1.60791500	1.66210400	0.29660000
O	-1.56762700	2.70826300	0.81214000
Br	3.40887600	-0.38070200	-0.65965900
F	2.84616700	-0.03071100	1.94624500
Cl	-2.47226500	-1.80844800	1.01687800
Cl	-3.83098100	-0.34099500	-1.07367900

Scl2_5_NO2

E = -4106.2985561



1 1

C	-0.27263800	-0.67225600	1.09880700
C	-1.09188300	-0.61937500	-0.17520100
C	-1.22987700	1.87553300	0.41113300
C	0.27534700	1.77978900	0.66468700
H	-0.78430300	-1.26341200	-0.99440800
H	-0.91099400	-0.51603900	1.97148600
H	0.18178800	-1.65488500	1.23344000
H	-1.47651000	2.86008600	0.00991800
H	-1.70001600	1.79982600	1.39576900

H	0.67359300	2.63687700	1.22182500
C	-1.64399500	0.76495100	-0.53473300
C	-2.56146800	-0.33631600	-0.12036800
C	0.80068400	0.42629300	1.17470300
C	2.07030600	0.22831400	0.34244400
H	-1.69652900	1.02895400	-1.58794400
H	1.13620700	0.53318100	2.20854300
F	3.12599200	0.80666100	0.94010500
Br	2.55683000	-1.52418400	-0.20580100
Cl	-3.42900500	-0.27002300	1.41212700
Cl	-3.55703900	-1.05226700	-1.39027300
O	1.88860500	0.97941600	-0.89470700
N	0.95900600	1.89942300	-0.68868700
O	0.72697600	2.66599300	-1.53480200

References and notes

[1] The M06-2X functional has demonstrated good thermodynamic data for organic reactions. For more details, see: (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.*, 2008, **120**, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.*, 2008, **41**, 157.

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