Supplementary Information

Fluorocyclohexanes: Synthesis and structure of all-*syn*-1,2,4,5-tetrafluorocyclohexane

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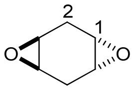
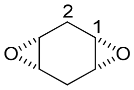
General Experimental

All chemicals were purchased from Acros, Sigma Aldrich, Alfa Aeser, Fisher Scientific, Fluorochem or Merck. All non-aqueous reactions were carried out in oven-dried glassware or teflon under an inert argon atmosphere using a double vacuum manifold with the inert gas passing through a bed of silica gel and molecular sieves. Anhydrous CH_2Cl_2 was obtained for a MBraun MB SPS-800 solvent purification system, where the solvent was dried by passage through activated filter columns and dispensed under an atmosphere of argon gas. All NMR spectra were recorded using either a Bruker Avance II 400, Bruker Avance 300 or 500 spectrometers. Using the deuterated solvent for an internal deuterium lock. ^{1}H NMR spectra were recorded at either 300, 400 or 500 MHz. ^{13}C NMR spectra were recorded using the DEPTQ pulse sequence and broadband proton decoupling at either 75, 100 or 126 MHz. ^{19}F NMR spectra were recorded at 282, 376 or 470 MHz. All chemical shifts, δ, are stated in units of parts per million (ppm), relative to a standard reference point, for ^{1}H NMR and ^{13}C NMR the reference point is TMS, where δ_H and δ_C is 0.00 ppm. For ^{19}F NMR the reference point is CCl_3F, where δ_F is 0.00 ppm. All spectrum are referenced to the residual solvent signal of the deuterated solvent. Melting points were determined using a Griffin MPA350 melting point apparatus and are uncorrected. GC-MS analyses were run under automation, injecting 1 μL samples using a Agilent 7683 series injector, into a Agilent 6890 series GC system fitted with a Supelco MDN-35 capillary column (30.0 m × 250.00 μm. Film thickness – 0.25 μm). Carrier gas was helium (flow rate – 1.1 mL min^{-1}). The column was heated at 50 °C for 10 min then the temperature was slowly increased to 280 °C over 11.5 min, where the temperature was held for 5 min. Detection was carried out by an Agilent 5973 network mass selective detector. High and low resolution mass spectra were obtained by EPSRC National Mass Spectrometry Service Centre Swansea and were obtained using electron ionization on a Finnigan MAT 95 XP. Thin layer chromatography was carried out on aluminium backed Merck TLC silica gel 60 F_{254} plates. These plates were visualised using UV light at a wavelength of 254 nm, potassium permanganate or phosphomolybdic acid.

1,4-Cyclohexadiene diepoxide 4[1,2]

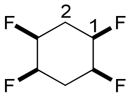


A solution of 1,4-cyclohexadiene **3** (6.0 mL, 5.14 g, 64.1 mmol, eq 1) in CH_2Cl_2 (13 mL) was added dropwise to a solution of *m*CPBA (70-77% dispersion in water, 33.2 g, 134.6 mmol, eq 2.1) in CH_2Cl_2 (125 mL) at -15 °C, over 1 h. The reaction was stirred at -10 °C for 6 h, during which time a colourless precipitate formed. CH_2Cl_2 (100 mL) was added to the reaction and the resulting solution was stirred for 16 h, whilst warming slowly to RT. The precipitate was removed by filtration. The filtrate was washed with aqueous sodium hydroxide solution (10% *w/v*, 100 mL) and the aqueous was re-extracted with CH_2Cl_2 (3 × 50 mL). The combined organic layers were dried over magnesium sulfate, filtered and concentrated *in vacuo* to give a colourless solid. This solid was purified by silica gel column chromatography, eluting with ethyl acetate:hexane (1:9 → 0:1), to yield *anti*-1,4-cyclohexadiene diepoxide (1.4 g, 20%), as a colourless solid: **mp** 105-107 °C [lit.[1] 108-109 °C]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 3.11-3.09 (4H, m, $C\underline{H}O$), 3.36-3.34 (4H, m, $C\underline{H}_2$). **MS** (GCMS-EI) *m/z* 112 ($[M]^{+\bullet}$, 2.5%), 83 (25%), 55 (100%).

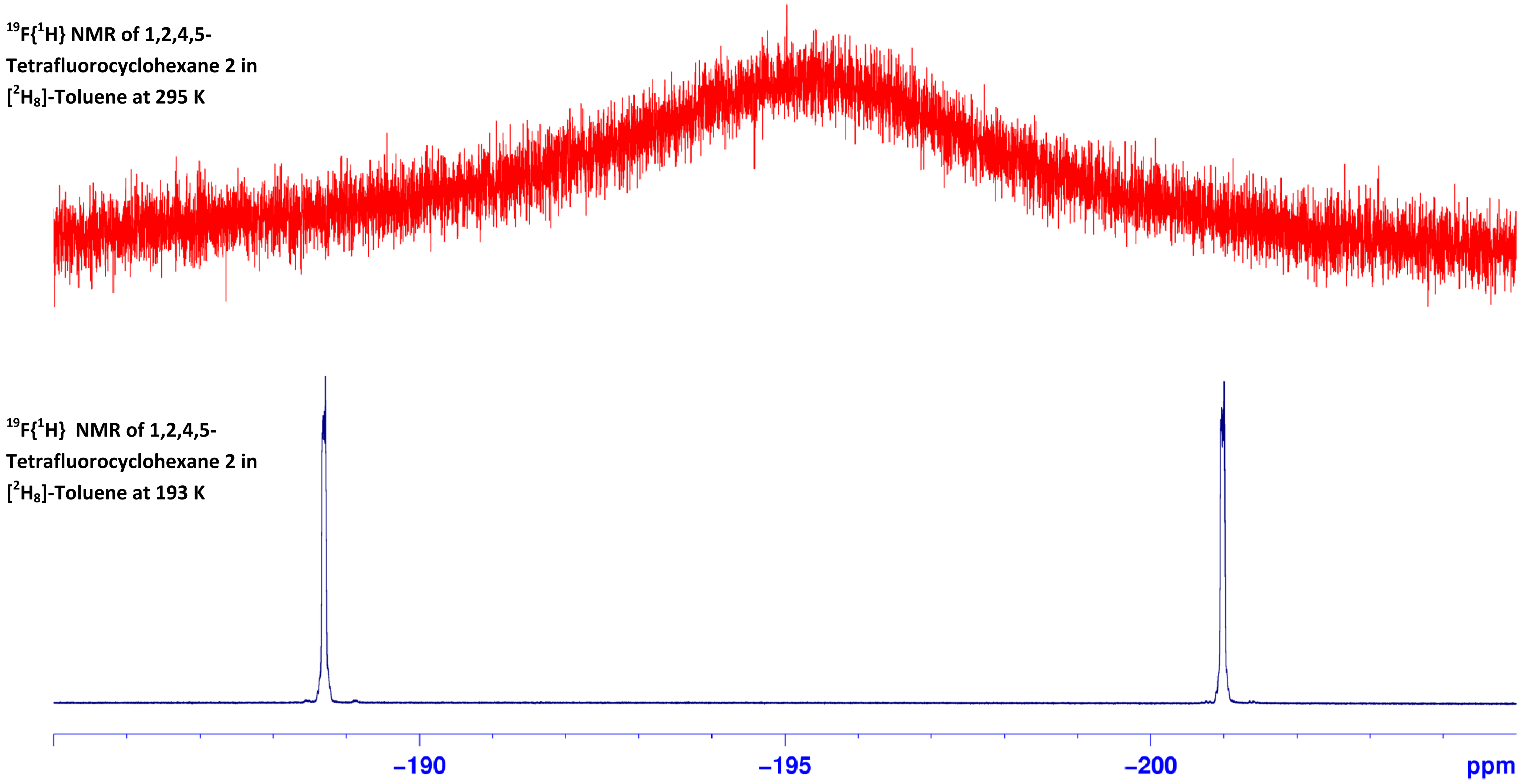


Further elution provided *syn*-1,4-cyclohexadiene diepoxide **4** (3.8 g, 52%), as a colourless solid: **mp** 59-60 °C [lit.[2] 59-60 °C]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 3.13-3.09 (4H, m, $C\underline{H}O$-1), 2.78 (2H, dt, *J* 17.1, 0.7 Hz, $C\underline{H}_AH_B$-2), 2.33-2.23 (2H, m, $CH_A\underline{H}_B$-2); **MS** (GCMS-EI) *m/z* 112 ($[M]^{+\bullet}$, 25%), 83 (20%), 55 (100%).

All-*syn*-1,2,4,5-tetrafluorocyclohexane 2

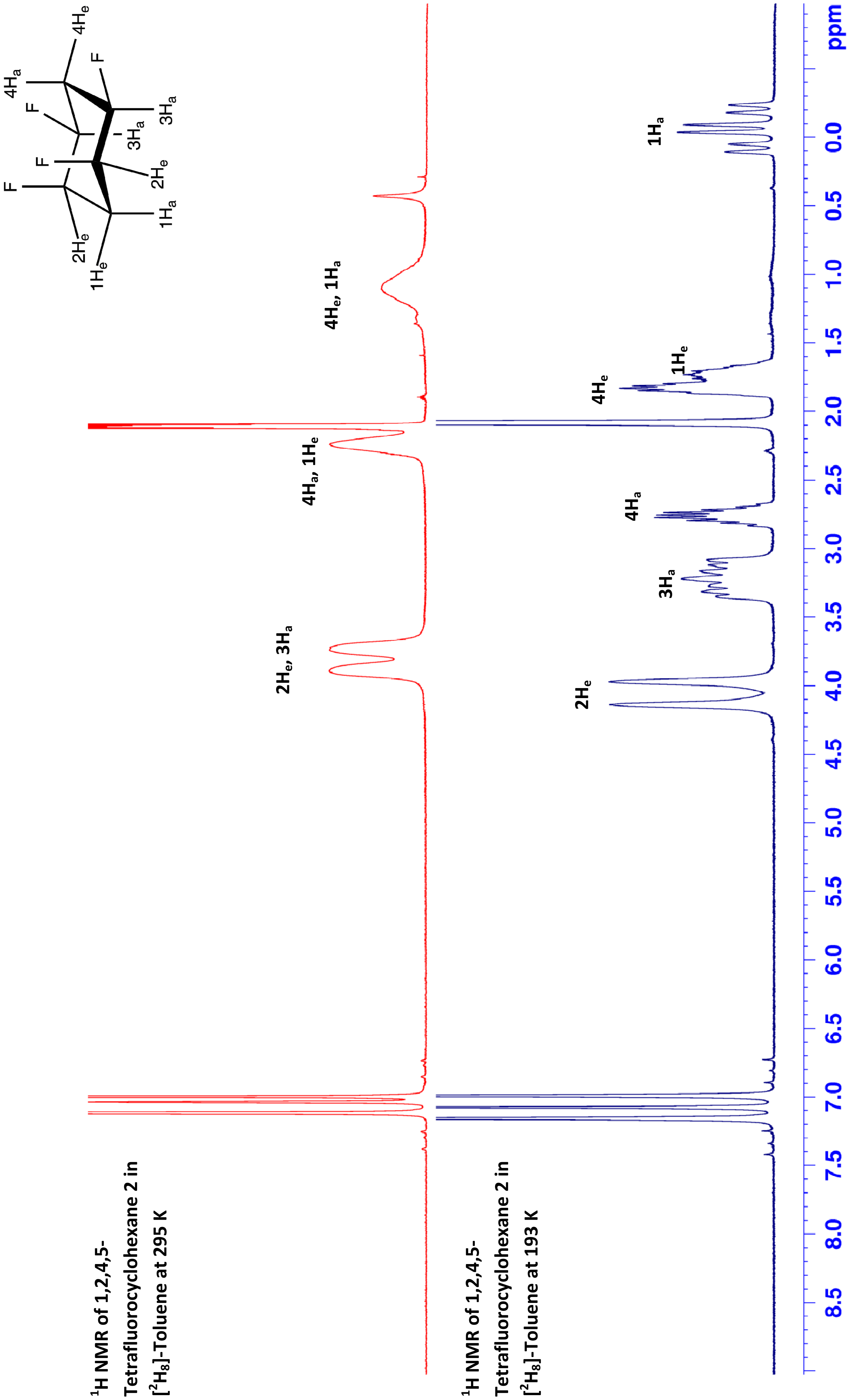


A solution of *syn*-1,4-cyclohexadiene diepoxide **4** (210 mg, 1.88 mmol, eq 1) in diethylsulfur trifluoride (DAST) (4.0 mL, 4.9 g, 30.3 mmol, eq 16) was heated to 70 °C and left to stir for 72 h. The reaction was cooled to room temperature and quenched with sat. aq. $NaHCO_3$ (50 mL). This aqueous solution was extracted with ethyl acetate (4 × 50 mL). The combined organics were dried over sodium sulfate and concentrated *in vacuo* to give the crude product, which was purified by silica gel column chromatography, eluting with chloroform. This was further purified silica gel column chromatography, eluting with acetone:cyclohexane (1:9), to yield the pure all-*syn*-1,2,4,5-tetrafluorocyclohexane **2** (71 mg, 24%) as a colourless crystalline solid: **mp** 107-109 °C; **^{1}H NMR RT** (300 MHz, CD_2Cl_2) δ_H 4.89-4.53 (4H, m, $C\underline{H}F$-1), 2.70-2.49 (2H, m, $C\underline{H}_AH_B$-2), 2.13-1.85 (2H, m, $CH_A\underline{H}_B$-2); **^{1}H NMR 193K** (300 MHz, CD_2Cl_2) δ_H 4.94 (2H, d, *J* 50.4 Hz, $2H_e$), 4.67-4.36 (2H, m, $3H_a$), 2.72-2.29 (1H, m, $4H_a$, $4H_e$, $1H_e$), 1.63 (1H, td, *J* 44.2, 16.7 Hz, $1H_a$); **^{1}H NMR 193K** (300 MHz, $C_6D_5CD_3$) δ_H 4.06 (2H, d, *J* 50.4 Hz, $2H_e$), 3.40-3.04 (2H, m, $3H_a$), 2.86-2.66 (1H, m, $4H_a$), 1.91-1.62 (2H, m, $4H_e$, $1H_e$), -0.06 (1H, td, *J* 43.2, 16.7 Hz, $1H_a$); **^{1}H{^{19}F} NMR 193K** (300 MHz, $C_6D_5CD_3$) δ_H 4.06 (2H, br. s, $2H_e$), 3.27-3.18 (2H, m, $3H_a$), 2.76 (1H, q, *J* 11.7 Hz, $4H_a$), 1.88-1.79 (1H, m, $4H_e$), 1.74 (1H, dt, *J* 16.7 Hz, $1H_e$) -0.06 (1H, d, *J* 16.7 Hz, $1H_a$); **^{13}C NMR** (126 MHz, $CDCl_3$) 87.5-85.2 (m, $\underline{C}HF$-1), 28.7-28.0 (m, $\underline{C}H_2$-2); **^{19}F{^{1}H} NMR** (282 MHz, CD_2Cl_2) δ_F -196.7 (4F, br. s); **HRMS** *m/z* (EI) [Found: $[M]^{+\bullet}$ 156.0555. $C_6H_8F_4^{+\bullet}$ requires *m/z* 156.0557; **MS** (EI) *m/z* 156 ($[M]^{+\bullet}$, 10%), 136 ($[M-HF]^{+\bullet}$, 5%), 123 (25%), 105 (35%), 77 (90%), 56 (100%).



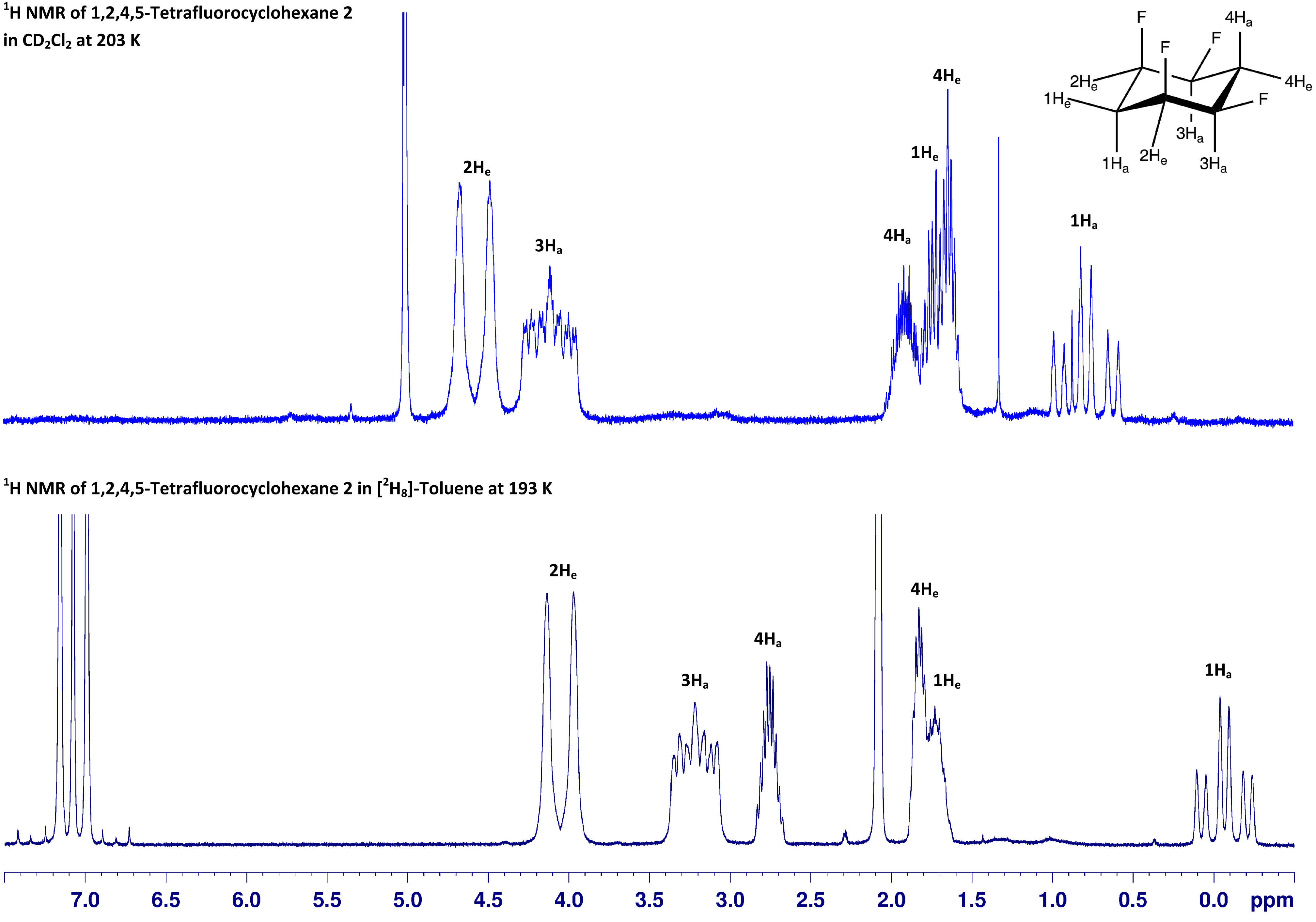
$^{19}F\{^1H\}$ NMR of 1,2,4,5-
Tetrafluorocyclohexane 2 in
$[^2H_8]$-Toluene at 295 K

$^{19}F\{^1H\}$ NMR of 1,2,4,5-
Tetrafluorocyclohexane 2 in
$[^2H_8]$-Toluene at 193 K



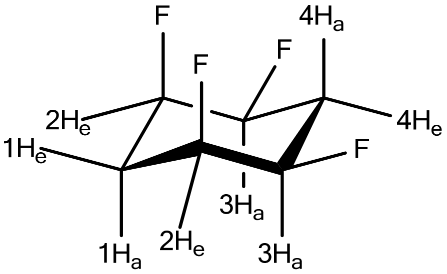
^{1}H NMR of 1,2,4,5-Tetrafluorocyclohexane 2 in [^{2}H$_8$]-Toluene at 295 K

^{1}H NMR of 1,2,4,5-Tetrafluorocyclohexane 2 in [^{2}H$_8$]-Toluene at 193 K



^{1}H NMR of 1,2,4,5-Tetrafluorocyclohexane 2 in CD_2Cl_2 at 203 K

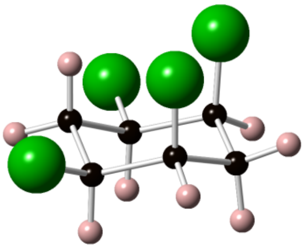
^{1}H NMR of 1,2,4,5-Tetrafluorocyclohexane 2 in [$^2H_8$]-Toluene at 193 K



Proton Signal	δ CD_2Cl_2 (ppm)	δ [$^2H_8$]-Toluene (ppm)	Δδ (ppm)
1H$_a$	1.63	-0.06	+1.69
1H$_e$	2.46	1.74	+0.72
2H$_e$	4.94	4.06	+0.88
3H$_a$	4.53	3.22	+1.31
4H$_a$	2.61	2.76	-0.15
4H$_e$	2.37	1.84	+0.53

Table 1. The ^{1}H NMR assignments in CD_2Cl_2 and [$^2H_8$]-toluene and difference in chemical shift between the two solvents

Crystallographic Details for structure **2**



A. Crystal Data

Empirical Formula	$C_6H_8F_4$
Formula Weight	156.12
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.200 X 0.100 X 0.020 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 5.589(2) Å
	b = 10.768(3) Å
	c = 11.185(4) Å
	□ = 101.316(13) ^{o}
	V = 660.1(4) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.571 g/cm^3
F_{000}	320.00
□(CuK□)	15.383 cm^{-1}

B. Intensity Measurements

Diffractometer	Saturn70
Radiation	CuK□ (□ = 1.54187 Å)
Voltage, Current	40kV, 20mA
Temperature	-100.0^{o}C
Detector Aperture	70 x 70 mm
Pixel Size	0.034 mm
2□$_{max}$	135.3^o
No. of Reflections Measured	Total: 7327
	Unique: 1146 (R_{int} = 0.0778)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\square$ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	w = 1/ [$\square^2(Fo^2) + (0.1197 \cdot P)^2$ + 1.8093 · P] where P = $(Max(Fo^2,0) + 2Fc^2)/3$
$2\square_{max}$ cutoff	135.3°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	1146
No. Variables	91
Reflection/Parameter Ratio	12.59
Residuals: R1 (I>2.00□(I))	0.0934
Residuals: R (All reflections)	0.0986
Residuals: wR2 (All reflections)	0.2750
Goodness of Fit Indicator	1.191
Max Shift/Error in Final Cycle	0.056
Maximum peak in Final Diff. Map	0.40 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.34 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
F1	0.8488(6)	0.3124(4)	0.4469(3)	4.54(9)
F2	0.4516(7)	0.3443(4)	0.5451(3)	4.43(8)
F4	0.3700(7)	-0.0166(3)	0.2987(3)	4.58(8)
F5	0.8045(5)	0.0965(3)	0.3044(3)	3.84(7)
C1	0.6296(9)	0.3464(5)	0.3705(5)	3.23(10)
C2	0.4225(9)	0.2988(5)	0.4264(4)	3.04(10)
C3	0.4092(9)	0.1598(5)	0.4283(5)	2.93(9)
C4	0.3823(8)	0.1128(5)	0.2989(5)	2.92(9)
C5	0.5921(8)	0.1522(5)	0.2411(5)	2.86(9)
C6	0.6197(10)	0.2918(5)	0.2451(5)	3.22(10)

$B_{eq} = 8/3\ \square^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\square + 2U_{13}(aa^*cc^*)\cos\square + 2U_{23}(bb^*cc^*)\cos\square)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.6200	0.4390	0.3643	3.87
H2	0.2656	0.3315	0.3779	3.64
H3A	0.2679	0.1330	0.4631	3.52
H3B	0.5594	0.1255	0.4794	3.52
H4	0.2273	0.1463	0.2493	3.51
H5	0.5612	0.1238	0.1543	3.43
H6A	0.4807	0.3292	0.1878	3.87
H6B	0.7710	0.3144	0.2167	3.87

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	0.038(2)	0.072(3)	0.060(2)	-0.013(2)	0.004(2)	-0.015(2)
F2	0.073(3)	0.057(2)	0.045(2)	-0.004(2)	0.025(2)	-0.014(2)
F4	0.071(3)	0.036(2)	0.067(2)	-0.016(2)	0.015(2)	-0.011(2)
F5	0.036(2)	0.048(2)	0.062(2)	0.0119(13)	0.0098(13)	-0.002(2)
C1	0.043(3)	0.033(3)	0.049(3)	-0.004(2)	0.014(3)	-0.002(2)
C2	0.042(3)	0.041(3)	0.033(3)	0.006(2)	0.010(2)	-0.004(2)
C3	0.035(3)	0.038(3)	0.040(3)	-0.002(2)	0.012(2)	0.003(2)
C4	0.030(3)	0.037(3)	0.043(3)	-0.004(2)	0.004(2)	-0.004(2)
C5	0.031(3)	0.039(3)	0.038(3)	0.004(2)	0.005(2)	-0.003(2)
C6	0.045(3)	0.040(3)	0.042(3)	0.002(2)	0.019(2)	0.005(2)

The general temperature factor expression: $\exp(-2□^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
F1	C1	1.398(6)	F2	C2	1.395(6)
F4	C4	1.395(6)	F5	C5	1.393(5)
C1	C2	1.509(8)	C1	C6	1.512(8)
C2	C3	1.499(7)	C3	C4	1.513(7)
C4	C5	1.507(7)	C5	C6	1.511(7)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1	1.000	C2	H2	1.000
C3	H3A	0.990	C3	H3B	0.990
C4	H4	1.000	C5	H5	1.000
C6	H6A	0.990	C6	H6B	0.990

Table 6. Bond angles (^{0})

atom	atom	atom	angle	atom	atom	atom	angle
F1	C1	C2	108.0(4)	F1	C1	C6	109.5(5)
C2	C1	C6	111.2(4)	F2	C2	C1	108.6(4)
F2	C2	C3	109.5(4)	C1	C2	C3	112.9(5)
C2	C3	C4	108.5(4)	F4	C4	C3	109.4(4)
F4	C4	C5	108.9(4)	C3	C4	C5	112.1(4)
F5	C5	C4	108.5(4)	F5	C5	C6	110.0(4)
C4	C5	C6	110.6(5)	C1	C6	C5	113.5(5)

Table 7. Bond angles involving hydrogens (^{0})

atom	atom	atom	angle	atom	atom	atom	angle
F1	C1	H1	109.4	C2	C1	H1	109.4
C6	C1	H1	109.4	F2	C2	H2	108.6
C1	C2	H2	108.6	C3	C2	H2	108.6
C2	C3	H3A	110.0	C2	C3	H3B	110.0
C4	C3	H3A	110.0	C4	C3	H3B	110.0
H3A	C3	H3B	108.4	F4	C4	H4	108.8
C3	C4	H4	108.8	C5	C4	H4	108.8
F5	C5	H5	109.2	C4	C5	H5	109.2
C6	C5	H5	109.2	C1	C6	H6A	108.9
C1	C6	H6B	108.9	C5	C6	H6A	108.9
C5	C6	H6B	108.9	H6A	C6	H6B	107.7

Table 8. Torsion Angles(^{0})

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
F1	C1	C2	F2	55.3(5)	F1	C1	C2	C3	-66.4(5)
F1	C1	C6	C5	69.4(5)	C2	C1	C6	C5	-49.8(5)
C6	C1	C2	F2	175.4(4)	C6	C1	C2	C3	53.7(5)
F2	C2	C3	C4	-179.0(4)	C1	C2	C3	C4	-57.8(5)
C2	C3	C4	F4	179.9(4)	C2	C3	C4	C5	59.1(5)
F4	C4	C5	F5	-56.5(5)	F4	C4	C5	C6	-177.2(3)
C3	C4	C5	F5	64.6(5)	C3	C4	C5	C6	-56.1(5)
F5	C5	C6	C1	-68.7(5)	C4	C5	C6	C1	51.2(5)

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F1	F2	2.685(5)	F1	F5	2.802(5)
F1	C3	2.929(6)	F1	C4	3.531(6)
F1	C5	3.006(6)	F4	F5	2.706(5)
F5	C1	3.004(6)	F5	C2	3.508(6)
F5	C3	2.910(6)	C1	C4	2.906(7)
C2	C5	2.908(7)	C3	C6	2.924(8)

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F1	H2	3.206	F1	H3B	2.652
F1	H6A	3.213	F1	H6B	2.525
F2	H1	2.600	F2	H3A	2.589
F2	H3B	2.575	F4	H3A	2.591
F4	H3B	2.590	F4	H5	2.591
F5	H3B	2.619	F5	H4	3.208
F5	H6A	3.214	F5	H6B	2.535
C1	H3A	3.356	C1	H3B	2.736
C1	H4	3.215	C1	H5	3.372
C2	H4	2.639	C2	H6A	2.770
C2	H6B	3.333	C3	H1	3.357
C3	H5	3.359	C3	H6A	3.338
C4	H2	2.642	C4	H6A	2.747
C4	H6B	3.326	C5	H1	3.372
C5	H2	3.240	C5	H3A	3.355
C5	H3B	2.723	C6	H2	2.731
C6	H3B	3.247	C6	H4	2.703
H1	H2	2.325	H1	H6A	2.301
H1	H6B	2.405	H2	H3A	2.339
H2	H3B	2.859	H2	H4	2.444
H2	H6A	2.640	H3A	H4	2.362
H3B	H4	2.872	H4	H5	2.334
H4	H6A	2.596	H5	H6A	2.302
H5	H6B	2.398			

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F1	F2^{1}	3.350(5)	F1	C2^{1}	3.262(6)
F1	C3^{1}	3.579(6)	F1	C5^{2}	3.327(6)
F1	C6^{2}	3.563(6)	F2	F1^{3}	3.350(5)
F2	F2^{4}	3.572(5)	F2	F5^{5}	3.230(5)
F2	C1^{4}	3.515(6)	F2	C4^{2}	3.374(6)
F2	C5^{5}	3.252(7)	F2	C6^{5}	3.496(7)
F4	F5^{3}	3.399(5)	F4	C1^{6}	3.388(6)
F4	C2^{6}	3.368(6)	F4	C3^{7}	3.428(6)
F4	C6^{6}	3.385(7)	F5	F2^{8}	3.230(5)
F5	F4^{1}	3.399(5)	F5	C1^{9}	3.391(6)
F5	C3^{1}	3.460(6)	F5	C4^{1}	3.247(6)
F5	C6^{9}	3.368(6)	C1	F2^{4}	3.515(6)
C1	F4^{10}	3.388(6)	C1	F5^{11}	3.391(6)
C2	F1^{3}	3.262(6)	C2	F4^{10}	3.368(6)
C3	F1^{3}	3.579(6)	C3	F4^{7}	3.428(6)
C3	F5^{3}	3.460(6)	C4	F2^{12}	3.374(6)
C4	F5^{3}	3.247(6)	C5	F1^{12}	3.327(6)
C5	F2^{8}	3.252(7)	C6	F1^{12}	3.563(6)
C6	F2^{8}	3.496(7)	C6	F4^{10}	3.385(7)
C6	F5^{11}	3.368(6)			

Symmetry Operators:

(1) X+1,Y,Z
(2) X+1/2,-Y+1/2,Z+1/2
(3) X-1,Y,Z
(4) -X+1,-Y+1,-Z+1
(5) X+1/2-1,-Y+1/2,Z+1/2
(6) -X+1/2,Y+1/2-1,-Z+1/2
(7) -X+1,-Y,-Z+1
(8) X+1/2,-Y+1/2,Z+1/2-1
(9) -X+1/2+1,Y+1/2-1,-Z+1/2
(10) -X+1/2,Y+1/2,-Z+1/2
(11) -X+1/2+1,Y+1/2,-Z+1/2
(12) X+1/2-1,-Y+1/2,Z+1/2-1

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F1	H2^{1}	2.602	F1	H3A^{1}	3.014
F1	H5^{2}	2.486	F1	H6A^{2}	3.058
F2	H1^{3}	2.606	F2	H4^{2}	2.494
F2	H5^{4}	2.724	F2	H5^{2}	3.404
F2	H6A^{2}	3.596	F2	H6B^{4}	2.896
F4	H1^{5}	3.016	F4	H2^{5}	2.562
F4	H3A^{6}	3.263	F4	H3B^{6}	2.703
F4	H6A^{5}	2.596	F4	H6B^{7}	2.740
F5	H1^{7}	2.632	F5	H2^{1}	3.590
F5	H3A^{1}	2.865	F5	H4^{1}	2.612
F5	H6A^{7}	3.113	F5	H6B^{7}	3.070
C1	H2^{1}	3.543	C1	H5^{8}	3.489
C3	H3B^{6}	3.235	C3	H6B^{4}	3.473
C4	H1^{5}	3.565	C4	H3B^{6}	3.538
C5	H1^{7}	3.162	C5	H4^{1}	3.534
C6	H3A^{9}	3.508	H1	F2^{3}	2.606
H1	F4^{10}	3.016	H1	F5^{8}	2.632
H1	C4^{10}	3.565	H1	C5^{8}	3.162
H1	H4^{10}	3.066	H1	H5^{8}	2.707
H2	F1^{11}	2.602	H2	F4^{10}	2.562
H2	F5^{11}	3.590	H2	C1^{11}	3.543
H2	H5^{4}	3.533	H2	H6B^{11}	2.995
H3A	F1^{11}	3.014	H3A	F4^{6}	3.263
H3A	F5^{11}	2.865	H3A	C6^{4}	3.508
H3A	H3B^{6}	2.975	H3A	H6A^{4}	3.262
H3A	H6B^{4}	2.889	H3B	F4^{6}	2.703
H3B	C3^{6}	3.235	H3B	C4^{6}	3.538
H3B	H3A^{6}	2.975	H3B	H3B^{6}	2.843
H3B	H6A^{2}	3.010	H3B	H6B^{4}	3.426
H4	F2^{12}	2.494	H4	F5^{11}	2.612
H4	C5^{11}	3.534	H4	H1^{5}	3.066
H4	H6B^{11}	3.090	H5	F1^{12}	2.486
H5	F2^{12}	3.404	H5	F2^{9}	2.724
H5	C1^{7}	3.489	H5	H1^{7}	2.707
H5	H2^{9}	3.533	H6A	F1^{12}	3.058
H6A	F2^{12}	3.596	H6A	F4^{10}	2.596
H6A	F5^{8}	3.113	H6A	H3A^{9}	3.262

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H6A	H3B^{12}	3.010	H6B	F2^{9}	2.896
H6B	F4^{8}	2.740	H6B	F5^{8}	3.070
H6B	C3^{9}	3.473	H6B	H2^{1}	2.995
H6B	H3A^{9}	2.889	H6B	H3B^{9}	3.426
H6B	H4^{1}	3.090			

Symmetry Operators:

(1) X+1,Y,Z
(2) X+1/2,-Y+1/2,Z+1/2
(3) -X+1,-Y+1,-Z+1
(4) X+1/2-1,-Y+1/2,Z+1/2
(5) -X+1/2,Y+1/2-1,-Z+1/2
(6) -X+1,-Y,-Z+1
(7) -X+1/2+1,Y+1/2-1,-Z+1/2
(8) -X+1/2+1,Y+1/2,-Z+1/2
(9) X+1/2,-Y+1/2,Z+1/2-1
(10) -X+1/2,Y+1/2,-Z+1/2
(11) X-1,Y,Z
(12) X+1/2-1,-Y+1/2,Z+1/2-1