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Supporting Information

Understanding the Conformational Behavior of Fluorinated Piperidines: The Origin of the Axial-F Preference

Zackaria Nairoukh[+],* Felix Strieth-Kalthoff[+], Klaus Bergander, and Frank Glorius*[a]

Understanding the conformational behavior of fluorinated piperidines: The origin of the axial-F orientation

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Supplementary Information

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Materials and Methods

All trifluoroacetyl-(TFA) and *tert*-butyloxycarbonyl-(Boc)-fluoropiperidine derivatives were prepared according to previously published procedures.[1] The preparation of acetyl-(Ac)- and pivaloyl-(Piv)-fluoropiperidine derivatives as well as the preparation of fluoropiperidinium hydrochloride salts and non-protonated fluoropiperidine derivatives is described in the following section.

^{1}H and ^{13}C, and ^{19}F NMR spectra were recorded on a Bruker Avance II 300 or Avance II 400, Agilent DD2 500 or Agilent DD2 600 in the indicated solvents. Chemical shifts (δ) are given in ppm relative to TMS. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; CD_2Cl_2: δ_H = 5.32 ppm, δ_C = 54.0 ppm; C_6D_6: δ_H = 7.16 ppm, δ_C = 128.06 ppm; D_2O: δ_H = 4.79 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.5 ppm). ^{19}F NMR spectra are referenced according to the proton resonance of TMS as the primary reference for the unified chemical shift scale (IUPAC recommendation 2001). ESI mass spectra were recorded on a Bruker Daltonics MicroTof spectrometer.

Typical NMR sample contains 20 mg of the measured compounds. For literature known compounds, only ^{1}H NMR spectra in different deuterated solvents are presented. For newly synthesized compounds, fully detailed NMR spectra and ESI-MS are given.

The experimental determination of the axial or equatorial orientation of the fluorine atoms on the piperidine ring was done through NMR studies. It has been shown that the vicinal $^{3}J(^{19}F,^{1}H)$ coupling constants provide useful insight into conformational structure, as large values of $^{3}J(^{19}F,^{1}H_a)$ indicate axial preference and small values of $^{3}J(^{19}F,^{1}H_a)$ indicate equatorial preference.[1] For determining the $^{3}J(^{19}F,^{1}H_a)$ we applied selective, multi-selective and band-selective decoupling schemes. This was done using the Pbox provided by Vnmrj of Agilent.

Computations were carried out using the ORCA 4.1.1 software package, as developed by Neese and co-workers.[2] All structures are given in the .xyz format and were visualized using *Jmol*.[3] Gas phase geometries of the respective conformers were optimized using the M06-2X hybrid functional[4] in Ahlrich's def2-TZVPP basis set.[5] All conformers were confirmed to be local minima on the respective potential energy surface by the absence of negative eigenvalues of the Hessian after numerical harmonic frequency analysis at the same level of computation. No symmetry of internal coordinate constraints were applied. Higher energy conformers (in particular, rotamers of the respective acetyl-, pivaloyl- or carbamoyl-protected amines) were taken into account. The

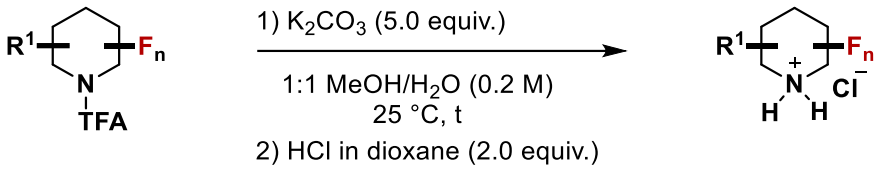
electronic energy of the previously optimized geometries was then determined by an additional single-point calculation on the M06-2X / def2-QZVPP level.[4, 5] The reported free energy values (in E_h and kcal mol^{-1}) were then obtained as the sum of the single point electronic energies and the respective free energy corrections (ZPVE, thermal corrections, enthalpy correction, entropy correction), as obtained from the harmonic frequency analysis. Geometries and free energies for the conformers in solution were obtained accordingly. For both geometry optimization and single point calculation, solvation effects were included using the CPCM continuum solvation model (presets for benzene, dichloromethane, chloroform, dimethyl sulfoxide and water, respectively).[6] NBO analysis was performed using the NBO 6.0 software.[7] The difference in electronic energies between two conformers was attributed to a sum of hyperconjugative, steric and electrostatic contributions.

$$\Delta E_{el} = \Delta E_{\mathrm{hyperconj}} + \underbrace{\Delta E_{\mathrm{steric}} + \Delta E_{\mathrm{electrostat}}}_{\Delta E_{\mathrm{loc}}}$$

Hyperconjugative stabilization was quantified by subtracting the actual electronic energy from the energy of a hypothetical fully localized structure E_{loc}, deleting all antibonding orbitals from the electronic energy computation ($DEL LEWIS keyword). Steric contributions were obtained using the NBO/NLMO steric analysis ($NBO STERIC keyword). The residual difference in electronic energies was attributed to electrostatic interactions, neglecting potential coupling between steric and electrostatic interactions, and potential non-Lewis electrostatic interactions. Individual hyperconjugative interactions were extracted from the result of a second order perturbation theory analysis of the Fock matrix within the basis of NBOs.

Preparation of Fluoropiperidine Derivatives

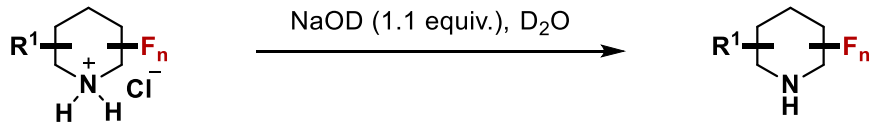
Preparation of fluoropiperidinium hydrochloride salts (**1B**–**12B**).



Following a literature procedure,[1] K_2CO_3 (5.0 equiv) was added in one portion to a solution of TFA-fluoropiperidine derivative (**1A–12A**) (1.0 equiv.) in 1:1 methanol/water (0.2 M) at room temperature. After stirring the solution for the indicated time, the reaction mixture was acidified with 2 M aqueous solution of HCl. After removal of all volatiles, 2 M aqueous solution of NaOH and CH_2Cl_2 (5 mL) were added. The organic layer was separated and the aqueous layer was further extracted with CH_2Cl_2 (3×5 mL). The organic layers were combined, dried over $MgSO_4$ and filtrated. HCl (4 M in 1,4-dioxane, 2.0 equiv.) was added to the filtrate and all volatiles were removed to yield the corresponding fluoropiperidinium hydrochloride (**1B**–**12B**) as a white solid. NMR samples were prepared by dissolving the fluoropiperidinium adducts in D_2O.

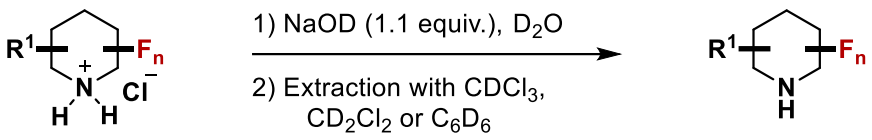
Preparation of non-protonated fluoropiperidine derivatives (**1C**–**12C**).

General procedure A



To a solution of fluoropiperidinium hydrochloride salt (**1B**–**12B**, 1.0 equiv.) in D_2O (1 mL) was added NaOD (1.1 equiv.) at room temperature. The mixture was then transferred to NMR tube and submitted for measurements.

General procedure B



To a solution of fluoropiperidinium hydrochloride salt (**1B**–**12B**, 1.0 equiv.) in D_2O (1 mL) was added NaOD (1.1 equiv.) at room temperature. The aqueous solution was then extracted with a deuterated solvent ($CDCl_3$, CD_2Cl_2 or C_6D_6), dried over $MgSO_4$ and transferred to NMR tube for the required measurements.

Preparation of 1-(cis-3,5-difluoropiperidin-1-yl)ethan-1-one (**13**).

To a solution of *cis*-3,5-difluoropiperidine hydrochloride **2B** (0.157 g, 1.0 mmol, 1.0 equiv.) in H_2O (1 mL) was added 1M NaOH (1.1 mL, 1.1 mmol, 1.1 equiv.) at room temperature. The aqueous solution was then extracted with CH_2Cl_2 (3×5 mL), dried over $MgSO_4$ and filtrated to deliver the non-protonated fluoropiperidine derivative in CH_2Cl_2 solution.

To the prepared solution, acetyl chloride (0.117 g, 1.5 mmol, 1.5 equiv.) and triethylamine (0.42 mL, 3.0 mmol, 3.0 equiv.) were added at room temperature. Upon the completion of the reaction (followed by TLC), water (10 mL) was added. The organic layer was separated and the aqueous layer was further extracted with CH_2Cl_2 (3×5 mL). The organic layers were combined, dried over $MgSO_4$, filtrated and concentrated under reduced pressure. The crude was then submitted to column chromatography (0-100% ethyl acetate in pentane) to obtain the final product as a white solid (0.15 g, 0.92 mmol, 92%).

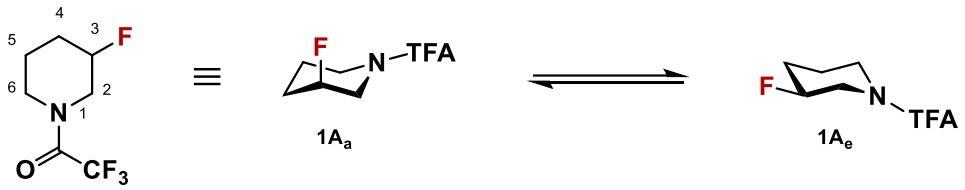
Preparation of 1-(cis-3,5-difluoropiperidin-1-yl)-2,2-dimethylpropan-1-one (**14**).

To a solution of *cis*-3,5-difluoropiperidine hydrochloride **2B** (0.504 g, 3.2 mmol, 1.0 equiv.) in H_2O (2 mL) was added 1M NaOH (3.5 mL, 3.5 mmol, 1.1 equiv.) at room temperature. The aqueous solution was then extracted with CH_2Cl_2 (3×5 mL), dried over $MgSO_4$ and filtrated to deliver the non-protonated fluoropiperidine derivative in CH_2Cl_2 solution.

To the prepared solution, pivaloyl chloride (1.1 g, 9.6 mmol, 3.0 equiv.) and triethylamine (1.3 mL, 9.6 mmol, 3.0 equiv.) were added at room temperature. Upon the completion of the reaction (followed by TLC), water (10 mL) was added. The organic layer was separated and the

aqueous layer was further extracted with CH_2Cl_2 (3×5 mL). The organic layers were combined, dried over $MgSO_4$, filtrated and concentrated under reduced pressure. The crude was then submitted to column chromatography (0-10% ethyl acetate in pentane) to obtain the final product as a white solid (0.612 g, 2.9 mmol, 90%).

2,2,2-Trifluoro-1-(3-fluoropiperidin-1-yl)ethan-1-one (1A)



This compound was prepared following a recent literature procedure.[1]

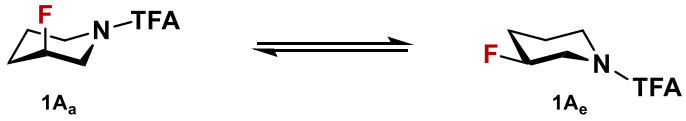
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **Toluene-*d*$_8$**: The orientation of the fluorine atom was assigned as axial due to the large value of ^3J(F,H$_a$).[1] [**Rot A: ^3J(2-H$_a$,3-F) = 26.0 Hz, Rot B: ^3J(2-H$_a$,3-F) = 26.0 Hz**]

Computational observation

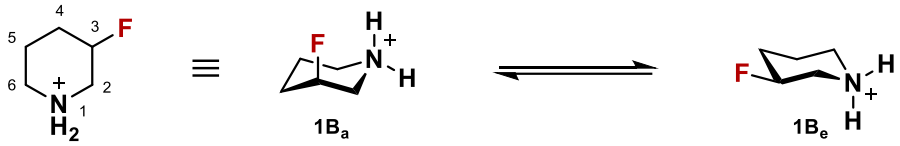
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE$_{elect}$	ΔE$_{hyperc}$	ΔE$_{steric}$	μ$_a$	μ$_e$	Experimental
Toluene	+0.1	+6.5	+3.3	–9.6	6.8	4.3	axial
gas phase	–0.4	+9.4	+2.4	–12.1	5.6	3.6	-

All values are given in kcal/mol at 298 K.

3-Fluoropiperidine hydrochloride (1B)



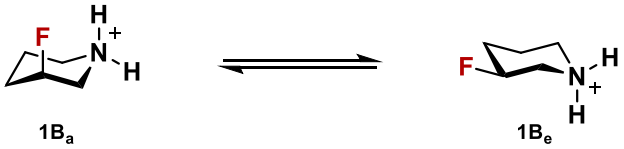
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large value of $^3J(F,H_a)$.[1] [***^3J*(2-H_a,3-F) = 38.7 Hz**]

Computational observation

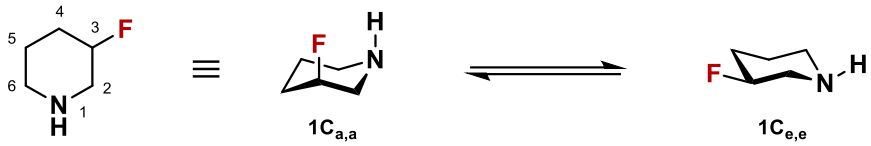
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+1.8	+12.6	+3.8	–14.4	6.9	9.0	axial
gas phase	+4.8	+22.1	–0.1	–16.8	5.0	7.0	-

All values are given in kcal/mol at 298 K.

3-Fluoropiperidine (1C)



The preparation of this compound is described in the previous section.

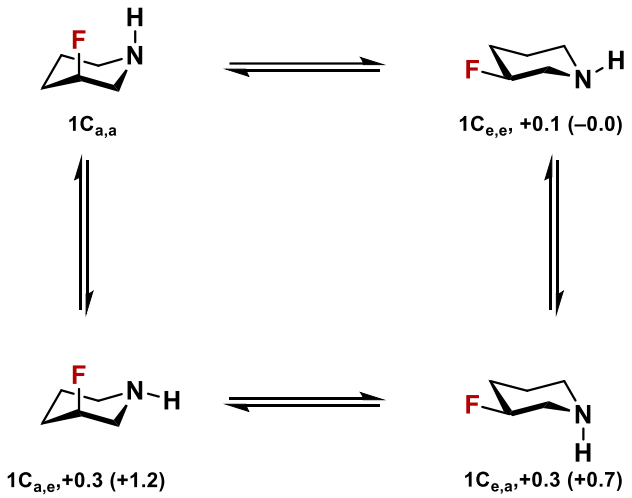
Experimental observation

In **D_2O**: Due to peaks overlapping in NMR spectra, we could not verify the orientation of the fluorine atom through $^3J(F,H_a)$. Therefore we conducted additional NMR studies that includes $^1H\{^{19}F\}$ NMR with homo-decoupling of proton at two different positions 4-H and 2-H (separately). From these experiments, we found that the vicinal coupling constants $^3J(3\text{-}H_e,2\text{-}H_a)$, $^3J(3\text{-}H_e,2\text{-}H_{eq})$, $^3J(3\text{-}H_e,4\text{-}H_a)$ and $^3J(3\text{-}H_e,4\text{-}H_e)$ are of small values (~4.4 Hz). In addition, we could not observe any axial-axial interaction between 3-H and 4-H/2-H. Accordingly, we believe that the axial orientation of the fluorine atom in this case is dominant.

^{1}H NMR (500 MHz, D_2O, 299 K) δ 4.79 (d, *J* = 47.3 Hz, 1H overlaps with solvent), 3.04 – 2.91 (m, 2H), 2.89 – 2.81 (m, 1H), 2.78 – 2.69 (m, 1H), 1.97 – 1.75 (m, 3H), 1.61 – 1.52 (m, 1H); **^{1}H{^{19}F} NMR** (500 MHz, D_2O, 299 K) δ 4.79 (s, 1H overlaps with solvent), 3.07 – 2.92 (m, 2H), 2.90 – 2.81 (m, 1H), 2.78 – 2.69 (m, 1H), 2.00 – 1.76 (m, 3H), 1.60 – 1.51 (m, 1H); **^{13}C NMR** (126 MHz, D_2O, 299 K) δ 88.49 (d, *J* = 166.3 Hz), 48.24 (d, *J* = 21.9 Hz), 44.14, 28.58 (d, *J* = 19.8 Hz), 20.89 (d, *J* = 3.9 Hz); **^{13}C{sel-^{19}F at -183 ppm} NMR** (126 MHz, D_2O, 299 K) δ 88.49, 48.24, 44.14, 28.58, 20.89; **^{19}F NMR** (470 MHz, D_2O, 299 K) δ -183.33; **^{19}F{^{1}H} NMR** (470 MHz, D_2O, 299 K) δ -183.33.

Computational observation

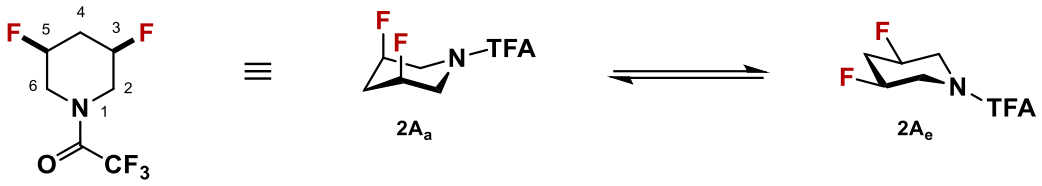
The calculated ΔG is presented as follows: ΔG in water (ΔG gas phase) and are given for the energetically lowest conformers.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+0.1	+12.7	+5.1	–17.7	2.3	2.9	axial dominant
gas phase	–0.0	+6.9	+4.8	–11.7	1.6	2.2	-

All values are given in kcal/mol at 298 K.

1-(*cis*-3,5-Difluoropiperidin-1-yl)-2,2,2-trifluoroethan-1-one (2A)



For this particular sample we conducted several computations and NMR experiments in different solvents in order to investigate the effect of solvent's dipole moment on the orientation of the fluorine atoms.

This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**^3J(2-H_a,3-F) = 32.1 Hz, ^3J(4-H_a,3-F) = 36.1 Hz, ^3J(4-H_a,5-F) = 36.1 Hz, ^3J(6-H_a,5-F) = 30.6 Hz**]

In **DMSO**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H_a,3-F) = 38.6 Hz, ^3J(4-H_a,3-F) = 44.4 Hz, ^3J(4-H_a,5-F) = 44.4 Hz, ^3J(6-H_a,5-F) = 40.1 Hz**]

^{1}H NMR (500 MHz, DMSO-d_6, 299 K) δ 4.95 (dm, *J* = 46.0 Hz, 1H), 4.90 (dm, *J* = 46.0 Hz, 1H), 4.56 (ddq, *J* = 14.8, 12.4, 2.5 Hz, 1H), 4.09 (dddd, *J* = 13.0, 9.3, 4.9, 2.5 Hz, 1H), 3.62 (ddd, *J* = 38.6, 15.1, 1.5 Hz, 1H), 3.23 (dd, *J* = 40.1, 14.5 Hz, 1H), 2.30 (dtt, *J* = 17.3, 12.4, 2.5 Hz, 1H), 2.10 (tdt, *J* = 44.4, 16.2, 3.3 Hz, 1H); **^{1}H{^{19}F} NMR** (500 MHz, DMSO-d_6, 299 K) δ 4.96 (bs, 1H), 4.91 (bs, 1H), 4.56 (dq, *J* = 14.6, 2.5 Hz, 1H), 4.09 (dm, *J* = 15.1 Hz, 1H), 3.62 (d, *J* = 15.0 Hz, 1H), 3.23 (d, *J* = 14.5 Hz, 1H), 2.30 (dp, *J* = 16.2, 2.5 Hz, 1H), 2.10 (dt, *J* = 16.2, 3.3 Hz, 1H).

In **CD_2Cl_2**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H_a,3-F) = 32.9 Hz, ^3J(4-H_a,3-F) = 38.8 Hz, ^3J(4-H_a,5-F) = 38.8 Hz, ^3J(6-H_a,5-F) = 34.6 Hz**]

^{1}H NMR (500 MHz, CD_2Cl_2, 299 K) δ 4.86 (dm, *J* = 45.1 Hz, 1H), 4.79 (dm, *J* = 45.7 Hz, 1H), 4.66 – 4.58 (m, 1H), 4.21 – 4.12 (m, 1H), 3.46 (dd, *J* = 32.9, 14.9 Hz, 1H), 3.18 (ddm, *J* = 34.6,

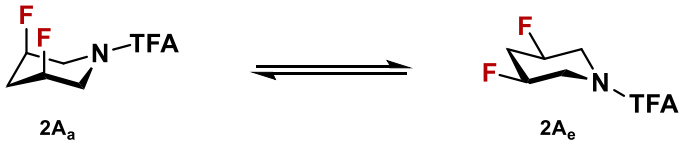
14.5 Hz, 1H), 2.52 – 2.38 (m, 1H), 2.03 (tdm, *J* = 38.8, 15.8 Hz, 1H); **^{1}H{^{19}F} NMR** (500 MHz, CD_2Cl_2, 299 K) δ 4.89 – 4.85 (m, 1H), 4.83 – 4.76 (m, 1H), 4.62 (dm, *J* = 14.5 Hz, 1H), 4.16 (dm, *J* = 14.9 Hz, 1H), 3.46 (d, *J* = 15.0 Hz, 1H), 3.17 (dd, *J* = 14.5, 3.6 Hz, 1H), 2.46 (dm, *J* = 15.8 Hz, 1H), 2.02 (dm, *J* = 15.8 Hz, 1H).

In **C_6D_6**: The orientation of the fluorine atoms was assigned as axial due to the large values of ^{3}J(F,H_a). [***^{3}J*(2-H_a,3-F) = 29.6 Hz, *^{3}J*(4-H_a,3-F) = 34.1 Hz, *^{3}J*(4-H_a,5-F) = 34.1 Hz, *^{3}J*(6-H_a,5-F) = 30.6 Hz**]

^{1}H NMR (500 MHz, C_6D_6, 299 K) δ 4.03 – 3.95 (m, 1H), 3.82 (dm, *J* = 45.0 Hz, 1H overlaps with 5-H_e), 3.74 (dm, *J* = 45.7 Hz, 1H overlaps with 3-H_e), 3.45 – 3.35 (m, 1H), 2.46 (dm, *J* = 29.6 Hz, 1H overlaps with 6-H_a), 2.40 (dm, *J* = 30.6 Hz, 1H overlaps with 2-H_a), 1.75 – 1.63 (m, 1H), 0.90 (tdt, *J* = 34.1, 15.1, 3.7 Hz, 1H); **^{1}H{^{19}F} NMR** (500 MHz, C_6D_6, 299 K) δ 3.99 (dm, *J* = 14.2 Hz, 1H), 3.85 – 3.81 (m, 1H), 3.78 – 3.73 (m, 1H), 3.40 (dm *J* = 14.7 Hz, 1H), 2.47 (dd, *J* = 14.7, 2.4 Hz, 1H), 2.40 (dd, *J* = 14.2, 2.4 Hz, 1H), 1.69 (dtt, *J* = 15.1, 4.5, 1.7 Hz, 1H), 0.90 (dt, *J* = 15.1, 3.7 Hz, 1H).

<u>Computational observation</u>

The calculated ΔG is given for the energetically lowest conformers.

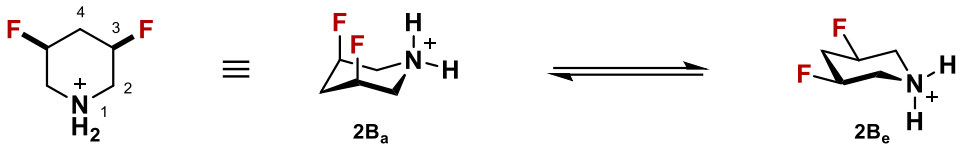


$2A_a$ **$2A_e$**

Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
DMSO	+2.0	+10.6	+12.1	–20.8	9.8	3.3	axial
CH_2Cl_2	+1.4	+8.5	+11.9	–19.0	9.3	3.2	axial
$CHCl_3$	+0.9	+8.1	+11.7	–18.8	8.9	3.0	axial
C_6H_6	+0.1	+12.4	+11.4	–23.7	8.1	2.7	axial
gas phase	–1.4	+12.5	+11.0	–24.8	6.6	2.2	-

All values are given in kcal/mol at 298 K.

***cis*-3,5-Difluoropiperidine hydrochloride (2B)**



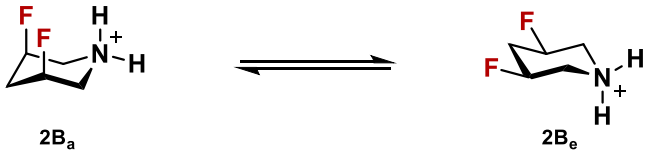
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [^{3}***J*(2-H$_a$,3-F) = 39.5 Hz, ^{3}*J*(4-H$_a$,3-F) = 46.7 Hz**]

Computational observation

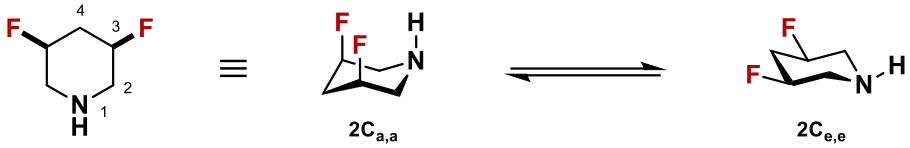
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+3.9	+14.7	+11.0	–21.1	9.1	10.1	axial
gas phase	+8.6	+33.9	+5.4	–30.3	6.8	7.8	-

All values are given in kcal/mol at 298 K.

***cis*-3,5-Difluoropiperidine (2C)**



For this particular sample we conducted NMR experiments in different solvents in order to investigate the effect of solvent's dipole moment on the orientation of the fluorine atoms.

The preparation of this compound is described in the previous section.

Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of ^3J(F,H_a). [***^3J*(2-H_a,3-F) = 40.2 Hz, ^3J(4-H_a,3-F) = 44.2 Hz**]

^{1}H NMR (500 MHz, D_2O, 299 K) δ 4.81 (dm, *J* = 46.6 Hz, 2H overlap with solvent), 3.23 – 3.13 (m, 2H), 2.85 (dd, *J* = 40.2, 14.6 Hz, 2H), 2.47 – 2.35 (m, 1H), 2.10 (tdt, *J* = 44.2, 16.1, 3.3 Hz, 1H); **^{1}H{^{19}F} NMR** (500 MHz, D_2O, 299 K) δ 4.85 – 4.81 (m, 2H), 3.18 (dm, *J* = 14.9 Hz, 2H), 2.86 (d, *J* = 14.8 Hz, 2H), 2.40 (dm, *J* = 16.1 Hz, 1H), 2.10 (dt, *J* = 16.8, 3.3 Hz, 1H); **^{13}C NMR** (126 MHz, D_2O, 299 K) δ 86.68 (d, *J* = 168.3 Hz), 47.35 – 47.03 (m), 32.20 (t, *J* = 20.1 Hz); **^{13}C{sel-^{19}F at -181 ppm} NMR** (126 MHz, D_2O, 299 K) δ 86.68, 47.19, 32.20; **^{19}F NMR** (470 MHz, D_2O, 299 K) δ -181.73 – -182.13 (m); **^{19}F{^{1}H} NMR** (470 MHz, D_2O, 299 K) δ -181.94.

In **DMSO**: The orientation of the fluorine atoms was assigned as axial due to the large value of ^3J(F,H_a). [***^3J*(2-H_a,3-F) = 31.9 Hz**]

It should be noted that the NMR sample contained small amount of water that were needed for the preparation of the non-protonated piperidine.

^{1}H NMR (600 MHz, DMSO-d_6, 299 K) δ 4.57 (dm, *J* = 47.1 Hz, 2H), 2.81 (ddt, *J* = 13.6, 11.8, 2.6 Hz, 2H), 2.72 (dd, *J* = 31.9, 14.2 Hz, 2H), 2.14 – 1.93 (m, 2H); **^{1}H{^{19}F} NMR** (600 MHz, DMSO-d_6, 299 K) δ 4.60 – 4.52 (m, 2H), 2.82 (dd, *J* = 14.3, 4.2 Hz, 2H), 2.72 (d, *J* = 14.4 Hz, 2H), 2.07 – 2.00 (m, 2H).

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [***^3J*(2-H_a,3-F) = 30.1 Hz, *^3J*(4-H_a,3-F) = 34.5 Hz**]

^{1}H NMR (600 MHz, CD_2Cl_2, 299 K) δ 4.57 (dm, *J* = 46.0 Hz, 2H), 3.14 – 3.05 (m, 2H), 2.91 (ddd, *J* = 30.1, 14.3, 2.2 Hz, 2H), 2.35 – 2.23 (m, 1H), 2.06 (tdt, *J* = 34.5, 14.9, 3.6 Hz, 1H); **^{1}H{^{19}F} NMR** (600 MHz, CD_2Cl_2, 299 K) δ 4.62 – 4.55 (m, 2H), 3.09 (ddd, *J* = 14.3, 4.4, 1.9 Hz, 2H), 2.91 (d, *J* = 14.3 Hz, 2H), 2.29 (dm, *J* = 14.8 Hz, 1H), 2.06 (dt, *J* = 14.9, 3.6 Hz, 1H).

In **CD_2Cl_2**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [***^3J*(2-H_a,3-F) = 28.5 Hz, *^3J*(4-H_a,3-F) = 33.5 Hz**]

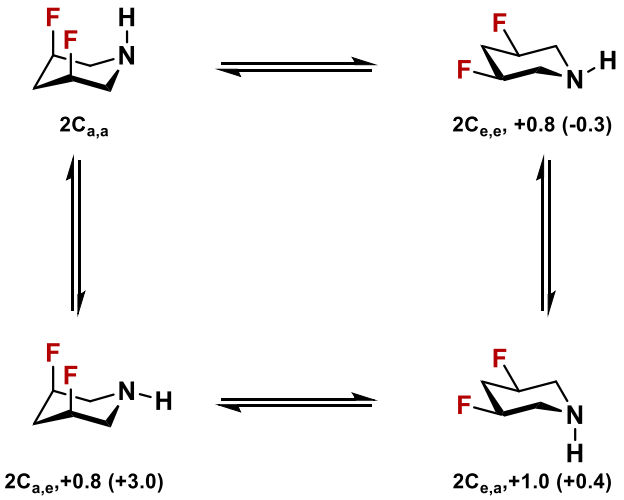
^{1}H NMR (600 MHz, CD_2Cl_2, 299 K) δ 4.53 (dm, *J* = 47.2 Hz, 2H), 3.03 – 2.96 (m, 2H), 2.89 (dm, *J* = 28.5 Hz, 2H), 2.25 – 2.15 (m, 1H), 2.07 (tdt, *J* = 33.5, 14.6, 3.6 Hz, 1H); **^{1}H{^{19}F} NMR** (600 MHz, CD_2Cl_2, 299 K) δ 4.56 – 4.50 (m, 2H), 3.00 (ddd, *J* = 14.1, 4.8, 1.8 Hz, 2H), 2.90 (dd, *J* = 14.2, 2.5 Hz, 2H), 2.19 (dtt, *J* = 14.7, 5.1, 1.9 Hz, 1H), 2.08 (dt, *J* = 14.6, 3.6 Hz, 1H).

In **C_6D_6**: The dominant orientation of the fluorine atoms is assigned to be axial based on the values of $^3J(F,H_a)$. [***^3J*(2-H_a,3-F) = 21.2 Hz, *^3J*(4-H_a,3-F) = 25.5 Hz**]

^{1}H NMR (600 MHz, C_6D_6, 299 K) δ 3.92 (dm, *J* = 47.6 Hz, 2H), 2.54 – 2.48 (m, 2H), 2.43 (dd, *J* = 21.2, 13.3 Hz, 2H), 1.83 – 1.72 (m, 1H), 1.59 (tdt, *J* = 25.5, 14.0, 3.9 Hz, 1H); **^{1}H{^{19}F} NMR** (600 MHz, C_6D_6, 299 K) δ 3.94 – 3.90 (m, 2H), 2.51 (ddd, *J* = 13.4, 6.1, 1.3 Hz, 2H), 2.42 (dd, *J* = 13.3, 3.3 Hz, 2H), 1.81 – 1.74 (m, 1H), 1.59 (dt, *J* = 13.6, 4.0 Hz, 1H).

Computational observation

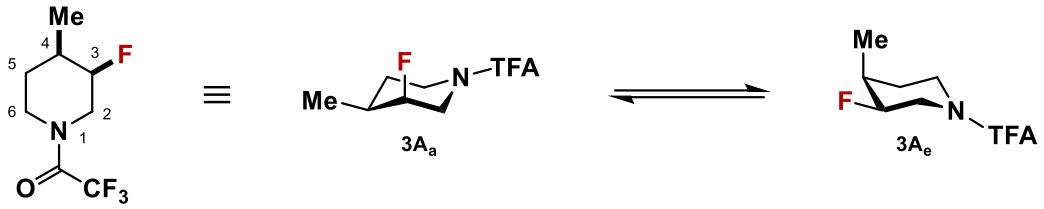
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE$_{elect}$	ΔE$_{hyperc}$	ΔE$_{steric}$	μ$_{a,a}$	μ$_{e,e}$	Experimental
DMSO	+0.8	+20.8	+10.8	–30.7	4.4	2.8	axial
H_2O	+0.8	+20.8	+10.8	–30.7	4.4	2.8	axial
CH_2Cl_2	+0.6	+20.8	+10.9	–30.9	4.3	2.8	axial
$CHCl_3$	+0.5	+20.5	+11.0	–30.9	4.1	2.7	axial
C_6H_6	+0.2	+20.2	+11.1	–31.0	3.7	2.6	axial
gas phase	–0.3	+20.6	+11.3	–32.1	3.1	2.3	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-3-fluoro-4-methylpiperidin-1-yl)ethan-1-one (3A)



This compound was prepared following a recent literature procedure.[1]

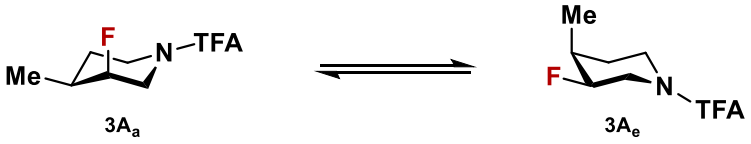
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as axial due to the large value of $^3J(F,H_a)$.[1] [**Rot A: ^3J(2-H$_a$,3-F) = 38.3 Hz, Rot B: ^3J(2-H$_a$,3-F) = 36.6 Hz**]

Computational observation

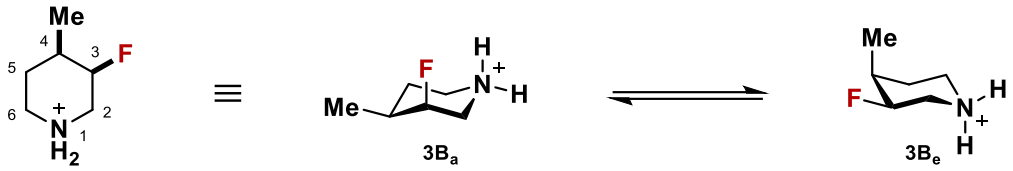
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+2.3	–0.8	+5.0	–2.1	7.5	5.8	axial
gas phase	+1.8	+0.5	+4.4	–3.3	5.6	4.4	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-4-methylpiperidine hydrochloride (3B)**



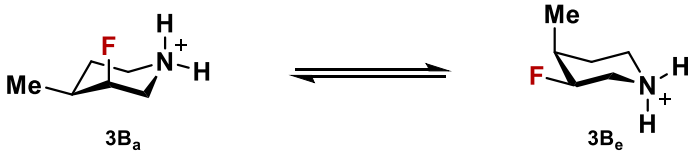
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [***^3J*(2-H_a,3-F) = 36.6 Hz, *^3J*(4-H_a,3-F) = 36.5 Hz**]

Computational observation

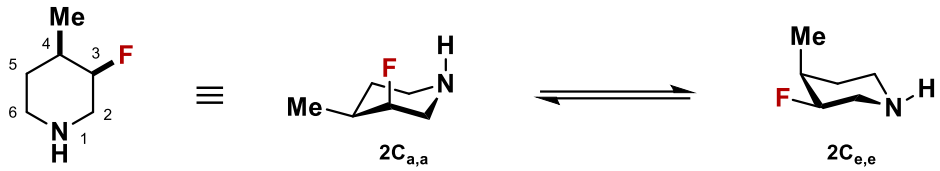
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+3.6	+8.5	+3.0	–8.0	8.3	9.7	axial
gas phase	+6.2	+16.3	–0.8	–9.3	6.0	7.4	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-4-methylpiperidine (3C)**



The preparation of this compound is described in the previous section.

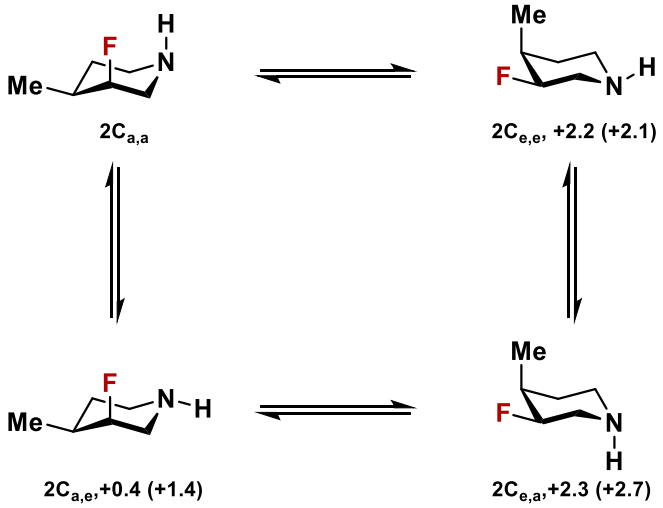
Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large values of ^{3}J(F,H_a). [***^{3}J*(2-H_a,3-F) = 42.3 Hz, *^{3}J*(4-H_a,3-F) = 37.3 Hz**]

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.56 (d, *J* = 48.3 Hz, 1H), 3.12 (t, *J* = 13.0 Hz, 1H), 2.91 (dm, *J* = 12.9 Hz, 1H), 2.65 (dd, *J* = 42.3, 14.3 Hz, 1H), 2.50 (tdd, *J* = 12.5, 3.3, 1.4 Hz, 1H), 1.70 (dm, *J* = 37.3 Hz, 1H), 1.50 – 1.34 (m, 2H), 0.96 (d, *J* = 6.9 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.56 (bs, 1H), 3.12 (d, *J* = 13.8 Hz, 1H), 2.91 (d, *J* = 12.9 Hz, 1H), 2.65 (bs, 1H), 2.50 (td, *J* = 12.6, 3.2 Hz, 1H), 1.70 (bs, 1H), 1.49 – 1.33 (m, 2H), 0.96 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 92.05 (d, *J* = 169.6 Hz), 48.81 – 47.93 (m), 44.21, 33.08 (d, *J* = 20.2 Hz), 28.13, 16.93; **^{13}C{sel-^{19}F at -202 ppm} NMR** (151 MHz, D_2O, 299 K) δ 92.02, 48.37, 44.20, 33.08, 28.12, 16.98; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -202.43; **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -202.43.

Computational observation

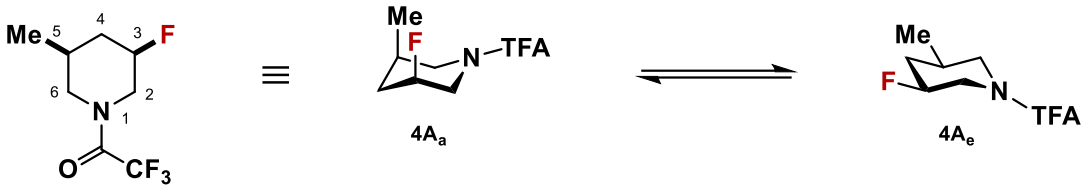
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+2.2	+13.5	+5.8	–17.4	2.3	2.8	axial
gas phase	+2.1	+12.4	+5.6	–16.1	1.6	2.1	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-3-fluoro-5-methylpiperidin-1-yl)ethan-1-one (4A)



This compound was prepared following a recent literature procedure.[1]

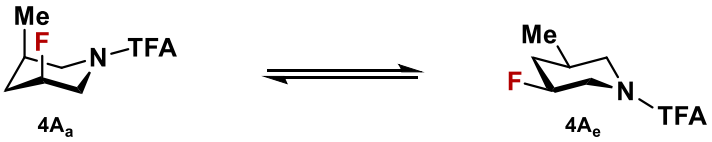
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$.[1] [**Rot A: ^3J(2-H$_a$,3-F) = 4.4 Hz, ^3J(4-H$_a$,3-F) = 12.0 Hz, Rot B: ^3J(2-H$_a$,3-F) = 5.1 Hz, ^3J(4-H$_a$,3-F) = 12.0 Hz**]

Computational observation

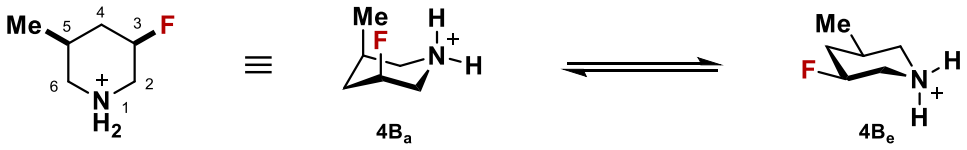
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	–1.2	–3.6	+6.7	–3.8	7.5	5.6	equatorial
gas phase	–1.7	–3.2	+5.9	–3.9	5.5	4.3	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-5-methylpiperidine hydrochloride (4B)**



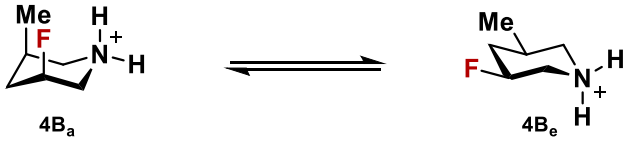
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: Due to peaks overlapping and broadening in NMR spectra, we could not verify the orientation of the fluorine atom through $^3J(F,H_a)$ values. Therefore additional NMR studies that includes NOE and HF/FH-HetNOE experiments were conducted.[1] All those experiments showed unequivocally that the fluorine atom adopts equatorial orientation.[1]

Computational observation

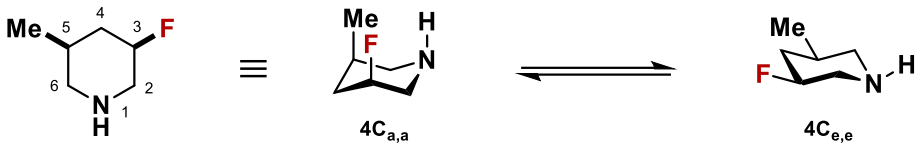
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	–0.4	+10.3	+6.6	–16.7	7.4	8.9	equatorial
gas phase	+2.9	+23.4	+2.4	–22.5	5.3	6.8	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-5-methylpiperidine (4C)**



The preparation of this compound is described in the previous section.

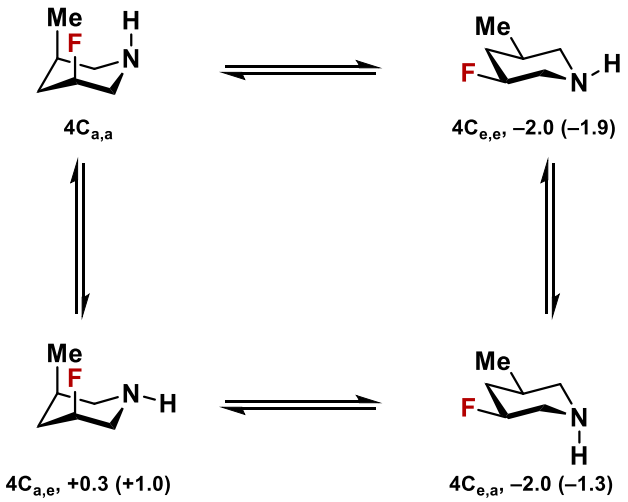
Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$. [^{3}***J*(2-H$_a$,3-F) = 5.7 Hz, ^{3}*J*(4-H$_a$,3-F) = 10.6 Hz**]

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.64 (dtt, *J* = 48.6, 10.0, 4.7 Hz, 1H), 3.24 – 3.19 (m, 1H), 2.85 (dt, *J* = 12.5, 4.1 Hz, 1H), 2.46 (ddd, *J* = 11.8, 10.0, 5.7 Hz, 1H), 2.25 – 2.17 (m, 1H), 2.08 (dd, *J* = 12.6, 10.8 Hz, 1H), 1.73 – 1.63 (m, 1H), 1.31 – 1.20 (m, 1H), 0.95 (dd, *J* = 6.7, 1.1 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.72 – 4.55 (m, 1H), 3.21 (dd, *J* = 11.6, 3.9 Hz, 1H), 2.85 (dd, *J* = 12.7, 4.1 Hz, 1H), 2.46 (dd, *J* = 12.0, 9.8 Hz, 1H), 2.24 – 2.19 (m, 1H), 2.08 (dd, *J* = 12.6, 10.8 Hz, 1H), 1.72 – 1.63 (m, 1H), 1.29 – 1.21 (m, 1H), 0.95 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 89.89 (d, *J* = 168.7 Hz), 51.18 (d, *J* = 1.8 Hz), 48.50 (d, *J* = 24.2 Hz), 38.73 (d, *J* = 16.1 Hz), 30.29 (d, *J* = 9.3 Hz), 18.09 (d, *J* = 1.1 Hz); **^{13}C{sel-^{19}F at -175 ppm} NMR** (151 MHz, D_2O, 299 K) δ 89.85, 51.16, 48.49, 38.72, 30.28, 18.07; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -175.97 (dd, *J* = 48.4, 4.7 Hz); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -175.97.

Computational observation

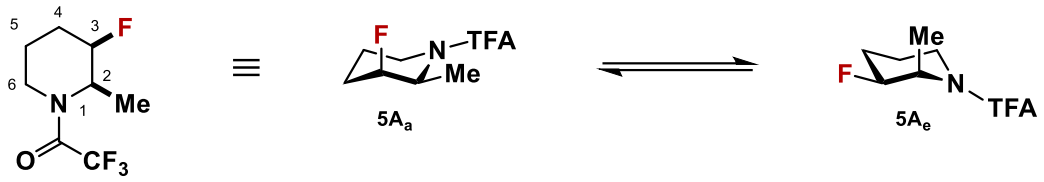
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	–2.0	+13.0	+7.2	–21.7	2.4	2.8	equatorial
gas phase	–1.9	+6.6	+7.1	–15.1	1.6	2.2	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-3-fluoro-2-methylpiperidin-1-yl)ethan-1-one (5A)



This compound was prepared following a recent literature procedure.[1]

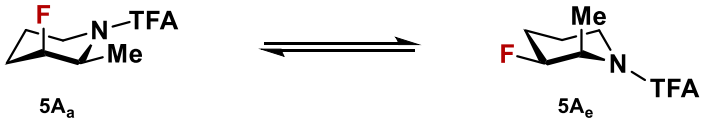
Experimental observation

The product was present as a ~1.5:1 mixture of amide bond rotamers.

In **$CDCl_3$**: Due to peaks overlapping and broadening in NMR spectra, we could not verify the orientation of the fluorine atom through $^3J(F,H_a)$ values. Therefore additional NMR studies that includes NOE and HF/FH-HetNOE experiments were conducted.[1] All those experiments showed unequivocally that the fluorine atom adopts equatorial orientation.[1]

Computational observation

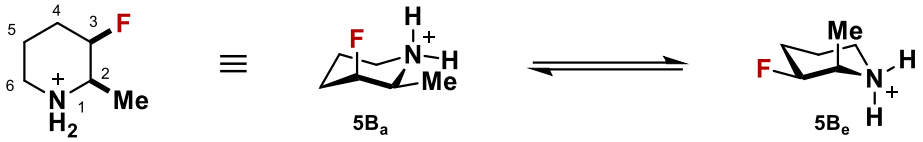
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	–3.7	–5.1	+3.8	–2.1	7.7	5.6	equatorial
gas phase	–4.3	–6.4	+5.1	–2.6	5.6	4.1	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-2-methylpiperidine hydrochloride (5B)**



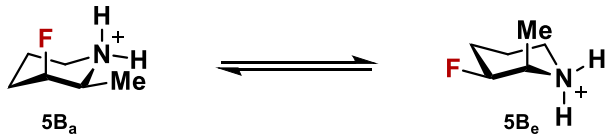
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [***^3J*(2-H_a,3-F) = 31.5 Hz, *^3J*(4-H_a,3-F) = 46.0 Hz**]

Computational observation

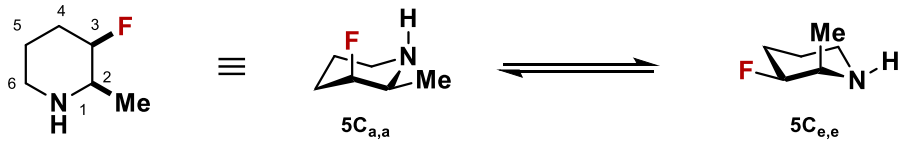
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+3.3	+10.2	+3.6	–10.5	6.3	8.7	axial
gas phase	+6.2	+15.1	–0.0	–8.8	4.5	6.6	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-2-methylpiperidine (5C)**



$5C_{a,a}$ $5C_{e,e}$

The preparation of this compound is described in the previous section.

Experimental observation

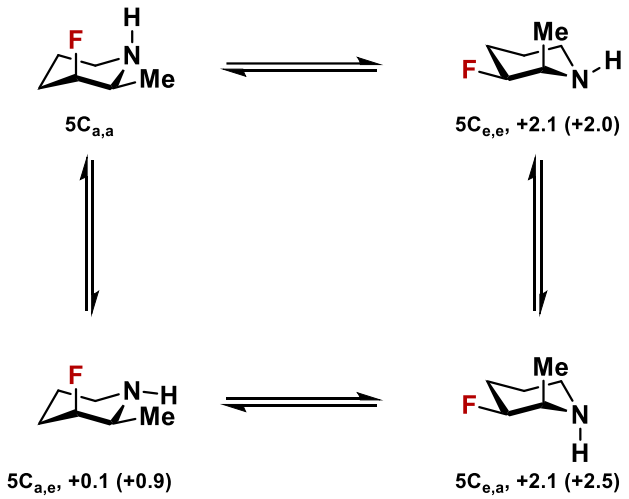
In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large value of $^3J(F,H_a)$. [^{3}***J*(2-H$_a$,3-F) = 32.3 Hz**]

NMR spectra contain traces of the corresponding piperidine carboxylic acid due to a fast reaction of the free amine with carbon dioxide.

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.61 (d, *J* = 49.8 Hz, 1H), 2.98 – 2.91 (m, 1H), 2.76 (dqd, *J* = 32.3, 6.8, 1.4 Hz, 1H), 2.63 – 2.56 (m, 1H), 2.12 – 2.04 (m, 1H), 1.76 – 1.60 (m, 2H), 1.50 – 1.44 (m, 1H), 1.10 (d, *J* = 6.8 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.61 (bs, 1H), 2.97 – 2.91 (m, 1H), 2.76 (q, *J* = 6.8 Hz, 1H), 2.59 (td, *J* = 12.5, 3.1 Hz, 1H), 2.12 – 2.05 (m, 1H), 1.76 – 1.60 (m, 2H), 1.49 – 1.44 (m, 1H), 1.10 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 91.28 (d, *J* = 166.0 Hz), 52.63 (d, *J* = 19.2 Hz), 44.49, 28.68 (d, *J* = 21.1 Hz), 19.29, 16.77 (d, *J* = 4.9 Hz); **^{13}C{sel-^{19}F at -201 ppm} NMR** (151 MHz, D_2O, 299 K) δ 91.27, 52.62, 44.48, 28.67, 19.27, 16.74; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -201.54; **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -201.54.

Computational observation

The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



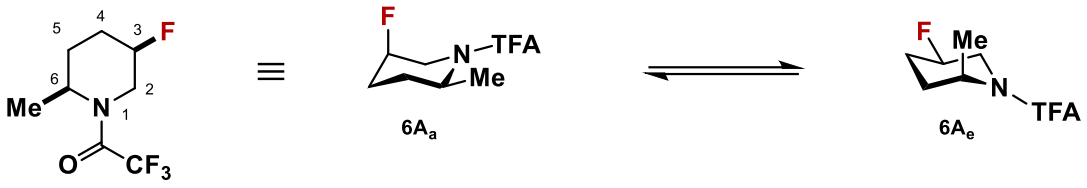
$5C_{a,a}$ **$5C_{e,e}$, +2.1 (+2.0)**

$5C_{a,e}$, +0.1 (+0.9) **$5C_{e,a}$, +2.1 (+2.5)**

Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+2.1	+18.4	+3.1	–19.6	2.4	2.8	axial
gas phase	+2.0	+11.8	+2.8	–12.8	1.6	2.0	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-5-fluoro-2-methylpiperidin-1-yl)ethan-1-one (6A)



This compound was prepared following a recent literature procedure.[1]

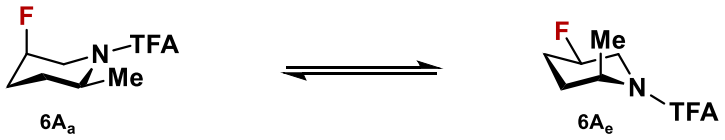
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$.[1] [**Rot A: ^3J(2-H_a,3-F) = 5.8 Hz, Rot B: ^3J(2-H_a,3-F) = 5.8 Hz**]

Computational observation

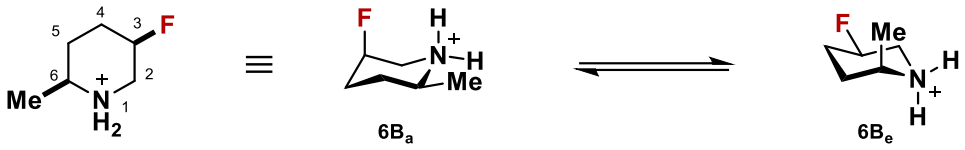
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	–3.3	+13.4	+1.1	–17.5	7.6	4.8	equatorial
gas phase	–3.7	+22.5	–0.6	–25.3	5.6	3.7	-

All values are given in kcal/mol at 298 K.

***cis*-5-Fluoro-2-methylpiperidine hydrochloride (6B)**



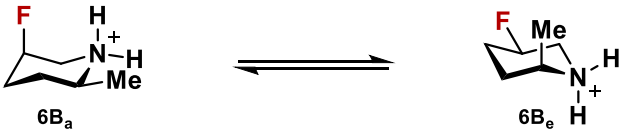
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large value of $^3J(F,H_a)$.[1] [^{3}***J*****(2-H$_a$,3-F) = 40.7 Hz**]

Computational observation

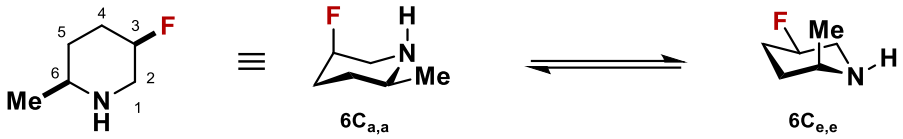
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+3.5	+11.2	+4.3	–11.9	5.9	8.3	axial
gas phase	+6.8	+22.2	+1.4	–16.8	4.3	6.3	-

All values are given in kcal/mol at 298 K.

***cis*-5-Fluoro-2-methylpiperidine (6C)**



The preparation of this compound is described in the previous section.

Experimental observation

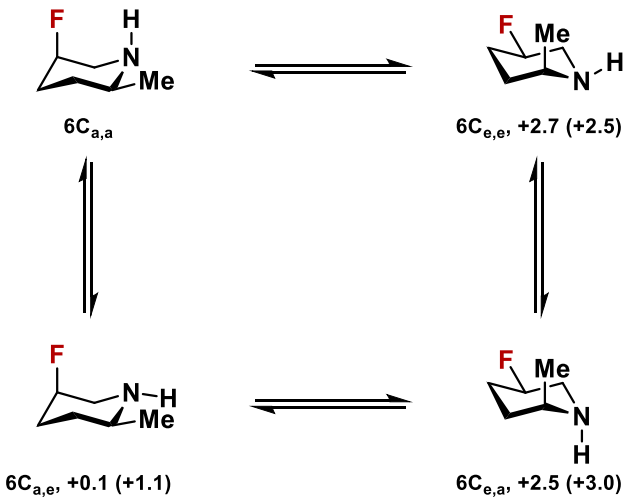
In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large values of ^3J(F,H_a). [***^3J*(2-H_a,3-F) = 43.3 Hz, *^3J*(4-H_a,3-F) = 48.1 Hz**]

NMR spectra contain traces of the corresponding piperidine carboxylic acid due to a fast reaction of the free amine with carbon dioxide.

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.76 (d, *J* = 47.7 Hz, 1H overlaps with solvent), 3.14 (ddt, *J* = 14.8, 12.3, 2.7 Hz, 1H), 2.75 (ddd, *J* = 43.3, 14.3, 1.5 Hz, 1H), 2.67 – 2.59 (m, 1H), 2.03 (ddt, *J* = 14.8, 11.5, 3.2 Hz, 1H), 1.68 (dtdd, *J* = 48.1, 14.8, 4.9, 2.3 Hz, 1H), 1.54 (ddt, *J* = 13.5, 5.1, 2.7 Hz, 1H), 1.36 (tdd, *J* = 13.5, 11.3, 4.1 Hz, 1H), 1.04 (d, *J* = 6.4 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.76 (s, 1H), 3.14 (d, *J* = 14.2 Hz, 1H), 2.81 – 2.70 (m, 1H), 2.63 (dtd, *J* = 12.7, 6.4, 2.7 Hz, 1H), 2.03 (dm, *J* = 14.6 Hz, 1H), 1.77 – 1.61 (m, 1H), 1.57 – 1.51 (m, 1H), 1.36 (tdd, *J* = 13.5, 11.3, 4.1 Hz, 1H), 1.04 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 87.77 (d, *J* = 163.3 Hz), 50.21, 48.32 (dm, *J* = 20.2 Hz), 28.22 (d, *J* = 20.9 Hz), 27.71, 21.19; **^{13}C{sel-^{19}F at -186 ppm} NMR** (151 MHz, D_2O, 299 K) δ 87.74, 50.20, 48.31, 28.21, 27.70, 21.14; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -186.43 (qt, *J* = 49.2, 12.2 Hz); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -186.43.

Computational observation

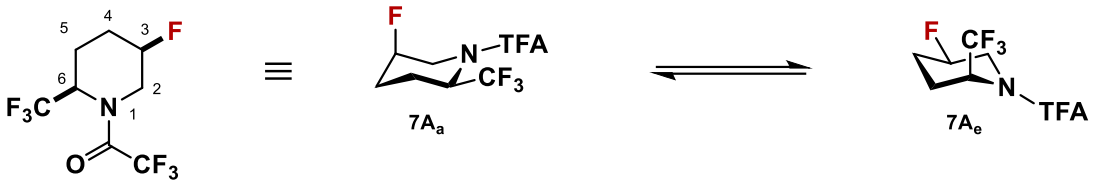
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE$_{elect}$	ΔE$_{hyperc}$	ΔE$_{steric}$	μ$_{a,a}$	μ$_{e,e}$	Experimental
H_2O	+2.7	+11.7	+4.0	–13.4	2.4	2.9	axial
gas phase	+2.5	+11.6	+4.3	–13.5	1.6	2.3	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-5-fluoro-2-(trifluoromethyl)piperidin-1-yl)ethan-1-one (7A)



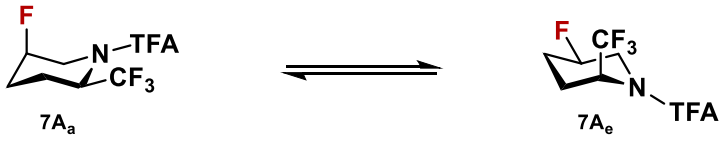
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$.[1] [^{3}***J*****(2-H$_a$,3-F) = 5.8 Hz**]

Computational observation

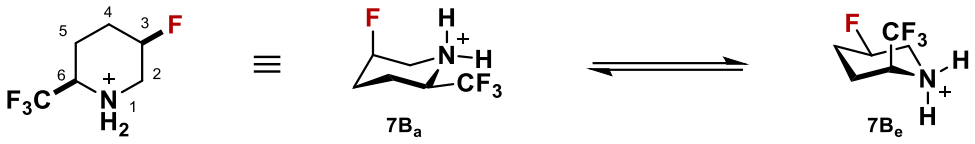
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	–4.4	+19.6	+1.6	–25.6	8.4	4.0	equatorial
gas phase	–6.0	+20.8	–0.4	–26.4	6.2	2.9	-

All values are given in kcal/mol at 298 K.

***cis*-5-Fluoro-2-(trifluoromethyl)piperidine hydrochloride (7B)**



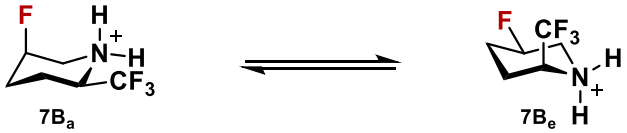
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**^3J(2-H_a,3-F) = 39.7 Hz, ^3J(4-H_a,3-F) = 45.0 Hz**]

Computational observation

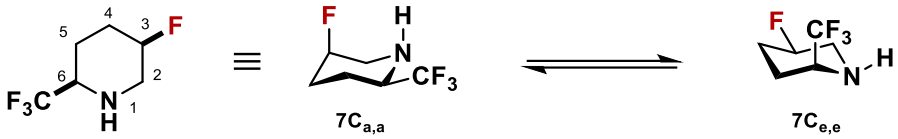
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+5.2	+19.5	+2.3	–17.3	7.7	9.4	axial
gas phase	+7.7	+27.6	–0.8	–19.2	6.3	7.0	-

All values are given in kcal/mol at 298 K.

***cis*-5-Fluoro-2-(trifluoromethyl)piperidine (7C)**



The preparation of this compound is described in the previous section.

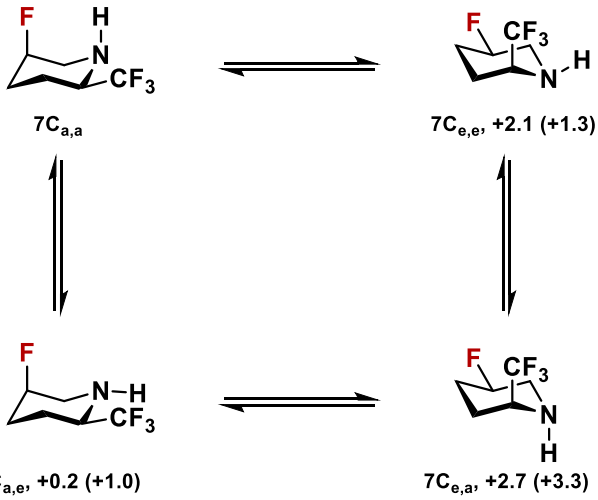
Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large value of $^{3}J(F,H_a)$. [^{3}***J*(2-H$_a$,3-F) = 41.9 Hz**]

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.82 (d, *J* = 45.0 Hz, 1H overlaps with solvent), 3.34 (ddt, *J* = 14.9, 10.3, 5.0 Hz, 1H), 3.27 (ddt, *J* = 14.6, 11.9, 2.7 Hz, 1H), 2.85 (dd, *J* = 41.9, 14.4 Hz, 1H), 2.23 – 2.15 (m, 1H), 1.86 – 1.69 (m, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.83 (bs, 1H), 3.39 – 3.31 (m, 1H), 3.27 (d, *J* = 14.4 Hz, 1H), 2.85 (dd, *J* = 14.4, 1.4 Hz, 1H), 2.22 – 2.17 (m, 1H), 1.84 – 1.73 (m, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 125.44 (q, *J* = 278.6 Hz), 86.51 (d, *J* = 166.2 Hz), 55.97 (q, *J* = 29.2 Hz), 47.63 (d, *J* = 20.2 Hz), 26.68 (d, *J* = 21.1 Hz), 18.65 (d, *J* = 1.7 Hz); **^{13}C{sel-^{19}F at -187 ppm} NMR** (151 MHz, D_2O, 299 K) δ 125.45 (q, *J* = 278.3 Hz), 86.50, 55.97 (q, *J* = 29.0 Hz), 47.64, 26.68, 18.65; **^{19}F NMR** (564 MHz, D_2O, 299 K) -77.19 (d, *J* = 7.2 Hz), -186.68 – -188.85 (m); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -77.19, -187.79.

Computational observation

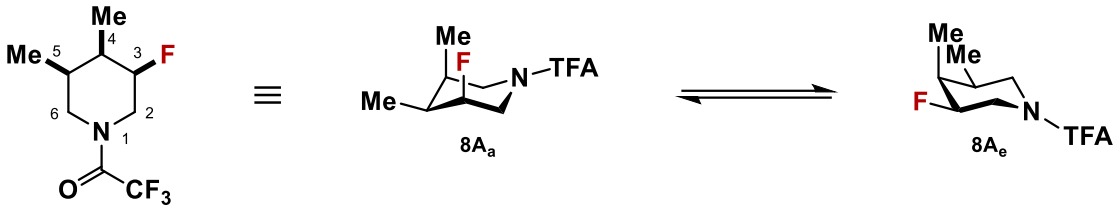
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+2.1	+32.5	–2.2	–28.4	4.7	2.8	axial
gas phase	+1.3	+30.7	–0.6	–29.0	3.4	2.1	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-3-fluoro-4,5-dimethylpiperidin-1-yl)ethan-1-one (8A)



This compound was prepared following a recent literature procedure.[1]

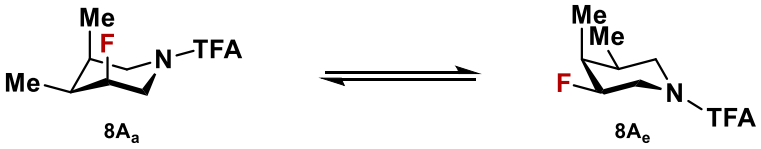
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**Rot A: ^3J(2-H$_a$,3-F) = 30.4 Hz, ^3J(4-H$_a$,3-F) = 27.0 Hz, Rot B: ^3J(2-H$_a$,3-F) = 30.4 Hz, ^3J(4-H$_a$,3-F) = 27.0 Hz**]

Computational observation

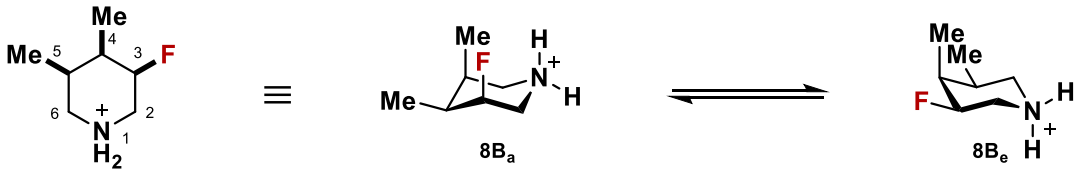
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+0.6	–0.3	+7.3	–6.2	7.4	5.8	axial
gas phase	+0.2	–3.6	+7.0	–3.1	5.4	4.8	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-4,5-dimethylpiperidine hydrochloride (8B)**



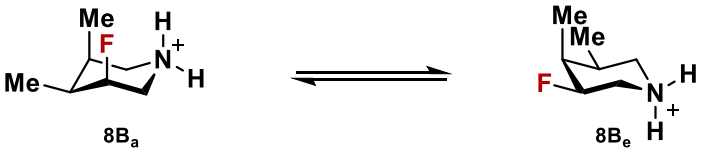
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large value of $^3J(F,H_a)$.[1] [^{3}***J*****(2-H$_a$,3-F) = 34.3 Hz**]

Computational observation

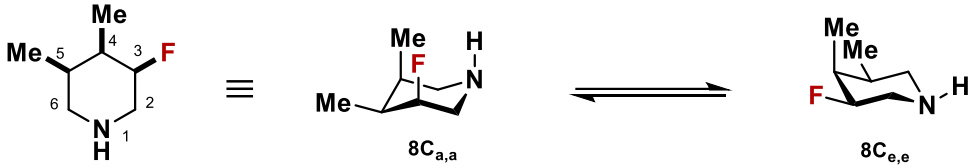
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+1.1	+17.0	+6.3	–21.8	8.5	9.6	axial
gas phase	+4.2	+24.5	+2.5	–22.7	6.0	7.1	-

All values are given in kcal/mol at 298 K.

***cis*-3-Fluoro-4,5-dimethylpiperidine (8C)**



The preparation of this compound is described in the previous section.

Experimental observation

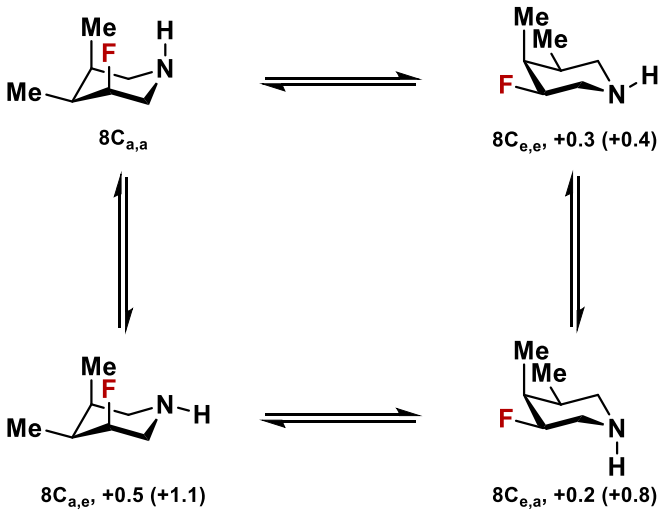
In **D_2O**: The dominant orientation of the fluorine atoms is assigned to be axial based on the values of ^{3}J(F,H$_a$). [***^{3}J*(2-H$_a$,3-F) = 26.0 Hz, *^{3}J*(4-H$_a$,3-F) = 26.3 Hz**]

NMR spectra contain mixture of diastereomers originated from the recently reported procedure (*d.r.* 95:5:0).[1] Only the signals of the major diastereomer are listed. The NMR spectra also contain traces of the corresponding piperidine carboxylic acid due to a fast reaction of the free amine with carbon dioxide.

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.64 (ddt, *J* = 48.0, 6.6, 3.4 Hz, 1H), 2.95 (ddd, *J* = 13.7, 9.4, 6.4 Hz, 1H), 2.79 (ddd, *J* = 26.0, 13.6, 3.3 Hz, 1H), 2.67 – 2.58 (m, 2H), 2.06 (dm, *J* = 26.3 Hz, 1H), 1.75 (ddp, *J* = 11.5, 7.1, 4.4, 3.6 Hz, 1H), 0.97 (d, *J* = 7.2 Hz, 3H), 0.95 (dd, *J* = 7.3, 1.8 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.64 (bs, 1H), 2.95 (dd, *J* = 13.5, 6.4 Hz, 1H), 2.78 (dd, *J* = 13.7, 3.2 Hz, 1H), 2.67 – 2.58 (m, 2H), 2.12 – 2.01 (m, 1H), 1.75 (ddt, *J* = 9.8, 7.0, 3.5 Hz, 1H), 0.97 (d, *J* = 7.2 Hz, 3H), 0.95 (d, *J* = 7.3 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 93.10 (d, *J* = 171.0 Hz), 48.08, 45.64 (dm, *J* = 20.5 Hz), 35.71 (d, *J* = 17.2 Hz), 32.27 (d, *J* = 1.9 Hz), 13.84 (d, *J* = 3.5 Hz), 9.86 (bs); **^{13}C{sel-^{19}F at -188 ppm} NMR** (151 MHz, D_2O, 299 K) δ 93.08, 48.07, 45.64, 35.70, 32.26, 13.83, 9.88; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -188.53 (bs); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -188.56 (bs).

Computational observation

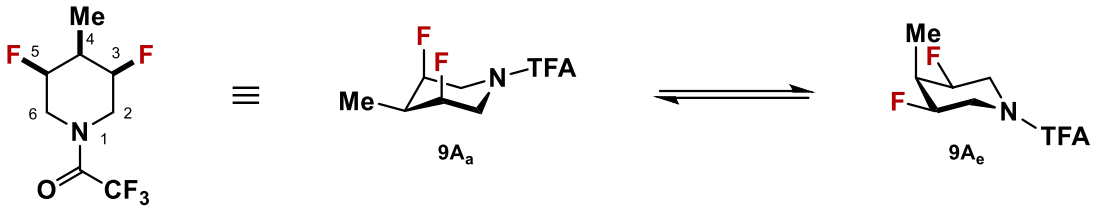
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+0.3	+20.1	+8.6	–28.4	2.4	2.8	axial
gas phase	+0.4	+17.6	+8.5	–25.8	1.6	2.1	-

All values are given in kcal/mol at 298 K.

1-(*cis*-3,5-Difluoro-4-methylpiperidin-1-yl)-2,2,2-trifluoroethan-1-one (9A)



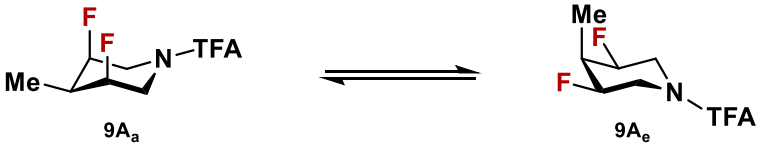
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**^3J(2-H_a,3-F) = 37.8 Hz, ^3J(4-H_a,3-F) = 34.9 Hz, ^3J(4-H_a,5-F) = 34.9 Hz, ^3J(6-H_a,5-F) = 35.6 Hz**]

Computational observation

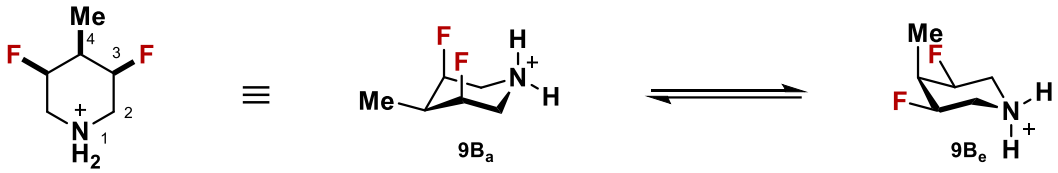
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+2.2	+8.1	+12.2	–18.2	8.7	3.4	axial
gas phase	+0.1	+5.0	+12.2	–17.4	6.3	2.6	-

All values are given in kcal/mol at 298 K.

***cis*-3,5-Difluoro-4-methylpiperidine hydrochloride (9B)**



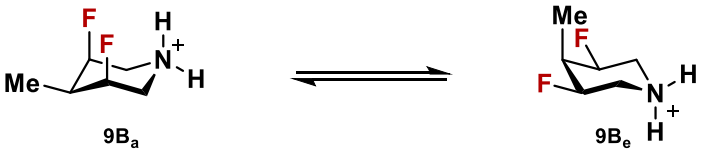
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [***^3J*(2-H_a,3-F) = 40.9 Hz, *^3J*(4-H_a,3-F) = 38.1 Hz**]

Computational observation

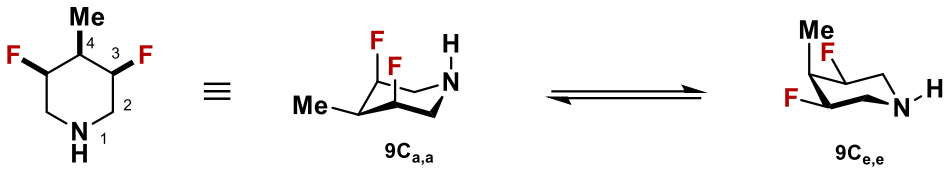
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+5.1	+11.5	+10.4	–16.3	10.0	10.6	axial
gas phase	+9.5	+21.8	+4.9	–17.1	7.2	8.0	-

All values are given in kcal/mol at 298 K.

***cis*-3,5-Difluoro-4-methylpiperidine (9C)**



The preparation of this compound is described in the previous section.

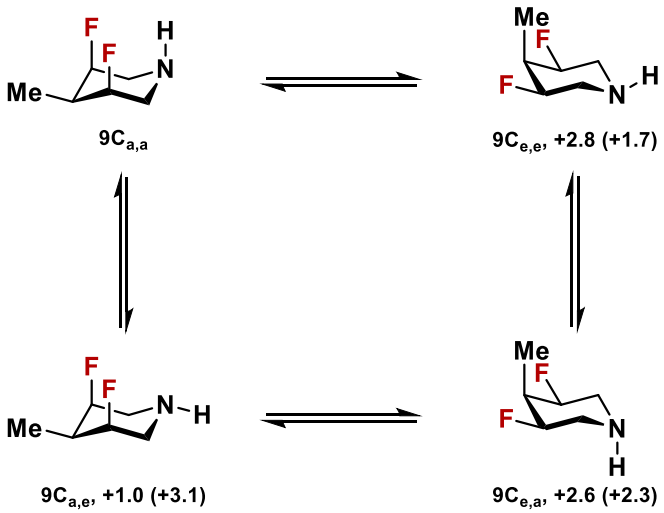
Experimental observation

In **D_2O**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^{3}J(F,H_a)$. [***^{3}J*(2-H_a,3-F) = 43.3 Hz, *^{3}J*(4-H_a,3-F) = 39.4 Hz**]

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.63 (dd, *J* = 47.9, 2.2 Hz, 2H), 3.24 (t, *J* = 13.5 Hz, 2H), 2.76 (dd, *J* = 43.3, 14.8 Hz, 2H), 1.95 (tm, *J* = 39.4 Hz, 1H), 1.16 (d, *J* = 7.2 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.64 – 4.61 (m, 2H), 3.24 (d, *J* = 14.9 Hz, 2H), 2.76 (d, *J* = 15.1 Hz, 2H), 1.98 – 1.91 (m, 1H), 1.16 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 90.65 (d, *J* = 173.3 Hz), 47.84 – 47.51 (m), 35.29 (t, *J* = 19.2 Hz), 12.48; **^{13}C{sel-^{19}F at -197 ppm} NMR** (151 MHz, D_2O, 299 K) δ 90.64, 47.69, 35.28, 12.46; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -196.89 – -197.33 (m); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -197.11.

Computational observation

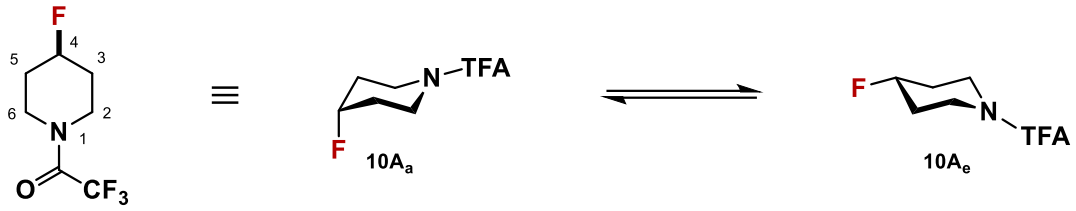
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	+2.8	+19.0	+12.0	–28.4	4.4	2.6	axial
gas phase	+1.7	+18.6	+12.8	–29.8	2.9	2.0	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(4-fluoropiperidin-1-yl)ethan-1-one (10A)



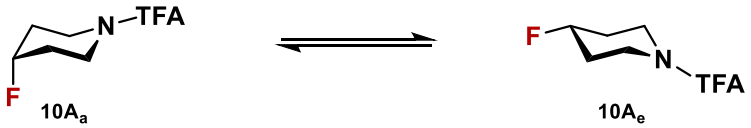
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [***^3J*(3-H_a,4-F) = 34.5 Hz, *^3J*(5-H_a,4-F) = 34.5 Hz**]

Computational observation

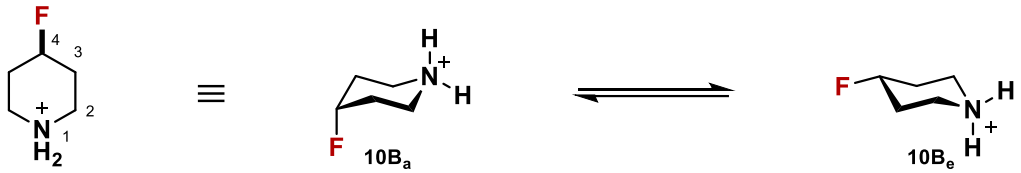
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+0.4	+6.7	+1.6	–8.1	5.0	4.9	axial
gas phase	+0.7	+9.6	+0.6	–9.5	3.9	3.7	-

All values are given in kcal/mol at 298 K.

4-Fluoropiperidine hydrochloride (10B)



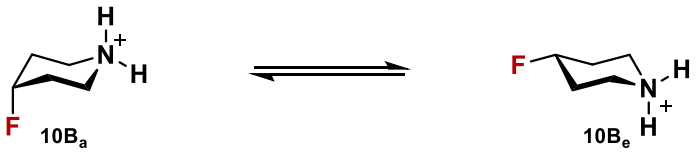
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: Due to peaks overlapping and broadening in NMR spectra, we could not verify the orientation of the fluorine atom through $^3J(F,H_a)$ values. Therefore additional NMR studies that includes NOE and HF/FH-HetNOE experiments were conducted.[1] All those experiments showed a dynamic behavior where the equilibrium favors equatorial fluorine orientation.[1]

Computational observation

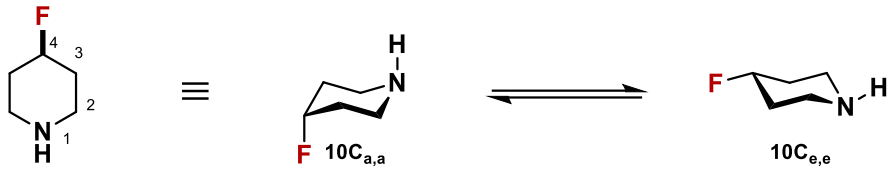
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+1.0	+12.4	2.5	–14.2	8.5	10.2	equatorial dominant
gas phase	+3.0	+21.5	–0.1	–18.2	6.4	8.0	-

All values are given in kcal/mol at 298 K.

4-Fluoropiperidine (10C)



The preparation of this compound is described in the previous section.

Experimental observation

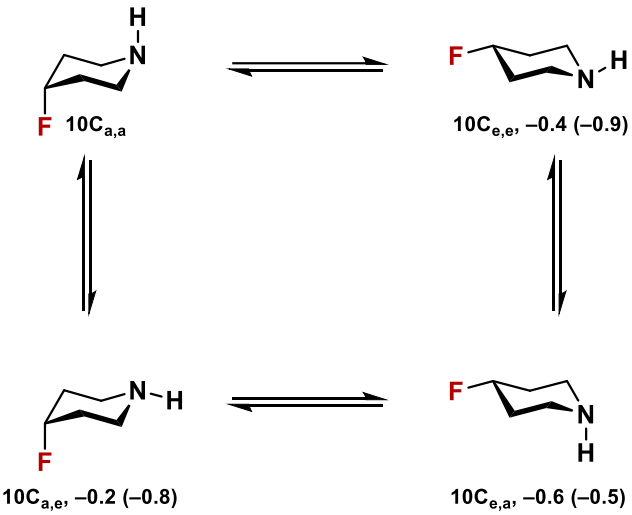
In **D_2O**: The orientation of the fluorine atom was assigned as equatorial due to the small value of $^{3}J(F,H_a)$. [***^{3}J*(3-H_a,4-F) = 10.6 Hz**]

The NMR spectra contain traces of defluorinated side-product, originated from the recently reported procedure,[1] which were inseparable from the product.

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.91 (dtt, *J* = 48.3, 7.3, 3.5 Hz, 1H), 3.08 (ddt, *J* = 11.7, 7.3, 3.4 Hz, 2H), 2.81 (ddd, *J* = 12.4, 7.5, 4.0 Hz, 2H), 1.99 (dddd, *J* = 25.5, 12.1, 8.2, 3.8 Hz, 2H), 1.81 (dddd, *J* = 21.1, 10.6, 7.4, 4.4 Hz, 2H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.90 (bs, 1H), 3.08 (ddd, *J* = 12.3, 8.0, 3.9 Hz, 2H), 2.81 (ddd, *J* = 12.4, 7.5, 4.0 Hz, 2H), 2.04 – 1.95 (m, 2H), 1.85 – 1.76 (m, 2H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 89.49 (d, *J* = 166.3 Hz), 41.13 (d, *J* = 6.6 Hz), 30.44 (d, *J* = 19.0 Hz); **^{13}C{sel-^{19}F at -176 ppm} NMR** (151 MHz, D_2O, 299 K) δ 89.50, 41.13, 30.44; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -176.16 (bs); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -176.16 (bs).

Computational observation

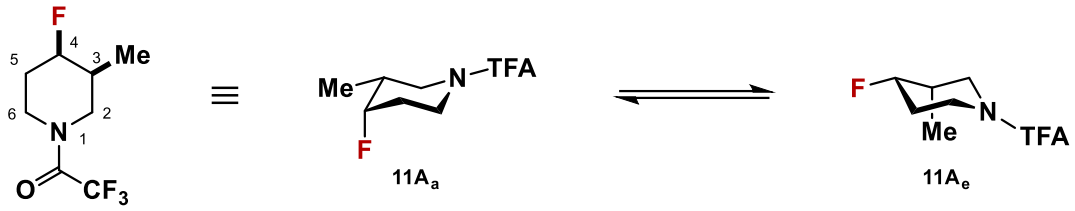
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	–0.4	+17.1	+2.8	–20.6	3.4	3.6	equatorial
gas phase	–0.9	+8.1	+1.9	–10.8	2.4	2.7	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-4-fluoro-3-methylpiperidin-1-yl)ethan-1-one (11A)



This compound was prepared following a recent literature procedure.[1]

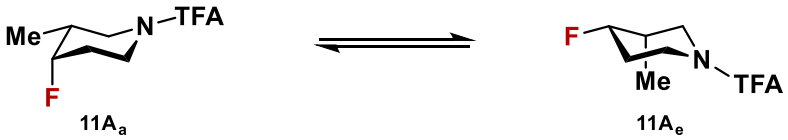
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**Rot A: ^3J(3-H$_a$,4-F) = 33.5 Hz, ^3J(5-H$_a$,4-F) = 41.2 Hz, Rot B: ^3J(3-H$_a$,4-F) = 33.5 Hz, ^3J(5-H$_a$,4-F) = 41.2 Hz**]

Computational observation

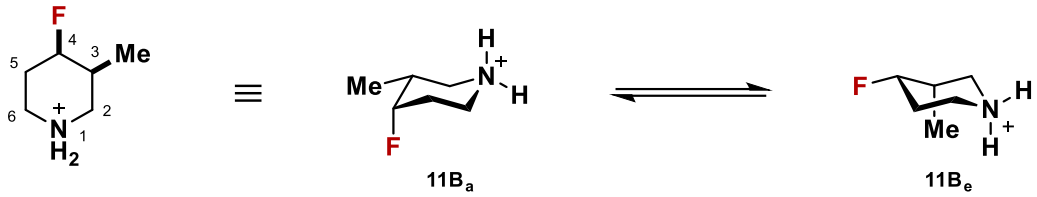
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+1.7	+4.2	+1.2	–4.4	5.0	4.7	axial
gas phase	+1.8	+0.7	+0.4	+0.2	3.9	3.4	-

All values are given in kcal/mol at 298 K.

***cis*-4-Fluoro-3-methylpiperidine hydrochloride (11B)**



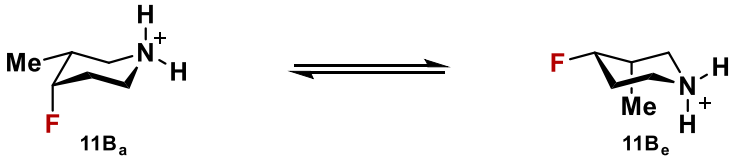
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [***^3J*(3-H_a,4-F) = 34.5 Hz, *^3J*(5-H_a,4-F) = 43.3 Hz**]

Computational observation

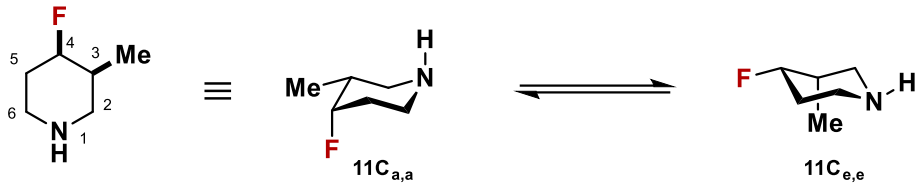
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	+2.3	+7.1	+0.8	–5.5	9.1	10.3	axial
gas phase	+3.9	+8.1	–1.6	–2.7	6.7	7.8	-

All values are given in kcal/mol at 298 K.

***cis*-4-Fluoro-3-methylpiperidine (11C)**



The preparation of this compound is described in the previous section.

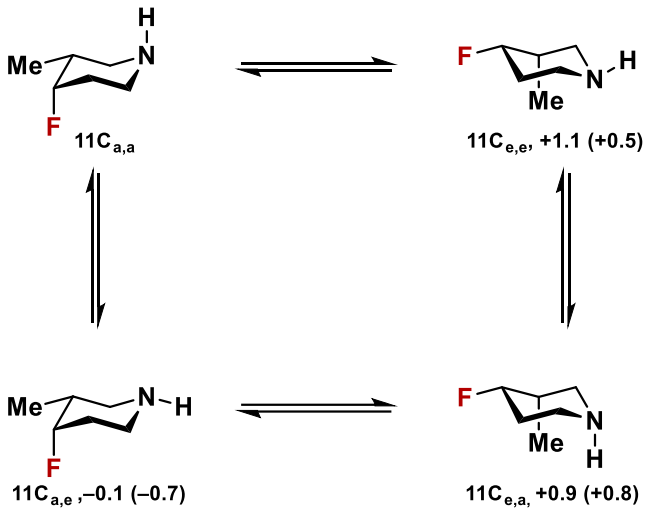
Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$. [^{3}***J*(3-H$_a$,4-F) = 35.6 Hz,** ^{3}***J*(5-H$_a$,4-F) = 43.0 Hz**]

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.85 (dm, *J* = 49.2 Hz, 1H), 2.79 – 2.72 (m, 3H), 2.55 (ddd, *J* = 12.6, 10.9, 1.6 Hz, 1H), 2.01 – 1.93 (m, 1H), 1.83 (dm, *J* = 35.6 Hz, 1H overlaps with 5-H$_a$), 1.72 (dm, *J* = 43.0 Hz, 1H overlaps with 3-H$_a$), 0.95 (d, *J* = 7.0 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.85 (bs, 1H), 2.79 – 2.72 (m, 3H), 2.55 (dd, *J* = 12.7, 11.0 Hz, 1H), 1.97 (dq, *J* = 14.6, 3.4 Hz, 1H), 1.87 – 1.79 (m, 1H), 1.77 – 1.68 (m, 1H), 0.95 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 92.99 (d, *J* = 166.5 Hz), 46.47 (d, *J* = 2.2 Hz), 39.25, 34.18 (d, *J* = 19.2 Hz), 30.12 (d, *J* = 20.2 Hz), 13.66 (d, *J* = 4.3 Hz); **^{13}C{sel-^{19}F at -198 ppm} NMR** (151 MHz, D_2O, 299 K) δ 92.99, 46.47, 39.25, 34.18, 30.12, 13.66; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -198.52 (bs); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -198.62 (bs).

Computational observation

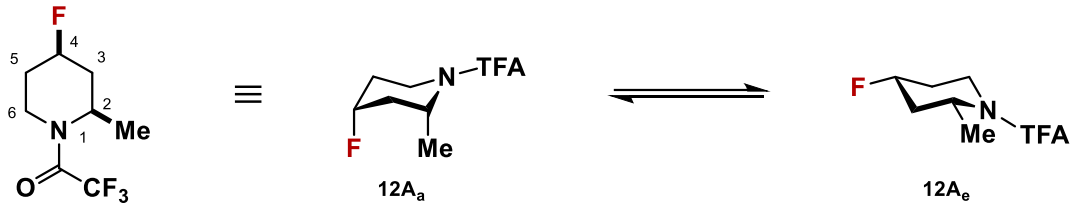
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE$_{elect}$	ΔE$_{hyperc}$	ΔE$_{steric}$	μ$_{a,a}$	μ$_{e,e}$	Experimental
H_2O	+1.1	–4.9	+2.8	+2.8	3.5	3.6	axial
gas phase	+0.5	+4.8	+2.1	–6.6	2.3	2.6	-

All values are given in kcal/mol at 298 K.

2,2,2-Trifluoro-1-(*cis*-4-fluoro-2-methylpiperidin-1-yl)ethan-1-one (12A)



This compound was prepared following a recent literature procedure.[1]

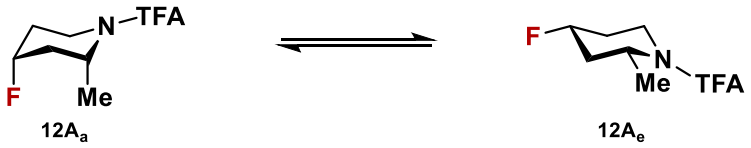
Experimental observation

The product was present as a ~1:1 mixture of amide bond rotamers.

In **$CDCl_3$**: The orientation of the fluorine atom was assigned as axial due to the large values of $^3J(F,H_a)$.[1] [**Rot A: ^3J(3-H$_a$,4-F) = 47.0 Hz, ^3J(5-H$_a$,4-F) = 44.0 Hz, Rot B: ^3J(3-H$_a$,4-F) = 47.0 Hz, ^3J(5-H$_a$,4-F) = 44.0 Hz**]

Computational observation

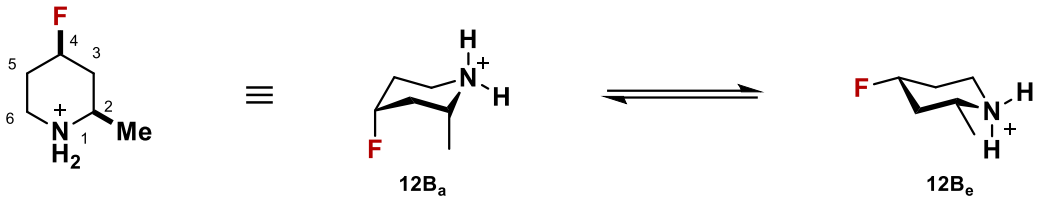
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
$CHCl_3$	+3.6	+11.8	+4.1	–12.4	5.1	5.4	axial
gas phase	+3.7	+15.2	+3.5	–15.1	4.0	3.9	-

All values are given in kcal/mol at 298 K.

***cis*-4-Fluoro-2-methylpiperidine hydrochloride (12B)**



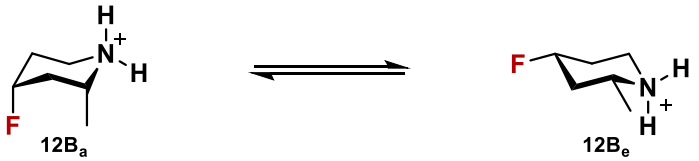
This compound was prepared following a recent literature procedure.[1]

Experimental observation

In **D_2O**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$.[1] [***^3J*(3-H_a,4-F) = 10.5 Hz, *^3J*(5-H_a,4-F) = 10.0 Hz**]

Computational observation

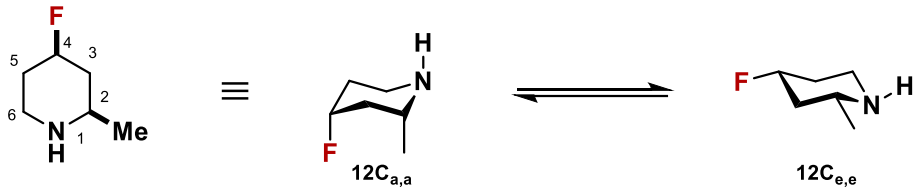
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
H_2O	–1.7	+4.7	+3.7	–9.6	8.4	9.2	equatorial
gas phase	+0.4	+15.5	+1.1	–15.8	6.1	7.1	-

All values are given in kcal/mol at 298 K.

***cis*-4-Fluoro-2-methylpiperidine (12C)**



The preparation of this compound is described in the previous section.

Experimental observation

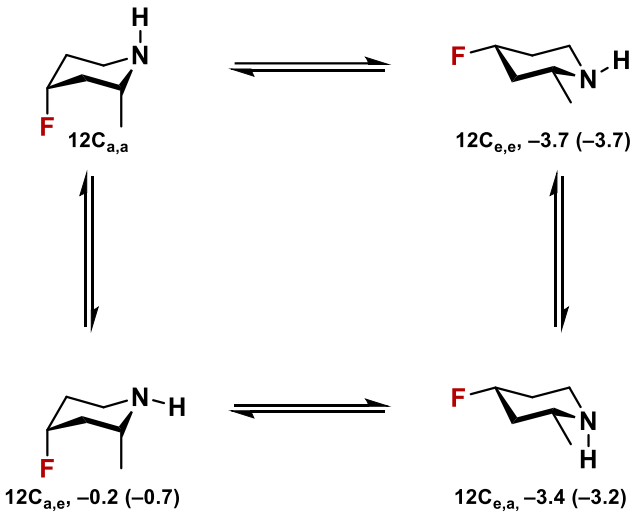
In **D_2O**: The orientation of the fluorine atom was assigned as equatorial due to the small values of $^3J(F,H_a)$. [^{3}***J*(3-H$_a$,4-F) = 11.5 Hz,** ^{3}***J*(5-H$_a$,4-F) = 10.1 Hz**]

NMR spectra contain mixture of diastereomers originated from the recently reported procedure (*d.r.* 92:8).[1] Only the signals of the major diastereomer are listed.

^{1}H NMR (600 MHz, D_2O, 299 K) δ 4.70 (dm, *J* = 49.1 Hz, 1H), 3.09 – 3.00 (m, 1H), 2.70 – 2.61 (m, 1H), 2.54 (tm, *J* = 12.8 Hz, 1H), 2.17 – 2.11 (m, 1H), 2.10 – 2.04 (m, 1H), 1.47 (dm, *J* = 10.1 Hz, 1H), 1.21 (dm, *J* = 11.5 Hz, 1H), 1.10 (d, *J* = 6.4 Hz, 3H); **^{1}H{^{19}F} NMR** (600 MHz, D_2O, 299 K) δ 4.70 (tt, *J* = 10.8, 5.0 Hz, 1H), 3.05 (ddd, *J* = 13.0, 4.8, 2.7 Hz, 1H), 2.65 (tdd, *J* = 12.7, 6.3, 2.4 Hz, 1H), 2.54 (td, *J* = 13.0, 2.7 Hz, 1H), 2.13 (ddt, *J* = 11.6, 4.7, 2.1 Hz, 1H), 2.07 (ddt, *J* = 11.7, 4.9, 2.4 Hz, 1H), 1.47 (qd, *J* = 12.0, 4.7 Hz, 1H), 1.21 (q, *J* = 11.4 Hz, 1H), 1.10 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (151 MHz, D_2O, 299 K) δ 92.02 (d, *J* = 167.0 Hz), 49.40 (d, *J* = 12.0 Hz), 42.32 (d, *J* = 12.7 Hz), 39.88 (d, *J* = 16.0 Hz), 31.64 (d, *J* = 17.1 Hz), 20.89 (d, *J* = 1.4 Hz); **^{13}C{sel-^{19}F at -166 ppm} NMR** (151 MHz, D_2O, 299 K) δ 92.02, 49.40, 42.32, 39.89, 31.64, 20.92; **^{19}F NMR** (564 MHz, D_2O, 299 K) δ -166.35 (dm, *J* = 50.0 Hz); **^{19}F{^{1}H} NMR** (564 MHz, D_2O, 299 K) δ -166.35.

Computational observation

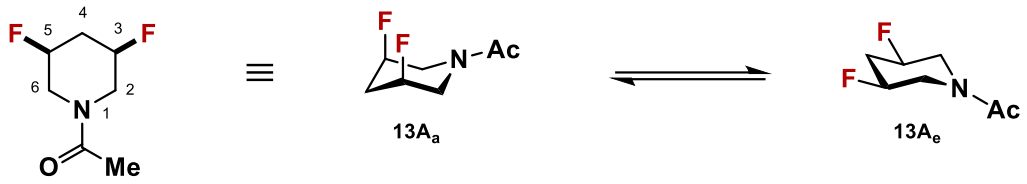
The calculated ΔG values in different solvents for the energetically lowest conformers are presented. In the scheme, the values of ΔG in water (ΔG gas phase) are given.



Solvent	ΔG(a,a→e,e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
H_2O	–3.7	+4.0	+3.8	–11.1	3.4	3.8	equatorial
gas phase	–3.7	+5.3	+2.4	–11.1	2.3	2.7	-

All values are given in kcal/mol at 298 K.

1-(*cis*-3,5-Difluoropiperidin-1-yl)ethan-1-one (13)



For this particular sample we conducted NMR experiments in different solvents in order to investigate the effect of solvent's dipole moment on the orientation of the fluorine atoms.

The preparation of this compound is described in the previous section.

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H$_a$,3-F) = 29.0 Hz, ^3J(6-H$_a$,5-F) = 29.9 Hz, ^3J(4-H$_a$,3-F) = 33.5 Hz, ^3J(4-H$_a$,5-F) = 33.5 Hz**]

^{1}H NMR (600 MHz, $CDCl_3$, 299 K) δ 4.71 (d, *J* = 46.5 Hz, 2H), 4.43 – 4.35 (m, 1H), 3.90 – 3.82 (m, 1H), 3.46 (dd, *J* = 29.0, 14.5 Hz, 1H), 3.27 (dd, *J* = 29.9, 14.3 Hz, 1H), 2.38 – 2.28 (m, 1H), 2.14 (s, 3H), 2.06 (tdt, *J* = 33.5, 15.0, 3.2 Hz, 1H overlaps with Me); **^{1}H{^{19}F} NMR** (600 MHz, $CDCl_3$, 299 K) δ 4.74 – 4.67 (m, 2H), 4.40 (dm, *J* = 14.2 Hz, 1H), 3.86 (dd, *J* = 14.4, 4.6 Hz, 1H), 3.46 (d, *J* = 14.5 Hz, 1H), 3.27 (d, *J* = 14.2 Hz, 1H), 2.33 (dm, *J* = 15.0 Hz, 1H), 2.14 (s, 3H), 2.07 (dt, *J* = 14.9, 3.2 Hz, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$, 299 K) δ 170.44, 84.52 (d, *J* = 178.2 Hz), 84.36 (d, *J* = 179.5 Hz), 49.83 (d, *J* = 23.4 Hz), 44.88 (d, *J* = 23.8 Hz), 34.44 (t, *J* = 20.9 Hz), 21.45; **^{13}C{sel-^{19}F at -183 ppm} NMR** (151 MHz, $CDCl_3$, 299 K) δ 170.44, 84.53, 84.37, 49.83, 44.88, 34.44, 21.45; **^{19}F NMR** (564 MHz, $CDCl_3$, 299 K) δ -182.77 – -183.32 (m); **^{19}F{^{1}H} NMR** (564 MHz, $CDCl_3$, 299 K) δ -182.99 (d, *J* = 11.1 Hz), -183.10 (d, *J* = 11.1 Hz).

ESI-MS: calculated $[C_7H_{11}NOF_2 + Na]^+$: 186.0701, found 186.0717.

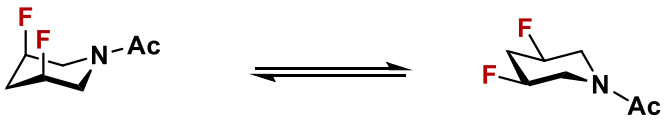
In **DMSO**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H$_a$,3-F) = 36.2 Hz, ^3J(6-H$_a$,5-F) = 37.5 Hz, ^3J(4-H$_a$,3-F) = 40.6 Hz, ^3J(4-H$_a$,5-F) = 40.6 Hz**]

^{1}H NMR (600 MHz, DMSO-d_6, 299 K) δ 4.81 (dm, *J* = 46.7 Hz, 1H), 4.76 (dm, *J* = 46.5 Hz, 1H), 4.44 (dddt, *J* = 14.4, 12.4, 3.8, 2.0 Hz, 1H), 3.96 (dddt, *J* = 15.0, 11.2, 3.8, 2.0 Hz, 1H), 3.42 (ddd,

J = 36.2, 14.9, 1.9 Hz, 1H), 3.01 (ddd, *J* = 37.5, 14.2, 2.1 Hz, 1H), 2.24 – 2.15 (m, 1H overlaps with 4-H_a), 2.07 (tdt, *J* = 40.6, 15.6, 3.3 Hz, 1H overlaps with 4-H_e and Me), 2.01 (s, 3H overlaps with 4-H_a); **$^1H\{^{19}F\}$ NMR** (600 MHz, DMSO-d_6, 299 K) δ 4.83 – 4.79 (m, 1H), 4.78 – 4.75 (m, 1H), 4.44 (ddt, *J* = 14.3, 3.8, 2.0 Hz, 1H), 3.96 (ddt, *J* = 14.9, 3.9, 2.0 Hz, 1H), 3.42 (dd, *J* = 14.8, 1.9 Hz, 1H), 3.01 (dd, *J* = 14.2, 2.0 Hz, 1H), 2.19 (dtt, *J* = 15.6, 3.5, 2.1 Hz, 1H), 2.07 (dt, *J* = 15.5, 3.4 Hz, 1H), 2.01 (s, 3H).

Computational observation

The calculated ΔG is given for the energetically lowest conformers.

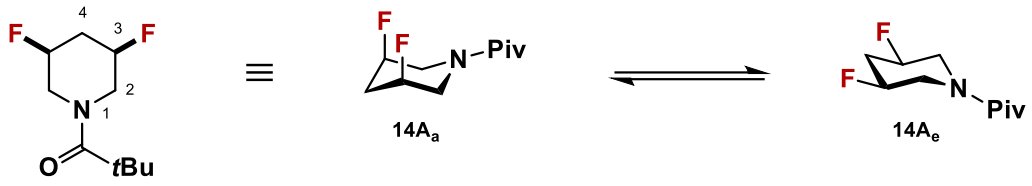


13A$_a$ **13A$_e$**

Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
DMSO	+1.1	+14.7	+10.4	–23.6	+8.9	+4.2	axial
$CHCl_3$	+0.4	+18.5	+9.7	–27.6	+8.1	+3.8	axial
gas phase	–1.6	+21.1	+8.6	–30.8	5.8	2.8	-

All values are given in kcal/mol at 298 K.

1-(*cis*-3,5-Difluoropiperidin-1-yl)-2,2-dimethylpropan-1-one (14)



For this particular sample we conducted NMR experiments in deuterated solvents in order to investigate the effect of solvent's dipole moment on the orientation of the fluorine atoms.

The preparation of this compound is described in the previous section.

Experimental observation

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as equatorial due to the small values of $^3J(F,H_a)$. [**^3J(2-H$_a$,3-F) = 7.3 Hz, ^3J(4-H$_a$,3-F) = 8.0 Hz**]

^{1}H NMR (500 MHz, $CDCl_3$, 299 K) δ 4.63 (ddq, *J* = 46.3, 7.0, 3.5 Hz, 2H), 3.86 (ddd, *J* = 20.7, 13.5, 3.4 Hz, 2H), 3.75 (dt, *J* = 14.1, 7.3 Hz, 2H), 2.42 – 2.24 (m, 1H), 2.15 (dm, *J* = 8.0 Hz, 1H), 1.31 (s, 9H); **^{1}H{^{19}F} NMR** (500 MHz, $CDCl_3$, 299 K) δ 4.63 (tt, *J* = 7.0, 3.8 Hz, 2H), 3.86 (dm, *J* = 13.6 Hz, 2H), 3.75 (dd, *J* = 13.7, 6.8 Hz, 2H), 2.32 (dt, *J* = 13.6, 4.1 Hz, 1H), 2.15 (dtt, *J* = 13.7, 6.9, 0.9 Hz, 1H), 1.31 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$, 299 K) δ 177.74, 84.41 (d, *J* = 180.2 Hz), 48.34 (d, *J* = 25.3 Hz), 39.15, 35.94 (t, *J* = 20.6 Hz), 28.62; **^{13}C{sel-^{19}F at -183 ppm} NMR** (126 MHz, $CDCl_3$, 299 K) δ 177.74, 84.43, 48.34, 39.15, 35.94, 28.62; **^{19}F NMR** (470 MHz, $CDCl_3$, 299 K) δ -182.32 – -183.44 (m); **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$, 299 K) δ -183.11.

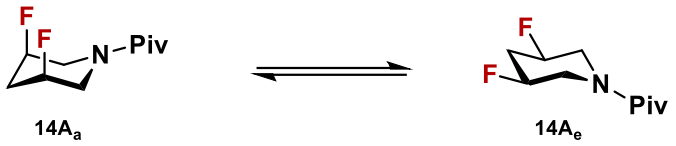
ESI-MS: calculated $[C_{10}H_{17}NOF_2 + Na]^+$: 228.1170, found 228.1184.

In **DMSO**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H$_a$,3-F) = 34.1 Hz, ^3J(4-H$_a$,3-F) = 38.5 Hz]**

^{1}H NMR (600 MHz, DMSO-d_6, 299 K) δ 4.79 (dqd, *J* = 46.6, 3.8, 1.9 Hz, 2H), 4.38 – 4.30 (m, 2H), 3.27 (dd, *J* = 34.1, 14.0 Hz, 2H), 2.19 – 2.15 (m, 1H overlaps with 4-H$_a$), 2.07 (tdt, *J* = 38.5, 15.3, 3.5 Hz, 1H overlaps with 4-H$_e$), 1.21 (s, 9H); **^{1}H{^{19}F} NMR** (600 MHz, DMSO-d_6, 299 K) δ 4.82 – 4.76 (m, 2H), 4.34 (dm, *J* = 14.9 Hz, 2H), 3.27 (d, *J* = 14.4 Hz, 2H), 2.17 (dtt, *J* = 15.2, 3.7, 1.8 Hz, 1H), 2.10 (dt, *J* = 15.3, 3.7 Hz, 1H), 1.21 (s, 9H).

Computational observation

The calculated ΔG is given for the energetically lowest conformers.

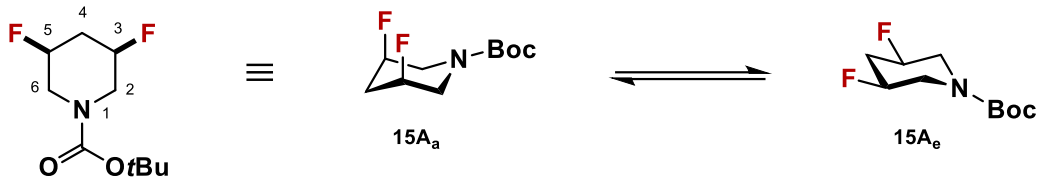


$14A_a$ $14A_e$

Solvent	$\Delta G(a \rightarrow e)$	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
DMSO	+0.5	+23.6	+11.6	–34.5	8.4	4.2	axial
$CHCl_3$	–1.0	+17.2	+11.8	–29.2	7.6	3.8	equatorial
gas phase	–2.3	+7.6	+13.4	–23.2	5.2	2.8	-

All values are given in kcal/mol at 298 K.

tert-Butyl _cis_-3,5-difluoropiperidine-1-carboxylate (15)



For this particular sample we conducted several computations and NMR experiments in different solvents in order to investigate the effect of solvent's dipole moment on the orientation of the fluorine atoms.

This compound was prepared following a recent literature procedure.[1]

Experimental observation

Broadening in NMR spectra was observed due to the dynamic behavior of the Boc group.

In **$CDCl_3$**: The orientation of the fluorine atoms was assigned as equatorial due to the small values of $^3J(F,H_a)$. [**^3J(4-H_a,3-F) = 12.5 Hz, ^3J(4-H_a,5-F) = 12.5 Hz**]

^{1}H NMR (600 MHz, $CDCl_3$, 299 K) δ 4.61 (d, *J* = 46.8 Hz, 2H), 3.71 – 3.54 (m, 4H), 2.21 (tdt, *J* = 25.2, 13.8, 4.1 Hz, 1H overlaps with 4-H_a), 2.12 (dm, *J* = 12.5 Hz, 1H overlaps with 4-H_e), 1.46 (s, 9H); **^{1}H{^{19}F} NMR** (600 MHz, $CDCl_3$, 299 K) δ 4.61 (s, 2H), 3.65 – 3.56 (m, 4H), 2.21 (dt, *J* = 13.9, 4.0 Hz, 1H), 2.12 (dt, *J* = 13.4, 6.6 Hz, 1H), 1.46 (s, 9H); **^{13}C NMR** (151 MHz, $CDCl_3$, 299 K) δ 154.99, 84.37 (d, *J* = 173.0 Hz), 80.75, 47.78 (bs), 46.70 (bs), 35.51 (t, *J* = 20.6 Hz), 28.42; **^{13}C{sel-^{19}F at -183 ppm} NMR** (151 MHz, $CDCl_3$, 299 K) δ 154.98, 84.37, 80.74, 47.69 (bs), 46.60 (bs), 35.51, 28.42; **^{19}F NMR** (564 MHz, $CDCl_3$, 299 K) δ -183.37 (bs); **^{19}F{^{1}H} NMR** (564 MHz, $CDCl_3$, 299 K) δ -183.36 (bs).

ESI-MS: calculated $[C_{10}H_{17}NO_2F_2 + Na]^+$: 244.1125, found 244.1125.

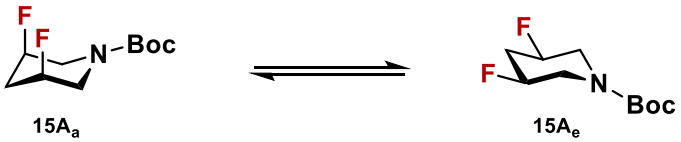
In **DMSO**: The orientation of the fluorine atoms was assigned as axial due to the large values of $^3J(F,H_a)$. [**^3J(2-H_a,3-F) = 33.8 Hz, ^3J(4-H_a,3-F) = 40.4 Hz, ^3J(4-H_a,5-F) = 40.4 Hz, ^3J(6-H_a,5-F) = 33.8 Hz**]

^{1}H NMR (600 MHz, DMSO-d_6, 299 K) δ 4.74 (d, *J* = 46.7 Hz, 2H), 4.04 (bs, 2H), 3.15 (tm, *J* = 33.8 Hz, 2H), 2.16 (ddddt, *J* = 15.9, 12.3, 10.2, 3.7, 1.7 Hz, 1H), 2.02 (tdt, *J* = 40.4, 15.5, 3.4 Hz,

1H), 1.40 (s, 9H); **^{1}H{^{19}F} NMR** (600 MHz, DMSO-d_6, 299 K) δ 4.74 (s, 2H), 4.04 (bs, 2H), 3.26 – 3.03 (m, 2H), 2.16 (dtt, J = 15.5, 3.8, 2.0 Hz, 1H), 2.02 (dt, J = 15.6, 3.5 Hz, 1H), 1.40 (s, 9H).

Computational observation

The calculated ΔG is given for the energetically lowest conformers.

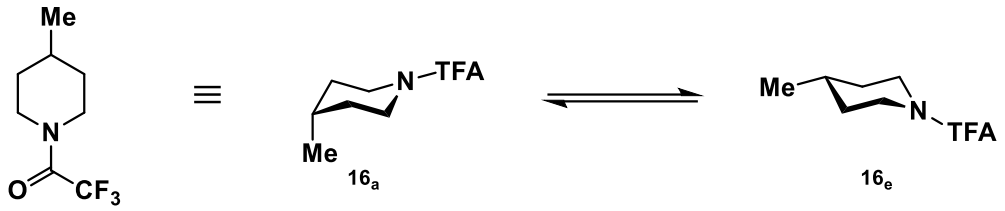


15A$_a$ **15A$_e$**

Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	μ_a	μ_e	Experimental
DMSO	+0.7	+30.4	+12.9	–42.5	6.5	3.3	axial
$CHCl_3$	–1.0	+30.0	+12.8	–42.7	5.9	3.1	equatorial
gas phase	–2.4	+36.9	+12.4	–51.3	4.2	2.4	-

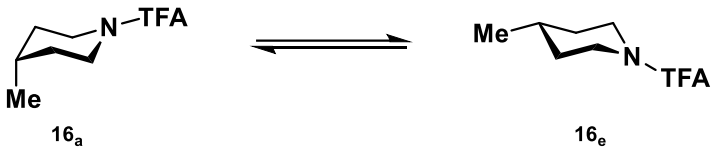
All values are given in kcal/mol at 298 K.

1-(4-Methylpiperidin-1-yl)-2,2,2-trifluoromethylethan-1-one (16)



Computational observation

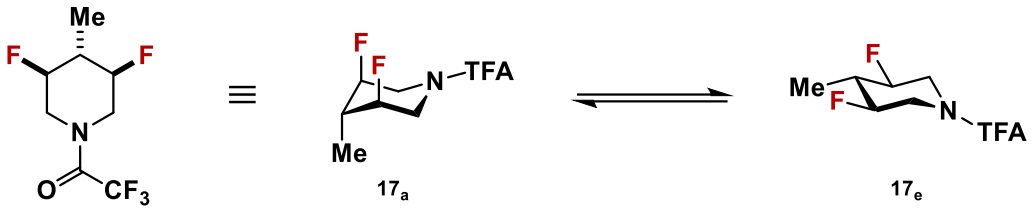
The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
DMSO	–2.0	+4.7	–0.9	–5.4	6.8	6.8	-
H_2O	–1.9	+4.7	–0.9	–5.4	6.8	6.8	-
CH_2Cl_2	–1.8	+4.3	–1.0	–5.0	6.5	6.5	-
$CHCl_3$	–1.9	+1.8	–0.9	–2.6	6.3	6.3	-
C_6H_6	–2.0	+3.8	–1.1	–4.5	5.8	5.8	-
gas phase	–2.0	+0.6	–1.1	–1.2	4.9	4.8	-

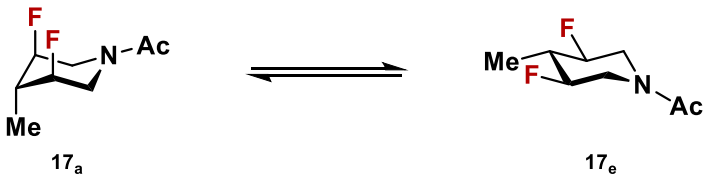
All values are given in kcal/mol at 298 K.

1-(*cis*-3,5-Difluoro-*trans*-4-methylpiperidin-1-yl)-2,2,2-trifluoromethylethan-1-one (17)



Computational observation

The calculated ΔG is given for the energetically lowest conformers.



Solvent	ΔG(a→e)	ΔE_{elect}	ΔE_{hyperc}	ΔE_{steric}	$\mu_{a,a}$	$\mu_{e,e}$	Experimental
DMSO	+0.5	+2.7	+9.1	–11.2	9.8	3.5	-
H_2O	+0.6	+2.7	+9.1	–11.3	9.9	3.5	-
CH_2Cl_2	–0.0	+0.6	+8.9	–9.4	9.5	3.4	-
$CHCl_3$	–0.4	+0.5	+8.8	–9.6	9.1	3.2	-
C_6H_6	–2.0	–0.7	+8.6	–9.1	8.2	2.9	-
gas phase	–2.9	+3.8	+8.6	–15.1	6.7	2.4	-

All values are given in kcal/mol at 298 K.

References

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Computational Data

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
1A_a	Gas Phase	-801.6259459	0.1689493	0.01133137	0.00094421	-0.04919698
1A_a	Toluene	-801.634133	0.16864346	0.01132307	0.00094421	-0.04913137
1A_e	Gas Phase	-801.6263801	0.16880073	0.01140211	0.00094421	-0.04938804
1A_e	Toluene	-801.6338477	0.16851314	0.01140735	0.00094421	-0.04938029
1B_a	Gas Phase	-351.530378	0.16835041	0.00624385	0.00094421	-0.03711602
1B_a	Water	-351.6326598	0.1682198	0.00631765	0.00094421	-0.03732519
1B_e	Gas Phase	-351.5221225	0.16801694	0.00635132	0.00094421	-0.03742287
1B_e	Water	-351.6295947	0.16811267	0.00635205	0.00094421	-0.03743271
1C_ae	Gas Phase	-351.1597787	0.15296809	0.00622141	0.00094421	-0.03708196
1C_ae	Water	-351.1704709	0.15269654	0.00619851	0.00094421	-0.03702969
1C_aa	Gas Phase	-351.1619248	0.15313089	0.00621352	0.00094421	-0.0370766
1C_aa	Water	-351.1708822	0.15271469	0.00624126	0.00094421	-0.03713985
1C_ee	Gas Phase	-351.1618747	0.15305333	0.00622065	0.00094421	-0.03710172
1C_ee	Water	-351.1706597	0.1526886	0.00621756	0.00094421	-0.03709072
1C_ea	Gas Phase	-351.1605979	0.1529366	0.00626151	0.00094421	-0.03719315
1C_ea	Water	-351.1703391	0.15271284	0.00626188	0.00094421	-0.03719523
2A_a	Gas Phase	-900.8816604	0.16101833	0.01211917	0.00094421	-0.05100981
2A_a	Benzene	-900.892217	0.16080437	0.01211744	0.00094421	-0.0509751
2A_a	Dichloromethane	-900.9003424	0.16047975	0.01129392	0.00094421	-0.04922862
2A_a	Chloroform	-900.8978157	0.16066426	0.01212913	0.00094421	-0.05099004
2A_a	DMSO	-900.9029415	0.16055378	0.01212662	0.00094421	-0.05096904
2A_a	Water	-900.9032053	0.16053968	0.01212936	0.00094421	-0.0509735
2A_e	Gas Phase	-900.8836352	0.16096724	0.01222411	0.00094421	-0.05132188
2A_e	Benzene	-900.8919635	0.16070132	0.0122501	0.00094421	-0.05139424
2A_e	Dichloromethane	-900.8977977	0.16060495	0.01222449	0.00094421	-0.05128684
2A_e	Chloroform	-900.8960406	0.1606235	0.0122435	0.00094421	-0.05134876
2A_e	DMSO	-900.8995407	0.16053115	0.01223756	0.00094421	-0.05131627
2A_e	Water	-900.8997162	0.16052755	0.01223589	0.00094421	-0.05131139

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
2C_ee	Gas Phase	-450.4222648	0.14542198	0.00696804	0.00094421	-0.03917046
2C_ee	Benzene	-450.4283847	0.14527285	0.00695724	0.00094421	-0.03913491
2C_ee	Dichloromethane	-450.432526	0.1451169	0.00698024	0.00094421	-0.03919794
2C_ee	Chloroform	-450.4313016	0.14517539	0.00697341	0.00094421	-0.03918554
2C_ee	DMSO	-450.4337225	0.14508166	0.0069824	0.00094421	-0.03919916
2C_ee	Water	-450.433842	0.14508354	0.00698135	0.00094421	-0.03919725
2C_ea	Gas Phase	-450.4209177	0.14523881	0.00703444	0.00094421	-0.03931768
2C_ea	Benzene	-450.4275901	0.14519336	0.0070261	0.00094421	-0.03930381
2C_ea	Dichloromethane	-450.4321603	0.14515023	0.00702779	0.00094421	-0.03930885
2C_ea	Chloroform	-450.4307934	0.1451697	0.00702407	0.00094421	-0.03929919
2C_ea	DMSO	-450.4335054	0.14521798	0.00701602	0.00094421	-0.0392816
2C_ea	Water	-450.4336407	0.14522606	0.00701737	0.00094421	-0.03928451
2C_ae	Gas Phase	-450.4167679	0.14513902	0.00697708	0.00094421	-0.03910142
2C_ae	Benzene	-450.4252986	0.14509296	0.00694825	0.00094421	-0.03903571
2C_ae	Dichloromethane	-450.4317693	0.14505474	0.00693099	0.00094421	-0.03899219
2C_ae	Chloroform	-450.42977	0.14506082	0.00693872	0.00094421	-0.03901428
2C_ae	DMSO	-450.4337855	0.14506134	0.0069274	0.00094421	-0.03898338
2C_ae	Water	-450.4339923	0.14507976	0.00692276	0.00094421	-0.03897331
2C_aa	Gas Phase	-450.4218862	0.14546089	0.00694339	0.00094421	-0.03906333
2C_aa	Benzene	-450.4287983	0.14529905	0.00695349	0.00094421	-0.03907755
2C_aa	Dichloromethane	-450.4336555	0.14519819	0.00695935	0.00094421	-0.03908468
2C_aa	Chloroform	-450.432188	0.14522116	0.00695957	0.00094421	-0.03908697
2C_aa	DMSO	-450.4351093	0.14516262	0.00696186	0.00094421	-0.03908754
2C_aa	Water	-450.435256	0.14515752	0.00696235	0.00094421	-0.03908844
3A_a	Gas Phase	-840.9398689	0.19700024	0.0128136	0.00094421	-0.05224187
3A_a	Chloroform	-840.9516605	0.19653986	0.01282299	0.00094421	-0.05222229
3A_e	Gas Phase	-840.9373161	0.19726744	0.01279345	0.00094421	-0.05222211
3A_e	Chloroform	-840.9481592	0.19676352	0.01281713	0.00094421	-0.05223844
3B_a	Gas Phase	-390.8453896	0.19638613	0.00769226	0.00094421	-0.04024415
3B_a	Water	-390.9460341	0.19626065	0.00774314	0.00094421	-0.04039481

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
3B_e	Gas Phase	-390.8354585	0.19641687	0.00770118	0.00094421	-0.04028583
3B_e	Water	-390.9406814	0.19661467	0.00767359	0.00094421	-0.04023764
3C_ae	Gas Phase	-390.473243	0.18102694	0.00766429	0.00094421	-0.04019317
3C_ae	Water	-390.4838329	0.18069321	0.00764032	0.00094421	-0.04013868
3C_aa	Gas Phase	-390.4756426	0.18122548	0.00764256	0.00094421	-0.04016537
3C_aa	Water	-390.4844915	0.18081529	0.00765648	0.00094421	-0.04019514
3C_ee	Gas Phase	-390.4726544	0.1814969	0.00759222	0.00094421	-0.04003724
3C_ee	Water	-390.4813313	0.1810497	0.00757865	0.00094421	-0.03999378
3C_ea	Gas Phase	-390.4715489	0.18140172	0.00761779	0.00094421	-0.04008927
3C_ea	Water	-390.4810823	0.18105404	0.00761586	0.00094421	-0.04008262
4A_a	Gas Phase	-840.9380827	0.19724179	0.01264227	0.00094421	-0.05166772
4A_a	Chloroform	-840.9499255	0.19678333	0.01263207	0.00094421	-0.05162098
4A_e	Gas Phase	-840.9399186	0.19683157	0.01289392	0.00094421	-0.05241024
4A_e	Chloroform	-840.9508543	0.19638561	0.0129133	0.00094421	-0.05243683
4B_a	Gas Phase	-390.8426546	0.19648425	0.00763904	0.00094421	-0.04013884
4B_a	Water	-390.9429668	0.196368	0.00766209	0.00094421	-0.04021186
4B_e	Gas Phase	-390.8373315	0.19610864	0.00778239	0.00094421	-0.04058233
4B_e	Water	-390.9430543	0.19614016	0.00779374	0.00094421	-0.04062399
4C_ae	Gas Phase	-390.4714529	0.18128362	0.00754708	0.00094421	-0.03992141
4C_ae	Water	-390.480976	0.18071351	0.00758811	0.00094421	-0.04002575
4C_aa	Gas Phase	-390.4731709	0.18141371	0.0075465	0.00094421	-0.03993877
4C_aa	Water	-390.4819939	0.18107617	0.00750854	0.00094421	-0.03983668
4C_ee	Gas Phase	-390.4755312	0.18104879	0.00765437	0.00094421	-0.04026993
4C_ee	Water	-390.4844743	0.18059586	0.00765259	0.00094421	-0.04026001
4C_ea	Gas Phase	-390.474424	0.18094129	0.00770719	0.00094421	-0.04039216
4C_ea	Water	-390.4843432	0.18061678	0.00770578	0.00094421	-0.04038857
5A_a	Gas Phase	-840.9331314	0.19744122	0.01254499	0.00094421	-0.05139452
5A_a	Chloroform	-840.9447066	0.19690447	0.01258967	0.00094421	-0.05148371
5A_e	Gas Phase	-840.9391887	0.19713343	0.01281675	0.00094421	-0.05212767
5A_e	Chloroform	-840.9500709	0.19671024	0.01279687	0.00094421	-0.05209453

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
5B_a	Gas Phase	-390.8499078	0.19629763	0.00767043	0.00094421	-0.04016662
5B_a	Water	-390.9473783	0.19621357	0.00775075	0.00094421	-0.04038723
5B_e	Gas Phase	-390.8400293	0.19632459	0.00768476	0.00094421	-0.04023
5B_e	Water	-390.9427392	0.19660802	0.00756538	0.00094421	-0.03994581
5C_ae	Gas Phase	-390.4756708	0.18101751	0.00763667	0.00094421	-0.04012766
5C_ae	Water	-390.485658	0.18059096	0.00763065	0.00094421	-0.04011088
5C_aa	Gas Phase	-390.4771249	0.18114373	0.00765618	0.00094421	-0.04018013
5C_aa	Water	-390.4858376	0.18066476	0.00766511	0.00094421	-0.04019251
5C_ee	Gas Phase	-390.4742597	0.18133165	0.00760285	0.00094421	-0.04003301
5C_ee	Water	-390.482848	0.18086963	0.007604	0.00094421	-0.04003428
5C_ea	Gas Phase	-390.4733895	0.18135162	0.00760698	0.00094421	-0.04005578
5C_ea	Water	-390.4828226	0.18094322	0.00761845	0.00094421	-0.04008603
6A_a	Gas Phase	-840.9338674	0.19712694	0.01257976	0.00094421	-0.05145692
6A_a	Chloroform	-840.9451703	0.19665764	0.01259902	0.00094421	-0.05148391
6A_e	Gas Phase	-840.93929	0.19707249	0.0128277	0.00094421	-0.05219499
6A_e	Chloroform	-840.9500191	0.19663466	0.01281918	0.00094421	-0.05214099
6B_a	Gas Phase	-390.8498803	0.19617696	0.00765589	0.00094421	-0.04018899
6B_a	Water	-390.9478147	0.19586991	0.0077484	0.00094421	-0.04043313
6B_e	Gas Phase	-390.8391004	0.19624634	0.00769377	0.00094421	-0.04029724
6B_e	Water	-390.9426872	0.19626881	0.00769224	0.00094421	-0.04030439
6C_ae	Gas Phase	-390.4758832	0.18091855	0.00762295	0.00094421	-0.04014556
6C_ae	Water	-390.4866601	0.18062266	0.00755101	0.00094421	-0.03996809
6C_aa	Gas Phase	-390.4777825	0.18104477	0.00762234	0.00094421	-0.04015211
6C_aa	Water	-390.4867059	0.18063117	0.00763115	0.00094421	-0.04017193
6C_ee	Gas Phase	-390.474037	0.18124917	0.00760484	0.00094421	-0.04009064
6C_ee	Water	-390.4827291	0.18082888	0.00759912	0.00094421	-0.04007788
6C_ea	Gas Phase	-390.4732172	0.18126088	0.00760814	0.00094421	-0.04011021
6C_ea	Water	-390.4830227	0.1808648	0.00762354	0.00094421	-0.04015494
7A_a	Gas Phase	-1138.728248	0.1741844	0.01455138	0.00094421	-0.05608935
7A_a	Chloroform	-1138.742016	0.17371648	0.01456243	0.00094421	-0.05609464

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
7A_e	Gas Phase	-1138.737738	0.17442237	0.01474117	0.00094421	-0.05662169
7A_e	Chloroform	-1138.748694	0.17381775	0.01480929	0.00094421	-0.05676251
7B_a	Gas Phase	-688.6338359	0.17345359	0.00957155	0.00094421	-0.0452195
7B_a	Water	-688.7390937	0.17305183	0.00977784	0.00094421	-0.04577268
7B_e	Gas Phase	-688.6215475	0.17339225	0.00959307	0.00094421	-0.04514972
7B_e	Water	-688.7320217	0.17380057	0.0095458	0.00094421	-0.04507791
7C_ae	Gas Phase	-688.2796547	0.1585795	0.00951651	0.00094421	-0.04513425
7C_ae	Water	-688.2929145	0.1581745	0.00951731	0.00094421	-0.04512443
7C_aa	Gas Phase	-688.2813934	0.15868262	0.00949823	0.00094421	-0.04510205
7C_aa	Water	-688.2931305	0.15815529	0.009526	0.00094421	-0.04515787
7C_ee	Gas Phase	-688.279636	0.15889365	0.00950529	0.00094421	-0.04498004
7C_ee	Water	-688.2899473	0.15823823	0.00954003	0.00094421	-0.0450408
7C_ea	Gas Phase	-688.2762702	0.15869289	0.00955005	0.00094421	-0.04505896
7C_ea	Water	-688.2891518	0.15828512	0.00954313	0.00094421	-0.04504776
8A_a	Gas Phase	-880.2507371	0.22539288	0.01411982	0.00094421	-0.05460079
8A_a	Chloroform	-880.2623052	0.22488707	0.01412995	0.00094421	-0.05462755
8A_e	Gas Phase	-880.2502769	0.22545207	0.01420171	0.00094421	-0.0549507
8A_e	Chloroform	-880.2610386	0.22490327	0.01422352	0.00094421	-0.05497025
8B_a	Gas Phase	-430.1567416	0.22480191	0.0089966	0.00094421	-0.04294869
8B_a	Water	-430.2552905	0.22463158	0.00906713	0.00094421	-0.04313992
8B_e	Gas Phase	-430.149895	0.22473285	0.00904227	0.00094421	-0.04309384
8B_e	Water	-430.2535374	0.22474703	0.00907088	0.00094421	-0.04318461
8C_ae	Gas Phase	-429.7840955	0.20952604	0.00894273	0.00094421	-0.04281757
8C_ae	Water	-429.7935556	0.20901332	0.00897776	0.00094421	-0.04290965
8C_aa	Gas Phase	-429.7859444	0.20969246	0.00892838	0.00094421	-0.04281282
8C_aa	Water	-429.7945978	0.20920188	0.00894512	0.00094421	-0.04284581
8C_ee	Gas Phase	-429.7853935	0.20972313	0.00893673	0.00094421	-0.04284051
8C_ee	Water	-429.7941218	0.20920212	0.00894845	0.00094421	-0.04287023
8C_ea	Gas Phase	-429.7845618	0.20966686	0.00895802	0.00094421	-0.04288716
8C_ea	Water	-429.7942459	0.20922986	0.00898115	0.00094421	-0.04294813

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
9A_a	Gas Phase	-940.1948588	0.18916859	0.01366254	0.00094421	-0.0541192
9A_a	Chloroform	-940.2104416	0.18883027	0.01363615	0.00094421	-0.05401677
9A_e	Gas Phase	-940.1950964	0.18950613	0.01361881	0.00094421	-0.05405058
9A_e	Chloroform	-940.2069659	0.18897225	0.01366124	0.00094421	-0.0541473
9B_a	Gas Phase	-490.0979344	0.18856093	0.00844122	0.00094421	-0.04214427
9B_a	Water	-490.2039846	0.18870557	0.00849228	0.00094421	-0.04227794
9B_e	Gas Phase	-490.0826093	0.18850663	0.0085208	0.00094421	-0.04238395
9B_e	Water	-490.1957649	0.18866672	0.00854106	0.00094421	-0.04245688
9C_ae	Gas Phase	-489.7300861	0.17331171	0.00844661	0.00094421	-0.04215687
9C_ae	Water	-489.7466928	0.1731928	0.00836933	0.00094421	-0.04196661
9C_aa	Gas Phase	-489.735469	0.17365755	0.00839375	0.00094421	-0.04208115
9C_aa	Water	-489.7482402	0.17330843	0.00841727	0.00094421	-0.04212243
9C_ee	Gas Phase	-489.7330015	0.17391362	0.00836761	0.00094421	-0.04202201
9C_ee	Water	-489.7439577	0.17342684	0.00839712	0.00094421	-0.04208546
9C_ea	Gas Phase	-489.7319796	0.1737738	0.0084125	0.00094421	-0.04211834
9C_ea	Water	-489.7441242	0.17341379	0.00845053	0.00094421	-0.04222066
10A_a	Gas Phase	-801.6284032	0.16896879	0.01137663	0.00094421	-0.04946828
10A_a	Chloroform	-801.6395066	0.16850184	0.01137936	0.00094421	-0.0494352
10A_e	Gas Phase	-801.6273874	0.16887529	0.01133477	0.00094421	-0.04927865
10A_e	Chloroform	-801.6390035	0.16851712	0.01135683	0.00094421	-0.04930666
10B_a	Gas Phase	-351.5301748	0.16823669	0.00627341	0.00094421	-0.03719035
10B_a	Water	-351.6347746	0.16811316	0.00637208	0.00094421	-0.03749039
10B_e	Gas Phase	-351.5250141	0.16804432	0.00632918	0.00094421	-0.03737591
10B_e	Water	-351.6334149	0.16823859	0.00629825	0.00094421	-0.0373068
10C_ae	Gas Phase	-351.1625006	0.15325032	0.0061813	0.00094421	-0.03700131
10C_ae	Water	-351.1713795	0.15276061	0.00618994	0.00094421	-0.03701612
10C_aa	Gas Phase	-351.1610358	0.15307855	0.00620771	0.00094421	-0.03705125
10C_aa	Water	-351.1708619	0.15269659	0.006236	0.00094421	-0.03712181
10C_ee	Gas Phase	-351.1623525	0.15304856	0.00621035	0.00094421	-0.03709128
10C_ee	Water	-351.1714528	0.15271887	0.00620835	0.00094421	-0.03708517

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
10C_ea	Gas Phase	-351.1617011	0.15298624	0.00623675	0.00094421	-0.0371581
10C_ea	Water	-351.1718592	0.1527355	0.00624111	0.00094421	-0.03716634
11A_a	Gas Phase	-840.9422407	0.19702256	0.01289005	0.00094421	-0.05248776
11A_a	Chloroform	-840.9530003	0.19638325	0.01295953	0.00094421	-0.05259982
11A_e	Gas Phase	-840.9401224	0.19729802	0.01269629	0.00094421	-0.05183244
11A_e	Chloroform	-840.9514582	0.19705445	0.01268718	0.00094421	-0.05179894
11B_a	Gas Phase	-390.8455476	0.19638472	0.00772018	0.00094421	-0.04030837
11B_a	Water	-390.947998	0.19640458	0.00773805	0.00094421	-0.04037977
11B_e	Gas Phase	-390.8394488	0.19644097	0.00768542	0.00094421	-0.04026069
11B_e	Water	-390.9445031	0.19652299	0.00772373	0.00094421	-0.04037976
11C_ae	Gas Phase	-390.4758974	0.18130604	0.00763625	0.00094421	-0.04013822
11C_ae	Water	-390.4846589	0.18076428	0.00764669	0.00094421	-0.04015891
11C_aa	Gas Phase	-390.4746895	0.18117078	0.00766404	0.00094421	-0.04019458
11C_aa	Water	-390.484392	0.18072055	0.00769225	0.00094421	-0.04026321
11C_ee	Gas Phase	-390.4742425	0.18137817	0.00759151	0.00094421	-0.04003891
11C_ee	Water	-390.4829239	0.18084404	0.00761397	0.00094421	-0.04008927
11C_ea	Gas Phase	-390.4736172	0.18140477	0.00759064	0.00094421	-0.04003769
11C_ea	Water	-390.4833872	0.1810943	0.00759572	0.00094421	-0.04005261
12A_a	Gas Phase	-840.9408223	0.19724261	0.01275249	0.00094421	-0.05207009
12A_a	Chloroform	-840.9516784	0.19671955	0.0127605	0.00094421	-0.05210527
12A_e	Gas Phase	-840.9351937	0.19721311	0.01260137	0.00094421	-0.05161401
12A_e	Chloroform	-840.9461902	0.19679629	0.01264337	0.00094421	-0.05177724
12B_a	Gas Phase	-390.8460162	0.1964402	0.00761188	0.00094421	-0.0400317
12B_a	Water	-390.9464266	0.19640999	0.00763112	0.00094421	-0.04010392
12B_e	Gas Phase	-390.8445704	0.19589943	0.00776609	0.00094421	-0.04053595
12B_e	Water	-390.9484908	0.19602502	0.00771969	0.00094421	-0.04040068
12C_ae	Gas Phase	-390.4741778	0.18142212	0.00754636	0.00094421	-0.03990905
12C_ae	Water	-390.4828002	0.18093447	0.00755173	0.00094421	-0.03992208
12C_aa	Gas Phase	-390.4729092	0.18134933	0.00755644	0.00094421	-0.03993927
12C_aa	Water	-390.4825491	0.18095488	0.00755639	0.00094421	-0.03994456

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
12C_ee	Gas Phase	-390.478286	0.18098152	0.00762949	0.00094421	-0.04022217
12C_ee	Water	-390.487877	0.18054816	0.0076358	0.00094421	-0.04023338
12C_ea	Gas Phase	-390.4773269	0.180909	0.00765765	0.00094421	-0.04029172
12C_ea	Water	-390.4873876	0.18060441	0.00765247	0.00094421	-0.04027854
13_e	Gas Phase	-603.0972636	0.1835471	0.01033272	0.00094421	-0.04693444
13_e	Chloroform	-603.1117176	0.18336318	0.01030775	0.00094421	-0.04681252
13_e	DMSO	-603.1159209	0.18333834	0.01028599	0.00094421	-0.04672462
13_a	Gas Phase	-603.0955554	0.18373162	0.01012498	0.00094421	-0.04614494
13_a	Chloroform	-603.1128621	0.18346349	0.01018112	0.00094421	-0.04629832
13_a	DMSO	-603.1182766	0.18349889	0.01009694	0.00094421	-0.04607357
14_a	Gas Phase	-721.0227066	0.26909697	0.0141355	0.00094421	-0.05425624
14_a	Chloroform	-721.0386691	0.26890454	0.01401152	0.00094421	-0.05391373
14_a	DMSO	-721.043748	0.26864042	0.01410023	0.00094421	-0.05408482
14_e	Gas Phase	-721.0261475	0.26900742	0.01424383	0.00094421	-0.05457529
14_e	Chloroform	-721.0389444	0.26838451	0.01440748	0.00094421	-0.05514869
14_e	DMSO	-721.0427078	0.26816454	0.01356182	0.00094421	-0.05320403
15_e	Gas Phase	-796.2833106	0.2733248	0.01528841	0.00094421	-0.05702432
15_e	Chloroform	-796.2947864	0.27247927	0.0154523	0.00094421	-0.05765734
15_e	DMSO	-796.2980458	0.27220275	0.01458901	0.00094421	-0.05553863
15_a	Gas Phase	-796.2803916	0.27360263	0.01500503	0.00094421	-0.05612973
15_a	Chloroform	-796.294654	0.2729218	0.01508514	0.00094421	-0.05634949
15_a	DMSO	-796.2990611	0.27267934	0.01516926	0.00094421	-0.05663547

Comp. No.	Solvent	Electronic Energy [E_h]	ZPVE [E_h]	Thermal Correction [E_h]	Enthalpy Correction [E_h]	Entropy Correction [E_h]
16_a	Gas Phase	-741.6777787	0.20495266	0.01195644	0.00094421	-0.05024991
16_a	Benzene	-741.6837267	0.20467546	0.01192003	0.00094421	-0.05013012
16_a	Dichloromethane	-741.6881253	0.20427648	0.01200668	0.00094421	-0.05032388
16_a	Chloroform	-741.6867806	0.20442826	0.01196373	0.00094421	-0.05021864
16_a	DMSO	-741.68948	0.20430079	0.01194774	0.00094421	-0.0501768
16_a	Water	-741.6896129	0.20424224	0.01194608	0.00094421	-0.05017117
16_e	Gas Phase	-741.6804458	0.20459883	0.01202547	0.00094421	-0.05043681
16_e	Benzene	-741.686371	0.20426839	0.01201741	0.00094421	-0.05038409
16_e	Dichloromethane	-741.6907413	0.20400414	0.01202506	0.00094421	-0.05036565
16_e	Chloroform	-741.6894009	0.20408999	0.01201979	0.00094421	-0.05036716
16_e	DMSO	-741.6920886	0.20392426	0.01203885	0.00094421	-0.05039664
16_e	Water	-741.6922254	0.20392097	0.01203781	0.00094421	-0.05039309
17_a	Gas Phase	-940.1937221	0.18934864	0.01356321	0.00094421	-0.05388173
17_a	Benzene	-940.2042222	0.18902016	0.01269026	0.00094421	-0.051956
17_a	Dichloromethane	-940.212114	0.18884457	0.01358664	0.00094421	-0.0538402
17_a	Chloroform	-940.2096648	0.1889022	0.01357705	0.00094421	-0.05385483
17_a	DMSO	-940.2144477	0.18882597	0.01353705	0.00094421	-0.05368567
17_a	Water	-940.2147229	0.18880469	0.01354923	0.00094421	-0.05376113
17_e	Gas Phase	-940.1980607	0.18916465	0.01367332	0.00094421	-0.05412402
17_e	Benzene	-940.2059744	0.18885374	0.01370735	0.00094421	-0.0541995
17_e	Dichloromethane	-940.2115064	0.18862292	0.01372987	0.00094421	-0.05424675
17_e	Chloroform	-940.2098409	0.18869868	0.01372265	0.00094421	-0.05423674
17_e	DMSO	-940.2131561	0.18865707	0.01369387	0.00094421	-0.05414439
17_e	Water	-940.2133225	0.18861600	0.01370394	0.00094421	-0.05417927

1A_a, Gas Phase

C	-5.32148868182699	2.09878327766517	0.22079697168556
C	-5.23346030419343	0.87802802348472	-0.68402663354220
C	-4.10695217206062	2.99348629428958	0.06145065498225
F	-5.39195216243847	1.66011122938655	1.53279694706958
H	-6.24366217325913	2.64162723360519	0.00670115144496
C	-2.82285639685548	2.19881356943477	0.27639690831311
H	-4.17688895881526	3.82839340301073	0.75838257719594
H	-4.12581889957939	3.40996537718733	-0.95036864039914
C	-2.79628009052503	0.96300075510301	-0.61556007377435
H	-2.75290511020031	1.88840540830251	1.31971514979651
H	-1.95242606041206	2.81935611244344	0.06006615862235
N	-4.00235804653050	0.16414611228502	-0.43394670873968
H	-1.93843379910639	0.33460593553143	-0.39816117676228
H	-2.74849333062755	1.26404525442352	-1.66757047459166
H	-5.24625009022098	1.21289802781311	-1.72631470094918
H	-6.09475344395353	0.24057737759436	-0.52619848954207
C	-3.89375569705770	-1.07479993372055	0.08794215198142
O	-2.85834431881585	-1.59107730834543	0.42036182066037
C	-5.19301631992636	-1.91760203178182	0.21720124928083
F	-5.81406740535775	-2.02788720170980	-0.96624958185170
F	-6.05749756436130	-1.38097761712174	1.08307346118588
F	-4.89787897387592	-3.13181929888108	0.63490127793350

1A_a, Toluene

C	-5.32300254625423	2.10270935505912	0.21368983007350
C	-5.23146809528845	0.87644659542880	-0.68038463706348
C	-4.10753510091177	2.99483601679528	0.06276139530000
F	-5.40725397097791	1.66791689639119	1.53347735232627
H	-6.24306688721223	2.64315465586453	-0.00922597887165
C	-2.82244125487348	2.20250043898443	0.27936510195647
H	-4.18035714770940	3.82916013079274	0.76015666499297
H	-4.12451183035151	3.41150876021881	-0.94850110906458
C	-2.79348818725388	0.96451463572913	-0.60856645631452
H	-2.74604896185516	1.89723658363215	1.32397007655331
H	-1.95424425284061	2.82306092068899	0.05549901265756
N	-3.99940771525307	0.16270557597211	-0.41673827318014
H	-1.93038254980908	0.34289604300652	-0.39525463898342
H	-2.75681866976669	1.26120269731702	-1.66126303369408
H	-5.23339350203494	1.20456151677494	-1.72364857260718
H	-6.09572277671212	0.24276091191446	-0.52545781822248
C	-3.89358087783506	-1.07848088838737	0.07705177239550
O	-2.85635732486096	-1.61543684086940	0.39129484745722
C	-5.19511497701802	-1.91611644417140	0.21624186065084
F	-5.82848726666876	-2.02861869653257	-0.95842763888079
F	-6.04889652053747	-1.38220446741847	1.09380693893491
F	-4.89795958397519	-3.13423439719099	0.63154330358377

1A_e, Gas Phase

C	-5.99242294614089	1.71215752892824	-1.28228139793338
C	-5.61857173331416	0.69399871090271	-0.21169802739316
C	-4.90975613298309	2.75888411102150	-1.44897143584107
F	-7.17265666057111	2.31821409798580	-0.89691245498612
H	-6.17647424186008	1.19043421941482	-2.22602238072229
C	-3.55768178694023	2.09807873627972	-1.70835832763652
H	-4.86562113727813	3.34406273162187	-0.52570739311305
H	-5.17639379075101	3.43961994260653	-2.25726041927700
C	-3.24613017926745	1.06311466664842	-0.63460650344428
H	-2.76916135003678	2.85126605729504	-1.72715310733123
H	-3.55527557486970	1.60557633107947	-2.68364462446297
N	-4.33761224140014	0.10179752500004	-0.53466330762011
H	-3.13405861488630	1.55470993464325	0.33692198844767
H	-2.33233179401556	0.51976602543548	-0.85310955636612
H	-6.39527225537491	-0.05591848396208	-0.12287030868174
H	-5.53648629121300	1.21219871408308	0.74878283844918
C	-4.08960145537598	-1.19524943659748	-0.80984111437144
O	-3.01016240520535	-1.64137530586430	-1.10223136116009
C	-5.28445870608269	-2.18309810031553	-0.74791521103368
F	-6.24373111777089	-1.83686186746366	-1.61743891262834
F	-5.83057973636134	-2.21968896209488	0.47281871113855
F	-4.87958984830122	-3.39879717664801	-1.05075769403280

1A_e, Toluene

C	-5.98754777140911	1.71211501096241	-1.28769700983232
C	-5.61768681484966	0.69227457195634	-0.21798723119531
C	-4.91006967561238	2.76322291099130	-1.44506939781205
F	-7.17608496168129	2.31397806646279	-0.89954314356681
H	-6.17233335916623	1.19750594596330	-2.23417491328523
C	-3.55833647324425	2.10292614344811	-1.70781157301941
H	-4.86502380816450	3.34176215003276	-0.51784417984305
H	-5.17461150919793	3.44590445382993	-2.25234145632831
C	-3.24483686859915	1.06381943203636	-0.63938259137672
H	-2.76994730303646	2.85595427820755	-1.71888246782919
H	-3.55675965435489	1.61727327122547	-2.68634572184645
N	-4.33655586736740	0.09793632522928	-0.54539315781804
H	-3.13922297063202	1.54809718379359	0.33556350829396
H	-2.32807723283688	0.52741887838732	-0.86004412729041
H	-6.39657269880970	-0.05522310177206	-0.12937221768286
H	-5.52781947356054	1.20728083956170	0.74265580839053
C	-4.09346091314616	-1.19425824991533	-0.80939107758956
O	-3.01235161494693	-1.65269889394573	-1.09769105628213
C	-5.28807164408118	-2.18261411802868	-0.74156624681621
F	-6.25054285170520	-1.84775172015798	-1.60942158233709
F	-5.82945636094667	-2.22094076788946	0.48032260408286
F	-4.87866017265147	-3.40109261037895	-1.04150276901617

1B_a, Gas Phase

C	-5.38118290670021	1.36934314817799	-0.43140692022412
C	-4.52223322225276	0.63943450131116	-1.44819197314312
C	-4.59926740703858	1.70997331714868	0.82157555120911
C	-3.98612578397298	0.44996960644944	1.42708812937993
C	-3.18405804462960	-0.33695184402030	0.40716031388013
N	-4.03932425923705	-0.61954115607277	-0.79879838398568
H	-4.77478860982288	-0.18185503972961	1.83966558654737
H	-3.32536266905015	0.70566563883217	2.25410330177953
H	-5.82675647914079	2.25207713059679	-0.88811169974140
F	-6.40038502114223	0.48529949343294	-0.10345967653538
H	-5.09552307012229	0.36977050397547	-2.33124499795217
H	-3.65140385885745	1.22707762990600	-1.73366328392586
H	-5.26144991556595	2.19267146239722	1.53858939906354
H	-3.82359749686467	2.43474274146696	0.56123370772022
H	-2.32432217291490	0.22584785458922	0.04403699434971
H	-2.84436599615786	-1.29232436897557	0.79887556907313
H	-3.52862480743946	-1.19233872604531	-1.47025211081058
H	-4.86632827909019	-1.15094189344048	-0.50821950668435

1B_a, Water

C	-5.37555643922067	1.38712407181652	-0.43140491814149
C	-4.54852078286180	0.61161954416939	-1.43167596066371
C	-4.59837170490645	1.70368995207591	0.82802343811486
C	-3.99800134778135	0.43666892283599	1.42746631795700
C	-3.17915024522280	-0.32474509878992	0.40455024243081
N	-4.02154608431824	-0.62284761985514	-0.79157098153346
H	-4.79089147952478	-0.20939359685206	1.80914395386754
H	-3.35150603825812	0.68377291602991	2.26798148427240
H	-5.75861921572923	2.28849357593033	-0.90617441392195
F	-6.47470851215403	0.58626158677941	-0.09745975824224
H	-5.14018534677284	0.31866618537971	-2.29350635242407
H	-3.69555735107182	1.20538291907956	-1.75433185102645
H	-5.25485196245337	2.19992487174503	1.54171127104505
H	-3.80693357393961	2.40866296055215	0.56252905922610
H	-2.33618438493716	0.26403070100636	0.04605383467883
H	-2.81865117710752	-1.27354752901347	0.78961550299619
H	-3.48163118316942	-1.15471287678285	-1.47329318651450
H	-4.80423317057079	-1.22113148610682	-0.51867768212089

1B_e, Gas Phase

C	-5.42960188539503	1.34929036811959	-0.43678253109944
C	-4.58251961231123	0.60733942243422	-1.45066176548275
C	-4.63400478845827	1.68644019806731	0.82263802710561
C	-4.02816970160602	0.43220911194469	1.41945004618730
C	-3.19888958988407	-0.33641588577229	0.39367951842883
N	-4.02958089048824	-0.64058199574366	-0.81521577931373

H	-4.81382483286770	-0.21563562271224	1.82455738665129
F	-3.17297826694542	0.74416608008981	2.43854746615075
H	-5.79956523844623	2.26063379093920	-0.90485688193505
H	-6.31255703283955	0.75235430110222	-0.18961693557757
H	-5.14678144010045	0.30589830012660	-2.32985346807124
H	-3.72055130205703	1.19619290903586	-1.76314442473022
H	-5.27542248017743	2.16585929352477	1.56067526593112
H	-3.82699134988010	2.38496158803321	0.58844992754927
H	-2.36162556130896	0.2744577090140	0.06341281657152
H	-2.82608175222444	-1.27131139979755	0.80422063638614
H	-3.46875210101378	-1.15892482280092	-1.49279518042522
H	-4.80718217399604	-1.25200140749221	-0.55373412432661

1B_e, Water

C	-5.42759802503277	1.35038959541414	-0.43246588337256
C	-4.58290833228645	0.60153090985723	-1.44201390751592
C	-4.62694802709966	1.69206380295992	0.82222131384889
C	-4.03886008367953	0.42889994221555	1.40747757321915
C	-3.20438309715454	-0.32997037051055	0.38814058903438
N	-4.02706794428749	-0.63259727038354	-0.81129525357689
H	-4.82657176273055	-0.21625786131229	1.80314724119494
F	-3.19006162190629	0.73684386937044	2.46182155236797
H	-5.79610241723680	2.26040991370579	-0.90280927873262
H	-6.30083439691646	0.74713373102735	-0.17266903672690
H	-5.15586877976044	0.29009296216539	-2.31012745139329
H	-3.72750055711136	1.19162427336848	-1.76669505562699
H	-5.26407159058250	2.17749044449181	1.56050360258523
H	-3.81111373374405	2.37465940642960	0.57210643424254
H	-2.36889336198246	0.28540883588985	0.05855898361725
H	-2.83688737345560	-1.26712705785038	0.79458529295217
H	-3.45769386716619	-1.13934106103095	-1.48915315380737
H	-4.79171502786685	-1.26333406580782	-0.56236356230998

1C_ae, Gas Phase

C	-5.37619641053129	1.38114859883258	-0.43490158055643
C	-4.53620190300241	0.57695543317770	-1.41300765161446
C	-4.59609159035918	1.69337305561255	0.82930783732564
C	-3.99539622868178	0.42205724691733	1.41975326607591
C	-3.16916028718600	-0.30839885248439	0.36878722220017
N	-4.00607986437508	-0.61044843314175	-0.77797131155445
H	-4.79891165878840	-0.23515662157435	1.75558178570150
H	-3.37487954130627	0.66220116459185	2.28404656581569
H	-5.71167595774963	2.30150732816973	-0.91857648908795
F	-6.51584096879013	0.66515573824053	-0.09910665608016
H	-5.15594657028107	0.28765957546387	-2.26149252131774
H	-3.74713777933170	1.25480677363129	-1.78275802197504
H	-5.24833443139391	2.19746988041759	1.54313162735802
H	-3.79669609351475	2.39303926185433	0.56602154210120
H	-2.30159111672064	0.31850589478672	0.09928869597895
H	-2.78619831488737	-1.24414083090552	0.77604765134065
H	-3.52236128310041	-1.19176521359008	-1.44642196171152

1C_ae, Water

C	-5.36800682641342	1.38681335093588	-0.43867474484200
C	-4.53657404572189	0.57566810488824	-1.41207323224505
C	-4.60073925926293	1.69185910081705	0.83141810623267
C	-3.99367632532601	0.42338619985554	1.42283840228150
C	-3.17875047670179	-0.31436600709610	0.36901797257845
N	-4.02520467713703	-0.62710846711774	-0.77599911642520
H	-4.78900829188756	-0.23224526120606	1.78398015438385
H	-3.36059148306034	0.67269255683541	2.27510073401116
H	-5.71121407445636	2.30297106198034	-0.91969917898803
F	-6.52261915919166	0.65912321957315	-0.10574387748699
H	-5.14780905346371	0.30104579021804	-2.27163587540144
H	-3.73236607823497	1.23887824628569	-1.76666570149127
H	-5.25507151555514	2.19616384010344	1.54354381013929
H	-3.80336670778413	2.39301123262722	0.56877869500667
H	-2.32119663071054	0.31328103818904	0.07944719862483
H	-2.78578714008119	-1.24554409711020	0.77682345048791
H	-3.50671825501135	-1.17165990977895	-1.45272679686637

1C_aa, Gas Phase

C	-5.38332762699692	1.38967080844080	-0.42589557297850
C	-4.55125895609074	0.57280405778189	-1.40190836219068
C	-4.59686388323770	1.71090180576678	0.83188090345474
C	-3.99878771598035	0.44319794622351	1.43735365354468
C	-3.21831935716276	-0.33623564238659	0.38024296781582
N	-3.99860648456596	-0.63093176481786	-0.81248011163631
H	-4.80449810724636	-0.18692615350194	1.82117020765280
H	-3.35303657281529	0.69353105191865	2.28091151434021
H	-5.75815519430211	2.29902690104577	-0.90062413930059
F	-6.49851469330322	0.62822757822667	-0.07408161029492
H	-5.15552938765619	0.30762386537211	-2.26949512142385
H	-3.72495050054220	1.19850257718894	-1.75595730726650
H	-5.24169274043857	2.22551242086517	1.54487199441029
H	-3.79642602470845	2.40467502267139	0.55643680206848
H	-2.34639573387808	0.24832555211592	0.06586415755451
H	-2.83941887083874	-1.27266527014903	0.79011904813197
H	-4.75281815023635	-1.26731075676217	-0.58350902388215

1C_aa, Water

C	-5.37432647923573	1.39655489396221	-0.43093613514302
C	-4.55380551803506	0.56859805032783	-1.40349032834148
C	-4.59994068947921	1.70491051700440	0.83424289041512
C	-3.99897775525811	0.43692928208187	1.43587941424125
C	-3.21111886911819	-0.33302838992706	0.37968205337668
N	-3.99964445459848	-0.63906709864769	-0.81100373173978
H	-4.79767477286975	-0.20421060925914	1.81749600205658
H	-3.35415115901680	0.68897469871542	2.27929113140709
H	-5.73637663243034	2.30742345552966	-0.90865293130543
F	-6.51567723385557	0.64657345883784	-0.08656627542450
H	-5.16432829686426	0.30407262142405	-2.26704349021782
H	-3.72948841669737	1.19382132220505	-1.76040418276588
H	-5.24939901785735	2.21621020111127	1.54578735365295
H	-3.80027926722877	2.40124337590694	0.56524310078383
H	-2.35041722400606	0.26453911142380	0.06071599031484
H	-2.82308526156607	-1.26484251579139	0.79137436665208
H	-4.75990895188288	-1.26077237490503	-0.55671522796251

1C_ee, Gas Phase

C	-5.41969279523247	1.35514028713711	-0.44788299028893
C	-4.55052001594963	0.58398067912551	-1.43230081469529
C	-4.63363340499944	1.67925572579942	0.82154638837976
C	-4.02595101903969	0.41677782279080	1.39665978464326
C	-3.19952907095489	-0.31300630866887	0.35061919506189
N	-4.04415512614800	-0.61668817612041	-0.78898425741357
H	-4.80684019325343	-0.24768906889361	1.77471318725841
F	-3.20209195617019	0.74184951750300	2.46434980269972
H	-5.78193779438680	2.27486011169410	-0.90884587482818
H	-6.29196411221683	0.74570372378279	-0.20035913083670
H	-5.13601128362544	0.29353055557407	-2.30478904675403
H	-3.73662875635171	1.24184292280353	-1.77863913621291
H	-5.26614618774376	2.16291548480293	1.56672273358505
H	-3.81562502081951	2.36658513317982	0.58608136629127
H	-2.34440004684876	0.33264841364746	0.09458308042373
H	-2.81257779014637	-1.23882165420690	0.77528673822322
H	-3.55899542611308	-1.20774516995075	-1.44829102553669

1C_ee, Water

C	-5.42016405755767	1.35492012335193	-0.44595345287008
C	-4.55525598915239	0.57938874102458	-1.42957284364705
C	-4.63198588106071	1.68103447650457	0.82241349640925
C	-4.03316488704750	0.41473777497633	1.39131146410648
C	-3.20326823668504	-0.31540963236551	0.35119322279884
N	-4.04888147911118	-0.62884452324981	-0.78929853697847
H	-4.81264769563751	-0.24387909105887	1.77980953733785
F	-3.20033721705279	0.73752471620768	2.47020806111585
H	-5.77606928995301	2.27573725026333	-0.90884103645938
H	-6.29756176526196	0.75421997416730	-0.19304395080176
H	-5.13969543822965	0.29257499013787	-2.30368427585382
H	-3.73530176353416	1.22895500500352	-1.77197722225025
H	-5.26575244683024	2.16633066903357	1.56556532891314

H	-3.81214381739395	2.36354473239053	0.57898886135220
H	-2.35586407009132	0.33378511416012	0.08246034600702
H	-2.80907245422863	-1.23806603733925	0.77634199891957
H	-3.52953351117231	-1.18541428320790	-1.45545099809938

1C_ea, Gas Phase

C	-5.43634173331009	1.36838339098993	-0.43246689575380
C	-4.58555827280096	0.56302538902835	-1.41216928326851
C	-4.63021338223688	1.69390635152229	0.82443004714573
C	-4.03519715818233	0.43045465466590	1.41315797934160
C	-3.23664443466339	-0.33735937289317	0.36879184272578
N	-4.01092518541287	-0.63534677891809	-0.82219464555994
H	-4.82774548736244	-0.21080142663592	1.81364915486522
F	-3.20139169042114	0.75835364716127	2.47259529096088
H	-5.79309550896914	2.28771419509476	-0.90063364711887
H	-6.32089731621361	0.78096672682060	-0.16723047642629
H	-5.16420142827467	0.27875176062709	-2.29139834705838
H	-3.75596338764794	1.18474180605483	-1.76529618284600
H	-5.24480415901749	2.19760067435757	1.57120151424890
H	-3.80461019425483	2.36525639382785	0.56999491429238
H	-2.37891040359934	0.27803557124415	0.07864228444124
H	-2.84583346246042	-1.26081517086046	0.79549209517864
H	-4.73563679517247	-1.31282781208695	-0.61938564516855

1C_ea, Water

C	-5.43313611492518	1.36469755973587	-0.43355693419930
C	-4.58166669688759	0.56510341828104	-1.41511148718766
C	-4.62847410134264	1.69332772519720	0.82396792073797
C	-4.04120040411698	0.42595973105332	1.40378616234178
C	-3.23156257387481	-0.33532820439980	0.36641427054119
N	-4.01044727191218	-0.64134599353018	-0.82417701500718
H	-4.82911520254764	-0.21694237318645	1.80457325655709
F	-3.20096129727842	0.75023056217855	2.47820502482509
H	-5.79045176391247	2.28346467611659	-0.90134640399825
H	-6.31306492064244	0.77175338709369	-0.16744298110217
H	-5.16564333092795	0.28178322175048	-2.29091305543600
H	-3.75154983965863	1.18725140414878	-1.76533545767191
H	-5.24948658079710	2.19264282116866	1.56858742765446
H	-3.80352871736703	2.36479794404098	0.56676666787329
H	-2.37974035530205	0.28696242276425	0.07310785953628
H	-2.84147322599829	-1.25738842263342	0.79716970109466
H	-4.75646760250859	-1.28692987977955	-0.58751495655931

2A_a, Gas Phase

C	-5.49547788491601	1.20136414606274	0.36670195753307
C	-5.05203416406787	0.68438709051080	-0.99211531142127
C	-4.31316230226270	1.65615610309422	1.20753378507599
C	-3.18778059226802	0.63581833375096	1.23806781704885
C	-2.81836980897996	0.17259687015943	-0.16278226215226
N	-3.99266868225212	-0.29902628505498	-0.85974773078820
C	-4.20849192282403	-1.55128497394068	-1.32124725947614
O	-5.21703034989721	-1.91302994523473	-1.86537580609417
C	-3.05262614028086	-2.57906804104932	-1.17940875073376
F	-1.95757359377885	-2.15529916508462	-1.82897715937758
F	-3.41496702643112	-3.73171427123294	-1.70280411526310
F	-2.71602412099266	-2.78740861242379	0.09505383864382
H	-5.89013741201274	0.22752696302279	-1.50981206971380
H	-4.68672427933247	1.52886319947613	-1.58714892605308
H	-2.39189451335894	1.01790843186051	-0.71430373501257
H	-2.06226984522235	-0.60056889260848	-0.10142708681464
H	-6.19103991378920	2.03130057880733	0.21966719889395
F	-6.17967761457146	0.20251040472207	1.02663351491863
H	-4.64177835270379	1.88129317975319	2.22141300990980
H	-3.92084763911737	2.58038370909854	0.77309149592530
F	-3.56944579854076	-0.46365802037320	1.97690984170049
H	-2.30381804239948	1.06311919668404	1.71597775325067

2A_a, Benzene

C	-5.49331044478235	1.20338364227745	0.36343521543200
C	-5.05119738479974	0.68957285676452	-0.99515626299417
C	-4.31444452537740	1.65226070999950	1.20864320865379
C	-3.18649819275991	0.63731388104599	1.23257649754046
C	-2.81703432563172	0.17578187867252	-0.16711988840773
N	-3.99536639874543	-0.30137376957429	-0.86007937553813
C	-4.20820377982387	-1.54799794250357	-1.31369498165932
O	-5.22158412192675	-1.92317434237425	-1.85144378337024
C	-3.05137364496482	-2.57555831339262	-1.17442436522882
F	-1.95635809517151	-2.16028999385443	-1.82508086371757
F	-3.41858584110332	-3.73026396886846	-1.69785413969366
F	-2.71599243843819	-2.78897511424423	0.09947043374536
H	-5.89117456121757	0.24488873608333	-1.51900592071624
H	-4.67426967424841	1.53252899804687	-1.58239120648982
H	-2.40094782485481	1.02298627656609	-0.72053765169355
H	-2.05551792990363	-0.59192508364160	-0.10808234850359
H	-6.19206553812722	2.02942964289131	0.22099658423427
F	-6.18046919864250	0.19324737481675	1.02000590899364
H	-4.64314703883196	1.87376749855584	2.22333125202034
H	-3.92379857369213	2.57873918142123	0.77893265487394
F	-3.56859812259583	-0.47252442640897	1.97004537946125
H	-2.30390234436089	1.06035227772103	1.71333365305780

2A_a, Dichloromethane

C	-5.49142537618273	1.20143269200387	0.35680679852920
C	-5.04548354128812	0.70024097404201	-1.00380340354126
C	-4.31779527441729	1.64199450317750	1.21091734720176
C	-3.18496199394940	0.63435241646571	1.22469420559098
C	-2.81223357894701	0.18470658403579	-0.17690063151650
N	-3.99229890346521	-0.29662230364325	-0.86919791258420
C	-4.21129380849534	-1.54433286774124	-1.29696477345741
O	-5.23602469921678	-1.93471340859059	-1.81225920529330
C	-3.05312219752292	-2.57150160762659	-1.16321654437160
F	-1.96296645840449	-2.16743360721525	-1.82435811721563
F	-3.42933525504199	-3.73055423957509	-1.67781711408719
F	-2.71022184521497	-2.78301961601433	0.10898123634899
H	-5.88408082408374	0.26839412939136	-1.53952396528719
H	-4.65675699413035	1.54606999170635	-1.57694490855195
H	-2.40795904702411	1.03847224488035	-0.72647960319367
H	-2.04343716974306	-0.57612309278911	-0.12555373477936
H	-6.19382087517988	2.02434861763230	0.22233914634265
F	-6.18026810377785	0.17574417702807	1.00137512004984
H	-4.64886049414013	1.85298957974560	2.22709779339317
H	-3.93006469685995	2.57429897924258	0.79229593610566
F	-3.56602549378412	-0.48999354624481	1.95233864177885
H	-2.30540336913051	1.05341940008877	1.71207368853815

2A_a, Chloroform

C	-5.49205319180212	1.20130006413972	0.35835594340562
C	-5.04657252819309	0.69785851032854	-1.00206529661224
C	-4.31708389613248	1.64433734103503	1.21026335785888
C	-3.18535248225441	0.63479088186227	1.22669218779463
C	-2.81317661371867	0.18266033164413	-0.17462369668364
N	-3.99231680289206	-0.29704358403111	-0.86799200300539
C	-4.21087445962244	-1.54526991785251	-1.30080418091291
O	-5.23312867646487	-1.93149423752897	-1.82067128613024
C	-3.05313657826535	-2.57263823026593	-1.16567955938250
F	-1.96192144055215	-2.16553488584820	-1.82476560780874
F	-3.42711806893538	-3.73055492859162	-1.68213968606452
F	-2.71142881242461	-2.78412976683622	0.10680445066521
H	-5.88524410755102	0.26249979020230	-1.53509152362099
H	-4.66136667122730	1.54360942571421	-1.57827454609916
H	-2.40528350692088	1.03495865230322	-0.72450356758627
H	-2.04636821975985	-0.58010102306996	-0.12133145469304
H	-6.19363463946426	2.02503052649041	0.22214716776132
F	-6.17976839880838	0.17939832534876	1.00553324613178
H	-4.64768098281087	1.85760357175089	2.22612840402299
H	-3.92873929521667	2.57530626399068	0.78899864067397
F	-3.56644455971925	-0.48567728705346	1.95652893621840
H	-2.30514606726385	1.05526017626781	1.71239007406683

2A_a, DMSO

C	-5.49078800142334	1.19766001790688	0.35164830643153
C	-5.03995969098377	0.70865435134331	-1.01134935848757
C	-4.32062713543774	1.63337531064269	1.21229856970188

C	-3.18393794235160	0.63050578798050	1.21934002939565
C	-2.80783899367855	0.19197536231145	-0.18470443718721
N	-3.98732380255106	-0.29011814410523	-0.87913438123771
C	-4.21460160364306	-1.54179847033841	-1.28392106100904
O	-5.24846948818835	-1.93992771756491	-1.77842888778426
C	-3.05607998694507	-2.56918075633451	-1.15403163400302
F	-1.97061625358584	-2.17220663735273	-1.82547915669094
F	-3.43888681453971	-3.73126334127422	-1.65939645490695
F	-2.70456514815278	-2.77565593383174	0.11659519098774
H	-5.87617399638429	0.28401427955190	-1.55625060543876
H	-4.64565464287018	1.55863764936949	-1.57356446496094
H	-2.40936635080547	1.05117749506804	-0.72901022936896
H	-2.03480589029625	-0.56497285962632	-0.13942396190085
H	-6.19581914801966	2.01887528437097	0.22342512666072
F	-6.17865734047800	0.16153020960882	0.98538702170287
H	-4.65402652767727	1.83507499938713	2.22963479291538
H	-3.93541638420924	2.57046798279074	0.80253658806326
F	-3.56338222428093	-0.50268491752252	1.93799723297351
H	-2.30684263349780	1.04803004761866	1.71173177414367

2A_a, Water

C	-5.49070707117576	1.19736799904005	0.35109661007657
C	-5.03935266153654	0.70941752657847	-1.01204021693812
C	-4.32095406100442	1.63263058333463	1.21244461188709
C	-3.18382339706869	0.63031166674251	1.21887140257162
C	-2.80738903265819	0.19262595015247	-0.18533205318376
N	-3.98688789657876	-0.28960572656631	-0.87980264069864
C	-4.21495830722294	-1.54160299975969	-1.28250454530009
O	-5.24974289206749	-1.94034249542814	-1.77498993283194
C	-3.05637301913228	-2.56899965643722	-1.15335471639950
F	-1.97146704244371	-2.17255799484905	-1.82582880118969
F	-3.43985188115585	-3.73129142236054	-1.65796336006676
F	-2.70388966300996	-2.77517113184730	0.11705575977840
H	-5.87530132233790	0.28541734955535	-1.55783495421885
H	-4.64436676049308	1.55965478691776	-1.57332031523669
H	-2.40944569388143	1.05219853195662	-0.72936049279210
H	-2.03404981025760	-0.56403702940161	-0.14044850755461
H	-6.19610333069205	2.01831794894466	0.22346770157971
F	-6.17851114425183	0.16018253657070	0.98374644918019
H	-4.65461314929197	1.83342336844228	2.22987297467195
H	-3.93602722533388	2.57022323981849	0.80357250513716
F	-3.56304072884438	-0.50368701453796	1.93678228324063
H	-2.30698390956128	1.04769398313385	1.71177023828742

2A_e, Gas Phase

C	-5.48730074357699	1.18065010181729	0.25018098511048
C	-4.98977050454420	0.62399073505034	-1.07720761992831
C	-4.34116719684203	1.73518525954965	1.07666646277810
C	-3.23826035079541	0.70480565063605	1.24447011887264
C	-2.80685456690662	0.13341542015928	-0.09993668033862
N	-3.96807056021272	-0.36897358150121	-0.81744076486605
C	-3.97587966437698	-1.66102386312631	-1.22104866411845
O	-3.09693307466571	-2.45026391003948	-1.00055850542645
C	-5.20721672280481	-2.15619404281650	-2.02765964435058
F	-6.33760485007272	-2.02375144000390	-1.32139685180329
F	-5.06129261429879	-3.42814545657443	-2.33112046244420
F	-5.35056376592440	-1.47035886962049	-3.16714647255704
H	-5.81776028448859	0.20556029596093	-1.63635170627428
H	-4.55930241475682	1.44107761736653	-1.66443494711938
H	-2.33591826017131	0.93196613762794	-0.68182061048545
H	-2.09393890885420	-0.67428397069479	0.03224336007438
F	-6.38724314208887	2.19084224352994	-0.01656424737597
H	-6.01980721408293	0.39351950680112	0.79145781995588
H	-4.70114288577197	2.06948488968234	2.04906345278722
H	-3.92567842528040	2.59940550271330	0.55143201950860
H	-3.55476143083837	-0.10770131262585	1.90353690946735
F	-2.14270241864515	1.30813308610821	1.82799604853343

2A_e, Benzene

C	-5.48440170332886	1.17750256892232	0.25363999951856
C	-4.99034301475303	0.62192513577160	-1.07507232004268
C	-4.33957731938791	1.73882368149361	1.07558344299164
C	-3.24194375310732	0.70473454889282	1.24449624891695
C	-2.80657089650239	0.13315592819999	-0.09805926466085
N	-3.96830197172695	-0.37342295681905	-0.81500785136882
C	-3.97795354790196	-1.65734601275218	-1.22063613275597
O	-3.09842391267077	-2.45449783030147	-1.00646321792438
C	-5.20825540878908	-2.15225845095559	-2.02972735047600
F	-6.34077753907631	-2.02731030128067	-1.32862685345208
F	-5.05712715799381	-3.42675745557667	-2.33415456781106
F	-5.35041694009460	-1.47057282408937	-3.17063194636476
H	-5.82000884685118	0.20532413864728	-1.63288435190949
H	-4.55518613761730	1.43555541212208	-1.66218203704020
H	-2.34198729582890	0.93100335655587	-0.68471186524079
H	-2.09051123103005	-0.67041846427618	0.03860212106933
F	-6.38870710033895	2.18956200705708	-0.01695173067895
H	-6.01753793942141	0.39527266366986	0.79928859421300
H	-4.69950205411419	2.07294761445126	2.04800590651906
H	-3.92341633284738	2.59910696822966	0.54447686811697
H	-3.55798971795096	-0.10357871008516	1.90709567826288
F	-2.14023017866668	1.30858898212288	1.82828063011766

2A_e, Dichloromethane

C	-5.48236399961090	1.17640530419264	0.25707338758549
C	-4.99187269732562	0.61932482331600	-1.07200565963137
C	-4.33765296531952	1.74321519590598	1.07417438438208
C	-3.24511247881649	0.70544569025600	1.24531301425817
C	-2.80738956607184	0.13175693857135	-0.09524607391508
N	-3.96974880957233	-0.37801584008843	-0.81128058864377
C	-3.97866650271224	-1.65473917739540	-1.22218373576076
O	-3.09635446757276	-2.45662731183887	-1.01651663459926
C	-5.20849335839142	-2.14943995796257	-2.03246273640677
F	-6.34189303425663	-2.03211602140694	-1.33423111851639
F	-5.05245161226728	-3.42556479829736	-2.33932278926890
F	-5.35086966192932	-1.46971327852972	-3.17347051601008
H	-5.82322581786192	0.20334486076807	-1.62758268813408
H	-4.55312841250633	1.42923021814441	-1.66059496104431
H	-2.34676353987292	0.92794434614515	-0.68640971628455
H	-2.08991098139626	-0.66939358082562	0.04561642818500
F	-6.38936907695811	2.18966794247967	-0.01750636337979
H	-6.01573493687459	0.39880381569198	0.80766079381043
H	-4.69700869625266	2.07884036193368	2.04623691851858
H	-3.92038524574296	2.59918695771587	0.53709459092915
H	-3.56258999892757	-0.09865605139679	1.91114915206799
F	-2.13818413976032	1.30843956262086	1.82885491185824

2A_e, Chloroform

C	-5.48298594375173	1.17627238173013	0.25561761375052
C	-4.99090796489319	0.62072076903535	-1.07366096054751
C	-4.33853609126418	1.74107803699770	1.07486838748552
C	-3.24393310166350	0.70482659042188	1.24472070356538
C	-2.80669983752016	0.13286599005541	-0.09686183582743
N	-3.96864143037587	-0.37588564206058	-0.81350086175048
C	-3.97886739234940	-1.65541963814030	-1.22079408264700
O	-3.09852015877281	-2.45651607511163	-1.01050647052338
C	-5.20869602847847	-2.15020604396907	-2.03097753769520
F	-6.34204540013070	-2.02972199020806	-1.33231083957083
F	-5.05452351786314	-3.42609172625699	-2.33623912678789
F	-5.35039838225829	-1.47058890413281	-3.17242338311598
H	-5.82145663076094	0.20485825598787	-1.63059019229984
H	-4.55331237625315	1.43229177434976	-1.66108571313925
H	-2.34532300974825	0.93021456450860	-0.68610809695919
H	-2.08918596624794	-0.66873672009174	0.04205833760916
F	-6.38936282854867	2.18912690840130	-0.01710553093338
H	-6.01620803987598	0.39662380359948	0.80388931018838
H	-4.69828765956686	2.07550755883226	2.04721954209412
H	-3.92184432317154	2.59900668171806	0.54040953818851
H	-3.56050110967000	-0.10118581032027	1.90903980067485
F	-2.13893280683520	1.30829923465362	1.82870139824093

2A_e, DMSO

C	-5.48175967671952	1.17602724705925	0.25802221679237
C	-4.99224249277183	0.61872097768259	-1.07124268705880
C	-4.33710603257616	1.74438753865249	1.07379860911676
C	-3.24608249939098	0.70551659850607	1.24549411032636
C	-2.80755620186928	0.13155234995402	-0.09459902176874

N	-3.96999754759197	-0.37920229175506	-0.81048268523852
C	-3.97894054154612	-1.65385812495419	-1.22250673609968
O	-3.09590165901880	-2.45731359452962	-1.01907712357951
C	-5.20865050603948	-2.14854700392342	-2.03306036000901
F	-6.34226717288723	-2.03323031899958	-1.33576884693970
F	-5.05121136076493	-3.42534271711109	-2.34026641475998
F	-5.35090445345356	-1.46981609224981	-3.17430958171553
H	-5.82400780191579	0.20297741948586	-1.62632806589258
H	-4.55238838185646	1.42758545898309	-1.66011949110357
H	-2.34831726743371	0.92744166998769	-0.68698408436495
H	-2.08951604950565	-0.66879106946038	0.04731127594197
F	-6.38960399070306	2.18959692960870	-0.01759293486731
H	-6.01513260417165	0.39964686058521	0.80992353183993
H	-4.69634311513694	2.08028395562101	2.04579431879449
H	-3.91951098056738	2.59916641375359	0.53509632833780
H	-3.56409177788749	-0.09750338891547	1.91204755347686
F	-2.13763788619197	1.30804118201900	1.82921008877134

2A_e, Water

C	-5.48170027830551	1.17597071089433	0.25809733806368
C	-4.99225365255543	0.61869550064658	-1.07120280796377
C	-4.33706571257470	1.74446584016547	1.07377377422463
C	-3.24617493598679	0.70550113176398	1.24549936606203
C	-2.80755246718672	0.13156635359466	-0.09456916076630
N	-3.96998908127178	-0.37928204357258	-0.81045887497197
C	-3.97898353253492	-1.65375609887288	-1.22250619266644
O	-3.09590719221354	-2.45739608590783	-1.01922956122420
C	-5.20868214235572	-2.14845452088098	-2.03308302942917
F	-6.34231977591200	-2.03329406387209	-1.33589509011239
F	-5.05112252102664	-3.42533801359477	-2.34026452193243
F	-5.35090840899495	-1.46988376554823	-3.17439027865985
H	-5.82404577542305	0.20299478922684	-1.62627322643930
H	-4.55228751272492	1.42748111263188	-1.66007322980652
H	-2.34847030412557	0.92745767071624	-0.68704267066669
H	-2.08943454100609	-0.66868303986952	0.04741383699482
F	-6.38963303506775	2.18957044551868	-0.01759214576890
H	-6.01506667236533	0.39967921118592	0.81008999461621
H	-4.69630242072037	2.08035608129864	2.04577055389848
H	-3.91944718332112	2.59915455848352	0.53494938063199
H	-3.56422914078497	-0.09744287858633	1.91208968220038
F	-2.13759371354212	1.30797710457841	1.82925686371573

2C_ee, Gas Phase

C	-5.50478699130178	1.27851878588881	-0.38425569971181
C	-4.62354315194148	0.55052243472327	-1.38549771151688
C	-4.72266937119995	1.63288590792131	0.86849804456875
C	-4.01896237532667	0.41250317449696	1.43612532196774
C	-3.19399409836644	-0.28383208181569	0.36669579007488
N	-4.07393177386846	-0.62344263785578	-0.73501067430544
H	-3.61905470480309	-1.23390454551928	-1.39682176885427
H	-5.22077636765058	0.24662026588099	-2.24433551307182
H	-4.73838530675017	-0.29409107537028	1.85615860906646
F	-3.18194719790860	0.81324676122076	2.46334286512325
H	-3.85190919746668	1.25504685865422	-1.73216538318969
F	-5.97988921616470	2.44322103259675	-0.96214963022465
H	-6.36923755512673	0.65577140458120	-0.14299858349171
H	-2.37667875138990	0.39374680108682	0.07541243966375
H	-2.75570769165301	-1.19238895038662	0.77787459401885
H	-5.37856108988486	2.07904063850790	1.61596826514360
H	-3.96200515919688	2.37033522538864	0.59837903473898

2C_ee, Benzene

C	-5.50426510764347	1.27508708901019	-0.38184732900011
C	-4.62510279904014	0.54883458809620	-1.38446177621847
C	-4.72202178143486	1.63399631986389	0.86852483136247
C	-4.02230284141668	0.41128390768486	1.43383294651783
C	-3.19598257169613	-0.28519502381475	0.36710272532258
N	-4.07663365697140	-0.62835422900168	-0.73512873944918
H	-3.60548215231643	-1.22200976919857	-1.40231794528330
H	-5.22141668963801	0.24574282846536	-2.24414319060730
H	-4.74096814480512	-0.29130074206760	1.86002603806427
F	-3.18079501803079	0.81423739591193	2.46475808506000
H	-3.84954765119857	1.25002146996477	-1.72761696370677
F	-5.98018775371588	2.44517332449163	-0.96283143049833
H	-6.37220751524927	0.65888061207598	-0.13953273352093
H	-2.38201893600951	0.39335708635109	0.07053250177794
H	-2.75632186925698	-1.19312549991883	0.77800110845512
H	-5.37814141827131	2.07985504653133	1.61598543467052
H	-3.95864409330544	2.36731559555417	0.59433643705365

2C_ee, Dichloromethane

C	-5.50395982292461	1.27271899873416	-0.38015050141963
C	-4.62618596638370	0.54763206664160	-1.38369172507972
C	-4.72149238145420	1.63477250139928	0.86849276849058
C	-4.02467022110422	0.41040904030587	1.43229259965093
C	-3.19737922025302	-0.28610256598300	0.36736717204426
N	-4.07844317868661	-0.63166520915562	-0.73518966117354
H	-3.59593178834279	-1.21320747118145	-1.40597897564793
H	-5.22176468118795	0.24496879914572	-2.24399798584040
H	-4.74316945505047	-0.28930474732473	1.86234633631658
F	-3.18027187653539	0.81494466616018	2.46605405434947
H	-3.84784354300571	1.24623172100524	-1.72466781471046
F	-5.98063284890728	2.44663928736085	-0.96311362343150
H	-6.37410103815229	0.66085441295894	-0.13671594656693
H	-2.38566162358797	0.39287553158597	0.06694040806962
H	-2.75667733213537	-1.19364744850154	0.77790719935337
H	-5.37769986419651	2.08057557458192	1.61596411592836
H	-3.95615515809187	2.36510484226660	0.59136157966693

2C_ee, Chloroform

C	-5.50404657363386	1.27342656228419	-0.38064764609195
C	-4.62587225309804	0.54798195973393	-1.38392270050420
C	-4.72163940732444	1.63455497814690	0.86849879243122
C	-4.02396849575401	0.41067954108340	1.43274905090269
C	-3.19697152976043	-0.28585111887059	0.36729359293328
N	-4.07788695352833	-0.63068192933625	-0.73518940695699
H	-3.59869650130228	-1.21579349331435	-1.40493958365174
H	-5.22171598246702	0.24519054317632	-2.24401198428021
H	-4.74253141496460	-0.28988954290799	1.86162507096086
F	-3.18042023875951	0.81471576609904	2.46564777827680
H	-3.84839844319582	1.24739119962726	-1.72557491051685
F	-5.98050350701435	2.44617547023451	-0.96304014237798
H	-6.37350721423017	0.66023809727487	-0.13753503491383
H	-2.38455070227166	0.39299313548389	0.06806958051115
H	-2.75662754339563	-1.19351749807956	0.77797887835313
H	-5.37780882026613	2.08039347486481	1.61596589431637
H	-3.95689441903370	2.36579285449960	0.59225277060823

2C_ee, DMSO

C	-5.50388344664023	1.27199396863767	-0.37963300665206
C	-4.62650006675729	0.54730069208188	-1.38345714115290
C	-4.72129511007881	1.63502258807821	0.86844827196614
C	-4.02538385097533	0.41015582825832	1.43183267657581
C	-3.19781244694700	-0.28638625661391	0.36745916175716
N	-4.07898193678030	-0.63263486411470	-0.73521697486008
H	-3.59308237928625	-1.21050418278005	-1.40705217457500
H	-5.22181030352012	0.24477358437099	-2.24398707822654
H	-4.74389015993336	-0.28866620066303	1.86301138508363
F	-3.18016521055085	0.81515143110692	2.46648507975220
H	-3.84730328368987	1.24509645217882	-1.72376726586557
F	-5.98090474520646	2.44703911968752	-0.96313651464314
H	-6.37462131283165	0.66135873158146	-0.13580293320830
H	-2.38673975793437	0.39266934417699	0.06586111097892
H	-2.75679192753585	-1.19382775620811	0.77786006848074
H	-5.37751109393442	2.08083416830111	1.61592969250902
H	-3.95536296739780	2.36442335191990	0.59038564207996

2C_ee, Water

C	-5.50387561576117	1.27192340902154	-0.37958328198857
C	-4.62653127105998	0.54726575232815	-1.38343303424276
C	-4.72127902367362	1.63504402073965	0.86844661391270
C	-4.02545404592758	0.41012826060848	1.43178815055973
C	-3.19785279079768	-0.28641053029777	0.36746636817241

N	-4.07903789500465	-0.63273250556162	-0.73521611180664
H	-3.59280922662588	-1.21024302101129	-1.40715353765311
H	-5.22181211176066	0.24475156328417	-2.24398669115066
H	-4.74395766611021	-0.28860777232962	1.86308035990586
F	-3.18015524897468	0.81517367692069	2.46653006650655
H	-3.84724625419469	1.24497778806258	-1.72367629361952
F	-5.98092080837398	2.44708576531663	-0.96314119340494
H	-6.37467980769057	0.66141851085657	-0.13571836330998
H	-2.38685169095322	0.39265803092551	0.06574580338391
H	-2.75679238950686	-1.19383932685036	0.77784967836576
H	-5.37749759122637	2.08085462041596	1.61592838025889
H	-3.95528656235818	2.36435175757072	0.59029308611035

2C_ea, Gas Phase

C	-5.52029632184291	1.29199637861722	-0.36454675994743
C	-4.66823488379466	0.52340550938029	-1.36486155081076
C	-4.71085112280706	1.65378568834084	0.86892735784208
C	-4.03514970987221	0.42599247502435	1.45502873369035
C	-3.23565200608012	-0.31188565410857	0.39038252417021
N	-4.03938163636014	-0.64082809561556	-0.77115438475923
H	-4.71442621170317	-1.36548141008678	-0.56511098363865
H	-5.26823104538235	0.22027839443901	-2.22224760877123
H	-4.77603936257498	-0.25261429922372	1.89033435331240
F	-3.19140440221460	0.81800695043962	2.48055920418213
H	-3.88449342760046	1.19327457381031	-1.73223151094168
F	-5.99418036231976	2.45235681530223	-0.95298491568900
H	-6.39358794222202	0.69058721075435	-0.09138649664009
H	-2.41179227379021	0.33456692336122	0.07212648714068
H	-2.79831263452701	-1.21987670050936	0.80421894439797
H	-5.34542868499694	2.13263395682602	1.61459042260171
H	-3.93487797191141	2.36539128324852	0.57421618386052

2C_ea, Benzene

C	-5.51820323467216	1.28675194324158	-0.36352028835746
C	-4.66572212337288	0.52461337390226	-1.36663736488061
C	-4.71031981934844	1.65337897019244	0.86833117996118
C	-4.03761843390052	0.42331189997136	1.45050354748358
C	-3.23281952918606	-0.31074213013244	0.38887047282967
N	-4.03880836650404	-0.64318035918951	-0.77271882570476
H	-4.72637561318410	-1.35207011088438	-0.54877592755418
H	-5.26755103017087	0.22141117245895	-2.22264362878075
H	-4.77607841262679	-0.25510647766357	1.88680559877968
F	-3.19121230279031	0.81679117896475	2.48206087837477
H	-3.88083530063210	1.19493449643155	-1.73045670876703
F	-5.99565499411787	2.45238168893107	-0.95396466504809
H	-6.39166868926351	0.68718751942113	-0.09233637850076
H	-2.41163085237118	0.33844605841460	0.06961332375503
H	-2.79714191793081	-1.21877267845863	0.80420853678438
H	-5.34733026519466	2.12867095153096	1.61427769179240
H	-3.93336911473373	2.36358250286788	0.57224255783292

2C_ea, Dichloromethane

C	-5.51689414162327	1.28316062895566	-0.36277211582572
C	-4.66413456031432	0.52540959869702	-1.36776479614883
C	-4.71008970876996	1.65302548114031	0.86797321398721
C	-4.03934859127441	0.42149222338483	1.44749763029345
C	-3.23101200117738	-0.31002874234431	0.38793707191417
N	-4.03826281794196	-0.64457483468921	-0.77382009183812
H	-4.73357911838721	-1.34320612433080	-0.53856607406558
H	-5.26753700477383	0.22191526200360	-2.22250799006878
H	-4.77602220434234	-0.25673857369712	1.88467415152357
F	-3.19040688343034	0.81658928549614	2.48266487965691
H	-3.87867679620545	1.19622721392310	-1.72948002933405
F	-5.99596162332389	2.45285858825536	-0.95488308050765
H	-6.39053691908115	0.68499434754153	-0.09298895499301
H	-2.41127291580094	0.34082384801516	0.06830126652129
H	-2.79710239157532	-1.21833081208692	0.80443032547480
H	-5.34897857077301	2.12553185547724	1.61413259293276
H	-3.93252375120522	2.36244075425841	0.57103200047753

2C_ea, Chloroform

C	-5.51726964964180	1.28423407139090	-0.36299399151284
C	-4.66459623672763	0.52517852859815	-1.36743886026424
C	-4.71012765487653	1.65315199991880	0.86807009997470
C	-4.03883769775610	0.42203119245497	1.44838191845316
C	-3.23153879797630	-0.31023061145056	0.38820736116795
N	-4.03842839614622	-0.64416968681864	-0.77349492021050
H	-4.73149330216819	-1.34581725041292	-0.54153524473915
H	-5.26751733851569	0.22177031650847	-2.22257468519093
H	-4.77608334061234	-0.25624567119293	1.88525838816207
F	-3.19073455741891	0.81655022264396	2.48254567486149
H	-3.87929995228255	1.19583694509790	-1.72976662549666
F	-5.99596936165980	2.45265498283032	-0.95458041145415
H	-6.39083603344538	0.68562243844757	-0.09276727739870
H	-2.41139925994289	0.34014948806751	0.06867389689083
H	-2.79704941309297	-1.21843187774599	0.80434666434804
H	-5.34842704673711	2.12653447537667	1.61416498330987
H	-3.93273196099961	2.36277043628580	0.57136302909904

2C_ea, DMSO

C	-5.51653519234336	1.28211061837346	-0.36254170161122
C	-4.66369461430029	0.52564835274570	-1.36807927637151
C	-4.71005394275268	1.65291380629381	0.86787857391695
C	-4.03985064905856	0.42097969482715	1.44662966910918
C	-3.23050569276988	-0.30985163892798	0.38769300768316
N	-4.03805502677374	-0.64493581199490	-0.77416268587594
H	-4.73550663731945	-1.34068664218846	-0.53579261879499
H	-5.26761684393014	0.22199057999060	-2.22238330007935
H	-4.77598507399139	-0.25718319276748	1.88409953603559
F	-3.19004211515994	0.81665811403947	2.48276579091877
H	-3.87812073067721	1.19665757640699	-1.72924622116298
F	-5.99592954429772	2.45308479920368	-0.95518816550504
H	-6.39024219505022	0.68437582712106	-0.09317720611046
H	-2.41110641439659	0.34143532114690	0.06800765115250
H	-2.79724156853430	-1.21828286620104	0.80454704821323
H	-5.34952992394301	2.12453888826173	1.61410625486990
H	-3.93232383470151	2.36213657366929	0.57070364361219

2C_ea, Water

C	-5.51650149305976	1.28199962183909	-0.36251524032071
C	-4.66364508644852	0.52567917312365	-1.36811017457310
C	-4.71004613932052	1.65290985850481	0.86786468475685
C	-4.03990011807953	0.42093798799745	1.44653896932133
C	-3.23046285485699	-0.30984536551206	0.38767232417725
N	-4.03803500866133	-0.64496904242851	-0.77420168747223
H	-4.73570123896101	-1.34043518358196	-0.53553553596144
H	-5.26761178995309	0.22201418077156	-2.22237895523420
H	-4.77598333385805	-0.25721105384938	1.88404643947666
F	-3.18998954391616	0.81668152888171	2.48276061692987
H	-3.87805783804581	1.19671317616589	-1.72920859516912
F	-5.99595424506458	2.45309332197090	-0.95521305579106
H	-6.39019754800279	0.68428666186756	-0.09318389131180
H	-2.41108132163761	0.34147096410935	0.06798889577570
H	-2.79728147892481	-1.21829467648160	0.80456717248584
H	-5.34958258401159	2.12443719698248	1.61410396191963
H	-3.93230837719787	2.36212164963906	0.57066407099053

2C_ae, Gas Phase

C	-5.46864901899963	1.34280956478042	-0.40679129644649
C	-4.60832156410684	0.56553908537068	-1.38954082453302
C	-4.69682872413433	1.66519164675588	0.86295016261593
C	-3.96269497657066	0.46439840594771	1.43842648027152
C	-3.17910586617475	-0.26742426736744	0.36124388644276
N	-4.04351328445573	-0.59892618650287	-0.74772766904431
H	-3.59081733226848	-1.21120380750785	-1.40862816301238
H	-5.22798734227598	0.25300301495478	-2.22921663228597
F	-4.86214574630839	-0.39912708702437	2.03136360124046
H	-3.27468963791088	0.79413380994362	2.22113950811800
H	-3.84166508560496	1.26280886351051	-1.77173128273010
H	-5.80419853070785	2.26975283246371	-0.87895081772173
F	-6.60110514495660	0.61564286464258	-0.09847305230139
H	-2.33657747891822	0.38575500967657	0.07227492626094
H	-2.76624429910259	-1.18159310244139	0.78616287313287

H	-5.36444470217230	2.09234217483408	1.61095821020379
H	-3.94946126533179	2.42484717796337	0.61466008978910

2C_ae, Benzene

C	-5.46439255775694	1.34535832473735	-0.40671275322651
C	-4.61023184393360	0.56334553600526	-1.38769882036572
C	-4.69554225973040	1.66712316447256	0.86278249278815
C	-3.96038283438289	0.46818011975203	1.43599009533764
C	-3.18218857803336	-0.26905210926166	0.36166104823553
N	-4.05277876605705	-0.60869071312082	-0.74485761683743
H	-3.57713937925811	-1.19719060270970	-1.41328614192904
H	-5.22710252859813	0.25665861801061	-2.23157904938558
F	-4.86924471004176	-0.40008052942405	2.02923106197003
H	-3.27697160946813	0.79201517188640	2.22308829831781
H	-3.83674951225228	1.25373743341914	-1.76376018847557
H	-5.80757595603087	2.26806438064282	-0.87815785822369
F	-6.60170009067343	0.61069224960866	-0.09251794492482
H	-2.34561606053857	0.38458457148100	0.06300246488328
H	-2.76279577520660	-1.17977152358182	0.78756216282761
H	-5.36074332397643	2.09840773151339	1.61073147333632
H	-3.94729421406144	2.42456817656880	0.61264127567198

2C_ae, Dichloromethane

C	-5.46111874798367	1.34717959911930	-0.40648056653742
C	-4.61194084053932	0.56161894156810	-1.38618946431549
C	-4.69436067754171	1.66859640504294	0.86253084551292
C	-3.95884792202140	0.47099988603385	1.43405278529819
C	-3.18462835946160	-0.27030045279495	0.36216494233936
N	-4.05947393747324	-0.61630709937325	-0.74298036501391
H	-3.56568536458626	-1.18500071573587	-1.41691671032900
H	-5.22680507848738	0.25954743654359	-2.23324188519909
F	-4.87564829746739	-0.40104953488782	2.02727413999243
H	-3.27892389311733	0.79014927408695	2.22463301113709
H	-3.83341581115214	1.24641687226924	-1.75785686767738
H	-5.81013647102105	2.26662108685726	-0.87757945188468
F	-6.60240712815739	0.60646122691206	-0.08731282970524
H	-2.35271523774442	0.38339947604091	0.05607553610680
H	-2.76001568966378	-1.17823572963299	0.78891211294049
H	-5.35717863588864	2.10389312914397	1.61040809704872
H	-3.94514790769326	2.42396019880671	0.61062667028620

2C_ae, Chloroform

C	-5.46220559298154	1.34657111867558	-0.40654185727484
C	-4.61136029314284	0.56224659388274	-1.38667709496017
C	-4.69474108213754	1.66815573288163	0.86258412182417
C	-3.95929334896749	0.47016517228390	1.43465220983419
C	-3.18388172206903	-0.26996009904369	0.36202196379200
N	-4.05739613911102	-0.61386581273181	-0.74357661736488
H	-3.56927973535162	-1.18882556498597	-1.41584845528196
H	-5.22678276430987	0.25873101815745	-2.23278863028397
F	-4.87357721400502	-0.40064089964621	2.02797353718214
H	-3.27826169902029	0.79079501997043	2.22411145819034
H	-3.83440649632615	1.24885854641081	-1.75961025007106
H	-5.80956444025038	2.26699237812385	-0.87768913372372
F	-6.60214133862827	0.60758978888032	-0.08896384754281
H	-2.35038772808573	0.38360251552426	0.05830904454741
H	-2.76109272467997	-1.17884780029905	0.78852393452616
H	-5.35823556567873	2.10224058039943	1.61051998846090
H	-3.94584211525448	2.42414171151632	0.61111962814605

2C_ae, DMSO

C	-5.46004027019351	1.34777867355927	-0.40641571489547
C	-4.61251902954012	0.56103628719522	-1.38571129330893
C	-4.69400634613466	1.66900110432919	0.86246067890706
C	-3.95840569896533	0.47184055860035	1.43345235729899
C	-3.18542556330307	-0.27066624967589	0.36233736930076
N	-4.06153138823021	-0.61873332392544	-0.74243295959256
H	-3.56198884779411	-1.18100172580365	-1.41799171472435
H	-5.22679225566405	0.26042402071247	-2.23373440248253
F	-4.87770299064433	-0.40152357496240	2.02673385879590
H	-3.27956040382336	0.78955914765111	2.22511274729180
H	-3.83241571605442	1.24399978588185	-1.75607823276059
H	-5.81081807041723	2.26622022414151	-0.87742817415050
F	-6.60271891396875	0.60523869311871	-0.08567783266853
H	-2.35505196408278	0.38309940746269	0.05388119195263
H	-2.75903052027168	-1.17766493777992	0.78933534372721
H	-5.35601997899488	2.10569005902390	1.61028598710446
H	-3.94442204191750	2.42365185047103	0.60999079020464

2C_ae, Water

C	-5.45993249280236	1.34783686642345	-0.40640514825838
C	-4.61257980711865	0.56098058381510	-1.38566234263010
C	-4.69396733572226	1.66904319114459	0.86245259561969
C	-3.95836388654853	0.47192673766521	1.43339117915640
C	-3.18550583932160	-0.27070293067385	0.36235795537508
N	-4.06173158231671	-0.61897462872648	-0.74238226174388
H	-3.56160380748831	-1.18058455073661	-1.41810373642803
H	-5.22679640702132	0.26051154642143	-2.23378055714447
F	-4.87792931015846	-0.40157404886008	2.02666386186224
H	-3.27963254749988	0.78949642050920	2.22516609789910
H	-3.83232824344453	1.24376602694029	-1.75590320943079
H	-5.81089339820544	2.26617464320464	-0.87740869459709
F	-6.60274962919578	0.60509127371764	-0.08550095290298
H	-2.35528263851782	0.38306604852518	0.05367500606067
H	-2.75893563683110	-1.17760999946924	0.78938045546564
H	-5.35588515546222	2.10589783689436	1.61027027372888
H	-3.94433228234499	2.42360498320515	0.60990947796799

2C_aa, Gas Phase

C	-5.47097876137534	1.35771671578347	-0.39663164729345
C	-4.63460383930349	0.54303454124519	-1.37071885329626
C	-4.69058217197634	1.68479067543584	0.86718312345597
C	-3.96596976609201	0.47994958112550	1.44734913392088
C	-3.21237294815964	-0.28593665344622	0.37154688212730
N	-4.04077668764428	-0.63324317080895	-0.76627576894878
H	-4.77106491100667	-1.27196299251279	-0.47406919915161
H	-5.25310156175406	0.24503545557483	-2.21705299073057
F	-4.88895919559416	-0.38279835869285	2.02327504239555
H	-3.28585197591205	0.79500246653540	2.24241018943031
H	-3.83090213298100	1.17825599172031	-1.75861464355216
H	-5.82559776009204	2.27650927485691	-0.86995914324974
F	-6.59544290824683	0.61283575472061	-0.06694387285313
H	-2.37940218688341	0.33231849748434	0.01968882817908
H	-2.78755609550398	-1.19195025862910	0.80313779726300
H	-5.35303574666132	2.12034202805009	1.61504972809058
H	-3.93906135081340	2.43809045155742	0.61237539421301

2C_aa, Benzene

C	-5.46777304438783	1.35886508416814	-0.39708363107202
C	-4.63561572516229	0.54333632105251	-1.37177151685213
C	-4.69016478862913	1.68436225410914	0.86664205708816
C	-3.96409810867657	0.48190457110385	1.44509850182922
C	-3.21148846825846	-0.28658526449046	0.37257294590398
N	-4.03891400629750	-0.63502795881056	-0.76859349012683
H	-4.76917185548015	-1.27451384488099	-0.47664504209218
H	-5.25533039085124	0.24622055432909	-2.21749832172931
F	-4.89287822797768	-0.38408634986696	2.02481826103629
H	-3.28610886631391	0.79412620171948	2.24140358021733
H	-3.83412859386410	1.18161311500981	-1.75771276218481
H	-5.82490066329782	2.27530679399864	-0.87020397731231
F	-6.59881790977794	0.61141689769341	-0.06420801828766
H	-2.37960442175684	0.33398955193962	0.02395965657417
H	-2.78724836685398	-1.19206242208324	0.80578078866336
H	-5.35080958826064	2.12296116460196	1.61447894732336
H	-3.93820697415394	2.43616333040658	0.61071202102137

2C_aa, Dichloromethane

C	-5.46520553534589	1.35962664112304	-0.39763325799476
C	-4.63592327646742	0.54354653338833	-1.37258148073794
C	-4.68995847733703	1.68377920727759	0.86618211581836

C	-3.96246759703109	0.48330502765411	1.44323102707051
C	-3.21073499206070	-0.28697772621433	0.37295537946078
N	-4.03856035797748	-0.63683115330604	-0.76973427825253
H	-4.77018869913780	-1.27421089480239	-0.47562956491596
H	-5.25607272242558	0.24788916303702	-2.21851586371766
F	-4.89550422637730	-0.38588554160999	2.02531983810379
H	-3.28623033986445	0.79331857424520	2.24071551914669
H	-3.83528789686134	1.18348505627119	-1.75630138942207
H	-5.82464253974548	2.27426487763406	-0.87048847473604
F	-6.60095645088947	0.60929627716916	-0.06279948061421
H	-2.38024755556263	0.33545264119371	0.02573083002949
H	-2.78600541373449	-1.19162754547630	0.80743026456367
H	-5.34926937002355	2.12458308279368	1.61399802496525
H	-3.93800454915829	2.43497577962195	0.60987079123262

2C_aa, Chloroform

C	-5.46601214110836	1.35938947187791	-0.39745296883172
C	-4.63583850322406	0.54348424744816	-1.37233035580435
C	-4.69001474239001	1.68398296520803	0.86631926238760
C	-3.96296352104884	0.48289411607800	1.44381016804623
C	-3.21096915863582	-0.28687208983384	0.37284941954897
N	-4.03861821647611	-0.63624637106262	-0.76941588028284
H	-4.76976081367094	-1.27441057952074	-0.47609602992213
H	-5.25586602890670	0.24739942050209	-2.21819077004609
F	-4.89467162722507	-0.38524839949929	2.02522558666411
H	-3.28618877845459	0.79356062995807	2.24093725805081
H	-3.83496781964096	1.18293608358104	-1.75675444963487
H	-5.82478891210774	2.27454953504838	-0.87040374000833
F	-6.60030080117749	0.60999437319739	-0.06319570677455
H	-2.37999168095207	0.33493197717432	0.02523745041512
H	-2.78648891072748	-1.19181039594128	0.80695605886132
H	-5.34974693245203	2.12408790038518	1.61414599565263
H	-3.93807141180176	2.43536711539920	0.61010870167804

2C_aa, DMSO

C	-5.46439247906829	1.35984366625463	-0.39782925126125
C	-4.63596882557855	0.54360517257920	-1.37282478146162
C	-4.68992592098310	1.68354943964797	0.86604032083576
C	-3.96194036361992	0.48372443625954	1.44263057868435
C	-3.21050816077213	-0.28708741216648	0.37302932788367
N	-4.03861616019593	-0.63747933583294	-0.77000138340918
H	-4.77084646297320	-1.27385246122004	-0.47492488139842
H	-5.25615000341853	0.24853532746011	-2.21894935280358
F	-4.89628580999275	-0.38658190428950	2.02541283352613
H	-3.28622267509678	0.79310886420153	2.24045302409097
H	-3.83546905054819	1.18397787063571	-1.75570910757643
H	-5.82451954260211	2.27395448045653	-0.87058389706051
F	-6.60159592812922	0.60847869678724	-0.06245545556035
H	-2.38056502742843	0.33597934642505	0.02609012227734
H	-2.78544700741062	-1.19140807557725	0.80788066908326
H	-5.34881555940755	2.12504428604724	1.61384841464013
H	-3.93799102277472	2.43459760233146	0.60964281950971

2C_aa, Water

C	-5.46430692299968	1.35986713244674	-0.39784980690490
C	-4.63597388539530	0.54360915434876	-1.37284966212548
C	-4.68992190006056	1.68352444358749	0.86602646239047
C	-3.96188761778667	0.48376542467832	1.44256990587170
C	-3.21048316884901	-0.28709579934326	0.37303626315685
N	-4.03862263056502	-0.63754711374317	-0.77002633821113
H	-4.77091706271226	-1.27381134446317	-0.47484452359344
H	-5.25616277405936	0.24859491589981	-2.21898866859041
F	-4.89636890192033	-0.38666009484451	2.02541343708077
H	-3.28622791319158	0.79308231508512	2.24043263293871
H	-3.83548832404133	1.18402361037222	-1.75565356025700
H	-5.82449983105839	2.27392640223133	-0.87059396484236
F	-6.60166241395646	0.60839983216940	-0.06242293333182
H	-2.38060084133402	0.33604117255232	0.02612290922549
H	-2.78537915825812	-1.19137997446135	0.80792358438542
H	-5.34876871825141	2.12509218538056	1.61383199376853
H	-3.93798793556052	2.43455773810340	0.60962226903856

3A_a, Gas Phase

C	-5.44550366907381	1.19405138930101	0.31043872632505
C	-5.04685627196144	0.62204667287035	-1.04003493234303
C	-4.24381475719489	1.73442572257075	1.07359974559617
C	-3.17608116294713	0.64684566895216	1.17025990220926
C	-2.80996938068274	0.11121088568718	-0.20689680939594
N	-3.99784740011896	-0.36954484238437	-0.88804153733569
C	-4.22561245533360	-1.62129288333338	-1.33397984798902
O	-5.21707289229398	-1.97559148041885	-1.91714388261915
C	-3.12530113730883	-2.68496977442765	-1.07398402400711
F	-2.86514550901390	-2.81265970828823	0.23353401696096
F	-1.97869959906623	-2.36815585459636	-1.69036327515819
F	-3.51868368051075	-3.85710403711291	-1.52685605893651
H	-5.89986311520877	0.15593235422599	-1.52382172899033
H	-4.68715295270579	1.44103705409058	-1.67216805790719
H	-2.37549898684093	0.91280084684762	-0.81458403945809
H	-2.06993018231161	-0.67588380253113	-0.13281302376129
H	-6.19322702298796	1.97862286499567	0.16627504422356
F	-6.04385406056683	0.18887523748600	1.05421027781911
C	-4.63782074415546	2.27967464905873	2.43699558267764
H	-3.84309615488841	2.55475573782889	0.46589452048767
H	-3.55167028597961	-0.17525425345962	1.78423815772100
H	-2.28317816711490	1.04301915620376	1.65564776290330
H	-5.09925025397934	1.49893510211888	3.04114830953922
H	-5.34858597527976	3.10175902183297	2.34325553198612
H	-3.76131418247433	2.64950427248198	2.96956963945247

3A_a, Chloroform

C	-5.44369926350448	1.20473772468360	0.29982514496613
C	-5.04227857728837	0.62967471046749	-1.04640457190754
C	-4.24608460734149	1.73069695128229	1.07490769293952
C	-3.17646668648884	0.64488650494288	1.16857402569450
C	-2.80850958406874	0.11204771956569	-0.20855549639792
N	-4.00173408971383	-0.37525681825940	-0.88570670158305
C	-4.23011205294670	-1.62102856829969	-1.31060384622281
O	-5.23647286475803	-1.99720046343221	-1.87210811714619
C	-3.12051355073061	-2.68047438312251	-1.07057651347274
F	-2.84579356509507	-2.82228900670422	0.23052306345731
F	-1.98440275851261	-2.36502530486500	-1.70126839072878
F	-3.52019522620571	-3.85483300145713	-1.52767613633381
H	-5.89874890757976	0.18167881438033	-1.53907749329057
H	-4.66127783982986	1.44267488406451	-1.67052827421374
H	-2.38727530269959	0.91458232498729	-0.82081018178616
H	-2.06293736535796	-0.66963933187021	-0.13508418803810
H	-6.18522705950115	1.99198044228410	0.15119680137691
F	-6.06366747685681	0.19376825199481	1.03652645734538
C	-4.64188620575039	2.27051071266156	2.44023536600564
H	-3.84438509942719	2.55438001258944	0.47391683611339
H	-3.54399572016363	-0.17864612428929	1.78621582034447
H	-2.28264542695161	1.04522897485950	1.64778470273258
H	-5.08662429555244	1.48486229170224	3.05140932500246
H	-5.36429679929947	3.08258254031724	2.34702590740840
H	-3.76579967437562	2.65314014151671	2.96463876773472

3A_e, Gas Phase

C	-5.46994851404299	0.99172527944880	0.12346310123420
C	-4.84204739253304	0.67393775608984	-1.22779824263646
C	-4.43604536680214	1.51622872570905	1.12724398864466
C	-3.28323391945578	0.51964996514373	1.20785510429205
C	-2.71006306441073	0.16506614939735	-0.16067110652153
N	-3.77113216399183	-0.28952678390241	-1.04538969195185
C	-3.73532965781814	-1.55146138128899	-1.51935478576539
O	-2.87301966293352	-2.35559494819704	-1.27631101282645
C	-4.88817675729607	-1.99492696312596	-2.46252639870861
F	-4.96682136647462	-1.21379158691013	-3.54646699913479
F	-6.07477424709121	-1.95197439660728	-1.83944681542055
F	-4.68797026880929	-3.23188735998188	-2.86635153689283
H	-5.58730815750376	0.29115756614045	-1.91374787069945
H	-4.41600887406090	1.57233206138346	-1.68147297443753
H	-2.23282725050876	1.04847799368545	-0.59258716433533
H	-1.96639848877443	-0.61985687408384	-0.06443115341360
H	-6.26194590666363	1.73062723421934	-0.00581529410191
H	-5.93391230973492	0.07747763518487	0.50255457405351
H	-4.90490018835421	1.55227846690390	2.11337272844201

C	-3.96205267592196	2.92479909336236	0.78355682668994
H	-3.62131981697559	-0.39670948008015	1.69911898704476
F	-2.25708594883053	1.04171009911502	1.97482522323784
H	-3.44271679292122	2.96965933604965	-0.17390334750346
H	-3.28131990615917	3.29873266537245	1.54539883515068
H	-4.81699130193155	3.59928974697194	0.72752502556011

3A_e, Chloroform

C	-5.47161901511679	0.99504143246315	0.13941084967410
C	-4.85328388888580	0.66208441065391	-1.21146084602758
C	-4.43289150098280	1.52841889974662	1.13329597215757
C	-3.29325354077765	0.52122690448020	1.21782904475985
C	-2.71957423267388	0.15359726204186	-0.14665844795617
N	-3.78559416935728	-0.31053309341892	-1.02389900578815
C	-3.73088383773239	-1.54500186964658	-1.53440080941166
O	-2.84830388059121	-2.34982239316038	-1.32945469185661
C	-4.88366223746635	-1.98820835034600	-2.47841054491649
F	-4.97279796910409	-1.20168173466550	-3.55558970597640
F	-6.06869594930127	-1.97522160072461	-1.85773955166766
F	-4.66491457990948	-3.22220918782207	-2.89908426787899
H	-5.60580313837089	0.28017353004706	-1.88954311765195
H	-4.41716181015677	1.54991631157020	-1.67406995034836
H	-2.24918682877707	1.03191552107346	-0.59474462448687
H	-1.97350393994786	-0.62689244690553	-0.03989779723189
H	-6.25924606053761	1.73624416261477	0.00154242741446
H	-5.93669852333714	0.08844152973031	0.53452035951182
H	-4.90091533727588	1.57596350203996	2.11898213833468
C	-3.95283450128237	2.93033613649995	0.77033516263194
H	-3.63577580826556	-0.38547341166631	1.72088936994895
F	-2.25120129299318	1.03936188104398	1.98053043730467
H	-3.42325526765649	2.95814094349204	-0.18230390472274
H	-3.28327018389972	3.32031639554312	1.53488686725085
H	-4.80902250560045	3.60128526331530	0.69367463693266

3B_a, Gas Phase

C	-5.42993332401969	1.27050777479790	-0.42109681956800
C	-4.57933056537978	0.56353824852171	-1.45975585950983
C	-4.62229783471579	1.66783935907157	0.80558460347840
C	-3.96016575166890	0.42054964612499	1.39417925295590
C	-3.15949221423096	-0.35319113025992	0.36403645571518
N	-4.03188843702179	-0.67300157313922	-0.81945813267207
H	-3.51574860241020	-1.22744426467661	-1.50196901726643
H	-4.82982810121469	-1.23493792208458	-0.50669733305933
H	-5.16897357885616	0.26731148837323	-2.32345457008424
H	-4.72614377888516	-0.22439417251289	1.83200405728748
H	-3.28836701997459	0.70183911258333	2.20489754823579
H	-3.73971900607031	1.18034439606406	-1.77543579638831
H	-5.92600442739999	2.13140462100280	-0.86999015318988
F	-6.40551201571051	0.35201371652500	-0.05243346058851
H	-2.32614746368784	0.23279040925678	-0.02306425871710
H	-2.78112282991039	-1.29416657830626	0.75531464306293
C	-5.48048956876374	2.39339660612288	1.83171006973522
H	-3.84064480685120	2.35104762979825	0.45477102910969
H	-6.31018934269652	1.76786448377467	2.15959860529631
H	-5.89033112473104	3.31429270120813	1.41741387568128
H	-4.88821020580075	2.65790544775419	2.70697526048551

3B_a, Water

C	-5.42961002696303	1.28560794127629	-0.42289934209994
C	-4.60255926837565	0.53641299971704	-1.44279906055647
C	-4.62600571603250	1.65868183484938	0.81135668790776
C	-3.97747680354756	0.40488625028830	1.39542226982493
C	-3.15773069171595	-0.34192985035938	0.36299631829201
N	-4.01107511486179	-0.67471447162848	-0.81544807056410
H	-3.46216694388976	-1.18161573532329	-1.50908435583764
H	-4.76122146855643	-1.30674090510520	-0.52834526899418
H	-5.20679014971246	0.21761053325437	-2.28666377401970
H	-4.74947609947422	-0.25466526232430	1.79960246247252
H	-3.32146906394580	0.67663876691606	2.22207161629635
H	-3.78255498701746	1.16000104241456	-1.79332165323963
H	-5.86499630887534	2.16743588481677	-0.89222151628684
F	-6.48449392262340	0.44503484216286	-0.04969370231058
H	-2.33879030895413	0.26824576794087	-0.01465409242968
H	-2.76190905732408	-1.27634850053656	0.74877398651782
C	-5.47347154565038	2.39772683924557	1.83557170194924
H	-3.83380091750239	2.32794295344123	0.46056399671348
H	-6.29399369973183	1.77112607873121	2.18621480841330
H	-5.89409690654699	3.30864682400015	1.40795805791729
H	-4.86685099869885	2.67552616622257	2.69772893003406

3B_e, Gas Phase

C	-5.48217838190564	1.17833932163102	-0.45670607257811
C	-4.64392435994611	0.44290898196898	-1.48336585515496
C	-4.68425574364962	1.56888309494579	0.79496358552282
C	-4.02799265783078	0.31614120162283	1.36670457170543
C	-3.20073098124849	-0.44522904717976	0.33343503189042
N	-4.05830619027624	-0.78776451272256	-0.84503556370683
H	-3.51190893451024	-1.31386274836910	-1.52805133506126
H	-4.82146546982430	-1.40093677064449	-0.54702129235142
H	-5.22861474988706	0.12233497811855	-2.34215959572921
H	-4.79833467595441	-0.34872606633500	1.77410541846443
F	-3.16846810567232	0.62670353025617	2.38390326918406
H	-3.80002572390437	1.03666157874816	-1.83078285341724
H	-2.38051175654914	0.17084727631649	-0.03080273151909
H	-2.80357524581453	-1.36500045131837	0.75519647353925
H	-5.39703898328103	1.92192249337294	1.54232779701612
C	-3.68502005704523	2.69052166052091	0.53614262148349
H	-6.34401858897639	0.55999514402409	-0.18804235288322
H	-5.88491207285102	2.07509098888080	-0.92808385068472
H	-2.93230989293583	2.43610367564103	-0.21174714719746
H	-3.16207398312057	2.95314028826371	1.45311775819513
H	-4.21010344481666	3.57849538225780	0.18557212328237

3B_e, Water

C	-5.48032590328183	1.18146509215347	-0.45036768207273
C	-4.64361230532196	0.44029789211908	-1.47369301028507
C	-4.68301548584132	1.57365471473723	0.80018324020721
C	-4.03891402873951	0.31262970872776	1.35679468683656
C	-3.20570588427502	-0.43757615473718	0.32883333412891
N	-4.05319650336552	-0.77683622283657	-0.84257682377578
H	-3.49618313543653	-1.28763911211117	-1.52748604537598
H	-4.80181804273951	-1.41298919694937	-0.56021190971693
H	-5.23806448331125	0.11042463746066	-2.32026645448759
H	-4.81182864558465	-0.35124258036257	1.75107809143053
F	-3.18787430468499	0.61818818730368	2.40918738623420
H	-3.80744317098898	1.03365481414859	-1.83794482230889
H	-2.38367253183788	0.17637862897771	-0.03297418621403
H	-2.81565612509748	-1.36062945505981	0.74662665799525
H	-5.39385898752156	1.92898358176796	1.54845998130086
C	-3.67831114369619	2.68839096004206	0.53224145087579
H	-6.33130593175118	0.55563670534725	-0.17105474339753
H	-5.88434643829103	2.07661731768570	-0.92268873297183
H	-2.93281294672146	2.41489957670473	-0.21507698334609
H	-3.15304662965084	2.96131139274250	1.44610492911419
H	-4.20477737186129	3.57094951213827	0.16850163582895

3C_ae, Gas Phase

C	-5.43273054528343	1.27508614414173	-0.42583579207112
C	-4.58737989178118	0.50369992433671	-1.42511929822128
C	-4.62570549239145	1.64643764571937	0.81145730417821
C	-3.97643674972745	0.38958359124345	1.38723726046660
C	-3.14728402263557	-0.32344273123004	0.32711231727972
N	-3.99324588189967	-0.65962600722665	-0.80290843199519
H	-3.49825800105744	-1.21862887510547	-1.48220651257219
H	-5.21632446012142	0.18670984922063	-2.25689397806749
H	-4.75852990191162	-0.28464036535231	1.74392069741675
H	-3.34874176839948	0.65458461046276	2.24032095739376
H	-3.83778307352100	1.21315215319649	-1.81678134884713
H	-5.82980255526458	2.17590674259206	-0.90243887933864
F	-6.52614288761513	0.50821696437768	-0.04945599052877
H	-2.30461914169936	0.32867966431813	0.03962463640245
H	-2.72759031521113	-1.24384053002391	0.73331431501944
C	-5.46537738075097	2.39661402492682	1.83359299437116
H	-3.82610129568476	2.30900968434612	0.45860413823267
H	-6.29790053156176	1.78010441296871	2.17207125214579
H	-5.87448970237891	3.31533022757170	1.40978890602288

H	-4.86395640110369	2.66454286951601	2.70308545271236

3C_ae, Water

C	-5.42480750960847	1.28212819555003	-0.43094781088892
C	-4.58562956280895	0.50419108858681	-1.42465473934977
C	-4.62985371832592	1.64452392787015	0.81307805399887
C	-3.97534228598678	0.39054714954397	1.38984588478239
C	-3.15793500227226	-0.33161006697156	0.32759125339593
N	-4.01275546869977	-0.67694855388592	-0.80115373778127
H	-3.48545853626173	-1.19875695063607	-1.48904539322007
H	-5.20542638738694	0.20444201667982	-2.26964859031762
H	-4.75066176397754	-0.27978740614924	1.77128958210396
H	-3.33534370723925	0.66439726540043	2.23065266724861
H	-3.81764021791224	1.19888042353649	-1.79855621391012
H	-5.82700493289081	2.17925519331000	-0.90508948957409
F	-6.53303565615856	0.50374879878935	-0.06027034599257
H	-2.32397550719620	0.31898095237658	0.02082014332047
H	-2.73070864532139	-1.24793021532323	0.73477508459600
C	-5.46939315772850	2.39517886280264	1.83533011915044
H	-3.83220481707878	2.30881899172346	0.46182679102827
H	-6.28942610527844	1.77340289603948	2.19652548936699
H	-5.89328304854553	3.30345080105538	1.40332827585521
H	-4.85851396932194	2.68056662970142	2.69279297618727

3C_aa, Gas Phase

C	-5.43512653895797	1.28716503891701	-0.41865075640972
C	-4.60059379971269	0.49761084283159	-1.41435286608239
C	-4.62605237816426	1.66360445568851	0.81506669827867
C	-3.97174938701846	0.41320318231285	1.40292368615557
C	-3.19406746821431	-0.35496124317561	0.33591637592508
N	-3.99120775664469	-0.68316956110784	-0.83593219269018
H	-4.71606408850765	-1.34552697058413	-0.58705343635762
H	-5.21745305479158	0.20805593490653	-2.26512988043259
H	-4.75202754862820	-0.23255083069261	1.81627954701119
H	-3.31367018854803	0.69385407277780	2.22870885286405
H	-3.80685407996603	1.15128417958178	-1.79150238351593
H	-5.86414079201468	2.17807794199165	-0.88550496065276
F	-6.50720603020997	0.48197058895662	-0.02951801244121
H	-2.34630085172088	0.25109774945562	-0.00251555042556
H	-2.77958757503326	-1.27592260920923	0.74624333111640
C	-5.47225899989343	2.40571804355601	1.83740681878105
H	-3.83085181039791	2.33022095584827	0.45954518377774
H	-6.30176458677099	1.77952441384137	2.16614611238155
H	-5.88596091491489	3.32396516267443	1.41773392198506
H	-4.87717214989013	2.66901865142939	2.71243951073159

3C_aa, Water

C	-5.42593561576171	1.29646073798278	-0.42565985903771
C	-4.60083097374252	0.49518107824316	-1.41640593860953
C	-4.62751868295063	1.65941257476311	0.81589976923416
C	-3.97208200310026	0.40886895693149	1.40130243482023
C	-3.18917174395717	-0.35326843798394	0.33613519462122
N	-3.99429565689742	-0.69128647308755	-0.83375658298782
H	-4.72797325002941	-1.33584205299921	-0.55923478491788
H	-5.22258678383465	0.20784969795237	-2.26453869148822
H	-4.74728910413506	-0.24464565326865	1.81320309640683
H	-3.31417796813334	0.69096508555807	2.22637299451561
H	-3.80645532180466	1.14622362415130	-1.79425857212470
H	-5.84066930295810	2.18985406449762	-0.89667806684768
F	-6.52461222635328	0.50201248805689	-0.04618944214177
H	-2.35038424437981	0.26179579107095	-0.00665726262777
H	-2.76954062920548	-1.27050650031459	0.74944127679323
C	-5.47530709829161	2.39909463877786	1.83921852158083
H	-3.83286010309474	2.32836596025615	0.46581723625584
H	-6.29128163458974	1.76520049938335	2.18870912446290
H	-5.90539481017395	3.30665914734945	1.41234345489977
H	-4.87174284660644	2.67984477267940	2.70318609719245

3C_ee, Gas Phase

C	-5.47320797736719	1.18593996695423	-0.46722318685084
C	-4.61478815024316	0.41997047428984	-1.46649687256561
C	-4.68671338317045	1.56684163253868	0.79471339727986
C	-4.02727124453835	0.30728996176333	1.34544980774821
C	-3.20185469055754	-0.42160755296042	0.29776584928666
N	-4.06527740977922	-0.76030116113580	-0.81901044998232
H	-3.58008505598180	-1.34715799340794	-1.48216181837856
H	-5.22965869636407	0.10171482207060	-2.30862639299749
H	-4.79684155535028	-0.37153020981139	1.72111961920910
F	-3.20390200125609	0.62935445130645	2.41534656525428
H	-3.82971767452534	1.07943574592454	-1.86609627406642
H	-2.35093662670425	0.21465343346338	0.01365549894912
H	-2.80355366854089	-1.33520358002211	0.73837649556328
H	-5.39421917585005	1.92176101900869	1.54869472275746
C	-3.68167327515284	2.68492887779352	0.53701154841212
H	-6.32124059320158	0.55382175149572	-0.19400016270342
H	-5.87275343401015	2.08967038645098	-0.93183987471684
H	-2.95658983117381	2.42002932758156	-0.23197297321117
H	-3.13201314879242	2.92619275515770	1.44508450997548
H	-4.20376240744052	3.58248589153846	0.20349999103713

3C_ee, Water

C	-5.47456942016063	1.18541221931488	-0.46238383681231
C	-4.61883260278201	0.41839706379059	-1.46229535805964
C	-4.68583698271775	1.56796397354596	0.79836114654518
C	-4.03533094782791	0.30361129525483	1.34144158197198
C	-3.20578965228007	-0.42381686295403	0.29848438580534
N	-4.06892896611223	-0.77093774814533	-0.82055038104946
H	-3.54933251285421	-1.31997050421590	-1.49284604900156
H	-5.23147062517967	0.10605860266949	-2.30796884244626
H	-4.80523909212942	-0.36994373692431	1.72381957644426
F	-3.20530793768391	0.61901278924496	2.42389534596977
H	-3.82680878697355	1.07098248749156	-1.85526612682839
H	-2.36289256601771	0.21627322229186	0.00297480208443
H	-2.80008516424044	-1.33463801346854	0.73833281173697
H	-5.39314291524040	1.92521058316062	1.55113360937759
C	-3.67837569915360	2.68257697306664	0.53262210150879
H	-6.32615742925070	0.55934826056607	-0.18416762934390
H	-5.87140881769420	2.08964657856530	-0.92755995282975
H	-2.95076458245002	2.40872341250603	-0.23100669999868
H	-3.13316211636864	2.94021254145393	1.43978415280498
H	-4.20262318288293	3.57416686278540	0.18648536212069

3C_ea, Gas Phase

C	-5.49136040192062	1.19775063619121	-0.45211701106064
C	-4.64582031895676	0.39999520237919	-1.44363859843824
C	-4.69102163853536	1.57677249552535	0.80232959634510
C	-4.03851628832382	0.31677745824543	1.36324689036289
C	-3.23770975764416	-0.44328049695848	0.31497671822600
N	-4.03445734317332	-0.78004437520561	-0.85162672874705
H	-4.74596358374184	-1.45969929613298	-0.61055037531543
H	-5.24792556861204	0.09214111609619	-2.29883625823956
H	-4.81607599204846	-0.34438958221648	1.76083456239574
F	-3.20686686130888	0.64358020678377	2.42571660995357
H	-3.84009334143798	1.02415849245636	-1.84021647052346
H	-2.39210706850722	0.17079677770292	-0.00648411076017
H	-2.82557884144197	-1.35153120126951	0.75420209478400
H	-5.38776336938655	1.94632761433952	1.55918690077586
C	-3.67613810380842	2.68237703571879	0.52859207836361
H	-6.35406424245113	0.58710909275344	-0.16822047651786
H	-5.88261844739962	2.10307562406960	-0.92274584062752
H	-2.95619091141360	2.40521169250056	-0.24129441291045
H	-3.12075594896555	2.92635350659822	1.43237102286791
H	-4.19175197092270	3.58195800042253	0.19071380906569

3C_ea, Water

C	-5.48836417334949	1.19452598031831	-0.45075078563799
C	-4.64281819382989	0.40392153118010	-1.44590526012639
C	-4.68864832283503	1.57560719705830	0.80370138079863
C	-4.04407728758583	0.31099472539645	1.35476730220699

C	-3.23308214682797	-0.44176397702989	0.31176130044816
N	-4.03457560748554	-0.78494513804273	-0.85453965461771
H	-4.76485014533213	-1.43557561630561	-0.58360648577510
H	-5.24998862570976	0.09858664584666	-2.29821139364713
H	-4.81849121585658	-0.35133640051054	1.75065532662369
F	-3.20663628758156	0.63058938333604	2.43197041937932
H	-3.83594218605517	1.02871029603078	-1.83878937881657
H	-2.39323096762577	0.17887335475329	-0.01260217352434
H	-2.82193856325568	-1.34934095915379	0.75369147999659
H	-5.38852359443599	1.94263626642284	1.55864627866161
C	-3.67441608613245	2.68157947184135	0.52735368118891
H	-6.34588509790100	0.57822064459785	-0.16554154932678
H	-5.88189797002101	2.09916658166736	-0.91985856514066
H	-2.94634910893141	2.39739947063554	-0.23258913333952
H	-3.12943013265359	2.94463694599416	1.43305972245614
H	-4.19363428659414	3.57295359596358	0.17322748819215

4A_a, Gas Phase

C	-5.32063049336662	1.67757617801567	0.54796178642108
C	-5.16179435138591	0.77450368828591	-0.67685186635826
C	-4.01139050504999	2.43055284505668	0.80187857055429
C	-5.79317068589127	0.88368933013287	1.76085641478462
H	-6.08655341971812	2.41524111220052	0.29688786434739
C	-2.80317077352875	1.51293281321855	0.86119864526217
H	-4.07112899291601	3.00688051535896	1.72608101518220
H	-3.83736200362426	3.14125731479495	-0.01194535113079
C	-2.75649990430487	0.56785138258753	-0.32653760472106
F	-2.83046440454224	0.76673196359218	2.02920826177716
H	-1.88187574998132	2.09955102009349	0.88186675901916
N	-4.02593328619052	-0.11315324256089	-0.51160864258013
H	-1.97643788256147	-0.17460577463641	-0.18899729125547
H	-2.53018559742452	1.15494066009562	-1.22374296422168
H	-4.98638082003521	1.38338801940143	-1.57062677794177
H	-6.06866098068237	0.20364657965984	-0.84208762166933
C	-4.03129348218651	-1.46096947224668	-0.55587417657582
O	-3.05459609759532	-2.15636827164205	-0.44882367515009
C	-5.39485364685087	-2.17151904354664	-0.77630741785036
F	-6.27743830012572	-1.86883728772563	0.18342982719092
F	-5.22362921638940	-3.47731317014679	-0.77265618287014
F	-5.93703534936831	-1.82944326161659	-1.95269890272270
H	-5.85115663260297	1.52499339863893	2.64020345453362
H	-5.10826006943900	0.06952716050039	1.99298063900698
H	-6.77937735423844	0.45651554248816	1.58002523696800

4A_a, Chloroform

C	-5.31766957395031	1.67220975639895	0.54856495027434
C	-5.16195605524306	0.77886323094643	-0.68331662042696
C	-4.00923735882080	2.42362180771485	0.80907485237546
C	-5.79503978964420	0.87308704400748	1.75615150397726
H	-6.08190645778595	2.41136567161726	0.29993900002490
C	-2.79700556416393	1.51419698433495	0.84796800667268
H	-4.06759034642810	2.98926444761981	1.73997603522501
H	-3.83845699595225	3.14348155829948	0.00353457338990
C	-2.75466561919164	0.57771367791495	-0.34387029645366
F	-2.81031753053168	0.74738534065129	2.01527269340536
H	-1.87804546290457	2.10120004790520	0.87002193947089
N	-4.02420350232441	-0.11405420481088	-0.51892134088829
H	-1.96060359600492	-0.15160212884323	-0.22422301493404
H	-2.55533264944513	1.17386742594316	-1.23904381347914
H	-4.97586074826301	1.39033714701736	-1.57058618809102
H	-6.07101831216350	0.21351311669258	-0.85412422821149
C	-4.04045277047807	-1.45028275249828	-0.52010704971566
O	-3.07210171561068	-2.16210795109172	-0.36036483438203
C	-5.39875118880840	-2.16171959982549	-0.77139949792752
F	-6.30365598957256	-1.86811620777172	0.16712741998308
F	-5.22099405641766	-3.47200359636650	-0.76112249674645
F	-5.91466616771453	-1.83127184857636	-1.96018225172213
H	-5.85103283001540	1.51234331060074	2.63751756880159
H	-5.11485619280938	0.05297223030334	1.98499389375162
H	-6.78385952575586	0.45330549181633	1.57093919562628

4A_e, Gas Phase

C	-5.35777216886636	2.14518523542154	0.20158376920497
C	-5.34693593346625	0.78647428020659	-0.49159763750300
C	-4.10066339760125	2.93712933771292	-0.09981952860126
H	-5.47813708325856	2.00666543834861	1.27926349086172
F	-6.46246482039927	2.84301304121939	-0.25184717749973
C	-2.84372070266521	2.12122971934170	0.20139990037274
H	-4.10453767183705	3.86795585650365	0.46950739038770
H	-4.11317864341616	3.20270063182780	-1.16250520616640
C	-2.91286966732125	0.79433546030227	-0.54790141083797
H	-2.82287369587951	1.88468642939930	1.27067445074771
C	-1.57272771826979	2.86826789616558	-0.16578104110474
N	-4.11720827065508	0.07501337997963	-0.18473518649012
H	-2.03137151542708	0.19644974373687	-0.34857530101691
H	-2.94160530362690	0.98635451201972	-1.62651350902818
H	-5.40529392681538	0.95281782730924	-1.57157815340519
H	-6.19522815992841	0.18572229363973	-0.17905021514205
C	-4.17923939212575	-1.09188453989332	0.48910734624515
O	-5.19481961476339	-1.62677839118759	0.85090059926453
C	-2.83497414759517	-1.80199544775385	0.81502627440207
F	-2.05486357875660	-1.03832040410382	1.59394500464767
F	-2.14602191405175	-2.09128829573240	-0.29533399350915
F	-3.06625366944261	-2.92891689548849	1.45506525667232
H	-1.55171789180561	3.09051285596983	-1.23465623482294
H	-0.69042490484371	2.27316480815756	0.07318578807235
H	-1.50144620718186	3.81086522689756	0.37570532424872

4A_e, Chloroform

C	-5.35106385837162	2.15513701238145	0.20535257557451
C	-5.34334546054104	0.78956971776552	-0.47206373036282
C	-4.10221818390316	2.94713743317910	-0.11506326691272
H	-5.47197834823492	2.03684346264057	1.28395524866208
F	-6.46919174507816	2.84226701739701	-0.25844229704589
C	-2.84670817295655	2.13663083672500	0.20610066886228
H	-4.10488519314132	3.88612859414645	0.44041386309591
H	-4.11188076178314	3.18874236141204	-1.18327588115011
C	-2.90687763078741	0.79698796368936	-0.51991250170485
H	-2.82972378627305	1.92427884649393	1.28021611651844
C	-1.57686376868127	2.87972824649759	-0.17380853634462
N	-4.11477770476570	0.07919248131619	-0.14778666331806
H	-2.02418009429955	0.20766967067867	-0.30224975783633
H	-2.93416562769589	0.96528111142800	-1.60126218055171
H	-5.38803504628353	0.93969491323417	-1.55437730414363
H	-6.19762684265222	0.19920184629608	-0.15807315327567
C	-4.17655968270690	-1.09906556620512	0.48247238359643
O	-5.19546317301599	-1.65888761025745	0.82284093317892
C	-2.83594088878822	-1.82066575472464	0.79825712046023
F	-2.05437759798090	-1.08932173545738	1.60074397282915
F	-2.14577323046783	-2.09509972711304	-0.31316402076571
F	-3.08128749526013	-2.96550769371339	1.41165713121146
H	-1.55799059989839	3.08259695570422	-1.24659826288852
H	-0.69401313050835	2.28980573376228	0.07613971938984
H	-1.51142197592471	3.83101388272343	0.35339782292140

4B_a, Gas Phase

C	-5.37169444385011	1.35528190571695	-0.50508886231781
C	-4.52838229875610	0.55984245780691	-1.49448660949698
C	-4.57292956947122	1.65368441639660	0.77149693176156
C	-3.88331817734129	0.43050050898243	1.34472419152197
C	-3.04325173473630	-0.28304686589981	0.30363088073081
N	-3.95316630422718	-0.65735132212569	-0.82276195538503
H	-5.11966231059244	0.21772651454938	-2.34119911542550
H	-3.67652206273211	1.13240310812396	-1.86009388195680
H	-5.22917555516508	2.07968057712311	1.53007641263202
H	-3.80054195989152	2.39983062346881	0.56624771195686
H	-2.26523505323487	0.36535458256169	-0.09579741135274
H	-2.60202638268324	-1.19005127185470	0.70804894713847
H	-3.46056796552787	-1.23687898500314	-1.50156231604703
H	-4.71592074066647	-1.22232037249246	-0.43509697764310
F	-4.82448109680916	-0.49817478588784	1.76703029791886
H	-3.26134342572151	0.69261647934424	2.20011026509318
H	-5.57496878274714	2.30890418022531	-0.99576161262730
C	-6.71607002687500	0.68271521014707	-0.23428042415939
H	-6.61831849773341	-0.30736645561746	0.21204202407120
H	-7.29599502785190	0.59555044023744	-1.15238114002181
H	-7.29471858338611	1.28020905419721	0.46879264360857

4B_a, Water

C	-5.37736418422571	1.35616249547129	-0.50423711485264
C	-4.52405938058506	0.57344177632356	-1.49164422518121
C	-4.57338710614793	1.66524181372514	0.76308716775306
C	-3.88556486944607	0.44951169668065	1.34811368030686
C	-3.08893093212529	-0.31063158693248	0.31378230003738
N	-3.95995243151230	-0.64758675543777	-0.84281524966180
H	-5.10078436035640	0.24465727540114	-2.35206270196430
H	-3.66948424199911	1.15580693826785	-1.83086596168978
H	-5.21519311092090	2.11397487503384	1.52161411864459
H	-3.79036658289572	2.39106840550385	0.53061991704575
H	-2.27595892252608	0.30796411151598	-0.06111720613518
H	-2.69084230796979	-1.23475615023208	0.72114458686847
H	-3.42546902008197	-1.18261618844327	-1.52639925603218
H	-4.71552374685866	-1.26279363219915	-0.53372783909223
F	-4.83843153285533	-0.43213451574790	1.87213903943397
H	-3.22430282380034	0.73187409823968	2.16572634372957
H	-5.59731083708649	2.30665359519032	-0.99281267693726
C	-6.70631066123006	0.66009271149926	-0.22259887876559
H	-6.57538493641059	-0.33727618087267	0.19764620477844
H	-7.28901489176716	0.57132995290708	-1.13925604443253
H	-7.28465311919906	1.23912526410570	0.49735379614662

4B_e, Gas Phase

C	-5.45427792442840	1.34054222173241	-0.48606921618633
C	-4.61400460692865	0.56956749656253	-1.49973023526816
C	-4.66757544975187	1.65109878690303	0.77020687426642
C	-4.05585303333124	0.38816688461368	1.37893536154146
C	-3.21487832350824	-0.34395786606981	0.34725265768233
N	-4.05003676386629	-0.66255740300983	-0.86354918554985
H	-4.86195256548007	-0.28485535757758	1.69573507149572
C	-3.20227317333190	0.71771046731262	2.59764594103193
F	-5.84028530618167	2.49283348438796	-1.11313756441456
H	-6.35825059608016	0.77193258585373	-0.24104086152165
H	-5.20280754955651	0.27677331675625	-2.36520150878695
H	-3.77182042656877	1.18190978625414	-1.81999351409065
H	-5.32041868604834	2.13545214549655	1.49642891472311
H	-3.87531937310336	2.36313075607136	0.52034366923575
H	-2.38844751283940	0.27640918799913	-0.00193298859733
H	-2.81920282881695	-1.28250917482564	0.73019250380132
H	-3.49321507290436	-1.17580384174073	-1.54813363376696
H	-4.81219021224860	-1.28511820041742	-0.58390745076158
H	-2.39650891501684	1.40412581495057	2.33269606184782
H	-2.76125346731547	-0.17674666349475	3.03655986541359
H	-3.81037821269287	1.19914557224180	3.36178923790458

4B_e, Water

C	-5.44995525996082	1.32742739227508	-0.47733513342176
C	-4.60933406494213	0.56821195397838	-1.49032526935513
C	-4.66287082082782	1.65943585197133	0.76894113185861
C	-4.05842543516503	0.39319290477415	1.37719174506663
C	-3.22248580193812	-0.34138646172875	0.34427313266079
N	-4.04684513899998	-0.65294286074162	-0.85941991408153
H	-4.87077040473931	-0.27260229480721	1.68616815405815
C	-3.20615263416743	0.71820110161171	2.59570139662441
F	-5.86727856927594	2.49385253391228	-1.10430755645411
H	-6.34627574459195	0.75533023435785	-0.22830031315824
H	-5.19914506108758	0.26637034353879	-2.35033566026013
H	-3.76895618687641	1.18113530643019	-1.81208070828398
H	-5.31280482353177	2.14809799782962	1.49542585482575
H	-3.86199783746736	2.35655169851828	0.50471867432618
H	-2.38960287126123	0.27225186874861	0.00120358654818
H	-2.84080920589548	-1.28384595468361	0.72767740478070
H	-3.48028513652347	-1.15289334036473	-1.54474964065089
H	-4.79977619875935	-1.29380537539151	-0.60070113461692
H	-2.39012141932873	1.39056709522011	2.32409698735235
H	-2.77676136327512	-0.18514766408717	3.02913619171132
H	-3.81029602138493	1.20924766863822	3.35811107046962

4C_ae, Gas Phase

C	-5.37353495094612	1.36370955778750	-0.51497385403349
C	-4.48941911228446	0.57451648541974	-1.48427524083930
C	-4.57393352935595	1.67182505992033	0.75586286556581
C	-3.89256255788304	0.44930122160945	1.34648342412022
C	-3.12549160168623	-0.31897181367745	0.28491712915893
N	-3.98542771212175	-0.62282829390299	-0.83758517050799
H	-5.07335381883360	0.28069174630407	-2.35774133900973
H	-3.67265215055984	1.22980977946011	-1.83174694257775
H	-5.21020064047750	2.13207084331201	1.51394633540481
H	-3.78443873298410	2.39115610261641	0.51662795126759
H	-2.26007577225996	0.30610018582841	0.00283589786374
H	-2.74656472114544	-1.24436117154557	0.71779705033811
H	-3.52398317037030	-1.23328546308987	-1.49530410178892
F	-4.83440290275032	-0.38362722740388	1.93521291970400
H	-3.20550912122784	0.75082285198409	2.14082631957263
H	-5.61067480736629	2.31791895456488	-0.99338594610201
C	-6.68325327110919	0.63823764088672	-0.22364262346393
H	-6.49508476114230	-0.36175111145138	0.16132096370753
H	-7.28313015534541	0.55215966055734	-1.13088868856172
H	-7.26882651015035	1.18298499082009	0.51845305018146

4C_ae, Water

C	-5.37526801393418	1.35796248705453	-0.51256965765440
C	-4.49561615005996	0.56298056704050	-1.47955388802487
C	-4.57759688978656	1.66523441146467	0.75948825117116
C	-3.88266211189371	0.45051972659779	1.34304717856632
C	-3.12225760922529	-0.32023435241183	0.28388347206679
N	-3.98824934079272	-0.64163086101202	-0.83636694688862
H	-5.07681386634512	0.27285323152791	-2.35606762897500
H	-3.67374343262967	1.21149556344633	-1.82148987291106
H	-5.21335507683486	2.12370403381843	1.51944122414883
H	-3.79008824680331	2.38617274287658	0.52124324236638
H	-2.26956674975503	0.31127305084470	-0.01249661076970
H	-2.72451963631066	-1.23775954281995	0.71702115120179
H	-3.48138875170328	-1.20435981946838	-1.50669164683018
F	-4.82891208511974	-0.39816797470913	1.94109088186161
H	-3.20076054473548	0.74892948174342	2.14014733830053
H	-5.60335539687741	2.31217604835397	-0.99418217573374
C	-6.69566261965750	0.65036634933280	-0.22463440182946
H	-6.52403329635746	-0.34508525989965	0.18089059007843
H	-7.28506957294195	0.55405786027152	-1.13801191505521
H	-7.28360060823611	1.21599225594780	0.50055141491039

4C_aa, Gas Phase

C	-5.38158216734614	1.36607674568950	-0.50397212349760
C	-4.52142324774851	0.53423641637144	-1.46495244877702
C	-4.57468175661505	1.67374012119431	0.76434770596319
C	-3.89392050470825	0.45167865026182	1.35563362762541
C	-3.13450331032911	-0.32665118986578	0.29437987050121
N	-3.94009708365871	-0.65470861453831	-0.86383534749039
H	-5.11105729322760	0.23633854209275	-2.33375185682415
H	-3.69367360028573	1.14806688327307	-1.83602582777969
H	-5.20599179990917	2.13998225987802	1.52309609206929
H	-3.78335565175861	2.38965318315824	0.52047120070031
H	-2.28776006280174	0.28438371890278	-0.03681342458632
H	-2.72855850654120	-1.23995768998214	0.72926745874814
H	-4.66121834286271	-1.31658542139477	-0.60597839532949
F	-4.85261667303443	-0.39742484973555	1.91096662943279
H	-3.22631420760605	0.74149171534727	2.17044988395085
H	-5.60317291991922	2.31874178119650	-0.99368453344824
C	-6.70796972862081	0.67160313256239	-0.21173589597046
H	-6.55618012210426	-0.32306576029336	0.20608632646144
H	-7.29442867086753	0.57404820074238	-1.12661377035058
H	-7.29653435005516	1.23754217513946	0.51091482860133

4C_aa, Water

C	-5.38195075271078	1.36364874999332	-0.50404050560851
C	-4.52010276555183	0.53891320333171	-1.46702021590341
C	-4.57621081414323	1.67261700398360	0.76392931943494
C	-3.88387510936343	0.45902537756168	1.35234456351681
C	-3.13649046201660	-0.33116597776712	0.29477770398150
N	-3.94765053601596	-0.66073945540521	-0.86558265888451
H	-5.10838506932926	0.24867142093483	-2.33933881149462

H	-3.68782343547104	1.15349980383138	-1.82469889967720
H	-5.20749207222729	2.13675119396504	1.52424818353643
H	-3.78755758994745	2.39053278953823	0.51968077551199
H	-2.28836634827096	0.27640170230958	-0.03632080943790
H	-2.73581389367289	-1.24441568550435	0.73494960509280
H	-4.68669965499323	-1.29810554979495	-0.59117986381051
F	-4.84232719869773	-0.39379030447644	1.93343367992155
H	-3.20968320870616	0.75112961418880	2.15856066461324
H	-5.60472198939828	2.31615662492654	-0.99225229536931
C	-6.70756925795522	0.66473327951414	-0.21712961909360
H	-6.55428730576812	-0.33683187130634	0.18519483187527
H	-7.29385434703920	0.57687790171111	-1.13332996056734
H	-7.29417818872132	1.22528017846446	0.51202431236240

4C_ee, Gas Phase

C	-5.44219363267079	1.31695295134887	-0.49594593460961
C	-4.56353341802956	0.56680217301526	-1.48237103490063
C	-4.67789555782341	1.64237667068300	0.77029800161210
C	-4.04980957137766	0.38583356189708	1.37583387005117
C	-3.23384736436580	-0.33963423636835	0.30978740036116
N	-4.06666752928050	-0.63556431672694	-0.84208227760230
H	-4.85338655497859	-0.29109941770042	1.68223957207935
C	-3.19599798107136	0.72510372634484	2.58881768603751
F	-5.87449357480048	2.49345553192271	-1.09098587972096
H	-6.32853874706403	0.71972178225675	-0.26861628854899
H	-5.14967652581459	0.29769192209882	-2.36056041712067
H	-3.76069557255661	1.25120859177267	-1.79952080413307
H	-5.33641690670471	2.13185133798882	1.49045738995319
H	-3.88571741376156	2.35387003029052	0.51244936460048
H	-2.36821222881299	0.29325550447337	0.04763250244970
H	-2.84751702256051	-1.27600220152991	0.71548157528070
H	-3.58066287894483	-1.22251523103627	-1.50424002426472
H	-2.37484691645050	1.38839524340573	2.30831118190115
H	-2.76549265992225	-0.17299428635640	3.03415294623492
H	-3.78554794300927	1.23080066221986	3.35423117033953

4C_ee, Water

C	-5.44163078413628	1.30932942267686	-0.49036076144939
C	-4.56572701145695	0.56419829590082	-1.47999263542496
C	-4.67888293185201	1.64408267991723	0.77127091820131
C	-4.05305966111407	0.38565315511260	1.37683410591034
C	-3.23942149534585	-0.34308771483272	0.31209972439150
N	-4.07158631064558	-0.64564145974351	-0.84439529590568
H	-4.85932595282332	-0.28494610781479	1.69116722306036
C	-3.19486700940340	0.72621220800468	2.58658612443214
F	-5.87882186518589	2.49504434544405	-1.09480886190376
H	-6.33431398076524	0.72316344404627	-0.26349401707550
H	-5.14776662441011	0.30004788772603	-2.36251644850351
H	-3.75462225769380	1.24183087539307	-1.78770379503102
H	-5.33678417982152	2.13178955832645	1.49322468526695
H	-3.88198636716088	2.34959615030857	0.51101252723974
H	-2.37793191056149	0.28916071341072	0.04126408464102
H	-2.85008340297371	-1.27741259710818	0.71892222519858
H	-3.55212619272761	-1.19682965758368	-1.51473386631334
H	-2.37065677774578	1.38285140506375	2.29849328537936
H	-2.76979866439154	-0.17429615422772	3.03263199850360
H	-3.78175661978496	1.23876354997952	3.34986877938227

4C_ea, Gas Phase

C	-5.45423337908562	1.33212647280812	-0.48332263735391
C	-4.60157152382584	0.54248469961155	-1.46636915461478
C	-4.67501434274791	1.65639578495600	0.77523132515335
C	-4.06697934588045	0.39675722501162	1.39546633314109
C	-3.27415880955682	-0.35926451014379	0.32756951831557
N	-4.03227674805777	-0.65385433081032	-0.87534845306916
H	-4.88270294430006	-0.25962317823475	1.72180304542750
C	-3.19728455822182	0.73054178817324	2.59835107604239
F	-5.87215635048320	2.51002768269037	-1.08687540386991
H	-6.35529828815468	0.76052197503033	-0.23698948183155
H	-5.18604873593766	0.27683459299272	-2.34687079867685
H	-3.78236572373153	1.18813949177301	-1.79886840702436
H	-5.31973936916920	2.16985359947253	1.49123009904388
H	-3.86995358942505	2.34822465657891	0.50420431001196
H	-2.40952544666024	0.24958960834980	0.03619359129452
H	-2.87992393132102	-1.29185635780054	0.73526567441361
H	-4.75240480802016	-1.33901327544586	-0.68319336635576
H	-2.38193494217884	1.39633547428983	2.30662224516219
H	-2.75586273135010	-0.16983938757327	3.02847842210965
H	-3.77344443189202	1.22990798827048	3.37781206268057

4C_ea, Water

C	-5.45029777159853	1.32143552969700	-0.47933648411130
C	-4.59792760539990	0.54370502949796	-1.46867963768077
C	-4.67267282543810	1.65766039670803	0.77333734215351
C	-4.06469147468607	0.39623123903604	1.39085821591939
C	-3.26725111991502	-0.35588317957760	0.32566615673702
N	-4.03227417330086	-0.65896163035232	-0.87756469156188
H	-4.88055328122895	-0.26152626785008	1.71120946694249
C	-3.19854000462800	0.72843767553019	2.59672745348029
F	-5.87865838214995	2.50784605555307	-1.09220097028374
H	-6.35085510401338	0.75198788788620	-0.23637037160480
H	-5.18701404540104	0.27888935661275	-2.34655457702219
H	-3.77662608045085	1.18997350754400	-1.79508073756588
H	-5.31954538034614	2.16431407822416	1.49236610781771
H	-3.86584399143312	2.34760364694549	0.50179828016875
H	-2.40624884306480	0.25633994985319	0.03157588015679
H	-2.87545870704176	-1.28727428317690	0.73779805441114
H	-4.77494641070836	-1.31196978458145	-0.65170429854441
H	-2.38148127575088	1.39380026518289	2.30753315081495
H	-2.76179533656723	-0.17499129228457	3.02573379504070
H	-3.78019818687704	1.22667181955195	3.37327786473222

5A_a, Gas Phase

C	-5.35156944613965	1.52792395526125	0.55258893582623
C	-5.05550002473412	0.88148605541547	-0.79604015885387
C	-4.11083534024932	2.21964842567233	1.10890262249906
C	-2.91156624208247	1.29040726482192	1.09203763761524
H	-4.28119420500294	2.57472986832429	2.12513598297369
H	-3.86211896220589	3.09173084469829	0.49686561948947
C	-2.70011841888429	0.68148666982358	-0.29429644009005
F	-3.11523790152011	0.26312462842068	1.99825749816711
H	-2.00400140410945	1.81767513054891	1.39671385866379
N	-3.92671067693156	-0.03339395642719	-0.67719096241124
C	-1.38184582877786	-0.06638754864989	-0.39359105067355
H	-2.64492332863389	1.52610520478295	-0.98928322314150
C	-4.05434456943486	-1.37156931597331	-0.53414250025538
O	-3.18317974885289	-2.13846230231790	-0.22314026395910
C	-5.45357512021448	-1.99100412413028	-0.83574095086604
F	-5.87564848103951	-1.70484999384462	-2.07430331938824
F	-6.38314254938169	-1.55099432635340	0.02467852970914
F	-5.39175537904637	-3.30177388186613	-0.72388486045993
H	-6.16902765518337	2.24113044125891	0.44576180725426
H	-5.67949971348004	0.75036960279242	1.24439478735514
H	-5.92676012689435	0.36929873282520	-1.18410682912599
H	-4.77912251205574	1.64308035018653	-1.53040269871275
H	-1.29758400355620	-0.60731509367328	-1.33303091945476
H	-1.25151651834788	-0.77202143502022	0.42002286306995
H	-0.58389184324106	0.67754480342349	-0.35227596523066

5A_a, Chloroform

C	-5.35102640485844	1.53042246383733	0.55625248018235
C	-5.05848239827673	0.87981372590034	-0.79051231919649
C	-4.10838481818539	2.21913848716943	1.11222151189152
C	-2.90475172576868	1.29937721311163	1.08999295466850
H	-4.27663929813574	2.57418747201324	2.12886739459639
H	-3.86067129293037	3.09046974193237	0.49993599212138
C	-2.70052240291694	0.67792016666619	-0.28909447725001
F	-3.09292967420362	0.26843366549863	2.01129596499144
H	-1.99855142271027	1.83104373436956	1.38515812233528
N	-3.93258037670308	-0.04335323228132	-0.65597565335580
C	-1.38163559067334	-0.06551234797895	-0.39742524538542
H	-2.65605550199367	1.51506336906338	-0.99099976644892
C	-4.06399901221463	-1.36933029629185	-0.51953705114261
O	-3.20085610554313	-2.14908038728791	-0.18738194024851
C	-5.45626369635103	-1.99009188034649	-0.85031846486100
F	-5.85934258045356	-1.70473873490306	-2.09298553218686

F	-6.40253997216699	-1.56899812277429	-0.00204688273825
F	-5.38773424888013	-3.30668144991720	-0.74610764549079
H	-6.16162026642067	2.24954504895461	0.44151062544340
H	-5.68960035635980	0.75877610737974	1.25033605378417
H	-5.93250146972674	0.37268389741337	-1.17862286919193
H	-4.76926851943901	1.63374461171339	-1.52521861964145
H	-1.30518105051226	-0.60878862992198	-1.33660665788305
H	-1.23336960850147	-0.76128289777974	0.42193235341001
H	-0.59016220607429	0.68520827445958	-0.37074032840333

5A_e, Gas Phase

C	-5.21965986631879	1.78490561473569	0.66499931661582
C	-5.14645535976138	0.82260905350617	-0.52468911108741
C	-3.90241564335368	2.46790482009921	0.95483238006518
C	-2.83368463585809	1.40543959173479	1.17876033606894
H	-4.01092196857453	3.11060509271175	1.82816114967513
H	-3.63327279293227	3.10517739968930	0.10890890237792
C	-2.73142731617377	0.48112188325925	-0.02348378541131
H	-3.07857329919610	0.80805245990320	2.06068575772185
H	-1.86283683754271	1.86706254416773	1.35579252120065
N	-4.02826905604260	-0.10964037427690	-0.32183334751586
H	-2.01013919548479	-0.30204700564939	0.17501531021140
H	-2.37726037852872	1.03923082058196	-0.89604229783036
C	-5.04646725009895	1.54121725981085	-1.86393983421315
H	-6.05241503502795	0.22138179124948	-0.52324889312081
C	-4.21186825711848	-1.37840648662533	-0.75159702221847
O	-5.24429900812758	-1.80778659756527	-1.19808578821640
C	-3.01623621609837	-2.36719627382066	-0.64822146985301
F	-2.00524506609483	-1.98944279527820	-1.44136895935530
F	-3.39791281241402	-3.57053493939685	-1.02360126408385
F	-2.54587327511008	-2.45663032232670	0.60235640137537
F	-6.19187441821884	2.73211210996373	0.39594199602209
H	-5.55016770886763	1.23015517834963	1.54717977098812
H	-4.11562327007214	2.09897118547991	-1.96452039392687
H	-5.87186037559299	2.24279872917394	-1.96777699018252
H	-5.10565095739070	0.81260926052271	-2.67101468530714

5A_e, Chloroform

C	-5.22480834696386	1.71904403702067	0.65276236361777
C	-5.13661376594976	0.84088880813108	-0.60048651235461
C	-3.92264760980063	2.40914978123673	0.98640675854476
C	-2.82425209915139	1.36068816168076	1.12766624509735
H	-4.04009259295805	2.97760440976342	1.90872173768552
H	-3.66991191478052	3.11398394990186	0.19069107146144
C	-2.72180669728695	0.51630166999921	-0.13230991224349
H	-3.03924913729182	0.70522562676050	1.97534579258683
H	-1.86312337924088	1.83796365781687	1.31367597091528
N	-4.01252242030303	-0.09216545427299	-0.43476543187945
H	-1.96553039999294	-0.24891893187487	-0.01353356248379
H	-2.42403551400445	1.13812519344244	-0.97963816840555
C	-5.01659812833364	1.64806365519640	-1.88597266923516
H	-6.04031907107843	0.23990558195984	-0.64916016430545
C	-4.22250132590048	-1.38986440674903	-0.68962863677475
O	-5.28060694245658	-1.87335992674874	-1.02980423157055
C	-3.02735128552890	-2.37316526394067	-0.53172651130374
F	-2.04404155212124	-2.10166877347613	-1.39613585741903
F	-3.43609492174710	-3.60870151346255	-0.76595913376539
F	-2.51373925457265	-2.34436380382737	0.70271838696469
F	-6.22090075931877	2.66825617926238	0.44292048737061
H	-5.54818588772883	1.10288330060938	1.49428911055192
H	-4.11547321984284	2.25931967573383	-1.91149184898704
H	-5.87540516882679	2.31026326197631	-1.97980783043538
H	-5.00459860481946	0.97421112386067	-2.74156745363279

5B_a, Gas Phase

C	-5.30245000103960	1.34087243303636	-0.40927694851086
C	-4.45407088251991	0.62424958808334	-1.45330532478753
C	-4.49204444530705	1.71718385795238	0.81300087349567
C	-3.84033489028377	0.47943867382439	1.42370927103133
C	-3.06765628134134	-0.32676911079303	0.39563844032510
N	-3.95131166868052	-0.62701432807634	-0.78125654713651
C	-5.20931230869411	0.27504429438845	-2.71279485055262
H	-3.57021307158012	1.22364311925841	-1.67504092156069
H	-5.13888622160076	2.20416541719527	1.54098394313471
H	-3.73758055274114	2.44871022447942	0.51256078224014
H	-2.21653967215877	0.22764269105150	0.00116731592347
H	-2.71736437713869	-1.27417125385490	0.79739835644651
H	-3.46127109319145	-1.20922906489665	-1.46086023350431
H	-4.77464090170823	-1.15270674657080	-0.46864402946445
H	-5.78601664674922	2.20569065292723	-0.86312408393400
F	-6.29333768460192	0.43947762736975	-0.03774018389446
H	-4.60542196091105	-0.14966312397720	1.88166569872576
H	-3.15172053200235	0.76471181435240	2.21753281463088
H	-6.11199363142443	-0.29103171534061	-2.48548541124911
H	-4.59010784885134	-0.29131910400822	-3.40829067116819
H	-5.50587532747421	1.19645405359886	-3.21175829019086

5B_a, Water

C	-5.28837993307852	1.37051550935102	-0.41759079132961
C	-4.46151666377202	0.61460117834246	-1.44361971748597
C	-4.48817584845815	1.71270157586821	0.81909802490763
C	-3.86075121438477	0.46077591126981	1.42201808437982
C	-3.06691336821608	-0.31589889174883	0.39117513567919
N	-3.93149046423157	-0.62048672448183	-0.78718688758797
C	-5.23120945647766	0.25213445891180	-2.69053365014418
H	-3.58921222221040	1.21938753769330	-1.69158261905534
H	-5.13387393317373	2.21118834058659	1.54094478129595
H	-3.71286783332001	2.42418085181408	0.52526476071378
H	-2.22673716971612	0.26234786038561	0.01028267216632
H	-2.70486477668882	-1.26282084456154	0.77953682114347
H	-3.40502425762561	-1.16537182887187	-1.47032654356846
H	-4.71688363455025	-1.20871463013466	-0.49664707226530
H	-5.70815597333902	2.25954335872513	-0.88613693497642
F	-6.35789360829031	0.54364366012252	-0.05398793298618
H	-4.63755888521270	-0.18181761923143	1.83962537455635
H	-3.19052274877224	0.72860443235743	2.23714965544687
H	-6.10812408743012	-0.34638561585730	-2.44759440928617
H	-4.60003802564991	-0.30122642575558	-3.38433036138432
H	-5.55795589540196	1.16847790521510	-3.17947839021949

5B_e, Gas Phase

C	-5.37879805157138	1.36485345394075	-0.43854993249419
C	-4.54720329878734	0.60214770623883	-1.45044104432100
C	-4.57693077821790	1.70560554533464	0.81608018729226
C	-3.98464703554929	0.44716214315472	1.41844848511581
C	-3.13242462717048	-0.34594405360422	0.41741680856248
N	-3.98611600853128	-0.63189271534800	-0.80017433986488
H	-5.21821197032631	2.18231172570311	1.55593373468964
H	-3.77773142633580	2.41154095697185	0.58475736598948
C	-1.85512083897703	0.36146877033865	0.02040321146867
H	-2.89768743603491	-1.32035178167735	0.84470274941610
H	-3.42511966305642	-1.15484241799959	-1.47485758478685
H	-4.76344105975246	-1.24028719887618	-0.53267445431038
H	-4.78759672135100	-0.19446714133531	1.79859521818341
F	-3.16647240363778	0.75232954441925	2.47181561081248
H	-5.74416667076776	2.27426244873292	-0.91354928713091
H	-6.26388877201636	0.77724916268397	-0.17750003090912
H	-5.13087344187332	0.27813928172551	-2.30891503132655
H	-3.69984082858934	1.18471064677344	-1.80474827955857
H	-2.02666140392737	1.36812588124010	-0.35462501440697
H	-1.30091232920821	-0.20621305948433	-0.72748991592448
H	-1.22915523431827	0.44696110106722	0.90590154350358

5B_e, Water

C	-5.37147905370215	1.36755087905366	-0.43759537663377
C	-4.53972417952531	0.59654134348764	-1.44175803152152
C	-4.57137588676922	1.70921144496651	0.81784120820733
C	-3.99504734107002	0.44232577284746	1.40871206579326
C	-3.13632277858941	-0.34142947230729	0.41418677885771
N	-3.98144758858713	-0.62633017911071	-0.79154243756877
H	-5.21419667306398	2.18671857406680	1.55626768228892
H	-3.76518343417289	2.40478974139507	0.57904672860176
C	-1.86043849483963	0.37129422587161	0.01839175006176
H	-2.89945417159596	-1.31414982043683	0.84004914636528
H	-3.42504678594925	-1.15290860801142	-1.46611971702738
H	-4.75195494484277	-1.24415292173849	-0.52876302980534

H	-4.79936902698961	-0.19999090159247	1.77479280543275
F	-3.18705515980383	0.74232168024855	2.49648336363484
H	-5.72916095685550	2.27745377950060	-0.91617458368881
H	-6.25101133993127	0.77645818946962	-0.17133728957788
H	-5.12831510481325	0.26206830477890	-2.29079840823593
H	-3.69790667044857	1.17942081940436	-1.80688814475603
H	-2.03727561413765	1.37846680052728	-0.35312674427395
H	-1.33090561897436	-0.19669979596137	-0.74572041136943
H	-1.22032917533825	0.44391014354049	0.89458264521521

5C_ae, Gas Phase

C	-5.27191402229245	1.39076427023461	-0.43100440782299
C	-4.43388339925708	0.60251799138947	-1.43367192687306
C	-4.48319212089023	1.70245026565255	0.82657014311330
C	-3.87725674095202	0.43140769523292	1.41088985121235
C	-3.06110329450710	-0.29717564153375	0.35164964698283
N	-3.90323848315624	-0.58618329613386	-0.79451905398950
C	-5.24368477535786	0.22458911430065	-2.65859642857471
H	-3.62467700688325	1.29327852177069	-1.73517193794825
H	-5.13042950366535	2.20516918611702	1.54599124881848
H	-3.68722250161680	2.40357863643281	0.55726169884074
H	-2.19112258219842	0.32576372415002	0.08200138124631
H	-2.68167627737712	-1.23775001038476	0.75112943226866
H	-3.42353705688933	-1.16514315830936	-1.46987638139560
H	-5.62182341343715	2.31048109491165	-0.90752090827382
F	-6.40311839704665	0.66432006929438	-0.08663869516377
H	-4.67733971223328	-0.22571430143228	1.75479970724826
H	-3.24800006292407	0.67171711201563	2.26878777219676
H	-6.09576437062751	-0.38544437166925	-2.36366549559576
H	-4.63431399441541	-0.34472721707353	-3.36182380826713
H	-5.60690228427269	1.11606031503440	-3.17053183802308

5C_ae, Water

C	-5.26839011122947	1.39119358622293	-0.43104207356975
C	-4.44113117276307	0.59424095558247	-1.43010232405927
C	-4.48575553206485	1.70123537394824	0.82742098301644
C	-3.87446537464621	0.43372850923709	1.41461340255196
C	-3.06789909542224	-0.30173908109034	0.35390744011298
N	-3.91801087580270	-0.60470399216203	-0.79069743757974
C	-5.24400397973158	0.22893423962717	-2.66357530861993
H	-3.62313613735496	1.27262670844407	-1.72563267582579
H	-5.13159260651335	2.20831698568158	1.54534036610042
H	-3.69114831327469	2.40125768064672	0.55366376407693
H	-2.20779293534620	0.32266860897765	0.06565544793256
H	-2.67789949920450	-1.23722159873273	0.75486374819855
H	-3.39922859501090	-1.14320791892761	-1.47383551915822
H	-5.62681288424886	2.30553813582885	-0.90677010649513
F	-6.41162989281178	0.65601119960172	-0.08036697278088
H	-4.66725801104926	-0.22157845834616	1.78159970316917
H	-3.23442315554006	0.68281563122096	2.26166489281732
H	-6.11031332800779	-0.37163546468351	-2.38721551737684
H	-4.63117348826591	-0.34668271462041	-3.35820704784840
H	-5.58813501171164	1.12816161354336	-3.17522476466236

5C_aa, Gas Phase

C	-5.29199889287462	1.38222403869983	-0.41680245348370
C	-4.45959108651634	0.58307048296515	-1.41709603237274
C	-4.48426046752409	1.72095613795320	0.82214261799402
C	-3.86687331718457	0.46394076535621	1.42965966732401
C	-3.11278844708032	-0.33108465324904	0.36531127613780
N	-3.91028447708604	-0.62180651085170	-0.81657174713157
C	-5.23951520275565	0.24446056229869	-2.67300512560704
H	-3.60929254998650	1.22001386814188	-1.69007179029631
H	-5.11710483912111	2.23958986396120	1.54294792823366
H	-3.69482894500722	2.41713060761538	0.52224801816024
H	-2.23712091082266	0.23903172683439	0.03619389195039
H	-2.74090941369922	-1.27018746057600	0.77566165676725
H	-4.67245026114317	-1.24788198314205	-0.57852007681072
H	-5.69684498594508	2.28345171566444	-0.88363857613625
F	-6.38502559890737	0.60050421635795	-0.03983455003272
H	-4.66004881701759	-0.16051756754031	1.84684320017519
H	-3.19761866211182	0.72946581700227	2.24998929653514
H	-6.10008664437311	-0.37992806275247	-2.43154615886604
H	-4.60153519179195	-0.29754853585839	-3.36899511407646
H	-5.60279128905158	1.14989497111936	-3.16013592846414

5C_aa, Water

C	-5.28063808414466	1.39140982779517	-0.42401818535281
C	-4.45916814686869	0.57856319260721	-1.41878932120211
C	-4.48443413587173	1.71653809984316	0.82298629431433
C	-3.86882350626748	0.45825443056355	1.42909415448389
C	-3.10763662913866	-0.33000573708554	0.36732140644511
N	-3.91297383211961	-0.63086155609139	-0.81302152896257
C	-5.24326135798392	0.24039813091679	-2.67256868677711
H	-3.60911256335498	1.21312589219759	-1.69392294452612
H	-5.12154309888698	2.23444962325179	1.54090435349168
H	-3.69325612467576	2.41275424952428	0.52979740626490
H	-2.24125078669557	0.25083400133561	0.03416052135539
H	-2.72922413400633	-1.26531793189588	0.78016660915689
H	-4.68335056362328	-1.23867690902459	-0.54941624731540
H	-5.66890902884592	2.29599103550602	-0.89455528221184
F	-6.40181558607246	0.62465372231128	-0.05461754125774
H	-4.65768495202241	-0.17469592154407	1.84296580076107
H	-3.20152102017250	0.72438144167471	2.25045902909053
H	-6.08129386109232	-0.41650878840960	-2.43596529669415
H	-4.59908563627552	-0.26645343747521	-3.39026460057847
H	-5.63598695188122	1.14594663399912	-3.13593594048547

5C_ee, Gas Phase

C	-5.37942591438599	1.36889780917727	-0.44176052417783
C	-4.52398126980586	0.58957123999242	-1.43103406757606
C	-4.57609808845976	1.70125565726565	0.81425156664057
C	-3.97910242911899	0.43377841059431	1.39019343599674
C	-3.14128511833474	-0.33509864745826	0.36787623856295
N	-4.00111936798237	-0.60181240666197	-0.78045307028470
H	-5.20268448314382	2.18039125425628	1.56738844861144
H	-3.76910208761307	2.39738665959051	0.57325465302721
C	-1.82824487117724	0.37231395604631	0.04034412956215
H	-2.90201139291078	-1.30174914201104	0.81715285584407
H	-3.52559600884837	-1.19935479517369	-1.44251768924695
H	-4.77742672620928	-0.22154921740927	1.74667482803629
F	-3.18606845594809	0.74776444242101	2.48552098578721
H	-5.75094023387065	2.28351540268670	-0.90530777077288
H	-6.24557967175470	0.75909568939858	-0.17366684408430
H	-5.12952145793765	0.27301456969064	-2.28062018146024
H	-3.73688474627922	1.25015151063851	-1.82310865849204
H	-1.98744631117619	1.35098097141498	-0.41088685025365
H	-1.25248713545854	-0.23268017215946	-0.66136230772728
H	-1.23554422958471	0.51058680770053	0.94316082200732

5C_ee, Water

C	-5.37715442822765	1.36860994849063	-0.44149023992526
C	-4.52363829277466	0.58412224044289	-1.42739445386748
C	-4.57506245564919	1.70319668298761	0.81543225049815
C	-3.98749233284174	0.43259436251758	1.38759935452520
C	-3.14356405619872	-0.33688839567838	0.37357591112717
N	-4.00256409720005	-0.61446491701741	-0.77740252317653
H	-5.20538981267478	2.18375666979071	1.56468607948219
H	-3.76633336847980	2.39544252143208	0.56910281860651
C	-1.83583072370508	0.37429533685362	0.03430048624648
H	-2.89674937173146	-1.30020654081265	0.82564213015002
H	-3.49220992494860	-1.17949504678985	-1.44495252482675
H	-4.78605661787454	-0.21749029442963	1.75089936724159
F	-3.19112204561220	0.74435382179379	2.49649178334658
H	-5.74092955397503	2.28414667509889	-0.90854141026806
H	-6.24934183171206	0.76790293246082	-0.17027449805896
H	-5.12620344194721	0.27097093305846	-2.28007784079616
H	-3.72949764866809	1.23665533182440	-1.81411073361723
H	-1.99994125690930	1.35933473708790	-0.40101667839854
H	-1.27733841007266	-0.22612618226161	-0.68489079750101
H	-1.22413032879717	0.49574918315016	0.92752151921208

5C_ea, Gas Phase

C	-5.38878697421703	1.38424494015091	-0.42960621815286
C	-4.54905379996220	0.56642038600689	-1.40850048540025
C	-4.57469076841789	1.71478953698938	0.82082290441949
C	-3.98628958447234	0.44760783861697	1.40907845525799
C	-3.16410006109727	-0.34271490406799	0.38676841145193
N	-3.95835523088080	-0.62030805405434	-0.80779344841620
H	-5.19043684772246	2.20824177553169	1.57340957449696
H	-3.76096587083899	2.39905720579667	0.56949305149249
C	-1.85761797806821	0.35584979852346	0.03377683199966
H	-2.91245570501641	-1.30687097397401	0.83333821508601
H	-4.68183835974062	-1.29655711154861	-0.59742028989489
H	-4.79412833977571	-0.19403396354255	1.77701653067708
F	-3.19626398429087	0.76538463621331	2.50597742690022
H	-5.74615988076084	2.30035714136422	-0.90353008565833
H	-6.27255768646245	0.80172801325062	-0.15088170043942
H	-5.14603108361518	0.25369402659762	-2.26555299431188
H	-3.74219795113776	1.18752077282383	-1.80572892374785
H	-2.01773930924804	1.33998503753428	-0.40519610799710
H	-1.30800752602110	-0.24847975994978	-0.68608975124239
H	-1.25016305825384	0.48764365773742	0.92725860347933

5C_ea, Water

C	-5.38431939360078	1.38219469729783	-0.43035413348782
C	-4.54569716788534	0.56757408474092	-1.41060106131321
C	-4.57118572251492	1.71365067706049	0.82089324043763
C	-3.99306104909419	0.44128596563895	1.40037834755582
C	-3.16045140008838	-0.34417103323869	0.38585640083501
N	-3.95947454697882	-0.62752603812583	-0.80843695198422
H	-5.19278340954683	2.20363940632393	1.57122185101900
H	-3.75703131018718	2.39701362892555	0.56742483723428
C	-1.85818216346995	0.36109355024955	0.03040488182185
H	-2.90930117549152	-1.30688545526677	0.83532879745479
H	-4.70360829267601	-1.27279553712647	-0.56599597854777
H	-4.79881192258949	-0.20078552787011	1.76586876797291
F	-3.20067754582278	0.75278853999930	2.51424778833870
H	-5.73905953588885	2.29873559279117	-0.90443434060576
H	-6.26582743349618	0.79748305590258	-0.15107523662110
H	-5.14829158705804	0.25597633245979	-2.26392605780702
H	-3.73780472072005	1.18819115237703	-1.80563371227918
H	-2.02443166423443	1.34147396860786	-0.41472180380885
H	-1.29869870847432	-0.24412091084909	-0.68241672589120
H	-1.24914125018195	0.49874385010201	0.92261108967612

6A_a, Gas Phase

C	-5.58116969620360	1.05703266168691	0.11361930661183
C	-4.84870271723792	0.68413667980728	-1.17069919150009
C	-4.61504077111808	1.48403400577474	1.20175642704247
C	-3.52419661247637	0.43692273549356	1.40232830739513
C	-2.85726283127750	0.08717560017572	0.07358432243895
N	-3.88080957597255	-0.35964953773765	-0.89161949902441
C	-4.18484250260682	-1.66968237774537	-1.05123950347371
O	-3.68959805930751	-2.58459615328182	-0.44959023747009
C	-5.19703770986528	-2.03023240495704	-2.18428095281321
F	-4.92711869300325	-1.36684162451054	-3.31707223427671
F	-6.45875100949551	-1.75416814763754	-1.84353312894964
F	-5.12177028834001	-3.32142155006953	-2.44464588229054
H	-2.48436077335003	1.01944752779629	-0.36612476592523
C	-1.65882831743285	-0.82959517313756	0.25365986437504
H	-6.31627976049219	1.83666715866187	-0.09318229308329
F	-6.27360958157742	-0.06401972277021	0.54461081017138
H	-5.16567756617331	1.66588835531328	2.12454061486151
H	-4.16503569704806	2.43420824502454	0.89801555376264
H	-3.94412760076330	-0.47479802984822	1.83245839705600
H	-2.76706861959337	0.80772109199500	2.09562955886100
H	-5.56142241158214	0.36831726780494	-1.92348096394208
H	-4.32270159769443	1.56180394221118	-1.55340636778592
H	-1.88680799530746	-1.67480923119393	0.89601431379847
H	-0.86054685574681	-0.24526091909342	0.71383550277529
H	-1.29623275633421	-1.21318039976248	-0.69827795861479

6A_a, Chloroform

C	-5.57766036979628	1.06630972241095	0.11108946195768
C	-4.84968314838212	0.67829923371440	-1.16861519639491
C	-4.61501440314451	1.48567709496407	1.20201220886475
C	-3.52375135790583	0.44014930178378	1.40751418828625
C	-2.85922953506792	0.08022292892812	0.08116585373773
N	-3.89283647228796	-0.37690809976505	-0.87468539968642
C	-4.17530051551430	-1.67387211711300	-1.06836165222088
O	-3.66234683799733	-2.61031599583636	-0.50009276393496
C	-5.20297089939245	-2.02469754410633	-2.19042671551038
F	-4.95782606022672	-1.35686426399661	-3.32328322128534
F	-6.46221620829130	-1.76695640953809	-1.82700903223551
F	-5.12495295824394	-3.31775336223386	-2.46430704935949
H	-2.49390114898366	1.00797908841238	-0.37033013677502
C	-1.65691235579446	-0.82897474624604	0.26412086053389
H	-6.30586386739165	1.84814115747764	-0.10255744032296
F	-6.28866145791973	-0.05482853367917	0.54451464445622
H	-5.16765140790269	1.66996588915622	2.12315623526528
H	-4.16388389362411	2.43407091820469	0.89707769667679
H	-3.93717833732851	-0.46801344112064	1.85237255935949
H	-2.76312551206106	0.82141456869476	2.09067232446079
H	-5.56550926548912	0.36971591543353	-1.92070190980404
H	-4.31134115942141	1.54618510384682	-1.55204186839843
H	-1.87515241447506	-1.66718485584847	0.91966694435658
H	-0.86486537833785	-0.23151131260559	0.71771753354732
H	-1.29116503502000	-1.21515024093815	-0.68576812557443

6A_e, Gas Phase

C	-5.44674043076812	1.23782193434707	0.28646800158793
C	-4.99781398869235	0.60180021160314	-1.03017045433333
C	-4.27334780118878	1.66502302029042	1.16401718158554
C	-3.34932703409851	0.48884101719549	1.38731231803956
C	-2.88761645440569	-0.10162785231361	0.06345830631540
N	-4.03437857948094	-0.47177395604968	-0.74240020108559
C	-4.22622740121422	-1.66785801756657	-1.33774267224362
O	-5.11789426382564	-1.91557019461932	-2.10896911001352
C	-3.24798201164196	-2.82190714445579	-0.98575422250198
F	-3.20852434970376	-3.04547319393546	0.33444806608727
F	-2.00236933387380	-2.55251689997230	-1.39493439906010
F	-3.63702323925793	-3.93403209762871	-1.57417685017220
H	-5.85301908149740	0.11528298080375	-1.49156908786541
C	-4.43715808373047	1.61158087716786	-2.02568975646175
H	-2.29149299104788	0.64997270315925	-0.46220473351683
H	-2.24890843065245	-0.95620960547468	0.24955064025778
H	-6.08345145140216	2.09530024195046	0.06462430994121
H	-6.06222080323230	0.51573403968132	0.82790077799608
H	-4.62808573397015	2.04628373560647	2.12135691457729
H	-3.70022854089462	2.46351823538774	0.68627935703659
H	-3.84631071681829	-0.28663390787766	1.97772932722371
F	-2.22480053324549	0.89348381731771	2.08071362438308
H	-3.56526008434370	2.13969789466399	-1.64013278072661
H	-5.19958980332600	2.35613648755941	-2.25638483410831
H	-4.15838885768740	1.11313567315968	-2.95329972294220

6A_e, Chloroform

C	-5.44630074568741	1.23646398577490	0.28407529752736
C	-4.99952493959730	0.60607222293411	-1.03533588336736
C	-4.27304927152965	1.66364381358728	1.16184257423276
C	-3.35742108267758	0.48300548040463	1.38062862435540
C	-2.88824774421214	-0.09996459405276	0.05647674353877
N	-4.03522699047718	-0.47359210112803	-0.75208283668830
C	-4.22901825480661	-1.66809204514129	-1.32476474027089
O	-5.13098581962637	-1.93730242170994	-2.08847974522739
C	-3.24356662882626	-2.81822458626209	-0.97767662080466
F	-3.19148347153844	-3.04613143551515	0.33921299934251
F	-2.00343035325042	-2.55547253067261	-1.40210323167551
F	-3.63984144101706	-3.93518743428454	-1.56325581215922
H	-5.85875741961260	0.12768467856796	-1.49582092879363
C	-4.43119728302144	1.61810092353292	-2.02297466791014
H	-2.30281666438092	0.65672977626725	-0.47170094384748
H	-2.24300004508301	-0.94992953416987	0.24033805313664
H	-6.08102308189517	2.09473014810430	0.06158796481246
H	-6.06019493437447	0.51347953248796	0.82547742479247
H	-4.63257257948435	2.04016071955692	2.11919107244572

H	-3.69953380058668	2.46155457010843	0.68374082110130
H	-3.85331417042980	-0.29073169814715	1.97186514751044
F	-2.22399834656494	0.88170507093174	2.08001380811437
H	-3.56525562449468	2.14700016854847	-1.62571398194289
H	-5.19687503832450	2.35916069616879	-2.25362246457319
H	-4.14152426850103	1.12514659410775	-2.95048867364954

6B_a, Gas Phase

C	-5.42984278330012	1.23729709461387	-0.39047107285102
C	-4.60936816777374	0.48922240993774	-1.42891104863178
C	-4.63785244520150	1.56321550151633	0.87125339341951
C	-3.98925893628778	0.31218659065491	1.42720631843646
C	-3.11332568225452	-0.36905274771728	0.39234575263843
N	-3.98788343476695	-0.72272081307758	-0.76532371834165
H	-3.46796152889987	-1.26203846559551	-1.45829883692731
H	-4.74107059193526	-1.32530962829827	-0.41671088674228
C	-5.42671808380552	0.03002819724939	-2.61402229540783
H	-3.75915036677445	1.09482149154819	-1.75000181339660
H	-2.32875334817228	0.29508679353105	0.03392163880267
H	-2.67499821318138	-1.28352154468362	0.78350301266941
H	-6.30792425135360	0.63943265167057	-0.13319724576567
H	-5.79999052529969	2.15118088833127	-0.85405657145649
H	-5.29059026614192	1.99748081330151	1.62685560483631
H	-3.85562004822706	2.29703146635322	0.66127620333052
H	-3.41040304686221	0.51662830060430	2.32676618220262
F	-4.97893016610702	-0.60880592919518	1.74470037631639
H	-4.82216763901074	-0.49753473547509	-3.35178791127810
H	-5.86538056004365	0.89820454225094	-3.10268109520432
H	-6.24527991460073	-0.61638287752075	-2.29254598664930

6B_a, Water

C	-5.44911886840393	1.21462318226168	-0.38274985430187
C	-4.61318225227120	0.48635958733064	-1.42082313350980
C	-4.64492922010606	1.56366967545286	0.86322189185161
C	-3.97479113867314	0.33238271532328	1.43139406767604
C	-3.14744090768598	-0.39194781635836	0.39476482897985
N	-3.99893345578832	-0.72442184043128	-0.77756395456603
H	-3.44257461432395	-1.23120509103407	-1.46665076744122
H	-4.74053963884233	-1.36582666697738	-0.48439749176341
C	-5.41532598397418	0.04892082803943	-2.62381424770613
H	-3.76624001446684	1.10359286887655	-1.72395162988501
H	-2.33877213803273	0.24628599690679	0.04509088472660
H	-2.73973786181270	-1.31815613651656	0.78809129048503
H	-6.30589734693042	0.59000589043558	-0.11683491552867
H	-5.84331541495944	2.11882003066791	-0.84494915953266
H	-5.28276212932979	2.01193263756259	1.62392783864189
H	-3.86459292266972	2.28853124273686	0.62022239259147
H	-3.34685793781866	0.57311349032882	2.28714555212163
F	-4.96134580911472	-0.55940574841392	1.86813062793135
H	-4.79108713935075	-0.47144098764615	-3.34919194187097
H	-5.84336305082800	0.92782235149380	-3.10282480321288
H	-6.23166215461711	-0.60720621003906	-2.31841747568686

6B_e, Gas Phase

C	-5.53424450992260	1.18323789711790	-0.36093502076935
C	-4.69772052653869	0.42628067287230	-1.38895420750602
C	-4.72951027785184	1.53962943488949	0.87236585100132
C	-4.07012846924052	0.29167306785780	1.45797380414411
C	-3.19547052358912	-0.44035109796523	0.44924864645681
N	-4.06270525061734	-0.77207024675220	-0.75599178137005
H	-3.49901896572808	-1.26347959316140	-1.45168874021928
H	-4.79308305324137	-1.42375615828227	-0.46022149430425
C	-1.96518436510819	0.32846791684166	0.01077940817542
H	-2.89503957562696	-1.40886048469863	0.84806324889101
H	-6.40966383052140	0.58593312629042	-0.08200787554106
F	-5.97925545597350	2.31142798153733	-0.99246309867569
H	-5.38629883272057	1.99450530460969	1.61234342751899
H	-3.98655683841150	2.29145083704553	0.60149894507147
H	-3.44601694186210	0.55919599210535	2.31016003979068
H	-4.83355820053370	-0.39129412680119	1.84161216619640
H	-5.30832741619890	0.08927308248759	-2.22294196283930
H	-3.90220034259010	1.06605313666200	-1.76418116986791
H	-1.41748534825853	-0.19052372905857	-0.77664193568248
H	-1.29790881597081	0.41772631435215	0.86679640959976
H	-2.19441245949416	1.33674067205028	-0.32746466007058

6B_e, Water

C	-5.53213091694137	1.16852930752267	-0.35302351298903
C	-4.69167877551452	0.43009237820069	-1.38230634677981
C	-4.72681564955762	1.54691246742939	0.86842477910518
C	-4.06935659559547	0.29847433754594	1.45476088283210
C	-3.20304456956059	-0.43697606429605	0.44235817406299
N	-4.05865233958639	-0.75944262737475	-0.75553000949348
H	-3.49635704541162	-1.24735524339213	-1.45391194365405
H	-4.78239207395234	-1.42321092235082	-0.47316135443012
C	-1.96362161864470	0.32370380473739	0.01632868297521
H	-2.91219253891112	-1.40629419258624	0.84141272840719
H	-6.39544066997997	0.56181060331207	-0.07047945538149
F	-6.01691528255678	2.30743603441315	-0.98126145029315
H	-5.38028470457312	2.00507471659790	1.60969408648374
H	-3.97736097949612	2.28698879511548	0.58231409177177
H	-3.44242709299115	0.56640720636279	2.30414746107577
H	-4.83821386418722	-0.38224356663921	1.82735305049406
H	-5.29876148346612	0.08514532639592	-2.21380803313863
H	-3.89923307564244	1.07506751416398	-1.75466893179034
H	-1.42870455875257	-0.20667167808294	-0.77111651271655
H	-1.30471984922306	0.40629389868457	0.87931739553618
H	-2.18548631545569	1.33151790424020	-0.32949378207755

6C_ae, Gas Phase

C	-5.44386598600272	1.21049820565204	-0.39150518759749
C	-4.57948054738933	0.48376218630107	-1.41832018357992
C	-4.64620243775690	1.55943203805268	0.85914264301716
C	-3.97906490201820	0.32165821745093	1.42840263232743
C	-3.17433296911227	-0.39778811807579	0.36030195049753
N	-4.00090332404159	-0.69322017481971	-0.78983838452569
H	-3.49661070585005	-1.25152861740122	-1.46485548129566
C	-5.40040714841048	0.05753716887908	-2.62131639055294
H	-3.79122795777344	1.18453352717844	-1.74929726691535
H	-2.31604337350829	0.25316749324062	0.12004856455378
H	-2.78435305114937	-1.32854442159632	0.77192213222486
H	-6.27577221108910	0.55644913624665	-0.12053646130944
H	-5.86145145160371	2.11377124183725	-0.83998856660609
H	-5.27978986268810	2.01537666490062	1.62062607647576
H	-3.86118427795339	2.28084809762439	0.61266587240772
H	-3.32379400195373	0.58307438712250	2.26242770170228
F	-4.95258313968440	-0.52780504464249	1.93297796761044
H	-4.78657175602799	-0.46958918015278	-3.35372410218301
H	-5.84731970684160	0.92205817406993	-3.11239238150469
H	-6.19757118914535	-0.61342098186789	-2.29873113474669

6C_ae, Water

C	-5.44770766586366	1.20886331572973	-0.39039410373948
C	-4.58730050884607	0.47211825678826	-1.41218888987446
C	-4.65197086145248	1.55563505270879	0.86270571743938
C	-3.96815740398714	0.32804906710731	1.42605842934333
C	-3.17340891970226	-0.39633542157358	0.35955650934391
N	-4.01498017451758	-0.71470415735628	-0.78180265233987
H	-3.47536592200286	-1.23383018159670	-1.46401656559683
C	-5.40235980403620	0.05829716411640	-2.62325002484527
H	-3.78694151746836	1.15889738038880	-1.73496713139247
H	-2.33141301114602	0.26139606414504	0.09481491947504
H	-2.76114671792158	-1.31660873280228	0.77309310698258
H	-6.29467060100419	0.56946980843228	-0.12647251585832
H	-5.85065301871138	2.11641380054385	-0.84307066049602
H	-5.28524707169494	2.00889099082188	1.62634849461593
H	-3.87005823343604	2.27965691013988	0.61703839868103
H	-3.31826547567952	0.58727177781852	2.26201118776707
F	-4.94555646185723	-0.54014110816371	1.93998660771693
H	-4.78939829469738	-0.49030346096380	-3.34029527100387
H	-5.81676045696839	0.93322919624499	-3.12487188463889
H	-6.22716787900671	-0.58599572252938	-2.31227367157971

6C_aa, Gas Phase

C	-5.45339944700565	1.23202317127429	-0.38175095390784
C	-4.60745292417157	0.45722134919513	-1.39513526188251
C	-4.64438481936257	1.57227542929950	0.86709864315813
C	-3.98202553254370	0.33225165495591	1.43667438602061
C	-3.19324434741328	-0.40528635565552	0.36737025139501
N	-3.98168535676895	-0.72219413471120	-0.80639749647684
H	-4.69786345214589	-1.39738687963513	-0.56002902494253
C	-5.41542080256489	0.04565355006745	-2.61148363275872
H	-3.78655329832997	1.10850131243733	-1.72226124484775
H	-2.35252249389726	0.22731472810127	0.06350662820966
H	-2.77723559096311	-1.32328063101730	0.78268033055976
H	-6.31129380827834	0.61331945923704	-0.10249886404308
H	-5.84626802520996	2.14350379063977	-0.83707884693460
H	-5.27016801528627	2.03649771553820	1.62991537410382
H	-3.85442943468436	2.28673991834160	0.61557507378755
H	-3.34510976496426	0.57933509910205	2.28874257197751
F	-4.97349454504485	-0.52865343553963	1.90841296948798
H	-4.78068410839440	-0.46095357062738	-3.33716880983611
H	-5.87530725185686	0.91191597753423	-3.08729633707649
H	-6.21406698111386	-0.64014814853760	-2.31867575599353

6C_aa, Water

C	-5.45877270347251	1.22042138840622	-0.38254759340352
C	-4.60842199825778	0.45331439920677	-1.39595644120832
C	-4.64927783712891	1.56817974900165	0.86390247737977
C	-3.96810074884355	0.34252592197618	1.43511407431059
C	-3.19584733619796	-0.41260858652893	0.36953216358631
N	-3.99318488191023	-0.73566444528695	-0.80290769984945
H	-4.72716310335721	-1.38619353116583	-0.53741266877289
C	-5.40969625629847	0.05410198637267	-2.62098648534258
H	-3.78272146914369	1.10417211339426	-1.70861528509635
H	-2.35467989243137	0.21496537782598	0.05968438940215
H	-2.78380339099356	-1.32867574515414	0.79318975987633
H	-6.31490061941216	0.59590063419373	-0.10842263858079
H	-5.85402137077274	2.13027578208376	-0.83823323657151
H	-5.27409071297961	2.03087090649086	1.62875352188066
H	-3.86571781312383	2.28695521904444	0.60711236299441
H	-3.31984624661068	0.60003485174100	2.27322390425941
F	-4.95535435290200	-0.52255767053413	1.94516670036025
H	-4.77155055586253	-0.43379001457458	-3.35793347268335
H	-5.87095931075102	0.92763671853029	-3.08236869258020
H	-6.20449939955019	-0.64121505502321	-2.34009513996088

6C_ee, Gas Phase

C	-5.54247238533095	1.15231455046734	-0.36024583551627
C	-4.66740153177576	0.43769317177310	-1.37497042907554
C	-4.73837879830879	1.54109684832817	0.86168770327662
C	-4.04811086992162	0.30761376062924	1.44344294895687
C	-3.21476142898492	-0.43458830415035	0.39629101607909
N	-4.07482599515244	-0.73002659563046	-0.74700957838392
H	-3.58551103142044	-1.29405875386683	-1.42786751048050
C	-1.92635707574210	0.31025716732515	0.04107548523903
H	-2.93178337997263	-1.39916767350523	0.82447997428446
H	-6.37882835706007	0.50734199376009	-0.07854610718541
F	-6.07332726853437	2.28912842365704	-0.95191176397963
H	-5.38844703733433	2.00502297597963	1.60435569283409
H	-4.00377358509513	2.29167932008149	0.55940379828924
H	-3.41475062921515	0.59395665607353	2.28435469687124
H	-4.80599242977394	-0.37953541578594	1.82605242059704
H	-5.28047358821667	0.11286373355454	-2.21535479122424
H	-3.93701750592503	1.16581771357176	-1.75599561968292
H	-1.35895559447937	-0.24927423263242	-0.70427522594220
H	-1.29709321975691	0.42805053401659	0.92436727825836
H	-2.12245828799938	1.30327412635356	-0.36283415321540

6C_ee, Water

C	-5.54092513135678	1.14358786507266	-0.35506059061375
C	-4.66728651129886	0.43591376590582	-1.37289721373901
C	-4.73872765783219	1.54413765661385	0.86091317371922
C	-4.05002411936986	0.30988190255404	1.44460124912695
C	-3.21837595858194	-0.43589772271245	0.39948003446054
N	-4.07729425188499	-0.73961369387911	-0.74919766757836
H	-3.55508978301749	-1.26560048422642	-1.43884484801956
C	-1.93208381785645	0.30670916003994	0.03707329364252
H	-2.93197044022333	-1.39794917931881	0.83003719589681
H	-6.38201357472973	0.50672786767414	-0.07248706760328
F	-6.08249327628414	2.28655597746917	-0.95648743210904
H	-5.38740639720352	2.00786371391077	1.60498620680570
H	-3.99944028426385	2.28843961682828	0.55400393258827
H	-3.41330319183968	0.59963040616549	2.28136647070973
H	-4.80995525572416	-0.37118295408867	1.83524856549503
H	-5.27513876099341	0.11690255145629	-2.21940599494624
H	-3.92768073745031	1.15967960983948	-1.74190450181865
H	-1.37443138959747	-0.25517920155034	-0.71389956779671
H	-1.29985028913345	0.41606736509887	0.91943449635934
H	-2.12722917135836	1.30278577714700	-0.36045973457950

6C_ea, Gas Phase

C	-5.54440723888623	1.17020819480989	-0.34890718307124
C	-4.69277956707711	0.41010581173302	-1.35543569442041
C	-4.73353825569315	1.55299347898607	0.87204442370987
C	-4.05939212005589	0.31658351787855	1.46739907643532
C	-3.23937079309129	-0.44087697265642	0.41401351372199
N	-4.03407367044534	-0.74815708133641	-0.77587249058354
H	-4.71642803532003	-1.46331463010470	-0.55757548550825
C	-1.96190006654365	0.30129789960618	0.03381454891200
H	-2.93982886825799	-1.40262836659671	0.83585024720096
H	-6.40259384383940	0.55603674531154	-0.05472068558662
F	-6.04929221145448	2.31358756746080	-0.95175470156284
H	-5.37745611279836	2.03517710500102	1.60815523094553
H	-3.98617347996675	2.28863407699940	0.56519564361671
H	-3.42658429595205	0.60030734019731	2.31074635551012
H	-4.82613228286963	-0.35883675084442	1.85886266375077
H	-5.30364170509496	0.08954051283134	-2.19909545299389
H	-3.93806806062747	1.09503519604241	-1.75014670093349
H	-1.41668743691877	-0.25789802020393	-0.72512896859275
H	-1.32144044238084	0.41998793193341	0.90835950612597
H	-2.16262151272661	1.29663644295165	-0.36208384667622

6C_ea, Water

C	-5.54156320996501	1.15963517532666	-0.34450173447452
C	-4.69044155164937	0.41340279012376	-1.35845518619382
C	-4.73187797842051	1.55307348976419	0.86997070355518
C	-4.05859295230785	0.31405450821670	1.46193538796901
C	-3.23612212878166	-0.44080245617755	0.41061813981079
N	-4.03657511503399	-0.75293740221406	-0.78047117141595
H	-4.74207201006211	-1.43701597077448	-0.52953683184968
C	-1.95921801368042	0.30230333888881	0.03239848652903
H	-2.94050723108487	-1.40208881678630	0.83513139216668
H	-6.39833546504410	0.54592941598949	-0.05386728077639
F	-6.06010680424484	2.31071446253020	-0.95438282115622
H	-5.37602272688595	2.02936706038698	1.60992056454410
H	-3.98247599075464	2.28658386736046	0.56163323855760
H	-3.42590238592486	0.59612625051633	2.30541607101500
H	-4.82698603331468	-0.36216565541205	1.84705021196341
H	-5.30448788668738	0.09621177258863	-2.20126923132313
H	-3.93229827542435	1.10015919661249	-1.74390317490221
H	-1.40001864181584	-0.26028173207632	-0.71534488564884
H	-1.32875576347980	0.42757303853302	0.91333426076533
H	-2.16004983543777	1.29457766660304	-0.37195613913539

7A_a, Gas Phase

C	-5.46371274550601	1.57921187873227	0.40971136785179
C	-4.96830282732472	0.98180006697679	-0.90338122829461
C	-4.33058161546097	2.21919245713745	1.18887768272937
C	-3.17451119741827	1.23950952738996	1.37767259022446
H	-4.70504440005897	2.56633346637615	2.15129649391743
H	-3.99196361631863	3.09933049158707	0.63426812128283
C	-2.77427036605278	0.65411484181187	0.02623864104449
N	-3.91501555378476	0.01570750784429	-0.63246513535212
C	-4.21075172806306	-1.29337761601261	-0.40110942235306
O	-3.56680595207382	-2.02526818867308	0.29341526810936
C	-5.41378362119894	-1.89724229577402	-1.18994399319338

F	-5.39585229496729	-1.51724767043493	-2.47340835971453
F	-6.58973451647026	-1.53172191183362	-0.67485041638981
F	-5.34215882332285	-3.21231340421090	-1.15057337361080
H	-6.26592978694241	2.29272802863718	0.21440989999877
F	-5.99556391757406	0.54877249306903	1.16773388296503
H	-2.50314425102836	1.47830887072347	-0.64035662204319
C	-1.46794136882766	-0.14625468082415	0.12623553528175
H	-3.46815771202791	0.42501196528139	2.04017557819396
H	-2.31878177292974	1.74385170420382	1.82736141284661
H	-5.78907839487356	0.51357361250153	-1.43432955601232
H	-4.56939670522351	1.77595231578962	-1.53781585576294
F	-1.32931535522057	-0.83532380753479	1.25015730490875
F	-0.46246629296870	0.75340268226591	0.11627989976898
F	-1.28102518436216	-0.95596233502972	-0.90931971639680

7A_a, Chloroform

C	-5.46260981471200	1.58729493809566	0.40590259244202
C	-4.96985751136491	0.97928984915273	-0.90041109348150
C	-4.33191216201635	2.22308278503197	1.18723582165441
C	-3.17267415170271	1.24822125843554	1.38081251439097
H	-4.70651636325263	2.57149376544828	2.14895887687987
H	-3.99418929980829	3.10081984440624	0.63018694696552
C	-2.77497470667162	0.65300403219308	0.03309369830041
N	-3.92183744173733	0.00580661321001	-0.61139314685391
C	-4.20209689266018	-1.29896047762230	-0.41632115522854
O	-3.54080262960161	-2.05792103075234	0.24494667317234
C	-5.41848372129286	-1.89412014063285	-1.19133188347366
F	-5.42272861245446	-1.51292753919724	-2.47196633389023
F	-6.58674640195611	-1.54158817129504	-0.65309579481688
F	-5.34332429768590	-3.21410205491547	-1.16147362537253
H	-6.26135426896446	2.30016553591871	0.20410655458444
F	-6.00719949948773	0.55477922216551	1.16986459204470
H	-2.51172493198878	1.47088869993010	-0.64287210585157
C	-1.47082862483608	-0.14285663274149	0.13255108019705
H	-3.45843072648965	0.44136374522259	2.05631977299264
H	-2.31877047092630	1.76530464389298	1.81879063226370
H	-5.79197897558087	0.51639091378151	-1.43278435816839
H	-4.55901238264721	1.76488394149820	-1.53502638825933
F	-1.33377435445744	-0.85294396645039	1.24885364047146
F	-0.46153079482276	0.75029215580242	0.14183499087231
F	-1.26993096288172	-0.94557193057842	-0.91050250183529

7A_e, Gas Phase

C	-5.37384456323784	1.72147630971147	0.47773897051460
C	-5.06848369469930	0.90597869836897	-0.78112308664320
C	-4.13141168700660	2.30917866812984	1.14591079467008
C	-3.07561984978118	1.24186974657340	1.34268291064631
H	-4.40031733739991	2.74274403422069	2.10894982848764
H	-3.69995243886817	3.10316988691542	0.53528153088493
C	-2.75264785280296	0.54977006539662	0.02655405797671
N	-3.96654072764758	-0.01547814703580	-0.54378819020378
C	-4.23901171981720	-1.34197278021786	-0.65640981020031
O	-5.27839723597490	-1.79145316807777	-1.05672469942568
C	-3.14440849774968	-2.35037267617055	-0.20908129310654
F	-2.01953561383694	-2.21217529569016	-0.91492867979428
F	-3.58261240339442	-3.58044688652096	-0.37005215523128
F	-2.84610429837426	-2.18291283178725	1.08671215242699
H	-6.08736545476366	2.50901860758711	0.23669666337267
H	-5.87466101967076	1.04505291432240	1.17346767167550
H	-5.93593916629687	0.29935246486334	-1.03624988173798
C	-4.84408530723467	1.77047871192501	-2.01878530593905
H	-2.33115888543954	1.27931928214195	-0.66534541128190
H	-2.00925289728217	-0.22143595674325	0.18371777934920
H	-3.40300158764552	0.49659897778007	2.07419264257699
F	-1.91345370033082	1.81500635511278	1.81601445268357
F	-3.83951480565323	2.64915136918406	-1.88361916730980
F	-5.94858850308662	2.47831515528490	-2.27556628742756
F	-4.57728075200517	1.02470649472557	-3.08757548696383

7A_e, Chloroform

C	-5.36834771648390	1.74428964041601	0.48673638829950
C	-5.07826318674059	0.90528729019829	-0.75924765622403
C	-4.12117265907894	2.33254494404640	1.14337953650115
C	-3.08830896219848	1.25082544888850	1.36099264909939
H	-4.39159548586360	2.78409704621181	2.09739739910898
H	-3.67824259699270	3.10920512272767	0.51832115121792
C	-2.76112705072593	0.54322793041174	0.05527199977157
N	-3.97746430906775	-0.02022987249067	-0.51709661015328
C	-4.22505258556281	-1.33711584995037	-0.68101344074186
O	-5.24605577253491	-1.79373406732937	-1.13339375027230
C	-3.13260769882883	-2.35007757723728	-0.23613064036167
F	-2.00287799599031	-2.20111248327587	-0.93054182648352
F	-3.57020837505351	-3.58053320719309	-0.42979510907632
F	-2.84645497186516	-2.21688155455738	1.06294702049379
H	-6.07556630684408	2.53364865339905	0.23488585930338
H	-5.87118081120639	1.08363083776604	1.19482992395360
H	-5.95654278656124	0.30725788339369	-0.99396883085079
C	-4.85565301372674	1.74244621998880	-2.01438488334045
H	-2.33270140427310	1.26210061398722	-0.64338151981024
H	-2.02285650565947	-0.23011140787434	0.22441465832689
H	-3.42907408248789	0.52378760423370	2.10251855524674
F	-1.91156050061396	1.81259232007001	1.83543057666619
F	-3.84276319014948	2.61451064589078	-1.91067278872776
F	-5.95494864060291	2.45392588201627	-2.28511398861090
F	-4.60256339088727	0.97135793626240	-3.07371467333598

7B_a, Gas Phase

C	-5.30844272664122	1.45988350820399	-0.35915459731360
C	-4.49778577470216	0.66624709928890	-1.36970052713444
C	-4.51480017926743	1.73300781243147	0.91650203752189
C	-3.94039010457307	0.44576924293747	1.47275111131856
C	-3.07212377008059	-0.26231818948120	0.44914494239733
N	-3.94334284999593	-0.57391898080233	-0.73050063347418
H	-5.16104312940432	2.19227759682916	1.66275863592631
H	-3.69441282151868	2.43029163235900	0.72943546046547
H	-3.43120723069014	-1.12294470286982	-1.42505012463734
H	-4.72543643131071	-1.15098482742711	-0.39666467427139
H	-5.61166419758794	2.39464139134118	-0.82806002830454
H	-6.21952902579780	0.91034087193289	-0.11605136688126
C	-5.32411456178951	0.21138907441327	-2.57006476379017
H	-3.64449716133111	1.23568021748972	-1.74248699310105
F	-4.97841947000376	-0.43022715609952	1.75225998136021
H	-3.37348868387898	0.61289918049348	2.38779397094280
H	-2.25173687167667	0.36783202036953	0.11002568521162
H	-2.68553058290142	-1.20195369654637	0.83466256030101
F	-6.30436848547920	-0.59910582243240	-2.16782506357032
F	-4.54856616621010	-0.47758672447932	-3.41140839931495
F	-5.83961977515922	1.24657045204799	-3.19694721365196

7B_a, Water

C	-5.33266414799742	1.41732094824966	-0.35224645666071
C	-4.50090125858613	0.64201839595290	-1.35931148230124
C	-4.52515317112785	1.72996856454205	0.90288390676705
C	-3.91851045389156	0.47254315413276	1.48360500328987
C	-3.09926961043931	-0.27800606215200	0.46043558174142
N	-3.95084621124944	-0.59054562968032	-0.72891760734420
H	-5.16074735837737	2.20446099293796	1.64871142143558
H	-3.71272332394276	2.42256988083807	0.67386725101449
H	-3.39346574790621	-1.11933600827359	-1.40321301505688
H	-4.71366582980485	-1.20733429944313	-0.43211261941265
H	-5.66631767081165	2.34070597472645	-0.82093776814058
H	-6.21880404248037	0.83641438607897	-0.09131847564258
C	-5.30759331529264	0.23970905017464	-2.58366530978436
H	-3.64810089596919	1.22538971263561	-1.70799644820354
F	-4.94603228849817	-0.37934595773165	1.89622571630326
H	-3.29609944213425	0.68902804670289	2.34988890378230
H	-2.26485465408427	0.32976735367652	0.11830924335799
H	-2.73454266390934	-1.22229724513794	0.85157368814973
F	-6.33829056751345	-0.54332251953461	-2.25255617845018
F	-4.55636105052918	-0.43822476128701	-3.45452132288240
F	-5.78557629545454	1.31630602259177	-3.19728403196236

7B_e, Gas Phase

C	-5.54480557166163	1.36085944235390	-0.31819601961937
C	-4.68119770085968	0.62336646136388	-1.33791770410275
C	-4.75181122771340	1.75855457281722	0.91080017226005

C	-4.03888102150632	0.54953228269323	1.51946241566490
C	-3.21144052070700	-0.25211647066174	0.52544723637809
N	-4.03487190170720	-0.57120313346841	-0.69283725793469
H	-5.42748694519609	2.18449497769982	1.65119290983898
H	-4.04456774942993	2.53817140427976	0.63184020813114
H	-3.44863029162991	-1.05688153799657	-1.37756328172118
H	-4.76385773753492	-1.23175361449431	-0.41049213383690
F	-6.02223181403622	2.46755024497791	-0.95950255162531
H	-6.40237488426415	0.73816373480053	-0.03746952709406
C	-1.89458582884236	0.40470052009767	0.09267411988795
H	-2.91931815867706	-1.21051097883152	0.95579793045639
H	-5.27468152597966	0.26580297917152	-2.17553691560095
H	-4.76968727435954	-0.12881031916256	1.96771934458026
H	-3.38157887249387	0.86104911344648	2.33143967615499
H	-3.88958528130768	1.27375017321725	-1.70270107117215
F	-2.04019003083547	1.66816203501691	-0.29300473682633
F	-1.38542378869309	-0.27930223369020	-0.93936181055622
F	-1.04737187256478	0.36536034636923	1.10155899673714

7B_e, Water

C	-5.54383905514661	1.35253609783839	-0.30810752901213
C	-4.69108620089197	0.62255125388871	-1.33392283229361
C	-4.74169760449100	1.76296012736724	0.90565198589742
C	-4.03323124463457	0.54886501691518	1.50616723280602
C	-3.21294726840367	-0.25089891069135	0.50518103672979
N	-4.03896714398391	-0.55928061998474	-0.69815580666700
H	-5.40805768128537	2.18984020327638	1.65375594585331
H	-4.02957219878666	2.53385174694612	0.61337575183187
H	-3.48367519099960	-1.06361712825665	-1.39397436332953
H	-4.76068857755321	-1.22417166042637	-0.40647343325624
F	-6.04764236623493	2.47486175733588	-0.94524327290461
H	-6.39460397902338	0.73162077506898	-0.01924857685238
C	-1.89394461545560	0.40052477754656	0.10252543436822
H	-2.93333895587003	-1.21275275121568	0.93254186826988
H	-5.29352611509254	0.25100067084052	-2.15686130507357
H	-4.77179547341227	-0.13403720006996	1.92957717905784
H	-3.38263378715826	0.85048064502169	2.32546701968380
H	-3.91079053958068	1.27558981585838	-1.71640269668926
F	-2.01575961059582	1.66615567260966	-0.30535747251476
F	-1.31795504728531	-0.28092900433943	-0.89200205343914
F	-1.06882734411458	0.39378871447049	1.14485588753405

7C_ae, Gas Phase

C	-5.33052998437363	1.40133893483788	-0.35456587544443
C	-4.47137911907797	0.64246108426863	-1.36176756599519
C	-4.52558688814046	1.72397757851092	0.89870967750949
C	-3.92266932090495	0.45964752468922	1.48059348508334
C	-3.12238183364738	-0.28395868296360	0.42722126944179
N	-3.92425473155761	-0.54829903107325	-0.75194624692363
H	-5.15314041921242	2.20782671145377	1.64712358608013
H	-3.70917054572140	2.41267923200677	0.66236657808015
H	-3.40437865115948	-1.09573109592305	-1.42376213678385
H	-5.71237143697003	2.31455119088234	-0.80984428713315
H	-6.17928182823067	0.77365195095852	-0.08208984748556
C	-5.29975431060246	0.23699861729494	-2.56772106042514
H	-3.69388623486024	1.32046435122610	-1.75371273336447
F	-4.93986032934525	-0.34985392925358	1.95762656259510
H	-3.27479521243052	0.69272995876119	2.32852543656263
H	-2.23379520136778	0.33263494326568	0.21273879769319
H	-2.78033275295376	-1.23284263096365	0.83832369618919
F	-6.37845729965239	-0.47291865435923	-2.24507911180498
F	-4.57412350924069	-0.50559001977385	-3.41907637792854
F	-5.71600039055090	1.31727196615424	-3.24048384594609

7C_ae, Water

C	-5.32534737014020	1.40895780846473	-0.35952954886482
C	-4.46994304306605	0.63664393808563	-1.36013640553392
C	-4.52693644683233	1.72178889127876	0.90052734919926
C	-3.92033020316152	0.46172766497701	1.47837551786662
C	-3.12486362274423	-0.28471835628859	0.43027771658889
N	-3.93374326272250	-0.56607215883311	-0.74996589766674
H	-5.15719573560407	2.20639871775081	1.64615214197168
H	-3.70712465784342	2.40705528308379	0.67039721452699
H	-3.36472201303899	-1.06879752234533	-1.42021315315547
H	-5.68182951918423	2.33160608706188	-0.81570470249262
H	-6.19367206421897	0.80346134264361	-0.09594286706295
C	-5.30049663467401	0.23565329467795	-2.56172033848023
H	-3.68264523991734	1.29949975060690	-1.75022078598075
F	-4.95037171043611	-0.36245447359953	1.95290813903100
H	-3.28312528842958	0.68701369312024	2.33350648211207
H	-2.24818989483222	0.33714829692285	0.20001826698440
H	-2.76774702577604	-1.22782909794859	0.84131234414579
F	-6.37549658004323	-0.49284544634136	-2.23664355589699
F	-4.58807198431271	-0.49761486551776	-3.43234124201453
F	-5.74429770302223	1.31041715220009	-3.22787667527768

7C_aa, Gas Phase

C	-5.34099849688281	1.43183179001673	-0.35454325571070
C	-4.50160004774296	0.60701310581378	-1.33151929317488
C	-4.51953428084256	1.74228416796135	0.89618974149734
C	-3.91599982120435	0.48199794524208	1.48750800150226
C	-3.15532784536025	-0.30583687308870	0.43325718025709
N	-3.96055345170475	-0.60132447389771	-0.73831015953254
H	-5.13332654918883	2.23966263642263	1.64707952052526
H	-3.69911202583591	2.42196537701158	0.64664040936951
H	-4.71957814959683	-1.22054017811494	-0.47446075111332
H	-5.68100601646467	2.35583941717800	-0.82092271416912
H	-6.22494305585861	0.85402049212810	-0.07587227068537
C	-5.28546157194060	0.23078391581716	-2.57518381901905
H	-3.65905605288634	1.21141412518813	-1.68633000385896
F	-4.94646966116828	-0.32562525597544	1.96341371413955
H	-3.27259279317574	0.71470938260274	2.33859283697607
H	-2.28184704690297	0.27705463300098	0.12480534923573
H	-2.79151951043913	-1.23984894576992	0.85972466707236
F	-6.25956089497585	-0.64607599509476	-2.29027598304351
F	-4.51367423576778	-0.32028260894739	-3.51012927431959
F	-5.86697849206077	1.30637734250562	-3.12199389594813

7C_aa, Water

C	-5.35424121509003	1.42064474617776	-0.35003814260188
C	-4.50897264303354	0.60445705182968	-1.32672008243657
C	-4.52646848942400	1.73644465975033	0.89560641744175
C	-3.89758244773095	0.49020994455069	1.48332516736245
C	-3.15606562914673	-0.31064054800056	0.42898306249954
N	-3.98069917552207	-0.61460107958158	-0.73488767970634
H	-5.13857365807742	2.22852591110406	1.65132127355581
H	-3.71543318058160	2.42284238961472	0.63771288958980
H	-4.75343064027313	-1.20345968677402	-0.43779945978750
H	-5.69469227511089	2.34671694162908	-0.81156186869457
H	-6.23615934102000	0.83851980655636	-0.07221655623837
C	-5.27441724845506	0.24151217061823	-2.58069974492762
H	-3.66191462362230	1.21015484619352	-1.66518325337696
F	-4.91954185301293	-0.32577517177234	1.99969495011574
H	-3.23963814004729	0.73408100558647	2.31767861710079
H	-2.28786968553794	0.27036985028618	0.10692957486887
H	-2.79119284578634	-1.24174699062585	0.86047298032888
F	-6.26722321267162	-0.62711078674965	-2.32854441195671
F	-4.49206912493413	-0.32451593831820	-3.50743774331298
F	-5.83295457092201	1.31879087792515	-3.14896598982414

7C_ee, Gas Phase

C	-5.55569020384134	1.33350911699343	-0.30943489692465
C	-4.67651565791121	0.63628797603343	-1.33243546590042
C	-4.74173404218902	1.75876099703175	0.89369259996835
C	-4.01019492337766	0.55539809254060	1.48933615983034
C	-3.21968128851011	-0.24719890204772	0.45468705944098
N	-4.03530532420250	-0.51049862763824	-0.70624855290082
H	-5.39466057763570	2.20518146710937	1.64429874327245
H	-4.03625361475177	2.52604644698443	0.57251385683410
H	-3.55937885551124	-1.09461618889763	-1.37756121827078
F	-6.12486297675480	2.44751432701711	-0.90266478625904
H	-6.37015475881061	0.66911164249341	-0.00835967838465
C	-1.86590794840434	0.38271794154761	0.13446342945386
H	-2.95263435387468	-1.20892459929673	0.90055689035494
H	-5.29663070484465	0.27385811635476	-2.15141611131436
H	-4.74355359590517	-0.12822484068345	1.92079937725767

H	-3.35175471708324	0.87095692358858	2.29817623557329
H	-3.97718361170845	1.37699803046519	-1.73777166447774
F	-1.94864981051810	1.63563547910136	-0.33199322596894
F	-1.22198570211568	-0.33729229482638	-0.79556567506021
F	-1.08360733204974	0.41639889612912	1.22046692347562

7C_ee, Water

C	-5.55318600463420	1.32793753446789	-0.30626596111964
C	-4.67661282380503	0.63448776525623	-1.33165411572210
C	-4.74319249369381	1.75934326888264	0.89427238124415
C	-4.01010900097464	0.55630397871106	1.48956107337889
C	-3.22157378923012	-0.24919467467887	0.45581762496456
N	-4.03865210703835	-0.51510487526103	-0.70565976502101
H	-5.39676112776786	2.19960148480602	1.64777450245366
H	-4.03769463689178	2.52752702875059	0.57373717111982
H	-3.56127539182225	-1.09466720683289	-1.38168163209198
F	-6.12448451576944	2.45290055368430	-0.90783133120117
H	-6.37567863572779	0.67455129127863	-0.00804413023799
C	-1.87055704375439	0.38034023995956	0.13266620432577
H	-2.95159713220368	-1.20876081333782	0.90292964145277
H	-5.29258273717755	0.27368002895049	-2.15423208972847
H	-4.74275236617793	-0.12622582588871	1.92317263323343
H	-3.35428527768863	0.87520130799461	2.29886332184430
H	-3.97170291441292	1.37260936749339	-1.73260108108794
F	-1.94479809690809	1.63760696365162	-0.33182505305675
F	-1.21884232342099	-0.33225153995034	-0.79976325358076
F	-1.08000158090058	0.41573412206263	1.21630385883045

7C_ea, Gas Phase

C	-5.57425451588622	1.35749836182805	-0.27256169085031
C	-4.72826283110564	0.62732300422549	-1.30462448705514
C	-4.72787169964769	1.77965890227196	0.90970423400379
C	-4.01924974400922	0.56491142604081	1.50833385816885
C	-3.24870188716992	-0.25051555584975	0.46151997452971
N	-3.99792183733190	-0.50472722704157	-0.75270222936628
H	-5.35526391437303	2.25641398801209	1.66320105028828
H	-4.00476760133084	2.52074352151437	0.56547576732735
H	-4.59826560043282	-1.30688382920899	-0.63218868685206
F	-6.13703004781361	2.47438847826835	-0.86731172959236
H	-6.39951618583814	0.71798536506265	0.05931556190751
C	-1.88697558889920	0.35569830989876	0.13196238162369
H	-2.99047126689298	-1.21920618093309	0.89351917016867
H	-5.35451543552137	0.26796190081241	-2.11987650110792
H	-4.76784760885012	-0.10610233745046	1.93789378280324
H	-3.36103279408127	0.86487099504478	2.32318839664704
H	-4.02400002516302	1.34387425359966	-1.73045918732078
F	-1.97144080947427	1.55645837050392	-0.45949029650496
F	-1.17864223355738	-0.43243684811168	-0.67354644845448
F	-1.16972837262136	0.52388510151224	1.25347707963617

7C_ea, Water

C	-5.57299639000181	1.34592049189871	-0.26989897176113
C	-4.72411127954824	0.63026220690891	-1.30656599053154
C	-4.73281715441421	1.78104913087509	0.90827035812706
C	-4.01959068868074	0.56809941042303	1.50453473326233
C	-3.24608861151541	-0.24703139493175	0.46177284742495
N	-3.99025567134297	-0.50521713688293	-0.75889480902543
H	-5.36394067727815	2.24694891014330	1.66535382789485
H	-4.01398508706674	2.52768551696032	0.56494278797174
H	-4.61754571313974	-1.28301581441998	-0.60089454587846
F	-6.14690171410478	2.47018880484470	-0.87353449635900
H	-6.39744874330772	0.70705771433922	0.05634890548367
C	-1.88606271239790	0.35119083611354	0.13444983948858
H	-2.99608533514692	-1.21559149352453	0.89777745072406
H	-5.35077183847209	0.26841688979508	-2.12033309637189
H	-4.76629217589031	-0.10738138622887	1.92757660405717
H	-3.36674977881437	0.86958268707518	2.32302170877138
H	-4.02242765009052	1.35387497717304	-1.72646263400503
F	-1.95115776167742	1.55729063784996	-0.45422139211659
F	-1.17913340100558	-0.43558558453599	-0.68539223326599
F	-1.15139761610438	0.50805459612399	1.24697910610927

8A_a, Gas Phase

C	-5.49967351429139	1.36069973752981	-0.01931461824505
C	-4.94320879322033	0.60894919517504	-1.21591646230291
C	-4.41321767731005	1.73034003572787	0.98254712644670
C	-3.54917618030946	0.51388029936608	1.35272782208288
C	-3.00544793110638	-0.12377473011380	0.07424512978805
N	-4.09378246581906	-0.49698775680204	-0.80961015416283
C	-4.31734204935890	-1.71156618866080	-1.35119250594221
O	-5.19198752048963	-1.96370621524115	-2.13891474451623
C	-3.37116229237096	-2.87155072174251	-0.93602326248657
F	-3.38536714852031	-3.07879574022579	0.38623543361732
F	-2.10565815516626	-2.62013726969722	-1.29750785640175
F	-3.74638220745675	-3.98761106561664	-1.52585236325630
C	-4.98318425089016	2.45845880819232	2.19087616203576
H	-3.75722609148998	2.42644885244766	0.44499531887608
C	-4.25768002388594	-0.52353391545056	2.21788427924644
H	-2.68541838366156	0.89219441412917	1.90708720053356
H	-5.75240904323864	0.22268925085163	-1.82831144134562
H	-4.35545384487091	1.31253006130769	-1.81665384768012
H	-5.99984149194070	2.26594275151119	-0.37518815432037
F	-6.47294489116655	0.58336425636753	0.59095672122656
H	-2.36684995835356	0.59124729321099	-0.45674838598482
H	-2.39910878371190	-0.98924573124573	0.31548943560281
H	-5.77263241349212	1.87766213074531	2.66480024045823
H	-5.40417208615847	3.42153111648683	1.89989222635862
H	-4.20213184751705	2.64131229882828	2.93031698644410
H	-5.08332688588282	-0.99036531100537	1.68293354356502
H	-4.66115319851937	-0.07434479109795	3.12402698399877
H	-3.55912086980077	-1.30690106497784	2.51179918636387

8A_a, Chloroform

C	-5.49314785483089	1.36768705963081	-0.02871798492558
C	-4.93254606953114	0.61951084422512	-1.22316250627268
C	-4.41607025011233	1.72758362136199	0.98315200623636
C	-3.55183220950768	0.51096857146127	1.35079389900987
C	-3.00059946010685	-0.12086130901977	0.07289025049352
N	-4.09072775665464	-0.49672722505469	-0.81504452055165
C	-4.33214646607498	-1.71023216418173	-1.32027711949062
O	-5.23809358802073	-1.98604706545013	-2.07715314929012
C	-3.36897720560853	-2.86570137027699	-0.93002685777302
F	-3.35548957107262	-3.08824987602907	0.38762346798151
F	-2.11473089879706	-2.61290940642797	-1.31984420180405
F	-3.75454243538733	-3.98356315989652	-1.52178510212944
C	-4.98883450095916	2.45360873467665	2.19166866679284
H	-3.75907681217873	2.42599138639251	0.45154459439849
C	-4.25794748004688	-0.53056590753945	2.21303157259448
H	-2.68942158405052	0.88857812214202	1.90619339256076
H	-5.73905863130708	0.25055714730867	-1.84811798547580
H	-4.32783283215645	1.31945193734192	-1.80753562585498
H	-5.99164274510685	2.27199785658019	-0.38414491166460
F	-6.47925482808490	0.58087850259069	0.57022794472055
H	-2.37103832103409	0.59787143242089	-0.45969085997438
H	-2.38997360331988	-0.98290291673188	0.31487093789278
H	-5.77042830673433	1.86925382244614	2.67510366758094
H	-5.41745918873935	3.41204855383135	1.89619620656232
H	-4.20401638198291	2.64463247717627	2.92520706879765
H	-5.07465861698338	-1.00868361305886	1.67286971068692
H	-4.67297602523806	-0.08077416524684	3.11397551967763
H	-3.55253637637262	-1.30467189067258	2.51573191922028

8A_e, Gas Phase

C	-5.44821095893474	1.15565304393099	-0.10480329720037
C	-4.69407038701665	0.65132772730399	-1.33247359007651
C	-4.46729504889139	1.57358880250257	1.00712852467415
C	-3.52749418119369	0.40314529144795	1.29114047803682
C	-2.83786005510041	-0.12257113112986	0.03596487337111
N	-3.83396005853413	-0.45708838892490	-0.96862071080747
C	-4.00273933953256	-1.74629470028314	-1.32551562669985
O	-3.34952046680877	-2.66900835765729	-0.91187729772883
C	-5.12040708060026	-2.06003831906833	-2.35976608785376
F	-4.93717036475828	-1.39586156243848	-3.50694823926528
F	-6.33059633415515	-1.73002317707474	-1.88446664533206
F	-5.13116984782528	-3.34786305857802	-2.63273024153690
H	-5.39358598618702	0.35848004547591	-2.10658670027492

H	-4.07007069735650	1.44643750591499	-1.75050594620453
H	-2.16891963878115	0.64572059685905	-0.35983581817755
H	-2.25486505330494	-1.00806909545861	0.26943640751332
C	-6.41625574424719	2.25860599706155	-0.50278950100901
H	-6.02861757275677	0.30594638569301	0.27099368439553
H	-4.08706504676945	-0.41371052651922	1.75497790321400
F	-2.54617079361917	0.78607181902487	2.18797896172449
H	-5.05109360612610	1.74562011977254	1.91618574514966
C	-3.70486705687101	2.85822823837478	0.69750679820112
H	-5.90387671737552	3.06526364499126	-1.02886675423812
H	-6.90943640898921	2.68450954899910	0.37122160917373
H	-7.18555870528998	1.86453283985678	-1.16760247798406
H	-3.13597556621300	2.79643609269878	-0.23085047262140
H	-3.00533338784561	3.08282422948065	1.50006033746592
H	-4.39333389491603	3.69739638774384	0.60936408409075

8A_e, Chloroform

C	-5.45352582789407	1.16083784421480	-0.08937024511502
C	-4.71241891740938	0.64118425339404	-1.31819012580053
C	-4.46465503190964	1.58510286374071	1.01314292551981
C	-3.53945001317503	0.40708671678655	1.29928857505356
C	-2.85234946764918	-0.12966112368292	0.04807247776213
N	-3.85731289301802	-0.47412266258279	-0.94721001020177
C	-3.99681841322573	-1.74525411614662	-1.33772246397979
O	-3.32187471342755	-2.67520494750467	-0.95321267405531
C	-5.10695482252257	-2.06099619868245	-2.37957117846904
F	-4.92795455271741	-1.38618279039106	-3.51936169569591
F	-6.32484977832350	-1.76525414759145	-1.91059850558994
F	-5.09143403975263	-3.35053373053410	-2.66944287526843
H	-5.42110151550355	0.34769274760351	-2.08343202341583
H	-4.08071066057440	1.42344975954776	-1.74648901558770
H	-2.19088154426866	0.63508131552873	-0.36532711022468
H	-2.26507507903327	-1.00931522747209	0.29015485154078
C	-6.41399342267847	2.26819921115750	-0.49417958478815
H	-6.03824963539874	0.32134757008805	0.30146406313497
H	-4.10319821017749	-0.39947188534828	1.77297288179647
F	-2.54361333315061	0.78345524763575	2.19483396543008
H	-5.04546389287126	1.76813568703180	1.92146657673349
C	-3.69519387649849	2.86098665785932	0.68496864933888
H	-5.89602369824060	3.06307295743875	-1.03257483283462
H	-6.89493440508510	2.70681714310174	0.38044844874184
H	-7.19072483115317	1.87237202370884	-1.14933483848530
H	-3.12663908083592	2.78208231007414	-0.24232062777796
H	-2.99737791539356	3.09885655101390	1.48588136555122
H	-4.38274042811194	3.69949597001055	0.58336302668671

8B_a, Gas Phase

C	-5.43279897469535	1.21801311953231	-0.50759097030802
C	-4.57835388731408	0.48794382381110	-1.52452247606867
C	-4.66584111025161	1.54386197555168	0.76716154777633
C	-3.99087517925445	0.29383201313193	1.36800069500382
C	-3.18808461982574	-0.44153612818461	0.30250623319743
N	-4.06804264852629	-0.75842439855789	-0.87510973535957
H	-3.56486897739639	-1.33198117711518	-1.55117329412411
H	-4.87646626648037	-1.30156110844000	-0.55495456909045
C	-5.54417018275148	2.28531426631244	1.76634014348112
H	-3.86373604371300	2.22287579574803	0.45439961789843
H	-3.25482251294170	0.65174647955175	2.09199753552298
C	-4.93503208206685	-0.65118012110555	2.10953981278494
H	-5.15921315366846	0.20842845674645	-2.39955035764382
H	-3.71819373423697	1.08471905910313	-1.82289380789254
F	-6.49797173823648	0.37047438183262	-0.23287281520452
H	-5.83676947681687	2.12645187860050	-0.95654824189487
H	-2.37155748915717	0.16639070608397	-0.08613082877779
H	-2.78837547648003	-1.38191903278500	0.67582651716336
H	-5.71326881811671	-1.07141285984481	1.47161879528099
H	-5.44629340117137	-0.12509922747698	2.91299686919727
H	-4.37401333971870	-1.46852113735589	2.56180425328047
H	-6.45732560047732	1.73342206307762	1.98275271757911
H	-5.82665201641359	3.26312590781489	1.37741515493220
H	-5.01054327028903	2.44279526396749	2.70386720326593

8B_a, Water

C	-5.43787098406545	1.22306777518140	-0.49784480047857
C	-4.60882191958474	0.45846038637662	-1.50294176648594
C	-4.66752009875955	1.54074821128062	0.77380674651851
C	-4.00150712537999	0.28940974753005	1.37404629478765
C	-3.18787014206254	-0.43004375977679	0.30829684325070
N	-4.04428674683731	-0.76125803671520	-0.86879884234960
H	-3.49837591089951	-1.27944986561934	-1.55651083497953
H	-4.80461933252637	-1.38377519428016	-0.58719529550137
C	-5.52585175360497	2.30450402995860	1.77221333346954
H	-3.85721802286506	2.20247735806870	0.44960922392408
H	-3.27553538724302	0.64273850583350	2.10983876458962
C	-4.95549055688152	-0.66389047204950	2.09009935455732
H	-5.20574306717116	0.15285054054901	-2.35676957221631
H	-3.77252281291624	1.06805131126767	-1.83921290346131
F	-6.56089862826763	0.44185485345867	-0.20241424520388
H	-5.79889533268959	2.13968554280546	-0.96445037027200
H	-2.38330099387222	0.19769302133991	-0.07070451385311
H	-2.77194387272316	-1.36329601045637	0.67841858318070
H	-5.69690515554992	-1.09853521490544	1.41953594844857
H	-5.49815366457785	-0.14501311559360	2.87869567965403
H	-4.39092672887366	-1.47543128614688	2.54894895169704
H	-6.43410898257382	1.75693011792310	2.02054706135551
H	-5.81444432762154	3.27294595622429	1.36259525509950
H	-4.97045845245319	2.47703559774569	2.69507110426887

8B_e, Gas Phase

C	-5.46601738688283	1.06390900419875	-0.47766967949466
C	-4.61400847897395	0.32738238253169	-1.49916982750301
C	-4.65792258184669	1.43449223475066	0.78179033703003
C	-4.01539396218857	0.16943027703020	1.34181661100191
C	-3.16714921531903	-0.56747758949866	0.30990923495969
N	-4.01435775550347	-0.90358315541404	-0.87630268923907
H	-3.45968130650685	-1.41332693269314	-1.56490760485117
H	-4.77076367322797	-1.52989892019014	-0.58913429262977
H	-5.20069562928125	0.00929927258879	-2.35870577337446
H	-3.77936881876770	0.93523090052007	-1.84729641533273
H	-2.35257632822291	0.06431914004652	-0.04032678826066
H	-2.76220019477923	-1.48772474243206	0.72303597225928
F	-3.18154741459283	0.45303612288153	2.38840692820730
H	-4.79640707969804	-0.50338700862396	1.71469213650093
H	-5.37609469564701	1.77804167100575	1.53026020498015
C	-3.64555420045699	2.55347556182477	0.56211433285135
H	-6.27240226839864	0.38491809293088	-0.17353201651467
C	-6.10646059618299	2.27944687048600	-1.13869604089665
H	-2.95641195307131	2.35967128501409	-0.26201335965804
H	-3.05434157915220	2.70626204964868	1.46243137091594
H	-4.15813218083961	3.48879535093792	0.34630558401993
H	-5.35439456914948	2.94270877484254	-1.56634562281040
H	-6.67538190342474	2.85035060947065	-0.40558466366653
H	-6.78840622788573	1.98399874814253	-1.93506793849467

8B_e, Water

C	-5.46366762446135	1.06687828270370	-0.47223585513163
C	-4.61219366301806	0.32719360643938	-1.49120730851043
C	-4.65695110562215	1.44097639634718	0.78637211411747
C	-4.02779516501245	0.16732386440057	1.33216764363851
C	-3.17403088880544	-0.56006725029777	0.30651233194375
N	-4.00959954119119	-0.89019513155846	-0.87513736207114
H	-3.44231533082001	-1.38260206497706	-1.56517120430508
H	-4.75108818949129	-1.54078051737659	-0.60740717702364
H	-5.20660907599244	-0.00015869834624	-2.34009088009707
H	-3.78473398073062	0.93537447651517	-1.85373847258241
H	-2.35520244486054	0.06767747494748	-0.03908689813751
H	-2.77946683509304	-1.48535219537586	0.71498526685350
F	-3.20269297397856	0.44679289638084	2.41202486247229
H	-4.81113251375632	-0.50306180060191	1.69374415808704
H	-5.37410425720768	1.78864193092086	1.53408432802950
C	-3.63649338938014	2.55078867164915	0.55702035437836
H	-6.26184245568374	0.38502908862608	-0.16076455093538
C	-6.10929614380830	2.27837783995207	-1.13178038645095
H	-2.95199772411632	2.33340866299154	-0.26397372304306
H	-3.04433753130009	2.71156687843455	1.45638712491296
H	-4.14619543087093	3.48468427006839	0.32542168831048

H	-5.35804895333183	2.93838481966254	-1.56710542781742
H	-6.67857697811176	2.85006516426956	-0.39835910117085
H	-6.78729780335576	1.96842333422487	-1.92665152546725

8C_ae, Gas Phase

C	-5.44376992748150	1.21291757300228	-0.49027089039399
C	-4.60175791060318	0.41956223168122	-1.47371424525571
C	-4.66357447818475	1.53860183284239	0.77802338291407
C	-3.99157567847418	0.28986642870016	1.37639270256515
C	-3.18107231332979	-0.40740190777368	0.28095447753127
N	-4.04404048454188	-0.75084839364078	-0.83350040783291
H	-3.57071415616713	-1.34078099228784	-1.50158944576626
C	-5.51150863309023	2.31617970151892	1.77446829248553
H	-3.84949200819496	2.19350251814186	0.44310547710147
H	-3.28237174350934	0.64577447325424	2.13074517704628
C	-4.95746648568252	-0.67672533894890	2.05526543643066
H	-5.22487927993380	0.11560842713683	-2.31449661712991
H	-3.82725933847494	1.10822929435738	-1.85425792355871
F	-6.59462469156646	0.49996542527301	-0.17950833355705
H	-5.77535985491258	2.14131097339519	-0.96468407495486
H	-2.35631121909033	0.25835502166141	-0.02572192444297
H	-2.73886526842667	-1.32305302440351	0.67620629361935
H	-5.63978883672602	-1.11801549124691	1.33201768580001
H	-5.54736568598026	-0.17623676652453	2.82300310091900
H	-4.40105830636019	-1.48163224232860	2.53799804993281
H	-6.42814882375574	1.77960248275565	2.01431699120127
H	-5.79030705038031	3.28946338169418	1.36770815424300
H	-4.96063782513325	2.48279439174004	2.70163864110249

8C_ae, Water

C	-5.43605813589013	1.21839628876526	-0.49694031253341
C	-4.59918373494564	0.42124049033219	-1.47629418898903
C	-4.66875468083812	1.53440262244908	0.77819648148723
C	-3.99654567332258	0.28543042163935	1.37538839358133
C	-3.19253787840470	-0.41704620602864	0.27975238100440
N	-4.05544849535606	-0.76545601599494	-0.84065555672114
H	-3.53837234442631	-1.30731602475212	-1.52051413075079
C	-5.51587403522154	2.31432823314822	1.77366213216873
H	-3.85474703038159	2.18961408678634	0.44640951868914
H	-3.28147291580679	0.64209112026431	2.12298705523814
C	-4.95692332605740	-0.67502436002343	2.07102054247503
H	-5.21342068223090	0.13303156135580	-2.32933641808862
H	-3.81187846073175	1.09990581100277	-1.84057243206233
F	-6.60285048725054	0.49843865308113	-0.19348795725280
H	-5.77011443074181	2.14452671547822	-0.96926814631155
H	-2.37359362311448	0.24815857561863	-0.03640225838402
H	-2.74568544843144	-1.33044252192927	0.67488410876832
H	-5.65773920016841	-1.11082501247154	1.36131856712942
H	-5.52888323250805	-0.17079750792362	2.85034061282377
H	-4.39647616838653	-1.48492005321355	2.54120282034215
H	-6.42239918873247	1.77101685674191	2.03845271204229
H	-5.81015225390394	3.27769378608102	1.35404374470473
H	-4.95283857314882	2.50059247959289	2.68991233063899

8C_aa, Gas Phase

C	-5.44631689890879	1.22270388840578	-0.49012031023383
C	-4.61495721745942	0.41415025992443	-1.47165264793292
C	-4.66732429963725	1.54359721262145	0.77956944349374
C	-3.99940479779406	0.29329521937829	1.38273051354056
C	-3.22395906027671	-0.44313030070007	0.28238682730623
N	-4.02217333575143	-0.77035894057216	-0.88673544384251
H	-4.74440612138769	-1.43990940835859	-0.65300828737714
C	-5.52002835964524	2.31771806413249	1.77428687755776
H	-3.85161810915263	2.19829555790128	0.44771812199117
H	-3.27380367303087	0.64796704269248	2.12261177381668
C	-4.96019538021897	-0.65484204198950	2.09496797964975
H	-5.22901011713914	0.13284276019590	-2.32715840176662
H	-3.80849938867840	1.05581952988101	-1.84285836395937
F	-6.58637892365865	0.48036221172660	-0.17467161446737
H	-5.79963621569949	2.14754837461053	-0.95558989986821
H	-2.39261067978072	0.18419457704309	-0.05714271052765
H	-2.78862375693139	-1.36154061578715	0.68003661530208
H	-5.69333363518112	-1.07661432106689	1.40827301307328
H	-5.51029879545086	-0.15146519875459	2.88903514493758
H	-4.40114368260507	-1.47598291267392	2.54655447945228
H	-6.43414217638149	1.77433600127835	2.00957225401589
H	-5.80383248004252	3.28903897812554	1.36672489059455
H	-4.97350289518807	2.48595406198567	2.70360974524405

8C_aa, Water

C	-5.43878161554749	1.23013811362014	-0.49391130868293
C	-4.61646672822124	0.41284135314405	-1.47254694247699
C	-4.66854726516255	1.54147665172901	0.78035028915083
C	-4.00163958004324	0.29064594062697	1.38196971143689
C	-3.22113654907795	-0.44133857573499	0.28421725982398
N	-4.02535509229107	-0.77754358407180	-0.88490380841159
H	-4.75868984386904	-1.42812193662659	-0.62683619840338
C	-5.51971696111360	2.31772369082626	1.77502502813838
H	-3.85272080700374	2.19618515304095	0.45118461899312
H	-3.27767833122495	0.64504653775861	2.12265681456743
C	-4.95957146024457	-0.66328186019478	2.09090173714507
H	-5.23475647424397	0.13345022437624	-2.32583308582459
H	-3.81051578030281	1.05347389448517	-1.84397906931714
F	-6.59948704834861	0.49606963798729	-0.18397239256941
H	-5.78235455412738	2.15488891539493	-0.96280931005813
H	-2.39723935310647	0.19333285061582	-0.05788243100214
H	-2.78204882940124	-1.35653033052443	0.68520176049206
H	-5.67685129073597	-1.10323591968677	1.39790804724905
H	-5.52420169867570	-0.15883618807611	2.87450682615423
H	-4.39428887092636	-1.47380657723111	2.55410920152700
H	-6.42603772957312	1.76972576143715	2.03108435782847
H	-5.81465546497628	3.28157491144691	1.35727905369119
H	-4.96245867178262	2.50010133565707	2.69541984054859

8C_ee, Gas Phase

C	-5.45866864169348	1.06562093882224	-0.48486948581549
C	-4.58572373472965	0.30461858627467	-1.48113315541525
C	-4.66168430948703	1.43144817637231	0.78310315500095
C	-4.01228282363095	0.16104191948548	1.32236140915405
C	-3.16627257865765	-0.54336727131905	0.27578939832594
N	-4.01864901868796	-0.87529085261980	-0.85083477420628
H	-3.52299175666717	-1.44408029019664	-1.52183503394108
H	-5.20131864412934	-0.01168273112776	-2.32493604174795
H	-3.81344839638849	0.98204971649421	-1.87899590456096
H	-2.32055513902338	0.10732792935028	0.00882148427537
H	-2.76215191274869	-1.45884675308589	0.70710787898730
F	-3.21254418768212	0.46024535947335	2.41673625521651
H	-4.78828471238065	-0.52640467577775	1.66774373711343
H	-5.37509178551804	1.77675294893119	1.53794384916267
C	-3.64364733977227	2.54699551844249	0.56242356740180
H	-6.25180707181796	0.37577329781145	-0.17962365554547
C	-6.10207182412842	2.28169093445995	-1.13765357690863
H	-2.98387973070996	2.34518264349589	-0.28155173540353
H	-3.02497763180305	2.67317539136207	1.44915787097341
H	-4.14930592351242	3.49209177757905	0.36884796164307
H	-5.35091609960437	2.94144629469410	-1.57482990665137
H	-6.67295837347105	2.86185242028249	-0.41071019588508
H	-6.78187836375587	1.97933872079569	-1.93510310117342

8C_ee, Water

C	-5.46011409783577	1.06520159014133	-0.48069115542824
C	-4.58933227071967	0.30386531034508	-1.47763047994382
C	-4.66118677168474	1.43312345539077	0.78622368854974
C	-4.02151400062022	0.15776389189493	1.31785195775643
C	-3.17088815962643	-0.54520300270925	0.27660386715087
N	-4.02128243568055	-0.88494169220480	-0.85357866639077
H	-3.49042413193298	-1.41379096419378	-1.53310853544136
H	-5.20272337254544	-0.00653470586332	-2.32493173131385
H	-3.81034277303226	0.97521043269992	-1.86837927295193
H	-2.33251011691672	0.10923537312283	-0.00041360380112
H	-2.75986641175367	-1.45807191201615	0.70723075419733
F	-3.21612419469712	0.44943170287819	2.42528293181441
H	-4.79864031384425	-0.52415470628510	1.66940859480003
H	-5.37481650014394	1.78136321268395	1.53913749121619
C	-3.63976819790618	2.54449263514573	0.55808453334601
H	-6.25672153465809	0.38119200317378	-0.17010361103583

C	-6.10265050074274	2.28097472013253	-1.13527069690054
H	-2.97667599145857	2.33194426185985	-0.28063643539377
H	-3.02513829313468	2.68610137090443	1.44612249753425
H	-4.14673009683555	3.48597677252277	0.35040526838243
H	-5.34999217562209	2.93556621511101	-1.57807927470150
H	-6.66846986868474	2.86451739255867	-0.40683569846017
H	-6.78519778992354	1.97371664270665	-1.92873242298479

8C_ea, Gas Phase

C	-5.47895455108928	1.07545202939813	-0.46695918896806
C	-4.62124397564974	0.28217347167776	-1.45692584204227
C	-4.66741337649571	1.44034703904001	0.79280975791955
C	-4.02265472700800	0.16972814685747	1.34021965385114
C	-3.20096030005962	-0.56276976875831	0.28979971124535
N	-3.98866807910003	-0.89378894990804	-0.88380982386443
H	-4.68646555079255	-1.59171685686107	-0.65623438774249
H	-5.22891566125817	-0.02469405318012	-2.31016300271986
H	-3.83112772008007	0.92605882052732	-1.85741698816117
H	-2.36350012566770	0.06957504824299	-0.01786473691288
H	-2.77800293332877	-1.47116575359062	0.71812707693152
F	-3.21405098673961	0.47314219162719	2.42738460033562
H	-4.80569658086088	-0.50231512963532	1.70742240515295
H	-5.36967154684525	1.79917235607020	1.55183050435813
C	-3.64074657509506	2.54509735978180	0.55643623956331
H	-6.28826695274961	0.40732075884062	-0.14813463520083
C	-6.10431305360875	2.29161570835814	-1.13596291576125
H	-2.99008051768559	2.33565001517574	-0.29308381967347
H	-3.01340540079983	2.66958533772319	1.43724113852339
H	-4.14019238256932	3.49388836289482	0.36511385418391
H	-5.33923347234332	2.94098209192312	-1.56468243159268
H	-6.68486522397980	2.88173038671351	-0.42506038560888
H	-6.76915030619334	1.98770138708143	-1.94554678381660

8C_ea, Water

C	-5.47433962221296	1.07403675254729	-0.46734857101967
C	-4.61521710876895	0.28872816890606	-1.46047511858039
C	-4.66411981574869	1.44106891355259	0.79296393202871
C	-4.02945612709062	0.16521021621166	1.33120371292953
C	-3.19788953164050	-0.56204192514673	0.28764254919958
N	-3.98864816038507	-0.89732769098137	-0.88744415140415
H	-4.70804714463675	-1.56539114003056	-0.63103618510240
H	-5.22637359114536	-0.01468048704076	-2.31218215940897
H	-3.82234529649786	0.93315370317192	-1.85415503105940
H	-2.36387364577265	0.07455660566368	-0.02092851880295
H	-2.77933491930348	-1.47113422077989	0.71926763332999
F	-3.21578167989408	0.46032620021883	2.43345665096776
H	-4.81076825633963	-0.50633128398387	1.69673857294458
H	-5.36994884193618	1.79841942814057	1.54903959720076
C	-3.63627771239559	2.54442264810717	0.55440818577475
H	-6.27819997234522	0.40068636663944	-0.14851521929474
C	-6.10685410243422	2.28800161678657	-1.13368382840201
H	-2.97746885200920	2.32493926411662	-0.28636262506365
H	-3.01771617103200	2.68639534064479	1.43962512676969
H	-4.13855700975933	3.48814570440183	0.34550613398996
H	-5.34604917074281	2.94124060665211	-1.56483132626081
H	-6.68748242190735	2.87296744298983	-0.41827310872042
H	-6.77283084600148	1.97737776921221	-1.94007625201575

9A_a, Gas Phase

C	-5.45512787027931	1.74095195247107	0.35706678056840
C	-5.15620419058618	0.82142409669314	-0.81399652655789
C	-4.18433055880674	2.35433880133483	0.93352908020464
C	-3.14573155628344	1.27936164157165	1.22393350274246
C	-4.45435103923639	3.23957996592982	2.13784482835228
H	-3.75952242334648	2.96863988384269	0.13042173274128
C	-2.88797496283584	0.40679736776603	0.00792761375217
N	-4.12571664628895	-0.14956776851917	-0.48989707698386
C	-4.35073709405174	-1.44772467504440	-0.79031464494911
O	-5.36873977490733	-1.87181059909165	-1.26880557025316
C	-3.19954978469821	-2.45703660019659	-0.52974071521990
F	-2.83893919945733	-2.49129385418475	0.75547880673064
F	-2.11541670238530	-2.13660285520320	-1.25256537319031
F	-3.57870160585890	-3.66742202756391	-0.88257917931353
H	-6.05416504145776	0.28740893731689	-1.10986546497504
H	-4.82393188615823	1.43717983902592	-1.65837764776797
F	-3.56066815074677	0.47832346669356	2.26736959493022
H	-2.20582449687302	1.74813281454362	1.52660408565382
H	-2.42353024598962	1.02258414338765	-0.77121944592636
H	-2.19073293720973	-0.37711343444831	0.27611938311893
H	-6.12163062746171	2.53779929264044	0.01425482144028
F	-6.13148786534694	1.03752486784881	1.33216774710245
H	-5.14410426956246	4.04311138186752	1.87816179274397
H	-3.52802660397386	3.69148321281170	2.49407160591508
H	-4.88948446619772	2.65934014850664	2.94854026914051

9A_a, Chloroform

C	-5.44825688954170	1.74034232625536	0.33825421917575
C	-5.14195985050280	0.84395746838995	-0.84620314952211
C	-4.18641640563803	2.34572715068341	0.93586614013699
C	-3.13514147870724	1.27869320719076	1.19808974099230
C	-4.46482028979119	3.20521147462850	2.15747773620749
H	-3.76664919760140	2.98243239271900	0.14920848822754
C	-2.87474845484509	0.42818736523378	-0.03081169882180
N	-4.11607234601109	-0.13757808794638	-0.52204757457449
C	-4.35679885906307	-1.43308142132212	-0.75997118032549
O	-5.39492161902348	-1.87956274194538	-1.19323634784245
C	-3.21056227081339	-2.44591554511654	-0.48800105223588
F	-2.83762999382833	-2.45344035582344	0.79393112956825
F	-2.13250366028369	-2.17145307431017	-1.23160428991132
F	-3.61367454828964	-3.66538619011394	-0.79972092319319
H	-6.04014067152824	0.32677051382697	-1.16688610451248
H	-4.78622134146332	1.47181481118636	-1.66866746577884
F	-3.54373040249061	0.44412511445562	2.23213601059573
H	-2.20011878072523	1.74567430745034	1.51065014301525
H	-2.43897967911816	1.06253975409692	-0.80802778383541
H	-2.15839115440988	-0.34590384401895	0.21357604789037
H	-6.12225686362572	2.53552456384904	0.01361572440818
F	-6.12778826526324	1.00047792756283	1.30028409247411
H	-5.15978468449952	4.00743624599384	1.90792485090707
H	-3.54060817937395	3.65695013161284	2.51906542959689
H	-4.89645051356195	2.61186650546140	2.96122781735754

9A_e, Gas Phase

C	-5.48697840765020	1.14233212479594	0.37672191333676
C	-5.08370817267993	0.57704390054743	-0.97896333702117
C	-4.30760358021308	1.77010140865258	1.11888191796802
C	-3.18438426697832	0.73630844687002	1.20859779984421
C	-2.82649057401570	0.14442973311034	-0.14965251287955
N	-4.02513898155249	-0.39132506585993	-0.77685398574753
C	-4.05658907133988	-1.70241404300478	-1.10777411091039
O	-3.15872074457921	-2.47795918303391	-0.91419420327073
C	-5.34359197923271	-2.24149915299540	-1.78956518325578
F	-6.41503506986186	-2.08207187982948	-1.00113334904849
F	-5.21104626467642	-3.52582639849319	-2.04342499408212
F	-5.58546411908515	-1.61177362297372	-2.94470707418260
H	-5.94664570456116	0.12779795877469	-1.45495584222258
H	-4.72339101963851	1.38014094881449	-1.62638386912629
H	-2.39388999314334	0.92013464329145	-0.78623539453525
H	-2.10045916384320	-0.65416180115269	-0.03452513220394
H	-3.46936060444655	-0.07449482111335	1.88416053105621
F	-2.05307848129560	1.32788269288658	1.73423084416377
H	-4.63897005356266	1.99246947295524	2.13590815123876
C	-3.84302042825114	3.06907678414192	0.47093663626630
F	-6.47119005696665	2.08839110339115	0.17841488849368
H	-5.92219543890370	0.33474631940358	0.97250096665472
H	-3.43679292794185	2.91695994070769	-0.52882605317763
H	-3.06483714760899	3.52706014366912	1.07706562328761
H	-4.67682774797172	3.76327034644423	0.39231576935401

9A_e, Chloroform

C	-5.48251928987853	1.13832033811716	0.38580012955400
C	-5.08552373894697	0.57291924728380	-0.97127291363372
C	-4.30550573658974	1.77654341801861	1.12041337251264
C	-3.18997112509796	0.73681771518718	1.21187083493644
C	-2.82806975137055	0.14271787691369	-0.14386563710139
N	-4.02782275604698	-0.40023802737642	-0.76779242320203

C	-4.06026305435480	-1.69788463564478	-1.10839564381474
O	-3.16083471537425	-2.48515230497698	-0.92630937057405
C	-5.34456815834385	-2.23563827778977	-1.79757335758250
F	-6.42105468648834	-2.09207953228208	-1.01757131624226
F	-5.20221592558960	-3.52277916694310	-2.05798240257561
F	-5.58281069988256	-1.60805872201961	-2.95271711033610
H	-5.95139171341149	0.12727997978948	-1.44504643928145
H	-4.71632941924513	1.36936969331707	-1.62049802247202
H	-2.40640794305108	0.91602404108828	-0.78943090848446
H	-2.09646524404705	-0.64903759394469	-0.02270513136135
H	-3.47560623689487	-0.06692240800102	1.89309571644373
F	-2.04881725503481	1.32719069480759	1.73561989819770
H	-4.63550621285757	2.00077381149951	2.13707080085783
C	-3.84042577428118	3.07070999378721	0.46292891810547
F	-6.47487731939869	2.08415539593629	0.18300517989753
H	-5.91542352128714	0.33728556675271	0.98948149020012
H	-3.43562628469583	2.91285057069126	-0.53653578792552
H	-3.06424557223143	3.53476257722594	1.06777604075382
H	-4.67312786559960	3.76668974856268	0.38317408312794

9B_a, Gas Phase

C	-5.45193866615970	1.36399006016270	-0.39389279031403
C	-4.62052417341690	0.60236747888402	-1.40929972729781
C	-4.65421734169565	1.72471275122165	0.85620157197702
C	-3.96027731788801	0.49434211303645	1.43374716093902
C	-3.15111985488633	-0.25503315275494	0.39170132874539
N	-4.07662524971798	-0.61578673493062	-0.72892100867075
C	-5.50457620776775	2.44335304785815	1.89294582024188
H	-3.85676731798076	2.40171032809504	0.52717350796554
H	-3.60966414287655	-1.22503500854274	-1.39998005871272
H	-4.86809419375394	-1.13815295028105	-0.33190835419805
H	-5.23168686252584	0.28122876808563	-2.24864692553573
F	-4.89427603564828	-0.40463739622564	1.91022469215948
H	-3.30873729285754	0.78000701637416	2.26099619449334
H	-3.77805989706306	1.19290733766211	-1.76575735102924
H	-5.85560109026851	2.26472704046198	-0.85875190757179
F	-6.50828763979698	0.53571075657287	-0.06856832383990
H	-2.35142868660286	0.36030904259785	-0.01744299912358
H	-2.74040214295434	-1.17232443310605	0.80529014948145
H	-6.31008922057616	1.80524274542524	2.24896913877272
H	-5.94088958300999	3.34664684054817	1.46758775234392
H	-4.89490708255286	2.73946434885503	2.74614212917385

9B_a, Water

C	-5.45825946458241	1.36240484292247	-0.38842028197239
C	-4.63967522346081	0.58824461931467	-1.39535728105083
C	-4.66213946872031	1.71613785509336	0.85913788668333
C	-3.96798908670128	0.49220607522695	1.43832967037409
C	-3.17393756454329	-0.26615961353654	0.40015501546430
N	-4.05390972728815	-0.61538373615773	-0.74692440270432
C	-5.49767980634613	2.45414758391714	1.89239640639998
H	-3.85964951985140	2.37918827649782	0.52019921464995
H	-3.52344786631043	-1.14943288977618	-1.43514188029097
H	-4.80504775809712	-1.23168878389950	-0.42647388615452
H	-5.25239398405402	0.25740376659892	-2.22817131619279
F	-4.91282873449625	-0.38539593275092	1.97005304141107
H	-3.30151406340152	0.78521001574899	2.24911610270753
H	-3.81680332325569	1.19779551801459	-1.76337409462385
H	-5.83793318914559	2.26700007916283	-0.86253986781150
F	-6.55826407550435	0.57590277251560	-0.04615386695422
H	-2.36407958605536	0.35187698659597	0.01820857713734
H	-2.77132325195565	-1.18763647594884	0.80899731354984
H	-6.30907873090647	1.82921635593110	2.26070080261427
H	-5.92608090442940	3.35599583308484	1.45503730854360
H	-4.87613467089435	2.74871685144446	2.73803553822011

9B_e, Gas Phase

C	-5.54252852205404	1.27824839638951	-0.50272262171501
C	-4.63698524200036	0.49781271005697	-1.45163360192472
C	-4.83958873223821	1.67236120729485	0.79752204204872
C	-4.25345972854503	0.41381597462306	1.43983484660123
C	-3.34750588928065	-0.36681902436826	0.49142326734990
N	-4.11682385517544	-0.71817431310383	-0.74616432277506
H	-3.52122013158488	-1.25379417604100	-1.37964763898764
H	-4.89805224756318	-1.33313508305734	-0.50148551845706
H	-5.17976747081585	0.17961778054128	-2.33825015803623
H	-3.77722024058348	1.09660654136894	-1.74633766300468
H	-2.49556057192717	0.23725583785983	0.18500815497818
H	-2.99468611596810	-1.28538951849218	0.95370990435501
H	-5.60802125689544	2.04996061077141	1.47536250140545
C	-3.80048610037288	2.76719937296938	0.59483577913362
F	-5.94686256790603	2.38920314812369	-1.18550667198824
H	-6.43581986256529	0.68161996714459	-0.28402573790411
H	-5.05882182961532	-0.24161721755984	1.79128255124494
F	-3.48670502756039	0.73914132921741	2.52158799766468
H	-2.98830113387317	2.47677211364072	-0.07308732308217
H	-3.36172937409121	3.03920657955819	1.55195209748588
H	-4.27501409938386	3.65110776306262	0.17521211560730

9B_e, Water

C	-5.54067222218610	1.26890842875274	-0.49359676418266
C	-4.63602659621625	0.49895789989335	-1.44228471625350
C	-4.83951787050552	1.67747951486300	0.79979301071082
C	-4.26357639516222	0.41222557738968	1.43108442070758
C	-3.35382442983604	-0.35981297140173	0.48916008670140
N	-4.11017074689123	-0.70345515862552	-0.74371101207665
H	-3.50040874519692	-1.22034757403962	-1.37845149851860
H	-4.87611302781672	-1.34308680995202	-0.51941078223305
H	-5.18410108249329	0.16780017933066	-2.31896824086612
H	-3.78141798275097	1.09785657149950	-1.74893644313315
H	-2.49517520964378	0.23672343712814	0.18924611458917
H	-3.01555996508991	-1.28443978016644	0.94651160904616
H	-5.60613797407931	2.05786283237325	1.47758885592871
C	-3.79135004082546	2.76181414470753	0.58659277616784
F	-5.97157038550967	2.39455261904475	-1.17202798591892
H	-6.42504875952657	0.66923632948569	-0.26833204806362
H	-5.07153135721260	-0.23915797232878	1.77113054122115
F	-3.50830497070545	0.74077409825194	2.54227777302343
H	-2.98959111069413	2.45227295048067	-0.08383794254304
H	-3.34564532022571	3.03606475262027	1.54063910306664
H	-4.25941580743212	3.64877093069294	0.16440314262642

9C_ae, Gas Phase

C	-5.46173496677802	1.35316368217072	-0.39609754814270
C	-4.61450930920961	0.56904482944749	-1.38420668127221
C	-4.66569408142099	1.70450269572243	0.85650489269216
C	-3.96568615519059	0.48012601141352	1.43707483293180
C	-3.18377380338321	-0.26443230477721	0.36799105951465
N	-4.04362561036881	-0.59381460073591	-0.74503529155596
C	-5.49900055539979	2.44520767454281	1.88885040523505
H	-3.86017014402523	2.36518558698550	0.51382522339907
H	-3.58403858677454	-1.19881881231732	-1.40815486030756
H	-5.24185875951191	0.25325862015016	-2.21706383362814
F	-4.88604868792165	-0.36654967188669	2.02353806785479
H	-3.28088829366254	0.79925249092604	2.22856229578502
H	-3.85279420253679	1.26591545472111	-1.77656738576726
H	-5.80933300633035	2.27539509211405	-0.87141821088690
F	-6.58865623010278	0.62806233780528	-0.06113726260391
H	-2.33446855735807	0.38175859000641	0.08358831152045
H	-2.77987096969771	-1.18064991735860	0.79734058465386
H	-6.30828550899941	1.81430282276176	2.24996121342339
H	-5.93190419111459	3.34841802519850	1.45683501938996
H	-4.88382838021340	2.73887139310994	2.74041916776445

9C_ae, Water

C	-5.45566364804336	1.35549301759801	-0.39685012155847
C	-4.61709218933014	0.56516767787212	-1.38073091831638
C	-4.66877296136213	1.70277838307930	0.85833708174124
C	-3.96237068320668	0.48373950742320	1.43310839709295
C	-3.18927523397965	-0.26701565473034	0.36804723709014
N	-4.06098174616400	-0.61367961148795	-0.74045578188112
C	-5.49763550368133	2.45008980965800	1.89006872807773
H	-3.86412954689393	2.36267303857697	0.51611647851473
H	-3.55555682702822	-1.16905906128537	-1.41760280747854
H	-5.23703137601195	0.26273317913527	-2.22407518182320
F	-4.89700691015383	-0.37695480131331	2.01998894882670

H	-3.28629290908570	0.79323032938428	2.23206831217572
H	-3.84081709315487	1.24853652134604	-1.75800770710179
H	-5.81609033537080	2.27056909872903	-0.86999433019292
F	-6.59304888356597	0.61417749009427	-0.05671673075565
H	-2.35411089900383	0.38229402855676	0.06356062591091
H	-2.76903247119770	-1.17535644025811	0.79847479748080
H	-6.31160088917826	1.83038979687047	2.26237820146962
H	-5.92469917245549	3.35290946830459	1.45161658785843
H	-4.87496072113216	2.74548422244678	2.73547818286912

9C_aa, Gas Phase

C	-5.45991080824701	1.37163851904429	-0.38993723137525
C	-4.63861920354830	0.54487574558879	-1.36605211043813
C	-4.66029013093719	1.72291433474418	0.86087194103240
C	-3.96309235388882	0.49791025664582	1.44436273607657
C	-3.21612732141307	-0.28325296936732	0.37557306645274
N	-4.04597319617019	-0.63098066544453	-0.76056217241643
C	-5.50097971235305	2.45342724514290	1.89451558477922
H	-3.85589574038379	2.38639909674133	0.52054511256225
H	-4.77641296128030	-1.26866325826346	-0.46707383450189
H	-5.26562762771121	0.24535244145310	-2.20553100587421
F	-4.90137921115285	-0.34862149395307	2.02141807601847
H	-3.28317249597793	0.80711751174293	2.24362615023461
H	-3.83560109413112	1.17470926988883	-1.76403808699908
H	-5.81882547830991	2.28847225150802	-0.86674767441972
F	-6.58477652930860	0.63564520244209	-0.03935151873141
H	-2.37776255155304	0.32660720994850	0.02187135998348
H	-2.79907801077817	-1.19001274555830	0.81307432350978
H	-6.30586559959736	1.81177337472005	2.24677471558991
H	-5.94076292308040	3.35483895562882	1.46637390161375
H	-4.89187705017770	2.74448971734703	2.75099666690293

9C_aa, Water

C	-5.45495662567927	1.37270583430357	-0.39186379058665
C	-4.63905951069792	0.54590015429152	-1.36830903701458
C	-4.66322058941673	1.71876664549111	0.86130648469292
C	-3.95941596111528	0.49972435452298	1.44053843583340
C	-3.21366349536907	-0.28380698546839	0.37648943589382
N	-4.04383592518508	-0.63508451261926	-0.76421774914255
C	-5.50115220515529	2.45348654620215	1.89474110078727
H	-3.86041086127192	2.38309182217352	0.52249306522592
H	-4.77687635648682	-1.26926444103823	-0.46675897389353
H	-5.26692795899927	0.25001829825987	-2.20844625974008
F	-4.90497833849659	-0.35676226632414	2.02470828857791
H	-3.28287549625656	0.80479744655121	2.24113595356072
H	-3.83852092063399	1.18077577690193	-1.76012738116305
H	-5.81705889052884	2.28577894645326	-0.86819726519172
F	-6.59281985098137	0.63055670781852	-0.04030151512773
H	-2.37903354115846	0.33155229912106	0.02705603836921
H	-2.79530204138172	-1.18851373636321	0.81698387189335
H	-6.31018930355848	1.82062927594996	2.25561627431804
H	-5.93584623885905	3.35486779461358	1.46137093801113
H	-4.88588588876830	2.74542003915900	2.74649208469619

9C_ee, Gas Phase

C	-5.52332791480280	1.26934631957569	-0.51496442156869
C	-4.59748514051885	0.49066227228386	-1.43541053806306
C	-4.84037094348412	1.66522075700586	0.79486215559367
C	-4.23828383314447	0.40716970734068	1.42213316977249
C	-3.34462524866526	-0.34870661667607	0.45225189838261
N	-4.13635673115215	-0.68347352562863	-0.71735311646826
H	-3.64236485105584	-1.31731343771473	-1.32715250439531
H	-5.15640481148501	0.17949966262351	-2.31725431594342
H	-3.78316341752760	1.15015449137762	-1.76630157332046
H	-2.46304233297660	0.26618612917024	0.22353539117036
H	-2.99978300423352	-1.26480861063801	0.93046336984232
H	-5.61083114128697	2.04071709080105	1.47321818062729
C	-3.80380623977084	2.76471894934820	0.59593423108471
F	-5.96013752548826	2.40843688509611	-1.17032603812917
H	-6.40411343927101	0.65764446273534	-0.30624918971093
H	-5.03536371169774	-0.26099051195853	1.75639218290110
F	-3.49991436165690	0.75665450178611	2.54034660896270
H	-3.00055869865019	2.46176789868168	-0.07455681001784
H	-3.35846805455739	3.03159591738100	1.55197482376599
H	-4.27725859857447	3.64788765740902	0.17239649551389

9C_ee, Water

C	-5.52479734481900	1.26213656518417	-0.50827854216136
C	-4.60075582915292	0.48937447850431	-1.43251539671592
C	-4.84108192880494	1.66790571284037	0.79664579197392
C	-4.24703438799590	0.40466737604261	1.41801427631678
C	-3.34881564452709	-0.34918658746450	0.45361026806661
N	-4.13922174085119	-0.69116041949621	-0.71875157477878
H	-3.60867594625317	-1.28941405217190	-1.33693710372822
H	-5.15676666625130	0.18018044079771	-2.31678011240377
H	-3.78036587473493	1.14340992748177	-1.75634612225724
H	-2.47234034787233	0.26787637671681	0.21537382706795
H	-2.99964137693326	-1.26389723818286	0.93109187544666
H	-5.61068158040414	2.04462460160458	1.47484970406890
C	-3.79849044215709	2.76119048919746	0.59076154503549
F	-5.96950843903773	2.40766672468022	-1.16923146314181
H	-6.40836403916505	0.65771233459997	-0.29592493907731
H	-5.04592268255654	-0.25700853286806	1.75725151399343
F	-3.50595105382927	0.75256077260563	2.54788038541998
H	-2.99863396270869	2.45206975294563	-0.08100998316131
H	-3.35085099161185	3.03337815018958	1.54482642608901
H	-4.26775972033358	3.64828312679270	0.16940962394697

9C_ea, Gas Phase

C	-5.54461327113793	1.28089759325348	-0.49758046316897
C	-4.63959274287525	0.47071069512740	-1.41534002392839
C	-4.84300089330051	1.67797535141267	0.80233296723761
C	-4.25789515900911	0.41765773490477	1.44175689732840
C	-3.38761421911023	-0.36839814150126	0.47096803778227
N	-4.10175157527382	-0.70107425412396	-0.74832241426948
H	-4.82474890460117	-1.38733015840742	-0.57361939568064
H	-5.19018201144035	0.16567150772378	-2.30460438761245
H	-3.80889725757959	1.09689294180105	-1.75008721394768
H	-2.50710306035219	0.22473221668459	0.21178442775817
H	-3.03099969949701	-1.28097473893108	0.94745598240963
H	-5.60135026340458	2.07483925218295	1.48221716913680
C	-3.79040293324324	2.75840150004691	0.58416095792383
F	-5.97826593363230	2.41953051036120	-1.15700921107521
H	-6.43652795127381	0.68782979412395	-0.26968242709713
H	-5.06893177627638	-0.22986836531894	1.79112210450474
F	-3.51468388610234	0.76572257827044	2.55790954712606
H	-2.99501959272689	2.43785000370209	-0.08785296153071
H	-3.33614360307089	3.02898402162050	1.53499214844915
H	-4.25399526609241	3.64409995706690	0.15491825865400

9C_ea, Water

C	-5.54175761181992	1.27098621945375	-0.49392603264046
C	-4.63496523622148	0.47335414035751	-1.41788646478819
C	-4.84249653358431	1.67800661521008	0.80210705265774
C	-4.26328901835206	0.41299319699447	1.43331907735612
C	-3.38235464840786	-0.36580247018952	0.46928362236847
N	-4.09927137325750	-0.70415226486649	-0.75117346296414
H	-4.84336978044420	-1.36290180737630	-0.55012417058407
H	-5.19027186515300	0.16733409620149	-2.30375699606223
H	-3.80334563502619	1.10094002613913	-1.74808032478541
H	-2.50508293215961	0.23176144246067	0.20889354581667
H	-3.03034817479656	-1.27867144236944	0.94835549340395
H	-5.60317475267734	2.07058182391091	1.48144218056415
C	-3.78809393187567	2.75687032271100	0.58202151246136
F	-5.98498885085213	2.41685681239766	-1.15846841491362
H	-6.43106884565739	0.67802396802728	-0.26765330040028
H	-5.07191790303408	-0.23455078919378	1.78046036693201
F	-3.51823389048674	0.75974447877925	2.56282906592720
H	-2.99367604581425	2.43500474338656	-0.09071056734937
H	-3.33405448445299	3.03193454305646	1.53229706011822
H	-4.24995848592671	3.64583634490931	0.15629075688186

10A_a, Gas Phase

C	-5.49324781692372	1.37914126383482	-0.08839416538179
C	-4.86764354502281	0.58978391110263	-1.23178586525016
C	-4.47014465034097	1.67274209456630	0.99200170373785
C	-3.78010194448774	0.40161102447590	1.44944776406432
C	-3.17445706803361	-0.34196695090718	0.26534482225528
N	-4.19509751704161	-0.60468528975683	-0.73376135457524
C	-4.47919158967193	-1.79236111774168	-1.30179073660231
O	-5.30026541454156	-1.96533799923491	-2.16655368226643
C	-3.69078146713869	-3.03471240983643	-0.80490459391536
F	-3.87929440346100	-3.24770715733378	0.50494000460950
F	-2.37534889266884	-2.89478862633680	-1.01162066739861
F	-4.09063844391347	-4.10982768278264	-1.45184965164969
H	-5.61683704502710	0.28294385212633	-1.95422035598426
H	-4.12984878400145	1.21437830945899	-1.74281639541247
H	-2.39373751023898	0.27233631394672	-0.19101299183528
H	-2.71834766789841	-1.26582592310925	0.59785483037343
H	-4.51500506763390	-0.23782239511382	1.94407275000619
H	-3.00031548239534	0.64435815379012	2.17068081432576
H	-4.92824116096856	2.19323834859040	1.83408232988748
F	-3.50569330909610	2.52935002118523	0.46542528348970
H	-5.90271805546355	2.31570673185388	-0.46818371922338
H	-6.31424316403066	0.80932552722198	0.35223387674547

10A_a, Chloroform

C	-5.49062641428588	1.37715656409479	-0.09253581917011
C	-4.86005985175973	0.59661568613852	-1.23880345530115
C	-4.48096530632912	1.66386707418063	0.99955107674473
C	-3.77707968858676	0.39771116968462	1.44281201811515
C	-3.16715358635722	-0.33693710182003	0.25611779075470
N	-4.18856007070410	-0.60433253292359	-0.74617303341121
C	-4.48042280297929	-1.78740484817726	-1.29155550154606
O	-5.31160653258012	-1.97650183304105	-2.15496091450976
C	-3.69478249368019	-3.03082301704828	-0.79181839615786
F	-3.87450507755677	-3.24336438230576	0.51663315738538
F	-2.38183350269055	-2.90804548842395	-1.01381816176369
F	-4.11034306899136	-4.10931195261312	-1.43420066128129
H	-5.60886888917853	0.30306389694814	-1.96602048473708
H	-4.11370353460956	1.21648876710550	-1.74155096754393
H	-2.39521762388284	0.28125527537708	-0.20773089354528
H	-2.70149669639135	-1.25615949460087	0.58755586065465
H	-4.50766129963440	-0.24665826084340	1.93683093286574
H	-2.99643070591792	0.63924374708575	2.16325342153374
H	-4.94934036404109	2.16778819691419	1.84436738893799
F	-3.51781433345727	2.54773607805961	0.49124826887635
H	-5.89993193281500	2.31414904480883	-0.47109113170292
H	-6.31279622357095	0.80434341139962	0.34107950480191

10A_e, Gas Phase

C	-5.44409327954467	1.31117801682576	-0.25151520409335
C	-4.62930741163746	0.67313520164881	-1.37341781966527
C	-4.55985050085291	1.58697764834259	0.94989921269704
C	-3.83180903502384	0.33493329391906	1.39928665692377
C	-3.07707458394048	-0.29321182867732	0.22953961769369
N	-3.97704431532209	-0.52831050702457	-0.89041472260168
C	-4.24846781573438	-1.79779506168250	-1.25342171950999
O	-3.75136097699828	-2.77659744630410	-0.75848927170510
C	-5.27410980487642	-2.01216158463061	-2.39953405733500
F	-4.87834328148330	-1.42189543847088	-3.53371424035044
F	-6.47532872511279	-1.51302890199180	-2.07581402514396
F	-5.41998678287000	-3.29855091619680	-2.63860829736313
H	-5.25681993513439	0.45453996451827	-2.22861215950160
H	-3.84868395471541	1.36135031526879	-1.71243576482505
H	-2.28089109320828	0.37647072084879	-0.10981077068518
H	-2.62765175458405	-1.23860327269143	0.51575641369185
H	-4.56321589887873	-0.37737881526122	1.78678007641783
H	-3.13721604491503	0.57573175747165	2.20481787225531
H	-5.90107720554979	2.23693300496227	-0.60026705219469
H	-6.24125675655449	0.62707114015417	0.04775573815299
F	-5.33479150706211	2.06957643708203	1.98975084711374
H	-3.83446933600111	2.37000627188903	0.70317867002822

10A_e, Chloroform

C	-5.44648249902060	1.31937736319281	-0.23774685592645
C	-4.65011828902283	0.66168691015183	-1.36044294483055
C	-4.54403264930471	1.60100710044885	0.94602168942063
C	-3.83036527813336	0.34785652994709	1.40877511701212
C	-3.09313085325191	-0.30345107486611	0.24154178702259
N	-4.00907688151593	-0.54675080687418	-0.86810329464046
C	-4.24977961264126	-1.80021300396568	-1.26235500469553
O	-3.73672871616289	-2.79309334354241	-0.79217307140855
C	-5.26143505158091	-2.01269216518687	-2.42169010445070
F	-4.86374400075939	-1.40751425297615	-3.54546131759878
F	-6.47623833160913	-1.54741425269731	-2.10954082753950
F	-5.37974433331604	-3.30371097736468	-2.68014172214610
H	-5.29094823725919	0.44623171137945	-2.20595005527138
H	-3.86179516080315	1.33342844160220	-1.70998240782028
H	-2.29940329197791	0.35617789721170	-0.11876480174019
H	-2.64551922596775	-1.24437024372252	0.54181335209747
H	-4.56701780898532	-0.34994144007215	1.81271377153046
H	-3.11887098014295	0.59017313089904	2.19859665006903
H	-5.89293317286930	2.24460892666019	-0.60026672936773
H	-6.24689214943961	0.64704036307661	0.07975034016375
F	-5.31132117446881	2.10552526292593	1.99535223314259
H	-3.81727230176704	2.37640792377236	0.68876419697758

10B_a, Gas Phase

C	-5.48694681226254	1.04611901329964	-0.46823400731261
C	-4.61842752956454	0.34619557496348	-1.49580277597288
C	-4.67760064239436	1.38498272587294	0.77335018248207
C	-4.04570394703100	0.13435472699748	1.36323207571419
C	-3.18143653940865	-0.56422356779289	0.33117677294260
N	-3.99882358657227	-0.88476851792486	-0.89105052660585
H	-3.41013924238952	-1.34753699008932	-1.58453701046344
H	-4.73601464869150	-1.54794555945120	-0.64161842497009
H	-5.17964709183032	0.03749355483508	-2.37361477472170
H	-3.79127005933020	0.98473828195174	-1.80153432710673
H	-2.37629109914043	0.08781741438084	-0.00342346566255
H	-2.76141614372492	-1.49516074721726	0.70235874530631
H	-6.34120797311861	0.42413617044696	-0.18868588176848
H	-5.88389637662015	1.95738958809213	-0.91385227376587
H	-5.29322084288916	1.89629030414968	1.51250979109934
F	-3.65858832115091	2.24222850907727	0.39792241811815
H	-3.42073398262559	0.39951400665420	2.21510783798533
H	-4.83008516125531	-0.53134448824593	1.73245564470220

10B_a, Water

C	-5.46993838076889	1.05475410329419	-0.47486353274457
C	-4.60518238038167	0.33699041942170	-1.49264884415547
C	-4.69252265422172	1.38288657956224	0.78384425053983
C	-4.03047641353465	0.14460703530980	1.35404668709896
C	-3.18375993686382	-0.56436822808804	0.31493814833383
N	-4.00882490064557	-0.88679125318083	-0.88443565358994
H	-3.43225921992717	-1.36486767707527	-1.57609556443772
H	-4.74951133110021	-1.54229352048221	-0.62936324948722
H	-5.17676549248290	0.02761499268156	-2.36179280378533
H	-3.77047721248965	0.95689020931523	-1.81330474137442
H	-2.37117885180011	0.06879628767592	-0.03458617055702
H	-2.77554634607378	-1.49584127502100	0.69393913288314
H	-6.32223321833564	0.42987323202927	-0.19905005813788
H	-5.86135547148395	1.96687770149992	-0.92277624572347
H	-5.33479616593951	1.85588804171396	1.52476442926064
F	-3.69382285006065	2.31078019728249	0.45921811711486
H	-3.40081673618328	0.41193069062776	2.20138647686051
H	-4.81198243770681	-0.52344753656670	1.72253962190127

10B_e, Gas Phase

C	-5.43635797871924	1.07447001860310	-0.49648451191756
C	-4.58966732709615	0.33590558805703	-1.51519691956601
C	-4.64164461981149	1.40958652399877	0.75732012559890
C	-3.99301906689031	0.16124410350274	1.33771676761398
C	-3.15961852130775	-0.56992993657221	0.30286611329347
N	-4.01102042090974	-0.90291428456373	-0.89046183677226

H	-3.46152811195208	-1.41810495138013	-1.57946485849184
H	-4.77309812498355	-1.51959749685593	-0.59822814938776
H	-5.16751793293885	0.03239860093717	-2.38432761889614
H	-3.73904764055631	0.93034587442222	-1.84852464788534
H	-2.34206941784252	0.04514318111785	-0.07298558267650
H	-2.75005307707145	-1.49925388403358	0.69019017848350
H	-6.30153732324707	0.47031921996315	-0.20958430984184
H	-5.81969045176891	1.98558208069074	-0.95460746865111
F	-5.49227324959520	1.93806982813914	1.68997637628150
H	-3.88034102505944	2.16388196692198	0.53354945345169
H	-3.35312758904350	0.42519129825379	2.17905279200879
H	-4.77982812120644	-0.49205773120209	1.72492409735453

10B_e, Water

C	-5.43974844910443	1.07009878750032	-0.48810981631350
C	-4.59028198550318	0.33137149371141	-1.50517249412380
C	-4.62972653243041	1.40745842490286	0.74712739535050
C	-4.00354771761945	0.16051699162755	1.33782376345086
C	-3.17002695666764	-0.56775564023892	0.30021094904807
N	-4.00632852917640	-0.89380031170077	-0.88942890529615
H	-3.44207398734919	-1.38839465187165	-1.58022217519300
H	-4.75380720961328	-1.53635936223897	-0.62091565416050
H	-5.17403280705049	0.02194533869413	-2.36616006146634
H	-3.74890186506684	0.93423436977498	-1.84293843259901
H	-2.34938630947623	0.04854090594520	-0.06304230350193
H	-2.77063409398739	-1.49922464175875	0.68834772287947
H	-6.28988921704603	0.45020231833368	-0.19336896647431
H	-5.82589168350676	1.97707840411980	-0.95091806086012
F	-5.47262261434153	1.98173033762762	1.69584646806365
H	-3.86312779895149	2.14948572790409	0.51363824656181
H	-3.36286438873716	0.41736455946132	2.18020268899844
H	-4.79854785437209	-0.49421305179389	1.70280963563586

10C_ae, Gas Phase

C	-5.46099156021046	1.05225873520659	-0.48567656608927
C	-4.57254191525516	0.32157614348375	-1.48441379831153
C	-4.68974819124585	1.37835300231614	0.77953585317141
C	-4.01963755671917	0.14043743689811	1.34577715648890
C	-3.18576402375922	-0.55700612782778	0.27855339620797
N	-4.02565983484216	-0.87634950415136	-0.86574850084479
H	-3.50464765275352	-1.41473354519410	-1.54394407432095
H	-5.15935539376546	0.03121585143154	-2.35568332343999
H	-3.78573601311101	1.01101560714093	-1.82323624858298
H	-2.34481760990227	0.09769151438574	0.00762292803246
H	-2.77227102424869	-1.48176254897610	0.68061686546678
H	-6.30478898442636	0.41278147734744	-0.21619657401760
H	-5.85449971876607	1.97168564217535	-0.92034754477094
H	-5.33787553979471	1.84652499812192	1.52278826188351
F	-3.70335610977906	2.31558115781981	0.46923693741797
H	-3.39942175917547	0.41865597582824	2.19847790380695
H	-4.79940711224534	-0.53918581600621	1.69738732790209

10C_ae, Water

C	-5.45916253095438	1.05465390462445	-0.48698284031128
C	-4.57487253668638	0.31621436226966	-1.48331948782825
C	-4.69898013957432	1.37315797348761	0.78421713675398
C	-4.01686670013578	0.14227908529428	1.34558681381210
C	-3.18972128151131	-0.56143243819473	0.27754030875318
N	-4.03188745046947	-0.88867331594571	-0.86702210198790
H	-3.48831205515411	-1.40100630605579	-1.55011713463001
H	-5.16011512205228	0.03343197991677	-2.35777955069549
H	-3.77710723760918	0.99288933666057	-1.82137262912448
H	-2.35103296320837	0.08885541702749	-0.00944389718651
H	-2.76995871686620	-1.48166495439682	0.68270759686342
H	-6.31171400794184	0.42658932145988	-0.21720318043856
H	-5.84677714224748	1.97549541145947	-0.92420311710676
H	-5.34783336448382	1.83811193929996	1.52635689862816
F	-3.70923803272308	2.32955493379484	0.48067047908991
H	-3.39191034648155	0.42266407906520	2.19425389579749
H	-4.79503037190042	-0.53238072976711	1.71086080961099

10C_aa, Gas Phase

C	-5.47603680053546	1.06539693845350	-0.47330073054945
C	-4.60263833031395	0.29912039107611	-1.46717662642346
C	-4.69165960589900	1.38870708650821	0.78627127701636
C	-4.02967397705795	0.15028535789599	1.36462701298587
C	-3.21981532964451	-0.57675723194784	0.29072269669023
N	-3.99268334156981	-0.89245886918332	-0.89964870541076
H	-4.70352485861848	-1.58156491979424	-0.68382698733413
H	-5.17897928503805	0.01962717068705	-2.34894380779159
H	-3.79525592904086	0.95262492012768	-1.80764173154704
H	-2.38589460419595	0.05958500722254	-0.01672042328659
H	-2.78916869089668	-1.49467881140697	0.69045552635250
H	-6.33785010373320	0.45208684785989	-0.19391470060034
H	-5.85524859236117	1.98916728656071	-0.91329410003915
H	-5.32737200044774	1.87459320265471	1.52858566100612
F	-3.69415911573242	2.30778331418131	0.45838073061377
H	-3.39846356384466	0.43476341082989	2.20808481777760
H	-4.81289587107011	-0.51246110172522	1.74444009054006

10C_aa, Water

C	-5.47064389788886	1.06443103633532	-0.47685702844961
C	-4.59834870059306	0.30018971504680	-1.47115575624883
C	-4.70000026068961	1.38134887821162	0.78904702037624
C	-4.02500899166739	0.15024708891599	1.35985865011320
C	-3.21490061661608	-0.57678058482633	0.28802047908826
N	-3.99497903103212	-0.89977974230112	-0.90167203317372
H	-4.72874133182501	-1.55518351769116	-0.65182983220089
H	-5.18157652450364	0.02359958468853	-2.34912922722040
H	-3.78681807663581	0.94804330945191	-1.81416731966320
H	-2.37932758517400	0.05517373626119	-0.02566604023663
H	-2.78923143137182	-1.49366297446032	0.69503285375141
H	-6.33071813499956	0.44820473880757	-0.20127697837308
H	-5.85157881577097	1.98732356036737	-0.91731534722897
H	-5.33929615516915	1.85998120878251	1.53054618207996
F	-3.70093488837884	2.32456236947442	0.47149953823335
H	-3.39377399594606	0.43352535482255	2.20378348501246
H	-4.80544156173801	-0.51540376188685	1.73838135414045

10C_ee, Gas Phase

C	-5.43543551066717	1.06495634280322	-0.49571082254545
C	-4.55856631964368	0.31754011014118	-1.49588741084928
C	-4.63398136720500	1.39855586470931	0.74588174915441
C	-3.99753274116040	0.15485509645855	1.33189963741830
C	-3.17303639361730	-0.55980278489146	0.26541672333162
N	-4.01499944379017	-0.87638405459733	-0.87407377661467
H	-3.51218153391074	-1.43606286747679	-1.54845904250755
H	-5.15343612406623	0.02613789549766	-2.36109683786262
H	-3.76561825009710	0.99522742905538	-1.85328705180418
H	-2.31990979299981	0.07969457842724	-0.01567712772163
H	-2.76697253429842	-1.48519211441158	0.67302484282910
H	-6.27547868971275	0.43114178602146	-0.20479625005743
H	-5.83085809753257	1.97855489663524	-0.94092649169526
F	-5.46142673860710	1.98933094313491	1.69081405182421
H	-3.85919151784240	2.13342375713236	0.50212638415824
H	-3.37169885139768	0.42215681710498	2.18404571858889
H	-4.79170609345147	-0.50780369574435	1.68142570435330

10C_ee, Water

C	-5.43768505164479	1.06448986950278	-0.49439640761368
C	-4.56270613772291	0.31333459381186	-1.49360921272357
C	-4.62862870864536	1.39516708105361	0.73997322184659
C	-3.99955420532199	0.15425935851390	1.33341037142374
C	-3.17808421552195	-0.56351191861773	0.26645332939271
N	-4.02258143725201	-0.88904432458634	-0.87440663465714
H	-3.48772565481613	-1.41242341742267	-1.55613544047025
H	-5.15522681867677	0.02975787586202	-2.36258781500158
H	-3.76265179893461	0.98399939255025	-1.84222592441654
H	-2.33289169195013	0.07847483714161	-0.02499404621176
H	-2.76487711132816	-1.48414655206727	0.67671450616681
H	-6.28117339986687	0.43453443694102	-0.20145465278211
H	-5.82648323752365	1.97795341449647	-0.94558356205450

F	-5.46263439822687	1.99605397011696	1.69493864465599
H	-3.85767157453303	2.13217955378717	0.50030832683758
H	-3.36650507634793	0.42108937387263	2.18031515306698
H	-4.79494948168684	-0.50583754495629	1.68800014254071

10C_ea, Gas Phase

C	-5.44718003184861	1.07962238663514	-0.48255605830008
C	-4.58861929910582	0.29352357915851	-1.47872758877086
C	-4.63587616206024	1.41028102101517	0.75326728288765
C	-4.00647095349546	0.16762675948090	1.34868086591018
C	-3.20760039954959	-0.58078444752301	0.27671888483724
N	-3.98406847546948	-0.89711962020237	-0.90865254187674
H	-4.69868340537517	-1.57992472980855	-0.68651679935883
H	-5.17885479255914	0.01180378397972	-2.35019148141627
H	-3.77611258416325	0.93048619471900	-1.84388463091262
H	-2.35866767533684	0.03310348746316	-0.04220932200995
H	-2.79044072610895	-1.50037530443460	0.68600948470202
H	-6.30422589341440	0.47153359907805	-0.18017373387623
H	-5.82971791446835	1.99565431726259	-0.93549569792105
F	-5.45423894108285	2.01563161499180	1.69836734646425
H	-3.85577383938865	2.13662687598988	0.50114106997736
H	-3.36900267036764	0.43786023680763	2.19202648729143
H	-4.80530623620556	-0.47724975461302	1.72510643237250

10C_ea, Water

C	-5.44655959660868	1.07599671395509	-0.48307183976811
C	-4.58559943491444	0.29573098983933	-1.48132645898956
C	-4.62960997926150	1.40512064554334	0.74573611472752
C	-4.00724306075360	0.16503995474418	1.34631477773001
C	-3.20364465351315	-0.57947715019296	0.27555323319641
N	-3.98589084976688	-0.90191404144235	-0.90969034093089
H	-4.71926283604073	-1.55701014162410	-0.65923808823797
H	-5.18085016224068	0.01798196723786	-2.35030295378064
H	-3.77297002137032	0.93555733412378	-1.83946778197516
H	-2.35922119404645	0.04007345286645	-0.04249396818184
H	-2.78882041808998	-1.49697037772357	0.69113570907080
H	-6.29759818725721	0.45804624041790	-0.18365114550936
H	-5.82870954014170	1.99006283830349	-0.94006686915351
F	-5.45740330316870	2.01733283383087	1.70140194103133
H	-3.85513576054665	2.13673862758936	0.50062103970978
H	-3.36675686860219	0.43198590764910	2.18830912654517
H	-4.80556413367713	-0.48599579511775	1.71314750451603

11A_a, Gas Phase

C	-5.47163782932372	1.35940738804640	-0.30074536535532
C	-4.72873457889554	0.59869246323683	-1.39418580688826
C	-4.57121552736142	1.62463221224388	0.89072461096125
C	-3.92866289739065	0.34079897567083	1.39739611800493
C	-3.18896122970442	-0.33963650113100	0.24769681245292
N	-4.09458126673316	-0.59736643030494	-0.85442703474472
C	-4.40242709975567	-1.79796559603501	-1.37832452748087
O	-5.18399972489799	-1.98127033383538	-2.27720278805490
C	-3.69201615076267	-3.04322659528640	-0.77998836958810
F	-3.97197358913277	-3.18864879610109	0.52365711909149
F	-2.36185628127600	-2.96071223445220	-0.90561745930148
F	-4.09120009029811	-4.13248498769951	-1.40296059678379
H	-5.40222286219884	0.29877311076770	-2.19052082550582
H	-3.95086954274446	1.23868958571491	-1.81808661023644
H	-2.38981196919126	0.31850284108162	-0.10603362361187
H	-2.72943204791810	-1.25719059823977	0.59442859344141
H	-4.74547110441674	-0.32077405883895	1.70396139140168
C	-3.00087225641051	0.58104228546723	2.57465933786976
H	-5.84138808708423	2.30596601898515	-0.69657508349569
H	-6.33355443055819	0.77933353904121	0.03598069217710
H	-5.11851286127191	2.12242564685357	1.69420579781200
F	-3.56186011364137	2.50091052009476	0.49423363077031
H	-2.18653780839687	1.24828241570818	2.29309532430907
H	-2.57141891325013	-0.35942961677375	2.92069947633440
H	-3.53889173738524	1.03335910578571	3.40767918642093

11A_a, Chloroform

C	-5.47153254417970	1.36452066027805	-0.29756160078787
C	-4.73533407871651	0.59613781764801	-1.38879863573606
C	-4.57565790486472	1.62834580253604	0.89494546223357
C	-3.93191901249429	0.34718019867455	1.40108473837757
C	-3.19975333733152	-0.34749555643656	0.25560899191606
N	-4.11113590887137	-0.60795242149070	-0.84599280279007
C	-4.39671053768696	-1.79812234803736	-1.37783080319480
O	-5.16770750859708	-1.99172283406334	-2.29444381153932
C	-3.68269084886998	-3.04472996965460	-0.78605966720402
F	-3.96889910423200	-3.21461919581798	0.51007922426395
F	-2.35387071770207	-2.96005337458713	-0.90790142991588
F	-4.07519150641162	-4.13134736939201	-1.42882678246872
H	-5.41306192479663	0.30876846365726	-2.18510318347429
H	-3.94601935573799	1.22093641085075	-1.81286431137076
H	-2.39776164540379	0.29825585639844	-0.11211402060302
H	-2.74643606442990	-1.26453753222235	0.61145804163655
H	-4.75185570606688	-0.30433261986044	1.71918798625850
C	-2.99597509853701	0.58851595888087	2.57212570468735
H	-5.83611986219884	2.30997054047372	-0.70023217780305
H	-6.33633915294773	0.79232791686845	0.04397047413490
H	-5.12330939893496	2.12575797137765	1.69661549743176
F	-3.56174279967869	2.51308654262828	0.49985979986088
H	-2.16828751500578	1.23459352324099	2.27901423861438
H	-2.58384232393768	-0.35505424773769	2.93054999102653
H	-3.52695614236628	1.06367980578708	3.39697907644584

11A_e, Gas Phase

C	-5.42562394203148	1.36338568855010	-0.31271337445271
C	-4.65191849716132	0.63128335935347	-1.41540433680308
C	-4.46660258918714	1.65361721818381	0.83715841702974
C	-3.80434257112374	0.39144556218310	1.35367970361534
C	-3.13180157211790	-0.36061030595131	0.20738917214676
N	-4.05893444852078	-0.58418666024275	-0.89399008225923
C	-4.32038644463594	-1.84801119658902	-1.28186951878628
O	-3.85550039153189	-2.83465008310075	-0.77048767129493
C	-5.27197871907616	-2.05181399811735	-2.49416238507439
F	-4.81074892460958	-1.43063500004888	-3.58674714878030
F	-6.50160512569735	-1.58173637057466	-2.24597662886378
F	-5.37780430506700	-3.33529616565652	-2.76909098944202
H	-5.31159687950376	0.41123189396695	-2.24712993582480
H	-3.84400192652464	1.26528783946854	-1.79491059100367
H	-2.28917534221354	0.22466659182989	-0.17541797448779
H	-2.75427182221833	-1.32243742234770	0.53890110550700
H	-5.75361677362222	2.32085588175729	-0.72353504648062
C	-6.64499861673815	0.56992214491205	0.13736512667616
H	-4.55308337460590	-0.24192811759320	1.83079663944283
H	-3.06064527230552	0.64900659893991	2.10844161807693
F	-5.14672366088159	2.27632835650861	1.87001174011242
H	-3.69973634637208	2.35747631975576	0.49618909176578
H	-6.37428881303858	-0.43724884867477	0.45631605756870
H	-7.35736227109928	0.47301501432641	-0.68093558944259
H	-7.13801137011612	1.06738169916103	0.97021260105453

11A_e, Chloroform

C	-5.42759184441725	1.36347792387318	-0.30832351158949
C	-4.66099131986665	0.62416932281417	-1.40990038555757
C	-4.45941945544814	1.65552634684386	0.83094925663362
C	-3.80530333346874	0.39530956170221	1.35751335705955
C	-3.13915314919902	-0.36661777604425	0.21494913708710
N	-4.07510947573877	-0.59725031152711	-0.88241777354807
C	-4.31723784621172	-1.84646386917534	-1.28967485894433
O	-3.84078343175188	-2.84734738739594	-0.79793716467255
C	-5.26425660080344	-2.04699031359915	-2.50595518549171
F	-4.80560407001867	-1.42134911926982	-3.59499889864028
F	-6.49964594658496	-1.59788815239101	-2.26172551533832
F	-5.35535850937184	-3.33501731872755	-2.79071282753088
H	-5.32556265253075	0.40965030941719	-2.23868436725195
H	-3.84644763228014	1.24743158349771	-1.78850888472957
H	-2.30273286095898	0.21603904401676	-0.18124985309586
H	-2.75824625827642	-1.32229927161561	0.55732824529843
H	-5.75052034033377	2.31796953583609	-0.72837688626814
C	-6.64885713725532	0.57673274327346	0.14874751073746
H	-4.55456118955427	-0.23206082197486	1.84196313750424

H	-3.05180150302785	0.65317206719646	2.10202037551306
F	-5.13670270337875	2.29190578935093	1.87027233729364
H	-3.69390234500773	2.35596642754619	0.48611806959801
H	-6.37935162656694	-0.42353247371070	0.49061062910119
H	-7.35353922330325	0.46698141269885	-0.67489005838317
H	-7.15207954464472	1.08883474736431	0.96697411521557

11B_a, Gas Phase

C	-5.51577249272795	1.04217001775287	-0.54250499511221
C	-4.65893985729486	0.33317784550226	-1.57311541877916
C	-4.69866492148117	1.37434909237704	0.69404315344044
C	-4.08089710490699	0.11893651882471	1.30108518245087
C	-3.21821598294296	-0.57068808786750	0.25546644743943
N	-4.03518148609477	-0.89357005602711	-0.96612188776987
H	-3.44895378001472	-1.35851540932391	-1.66010433172409
H	-4.77079477412949	-1.55601335306895	-0.71077741080745
H	-5.23063621730689	0.01873549865566	-2.44206030646093
H	-3.83451329010737	0.96820174382823	-1.89256950439389
H	-2.41375865989711	0.08666248503317	-0.07344423747814
H	-2.79458383891468	-1.50097063328804	0.62643356397568
H	-6.37327276641365	0.42817933353534	-0.25609713226217
H	-5.90746409065119	1.95602470515204	-0.98741157604811
H	-5.30381561714838	1.89728988460855	1.43531963564888
F	-3.67214403066931	2.22213034311388	0.31177020668857
C	-3.26347611015563	0.43323229219497	2.54569207341830
H	-4.90463977310683	-0.54892318056072	1.57775342393561
H	-2.48069780476476	1.15732830348540	2.32327982524021
H	-2.80227489815690	-0.46402580228789	2.95639925739610
H	-3.90686250311440	0.85835845835999	3.31501403120192

11B_a, Water

C	-5.50266988542642	1.04756191087937	-0.54861415948859
C	-4.64315192884136	0.32690259544712	-1.56816325735468
C	-4.72127731028047	1.37223418588837	0.70750737848627
C	-4.07547252894565	0.12700093784026	1.29494231329947
C	-3.22438200324708	-0.57029981289128	0.24553900234764
N	-4.04087476672097	-0.89283799364167	-0.95849561075616
H	-3.45926176569381	-1.36689367489183	-1.64881726025031
H	-4.77821396640171	-1.55345187987708	-0.70699996680973
H	-5.22046636146169	0.01170265684582	-2.43146342198596
H	-3.81205891593283	0.94675324967180	-1.89761722626176
H	-2.41133152392155	0.07086946934640	-0.09186275987612
H	-2.81318827190476	-1.50192571620279	0.62352734795023
H	-6.35761063573777	0.42746054232743	-0.27079698482100
H	-5.89029724570322	1.96185567664534	-0.99553565811762
H	-5.35703733939625	1.85562245752347	1.44922232216637
F	-3.71409629472702	2.28902087081644	0.37867641974101
C	-3.25246817743043	0.43847585913283	2.53497177648866
H	-4.89560705482785	-0.54187132249578	1.57353809670096
H	-2.44345302329807	1.13035956776601	2.30083483177024
H	-2.81889274990782	-0.47092275819990	2.94993917121903
H	-3.88374825019328	0.89445317806967	3.29771764555203

11B_e, Gas Phase

C	-5.42684577843098	1.06852873430752	-0.57605364672807
C	-4.53739384039450	0.35188404001675	-1.58323328843273
C	-4.61678644246847	1.39079701420209	0.68272974465878
C	-3.95694930154702	0.14903340968119	1.26683718684536
C	-3.12769168191064	-0.58311471752804	0.22851399576891
N	-3.97554847175436	-0.89971590620008	-0.97066377480916
H	-3.42839173470477	-1.41309744299760	-1.66215136030815
H	-4.74831678806639	-1.50871113319497	-0.69098054298672
H	-5.09389215839839	0.06577157800167	-2.47311050504360
H	-3.67884439350540	0.95445315627365	-1.87922078653818
H	-2.30546109249575	0.03008273653901	-0.14007089679539
H	-2.72514351817591	-1.51734905352791	0.61110555535175
C	-6.69721211180386	0.28437094814925	-0.26552267304560
H	-5.71310666637117	2.01429939667619	-1.04038392796667
H	-3.30646840324105	0.43236087742344	2.09354245595914
H	-4.72441411853288	-0.50891007565768	1.67926892915949
F	-5.44657141182530	1.93287962379160	1.62859223053130
H	-3.85510154758063	2.14027158191540	0.44545571924102
H	-6.50696187601787	-0.67972548026277	0.21272953714481
H	-7.27125278370106	0.10686012563332	-1.17429880139258
H	-7.32119587907362	0.85061058675797	0.42199484938628

11B_e, Water

C	-5.43050978135079	1.06946559808424	-0.57047677966274
C	-4.54482768561467	0.34184556983550	-1.57366438603006
C	-4.60604887198227	1.38810006883998	0.67235787732503
C	-3.97324843252554	0.14581387676293	1.26795064731343
C	-3.13874446078747	-0.57993199510291	0.22906417596523
N	-3.96745030600118	-0.89307718082188	-0.96960214202732
H	-3.39644845289979	-1.37465341618499	-1.66403222544012
H	-4.71215063815099	-1.54575965454930	-0.71887130474454
H	-5.10837372590217	0.04568763724849	-2.45401863426256
H	-3.69780405457213	0.95278879371979	-1.88105995499885
H	-2.31581331374520	0.03871825194860	-0.12514639375467
H	-2.74318734735869	-1.51517614326077	0.61178526496894
C	-6.69967601400264	0.28737027864249	-0.25308935759785
H	-5.71021936228061	2.01369712196910	-1.04074736035567
H	-3.32518346728607	0.42123594000304	2.09875486359516
H	-4.74968198426411	-0.51499472949893	1.65711254547456
F	-5.42381716602626	1.98163247253041	1.63057317635482
H	-3.83381064364076	2.11875973887974	0.42249590741741
H	-6.49355901023402	-0.68391381549246	0.19883951956974
H	-7.26959472041101	0.11938685253686	-1.16618412199324
H	-7.32340056096365	0.84458473391005	0.44303868288329

11C_ae, Gas Phase

C	-5.49315244268074	1.04402401645664	-0.56028549660532
C	-4.60737249640689	0.31310367801782	-1.56086769404510
C	-4.72096201027066	1.36562843243198	0.70458975055173
C	-4.06705712105976	0.12096860280174	1.28790990246873
C	-3.22986660930602	-0.56571192882737	0.21146905561570
N	-4.05702128819921	-0.88239430962843	-0.94185795921495
H	-3.52933528347558	-1.41742480417003	-1.61744507514808
H	-5.19812772874716	0.01927038778653	-2.42841159767306
H	-3.82391339874995	1.00336420320086	-1.90519478005414
H	-2.38690973254271	0.09508228242604	-0.04352698859279
H	-2.81603287569181	-1.49135977549750	0.61377053432305
H	-6.33897548024374	0.40734579647093	-0.29082143588855
H	-5.88435849684186	1.96505415583168	-0.99373351594700
H	-5.36376125669075	1.84330839333117	1.44846425815780
F	-3.72620595297345	2.29434349249889	0.39253176010569
C	-3.25076707769118	0.44091935351444	2.52990228548779
H	-4.88354594438081	-0.55835443903952	1.55212168076192
H	-2.44576753746471	1.13669612636871	2.29376726267287
H	-2.80959145848192	-0.46427344805527	2.94842703006422
H	-3.87512580810109	0.89749978408068	3.29934102295949

11C_ae, Water

C	-5.49378575953082	1.04392389377411	-0.56138247827572
C	-4.60802095732562	0.30978950894519	-1.55906353080255
C	-4.73420909416392	1.35993976494618	0.71019802476267
C	-4.06748489715810	0.12220361025702	1.28842382192831
C	-3.23483531541430	-0.56959433750323	0.21230522041415
N	-4.06108279290103	-0.89338076831128	-0.94380281070177
H	-3.50730416920530	-1.39874838274122	-1.62385305346758
H	-5.19390662923604	0.02474426109388	-2.43244388559834
H	-3.81378686045981	0.98976118173813	-1.89817748592800
H	-2.39400839903965	0.08839772693881	-0.05531534393933
H	-2.81550061642821	-1.49119874435348	0.61756262378256
H	-6.34641565635656	0.41521323408482	-0.29368897863551
H	-5.88164858592675	1.96562001791288	-0.99665221481348
H	-5.38028587563883	1.83179525638120	1.45253143207969
F	-3.73920016634301	2.30961485853602	0.40573941704707
C	-3.24488453018150	0.44253344470074	2.52661621536149
H	-4.88359268328961	-0.55272972487223	1.56547572893380
H	-2.42201992439506	1.11542757576403	2.28301415213341
H	-2.82410438532991	-0.46809617108986	2.95435080006152
H	-3.86177270167599	0.92187379379827	3.28831234565763

11C_aa, Gas Phase

C	-5.50752785752476	1.05925476294351	-0.54969012996898
C	-4.63483982080186	0.29114813954101	-1.54303203429672
C	-4.72485954012838	1.37556276926852	0.71164366602285
C	-4.08435985580884	0.12764947726612	1.30667252977307
C	-3.26835765143569	-0.58824009079729	0.22585282160311
N	-4.02471448637701	-0.89934172254406	-0.97462093082750
H	-4.73396295706953	-1.59325918687569	-0.76989763087799
H	-5.21296989960020	0.00939730745722	-2.42288463274205
H	-3.82854169905366	0.94439463424601	-1.88620857243389
H	-2.42963282036951	0.05358101937350	-0.06194111745947
H	-2.84043963606003	-1.50742936850541	0.62888346500912
H	-6.37323011460704	0.45037387292925	-0.27326726754476
H	-5.88080330656913	1.98542020718218	-0.98994592281094
H	-5.35489596956402	1.87248685364783	1.45374262151124
F	-3.71594514616094	2.28330516255329	0.38429462805999
C	-3.25030943521674	0.44894009286933	2.53585590961795
H	-4.90951155883464	-0.53443579296244	1.59441262377090
H	-2.46135194311603	1.15872260439170	2.28716690660791
H	-2.78363361114055	-0.45320871634712	2.93334005001523
H	-3.86352269056140	0.88749797436255	3.32433301697092

11C_aa, Water

C	-5.50437500540069	1.05608824957699	-0.55253026891527
C	-4.63023886273639	0.29336219274144	-1.54639846876578
C	-4.73509381303624	1.36912938038657	0.71451163507125
C	-4.08002654965165	0.12896231101324	1.30228079358608
C	-3.26244341947548	-0.58599750923473	0.22392300561039
N	-4.02473904203229	-0.90484518991972	-0.97658334323717
H	-4.75619018595915	-1.56724473682179	-0.73934076144891
H	-5.21320823500445	0.01419507844250	-2.42368328035363
H	-3.82082251732604	0.94330433352743	-1.89004680647530
H	-2.42315332565434	0.05366110542737	-0.06873252138823
H	-2.83852522970952	-1.50394612378563	0.63354179971273
H	-6.36648861989035	0.44155264914610	-0.28016443929448
H	-5.88223761805479	1.98046864645836	-0.99272081492901
H	-5.37025782235082	1.85735246662304	1.45558903551266
F	-3.72760033147654	2.30210012002014	0.39596649933697
C	-3.24651466066027	0.44786527234795	2.53282759537010
H	-4.90150464273005	-0.53616949762454	1.59003477530966
H	-2.43949264575960	1.13843751788717	2.28487563819189
H	-2.80131559847196	-0.46096800117253	2.93979296683708
H	-3.85918187461933	0.90451173496063	3.31156696026897

11C_ee, Gas Phase

C	-5.42694471208787	1.06754472829188	-0.57847729871064
C	-4.51807649132984	0.31811901021064	-1.55999283158815
C	-4.61063130707058	1.38453212665438	0.66989746424416
C	-3.96908673931941	0.14769856980588	1.26604109015894
C	-3.14004600175936	-0.56392688039245	0.20073632607503
N	-3.98257180264576	-0.87948115263776	-0.93805244764452
H	-3.48654890584392	-1.44519271959498	-1.61190792468284
H	-5.09723015782395	0.03152189351198	-2.43880964975596
H	-3.71829584240085	0.99861500273703	-1.89567918965406
H	-2.29064407020786	0.08116135785728	-0.08021897029622
H	-2.72912888879087	-1.48790162042431	0.60656332252601
C	-6.69703921676545	0.28713677568117	-0.26361327366755
H	-5.70527154807422	2.01938355922634	-1.03830742808509
H	-3.34145891896565	0.43347923226792	2.11081189117004
H	-4.74832698558072	-0.52135458251316	1.63369690928786
F	-5.41423060551951	1.99875257588339	1.62125436320679
H	-3.83001182757379	2.10714277418214	0.40931789446979
H	-6.46506776246301	-0.72306263504187	0.07001654618608
H	-7.31801357011019	0.20825653073234	-1.15659646350006
H	-7.27590464566719	0.78882545356215	0.51040967026039

11C_ee, Water

C	-5.42936294235583	1.06510296957511	-0.57439453367230
C	-4.52226443997828	0.31584040390349	-1.55725619941552
C	-4.60511870824017	1.37644258702524	0.66705722371259
C	-3.96845772249295	0.14088513587842	1.26549405937786
C	-3.14180401767938	-0.56910083962616	0.19707920525548
N	-3.98531750060534	-0.89093374202408	-0.94481220135869
H	-3.45254472088698	-1.41197012591685	-1.62957477411866
H	-5.09881165397881	0.03958459307808	-2.44068780868150
H	-3.71797973413867	0.99335016844526	-1.88260858977613
H	-2.30049621682819	0.08030044527925	-0.09107957572491
H	-2.72311584557678	-1.48927943429061	0.60282494841371
C	-6.70454424617066	0.29263236508852	-0.25892584992902
H	-5.70302448761665	2.01603451316725	-1.03832491585452
H	-3.33309378013889	0.42490367814302	2.10507125213932
H	-4.74640769867529	-0.52868098831799	1.63699020351312
F	-5.41213944914527	1.99824930985022	1.63124768548756
H	-3.82821355360046	2.10127748459661	0.41011159078983
H	-6.48352862305572	-0.69576927329136	0.14165628283810
H	-7.29243306678786	0.16245409014957	-1.16832572903197
H	-7.31587159204781	0.82992665928698	0.46554772603564

11C_ea, Gas Phase

C	-5.43646078472431	1.07406885779122	-0.56732798482654
C	-4.54139487399297	0.29793609774190	-1.54903168415968
C	-4.61318051606321	1.39197485162508	0.67512747575578
C	-3.97803164951816	0.15655945124849	1.28081254889383
C	-3.17634526268836	-0.59230266389892	0.21032083562311
N	-3.94015294158130	-0.89610029038575	-0.98591900667088
H	-4.64269160259431	-1.59846661848854	-0.79433737057127
H	-5.11790926670029	0.02460486124067	-2.43400333393259
H	-3.72564507543622	0.94438101550965	-1.88905421423492
H	-2.32197382358286	0.02073638175233	-0.09620951754482
H	-2.76773921362542	-1.51660202227908	0.61746378277290
C	-6.70915383401683	0.30113267602682	-0.24637768000717
H	-5.71511929785537	2.02346819959694	-1.03283883859501
H	-3.33358833356523	0.44645622165660	2.11227215177103
H	-4.76092005253795	-0.49119604931969	1.68111417439186
F	-5.41084719846716	2.01886224319758	1.62532212704976
H	-3.82900511635576	2.10790851919896	0.40685845029206
H	-6.49261221552865	-0.69262660782817	0.14775985129932
H	-7.30640016455815	0.17584826511130	-1.15038569366462
H	-7.31011877660748	0.82643661050261	0.49340392635783

11C_ea, Water

C	-5.43641352502071	1.07418998402723	-0.56562736930343
C	-4.54159202274222	0.30150495017228	-1.54993884826858
C	-4.60513423958799	1.38797123638058	0.66912058440404
C	-3.97885364962756	0.15336702777964	1.27872675976678
C	-3.17356749448251	-0.59110818182709	0.20865090815613
N	-3.94470330578649	-0.90058994527207	-0.98699351768649
H	-4.66569507487096	-1.57762594338125	-0.76547380947346
H	-5.12306309091559	0.03330960357209	-2.43295027570173
H	-3.72537098818190	0.94966253143249	-1.88354637600797
H	-2.32469913992329	0.02837245408094	-0.09802711378112
H	-2.76615329162078	-1.51355527191997	0.62034899832161
C	-6.70713890300425	0.29574685867632	-0.24742966031927
H	-5.71306973879437	2.02236635942191	-1.03411698690162
H	-3.33101432125581	0.43861162930884	2.10908155286879
H	-4.76150225920995	-0.50027560312408	1.67001408195470
F	-5.40542838024918	2.02573039005272	1.63083902067728
H	-3.82339503293797	2.10492719284269	0.40438454685130
H	-6.48747395530900	-0.69404683927272	0.15460687953293
H	-7.29313730129993	0.16188734202623	-1.15756699060038
H	-7.32188428517951	0.82263422502321	0.48086761551049

12A_a, Gas Phase

C	-5.35141246300015	1.51091190098500	-0.22744175154024
C	-4.75097492863428	0.58731432715781	-1.29049461705169
C	-4.48631126198562	1.68164107985408	1.00455445373019
C	-4.07980532005669	0.33307566849497	1.56012083635346
C	-3.39039948410220	-0.49663740405993	0.48896694666155
N	-4.25336876740094	-0.65139600875851	-0.67117720368673
C	-4.40417978259490	-1.79018083113426	-1.37768352025543
O	-4.96692806258518	-1.86894156004381	-2.44083516515922
C	-3.83504136499833	-3.10539182989043	-0.77624092085501
F	-4.33480044574165	-3.35218345873907	0.44222988733912
F	-2.50084063608902	-3.05790797635571	-0.66995592608268

F	-4.14241715471841	-4.12385509596380	-1.55313070467157
H	-5.55229958678453	0.28126492302615	-1.95873691084377
C	-3.67102531620021	1.25692228894074	-2.13439247392534
H	-2.46322607741942	-0.00352416139365	0.18604274340769
H	-3.12848683535203	-1.46785346272002	0.88925141811261
H	-4.97541230203009	-0.18733675216333	1.90713732748581
H	-3.41146486714357	0.46635869643793	2.41000076698571
H	-5.01032007185931	2.27281511654980	1.75693147024701
F	-3.33226119748956	2.39046154162238	0.67600472973402
H	-5.55136943739959	2.48584572980475	-0.67367060994789
H	-6.30862543033422	1.10195300431275	0.10450380836220
H	-2.80632662083395	1.54068787887198	-1.53755302058709
H	-4.07165680947495	2.16446744019435	-2.58714308563766
H	-3.35659577577121	0.58713894496984	-2.93368847817504

12A_a, Chloroform

C	-5.35603444450294	1.49267802846478	-0.23806440252682
C	-4.73117741056353	0.59432859483489	-1.30835009977205
C	-4.51108792426567	1.66288816603250	1.00586144785924
C	-4.06651911656572	0.32031910279730	1.54218284788779
C	-3.36012435497481	-0.48394082081135	0.46310127663469
N	-4.22238375960207	-0.64839691971820	-0.70013154855400
C	-4.42268013821989	-1.79359764674686	-1.36012477346411
O	-5.02454556936872	-1.89966787247535	-2.40835232634135
C	-3.86306144043875	-3.10697749247496	-0.74475501416363
F	-4.33312468417604	-3.32348612876829	0.48868404202231
F	-2.52720485268138	-3.09533386381404	-0.68185400278676
F	-4.21863445196493	-4.13678150019027	-1.49473325917476
H	-5.52363916987350	0.29322858385506	-1.98779398867518
C	-3.64632061325166	1.28699930101737	-2.12602764506762
H	-2.44910935354553	0.03182268908970	0.15243123516532
H	-3.06891329084242	-1.44944645683811	0.85602608809451
H	-4.94961645948426	-0.22185131248106	1.88731048084454
H	-3.39865310944799	0.45844381978230	2.39145742303879
H	-5.05777529516335	2.22534844536016	1.76220287040112
F	-3.36985452164647	2.41920568478222	0.70108738592086
H	-5.57176082723485	2.46815128232005	-0.67546463016047
H	-6.30733273798954	1.06104601319546	0.08047757103973
H	-2.79132523274623	1.56615981982743	-1.51315294163359
H	-4.05386055843277	2.19798561060629	-2.56524864712359
H	-3.31081168301698	0.63652487235297	-2.93316938946499

12A_e, Gas Phase

C	-5.34939520835138	1.33144649555853	-0.53303988188621
C	-4.38742822851261	0.60666016319802	-1.47428490752796
C	-4.70094313927076	1.57398612777928	0.81771811283284
C	-4.11010476941076	0.30219809958472	1.39672432944135
C	-3.17509492456623	-0.35510387937902	0.37924833679315
N	-3.93171157422477	-0.63088127463944	-0.85605891327744
C	-4.56226560488233	-1.81199900866670	-1.04181063560204
O	-4.52456673285091	-2.75614402230462	-0.29695749192992
C	-5.38216971320101	-1.98358190564477	-2.35617070708555
F	-4.68264438175669	-1.63593111123794	-3.44155257445337
F	-6.49530073946899	-1.23526475226587	-2.32946746336782
F	-5.74640869501485	-3.24206849265321	-2.49308183652623
H	-2.43982622281871	0.39323842760632	0.06599926387369
C	-2.39007624289128	-1.51441136164142	0.97074983932259
H	-4.91196581074424	-0.39609147158719	1.64988590217544
H	-3.56165194463914	0.53083120971938	2.31201072523912
H	-5.66527950010493	2.27812474890802	-0.97107941344308
H	-6.23793671616100	0.71288607849788	-0.38620387318192
F	-5.64284276732031	2.09086233617634	1.69036706482503
H	-3.91326271948189	2.32878690741374	0.71921150739474
H	-4.85827116666959	0.41248959065411	-2.43019031108224
H	-3.50507605595261	1.21900656922099	-1.67164882803328
H	-3.02375482429726	-2.19778586674802	1.52707578854114
H	-1.64215106845215	-1.09809452275993	1.64706123697864
H	-1.87322124895559	-2.08094908478919	0.19807472997932

12A_e, Chloroform

C	-5.35456264210378	1.33982797869985	-0.51977685164102
C	-4.40971924611465	0.59968894449719	-1.46510190362859
C	-4.68229268408126	1.58822074041204	0.81586078725311
C	-4.10437718067973	0.31703309572238	1.40445469611537
C	-3.18727227644417	-0.36107603552547	0.38467384517181
N	-3.96707464662694	-0.64190430025864	-0.83879510534767
C	-4.54560983366559	-1.82898615047023	-1.06564890578709
O	-4.46812119239260	-2.81006247430286	-0.36126949730140
C	-5.37313498864754	-1.98596871067898	-2.37780788013001
F	-4.68591191509244	-1.61842440661626	-3.46318527255926
F	-6.49913772601089	-1.26232545553617	-2.33721416694778
F	-5.71966883216936	-3.25276806989812	-2.53307448299669
H	-2.45085022777012	0.37606649904418	0.05270042326496
C	-2.40540315138113	-1.51606128858145	0.98565780878327
H	-4.91302617072624	-0.36758223789919	1.67406762166428
H	-3.53694052549428	0.54851332670745	2.30705578098319
H	-5.66080038119334	2.28442221530808	-0.96816766024500
H	-6.24606979612665	0.72968138061696	-0.35550267218500
F	-5.61507115055093	2.12667327992060	1.70209300022369
H	-3.89198927466255	2.33542381834589	0.70452378081466
H	-4.89211055702261	0.41050052685574	-2.41553170049456
H	-3.52071852779780	1.19810397975461	-1.66905262234201
H	-3.03822111259023	-2.19063337959593	1.55453542426028
H	-1.66032704856307	-1.08753422601461	1.65716553238986
H	-1.88493891209209	-2.08861905050703	0.21992002068160

12B_a, Gas Phase

C	-5.46175214780796	1.02002285875724	-0.48898905739059
C	-4.56552293517118	0.36059892676318	-1.51790326630336
C	-4.67736261035401	1.37163487472208	0.76328057111658
C	-3.97956850697016	0.14593418382087	1.33267341557521
C	-3.11221129344531	-0.59685679670286	0.32104670103148
N	-3.93783748838290	-0.86916384385647	-0.92691197164132
H	-3.33808925208423	-1.31555039661417	-1.62248659638105
H	-4.67531860262954	-1.53908231654792	-0.69966675120607
C	-1.82848064954602	0.11511322428033	-0.05846312301922
H	-2.87114984622712	-1.58517812865751	0.71125539219455
H	-3.34861688488775	0.43684639172740	2.17212611999309
H	-4.74769862487932	-0.52217718950403	1.73121193426162
H	-6.29395476673232	0.36316702209295	-0.22225235227918
H	-5.88942072177813	1.92312221181409	-0.92197079990831
H	-5.33333363951917	1.80738105929949	1.51642993604200
F	-3.73730909214424	2.33011197335448	0.42732410626294
H	-5.11194628282555	0.05476806564878	-2.40621833489367
H	-3.75370928761687	1.02159557814947	-1.81200163182973
H	-1.25333841677120	-0.45760124110151	-0.78666080661686
H	-1.21813455898418	0.21204552924101	0.83811991472969
H	-2.00205439124283	1.11927801331312	-0.43537339973781

12B_a, Water

C	-5.43827236984107	1.03355892064533	-0.49601194946165
C	-4.54874572153870	0.35065339018276	-1.51510612098783
C	-4.68601927562021	1.36539733489251	0.77605711465959
C	-3.97578281142964	0.14536291806062	1.33037720499210
C	-3.11473686076583	-0.59394010270811	0.31240121705126
N	-3.93958602183086	-0.87073038478187	-0.91547798352719
H	-3.35772534487255	-1.34047470193382	-1.60974051153114
H	-4.68037540990364	-1.53302379892395	-0.67907968421447
C	-1.83492003361145	0.12373021850970	-0.06992562495844
H	-2.86655623230092	-1.57674940981233	0.70718610123333
H	-3.34875205778744	0.42867934282701	2.17516710596252
H	-4.74613629696698	-0.52867881098395	1.71178330577567
H	-6.27608484736909	0.38237700285400	-0.23714631139855
H	-5.85110437710550	1.94137335589705	-0.93300063601583
H	-5.36305927748263	1.77324160187250	1.52493051605302
F	-3.75265653567665	2.37208568666652	0.49473356828398
H	-5.10866567127534	0.03503313389402	-2.38980294190193
H	-3.73343879467902	0.99438803785637	-1.83432952717072
H	-1.27074088120363	-0.45538996003875	-0.80039388602427
H	-1.22597484018702	0.22923149084065	0.82669338995638
H	-2.01747633855180	1.11988473418376	-0.46474434677584

12B_e, Gas Phase

C	-5.34266275915710	1.07264238129165	-0.50334917219774
C	-4.49640435807597	0.35823317033020	-1.54359356911422
C	-4.56108911957702	1.39408658978149	0.76074279113159

C	-3.91321936936684	0.14188850472415	1.33132686110257
C	-3.07502508408998	-0.57595803168698	0.29150746684954
N	-3.91731282474741	-0.88742288160670	-0.90954587793146
H	-3.36911755624571	-1.39581303986704	-1.60548334288043
H	-4.68884532160138	-1.50353867633633	-0.63865584092858
C	-5.26873195593736	-0.02762601517059	-2.78441800220372
H	-3.62431041720354	0.96100841161479	-1.80584907171709
H	-2.25264964103131	0.04216188036239	-0.06817492270925
H	-2.66962003356270	-1.51110965704684	0.66912117443032
H	-3.27813536619013	0.39803282690500	2.17842180803573
H	-4.70129370350933	-0.51690335176169	1.70624644659983
H	-6.20498693593707	0.45306092090903	-0.23592959337451
H	-5.73341302550588	1.98932316364611	-0.94478503208795
F	-5.42236976844500	1.90954349318788	1.69245109767734
H	-3.80134500270786	2.15423299906025	0.55283168360515
H	-6.12721343531326	-0.65265137724778	-2.53311604304198
H	-4.64345075402090	-0.55149169440537	-3.50778070522231
H	-5.64538356777424	0.87365038331640	-3.26463815602282

12B_e, Water

C	-5.34677760971689	1.06959349984117	-0.49908925908039
C	-4.49493193178371	0.35405241685223	-1.53549182005169
C	-4.55018473131766	1.39199805199920	0.74811378112342
C	-3.92599396949418	0.14005830303687	1.32836717719544
C	-3.08666977130553	-0.57367653992788	0.28641947445473
N	-3.91498010319250	-0.88046674480158	-0.91323647108189
H	-3.34659693329007	-1.37183664759157	-1.60437087247421
H	-4.66936571481688	-1.52278720904018	-0.65904970712845
C	-5.27221548400788	-0.02615837510924	-2.77418459511954
H	-3.63128235993433	0.96477102062076	-1.80137072694662
H	-2.26182560800544	0.04524329154869	-0.06210854301385
H	-2.69200848801779	-1.51195346315397	0.66285727946088
H	-3.28994261894184	0.38815336795600	2.17667883668782
H	-4.72210270930892	-0.52005558719422	1.68088313090415
H	-6.19631868091181	0.43690019604109	-0.22556709238082
H	-5.73671769253780	1.98299086586508	-0.94701190796990
F	-5.40501805922984	1.95193540910567	1.69495546892499
H	-3.78445674125850	2.13985281571591	0.53158503503848
H	-6.11777182225946	-0.66472240911377	-2.51564162163615
H	-4.63722885594116	-0.54633546562377	-3.49040933594770
H	-5.65419011472779	0.87779320297353	-3.24499823095869

12C_ae, Gas Phase

C	-5.42444947574738	1.03645905073249	-0.50206534828551
C	-4.51058314748787	0.34520246807239	-1.50357254694610
C	-4.66836682110172	1.35993471399248	0.77105222732601
C	-3.96925996571446	0.13048282168572	1.32071063167549
C	-3.13062047057446	-0.61452680374194	0.27766617967989
N	-3.95622974092714	-0.85876779115866	-0.90329222680853
H	-3.43001729338153	-1.38475099999801	-1.58836405568689
C	-1.79954213513037	0.07849499219723	-0.01881688720141
H	-2.90223785400748	-1.59654257752051	0.69942493200957
H	-3.34952046100640	0.41360186624641	2.17267116453608
H	-4.74915598209907	-0.54266133854171	1.68498609689067
H	-6.25084267355601	0.36870584521695	-0.24750732200248
H	-5.84105644042045	1.95225772805817	-0.92237421189709
H	-5.33740002912483	1.78139942689577	1.52395921223061
F	-3.72579612774360	2.35195590695927	0.49151732606640
H	-5.08442231185141	0.05431016189281	-2.38339039102715
H	-3.74509379030882	1.05952081184806	-1.83414071714174
H	-1.21328731059645	-0.52281032026093	-0.71581384750920
H	-1.21849226327894	0.19595506789508	0.89703375887584
H	-1.94370570594159	1.06851896952892	-0.44662397478445

12C_ae, Water

C	-5.42072085411542	1.03939412141430	-0.50330225794725
C	-4.50876521270148	0.34176502341180	-1.50170402054934
C	-4.67802850663820	1.35424822737338	0.77757506776130
C	-3.96889428756671	0.13139354325981	1.32326386048437
C	-3.13260045479432	-0.61626235248757	0.28088267436053
N	-3.95798582627851	-0.86933381280454	-0.90348615995846
H	-3.40641393520837	-1.36764790065910	-1.59176303662565
C	-1.80430358943177	0.07547866226385	-0.02783799275015
H	-2.89685640712100	-1.59410847544251	0.70699231407027
H	-3.34705757661059	0.41546699175882	2.17347405188432
H	-4.74770451340705	-0.53836535944216	1.69672311187467
H	-6.25665279550138	0.38251687051617	-0.25033521333712
H	-5.83101047902737	1.95694792287325	-0.92632392056159
H	-5.35048285116503	1.77057821950748	1.52795849395045
F	-3.73327587411565	2.36517594746449	0.50943147643129
H	-5.07966128398098	0.05773315275316	-2.38536494655727
H	-3.73325857072753	1.04556294624293	-1.82963401951913
H	-1.22225732340001	-0.53496788750077	-0.72028657708924
H	-1.22294394301201	0.20193097114636	0.88685231761231
H	-1.95120571519659	1.05923318835083	-0.47005522353430

12C_aa, Gas Phase

C	-5.42894364615358	1.05436138129497	-0.49113401289276
C	-4.53621929769466	0.31352372876256	-1.48474758587554
C	-4.66304213522385	1.36901700278805	0.78039016411404
C	-3.97980999460223	0.13408791275620	1.34260500434209
C	-3.16752176247891	-0.64128417969018	0.29207363939035
N	-3.93283041640292	-0.88783161381639	-0.93007874993489
H	-4.65118023759917	-1.57885228437452	-0.75076773628321
C	-1.83582459766144	0.03002952378150	-0.03036283704724
H	-2.93773375063492	-1.62381511297842	0.70980293709857
H	-3.35103135377908	0.41915565474078	2.18807829347926
H	-4.76820554454066	-0.51907404792932	1.72902602953274
H	-6.28433354469183	0.42439096094849	-0.22922127014060
H	-5.81708941951464	1.97962443242674	-0.91975176826791
H	-5.32280584703503	1.80825149098169	1.53101303137778
F	-3.70583479913935	2.34282343378844	0.48968639171965
H	-5.10081414541625	0.03902884577133	-2.37568817578252
H	-3.73723687503968	0.97962172269742	-1.81570506807286
H	-1.28028914639212	-0.57604852293241	-0.74452004351411
H	-1.24118207089778	0.13742366260432	0.87754104029345
H	-1.97068141510190	1.02580600837875	-0.44753928353628

12C_aa, Water

C	-5.42193653317470	1.05606929887545	-0.49309732421998
C	-4.53274973908008	0.31552997129206	-1.48819128047167
C	-4.66925779353847	1.36001050439660	0.78547460332890
C	-3.97899787876377	0.12915645935080	1.33942388937885
C	-3.16375298733278	-0.64144274755014	0.28995117491971
N	-3.93499312363242	-0.89431482152201	-0.93245556085035
H	-4.67641804363387	-1.55292092399939	-0.71811106008210
C	-1.83424051237137	0.03190009931955	-0.03602648014957
H	-2.93334889469302	-1.62159325872763	0.71160980586485
H	-3.35317249624196	0.40813538122615	2.18917610174111
H	-4.76720621483264	-0.52745143636236	1.71843108356297
H	-6.27824762721791	0.42657595016645	-0.23577311523994
H	-5.80855659607595	1.98209150571850	-0.92167018601896
H	-5.33188222744056	1.79384900259862	1.53440170948072
F	-3.70615884557223	2.35211738997425	0.50888071135858
H	-5.10647277412794	0.04285577680619	-2.37368199211657
H	-3.73094964648017	0.97625664842591	-1.82411714279090
H	-1.25968298527817	-0.58646396774230	-0.72595572463469
H	-1.25188327583653	0.16556388647938	0.87647916530844
H	-1.97270180467544	1.01431528127394	-0.48404837836938

12C_ee, Gas Phase

C	-5.33195958327591	1.08243377197532	-0.50955044451128
C	-4.46219960549647	0.34923898117412	-1.53054881815853
C	-4.55128681179563	1.38456295177670	0.75263186381546
C	-3.93086163440634	0.12555816681623	1.32040425380806
C	-3.09213398974921	-0.56118813216163	0.24810407655050
N	-3.91843337570435	-0.84874625628602	-0.91003312409386
H	-3.40782053222442	-1.39548142562750	-1.59110133496338
C	-5.26684988321172	-0.03322106216099	-2.75932270837937
H	-3.65140094085721	1.03401865728309	-1.83578329293565
H	-2.23445798930952	0.08399705678203	-0.00364955647031
H	-2.69224959384795	-1.49753931423019	0.63627851747527
H	-3.31871214420639	0.36863242207855	2.18946953119499
H	-4.73297867200752	-0.54347202248998	1.63826498962131
H	-6.18159887369803	0.44644219254494	-0.24769910899684
H	-5.71652680406047	2.00827435346398	-0.94059331421282

F	-5.39603958029305	1.95708062255179	1.69419861229589
H	-3.76958357348270	2.12217027960811	0.54242106191112
H	-6.09349870424081	-0.68339617017635	-2.47057875615016
H	-4.64880397762646	-0.56834657190988	-3.48231147295634
H	-5.67155373050585	0.85195149898769	-3.24964097484404

12C_ee, Water

C	-5.33642659023360	1.07725303117339	-0.50700673869314
C	-4.46798135030850	0.34150439194980	-1.52726958810558
C	-4.54683318847657	1.38024141577975	0.74640684784352
C	-3.93097446982505	0.12576899796141	1.32243272466690
C	-3.09513465628314	-0.56345764349946	0.24938639626637
N	-3.92462773526227	-0.86355766009450	-0.90930050471570
H	-3.37923273186653	-1.37211260842730	-1.59572850813353
C	-5.26927950325514	-0.03074669318270	-2.76103622489880
H	-3.65197222750202	1.01952233059335	-1.82560559695998
H	-2.24721012145425	0.08620992922943	-0.01461435327805
H	-2.68571951971745	-1.49388295328020	0.64083747412048
H	-3.31086686669739	0.37057950236219	2.18529531875044
H	-4.73300778009753	-0.54164939881951	1.64712824621295
H	-6.18672086783951	0.44218007616324	-0.24131155847038
H	-5.71748111240088	2.00159710886602	-0.94422091485625
F	-5.39838658487592	1.96232313466319	1.69820387204584
H	-3.77057533017802	2.12076108377203	0.53776127359511
H	-6.11510752260979	-0.66133469740107	-2.48090552465265
H	-4.65131428732309	-0.58051308315940	-3.47274265251137
H	-5.65009755379335	0.86228373535036	-3.25674998822615

12C_ea, Gas Phase

C	-5.35096865471396	1.08904483931469	-0.49563688733098
C	-4.49083617959779	0.32532331713958	-1.51170289910736
C	-4.55416461068419	1.39655815410709	0.75573263066699
C	-3.93206998062569	0.14471136341465	1.33751553510890
C	-3.12974510385626	-0.58786453751335	0.25842154888069
N	-3.89599977523793	-0.87416098797449	-0.94043002898981
H	-4.62251228314758	-1.55432957728050	-0.74212139450175
C	-5.27430895427336	-0.03322761185259	-2.76067535513861
H	-3.65316519093639	0.97085029038150	-1.80311367405258
H	-2.27212106167260	0.02435424008677	-0.03915325012180
H	-2.72440630384742	-1.51938428404513	0.65231071142125
H	-3.29749252212754	0.40101999494954	2.18733784467581
H	-4.73442280542436	-0.50329184623127	1.70054249725436
H	-6.21039554180283	0.46935655470852	-0.21970982655852
H	-5.73261300463113	2.01526446916292	-0.92951817445715
F	-5.38413784891807	1.98693049972621	1.70062359670303
H	-3.77127367743958	2.12716482515907	0.52585808303383
H	-6.10050017809107	-0.70363538061268	-2.51250095003933
H	-4.62919642881239	-0.53861111030596	-3.47812822175107
H	-5.69351989415985	0.85703678766542	-3.22905178569590

12C_ea, Water

C	-5.35142669612571	1.08237321650259	-0.49723117444898
C	-4.48811349111215	0.32223060389862	-1.51333646036845
C	-4.54779493772203	1.39169583489696	0.74595581792414
C	-3.93160909263938	0.14440147976336	1.33600401177752
C	-3.12682721267289	-0.58843953947581	0.25934439843963
N	-3.90108622278195	-0.88400509231827	-0.93742407005716
H	-4.64678160816348	-1.53472515968480	-0.70590396554158
C	-5.27336091281259	-0.02901007277854	-2.76337818168358
H	-3.64948707104771	0.96836444340990	-1.79727748886743
H	-2.27371424241076	0.02761047118429	-0.04106937951467
H	-2.72398754119605	-1.51703861461649	0.66174373194447
H	-3.29238433533196	0.40058147545586	2.18224813636035
H	-4.73272027850893	-0.50827995059789	1.69341214194137
H	-6.20500323301228	0.45452321112766	-0.22131980520467
H	-5.73232454971082	2.00604186740892	-0.93679272719879
F	-5.38688413659916	1.99087243679375	1.70017614378311
H	-3.77129071943964	2.12722673616628	0.52013905751419
H	-6.08999644775730	-0.71181466312287	-2.51780733562384
H	-4.62764491327059	-0.51492803829627	-3.49493721016114
H	-5.70141235768461	0.86542935428274	-3.21594564101448

13_e, Gas Phase

C	-5.52703409219049	1.02935549136378	0.40525231639111
C	-5.09226054391193	0.62713187592862	-0.99782735035010
C	-4.36121353585887	1.59883272233949	1.19322130445060
C	-3.17442862128621	0.64976219680509	1.18327101398434
C	-2.80843530200452	0.24918507704816	-0.23781117391529
N	-3.97849214341395	-0.28297318541305	-0.90533980897708
C	-3.96256040627514	-1.56643331300976	-1.38208004632726
O	-2.99475353396394	-2.27865447153557	-1.23912911188474
C	-5.18919877979375	-2.07318791570765	-2.10414562487040
H	-5.41080973931148	-1.47016902335766	-2.98406533457541
H	-6.06614203949495	-2.07392047429332	-1.45750207581451
H	-4.97213258636211	-3.09094293872800	-2.41232039691733
H	-5.92143748908641	0.17021621494739	-1.52793308626828
H	-4.79648258271537	1.53074932329444	-1.54245215355834
H	-2.44739440184741	1.13655624280439	-0.76865453446590
H	-2.03066140489766	-0.50798571683782	-0.24204823946252
F	-6.52125174338349	1.98289506145162	0.30337024765188
H	-5.95409610519252	0.15950543154230	0.91297576488373
H	-4.66523659422655	1.81909192254464	2.21597412627653
H	-4.05246299236831	2.53455858142519	0.71918541831878
H	-3.38211483550677	-0.24831118038429	1.77124471686002
F	-2.09057052690819	1.28207807777200	1.76120402857017

13_e, Chloroform

C	-5.52282984552047	1.02012545051187	0.40126571262455
C	-5.08883977888821	0.62257322596808	-1.00228229933477
C	-4.36343656060444	1.59727963005114	1.19150293920867
C	-3.18176595193195	0.64509807922527	1.18197227130908
C	-2.80578464187329	0.25161357693107	-0.23783972822361
N	-3.97240689854711	-0.28989019580479	-0.90654978125671
C	-3.96261466288359	-1.56117337616102	-1.38492012570666
O	-2.98452821778017	-2.27986256949468	-1.25423723187332
C	-5.19202858867347	-2.06718916382280	-2.09438584628240
H	-5.41847865872774	-1.45900652198265	-2.96930408988236
H	-6.06064197369663	-2.05922070259309	-1.43697697036145
H	-4.98848628992017	-3.08638563279851	-2.40745274575870
H	-5.91608659276928	0.16602240918895	-1.53417985527368
H	-4.78335698564668	1.52270757758923	-1.54499539935622
H	-2.45810083467505	1.14222127869564	-0.77035401429570
H	-2.01801480653667	-0.49413312669720	-0.23681573071867
F	-6.52074095412114	1.98038417812304	0.29390121206664
H	-5.95599542307374	0.15601829644106	0.90995537602575
H	-4.67126396374061	1.81138301806786	2.21439149766172
H	-4.05424969764085	2.53139987712075	0.71444725985771
H	-3.38894867024175	-0.25022533568002	1.77159368265084
F	-2.09057000250702	1.27760002712080	1.76565386691929

13_e, DMSO

C	-5.52196903678386	1.01857802630263	0.40115098668968
C	-5.08892671973740	0.61984786975871	-1.00206531033637
C	-4.36363242657411	1.59791416548546	1.19104853116094
C	-3.18419718921990	0.64408118265133	1.18243840112619
C	-2.80583723680790	0.25127495573641	-0.23678479576210
N	-3.97177272252128	-0.29355130546140	-0.90474000204558
C	-3.96174110069563	-1.55939632802843	-1.38776029802674
O	-2.97812010459868	-2.27828149679433	-1.26556500022407
C	-5.19211331039448	-2.06583312631640	-2.09248451663211
H	-5.41928072649977	-1.45721682022454	-2.96694660087287
H	-6.05886049325226	-2.05363622721185	-1.43287151458779
H	-4.99304960456683	-3.08594318170637	-2.40566899801533
H	-5.91590973443410	0.16287659336162	-1.53356191890589
H	-4.78046329815635	1.51788428128997	-1.54589232013096
H	-2.46204904349947	1.14224220899271	-0.77074540066100
H	-2.01531380170727	-0.49124280856507	-0.23384433926056
F	-6.51943505393125	1.98196167178798	0.29096747209115
H	-5.95768863361241	0.15738975720996	0.91157051240179
H	-4.67232173684126	1.81131590548963	2.21381727232472
H	-4.05391651111784	2.53087492815128	0.71205570916864
H	-3.39241707893716	-0.24978012930830	1.77320871825599
F	-2.09015443611083	1.27597987739901	1.76706341224226

13_a, Gas Phase

C	-5.48723039641856	1.09621703137242	0.35206539847604
C	-5.04271012007656	0.71201438985221	-1.05100151610493
C	-4.31380408259333	1.55374478184615	1.20631821111964
C	-3.12406678571702	0.60965147861424	1.14092442101734
C	-2.78166253510450	0.26037082732604	-0.29823606733899
N	-3.94313524399220	-0.22469697315158	-0.99495468402557
C	-4.17966301255361	-1.54390717431803	-1.28562300602054
O	-5.22403015279696	-1.89936215982468	-1.78023929232725
C	-3.08389072456078	-2.53766344971623	-0.98619616124067
H	-2.18254424743702	-2.32243645428998	-1.55983240952498
H	-3.46175115211308	-3.51528530885700	-1.26642331572387
H	-2.83434619996252	-2.53256793055064	0.07401540740986
H	-5.86384840496360	0.24807435078333	-1.58977926985903
H	-4.73155543740896	1.61599877441668	-1.58563357491934
H	-2.41105672958975	1.16210048961821	-0.79911453227833
H	-1.98664554334344	-0.47806457380826	-0.32011474270906
H	-6.23828054603825	1.88769317430616	0.29265817268203
F	-6.08714535957087	0.00393727881789	0.94652927715211
H	-4.63301111617705	1.68296801129073	2.23988068944045
H	-3.98529678766753	2.52933227921842	0.83571454039329
F	-3.41106077769828	-0.56479441068677	1.81496243510682
H	-2.25709464421608	1.05884556774069	1.62996001927499

13_a, Chloroform

C	-5.48544544698375	1.11121240980533	0.34615207371743
C	-5.04255521014306	0.71243910145350	-1.05051327890712
C	-4.31414642651423	1.55663999265763	1.20424117382757
C	-3.12915056297792	0.61038171441667	1.13981749620937
C	-2.78477629965872	0.24989724495902	-0.29395143193540
N	-3.95634987746436	-0.24332518083007	-0.97899542994757
C	-4.18263869352537	-1.55056187213966	-1.26200769749597
O	-5.24536588921576	-1.92467475535287	-1.73358021129346
C	-3.07257692772227	-2.53471685075737	-0.99867078530059
H	-2.18234888024718	-2.28753943463576	-1.57592402498215
H	-3.43175427989606	-3.51608222915909	-1.29085544985158
H	-2.80634874853715	-2.54408337422067	0.05733182601119
H	-5.87057496193273	0.27199529539375	-1.59620539886597
H	-4.70490161431229	1.60734148666708	-1.58049184295911
H	-2.42543463323457	1.14892191379267	-0.80295596368048
H	-1.98733348225821	-0.48475540855275	-0.31474384561158
H	-6.23260397589832	1.90302921968817	0.28309663303975
F	-6.10341119055571	0.01382878079247	0.94238241154771
H	-4.63389561404567	1.69227497244301	2.23690597217721
H	-3.98006820721133	2.52922591455371	0.83313162781643
F	-3.43089060706716	-0.56915927331876	1.82042850918172
H	-2.26125847059811	1.04988033234399	1.63128763730263

13_a, DMSO

C	-5.48475473370795	1.11706191380792	0.34432301110334
C	-5.04304600567259	0.71190460710204	-1.04993936233232
C	-4.31381517490316	1.55762687132464	1.20363080482410
C	-3.13121054312712	0.60971651386231	1.13954666663387
C	-2.78603629701167	0.24686036880755	-0.29268279669226
N	-3.96101977567689	-0.24948892068040	-0.97326094043457
C	-4.18327335582119	-1.55277356098911	-1.25440055075803
O	-5.25161075685763	-1.93394702117231	-1.71864828863287
C	-3.06830838898470	-2.53337674518343	-1.00270297021704
H	-2.18158989798629	-2.27567413522238	-1.58054361579482
H	-3.42092216665633	-3.51582001697182	-1.29959317272644
H	-2.79636151624846	-2.54779417942856	0.05175838666157
H	-5.87312462562798	0.27758164755174	-1.59679854634699
H	-4.69754312745592	1.60326366561726	-1.57972059486633
H	-2.43104977902428	1.14548531079788	-0.80400080608182
H	-1.98735148187762	-0.48605183079302	-0.31391408257711
H	-6.22930210957885	1.91035904754238	0.27929897137937
F	-6.11057656853267	0.01949368461459	0.94191948708815
H	-4.63372882366725	1.69607830109215	2.23590480616827
H	-3.97692008954864	2.52889605121507	0.83229250946334
F	-3.43942004206858	-0.57208536087300	1.82069978815261
H	-2.26286473996417	1.04485378797848	1.63271129598599

14_a, Gas Phase

C	-5.59058644526492	1.15956992338351	0.07159048110107
C	-4.67137902078739	0.93331765375704	-1.11586528920859
C	-4.79527377986688	1.40613022189840	1.34330512979352
C	-3.69853477919098	0.37709537654197	1.56089573008196
C	-2.88309293753663	0.14957639124633	0.29412501876972
N	-3.73186488950946	-0.13229009203769	-0.83328834434016
C	-3.85041781210439	-1.29851651824306	-1.55018076602118
O	-4.65987288269030	-1.35812483285288	-2.45034977468956
C	-2.94990289181359	-2.51579174748094	-1.27014092720254
C	-1.50236557347328	-2.19515311647928	-1.65887602909536
C	-3.44269427786374	-3.64027717779768	-2.18712063433513
C	-3.06715500959852	-3.03179738482594	0.17024979428441
H	-5.24803634223704	0.66299538688692	-1.99386934556656
H	-4.12475186199884	1.86125250662101	-1.32051806988406
H	-2.31533158603585	1.06711687054189	0.09180810006844
H	-2.16708873643387	-0.64325930030452	0.45568158947878
H	-6.24773813043777	2.00820299137294	-0.13235512113254
F	-6.39348970964445	0.04775029447512	0.23501356852296
H	-5.45947603212692	1.42770415057163	2.20661059200612
H	-4.32485638115175	2.39004365203999	1.25958984864365
F	-4.25936761251216	-0.82131673386688	1.96149257084461
H	-3.03123036856369	0.70222008788647	2.36241947843804
H	-4.10965637719727	-3.05219108090422	0.48820124545948
H	-2.51431296264571	-2.45286906641520	0.90408995161647
H	-2.68146397603158	-4.05144916358340	0.20455814612719
H	-3.41761593832777	-3.34114583585600	-3.23225446709871
H	-4.47028273143108	-3.91068213809539	-1.94760651426597
H	-2.80748091882701	-4.51601017850613	-2.04937489817820
H	-1.45184408918683	-1.91227188530560	-2.71157777148563
H	-0.88782691093216	-3.08625984657043	-1.52078535718643
H	-1.06092903457811	-1.38975940809798	-1.07390793554580

14_a, Chloroform

C	-5.57242262571252	1.19449595987565	0.05243500824526
C	-4.64929196531326	0.94519815070515	-1.12435740685732
C	-4.78822443710809	1.41567934674377	1.33225631605013
C	-3.70916482103125	0.37227530299450	1.55233347980214
C	-2.88229862326083	0.13665540490642	0.29708972377802
N	-3.73453711924033	-0.14460811195166	-0.83481457817275
C	-3.89399269149669	-1.32150871852651	-1.50177860996582
O	-4.76578560162437	-1.41308797398017	-2.35274844347092
C	-2.96161154862207	-2.52188794534348	-1.26009316979553
C	-1.52617781430352	-2.16064555545789	-1.65961821085784
C	-3.43231269669914	-3.64827905808280	-2.18592080585339
C	-3.04809630195388	-3.06288361365067	0.17363273463156
H	-5.22379291966696	0.70411102791032	-2.01082413790729
H	-4.07282045506768	1.85626796753159	-1.31093159569623
H	-2.31340284150429	1.04970067615172	0.09225306652892
H	-2.17090259947463	-0.65720707650762	0.46809866710260
H	-6.21108883442215	2.05322926348342	-0.15696469624340
F	-6.40952383643317	0.09102637564560	0.20247157065716
H	-5.45924439563549	1.44800927447129	2.19002889771887
H	-4.30060991251132	2.39103205421946	1.25717711769203
F	-4.30113393769563	-0.83018335889589	1.93125913088186
H	-3.04949478979032	0.67266012158199	2.36687506948743
H	-4.08922844599265	-3.15966922800981	0.48374822453037
H	-2.53786999473818	-2.45465972023815	0.91391466884858
H	-2.59394896556872	-4.05445300071357	0.19398845443220
H	-3.41726492012801	-3.33965160453761	-3.22928584775794
H	-4.44845515714630	-3.95510440547246	-1.94034556188499
H	-2.76974999786506	-4.50537024621526	-2.06168235020367
H	-1.49505463468191	-1.85384014621123	-2.70666009469759
H	-0.89367703767939	-3.04288169839281	-1.54843829567751
H	-1.09474007763212	-1.36060946403330	-1.06153832534491

14_a, DMSO

C	-5.56601481712195	1.20602276777555	0.04464401114047
C	-4.64077311802943	0.94871560073356	-1.12769667261819
C	-4.78650980607527	1.41816113963138	1.32775917249015
C	-3.71339291237522	0.37013142574938	1.54914397937621
C	-2.88144735019794	0.13277941981808	0.29839904578917
N	-3.73475219030437	-0.14880822742065	-0.83493946612262
C	-3.90891812212021	-1.32952680709310	-1.48305771639171

O	-4.80383626915902	-1.43286452862940	-2.31342124993888
C	-2.96561841797354	-2.52388220684914	-1.25614647943347
C	-1.53474478894396	-2.14908947271964	-1.65992207230084
C	-3.42979838136758	-3.64981037861932	-2.18563910185249
C	-3.04034455374889	-3.07353986683311	0.17509214231314
H	-5.21263207722768	0.71712880022958	-2.01807646130189
H	-4.05417126802982	1.85389293082568	-1.30766007515884
H	-2.31237812325714	1.04462994342293	0.09323151066529
H	-2.17143931483395	-0.66125728419263	0.47285556147022
H	-6.19774728091618	2.06868266022018	-0.16670050022937
F	-6.41550346656760	0.10596095765739	0.18898530005228
H	-5.46024895945336	1.45403693556537	2.18328677999901
H	-4.29326170513554	2.39065958659642	1.25621378490749
F	-4.31595732946651	-0.83391517136034	1.91909227024122
H	-3.05724502906568	0.66199239189394	2.36879817983264
H	-4.07943033639951	-3.19424498558786	0.48446157186442
H	-2.54254674793916	-2.45719420338900	0.91693187633271
H	-2.56510828320511	-4.05529091142773	0.19010283368411
H	-3.41963320388706	-3.33656577471777	-3.22797976874250
H	-4.44147817639460	-3.96920712984074	-1.93745761146384
H	-2.75801042455597	-4.50052395763964	-2.06795225272201
H	-1.51092952558050	-1.83330954874448	-2.70455848465783
H	-0.89635177321565	-3.02826764007394	-1.55905213364905
H	-1.10569624745156	-1.35168646498095	-1.05717797357498

14_e, Gas Phase

C	-5.42637897504943	0.57037204429924	0.92313335933030
C	-5.40662458602652	0.59649742942250	-0.60165473097382
C	-4.20836565825466	1.26590036984110	1.50506931665498
C	-2.92379259421523	0.73141510784467	0.89341216586333
C	-3.00008562896183	0.76760831481603	-0.62458898714571
N	-4.16660883386424	0.02615650302644	-1.07294531197108
C	-3.96265134098476	-1.23384250611207	-1.58856970265013
O	-2.83786616141506	-1.68484996106224	-1.62157745974133
C	-5.12284039381334	-2.05170223752976	-2.18504675128365
C	-5.86761990473597	-1.25768251400610	-3.26316166300794
C	-6.05786421430940	-2.57581954994861	-1.08725039429039
C	-4.50137549799863	-3.27557333650262	-2.86714173706989
H	-6.26481906187315	0.06557227925876	-0.98871010135861
H	-5.47702933503585	1.63686942788197	-0.93452918982154
H	-3.09552110905663	1.80834477271876	-0.94738898877417
H	-2.10939441046316	0.33245098293144	-1.06391634284986
F	-6.57118675273890	1.21026206904182	1.36000893994275
H	-5.48082374542433	-0.46909859785056	1.26164853454006
H	-4.19074954179904	1.15997113739957	2.58936555939795
H	-4.27720853697341	2.33110064273786	1.26768273056050
H	-2.71985138261704	-0.29251263784891	1.21829342766357
F	-1.86832236238507	1.51947008520370	1.31207292938794
H	-6.61720331766790	-1.90146057741200	-3.72596417765186
H	-5.17104677383588	-0.94545724007576	-4.04271021738304
H	-6.37454947044838	-0.36946859060440	-2.89455630701998
H	-6.76325170209233	-3.27951270746225	-1.53207436304030
H	-6.63886577811810	-1.80504838471812	-0.58571481494359
H	-5.48375820185569	-3.11663055945162	-0.33282124757361
H	-5.29458943203666	-3.87110891003824	-3.32137724059314
H	-3.96107735965928	-3.89396829811195	-2.15329402080852
H	-3.79697793629015	-2.97907455768865	-3.64236321338923

14_e, Chloroform

C	-5.43218014777942	0.58451370015283	0.92362405067375
C	-5.39230006854059	0.57120228239015	-0.59964212576939
C	-4.22704794218037	1.29842231303107	1.50741929408191
C	-2.94032970579456	0.73699405140473	0.93110356101543
C	-2.98589523045360	0.73620811415234	-0.58785509126864
N	-4.14516099322652	-0.02081961810417	-1.03188564352223
C	-3.94497226165750	-1.23255180256956	-1.63042082327847
O	-2.80700601973660	-1.65740849490886	-1.74959787469970
C	-5.11565728585496	-2.05290069071177	-2.19754341935137
C	-5.88449066486231	-1.25448631874466	-3.25715040639999
C	-6.02397237805345	-2.57914597736259	-1.07815677016058
C	-4.51840140704742	-3.27680404634115	-2.90048214429792
H	-6.24735488247563	0.03574761477142	-0.98426919737427
H	-5.44593453846136	1.60154790450933	-0.96359831668033
H	-3.07990366896508	1.76723844429435	-0.93976026600247
H	-2.08609181927513	0.29523890128360	-1.00020731729100
F	-6.58721989202458	1.24582432532888	1.32244790221663
H	-5.50039577089820	-0.44076868103693	1.29598595515980
H	-4.22752399888639	1.21863568060052	2.59394012432629
H	-4.28889504334299	2.35500577314632	1.23257807786831
H	-2.74590629458377	-0.27424784308223	1.29514448119493
F	-1.87887496622784	1.53409040382950	1.34395562712518
H	-6.64666404658611	-1.89850608478839	-3.69850391207716
H	-5.20573415892968	-0.94507080932898	-4.05376996103651
H	-6.38022215856390	-0.36602271115579	-2.87499285250035
H	-6.73870532645746	-3.28069985192741	-1.51114939998571
H	-6.59348346766728	-1.81004547275585	-0.56242672358955
H	-5.43252391344136	-3.12048329638369	-0.33751346963379
H	-5.33019410787536	-3.86645267150527	-3.32832874520324
H	-3.96300484307720	-3.90274838858489	-2.20399037185024
H	-3.84225299707337	-2.98232674960284	-3.70162424168933

14_e, DMSO

C	-5.43370115470315	0.59081900099285	0.92453543575242
C	-5.38824438383016	0.56234369097348	-0.59803838153081
C	-4.23224947178264	1.31131374172393	1.50710072667253
C	-2.94561253835451	0.73966519373092	0.94301326620839
C	-2.98184839483081	0.72453539033492	-0.57594155562357
N	-4.13921397475622	-0.03694420914338	-1.01845853041708
C	-3.94098854849493	-1.23337894095033	-1.64058226916562
O	-2.79981794145241	-1.65061800984790	-1.78368592057622
C	-5.11367801720281	-2.05388757718217	-2.20151113733480
C	-5.88975753646575	-1.25258299409446	-3.25415918453010
C	-6.01379902203514	-2.58308590352142	-1.07691206290454
C	-4.52287247276087	-3.27612394176268	-2.91262894728744
H	-6.24283089835635	0.02457592612308	-0.97970766040865
H	-5.43683356619261	1.58856242375966	-0.97366852281735
H	-3.07408920468889	1.75180114668117	-0.93887265174440
H	-2.07921588884662	0.28044225196251	-0.97806250496664
F	-6.59130258703235	1.25893463729292	1.31067937126166
H	-5.50589073513944	-0.42929585557989	1.30894071648435
H	-4.23846122072196	1.24190685337116	2.59426376064703
H	-4.29147840425060	2.36442301229045	1.21866173426847
H	-2.75504417775628	-0.26701813937626	1.32028498438049
F	-1.88132038576810	1.53925063773060	1.35172324746814
H	-6.65420938832726	-1.89665847870773	-3.69139383281636
H	-5.21638107701798	-0.94059652679894	-4.05445380775744
H	-6.38375014480697	-0.36589551301052	-2.86610489805140
H	-6.73321346094667	-3.28107820325577	-1.50782711249020
H	-6.57734086994568	-1.81481929799327	-0.55394194281282
H	-5.41730218515722	-3.12792649912827	-0.34290810942275
H	-5.33958936405396	-3.86429771508220	-3.33285551053170
H	-3.96196953625278	-3.90470340708863	-2.22264322867133
H	-3.85629344806890	-2.98048269444381	-3.72151547128229

15_e, Gas Phase

C	-5.14799601480612	1.78425389676159	0.75578229175338
C	-4.92265546624293	1.09047421794244	-0.58063333102458
C	-3.83470627055468	2.16610588201696	1.41244871226651
C	-2.92411823406077	0.95785505354798	1.52449071681901
C	-2.74283448005669	0.28104653795045	0.17588259016800
N	-4.03797179566092	-0.03801716904653	-0.38981787016068
C	-4.16985327403127	-1.23224847833475	-1.05235215454510
O	-3.32779268003211	-2.09437616373918	-1.02623439273816
C	-5.64037005933267	-2.48611150008073	-2.51566768458136
C	-7.01049193559678	-2.14826824446017	-3.08186094194878
C	-5.71994379461762	-3.73777379167913	-1.65495894139755
C	-4.62728123296658	-2.63147181906977	-3.64171860922006
H	-5.86765033376104	0.75314478495274	-0.99097892686323
H	-4.47850326620638	1.81666214098256	-1.27324876339360
H	-2.19496268182305	0.96704752963619	-0.48236352759664
H	-2.16894230669341	-0.63421841092400	0.27719104622135
F	-5.89311186708619	2.92654604225409	0.53115238146420
H	-5.73417996616349	1.13257028041456	1.40893373062863
H	-4.01152812120037	2.60499417238868	2.39398384258005
H	-3.33864909607457	2.91340469082538	0.78706043814154
H	-3.31579899759848	0.23695043928030	2.24676737847739
F	-1.68384215248633	1.36654546643418	1.97712826861885
H	-7.35366415844066	-2.95884670287788	-3.72392530777364
H	-6.96375730067597	-1.23236811708222	-3.67056674207869
H	-7.73213882120105	-2.01132871960760	-2.27685842786509

H	-6.10145077140943	-4.55957478996391	-2.26216210636315
H	-6.40837769096757	-3.58048403691986	-0.82403854508991
H	-4.74414470866800	-4.01235385960217	-1.26467712283694
H	-4.96726995303128	-3.40903210774845	-4.32648210114355
H	-3.64715379348831	-2.90396198506548	-3.26031799761588
H	-4.54909881422133	-1.69739523068629	-4.19931220258921
O	-5.32982996084390	-1.32116000849995	-1.70407570031312

15_e, Chloroform

C	-5.14842729985777	1.77241958952297	0.75191822743740
C	-4.91828206203577	1.08404423294679	-0.58537992094636
C	-3.84121109664693	2.16979587575171	1.40843246191223
C	-2.93242618601731	0.96285332169476	1.52548138031107
C	-2.73552845782805	0.28791157408430	0.17883115699591
N	-4.02618580238959	-0.04156453568455	-0.39358803392084
C	-4.15942787379301	-1.23358715784948	-1.04690470199182
O	-3.31412195179806	-2.10153101211814	-1.01668437655057
C	-5.63761751803173	-2.48991326577644	-2.51486679387642
C	-7.00747352900120	-2.13696073357752	-3.07200290903837
C	-5.72478213983126	-3.74378660510751	-1.65950311800908
C	-4.63160143956537	-2.63323435425010	-3.64637845929930
H	-5.86209449131980	0.74303050781808	-0.99470010129974
H	-4.47156048709371	1.80858729411372	-1.27636457583748
H	-2.19440471237027	0.97731452080147	-0.47995902902894
H	-2.15389699509344	-0.62065446008427	0.29098923472488
F	-5.90362533997124	2.91621588647326	0.52017521093126
H	-5.73493825657206	1.12409430552468	1.40566802727853
H	-4.02470966096583	2.60642109819457	2.38969513885013
H	-3.34741376630570	2.91405105766424	0.77754375782452
H	-3.32072980120105	0.24418546127430	2.24964640999601
F	-1.68729680247634	1.37757147617100	1.98423599419335
H	-7.35778534467363	-2.94143768637353	-3.71782340092658
H	-6.95525263492080	-1.21744181695327	-3.65499916713689
H	-7.72430223309080	-2.00118916427308	-2.26212933824110
H	-6.12542261264694	-4.55513189064080	-2.26828699887989
H	-6.40139734288789	-3.58061985580568	-0.81987177668663
H	-4.74902761754851	-4.03745615633379	-1.28288771169985
H	-4.98462642772734	-3.40123025658370	-4.33523385885139
H	-3.65190459574006	-2.92087204822866	-3.27468451788956
H	-4.54749478070426	-1.69430813677744	-4.19503133079170
O	-5.31510073989421	-1.32896706561787	-1.69676687955276

15_e, DMSO

C	-5.14924070424420	1.76767031758633	0.74984137064095
C	-4.91569965312490	1.08340348392266	-0.58874989383266
C	-3.84470195125116	2.16915458045861	1.40850643629482
C	-2.93549155690365	0.96317085167330	1.52565177730149
C	-2.73207265646996	0.29195090873309	0.17825109244631
N	-4.02035734350089	-0.04075053873737	-0.39803798005120
C	-4.15465269395582	-1.23284860530096	-1.04640978077667
O	-3.30799501895158	-2.10266721191020	-1.01400168988960
C	-5.63655049425283	-2.49099915740349	-2.51397355708436
C	-7.00624095510195	-2.13276044668284	-3.06794567120923
C	-5.72689899558813	-3.74490374066845	-1.65940721014615
C	-4.63346279316219	-2.63537672625148	-3.64760367820133
H	-5.85826997541393	0.74103365005407	-0.99956502896970
H	-4.46808652276143	1.80901809134923	-1.27750897013446
H	-2.19338123060579	0.98452614070499	-0.47877740959341
H	-2.14725622234928	-0.61424942186077	0.29181056493299
F	-5.90783407742499	2.91161314628869	0.51741302931460
H	-5.73589047610079	1.11845827147278	1.40195073008119
H	-4.03157444308766	2.60302993011126	2.39033278036008
H	-3.35146962807295	2.91423667335435	0.77810649962706
H	-3.32340881672884	0.24329029198007	2.24826791062115
F	-1.68983973510865	1.37939013612085	1.98849491241266
H	-7.35990988731768	-2.93559734810623	-3.71392509635387
H	-6.95179992814191	-1.21275067185312	-3.65003207616853
H	-7.72095913836736	-1.99589718401867	-2.25632036734329
H	-6.13392312797958	-4.55309315553512	-2.26807770346199
H	-6.39987853532561	-3.57901961519165	-0.81736548887003
H	-4.75157570422240	-4.04513349405769	-1.28671311164928
H	-4.99144915506563	-3.40056154123861	-4.33696535948572
H	-3.65388497513782	-2.92812134234798	-3.27942560806643
H	-4.54716330486846	-1.69551532811236	-4.19431194925777
O	-5.30915029941191	-1.33109094453330	-1.69493947348765

15_a, Gas Phase

C	-5.71651007623119	1.06605061363484	0.44324547035441
C	-5.22182553057889	1.09680207748727	-0.99602050888137
C	-4.66152128642139	1.59182527532806	1.40559730119452
C	-3.29027384974914	0.97073015208148	1.18591271252669
C	-2.90304110974324	0.98610027857964	-0.28416695937348
N	-3.94944739719963	0.41970797975013	-1.10261496172707
C	-3.97406784344504	-0.90384666259404	-1.46577439863474
O	-4.93727221959025	-1.43434185906683	-1.95578324082323
C	-2.72030502811723	-2.93957548544846	-1.14401613068460
C	-1.28691153112217	-3.16037358340969	-0.68879448529343
C	-2.96198671320346	-3.59524428797463	-2.49431076036085
C	-3.69693807042844	-3.42496367640839	-0.08279169063548
H	-5.93698970762439	0.60622453358433	-1.64943664183108
H	-5.10665954317911	2.13817570853449	-1.31198458126236
H	-2.74359240507901	2.02481039454070	-0.59184787830896
H	-1.97891616724546	0.43910353983591	-0.43488408985041
H	-6.63371756518259	1.65301196291799	0.53161383840785
F	-6.02899800409439	-0.23800793098445	0.77817882711669
H	-4.98246489576176	1.42994818719444	2.43424698506023
H	-4.57048379795413	2.67109182434400	1.25207012975522
F	-3.29559790656623	-0.34140768398420	1.62870753066901
H	-2.53718991094000	1.50343039675523	1.77100627937825
H	-4.72696703103658	-3.29083647952557	-0.40482299800652
H	-3.54306504374383	-2.87027946576560	0.84327894583782
H	-3.52359688771925	-4.48378193815388	0.10966759113931
H	-2.29379040250485	-3.16993076291031	-3.24383983837330
H	-3.99016374751574	-3.45725526374984	-2.81630320261606
H	-2.75312986903021	-4.66272538631309	-2.41300155397439
H	-0.59023062326669	-2.77144540972922	-1.43166498453848
H	-1.09846372829483	-4.22482344550180	-0.55443850250365
H	-1.11298153680073	-2.64888447560468	0.25814182231108
O	-2.80013057063013	-1.49607912744384	-1.24720002607160

15_a, Chloroform

C	-5.73127007747186	1.11728706749896	0.42129072130123
C	-5.20869114455871	1.11600988117461	-1.00550415308961
C	-4.68450616809518	1.61855101041600	1.40115110513465
C	-3.32376353003725	0.97150480467455	1.21020498536079
C	-2.90574725540431	0.96620714475426	-0.24934308678195
N	-3.95201606641528	0.40041640576850	-1.07542191762106
C	-3.98065899867513	-0.91160674935222	-1.44037121592450
O	-4.95155052165813	-1.44705539256439	-1.92908496146477
C	-2.71108880729230	-2.95366798368774	-1.15075418496012
C	-1.26410391500199	-3.16276791094711	-0.73516542999420
C	-2.97843353563427	-3.60887407834099	-2.49618796005711
C	-3.65313463336964	-3.45048938164445	-0.06486731008990
H	-5.92727855684350	0.64918924301868	-1.67126409322869
H	-5.05112978056859	2.14950057736992	-1.32336846641951
H	-2.73345079247501	1.99849950832739	-0.56510555065567
H	-1.98475631664223	0.40912515276230	-0.37682148201113
H	-6.63498753536182	1.72417846817974	0.48559733984143
F	-6.08925484741852	-0.18657278491123	0.75984605723796
H	-5.02882245179113	1.47445328231141	2.42495197303630
H	-4.56640265008665	2.69358552062952	1.24200935111942
F	-3.36905409236949	-0.34915051830623	1.65698308130628
H	-2.57099338371854	1.48441691809251	1.80950205069591
H	-4.69350336255661	-3.31687795344030	-0.35307473867947
H	-3.46896526254360	-2.90449491089795	0.86090799695368
H	-3.47171248885959	-4.51063354093040	0.11121501358828
H	-2.34665096627871	-3.16036919090074	-3.26389310536247
H	-4.01995448699638	-3.50343736500997	-2.78588856758198
H	-2.73428932444090	-4.66948014375382	-2.42628852449068
H	-0.59134241725016	-2.77077931064749	-1.49849318885576
H	-1.06607511634464	-4.22595603564486	-0.60510695389976
H	-1.06669169504969	-2.64852325330696	0.20582419009707
O	-2.80694981879016	-1.50897848069150	-1.24550897450467

15_a, DMSO

C	-5.73772717958485	1.13607538163459	0.40782999564915
C	-5.20026803820933	1.12507321220198	-1.01233627592316
C	-4.69681241660393	1.62488223506773	1.39872156533446

C	-3.34044143938808	0.96690888995620	1.22115345692429
C	-2.90643024724765	0.95816539858664	-0.23298885892232
N	-3.95022906979369	0.39517180416051	-1.06642393989145
C	-3.98085108472826	-0.91323642586151	-1.43158375480423
O	-4.95468312533004	-1.44988737437103	-1.91993563018003
C	-2.70651677568674	-2.95757149936825	-1.15196125661622
C	-1.25294149010478	-3.16322911223806	-0.75841627849288
C	-2.99078175225301	-3.61444765662412	-2.49313533057032
C	-3.63083390803277	-3.45606037801889	-0.05211490000317
H	-5.91751940083912	0.66843255022135	-1.68627045092696
H	-5.02532302610841	2.15588074672567	-1.32819749374707
H	-2.72801048267155	1.98899085906458	-0.54824383958735
H	-1.98673469824880	0.39719610457583	-0.35094853921678
H	-6.63551724643009	1.75171869277283	0.46152541848550
F	-6.11597858422010	-0.16714149544962	0.74359833367239
H	-5.05310418435660	1.48536801853335	2.41907358351282
H	-4.56696384004734	2.69853762314367	1.24092430210924
F	-3.40419592385068	-0.35765610757737	1.66454129186861
H	-2.58932514115403	1.46976539037605	1.82993994777334
H	-4.67570150992799	-3.31311288563741	-0.31966943182304
H	-3.42475576008287	-2.91859113874888	0.87397568753641
H	-3.45389548431410	-4.51880692051987	0.11209802176901
H	-2.38025519496866	-3.15557357451915	-3.27192043903952
H	-4.03904400338046	-3.52524170102704	-2.76326021965497
H	-2.72894104238723	-4.67113702195940	-2.42940043228186
H	-0.59282171599258	-2.77556047990534	-1.53492587529408
H	-1.05261179126374	-4.22561414392752	-0.62559903197822
H	-1.04034777977052	-2.64336177886496	0.17616484430457
O	-2.80766666302199	-1.51272721240257	-1.24424446998615

16_a, Gas Phase

C	-3.56702829499626	2.01289453560131	0.12776159093122
C	-3.63215350812117	0.88206348520035	-0.89285393685084
C	-2.30213873880407	2.86341707587739	-0.03441811218287
H	-3.58214910825392	1.56508217602221	1.12481026963057
H	-4.45702215804605	2.63773599599894	0.03459882671239
C	-1.06707365600074	1.95440900508794	-0.04981517950737
H	-2.22646820344517	3.51428798867775	0.83985272366083
C	-2.36901267423036	3.76253446956981	-1.26660738265974
C	-1.20550221829453	0.80568605386954	-1.04492109301736
H	-0.91341891234683	1.52709031378763	0.94409303718119
H	-0.17509258231234	2.53627153315398	-0.29275689192724
N	-2.43606409165628	0.06551432677891	-0.79525415703201
H	-3.67820974182776	1.28081112634706	-1.90977289736732
H	-4.52065111690119	0.28008015741713	-0.74590794843008
C	-2.35582145532307	-1.18820675672157	-0.31538406582611
O	-1.33058735052324	-1.79600420833147	-0.13192217879471
C	-3.68799783867129	-1.91225579418614	0.01937953780638
F	-4.48775937601054	-2.00274680656326	-1.05040493965252
F	-4.36415368246968	-1.26795719730721	0.98188751852484
F	-3.44316836649966	-3.13399159066943	0.44716400850531
H	-1.24245392321994	1.18460761641526	-2.06969674462882
H	-0.36978502026810	0.11732824222286	-0.96740932657555
H	-1.49748326977945	4.41655920287309	-1.31266280312225
H	-3.25936492170352	4.39203604838896	-1.23700559224729
H	-2.39980979029482	3.19273300048890	-2.19621426313067

16_a, Benzene

C	-3.56564143935819	2.01524936751410	0.12905696230919
C	-3.63105507324044	0.88160000841327	-0.88774903405529
C	-2.30156288813573	2.86621788191403	-0.03560923359439
H	-3.58071760964132	1.57251010174963	1.12844658684820
H	-4.45638966185325	2.63784895006769	0.03034943757008
C	-1.06632706609096	1.95775148884444	-0.04885320389106
H	-2.22594535588560	3.51772607314696	0.83803707710516
C	-2.36911092673486	3.76373152962668	-1.26903601325343
C	-1.20414085192897	0.80670687576417	-1.04081945942403
H	-0.91161309349022	1.53485422446386	0.94682259124308
H	-0.17491018670187	2.53782181413654	-0.29741528931919
N	-2.43357934496220	0.06296845482060	-0.78252808151483
H	-3.66868952738243	1.27508508124770	-1.90628174012495
H	-4.52148979685822	0.28242430346796	-0.74208444601272
C	-2.35854124312367	-1.18796015928571	-0.31680106542665
O	-1.33387055763594	-1.80902312983408	-0.13859597586975
C	-3.69111530363099	-1.91256387454458	0.01596290193245
F	-4.48890778528022	-2.00708253327675	-1.05389652059458
F	-4.36992929493717	-1.27680206255244	0.97979796222154
F	-3.44266320250061	-3.13774749118593	0.44185880284576
H	-1.25289871768944	1.18252078732158	-2.06559264322023
H	-0.36382653127456	0.12408264456948	-0.96828527025285
H	-1.49620297633708	4.41621997374638	-1.31537901585058
H	-3.25927541795987	4.39367003348564	-1.23714513904131
H	-2.40196614736617	3.19216965637870	-2.19772019062966

16_a, Dichloromethane

C	-3.56485832967399	2.01599747738180	0.12931024426769
C	-3.63017973410609	0.88128623420596	-0.88579067447429
C	-2.30129438178700	2.86729939806973	-0.03603828092519
H	-3.58067262878309	1.57617091919492	1.13002885282218
H	-4.45598789185478	2.63709625591621	0.02660797394163
C	-1.06583520881399	1.95938613538424	-0.04841750834198
H	-2.22584381962022	3.51849689927428	0.83771298439233
C	-2.36907729629132	3.76464208100696	-1.26959585780430
C	-1.20315006571053	0.80755144543006	-1.03920388910491
H	-0.91022485769878	1.53908340602935	0.94827757900703
H	-0.17501754703033	2.53853302396702	-0.30065413100627
N	-2.43165265858745	0.06094544968391	-0.77485596909794
H	-3.66096931515141	1.27160335005360	-1.90516974983584
H	-4.52211014178309	0.28400742907256	-0.74227384281936
C	-2.36073201673299	-1.18703564557751	-0.31764917055802
O	-1.33620890638054	-1.81818109201013	-0.14250821776879
C	-3.69356121623749	-1.91134207449394	0.01484402890133
F	-4.48973116339257	-2.01119631068021	-1.05451171005568
F	-4.37362968867186	-1.28050617755241	0.97889568573348
F	-3.44187976431639	-3.13864905490187	0.44165346524571
H	-1.26086489664881	1.18204973378213	-2.06347032195061
H	-0.35927521452284	0.12928559296080	-0.97140208267154
H	-1.49553925938300	4.41654070982995	-1.31507834696790
H	-3.25953051531727	4.39422542482800	-1.23605025508540
H	-2.40254348150412	3.19268938914455	-2.19812080584338

16_a, Chloroform

C	-3.56487136714766	2.01842572548214	0.13102157680486
C	-3.63022812069024	0.88186375629277	-0.88216317179748
C	-2.30139231212276	2.86942659356052	-0.03639049689546
H	-3.58016602283439	1.57992708000889	1.13232749566615
H	-4.45588963673692	2.63976829590628	0.02838992481780
C	-1.06600128732065	1.96144137288230	-0.04668577679285
H	-2.22593274544672	3.52339188246663	0.83533771146613
C	-2.36942786822464	3.76292530429741	-1.27269720992439
C	-1.20286449467484	0.80723898977850	-1.03494839397322
H	-0.91080826413511	1.54304986981832	0.95085856825139
H	-0.17512279963291	2.54053932848496	-0.29897088410159
N	-2.43210185325972	0.06260579014409	-0.77171516519551
H	-3.66426756363796	1.27118430510286	-1.90204813727618
H	-4.52168288318589	0.28453633404257	-0.73572619551057
C	-2.36039718273052	-1.18948293626180	-0.32112187252553
O	-1.33625396021513	-1.82067921163001	-0.15335268244308
C	-3.69306444666254	-1.91387712170022	0.01194003491565
F	-4.49278412709540	-2.00652864295637	-1.05581931122853
F	-4.36973630253316	-1.28537057924913	0.98058227921927
F	-3.44242321299341	-3.14274142753102	0.43232275125847
H	-1.25542799673993	1.17946951999203	-2.06055230306177
H	-0.36053934415855	0.12745496033550	-0.96221382893854
H	-1.49590375865653	4.41458629866111	-1.32130570472554
H	-3.25952887925819	4.39311078042376	-1.24145191231864
H	-2.40355356990622	3.18771373164786	-2.19907729569087

16_a, DMSO

C	-3.56439240420561	2.01944177769525	0.13158200911494
C	-3.62967245703115	0.88187591294486	-0.88013136663397
C	-2.30128773482037	2.87060169023890	-0.03666534320597
H	-3.58021296479092	1.58316486753606	1.13388697808014
H	-4.45561301441150	2.63982966514483	0.02621884085534
C	-1.06575986948807	1.96299950744984	-0.04584948652208
H	-2.22596710141596	3.52498689582652	0.83466897466993
C	-2.36954428696167	3.76296504062208	-1.27377739159007
C	-1.20206836708428	0.80776588775701	-1.03281117517744

H	-0.91012376920319	1.54679084458817	0.95258363495660
H	-0.17527187740467	2.54147345206745	-0.30055169106581
N	-2.43090090927968	0.06167746234243	-0.76594823254703
H	-3.65957840193254	1.26886888003894	-1.90066298524789
H	-4.52201013441765	0.28577312112770	-0.73453674967649
C	-2.36182337445312	-1.18931028697073	-0.32292333936702
O	-1.33772504725998	-1.82749621869551	-0.15929673096102
C	-3.69456634188685	-1.91332842611874	0.01051481883628
F	-4.49427251768878	-2.00817502697896	-1.05623757959477
F	-4.37078451236335	-1.28848740704364	0.98047051354745
F	-3.44185746853046	-3.14401268307815	0.43023997283447
H	-1.25929285606981	1.17857669242460	-2.05838276441605
H	-0.35789926774160	0.13035566891971	-0.96176930514976
H	-1.49544626934648	4.41392329921149	-1.32287641848492
H	-3.25961246590915	4.39323212211886	-1.24183931744998
H	-2.40468658630313	3.18648726083096	-2.19936586580489

16_a, Water

C	-3.56448350855462	2.01653421869555	0.12969536057828
C	-3.62978408901895	0.88124381626636	-0.88454606864856
C	-2.30116844324841	2.86796539400418	-0.03626463063145
H	-3.58050735477015	1.57797377057859	1.13098372863142
H	-4.45578890083509	2.63701936129991	0.02550006065173
C	-1.06558111024801	1.96030588387119	-0.04804180920976
H	-2.22576365860315	3.51938218877933	0.83727644952382
C	-2.36921070050970	3.76473423235896	-1.27022561767188
C	-1.20270142489570	0.80784562025694	-1.03801309844979
H	-0.90961503018040	1.54130567029882	0.94916782592589
H	-0.17499735172522	2.53905668952779	-0.30180310532582
N	-2.43087731132922	0.06034214585753	-0.77146545211226
H	-3.65817498283020	1.27021201508955	-1.90430123022580
H	-4.52213310572952	0.28453951662669	-0.74166903089556
C	-2.36155664267947	-1.18705140850199	-0.31833351778471
O	-1.33705989310303	-1.82189414923810	-0.14475299454208
C	-3.69455588308652	-1.91108809329694	0.01392545722082
F	-4.49034770663397	-2.01192408591275	-1.05516338402475
F	-4.37462395387699	-1.28242808731762	0.97864435187509
F	-3.44188693295254	-3.13948462724168	0.44025715654077
H	-1.26351849653669	1.18158122582880	-2.06221253554767
H	-0.35770315760833	0.13097235842358	-0.97162655695583
H	-1.49543999430444	4.41636074338037	-1.31588306305349
H	-3.25974082090295	4.39421515102604	-1.23616728939043
H	-2.40314954583671	3.19226044933885	-2.19844100647802

16_e, Gas Phase

C	-3.56501536990004	2.18352386646870	-0.03372073070302
C	-3.63661428590143	1.00175369208867	-0.99229568407128
C	-2.31035694854937	3.02191613831862	-0.27268196908164
H	-3.55714805870312	1.80192972971603	0.99239114060810
H	-4.45892797217822	2.79947877930763	-0.14765282007624
C	-1.07318886549771	2.12595526619787	-0.22681238962813
C	-2.21069541581957	4.16763115060523	0.72329321333371
H	-2.38003651125949	3.44292448994482	-1.28351339877032
C	-1.20941959547943	0.92841238644275	-1.16076101469103
H	-0.92424941095040	1.76427230753682	0.79535751607225
H	-0.18336144079447	2.69823521892369	-0.49901219301027
N	-2.43592436167336	0.19592064617816	-0.87437406752713
H	-3.69192906267126	1.36305115818596	-2.02408088597433
H	-4.52024448719518	0.40199347318857	-0.81172561219578
C	-2.34981647753884	-1.05033991892771	-0.37552957835348
O	-1.32272690407527	-1.65579329430769	-0.19642552338110
C	-3.67730457719073	-1.76707874394876	-0.00722732620288
F	-4.48948869748409	-1.88413422182569	-1.06509927073632
F	-4.34266029219909	-1.10091269221906	0.94765339944143
F	-3.42559407944563	-2.97796116047333	0.44630131090882
H	-1.33814376394633	4.79115390877494	0.52454779238516
H	-2.12180662310623	3.78127830982974	1.74097700471228
H	-3.09685177279442	4.80248975892310	0.68290992637460
H	-1.25693809330009	1.27122792319490	-2.19910745314396
H	-0.37146693234623	0.24561182856604	-1.06179138628944

16_e, Benzene

C	-3.56187300632126	2.18981037064067	-0.02368064839269
C	-3.63610337474103	1.00041052581197	-0.97172498315431
C	-2.30942688701423	3.02759481345112	-0.27411756707324
H	-3.55060612395104	1.81909596723491	1.00649458146126
H	-4.45733631183721	2.80187931628705	-0.14414280276530
C	-1.07223500889693	2.13275008574589	-0.21978920040944
C	-2.20922342020251	4.18363261551819	0.71014220248909
H	-2.38100154937024	3.43754830052546	-1.28898143093474
C	-1.20722583551904	0.92742040548483	-1.14314702523657
H	-0.92262839792871	1.78216564776668	0.80619802093007
H	-0.18292681333806	2.70099930944144	-0.50125234910043
N	-2.43347382197940	0.19347704919684	-0.84686488115722
H	-3.68900265841411	1.35137877015512	-2.00641954106308
H	-4.52075693827244	0.40455791949041	-0.78447166188074
C	-2.35442270618426	-1.05893359512654	-0.38524346643423
O	-1.32915259078308	-1.68406834322627	-0.22706313790603
C	-3.68250422683361	-1.77912090114933	-0.02492559745346
F	-4.49648360546158	-1.88300092463042	-1.08172649541847
F	-4.34622150268185	-1.13500491495254	0.94359794362686
F	-3.42776790636538	-3.00074247213744	0.40757414555324
H	-1.33652973921730	4.80464230817530	0.50308302562806
H	-2.11974346699506	3.80741215696921	1.73179096053528
H	-3.09606467786643	4.81738350716626	0.66237995122229
H	-1.26187773326694	1.26078363995249	-2.18356889362461
H	-0.36532169655831	0.25046844220868	-1.04252114944157

16_e, Dichloromethane

C	-3.56003657388536	2.19208759167786	-0.01849989163297
C	-3.63566866259034	0.99994375090152	-0.96231390794473
C	-2.30894925891804	3.02980989175520	-0.27446176282466
H	-3.54741839567238	1.82646770520645	1.01357391511177
H	-4.45637159501399	2.80176605753981	-0.14282889080028
C	-1.07156721703212	2.13586701181167	-0.21641096254737
C	-2.20852858189168	4.19062632545672	0.70431290542400
H	-2.38167122565000	3.43443417843685	-1.29102745916728
C	-1.20582705489016	0.92749425003581	-1.13545227713303
H	-0.92107768202188	1.79055553424442	0.81131188602110
H	-0.18290266041891	2.70208928411381	-0.50335161669562
N	-2.43169946496350	0.19153146830751	-0.83326580035409
H	-3.68490280121963	1.34604730005720	-1.99813955827409
H	-4.52130141301606	0.40631751102895	-0.77333601300719
C	-2.35748835870924	-1.06111554793901	-0.38912072076332
O	-1.33285094416687	-1.69829986667589	-0.23919855523586
C	-3.68594741338425	-1.78297308695976	-0.03324156779610
F	-4.49950791464490	-1.88345166278591	-1.08946810973531
F	-4.34968649788815	-1.15114231424547	0.94130291615682
F	-3.42817538125619	-3.01023080471413	0.39023996056499
H	-1.33586078234040	4.81040874120863	0.49278445351475
H	-2.11868578519781	3.81927367820965	1.72787179428597
H	-3.09595991540248	4.82344948649513	0.65264784112095
H	-1.26698252426671	1.25689213140472	-2.17619491563064
H	-0.36084189555895	0.25469138542827	-1.03611366265782

16_e, Chloroform

C	-3.56057088577882	2.19145213829180	-0.01998619209382
C	-3.63577897681021	1.00004499253050	-0.96497176683949
C	-2.30910016135113	3.02921324454101	-0.27439505426360
H	-3.54825283162159	1.82436165832901	1.01153867788689
H	-4.45667065800991	2.80182900828953	-0.14310461418940
C	-1.07176112986520	2.13501273844888	-0.21743978586809
C	-2.20872260514260	4.18864720495029	0.70597351560401
H	-2.38152691879644	3.43539178245147	-1.29047746851243
C	-1.20623887748362	0.92744630140067	-1.13763585085781
H	-0.92150395405538	1.78820892775472	0.80978569705663
H	-0.18291034661280	2.70183550578460	-0.50279958908224
N	-2.43222106830323	0.19212187934877	-0.83715501012945
H	-3.68619093549605	1.34753672203999	-2.00049140381803
H	-4.52111021860719	0.40575535803370	-0.77643641670452
C	-2.35655397406717	-1.06058654188364	-0.38794329302844
O	-1.33178951436749	-1.69415173814896	-0.23563511082659
C	-3.68493324202088	-1.78197918268975	-0.03088518021279
F	-4.49856765801638	-1.88327642652617	-1.08738957588647
F	-4.34878176004610	-1.14650916085876	0.94185406524995
F	-3.42817886788106	-3.00756818603841	0.39516784005699
H	-1.33606545927223	4.80881046729829	0.49572932059380
H	-2.11891614566211	3.81585864470426	1.72896267613173

H	-3.09598904212602	4.82174134753687	0.65552336109922
H	-1.26540901816136	1.25791610330073	-2.17833446238918
H	-0.36216575044503	0.25342721111058	-1.03783438167686

16_e, DMSO

C	-3.55954421204508	2.19256646678962	-0.01715550375969
C	-3.63555488382117	0.99989327702087	-0.96004818453838
C	-2.30881995759249	3.03027112845338	-0.27446961106660
H	-3.54670888193204	1.82821913224194	1.01539656296879
H	-4.45609067346742	2.80158135392787	-0.14264854967076
C	-1.07138364323464	2.13659100303645	-0.21545969043018
C	-2.20839321695779	4.19229581197629	0.70291433589961
H	-2.38180259750537	3.43351927920356	-1.29144025527928
C	-1.20540374561201	0.92759774254507	-1.13360032366187
H	-0.92067392399024	1.79257149176371	0.81269660421139
H	-0.18291549346228	2.70227767600906	-0.50386867294187
N	-2.43117930125156	0.19093523067548	-0.82981637082612
H	-3.68342750116718	1.34481664467028	-1.99611122051358
H	-4.52151593471260	0.40686995127153	-0.77092839155115
C	-2.35839801314451	-1.06143571089620	-0.39022230942282
O	-1.33383855644450	-1.70221033380671	-0.24248846070088
C	-3.68691329571324	-1.78360639841152	-0.03524709775124
F	-4.50038842309652	-1.88378724540356	-1.09111318480133
F	-4.35047130048665	-1.15496422993556	0.94082456280422
F	-3.42809997553515	-3.01235365463656	0.38625383268477
H	-1.33572235024929	4.81174121745575	0.49021730978516
H	-2.11854554880433	3.82222007952529	1.72698579147606
H	-3.09599847226966	4.82483199284649	0.65009817574958
H	-1.26857838177954	1.25615135576288	-2.17430187336955
H	-0.35954171572476	0.25594673791459	-1.03484747529426

16_e, Water

C	-3.55949741963058	2.19260566168169	-0.01703249695069
C	-3.63554308492709	0.99988973043001	-0.95984632475284
C	-2.30880666347915	3.03030978891030	-0.27446670743881
H	-3.54664976184129	1.82837329667863	1.01556332340580
H	-4.45606222027394	2.80155819439107	-0.14264120337090
C	-1.07136386121909	2.13665623095896	-0.21537273261748
C	-2.20837944928046	4.19244269871036	0.70279269997370
H	-2.38181310932698	3.43343359487768	-1.29147223210826
C	-1.20536396330392	0.92761197185372	-1.13343783980236
H	-0.92062687227768	1.79275494710175	0.81282258084381
H	-0.18291856494425	2.70229482832037	-0.50392663750871
N	-2.43112671709453	0.19087516642999	-0.82949503791745
H	-3.68327093853419	1.34470211499345	-1.99593062002526
H	-4.52153862732433	0.40692487712961	-0.77072526352836
C	-2.35848771190635	-1.06145000457789	-0.39031351640189
O	-1.33393080934126	-1.70257359606948	-0.24275827253929
C	-3.68701042767146	-1.78365044801765	-0.03542863525771
F	-4.50046486677788	-1.88382751287320	-1.09126341913233
F	-4.35056048273668	-1.15531597392381	0.94077920132761
F	-3.42808787488240	-3.01253995468836	0.38589935765709
H	-1.33570991109292	4.81185873639171	0.48998493360623
H	-2.11852946431540	3.82248252204957	1.72691087808374
H	-3.09600332973645	4.82494898896767	0.64987004706975
H	-1.26875388003374	1.25609561998762	-2.17412890069190
H	-0.35940998804798	0.25607852028624	-1.03476318192348

17_a, Gas Phase

C	-2.33810123019430	0.83990500615326	-0.79005925366117
C	-2.82498099044754	-0.53593802259353	-0.36510496031478
C	-0.91267360297886	1.11956938794360	-0.32428159219710
F	-3.19649215297155	1.78304480749171	-0.26593193552094
H	-2.39233624691045	0.91487973401831	-1.87896298168775
N	-2.67493342204320	-0.70036024338579	1.06303291671053
H	-2.24056591102708	-1.30342917627359	-0.88285638701439
H	-3.85928177452616	-0.65168236499708	-0.66427995544731
C	-0.75927245326865	0.83295905802613	1.16751351653918
C	-1.32282727746650	-0.52227450080005	1.56201413867428
F	-1.40300952950637	1.81065580503508	1.89669288650414
H	0.29951904765132	0.86632510013982	1.44034370021751
H	-0.72269302984966	2.18400908067917	-0.47444757020514
C	0.09768433450059	0.31589895674547	-1.14250318855323
H	-1.33793246751719	-0.61156663940202	2.64415708065998
H	-0.67890677590452	-1.31110195684931	1.15967506894724
C	-3.65554480133866	-0.99294443118950	1.94493223935836
O	-3.49334509377847	-1.12159123277670	3.12907916774585
C	-5.08477095078550	-1.22107780943112	1.38131585709727
F	-5.09439552042444	-2.23857865545114	0.50640789962455
F	-5.55926444545200	-0.14088650627353	0.75657039163249
F	-5.90813124092436	-1.52262720351114	2.36347803318380
H	-0.03462631091154	0.49813890191686	-2.20903639494817
H	0.00472048944257	-0.75863966000067	-0.98002237418599
H	1.11710135663250	0.59830256478578	-0.88127630315920

17_a, Benzene

C	-2.33919550739111	0.82436272800042	-0.79077515831416
C	-2.81776817930132	-0.55349036905626	-0.36757345530037
C	-0.91953453232620	1.11838114520916	-0.32062946736662
F	-3.21122127213435	1.76302812359435	-0.26205167641557
H	-2.39578126368100	0.90270734006761	-1.87784065075567
N	-2.67210434274946	-0.71158822365597	1.06466991565413
H	-2.22018887554322	-1.31596280778554	-0.87469055132486
H	-3.84794785419074	-0.68183899047343	-0.67500254134582
C	-0.76186883872036	0.82352398953881	1.16748040745086
C	-1.31442643016953	-0.53608951114833	1.55671635750236
F	-1.42208533164564	1.79391510982753	1.90604381783198
H	0.29381175107716	0.86912167427708	1.44454186981482
H	-0.73807618687340	2.18470503756639	-0.46731382825719
C	0.09914276989175	0.32885189481704	-1.14227378385149
H	-1.31408499198866	-0.63737140888130	2.63722992508802
H	-0.67574397559048	-1.31735739641539	1.13522302983605
C	-3.65260316027491	-0.98166425523816	1.94145485287798
O	-3.50156816698548	-1.09473639792828	3.13395243021225
C	-5.08383409969430	-1.20283403348153	1.37961940555724
F	-5.11079327591648	-2.22854886315148	0.51811792748204
F	-5.55147577356241	-0.12350791487090	0.74868201720179
F	-5.90994598349069	-1.48535324733172	2.36935693857502
H	-0.03079036289584	0.52561901106612	-2.20633176117394
H	0.00854129639969	-0.74762243145973	-0.99251502680519
H	1.11448258775694	0.61473979691354	-0.86964099417368

17_a, Dichloromethane

C	-2.34272798542789	0.80691081454185	-0.78809457600668
C	-2.80786094110555	-0.57691591038633	-0.37226509611553
C	-0.92868834832502	1.11621455389639	-0.31401897734894
F	-3.22926476517438	1.73457592979142	-0.24885375596812
H	-2.40276487120057	0.89377995820516	-1.87328161006874
N	-2.66668904886953	-0.73155290351949	1.06298434845775
H	-2.19538404551921	-1.33101809472333	-0.87160225724323
H	-3.83335882872697	-0.72114527317550	-0.68786634425254
C	-0.76430507319531	0.80913610117560	1.16976696552308
C	-1.30490058128249	-0.55680898451266	1.54938416560502
F	-1.43871206880186	1.76856736812411	1.92136614319263
H	0.28936214013187	0.86547137648634	1.44845947853402
H	-0.75866014024950	2.18535490730775	-0.45352193034340
C	0.09965558246979	0.34669202692166	-1.14276887413022
H	-1.29124227677099	-0.67320769761534	2.62782182943513
H	-0.66976801070513	-1.32884596874940	1.10852719154450
C	-3.65136760884888	-0.95890170695836	1.93774557936484
O	-3.51334759732289	-1.03461908838507	3.13924657599700
C	-5.08300992742403	-1.18112006513058	1.37648549180537
F	-5.12255002425524	-2.22040565449005	0.53565585441844
F	-5.54398868233381	-1.10799964521784	0.73021252981503
F	-5.91285271010678	-1.43872167978602	2.37358806031189
H	-0.03549969220973	0.55276817292883	-2.20423336368786
H	0.02264017049844	-0.73197712498612	-1.00219748314035
H	1.11022533475565	0.64475858825698	-0.86608994569911

17_a, Chloroform

C	-2.34146401216443	0.81247992747693	-0.78930031863465
C	-2.81129629704040	-0.56919331415182	-0.37077356638558
C	-0.92569904050071	1.11697013499734	-0.31629073139199
F	-3.22339075960194	1.74406549449776	-0.25397100781547
H	-2.40016297144870	0.89625636188496	-1.87511423357811
N	-2.66845130331547	-0.72509029768245	1.06348591837322
H	-2.20401770476325	-1.32626342291856	-0.87271260207284

H	-3.83844264291909	-0.70788340032642	-0.68356784014477
C	-0.76375973643660	0.81397099499333	1.16892987995059
C	-1.30787808111406	-0.55010275631786	1.55156807151756
F	-1.43423577327171	1.77680184727756	1.91612360880989
H	0.29042602708151	0.86729692978914	1.44744337683208
H	-0.75198607359644	2.18519619971463	-0.45829096910533
C	0.09981914758323	0.34083693854607	-1.14232786466939
H	-1.29837829354554	-0.66169950746416	2.63069426103757
H	-0.67154392660726	-1.32489986932870	1.11661154618443
C	-3.65158208877936	-0.96708307681613	1.93899629914298
O	-3.50913435929607	-1.05611030788460	3.13763074804823
C	-5.08332219618565	-1.18796320197619	1.37774704910067
F	-5.11966048578795	-2.22232351486683	0.52949455723401
F	-5.54601646127522	-0.11208745664648	0.73730456050881
F	-5.91186018924666	-1.45389468682057	2.37254609404186
H	-0.03404415765609	0.54277697051710	-2.20480556269202
H	0.01921840445365	-0.73703444148505	-0.99748854728988
H	1.11180297543420	0.63596745499100	-0.86748272700187

17_a, DMSO

C	-2.34400554115532	0.80175446056332	-0.78652523576289
C	-2.80446634776211	-0.58429036882936	-0.37372022752780
C	-0.93146795976755	1.11535849617260	-0.31178894982593
F	-3.23482335796850	1.72531804378840	-0.24271062964920
H	-2.40572695255298	0.89203666589622	-1.87104604702097
N	-2.66505794479048	-0.73775348071429	1.06252168427873
H	-2.18692267120182	-1.33540567380564	-0.87057025929356
H	-3.82830120310611	-0.73385539661447	-0.69213464556254
C	-0.76455329335296	0.80443927613594	1.17060754095444
C	-1.30227517302946	-0.56299076765759	1.54761069536500
F	-1.44208056729271	1.76094134272410	1.92665370053836
H	0.28870958949989	0.86306786245008	1.44925840660882
H	-0.76467093987402	2.18530313237877	-0.44899420498994
C	0.09932196907012	0.35201268142518	-1.14344273402736
H	-1.28489079835086	-0.68378569343466	2.62537828956947
H	-0.66837707260988	-1.33267990499585	1.10172166761183
C	-3.65129755220335	-0.95049466798738	1.93621958588882
O	-3.51789605777994	-1.01190236098043	3.14056128987064
C	-5.08262639823016	-1.17503205533866	1.37481776289466
F	-5.12465518875764	-2.21846342726542	0.54061280565801
F	-5.54272638697808	-0.10443312565829	0.72377373216669
F	-5.91351863899481	-1.42578844055468	2.37406271580352
H	-0.03773095068699	0.56174181254110	-2.20389149378034
H	0.02641531717084	-0.72746799502001	-1.00684771933115
H	1.10856412070485	0.65335958478105	-0.86567773043730

17_a, Water

C	-2.34409594198365	0.80121374375473	-0.78643443704453
C	-2.80418477818204	-0.58497631059377	-0.37380950540078
C	-0.93174405362692	1.11529106819802	-0.31157035929899
F	-3.23535000607236	1.72446579722485	-0.24238329749689
H	-2.40591233339291	0.89168496968808	-1.87091167401656
N	-2.66491614456652	-0.73824959650747	1.06251527856096
H	-2.18621367594310	-1.33586523024437	-0.87040829091796
H	-3.82788632597963	-0.73500298553298	-0.69243370955664
C	-0.76458218911434	0.80397406887780	1.17066525660020
C	-1.30200302325003	-0.56358442211171	1.54737245525826
F	-1.44240971630878	1.76020125137633	1.92714161239182
H	0.28863507664476	0.86286155909884	1.44934636154273
H	-0.76528579535657	2.18531258068304	-0.44853938064676
C	0.09932225760257	0.35257209812774	-1.14345355021031
H	-1.28417279523310	-0.68489243631788	2.62506401382501
H	-0.66829669192542	-1.33303184647829	1.10082563396203
C	-3.65128349248099	-0.94961553273534	1.93608739520331
O	-3.51835002550347	-1.00979236447626	3.14069698294766
C	-5.08258898529245	-1.17446278946973	1.37470709389754
F	-5.12483795283251	-2.21833470317347	0.54121775746967
F	-5.54266406714482	-0.10416816865208	0.72314344700584
F	-5.91358286276152	-1.42452870421205	2.37419181968511
H	-0.03771639633852	0.56286853786931	-2.20379198430692
H	0.02663190934449	-0.72700773407866	-1.00742786004834
H	1.10842800969781	0.65405714968534	-0.86536105940541

17_e, Gas Phase

C	-2.26227574036423	0.73881746422458	-0.88374538602330
C	-2.71886817123230	-0.64001984440490	-0.42819060672577
C	-0.87978385594319	1.09759657020430	-0.35248177318771
H	-2.99781133379667	1.48894928933516	-0.57647007632560
F	-2.22152685194332	0.74489253815171	-2.26510800889083
N	-2.62039708212977	-0.72651029730603	1.01914016950353
H	-2.06940102954547	-1.39497558459310	-0.87998495040706
H	-3.74467805535890	-0.82710190015501	-0.72995880398859
C	-0.79659745665011	0.84830530108440	1.14802961127201
C	-1.27794198894597	-0.54426866521646	1.52826380993611
H	-1.38293407354753	1.59455830635602	1.69447298309203
F	0.51834307439549	0.97370171975125	1.55106637574571
C	-0.50878974570637	2.53224269176418	-0.69471304668662
H	-0.17257403681320	0.40651044372348	-0.82557179096800
H	-1.22262432635485	3.22478685484644	-0.24295877199553
H	-0.51981553889700	2.68762318365756	-1.77182596268090
H	0.48360883142075	2.77310246318707	-0.31830828617348
H	-1.23576752866263	-0.67597247406742	2.60284025910968
H	-0.62043254117430	-1.28814227228927	1.06975627725122
C	-3.75382213113357	-0.84900572006565	1.74694358077529
O	-4.85990960759970	-0.92073866263760	1.28176358885690
C	-3.61005289994052	-0.90760182652256	3.29187422266751
F	-2.85254887566705	-1.94040900099485	3.67589171268722
F	-4.79535827571065	-1.03882788307808	3.84801823345862
F	-3.04950075869891	0.21331730504479	3.76669663969758

17_e, Benzene

C	-2.26084720095799	0.75156091251873	-0.88175959980705
C	-2.72937459302933	-0.62166321473303	-0.42233883034150
C	-0.87374909592096	1.09932487300713	-0.35799787857149
H	-2.98781783844220	1.51135522580060	-0.58159372178018
F	-2.22339060941896	0.74649444785699	-2.26783934438242
N	-2.63455368831228	-0.70102634219503	1.02697948792359
H	-2.08401954744643	-1.38462629447267	-0.86546183788806
H	-3.75485015146466	-0.80072884347253	-0.72863103935006
C	-0.80243400882603	0.86376451847437	1.14451521329583
C	-1.28943102923609	-0.52352296950997	1.53533527746133
H	-1.38286573579397	1.62009494453222	1.68149128684243
F	0.51536936672162	0.98278592113738	1.55474405667670
C	-0.48716837930757	2.52700692237184	-0.71267792112758
H	-0.17460952536198	0.39427835965391	-0.82198822245153
H	-1.19460409268987	3.23052718102836	-0.26829802016295
H	-0.49267411126497	2.67243333883729	-1.79146014426072
H	0.50794149146807	2.76056779458678	-0.33818933511017
H	-1.24708647769990	-0.64553850128472	2.61084594396351
H	-0.63892033141049	-1.27518568313383	1.08088916161124
C	-3.75495631348860	-0.86784404338163	1.75319762509612
O	-4.86528406129698	-0.97467723853928	1.29360221818023
C	-3.60916413839766	-0.93431171729347	3.29796935491277
F	-2.83786815242051	-1.95793575305056	3.67631591215435
F	-4.79604535902148	-1.09265808035914	3.85110917387309
F	-3.07305641698072	0.19035424162026	3.78668118324252

17_e, Dichloromethane

C	-2.26005138548997	0.76249982343587	-0.87984440965489
C	-2.73811171498634	-0.60603462540815	-0.41692334868301
C	-0.86898451329988	1.10037251678961	-0.36252187854228
H	-2.97949181217428	1.53007909022575	-0.58383997791678
F	-2.22675093609698	0.74908402564170	-2.26915846633516
N	-2.64590440193038	-0.68074294371312	1.03386169322434
H	-2.09658392545856	-1.37549866084474	-0.85358663257000
H	-3.76361872724621	-0.77812659318313	-0.72604953319148
C	-0.80739683207889	0.87760968640246	1.14177011324619
C	-1.29899187943100	-0.50511218027933	1.54201306872680
H	-1.38413589794308	1.64203012306822	1.66992090980118
F	0.51182278515175	0.99250653810201	1.55826538695740
C	-0.46832935935773	2.52130795097515	-0.72882073695414
H	-0.17723578642558	0.38299960396170	-0.81828956573705
H	-1.16969242163855	3.23496466772837	-0.29136494589560
H	-0.46944261990842	2.65733265490551	-1.80900388313102
H	0.52902920867441	2.74821477916856	-0.35580512313636
H	-1.25735149673583	-0.61806335602908	2.61839120499461
H	-0.65345765271645	-1.26327600952880	1.09226416122935
C	-3.75566320636958	-0.88208068773488	1.75814600558245

O	-4.86846959194319	-1.01527457463835	1.30200243522679
C	-3.60823999003564	-0.95800644796841	3.30257467131187
F	-2.82392298768760	-1.97318833449219	3.67409788773493
F	-4.79583285169419	-1.14208641987179	3.85250514001831
F	-3.09465200317779	0.16931937328708	3.80483582369358

17_e, Chloroform

C	-2.26020050948991	0.75896144835220	-0.88055835696760
C	-2.73539176412263	-0.61099806554081	-0.41873050461798
C	-0.87046661249648	1.10011696807900	-0.36105114346051
H	-2.98211753557322	1.52414371600487	-0.58363886323512
F	-2.22526217458836	0.74798579160207	-2.26891439996092
N	-2.64243385730826	-0.68698231240581	1.03160521010573
H	-2.09267702009015	-1.37851236757578	-0.85729933701288
H	-3.76088129025863	-0.78524266915066	-0.72703659234809
C	-0.80578538541038	0.87307000257962	1.14265495721440
C	-1.29600190044356	-0.51109567351499	1.53974638193695
H	-1.38347640507637	1.63496073342969	1.67379850439793
F	0.51309992584259	0.98907649976473	1.55709317910174
C	-0.47447818498366	2.52333482615431	-0.72345012976274
H	-0.17624133452954	0.38679009455609	-0.81949862863633
H	-1.17790775068838	3.23359116505414	-0.28368438309177
H	-0.47694745939779	2.66251481038117	-1.80318151245748
H	0.52214626832693	2.75246950496694	-0.34995555022938
H	-1.25403546070995	-0.62718544827639	2.61582142326292
H	-0.64906749806897	-1.26720964797198	1.08825331998970
C	-3.75546642124542	-0.87796755912934	1.75659590397747
O	-4.86752872207304	-1.00351002717176	1.29951035139400
C	-3.60848940170456	-0.95019032546156	3.30117318200070
F	-2.82876060801290	-1.96830317436304	3.67526176230198
F	-4.79594484929402	-1.12528636755346	3.85231398799116
F	-3.08714404860333	0.17629807719074	3.79861123810614

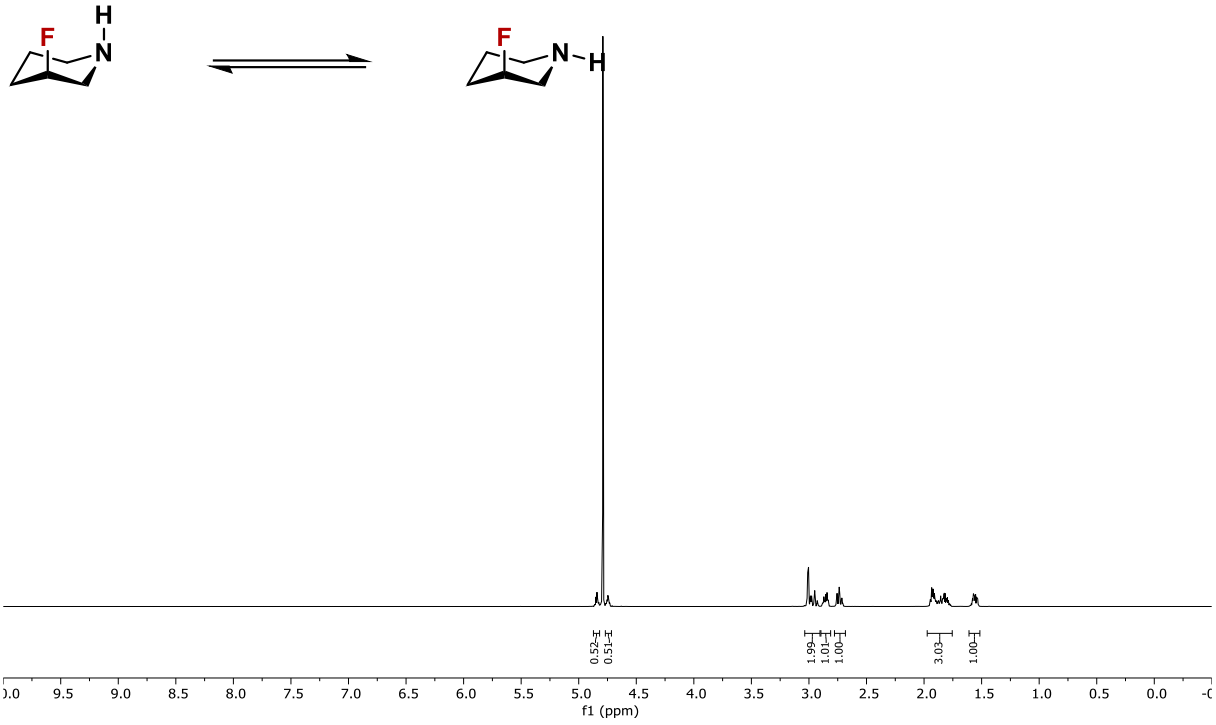
17_e, DMSO

C	-2.25991743443316	0.76615470704262	-0.87914916518403
C	-2.74101030271713	-0.60084768525336	-0.41499994980357
C	-0.86750611634193	1.10061645070899	-0.36400781769595
H	-2.97680043914724	1.53625268021481	-0.58418978316301
F	-2.22825312602849	0.75016884737544	-2.26940176990910
N	-2.64945941861099	-0.67437430352773	1.03620173566996
H	-2.10086307724385	-1.37237588859062	-0.84984440409957
H	-3.76661944960052	-0.77061473959300	-0.72475450462496
C	-0.80893241000089	0.88225416629344	1.14085802050337
C	-1.30208505929040	-0.49889121624747	1.54439758230426
H	-1.38451756061021	1.64933402109604	1.66602662480542
F	0.51063803867580	0.99586664689215	1.55926928145139
C	-0.46198340240035	2.51915731848967	-0.73429798513495
H	-0.17832001475925	0.37911729923257	-0.81704814444160
H	-1.16110239777563	3.23634199140911	-0.29912589332186
H	-0.46184480598768	2.65195863008873	-1.81493243110734
H	0.53617787420877	2.74367598939695	-0.36186125706869
H	-1.26088950236541	-0.60858853476831	2.62108972186617
H	-0.65794529092885	-1.25919715431096	1.09655208909397
C	-3.75581959196864	-0.88651074528459	1.75971104948957
O	-4.86928636643088	-1.02733503372262	1.30438463946361
C	-3.60800035757054	-0.96601696702718	3.30397721185447
F	-2.81839310726581	-1.97767951943016	3.67292661917302
F	-4.79561376017640	-1.16006524412814	3.85253318699311
F	-3.10311292123029	0.16242828364360	3.81112534288633

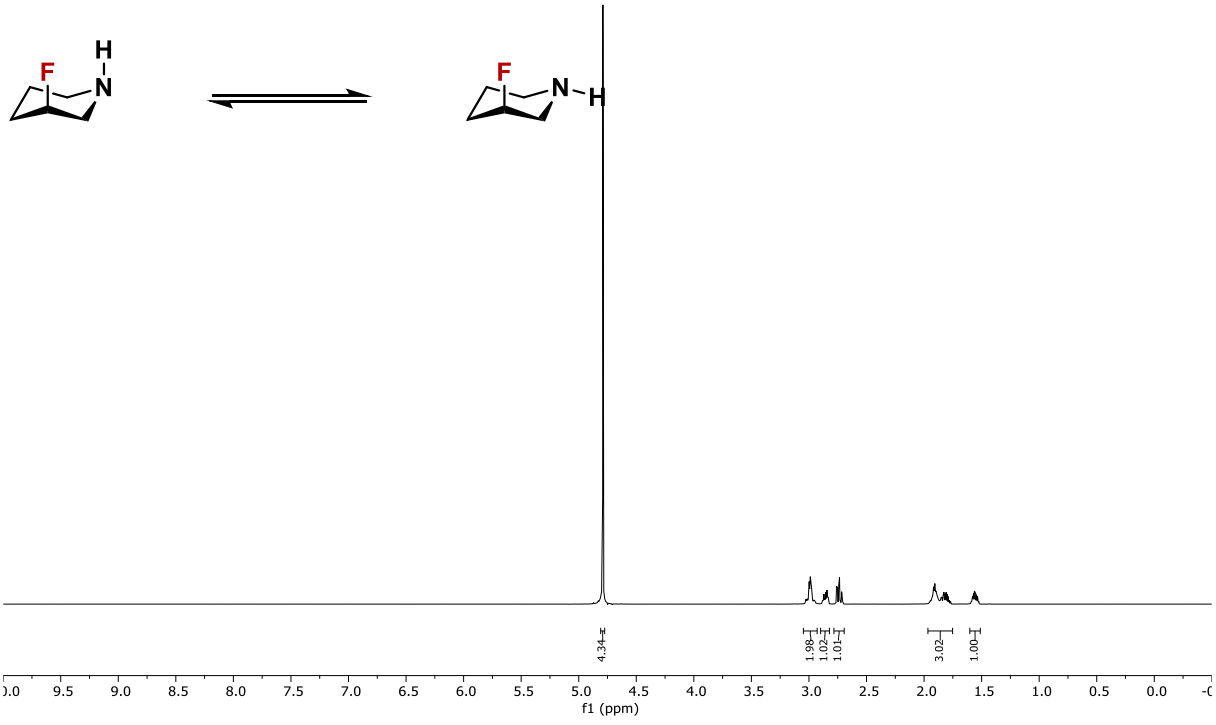
17_e, Water

C	-2.25990661543665	0.76647681419087	-0.87907795609433
C	-2.74125254367206	-0.60040116642493	-0.41483770210174
C	-0.86737661926818	1.10063782239035	-0.36413944022078
H	-2.97656800542397	1.53678482992239	-0.58419848137151
F	-2.22840070790796	0.75026875881314	-2.26942388283056
N	-2.64978163909962	-0.67381466506682	1.03640660364325
H	-2.10119971048229	-1.37210092942281	-0.84949264935733
H	-3.76685605568031	-0.76997741290036	-0.72467992807677
C	-0.80908464513914	0.88266718733744	1.14077735321576
C	-1.30236068642856	-0.49834956669058	1.54460380601619
H	-1.38457884720799	1.64997629198094	1.66567151161280
F	0.51052101324931	0.99617280238350	1.55937593955548
C	-0.46143350397754	2.51897008920827	-0.73477822196650
H	-0.17841897719578	0.37877443185442	-0.81693785904850
H	-1.16036467082776	3.23645876651007	-0.29981504571034
H	-0.46117012601199	2.65148608966034	-1.81545258313194
H	0.53679394510056	2.74328594625460	-0.36238385202653
H	-1.26120304394298	-0.60775525801992	2.62132268528610
H	-0.65835569758870	-1.25884459786242	1.09692030815375
C	-3.75581891532618	-0.88687870845576	1.75984282269324
O	-4.86936762353586	-1.02839932426249	1.30460970611822
C	-3.60795660372487	-0.96671650013582	3.30409257115482
F	-2.81797108532256	-1.97812536419977	3.67280945666930
F	-4.79558833369448	-1.16154834231113	3.85254103345760
F	-3.10376030145440	0.16178200524647	3.81168380436035

^{1}H NMR

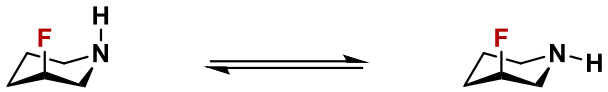


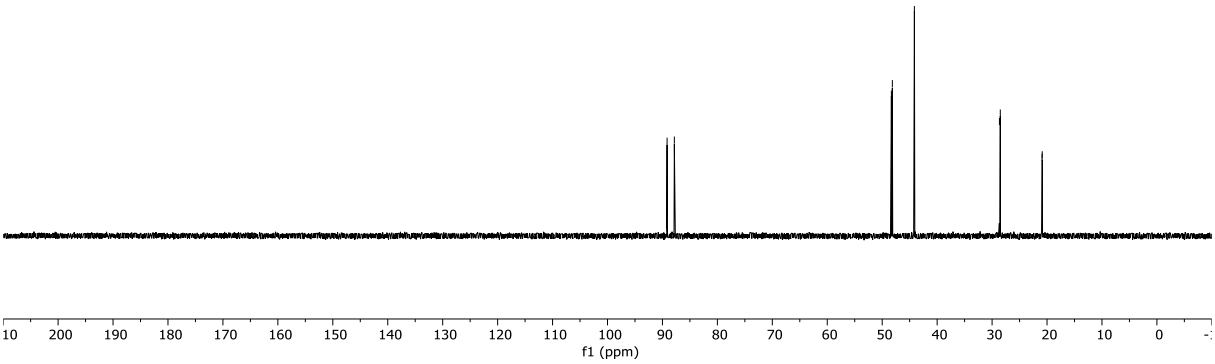
^{1}H{^{19}F} NMR



89.15
87.83
48.33
48.15
44.14
28.66
28.50
20.90
20.87

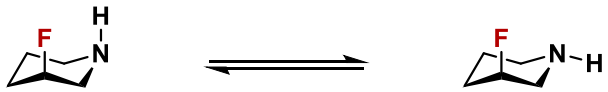
^{13}C NMR

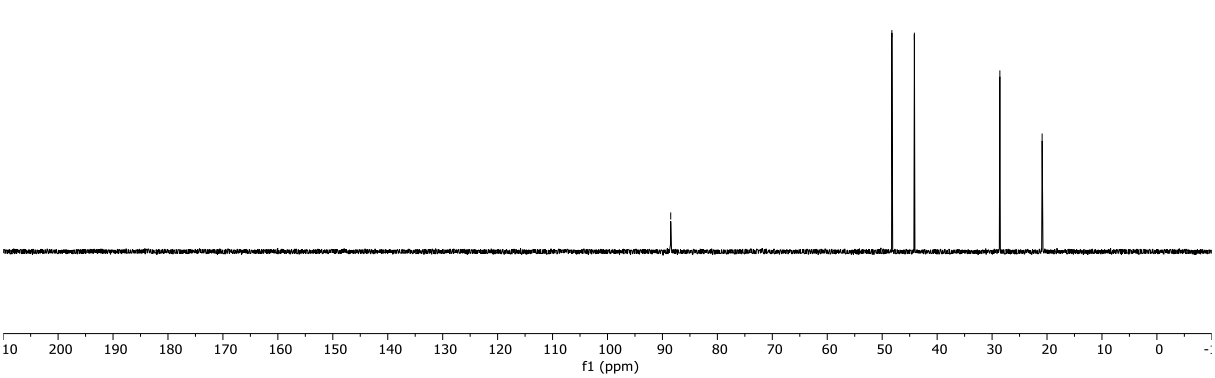




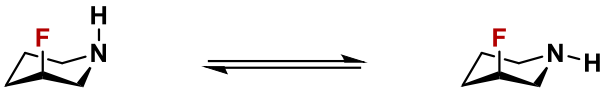
88.49
48.24
44.14
28.58
20.89

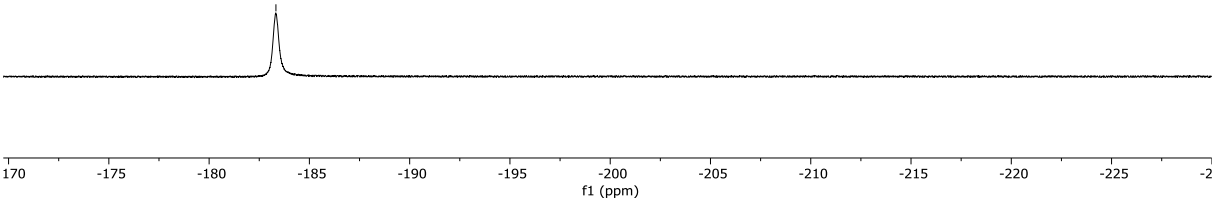
$^{13}C\{^{19}F\}$ NMR



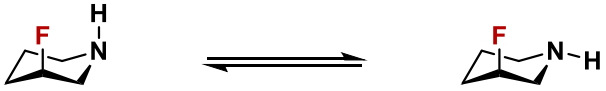


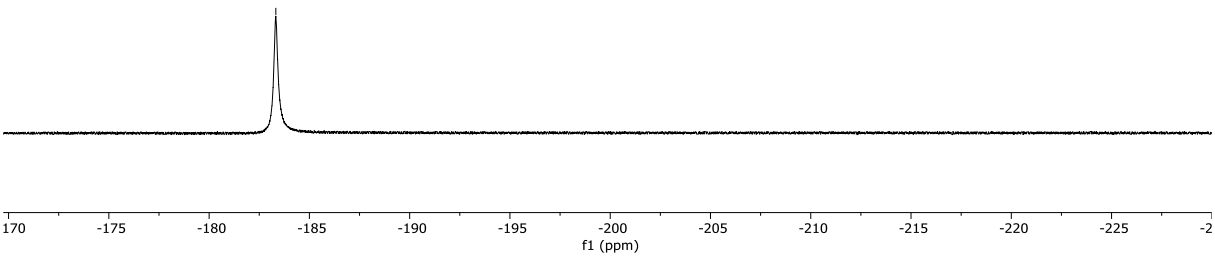
^{19}F NMR





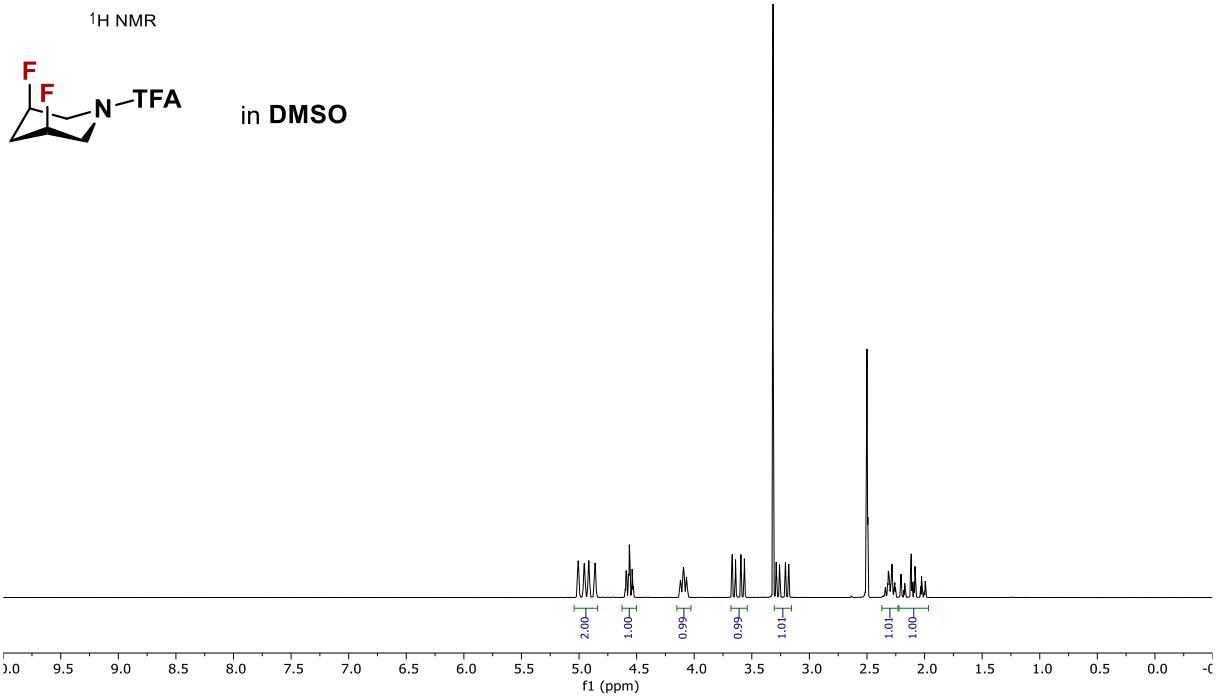
^{19}F{^{1}H} NMR



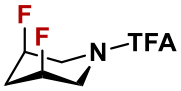


^{1}H NMR

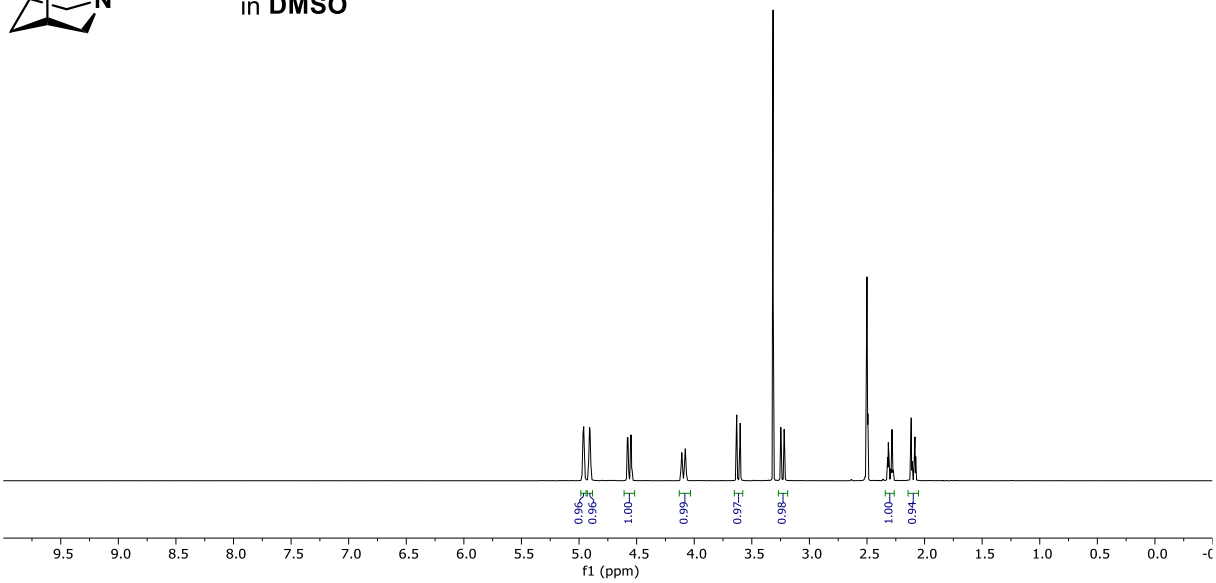
in **DMSO**



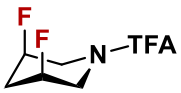
^{1}H{^{19}F} NMR



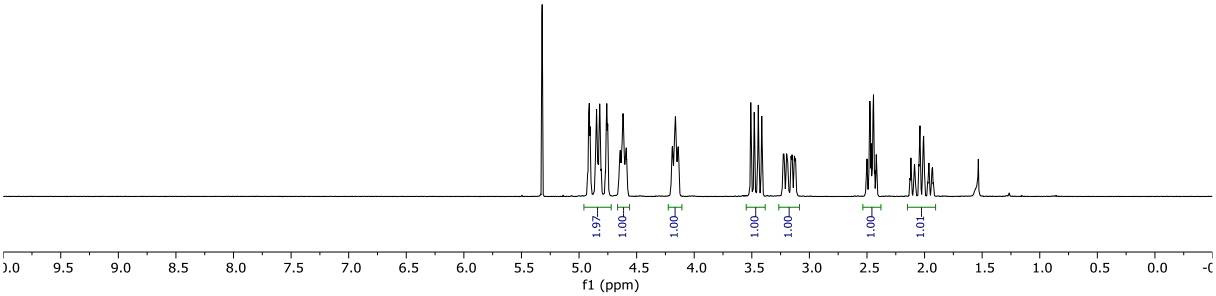
in **DMSO**



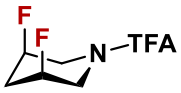
^{1}H NMR



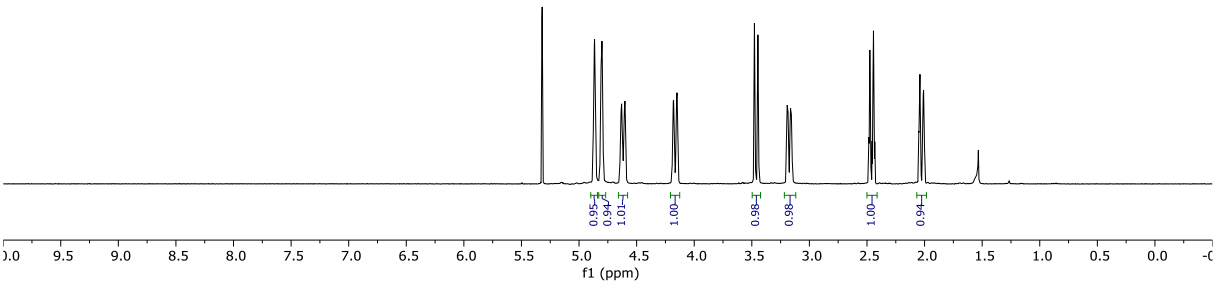
in CD_2Cl_2



^{1}H{^{19}F} NMR

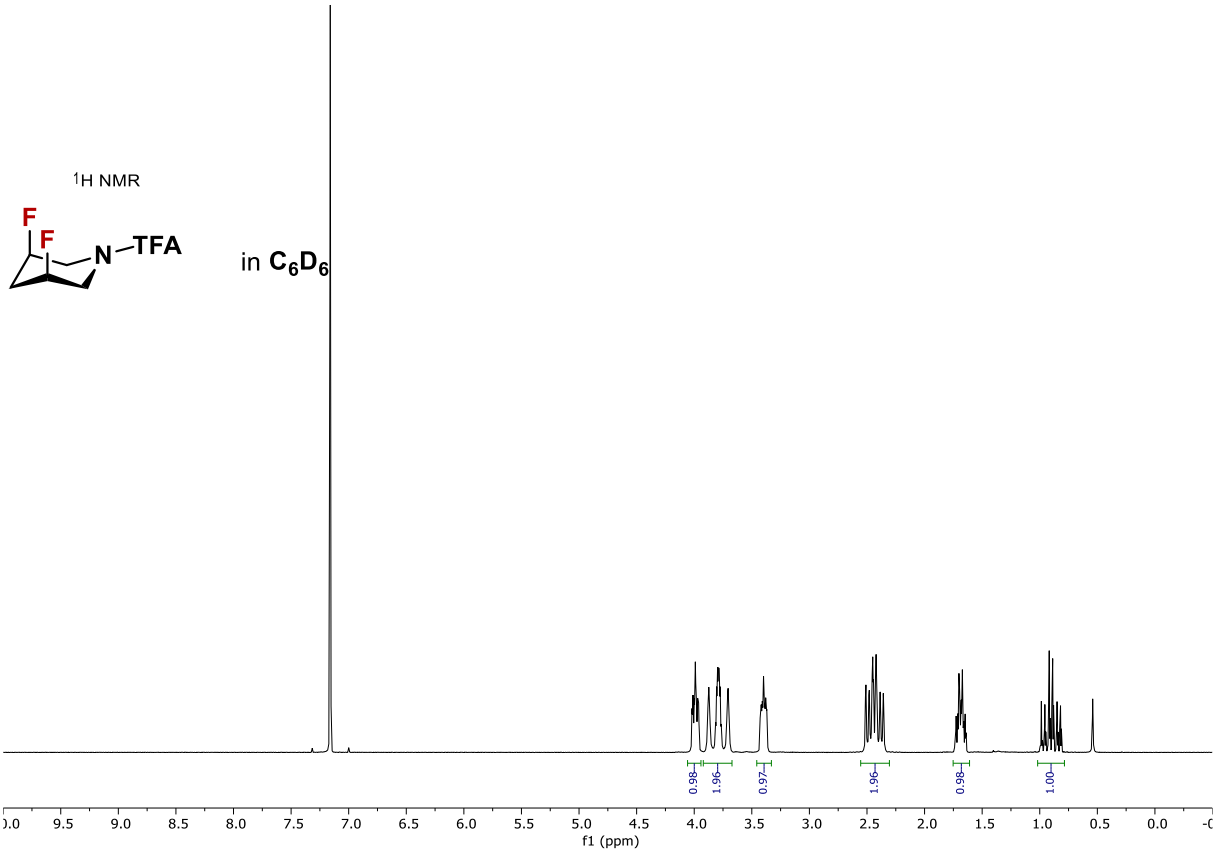


in CD_2Cl_2

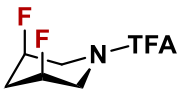


^{1}H NMR

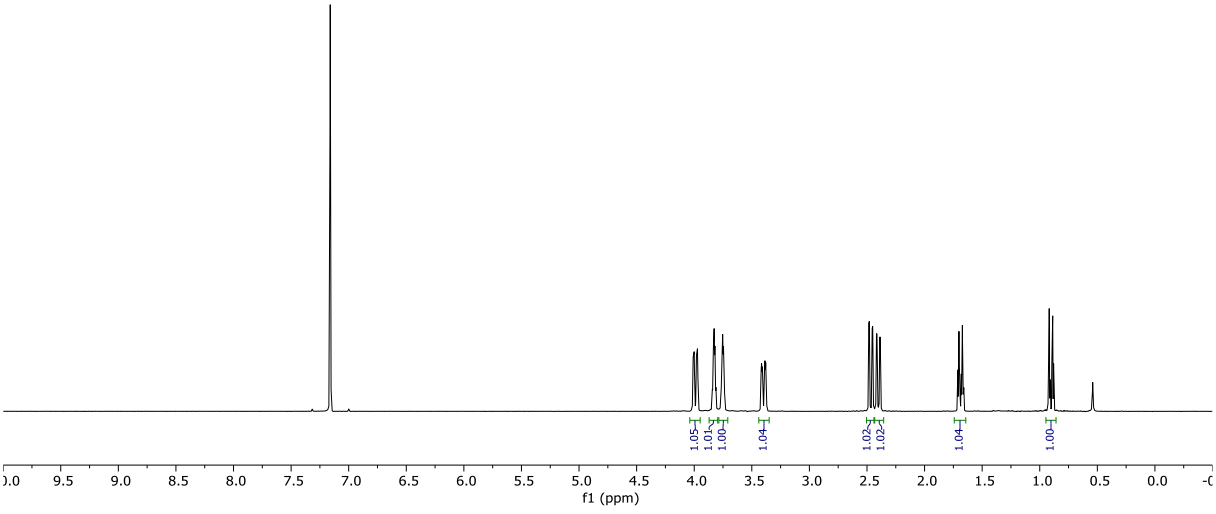
in C_6D_6



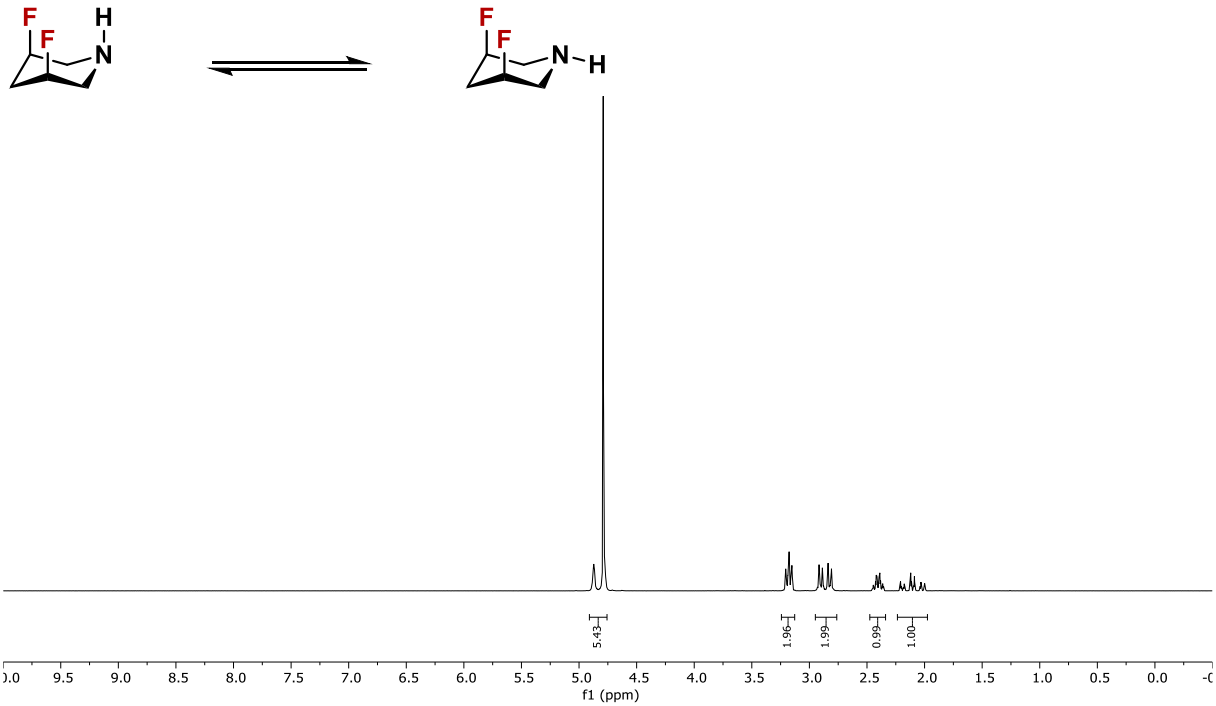
^{1}H{^{19}F} NMR



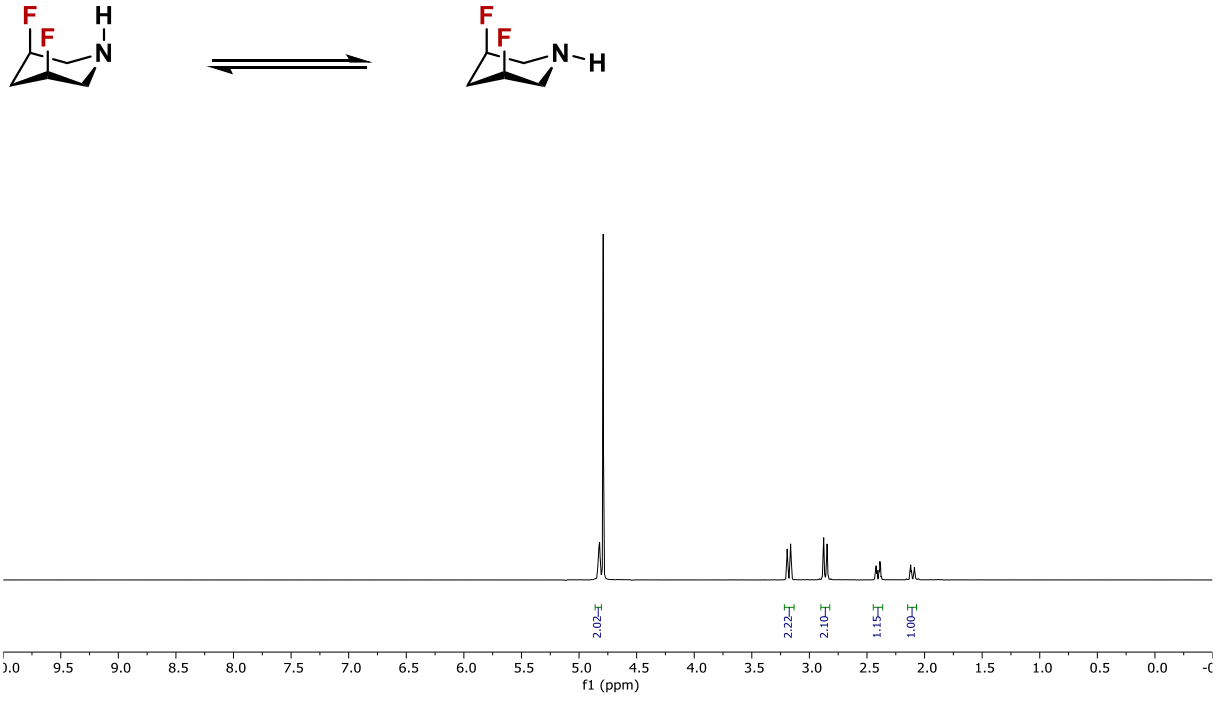
in C_6D_6



^{1}H NMR

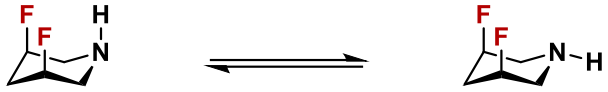


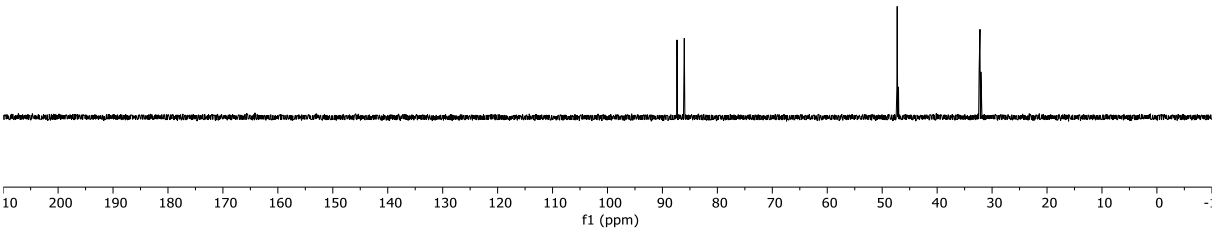
^{1}H{^{19}F} NMR



87.35
86.01
47.34
47.27
47.22
47.15
47.10
47.04
32.36
32.20
32.04

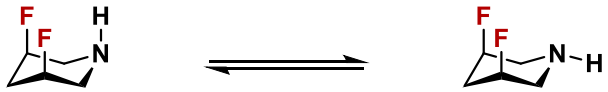
^{13}C NMR

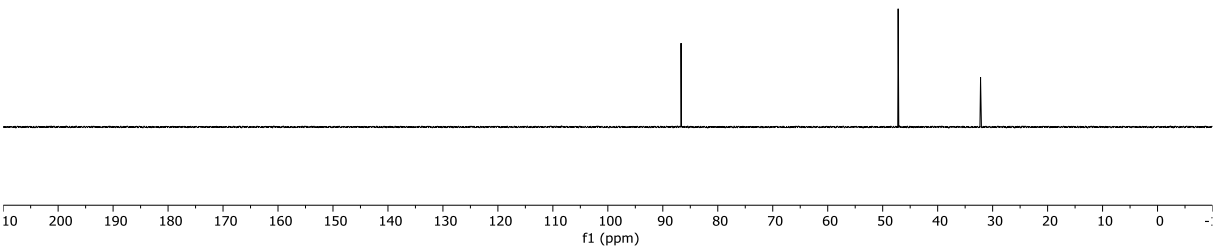




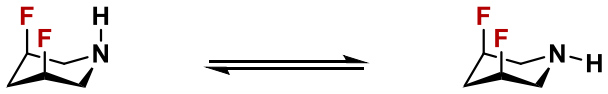
86.68
47.19
32.20

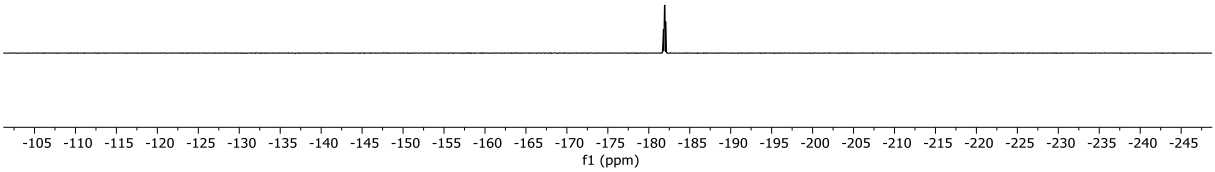
$^{13}C\{^{19}F\}$ NMR



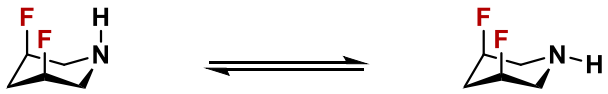


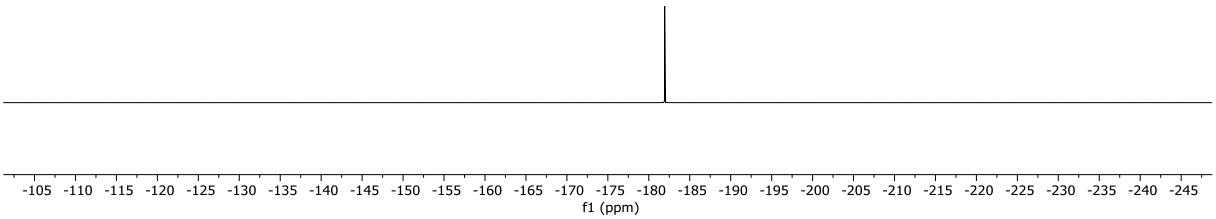
^{19}F NMR



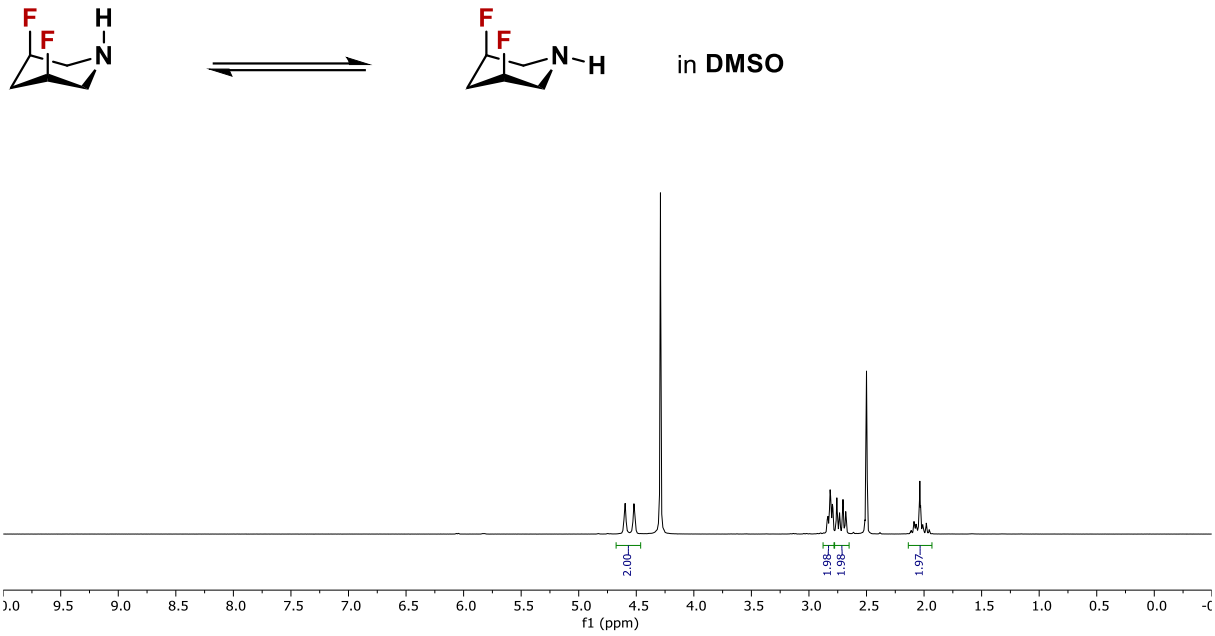


^{19}F{^{1}H} NMR

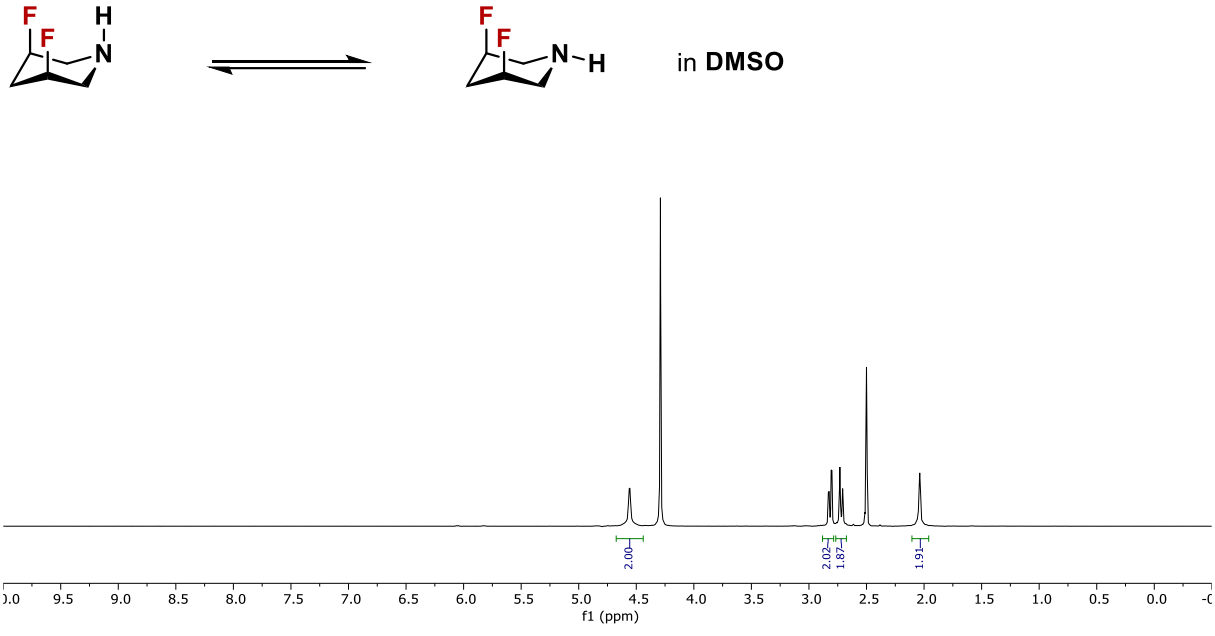




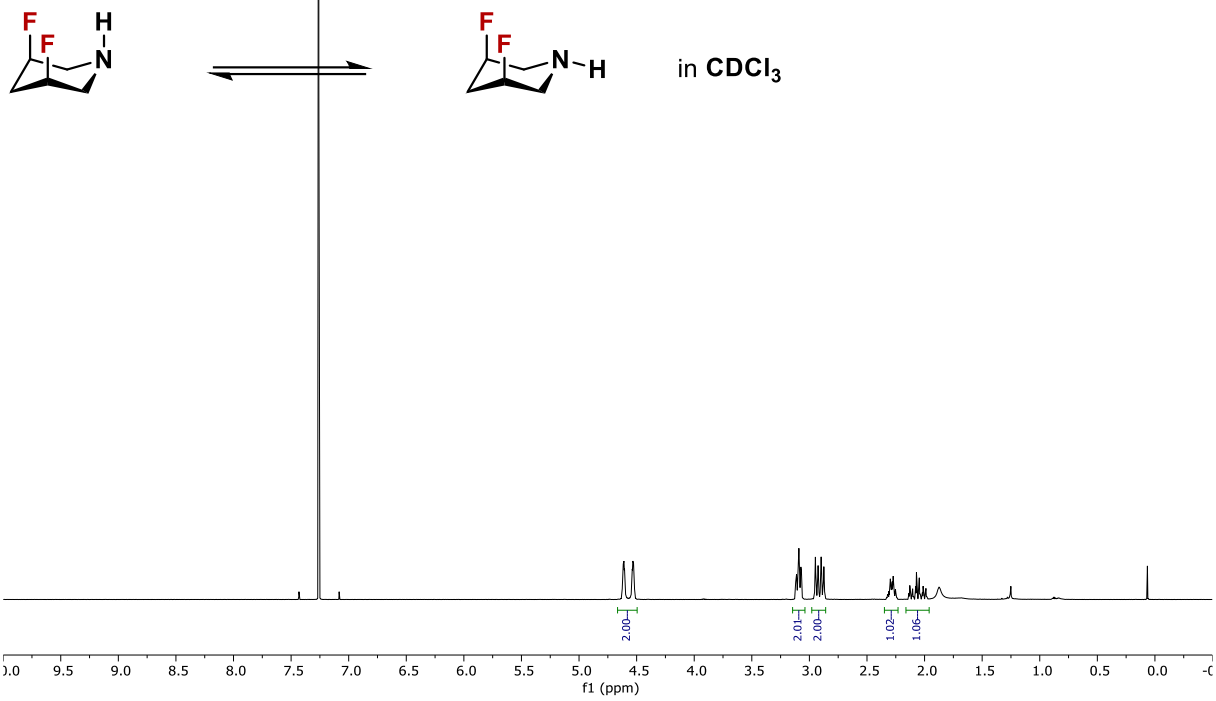
^{1}H NMR



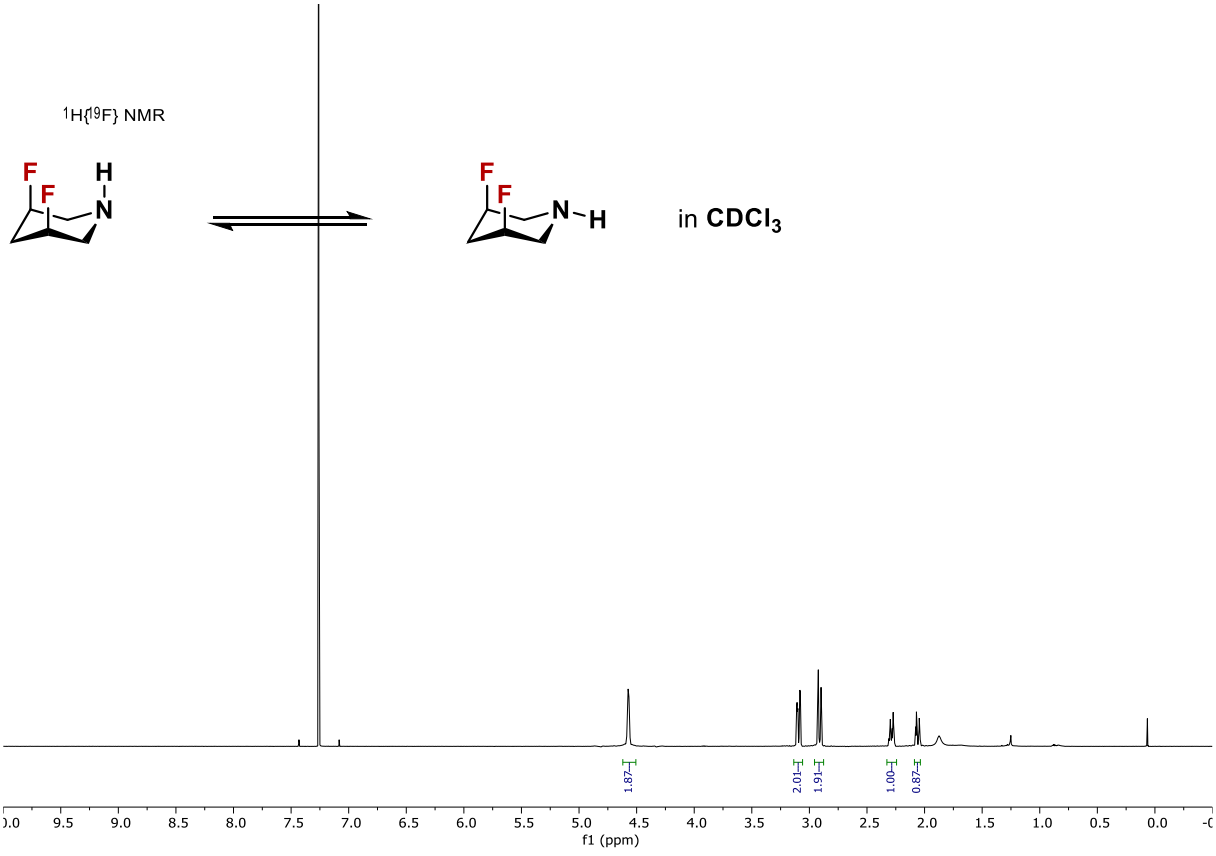
^{1}H{^{19}F} NMR



^{1}H NMR

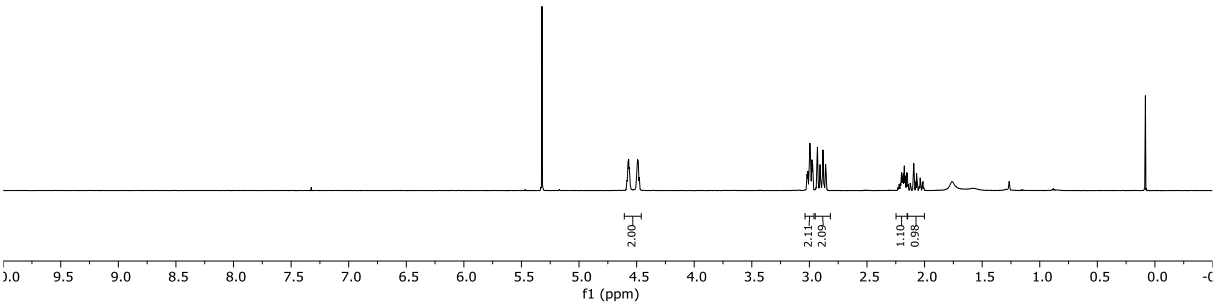


^{1}H{^{19}F} NMR



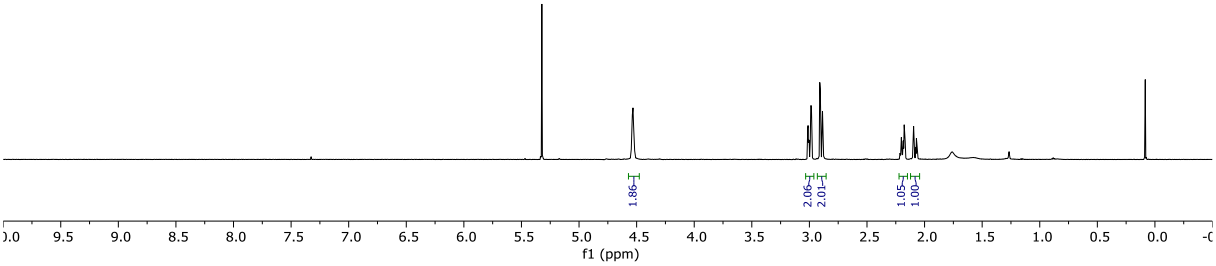
^{1}H NMR

in CD_2Cl_2

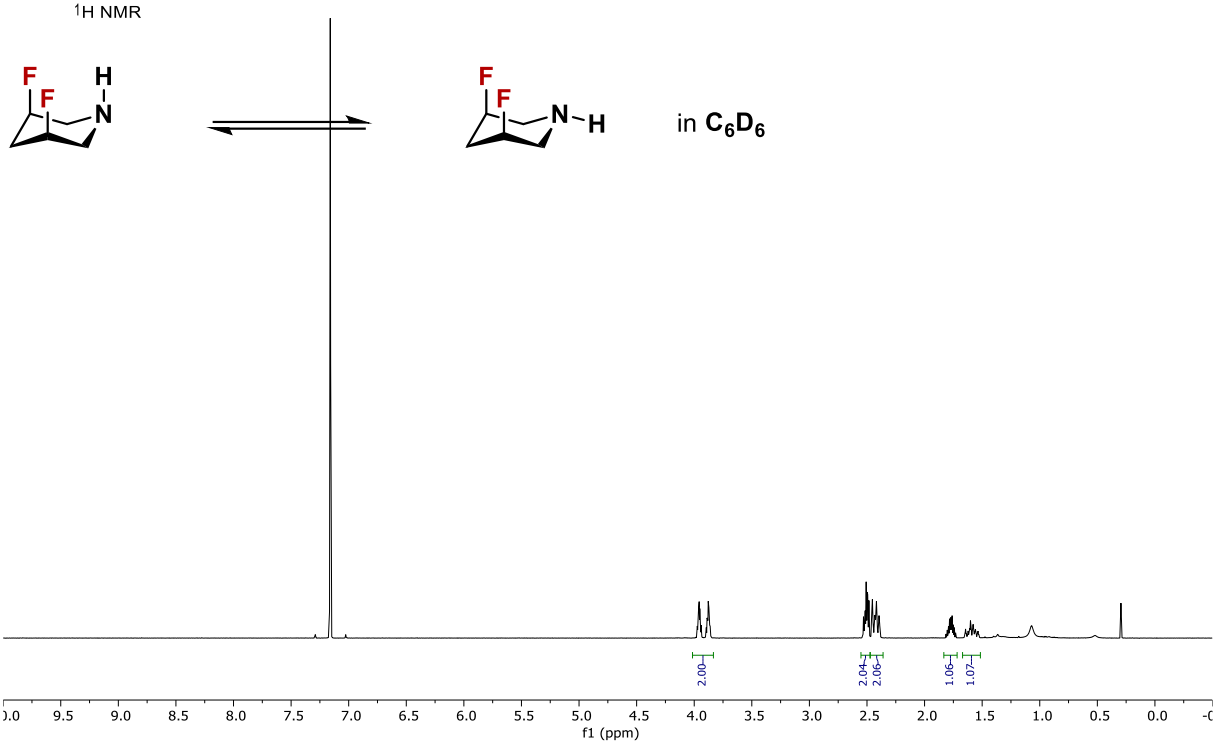


^{1}H{^{19}F} NMR

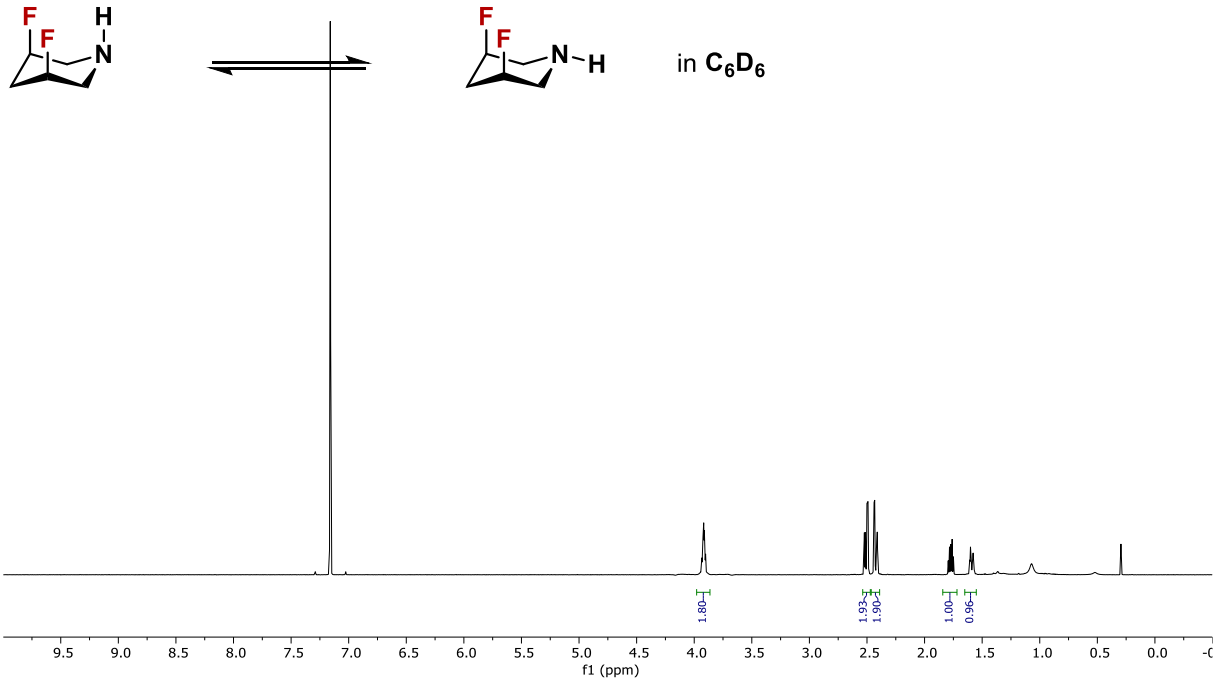
in CD_2Cl_2



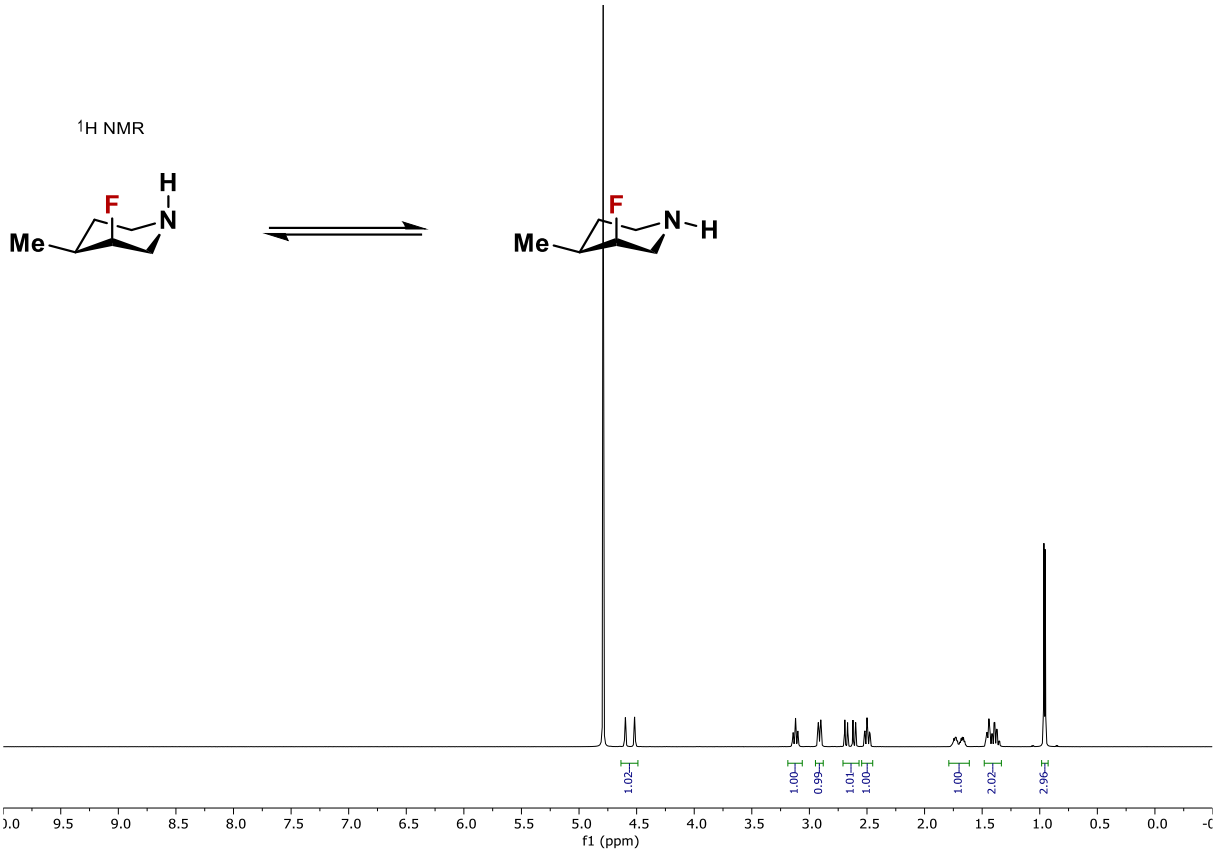
^{1}H NMR



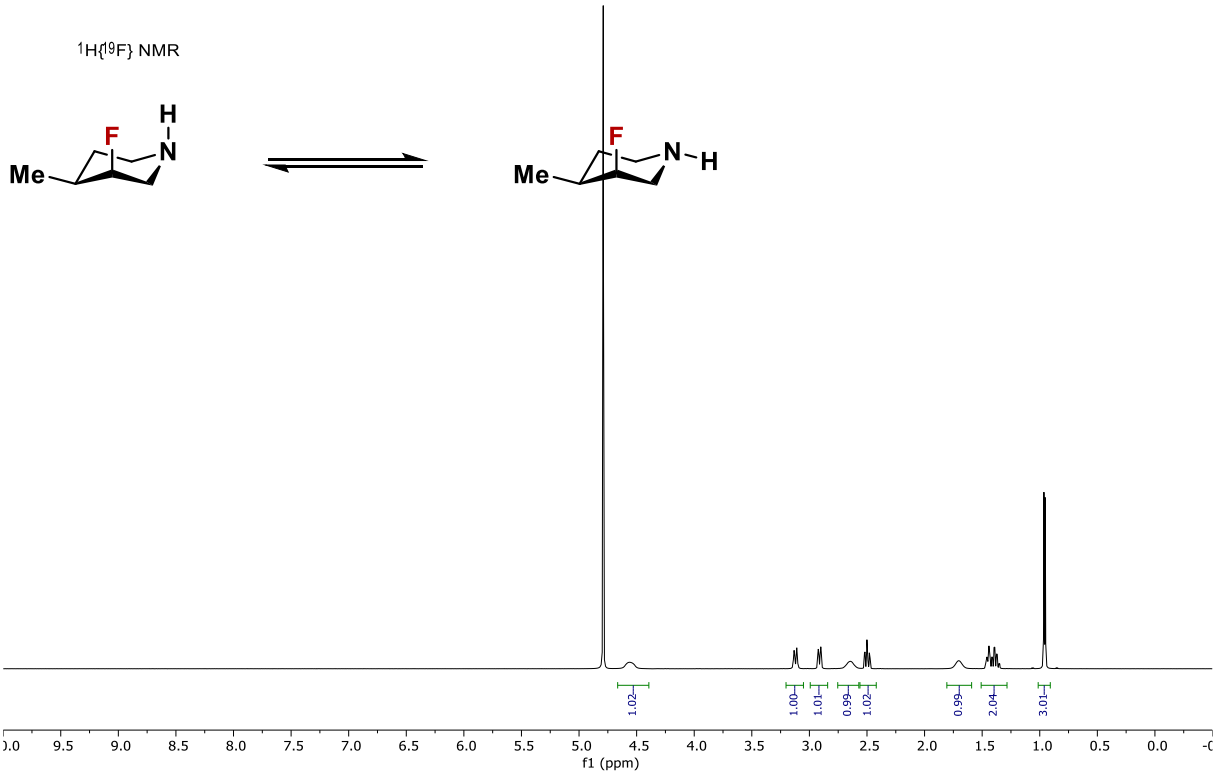
^{1}H{^{19}F} NMR



^{1}H NMR

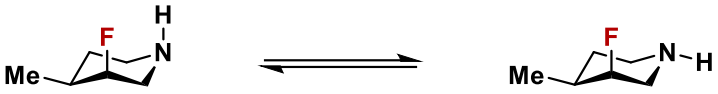


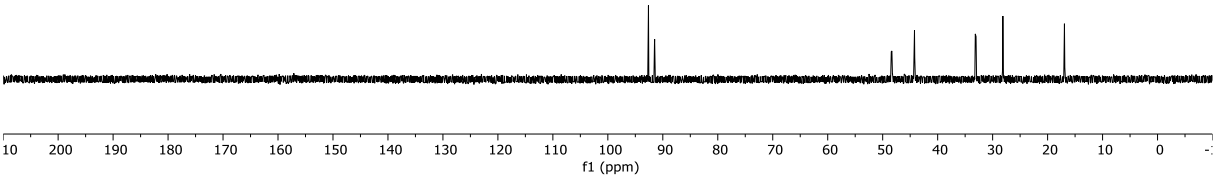
^{1}H{^{19}F} NMR



92.61
91.48
48.46
48.43
48.38
48.32
48.30
44.21
33.15
33.02
28.13
16.93

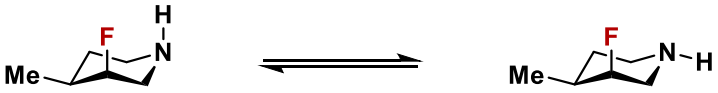
^{13}C NMR

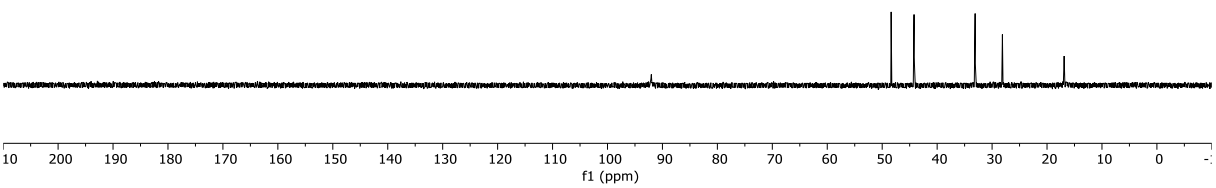




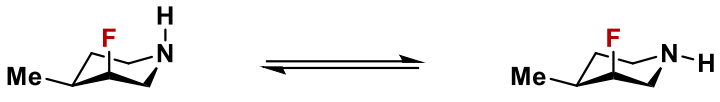
92.02
48.37
44.20
33.08
28.12
16.98

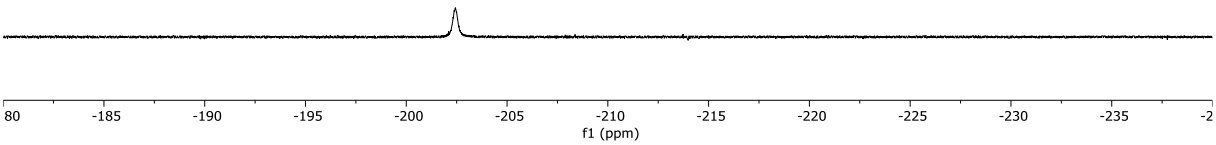
$^{13}C\{^{19}F\}$ NMR



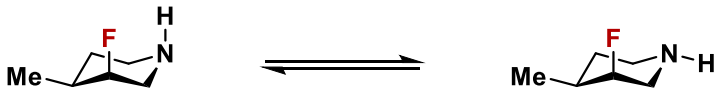


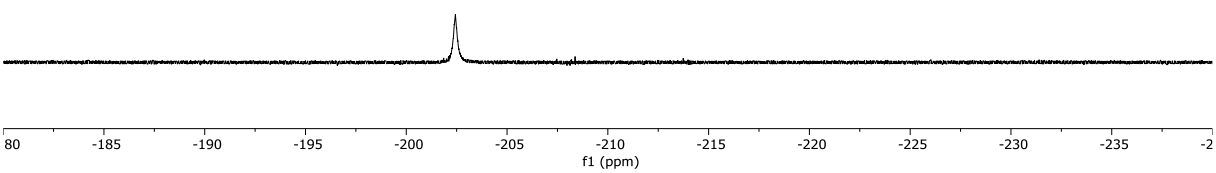
^{19}F NMR



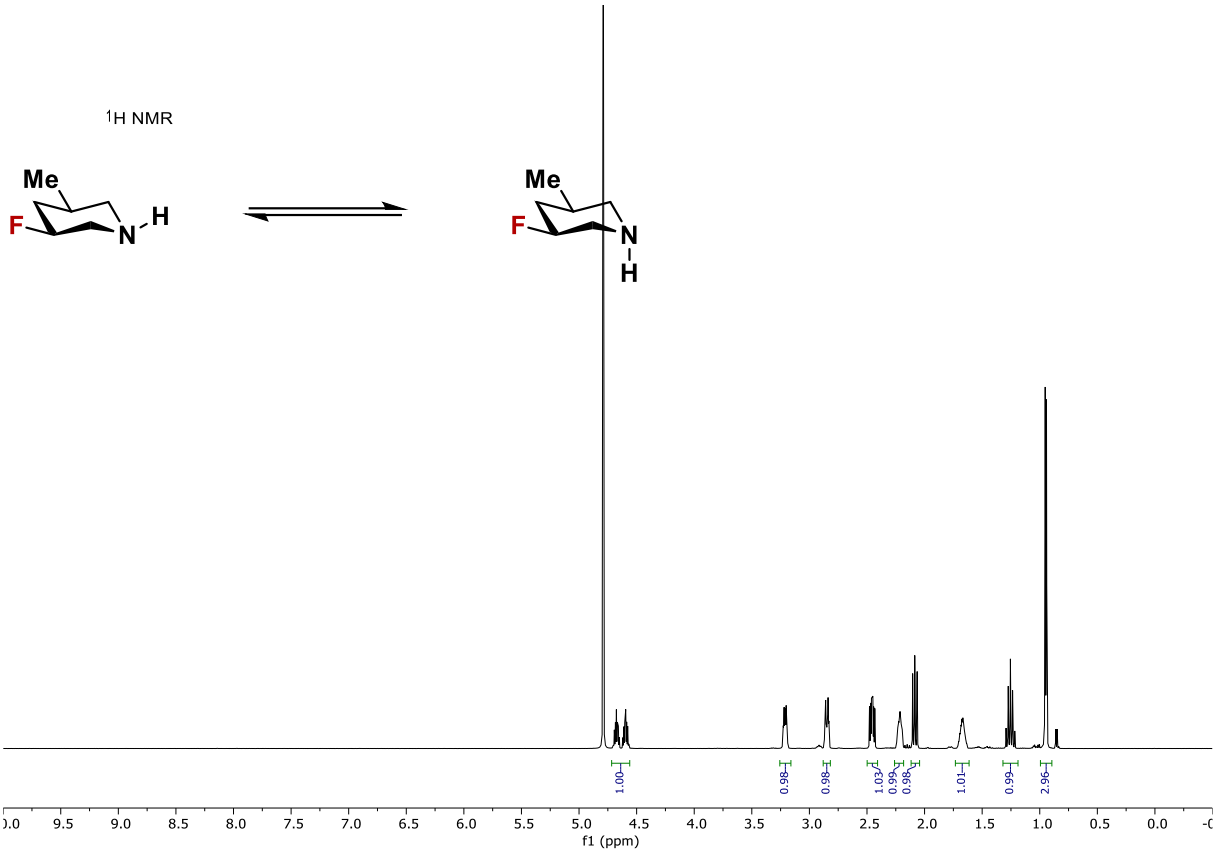


^{19}F{^{1}H} NMR

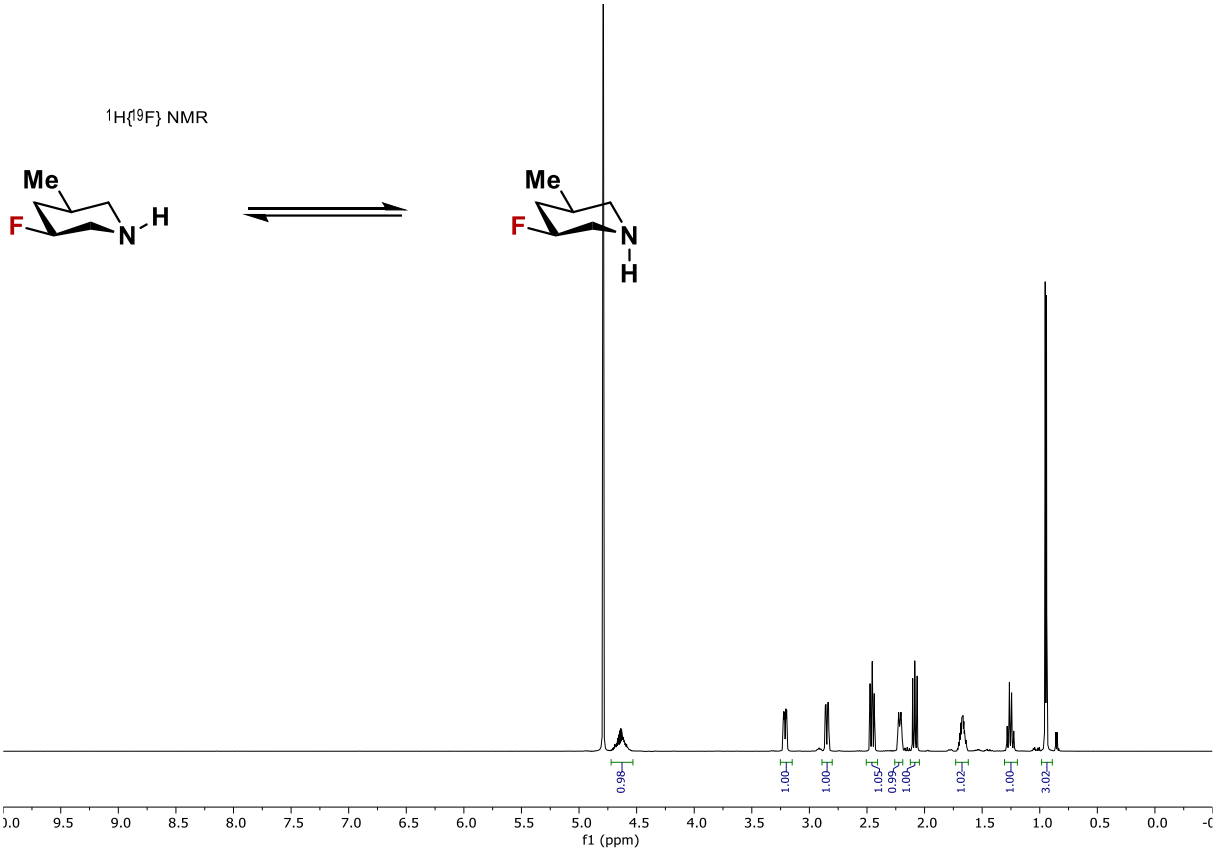




^{1}H NMR

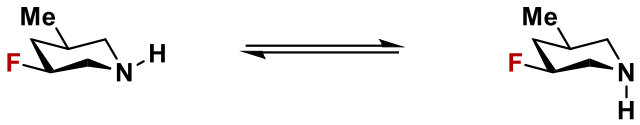


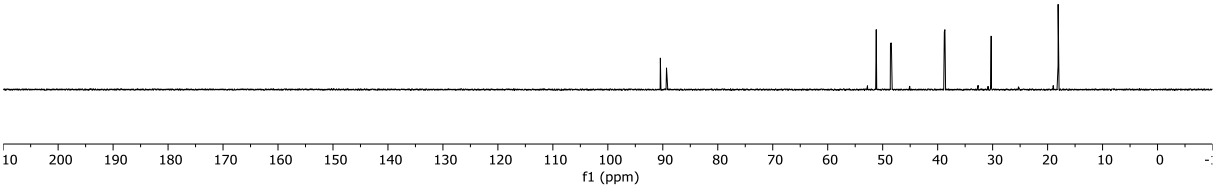
^{1}H{^{19}F} NMR



90.45
89.33
51.18
51.17
48.58
48.42
38.79
38.68
30.33
30.26
18.09
18.08

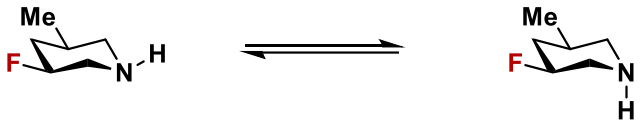
^{13}C NMR

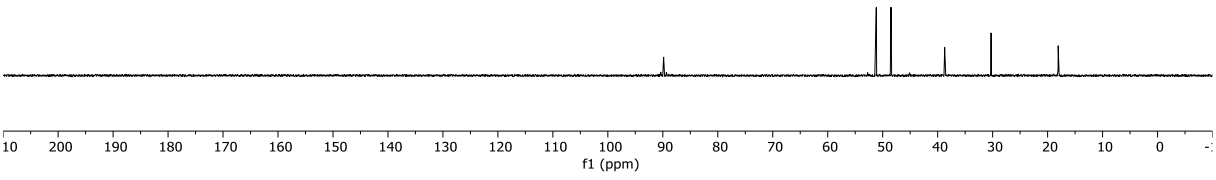




89.85
51.16
48.49
38.72
30.28
18.07

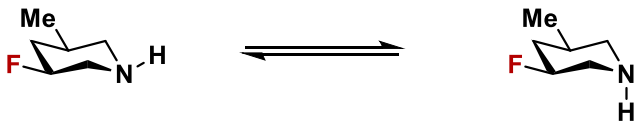
$^{13}C\{^{19}F\}$ NMR

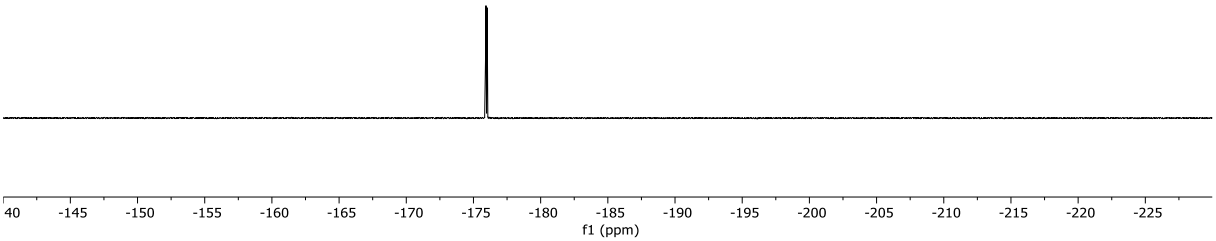




-175.92
-175.93
-176.01
-176.02

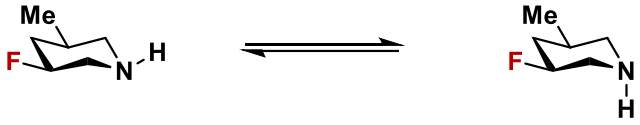
^{19}F NMR

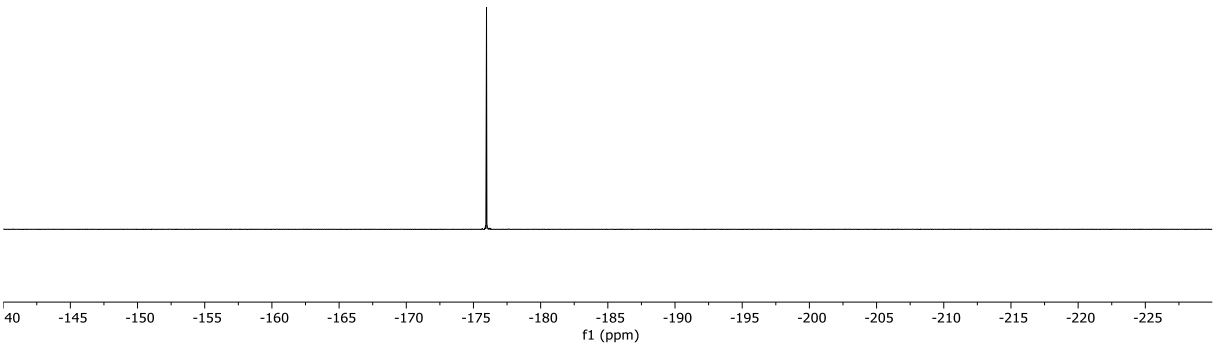




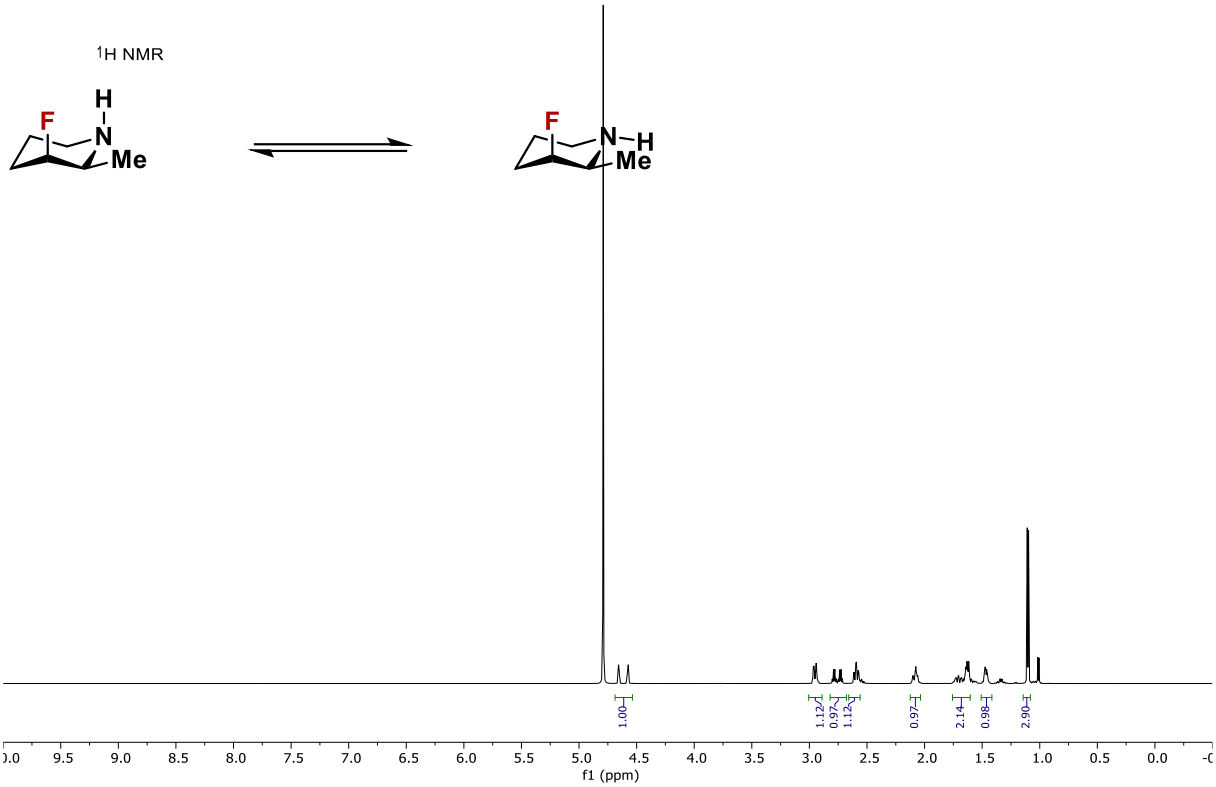
-175.97

^{19}F{^{1}H} NMR

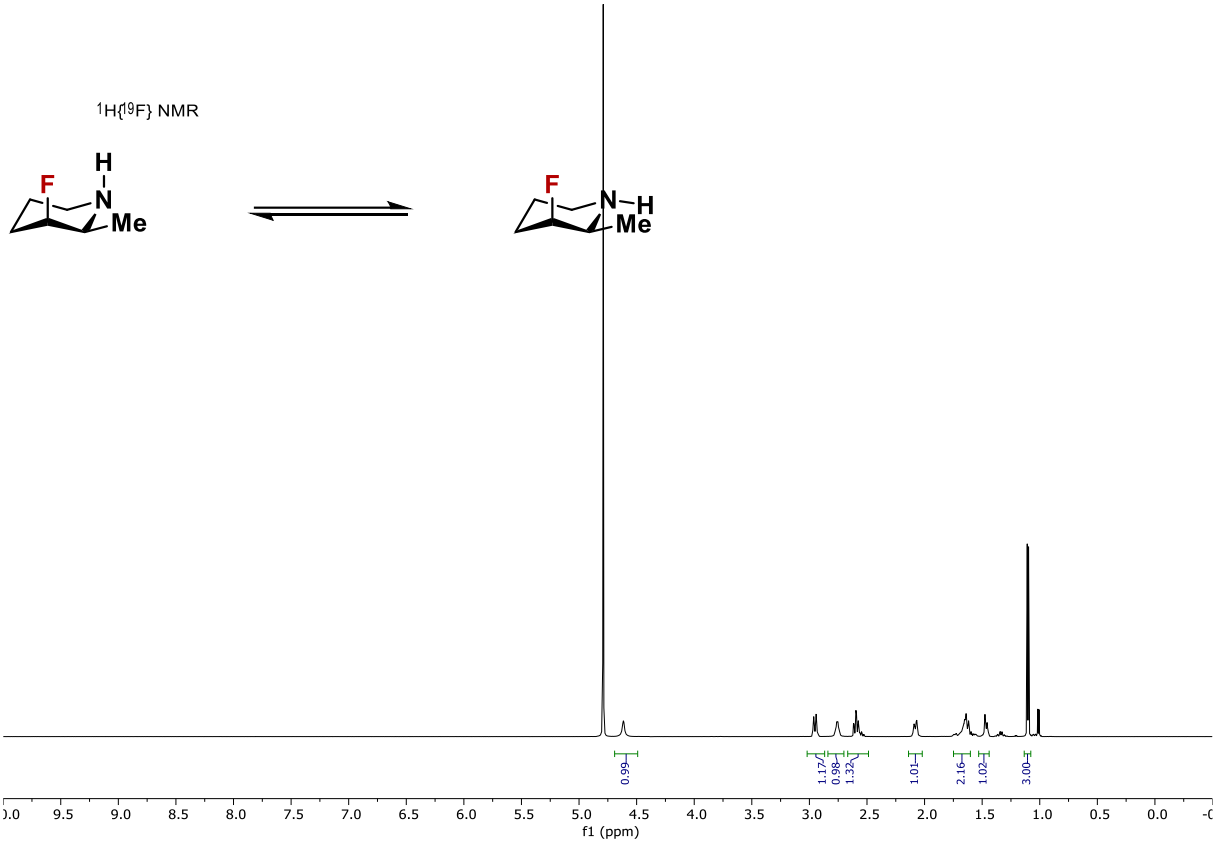




^{1}H NMR

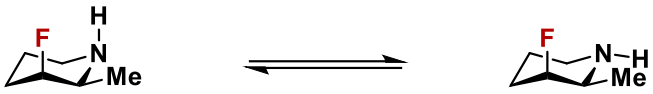


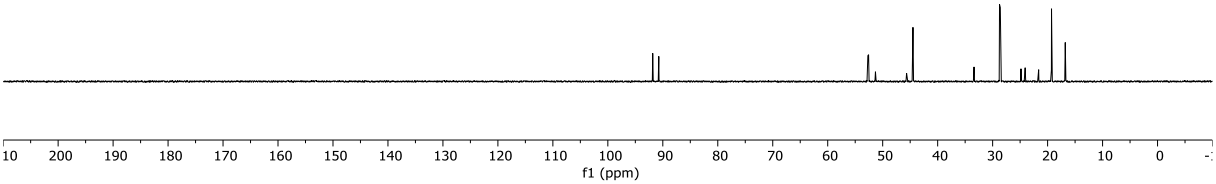
^{1}H{^{19}F} NMR



91.83
90.73
52.69
52.57
44.49
28.75
28.61
19.29
16.79
16.76

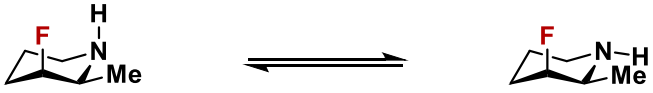
^{13}C NMR

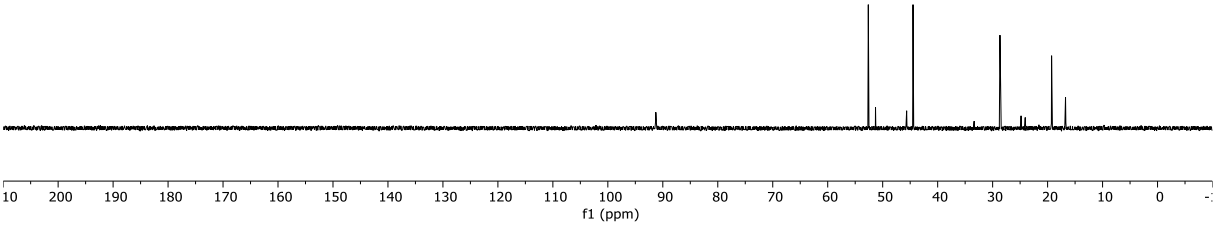




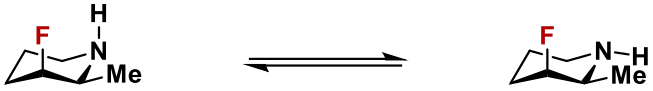
91.27
52.62
44.48
28.67
19.27
16.74

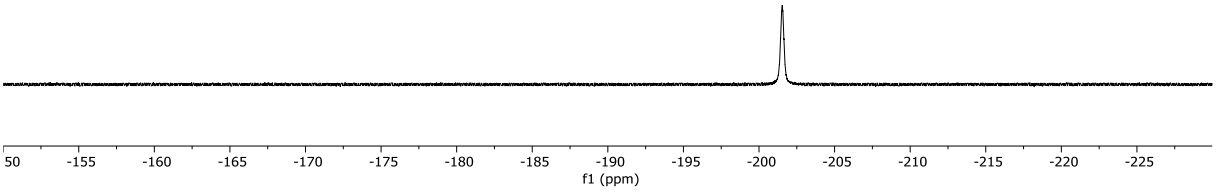
$^{13}C\{^{19}F\}$ NMR



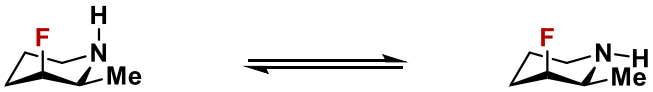


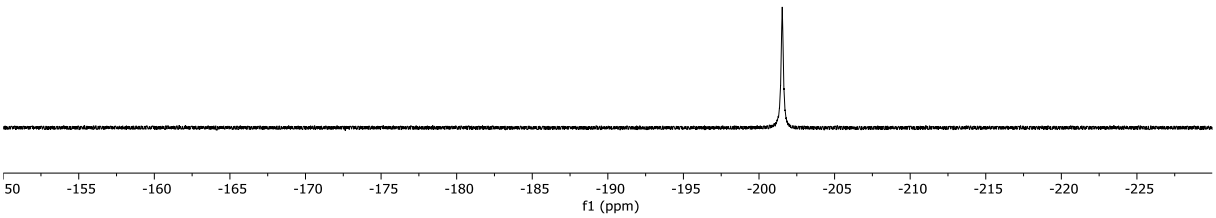
^{19}F NMR



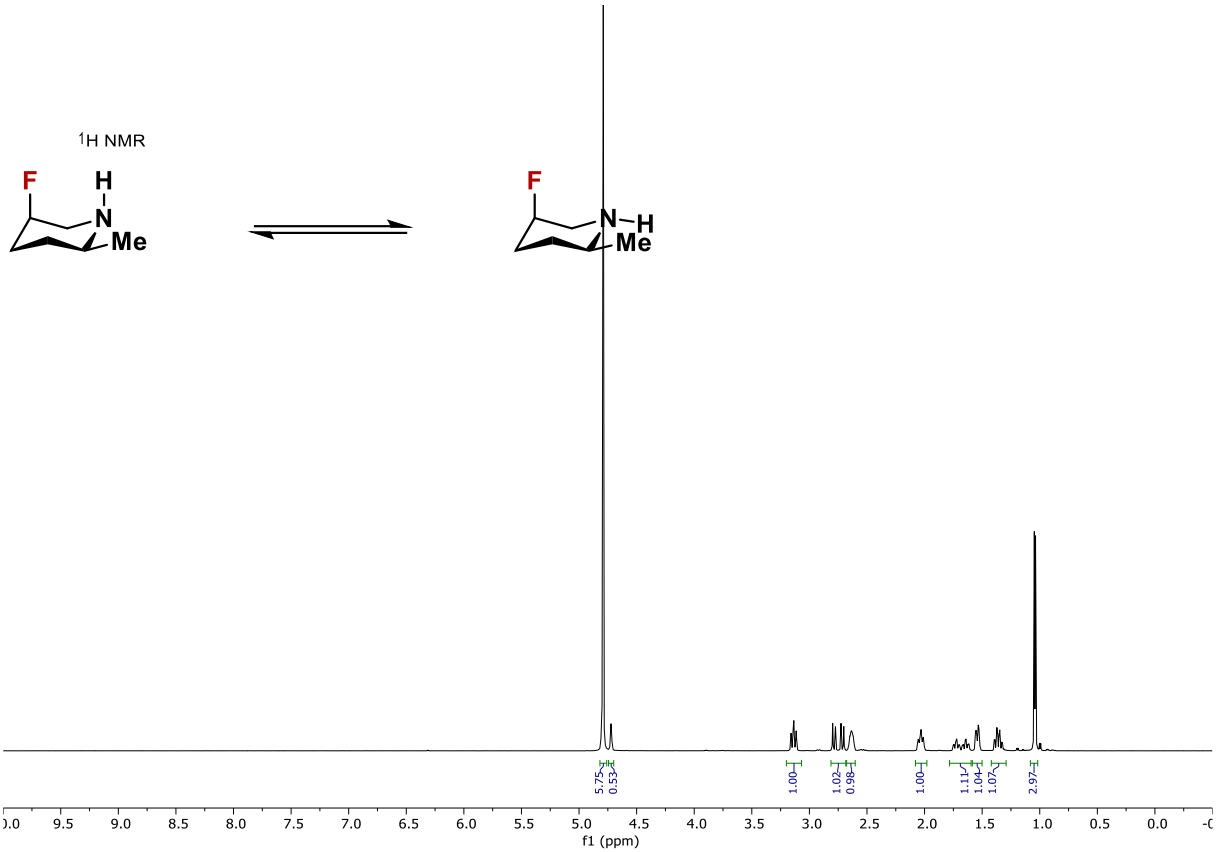


^{19}F{^{1}H} NMR

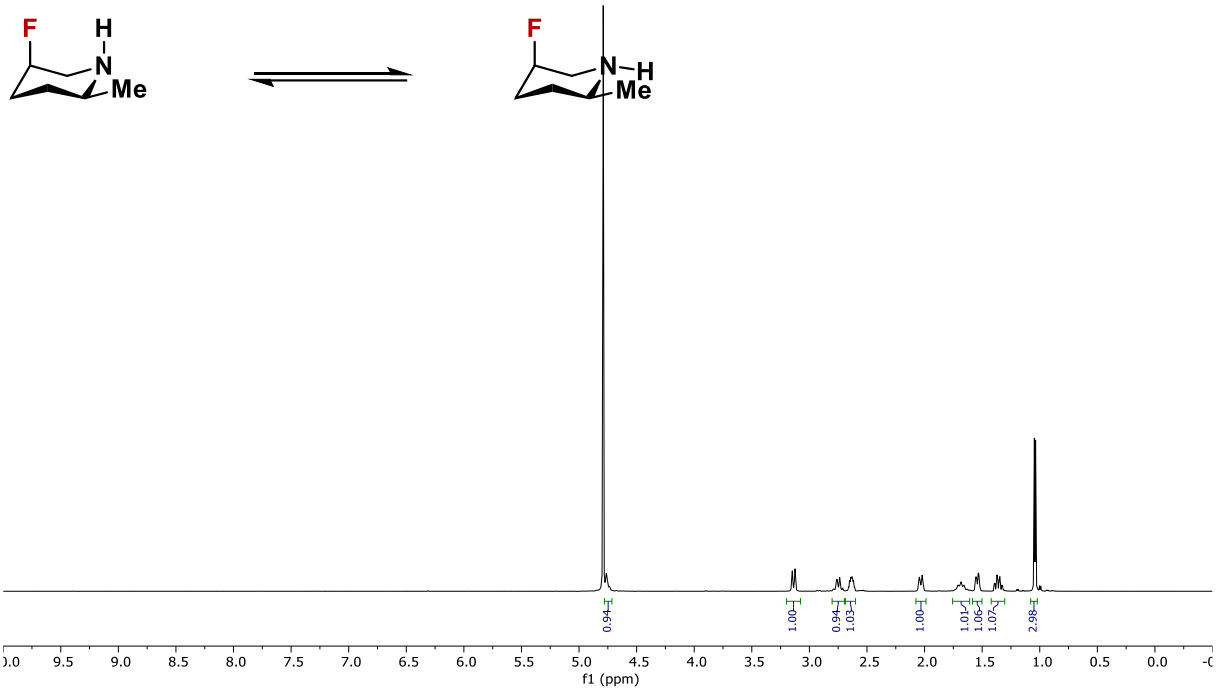




^{1}H NMR

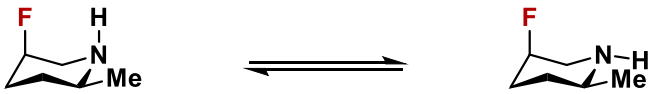


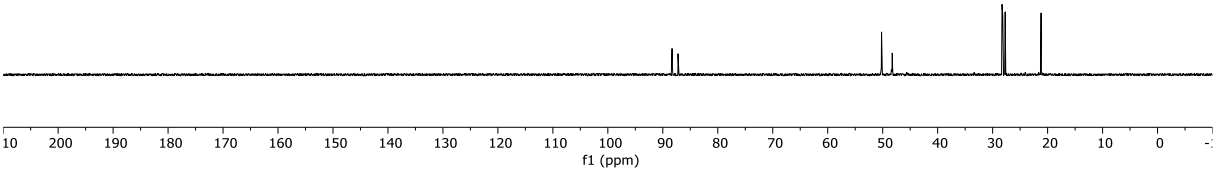
^{1}H{^{19}F} NMR



88.32
87.23
50.21
48.41
48.39
48.38
48.28
48.26
48.24
48.22
28.29
28.15
27.71
21.19

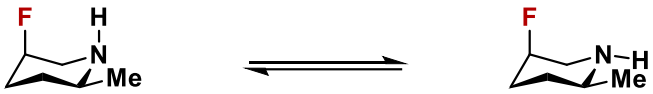
^{13}C NMR

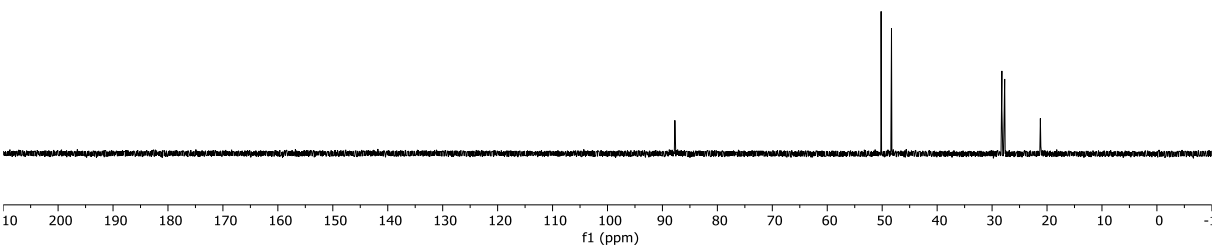




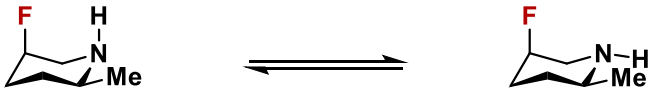
87.74
50.20
48.31
28.21
27.70
21.14

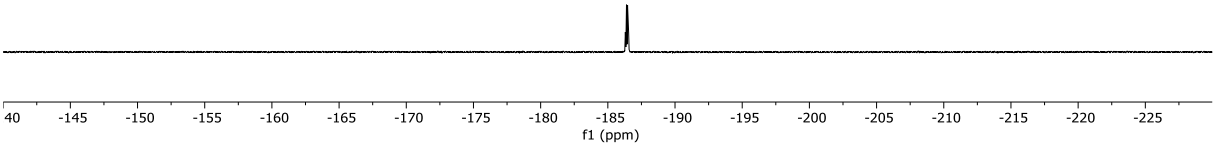
$^{13}C\{^{19}F\}$ NMR



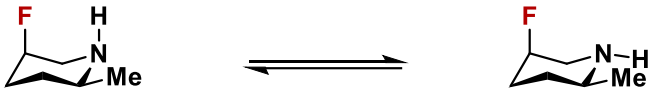


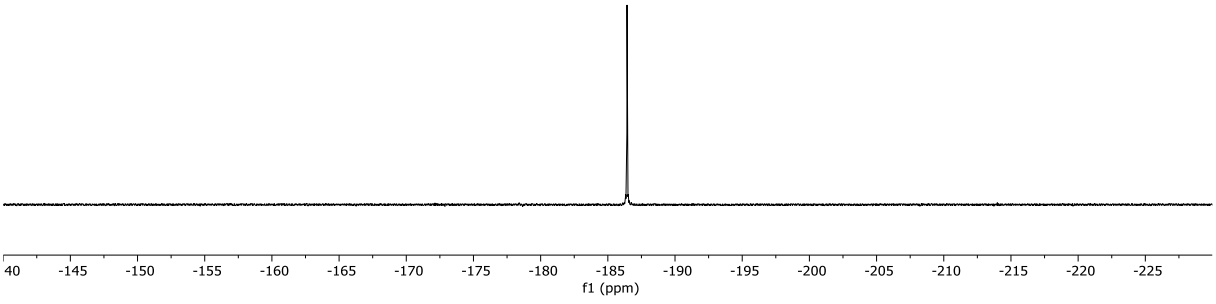
^{19}F NMR



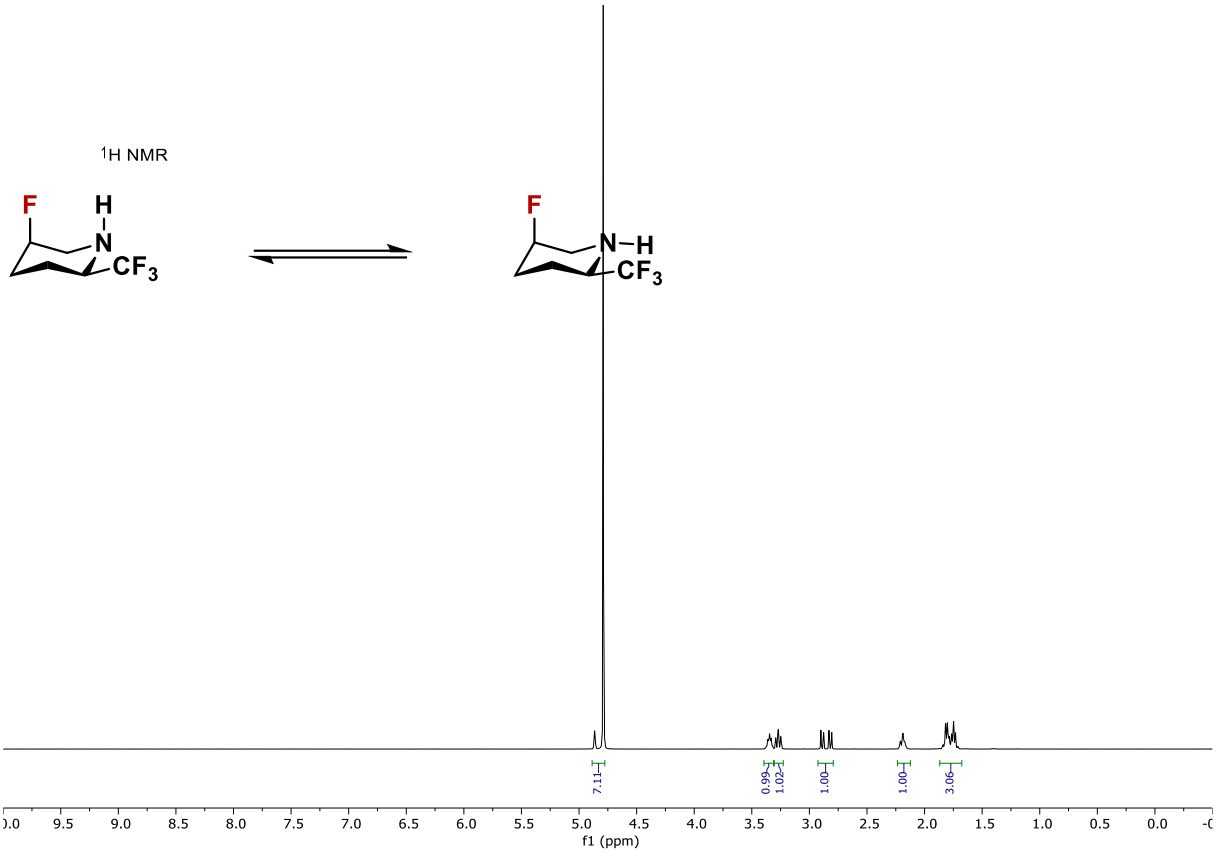


^{19}F{^{1}H} NMR

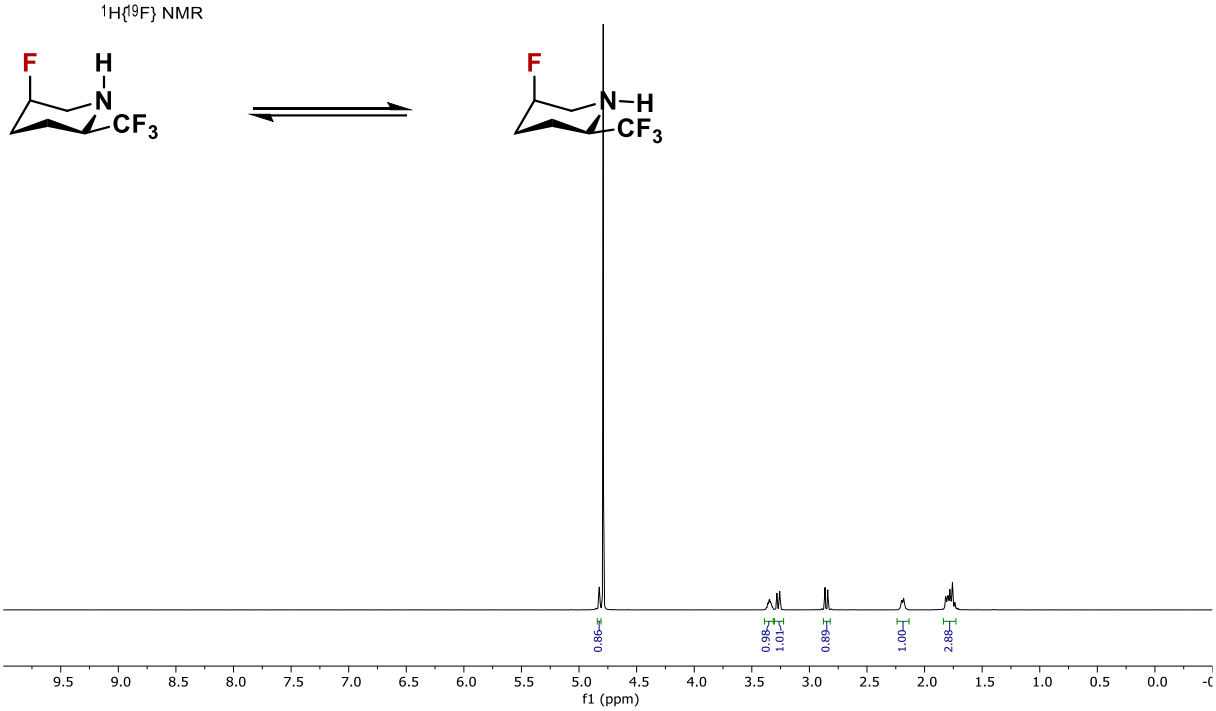




^{1}H NMR

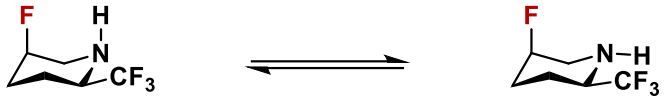


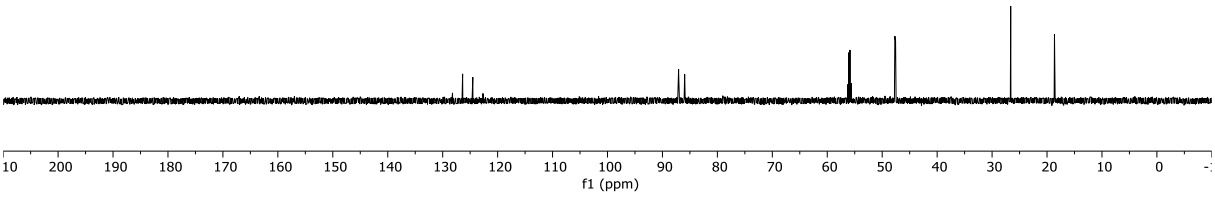
^{1}H{^{19}F} NMR



128.22
126.37
124.52
122.67
87.06
85.96
56.26
56.06
55.87
55.68
47.70
47.56
26.75
26.61
18.66
18.64

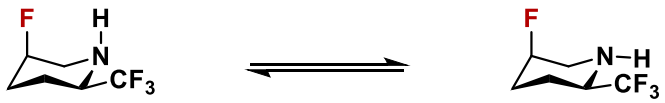
^{13}C NMR

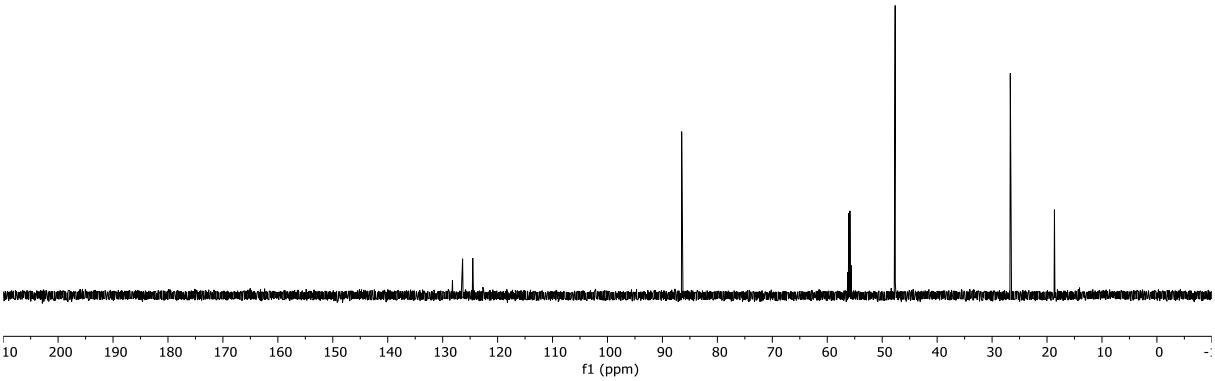




128.22
126.37
124.53
122.68
86.50
56.26
56.07
55.88
55.68
47.64
26.68
18.65

$^{13}C\{^{19}F\}$ NMR

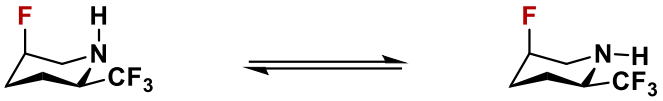


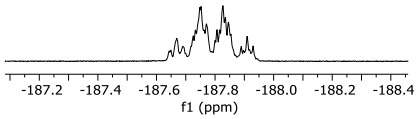


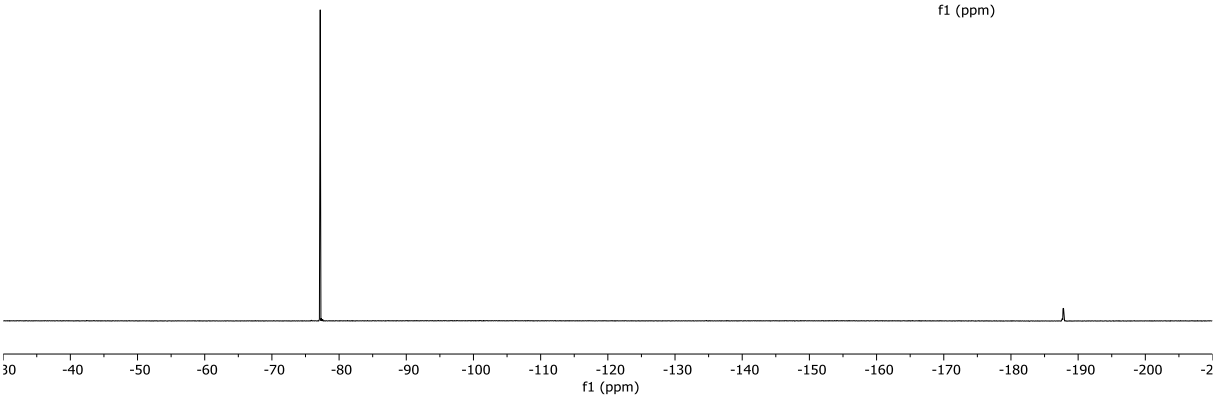
-77.18
-77.19

-187.64
-187.65
-187.66
-187.66
-187.67
-187.67
-187.68
-187.69
-187.69
-187.70
-187.72
-187.72
-187.73
-187.74
-187.75
-187.75
-187.76
-187.77
-187.77
-187.78
-187.80
-187.81
-187.81
-187.82
-187.83
-187.84
-187.85
-187.85
-187.86
-187.87
-187.89
-187.90
-187.91
-187.92
-187.93

^{19}F NMR



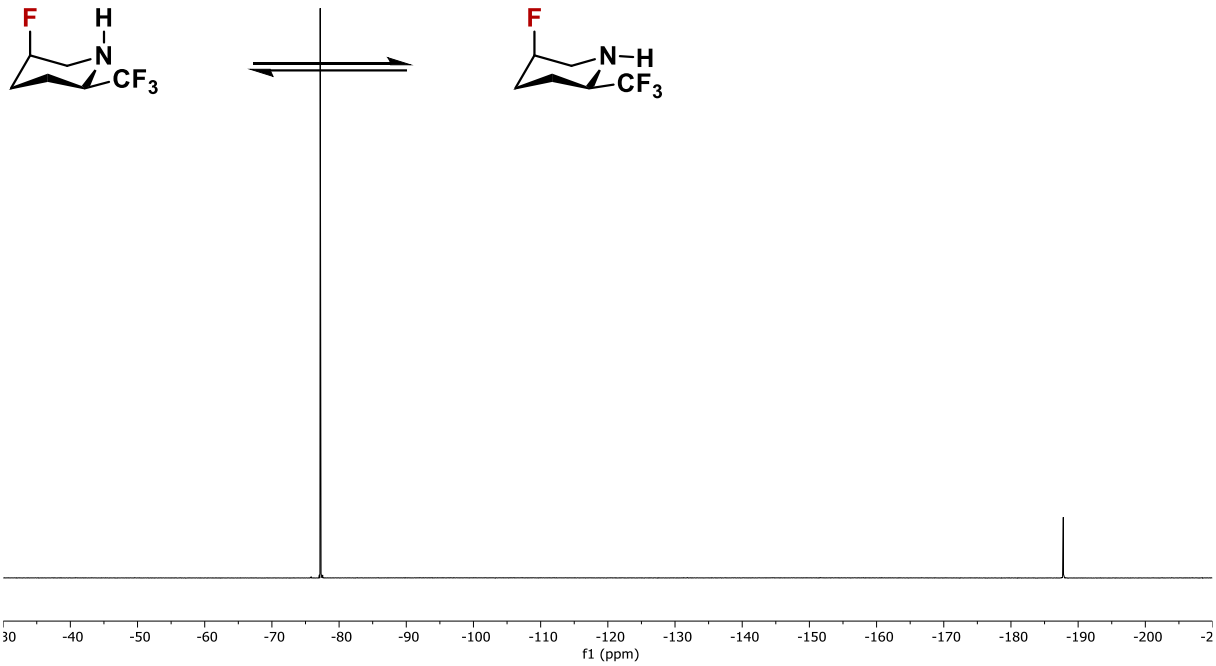




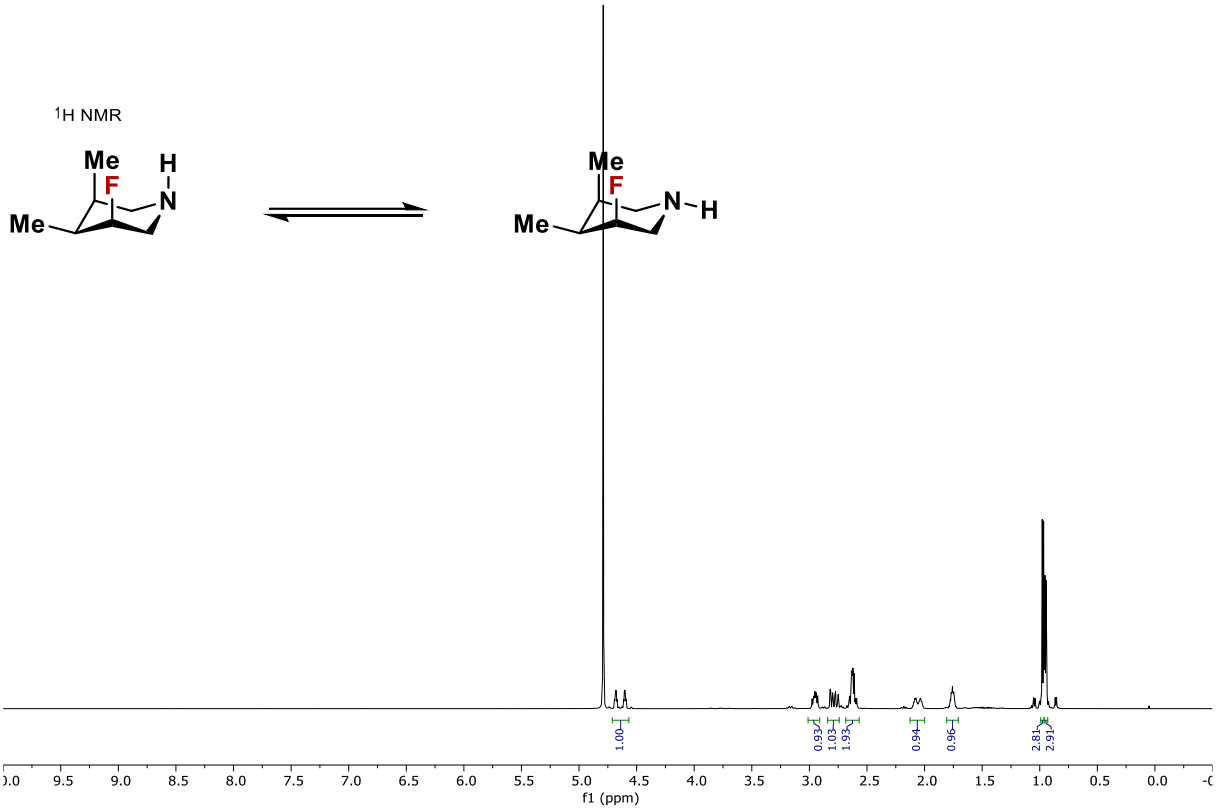
-77.19

-187.79

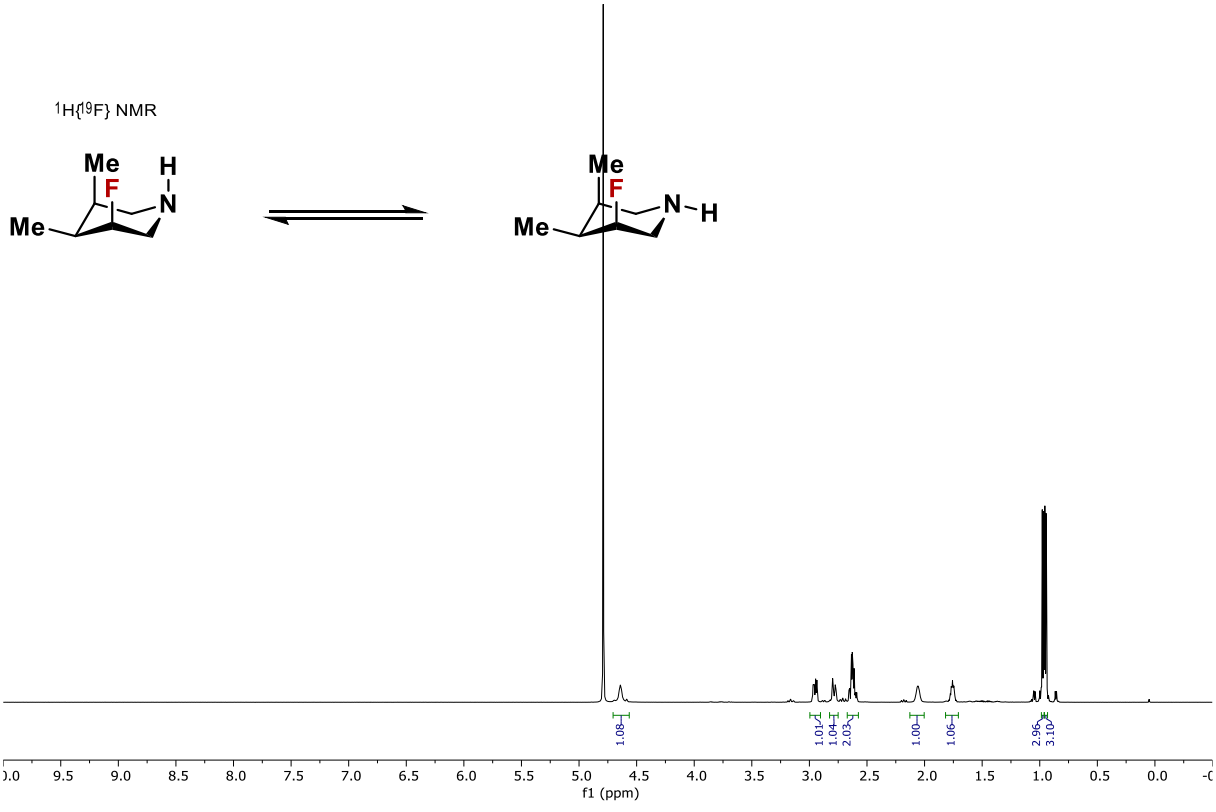
^{19}F{^{1}H} NMR



^{1}H NMR

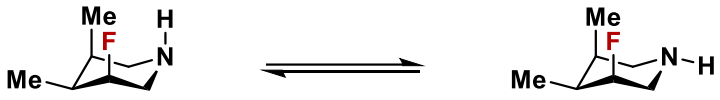


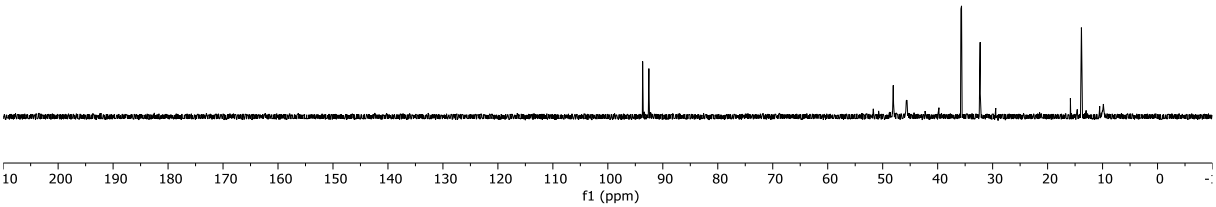
^{1}H{^{19}F} NMR



93.67
92.53
48.08
45.71
45.57
35.77
35.66
32.28
32.27
13.86
13.83
9.86

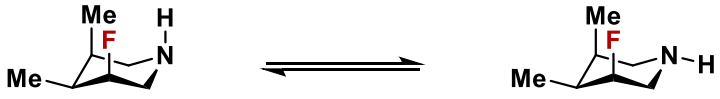
^{13}C NMR

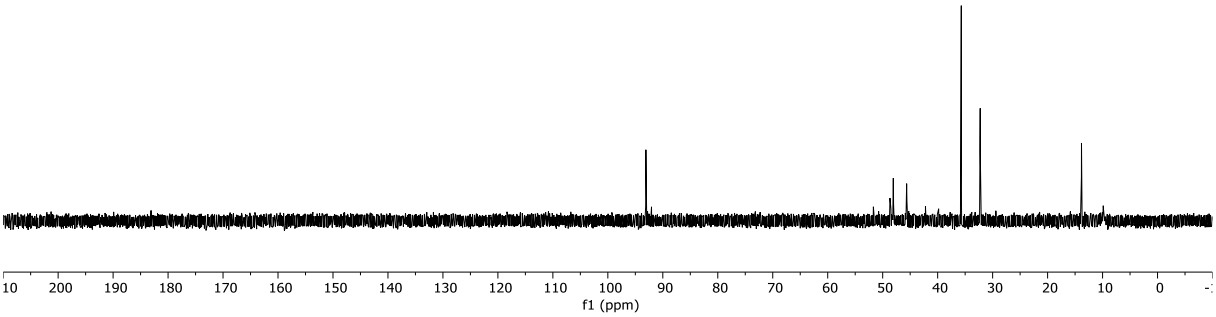




93.08
48.07
45.64
35.70
32.26
13.83
9.88

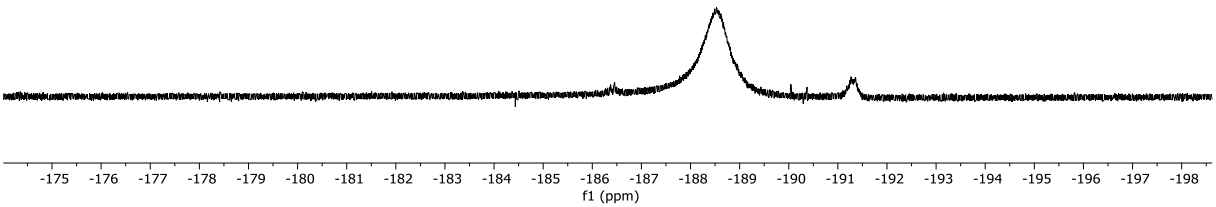
$^{13}C\{^{19}F\}$ NMR





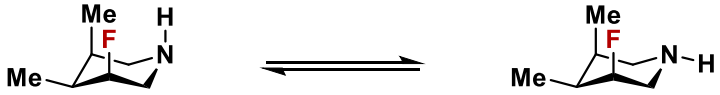
-188.53

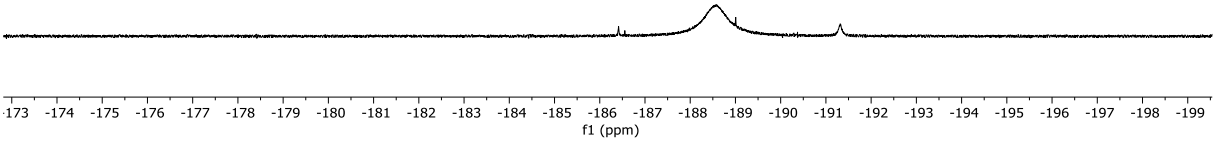
^{19}F NMR



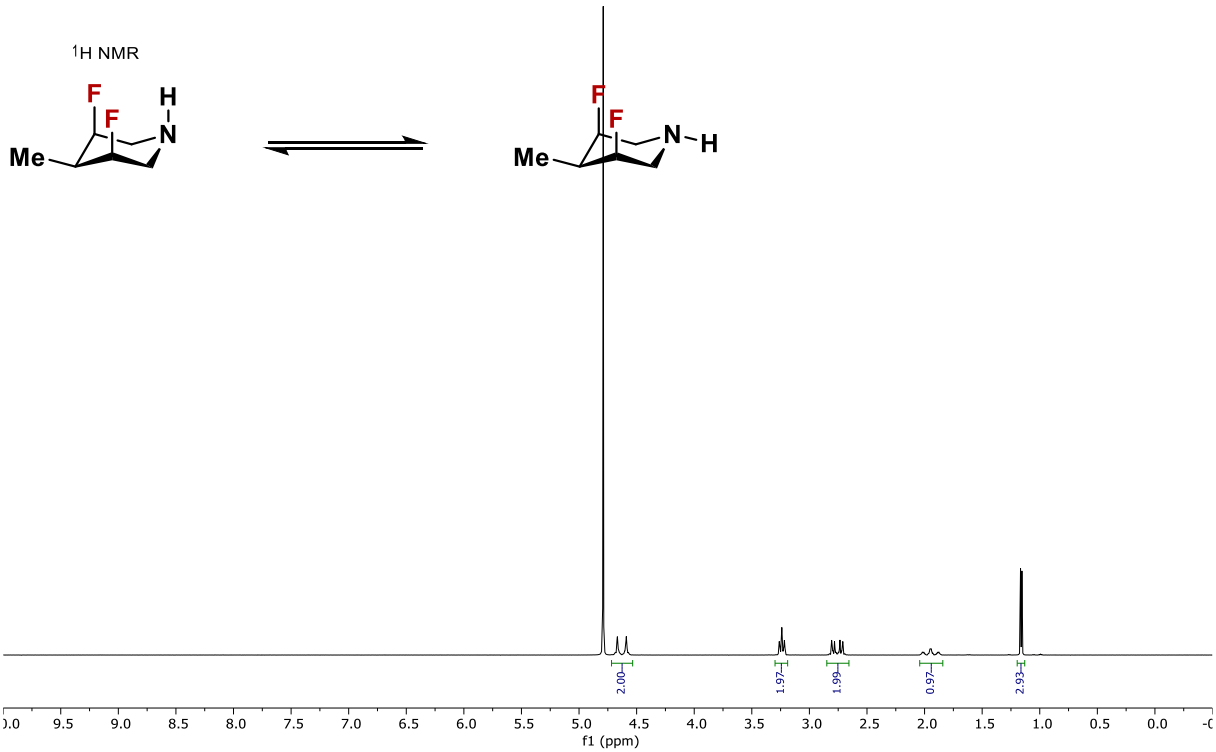
-188.56

^{19}F{^{1}H} NMR

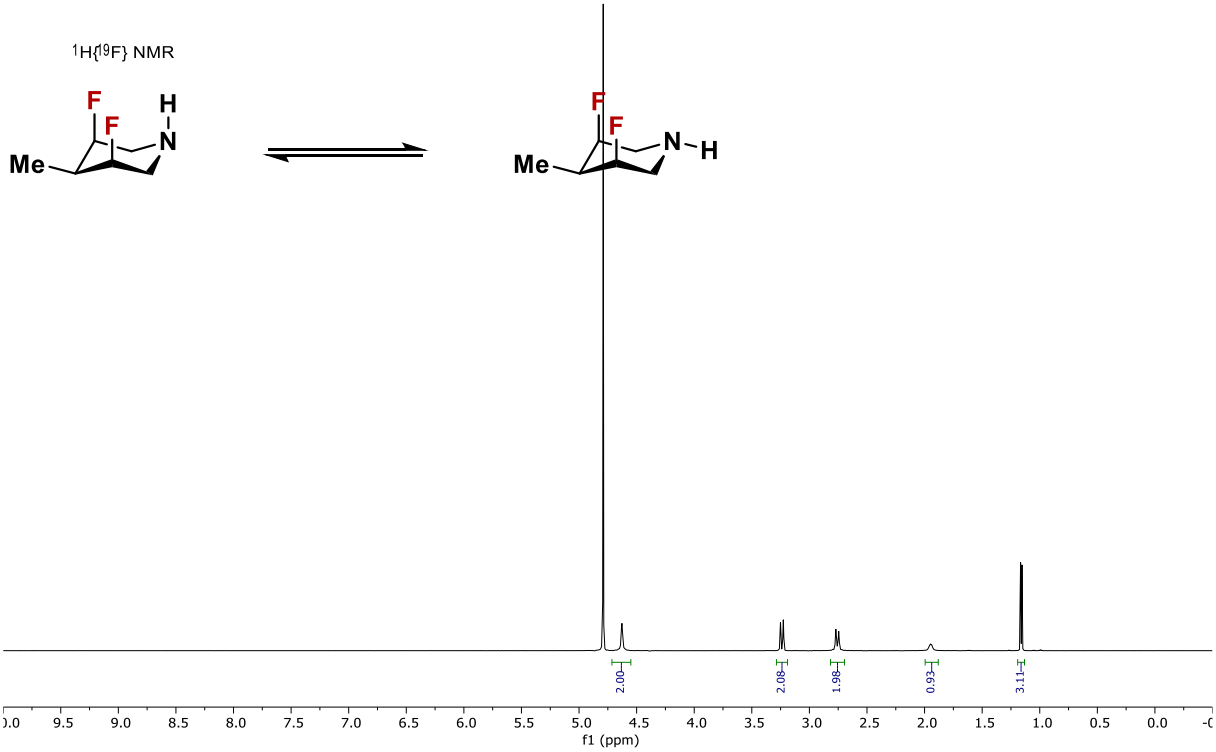




^{1}H NMR

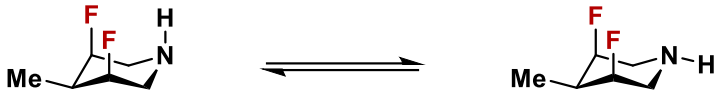


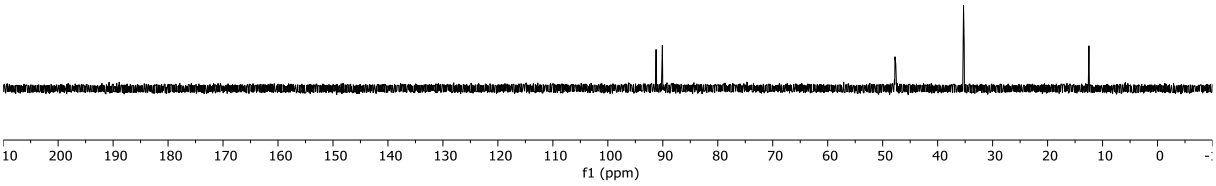
^{1}H{^{19}F} NMR



91.23
90.08
47.77
47.72
47.63
35.42
35.29
35.16
12.48

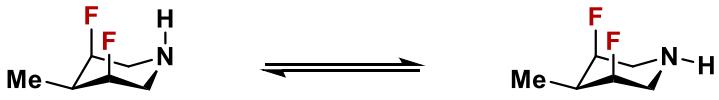
^{13}C NMR

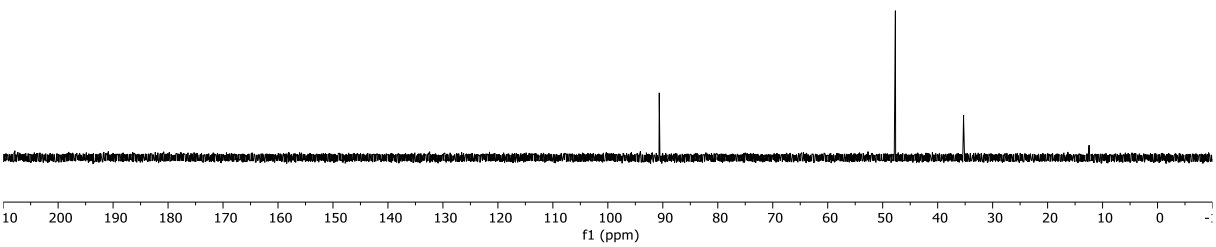




90.64
47.69
35.28
12.46

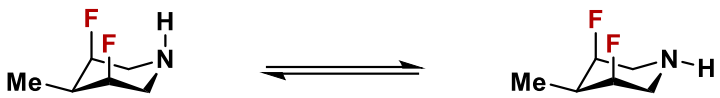
$^{13}C\{^{19}F\}$ NMR

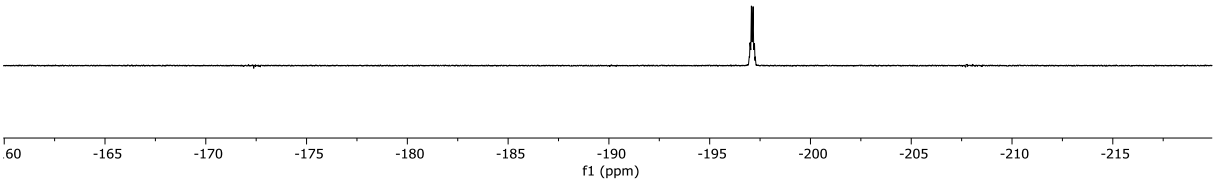




-196.96
-197.00
-197.02
-197.07
-197.07
-197.15
-197.15
-197.20
-197.22
-197.26

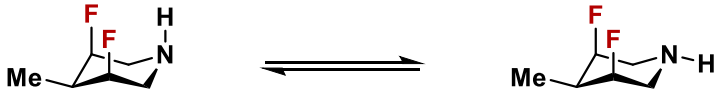
^{19}F NMR

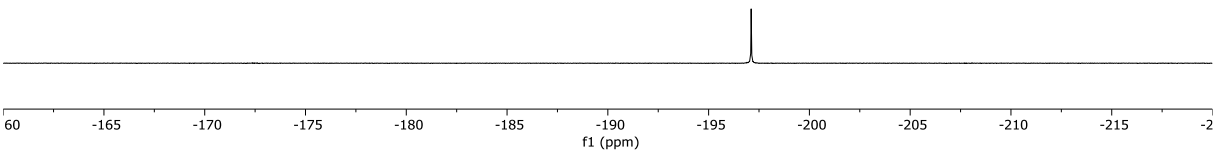




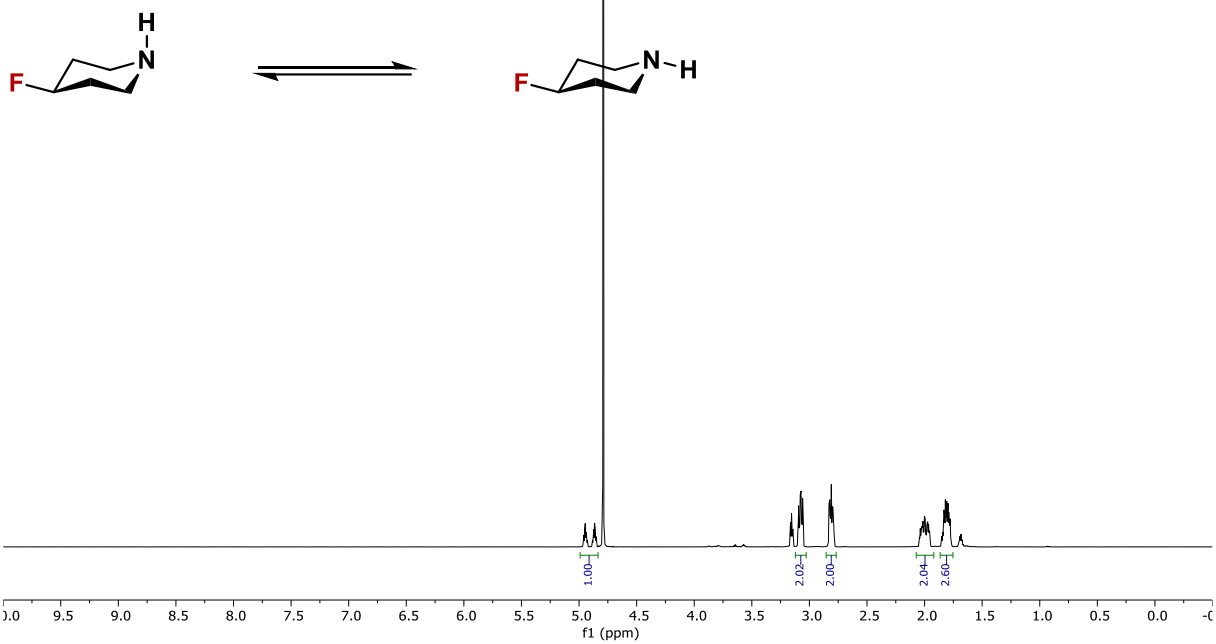
-197.11

^{19}F{^{1}H} NMR

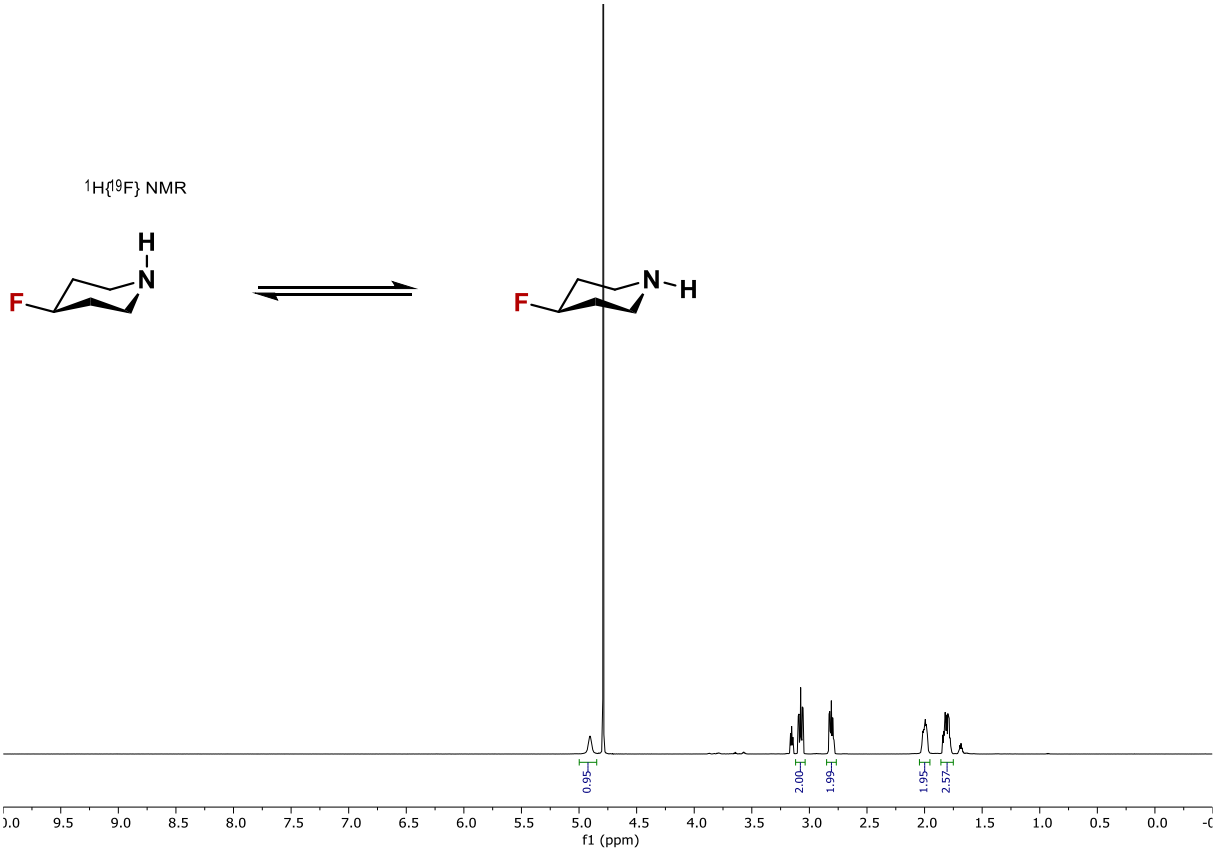




^{1}H NMR

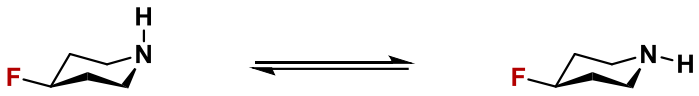


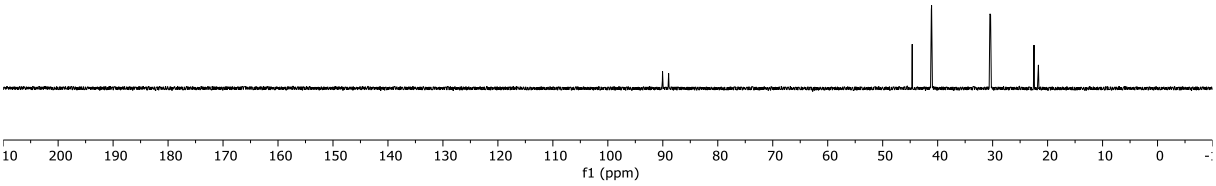
^{1}H{^{19}F} NMR



90.04
88.94
41.15
41.10
30.50
30.37

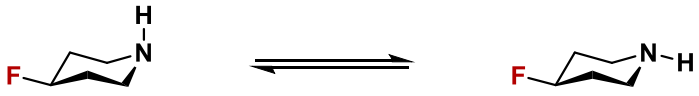
^{13}C NMR

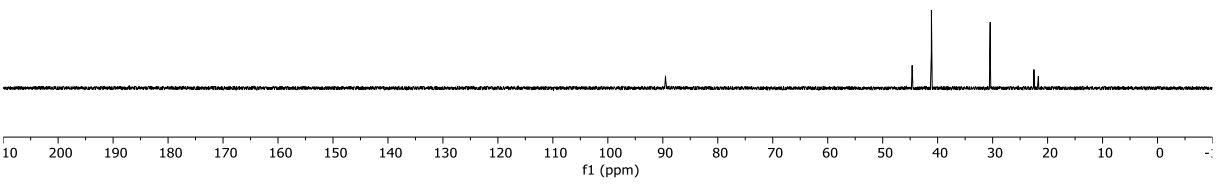




89.50
41.13
30.44

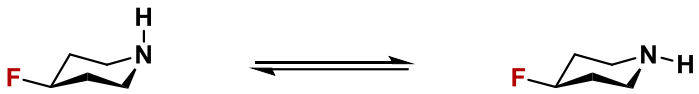
^{13}C{^{19}F} NMR

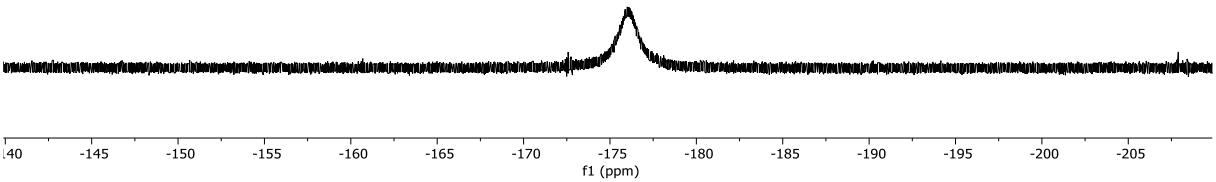




— -176.16

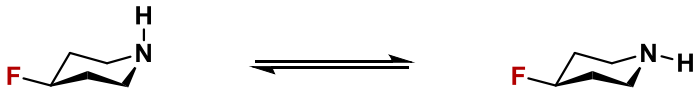
^{19}F NMR

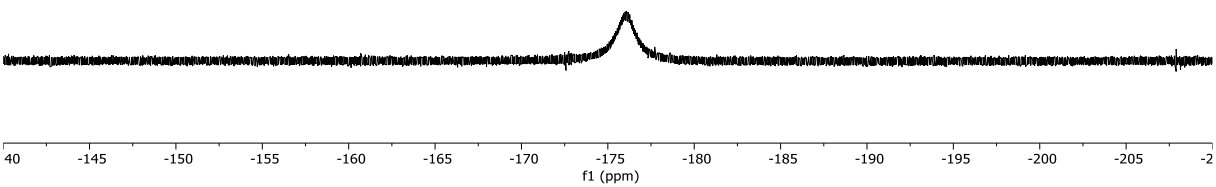




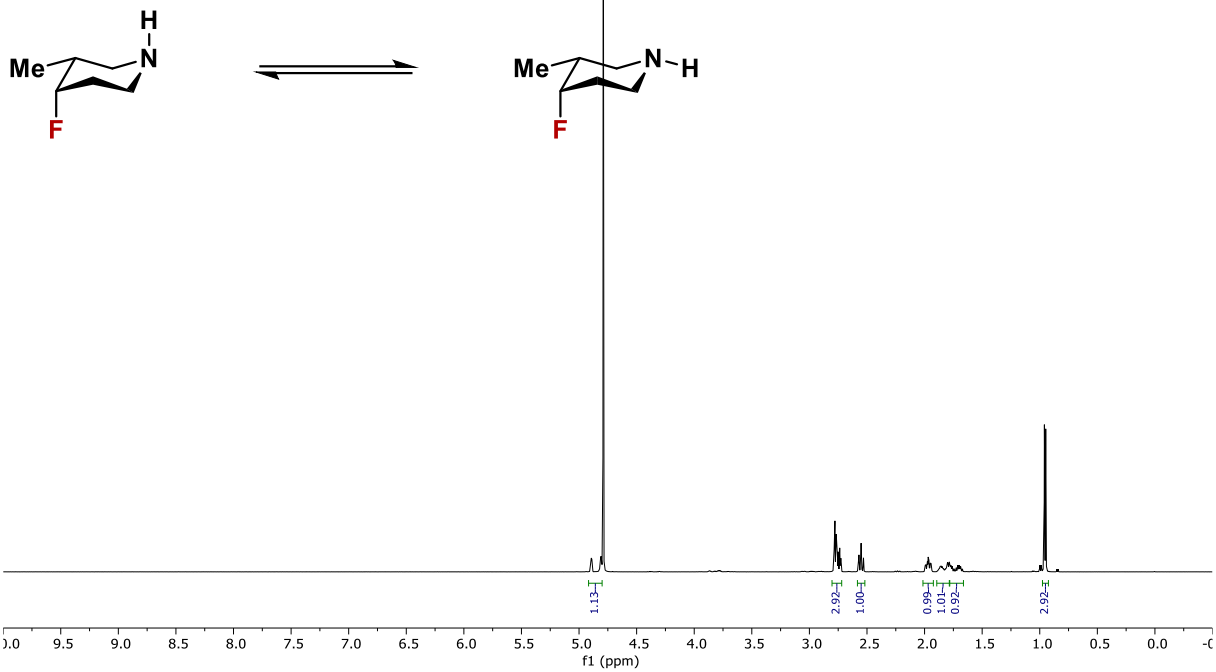
— -176.42

^{19}F{^{1}H} NMR

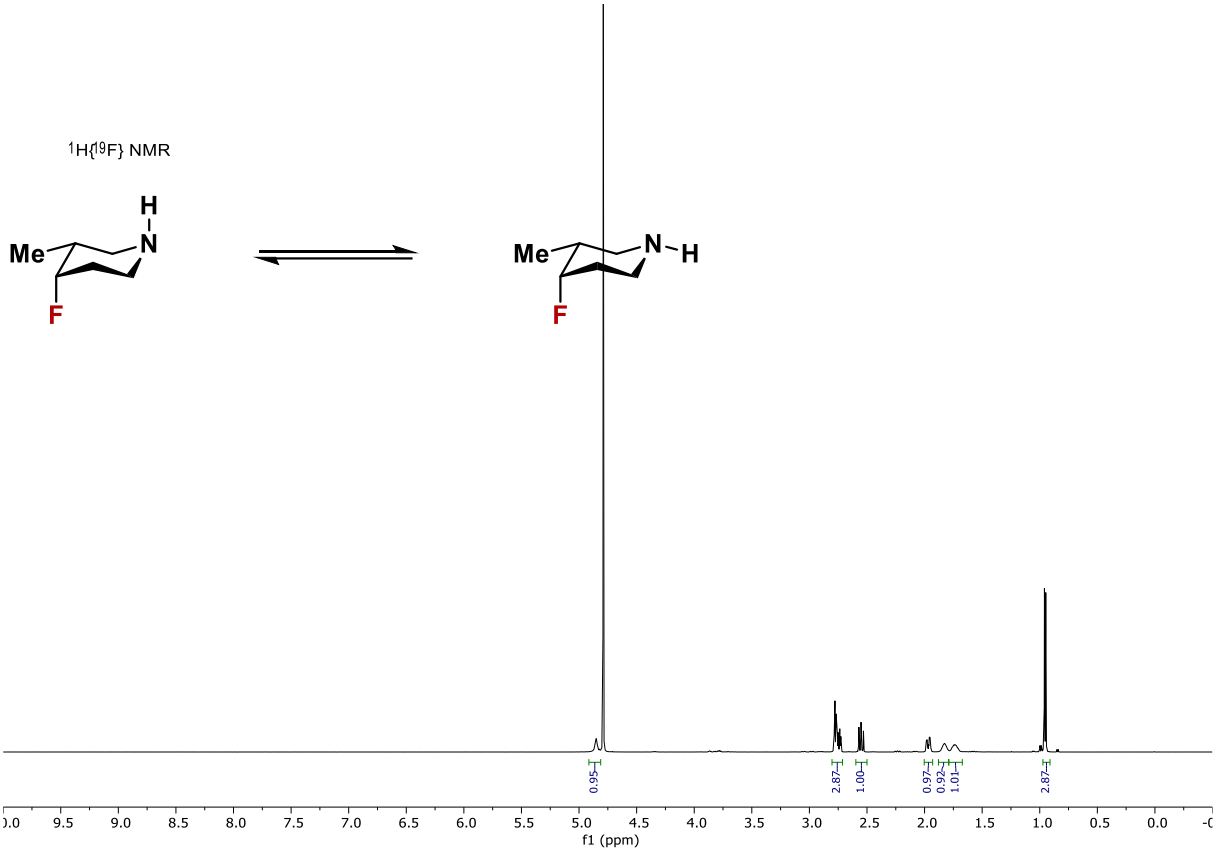




^{1}H NMR

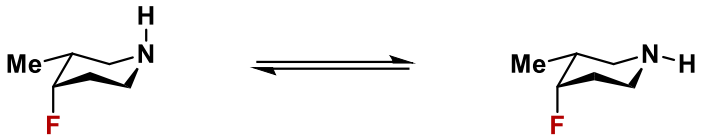


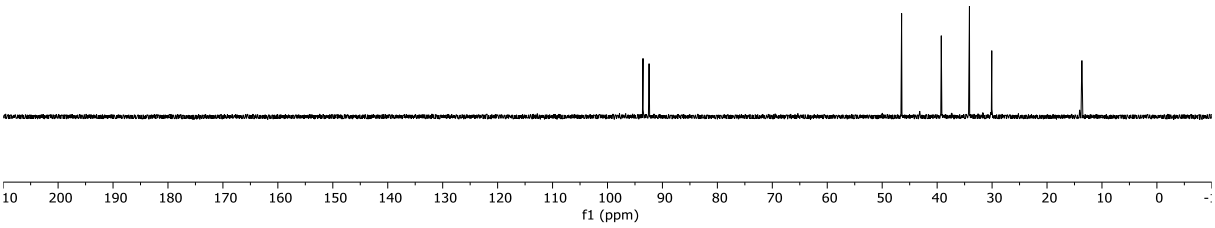
^{1}H{^{19}F} NMR



93.54
92.43
46.48
46.46
39.25
34.25
34.12
30.19
30.06
13.67
13.64

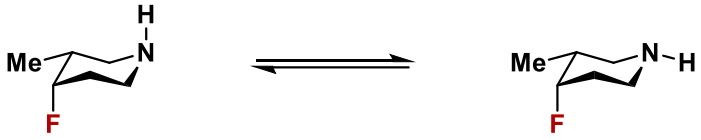
^{13}C NMR

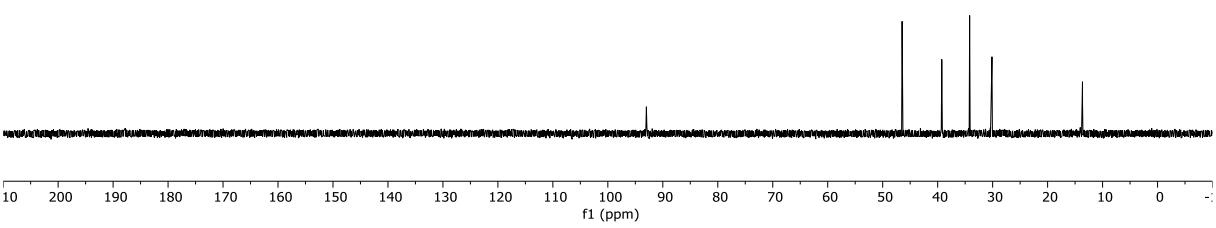




92.99
46.47
39.25
34.18
30.12
13.66

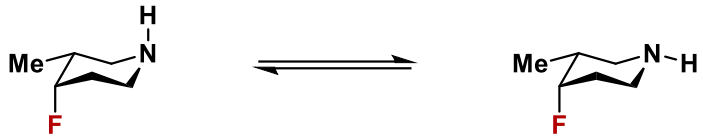
$^{13}C\{^{19}F\}$ NMR

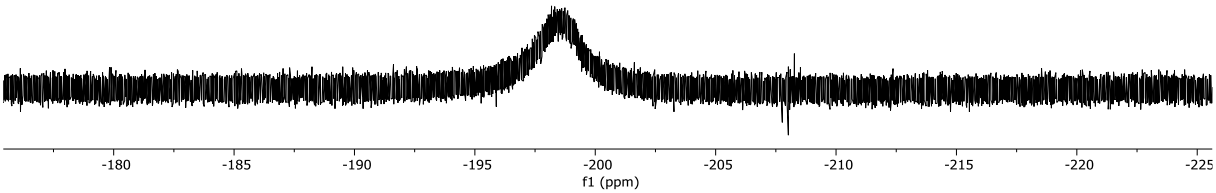




— -198.52

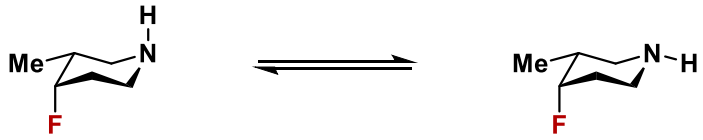
^{19}F NMR

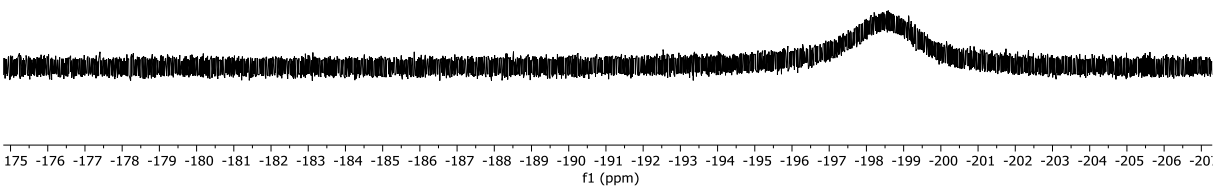




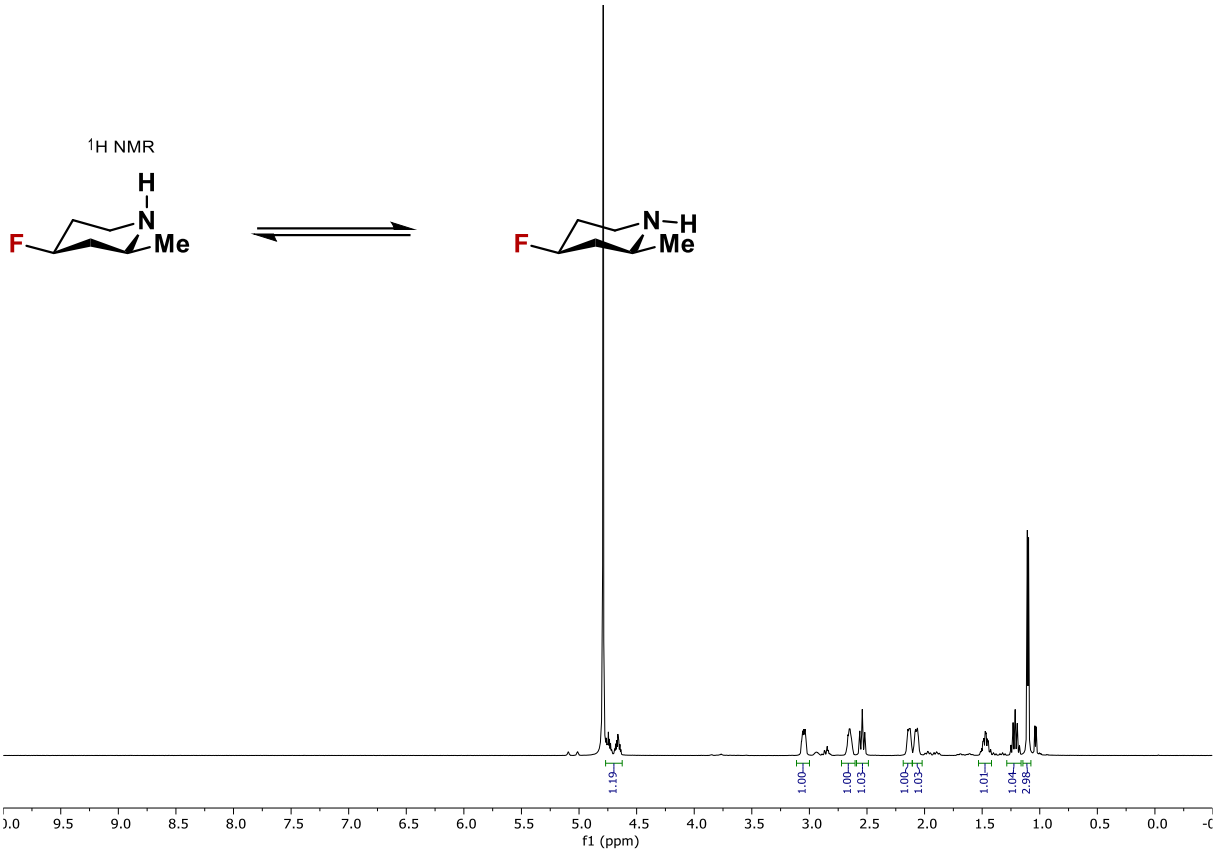
— -198.62

^{19}F{^{1}H} NMR

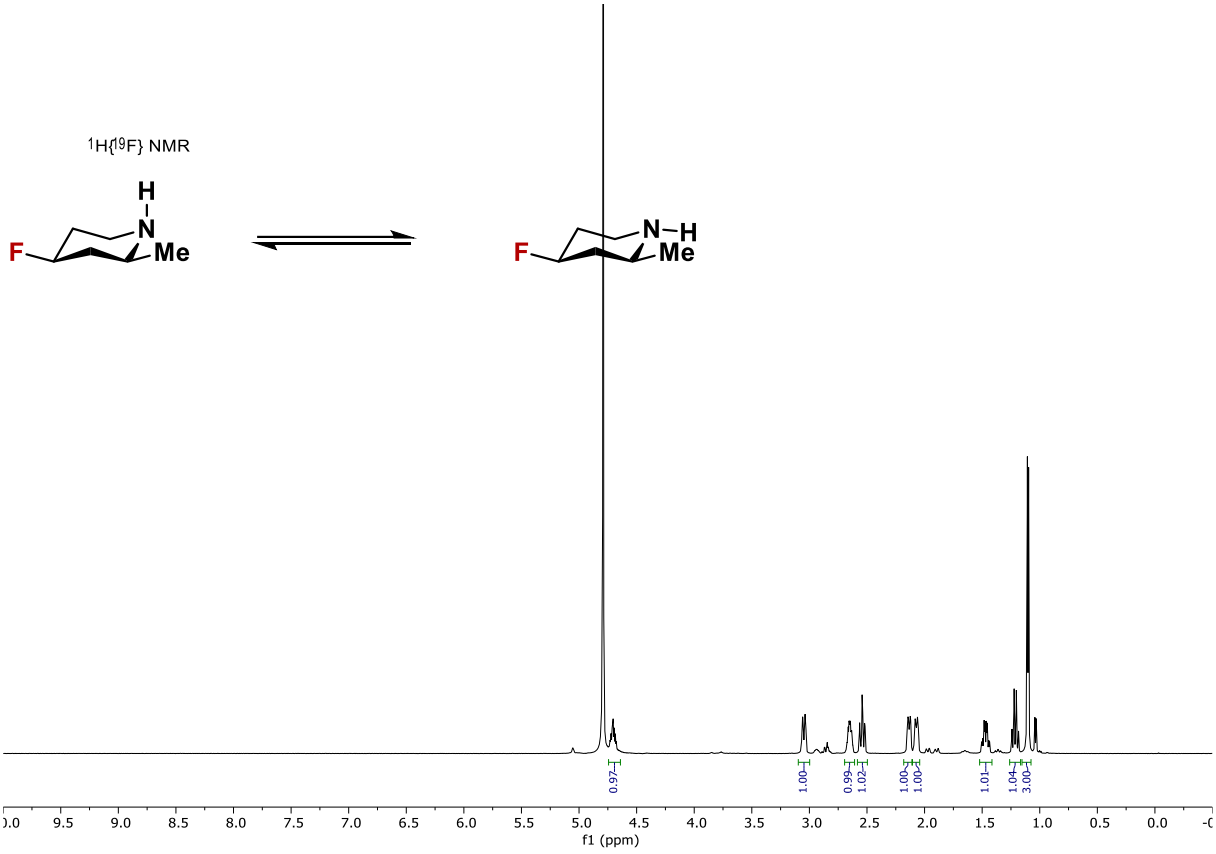




^{1}H NMR

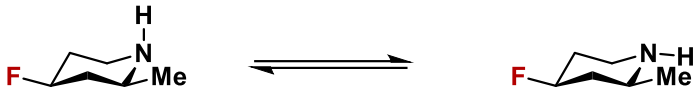


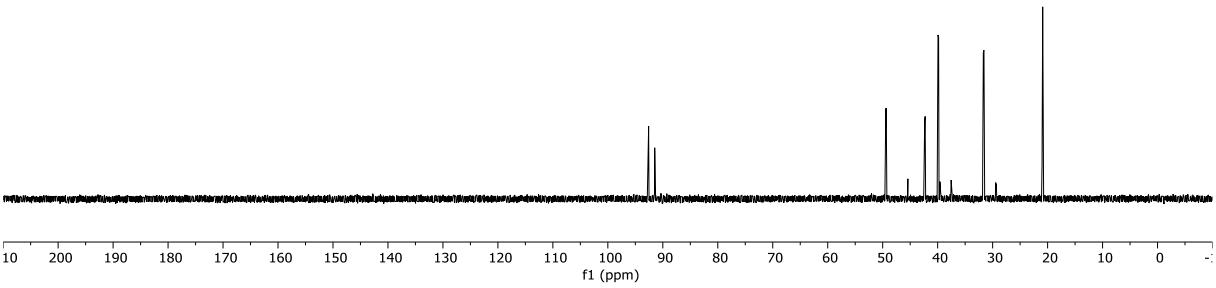
^{1}H{^{19}F} NMR



92.58
91.47
49.44
49.36
42.36
42.28
39.93
39.83
31.69
31.58
20.90
20.89

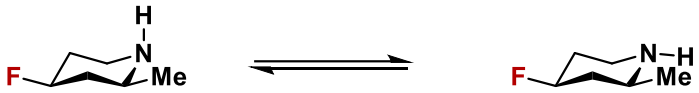
^{13}C NMR

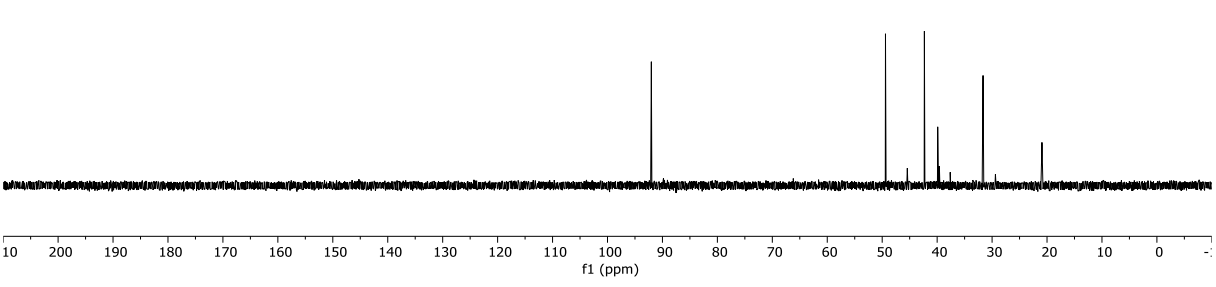




92.02
49.40
42.32
39.89
31.64
20.92

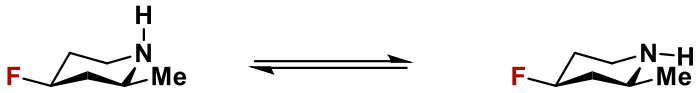
^{13}C{^{19}F} NMR

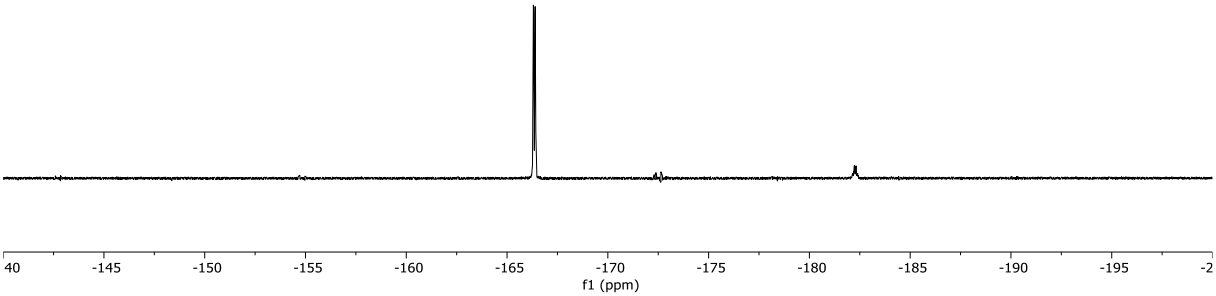




-166.31
-166.40

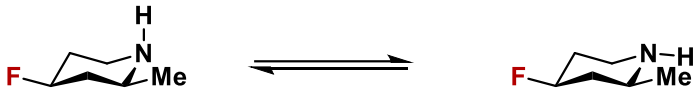
^{19}F NMR

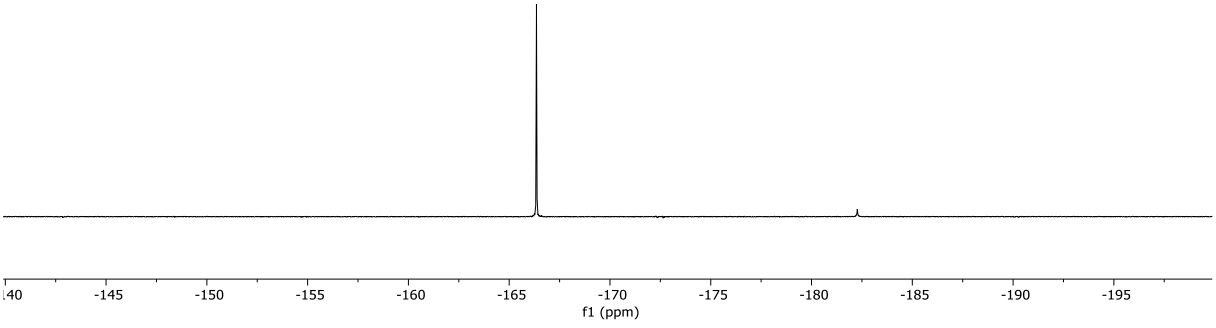




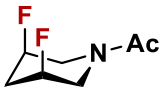
-166.35

^{19}F{^{1}H} NMR

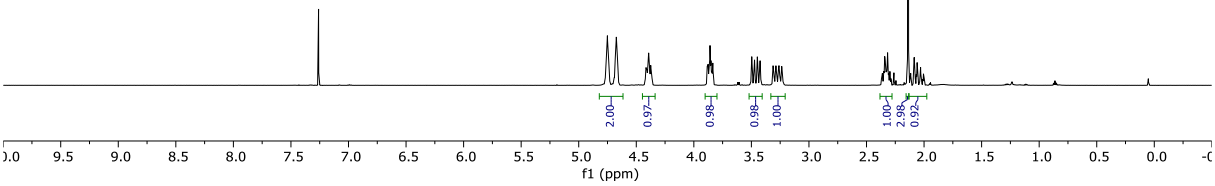




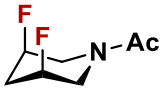
^{1}H NMR



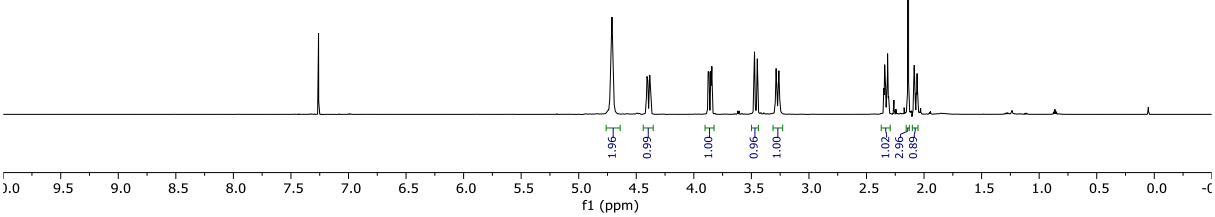
in **$CDCl_3$**



^{1}H{^{19}F} NMR

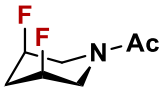


in **$CDCl_3$**

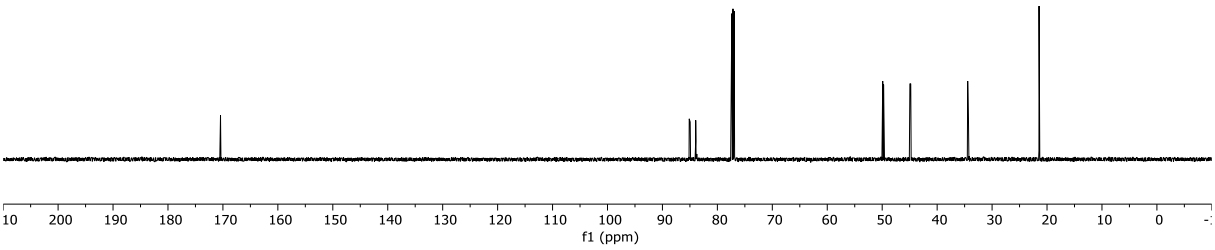


170.44
85.11
84.95
83.93
83.76
49.90
49.75
44.96
44.80
34.58
34.44
34.30
21.45

^{13}C NMR

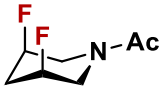


in **$CDCl_3$**

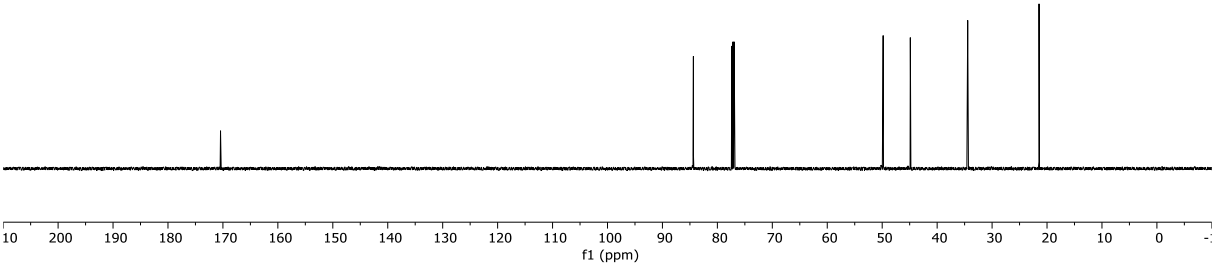


170.44
84.53
84.37
49.83
44.88
34.44
21.45

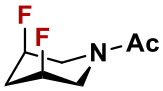
$^{13}C\{^{19}F\}$ NMR



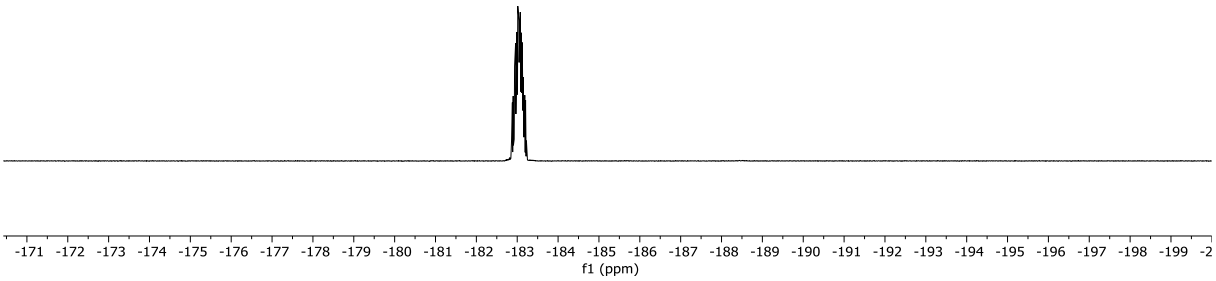
in **$CDCl_3$**



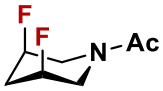
^{19}F NMR



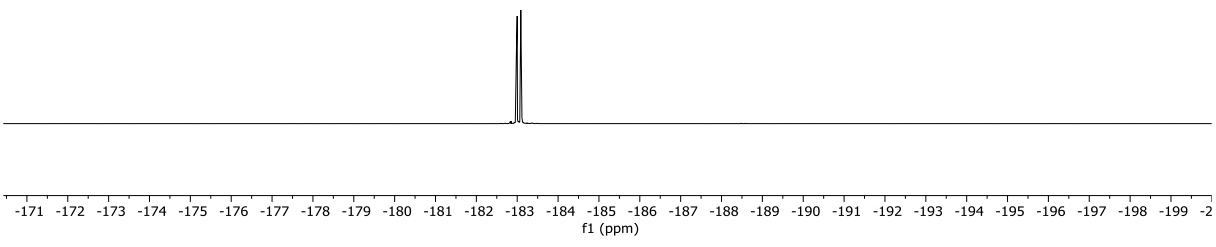
in **$CDCl_3$**



^{19}F{^{1}H} NMR

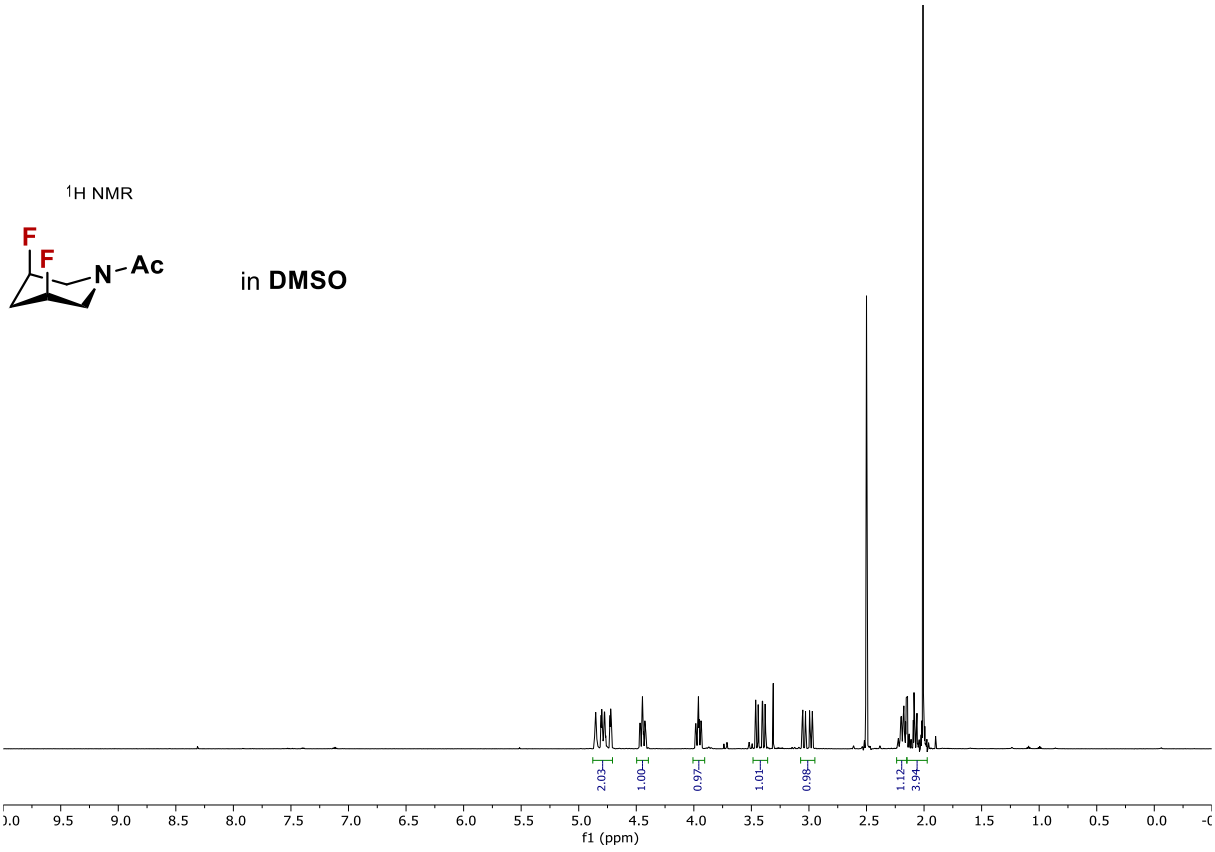


in **$CDCl_3$**



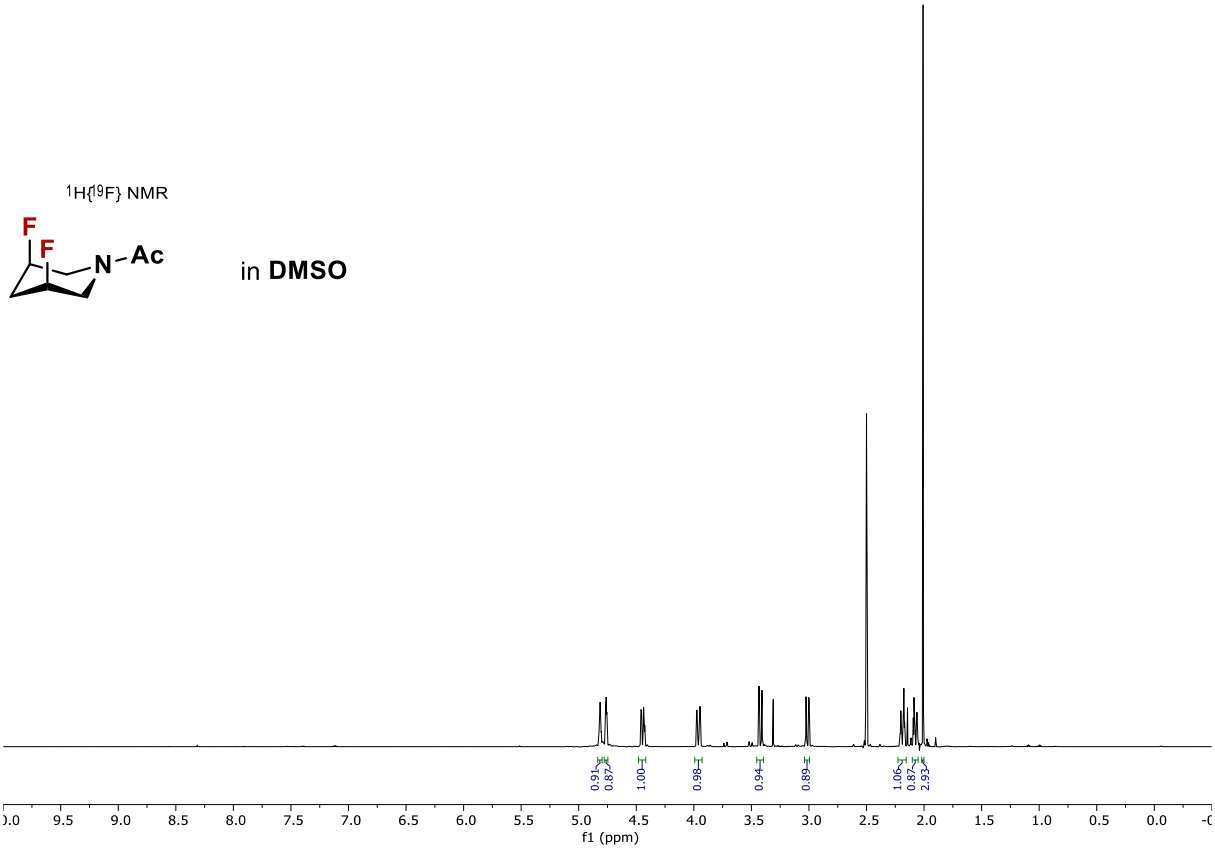
^{1}H NMR

in **DMSO**



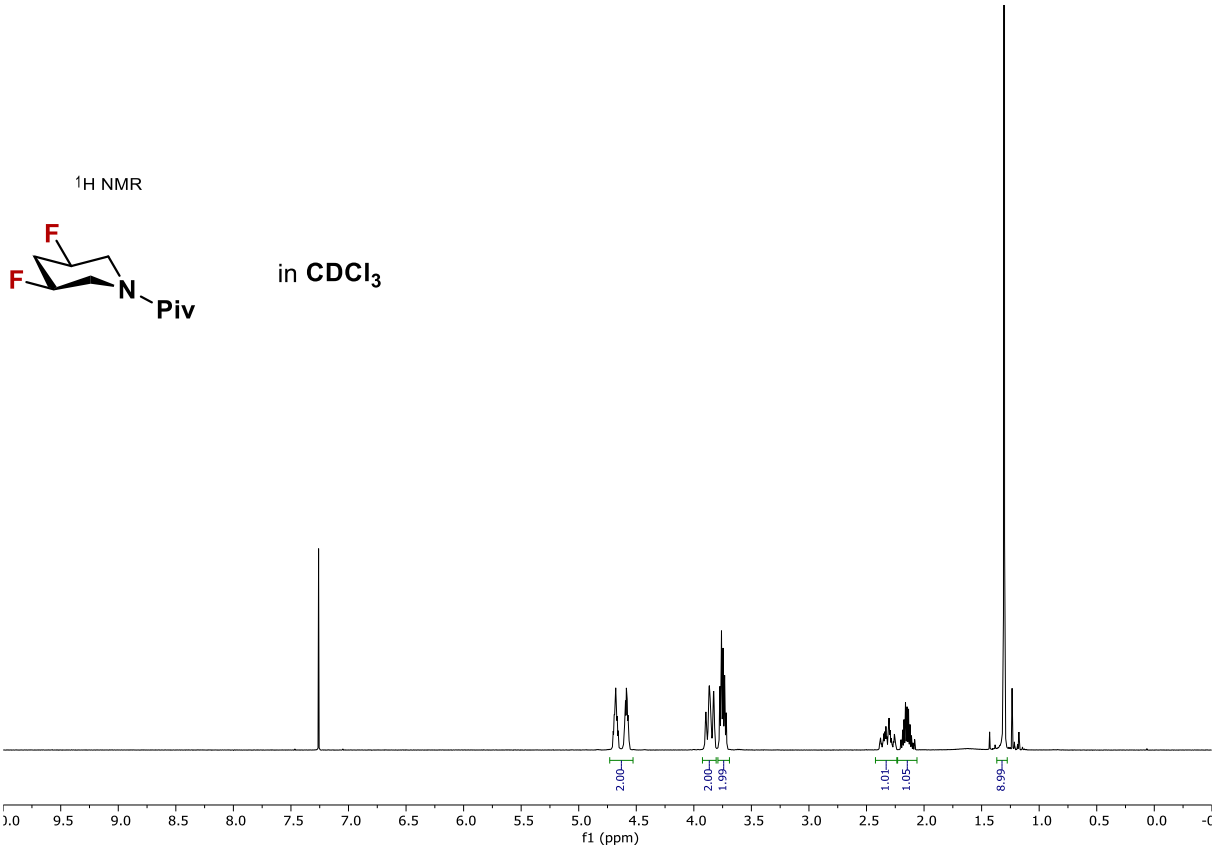
$^{1}H\{^{19}F\}$ NMR

in **DMSO**



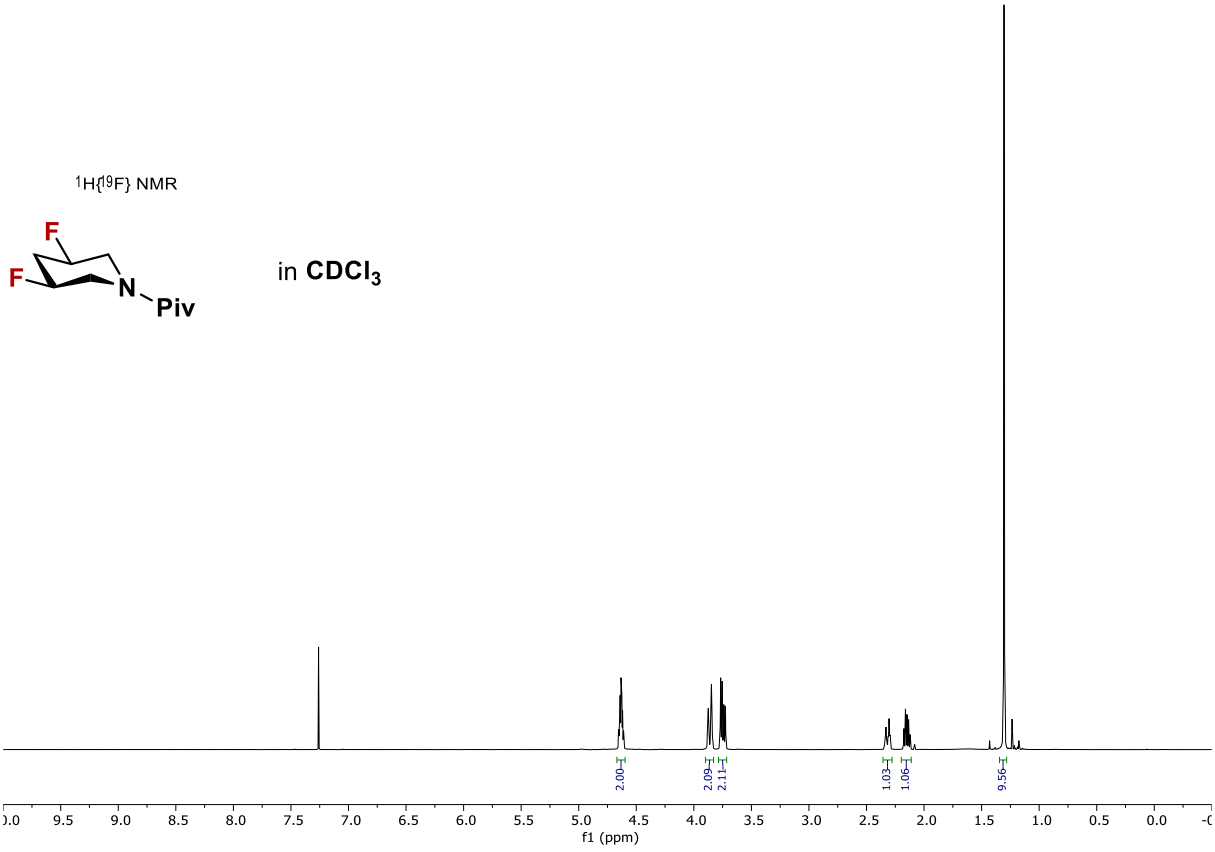
^{1}H NMR

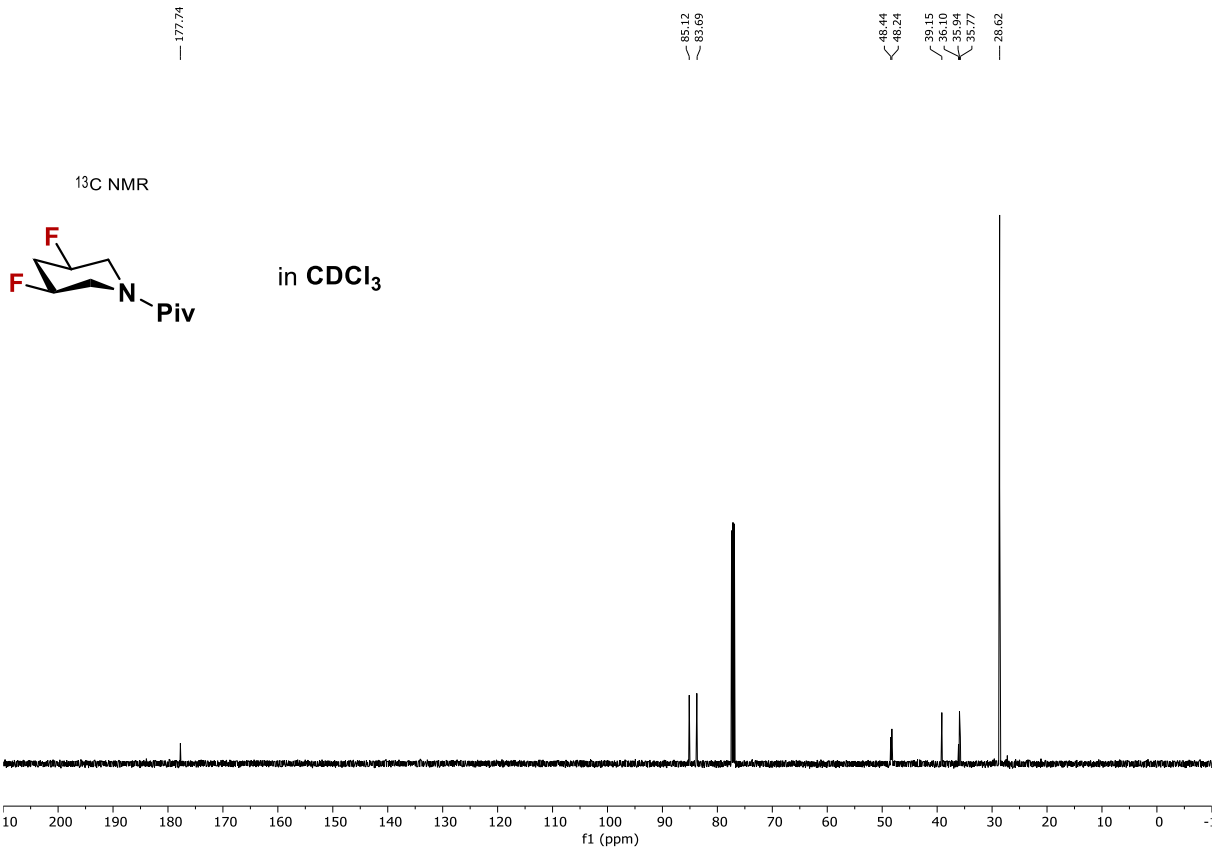
in **$CDCl_3$**

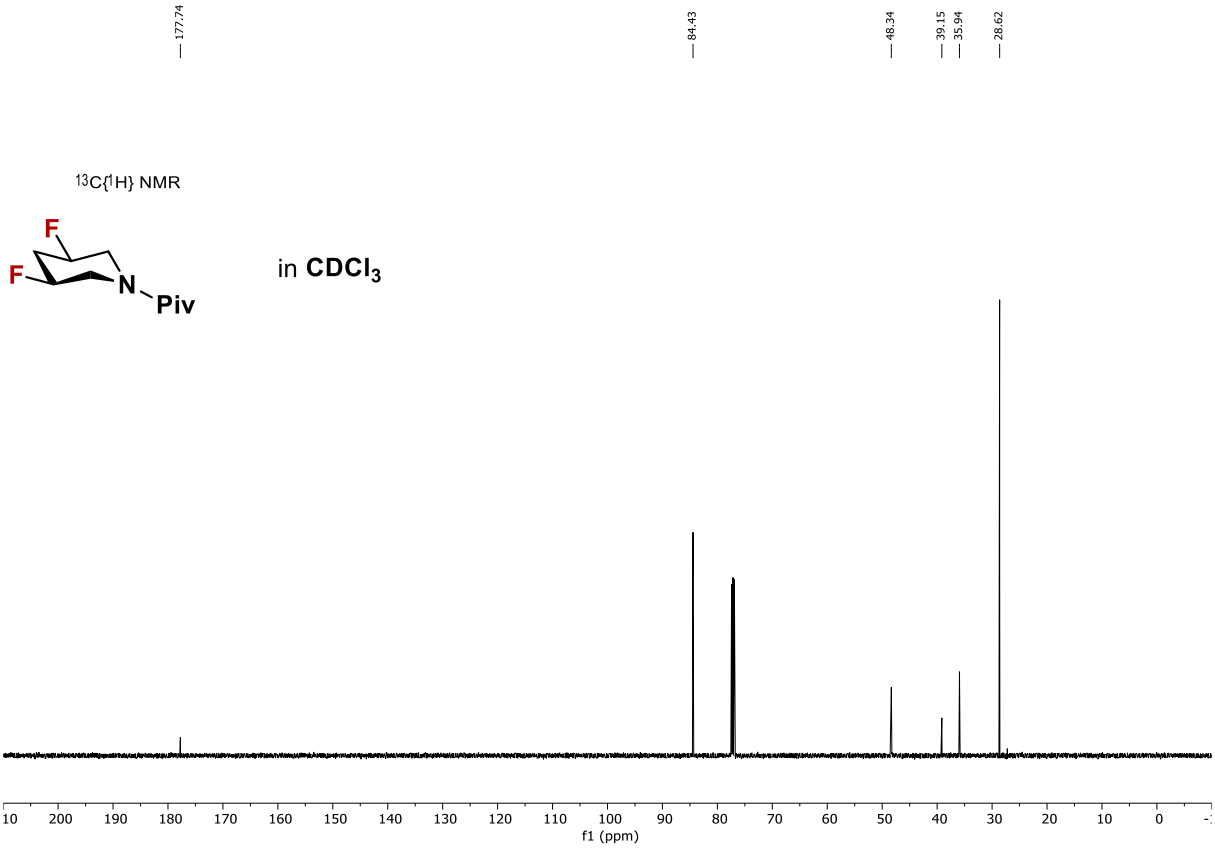


^{1}H{^{19}F} NMR

in **$CDCl_3$**

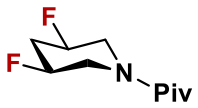



177.74
85.12
83.69
48.44
48.24
39.15
36.10
35.94
35.77
28.62
13C NMR
F
F
N
Piv
in CDCl3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

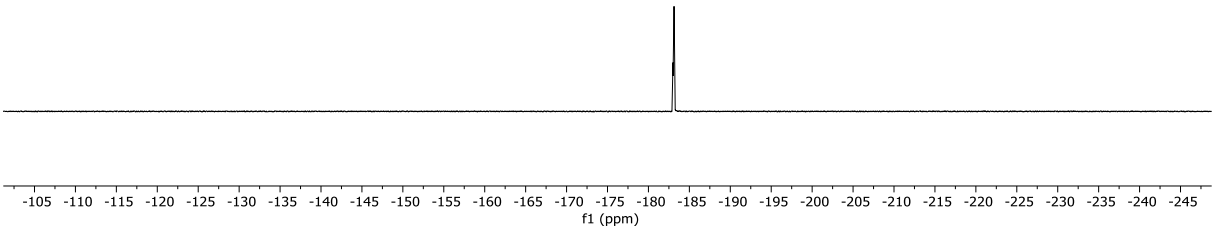

177.74
84.43
48.34
39.15
35.94
28.62
13C{1H} NMR
F
F
N
Piv
in CDCl3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

-182.98
-183.00
-183.01
-183.02
-183.03
-183.04
-183.05
-183.06
-183.07
-183.08
-183.09
-183.09
-183.10
-183.12
-183.13
-183.13
-183.14
-183.15
-183.17
-183.18
-183.19
-183.20
-183.21
-183.22
-183.24

^{19}F NMR

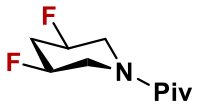


in **$CDCl_3$**

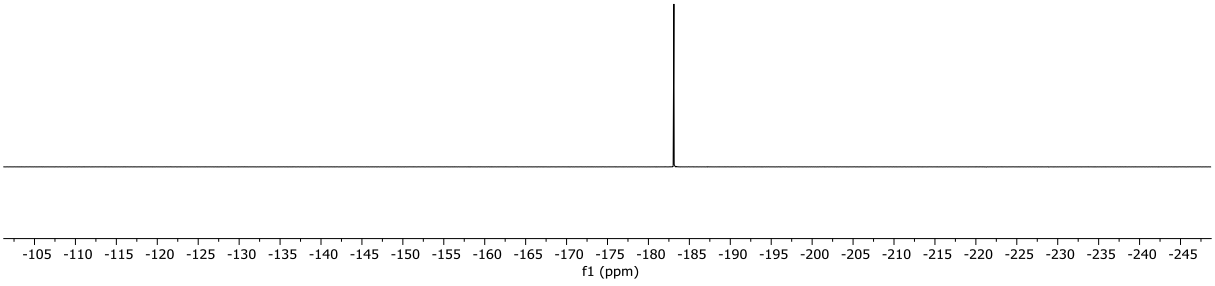


-183.11

^{19}F{^{1}H} NMR

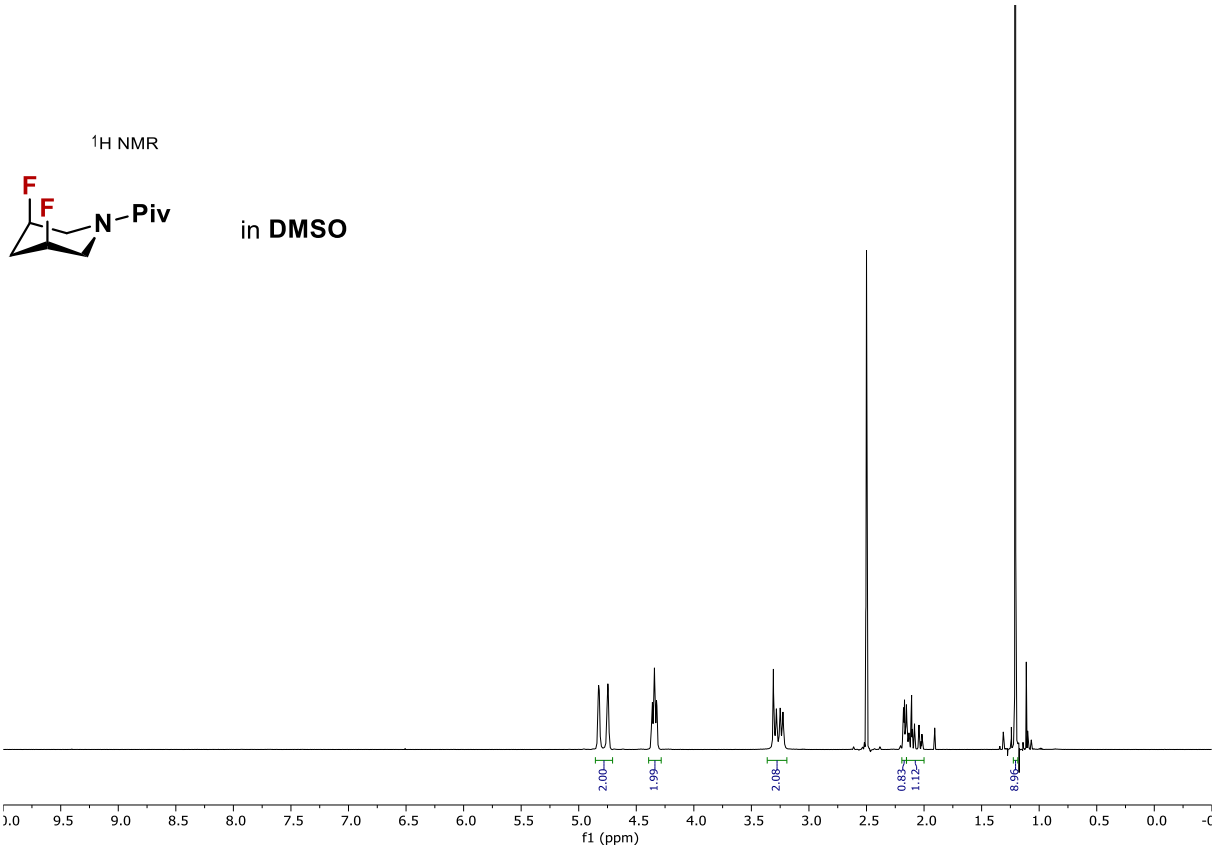


in **$CDCl_3$**



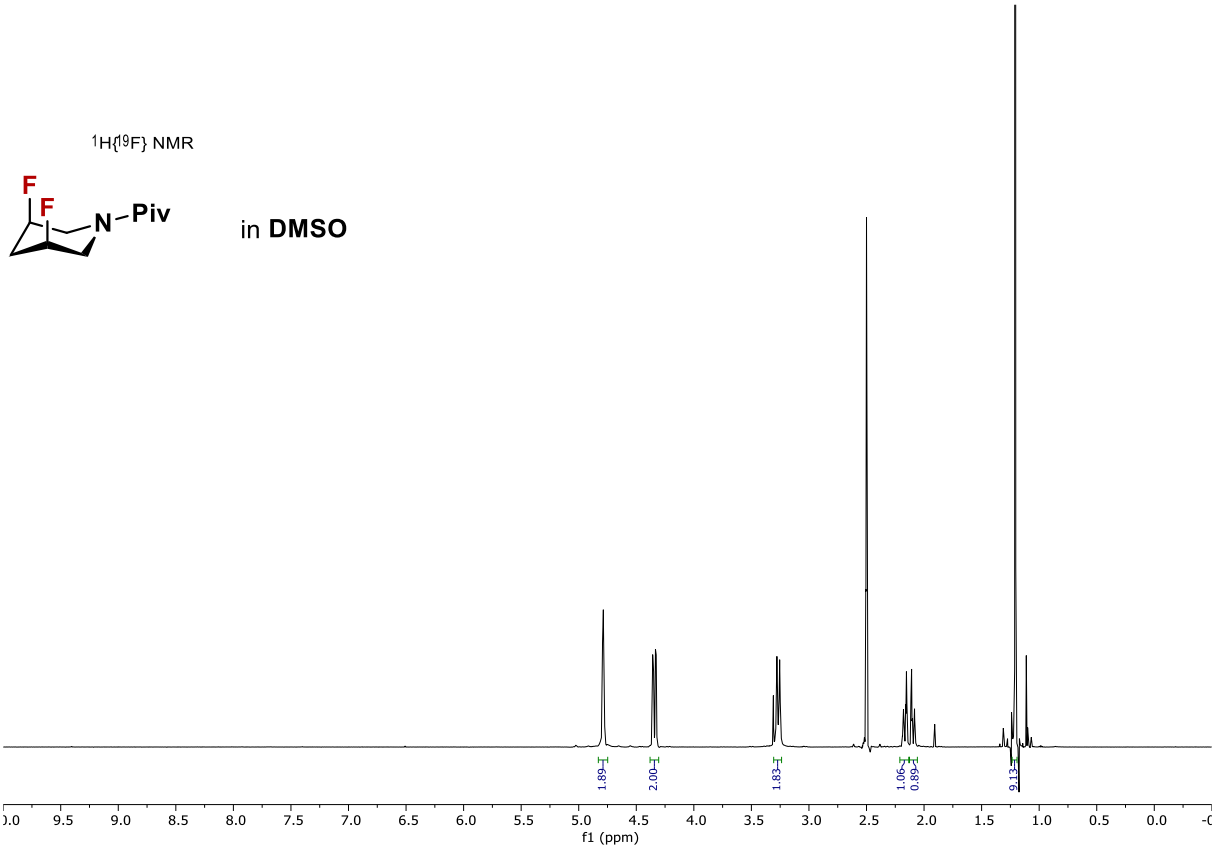
^{1}H NMR

in **DMSO**



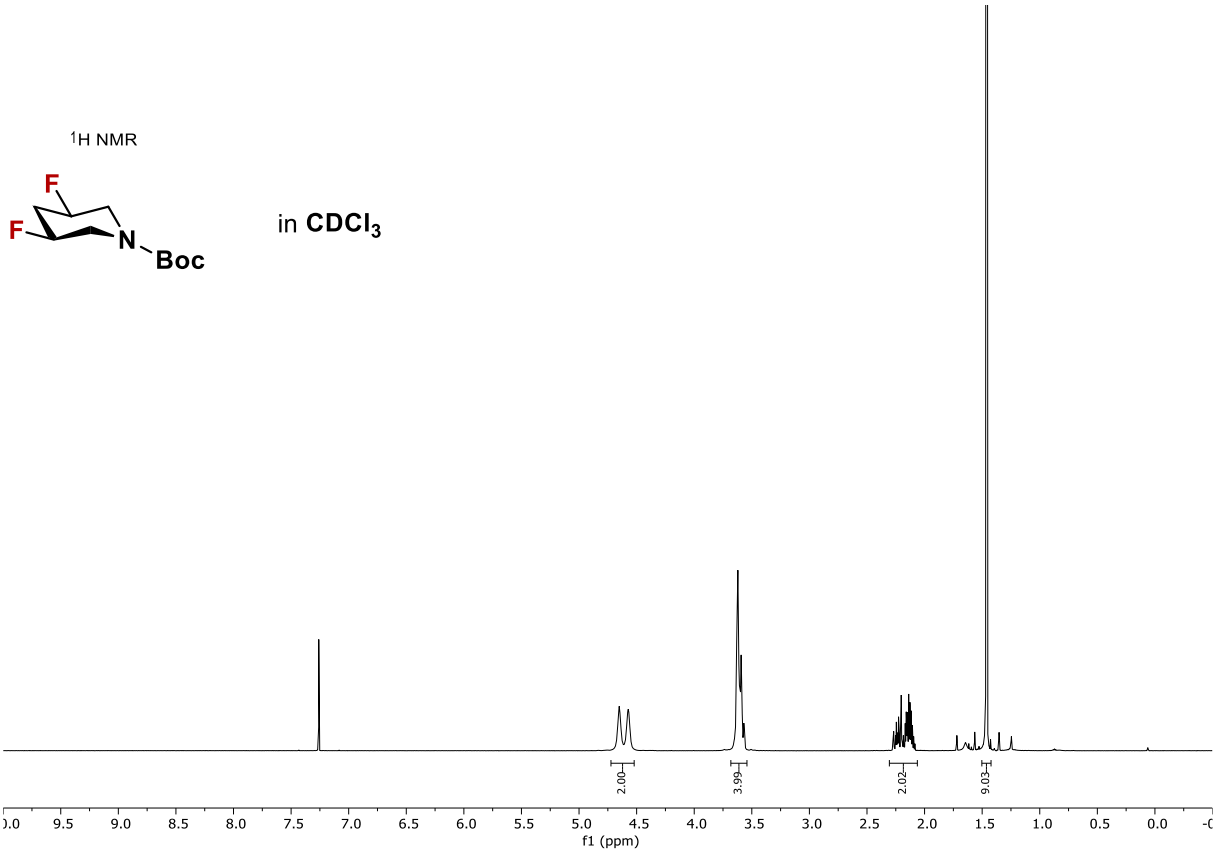
^{1}H{^{19}F} NMR

in **DMSO**



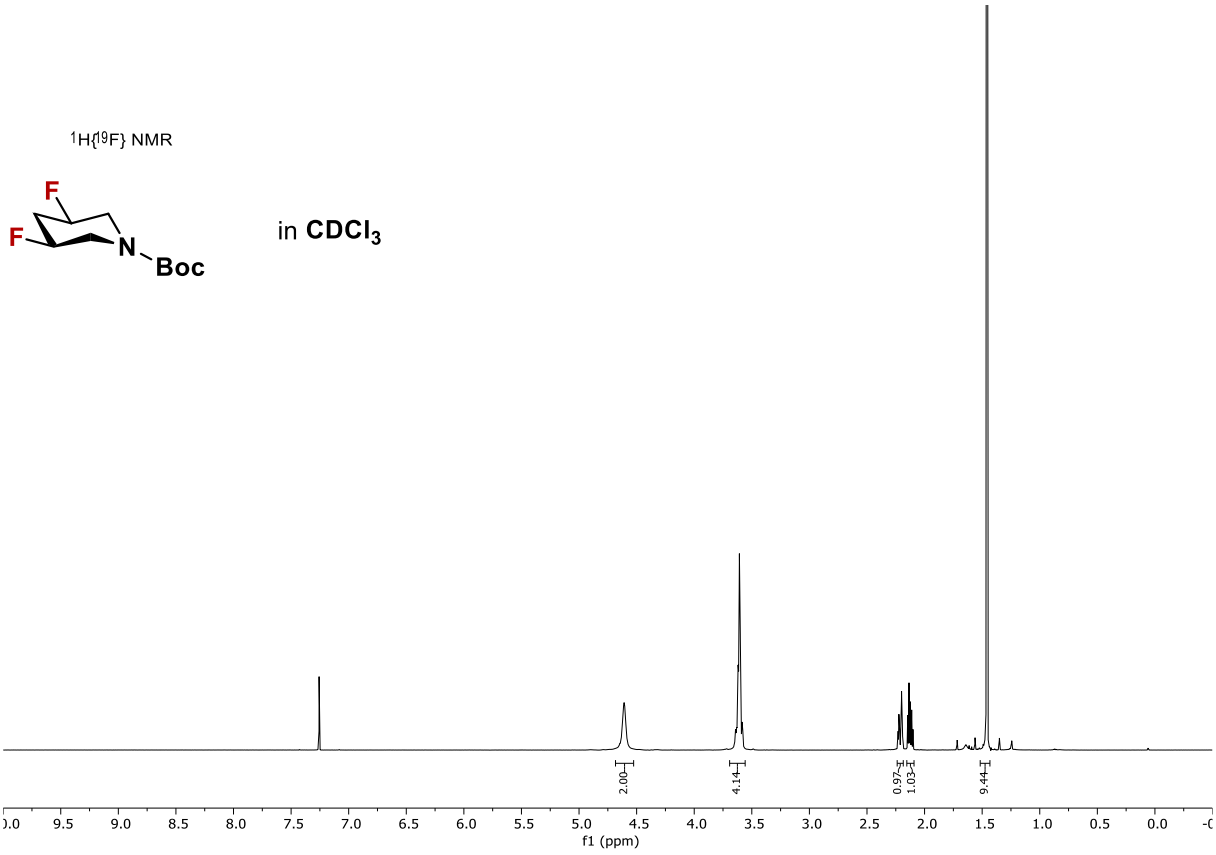
^{1}H NMR

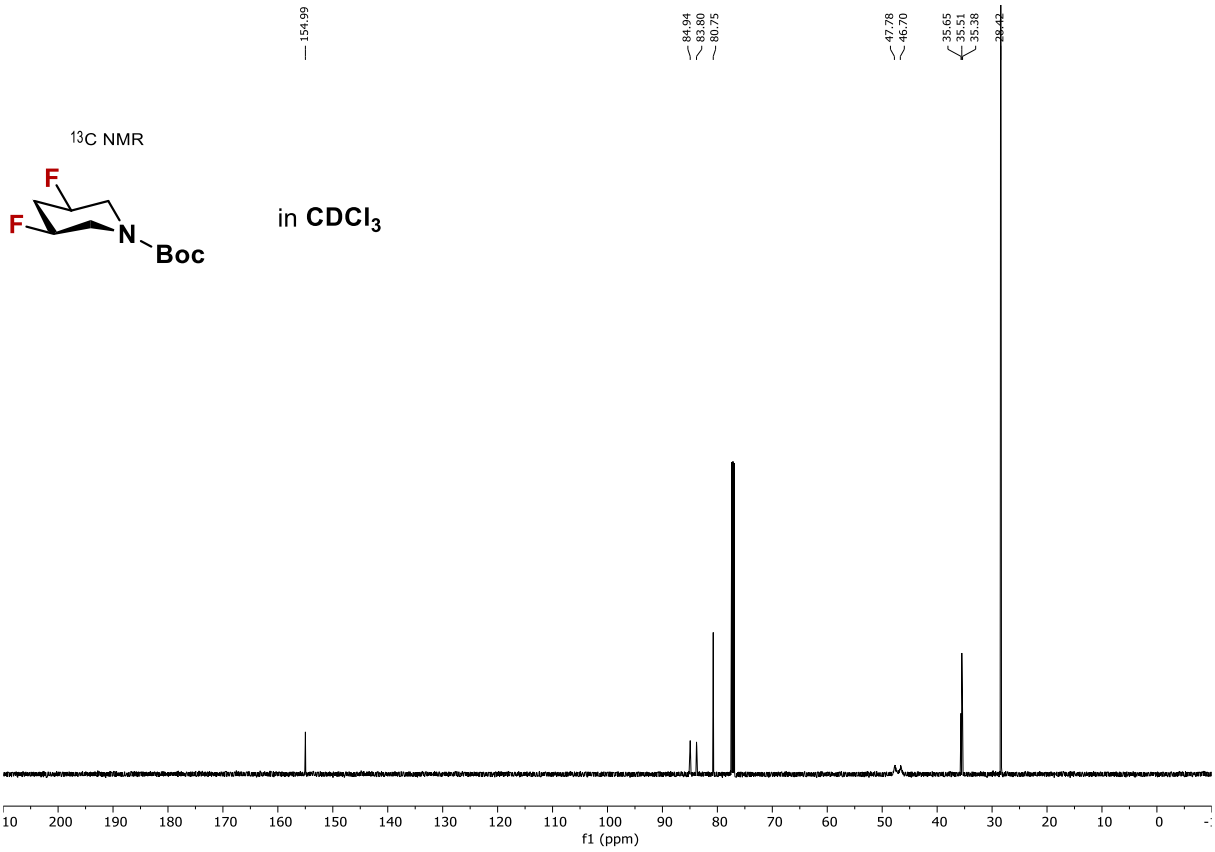
in **$CDCl_3$**

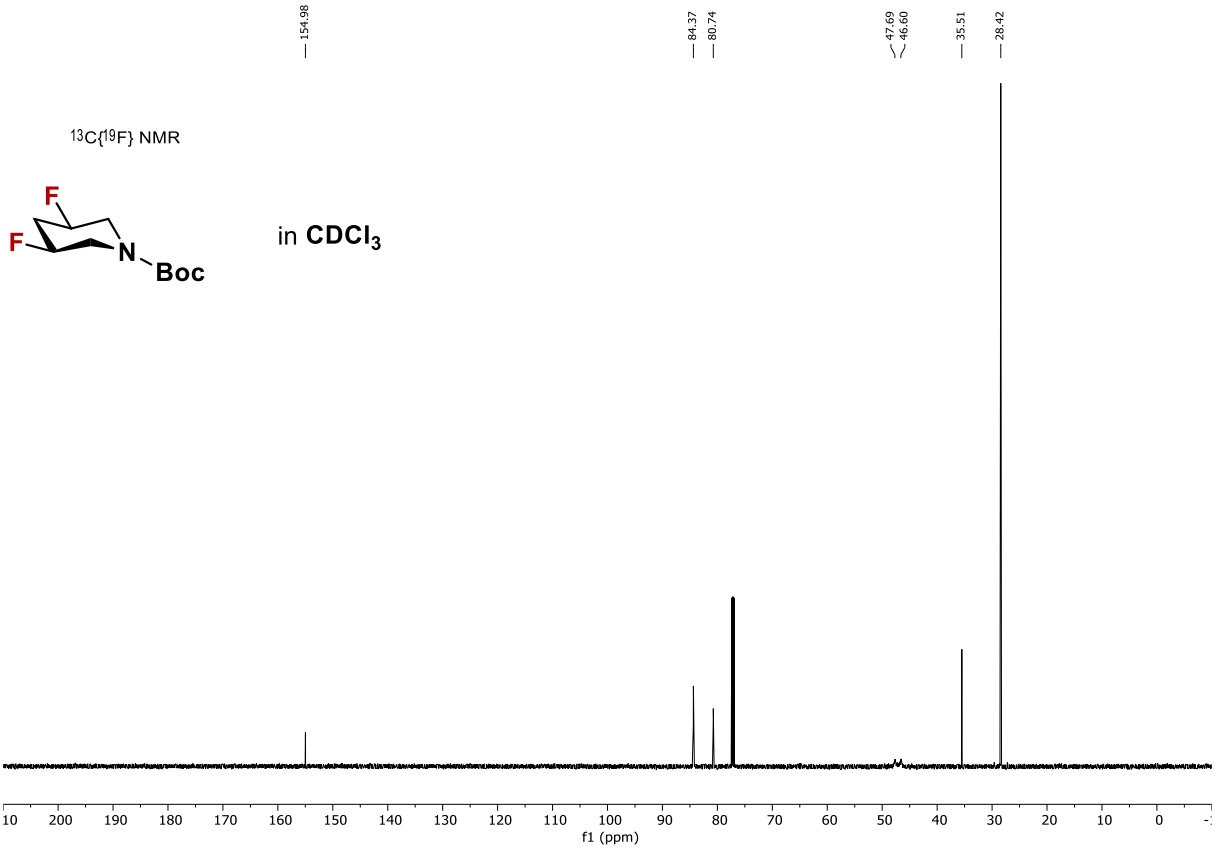


^{1}H{^{19}F} NMR

in **$CDCl_3$**

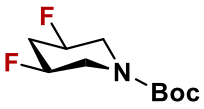



154.99
84.94
83.80
80.75
47.78
46.70
35.65
35.51
35.38
28.42
13C NMR
F
F
N
Boc
in CDCl3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

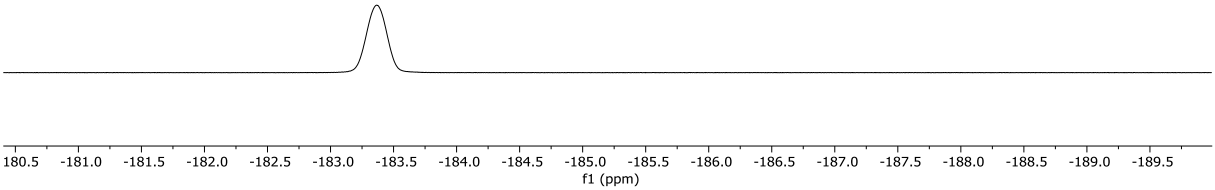

154.98
84.37
80.74
47.69
46.60
35.51
28.42
13C{19F} NMR
F
F
N
Boc
in CDCl3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

-183.37

^{19}F NMR

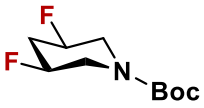


in **$CDCl_3$**

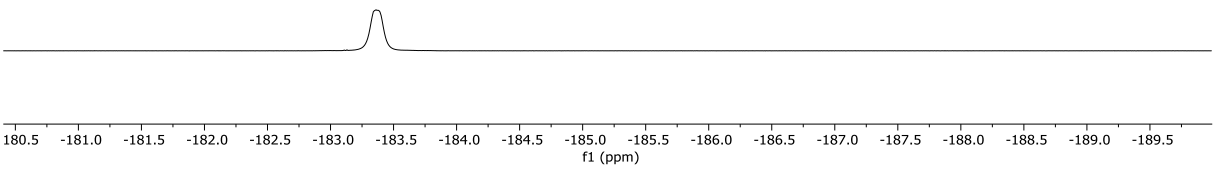


-183.36

^{19}F{^{1}H} NMR

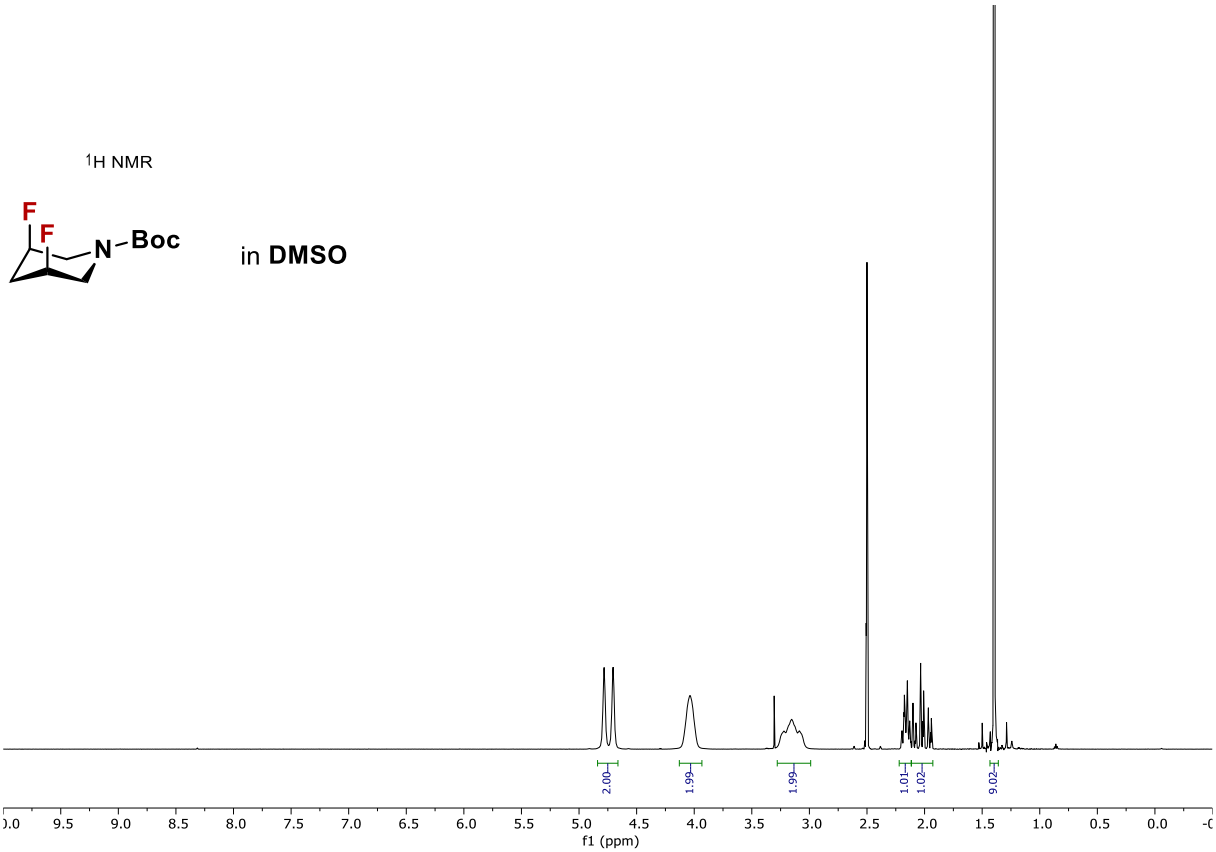


in **$CDCl_3$**



^{1}H NMR

in **DMSO**



^{1}H{^{19}F} NMR

in **DMSO**