Supporting information

From Cyclic (Alkyl)(Amino)Carbene (CAAC) Precursors to Fluorinating Reagents. Experimental and Theoretical Study.

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S1 Characterization of salts

S1.1 NMR spectroscopy

S1.1.1 ^{Me}CAAC(H)F (1)

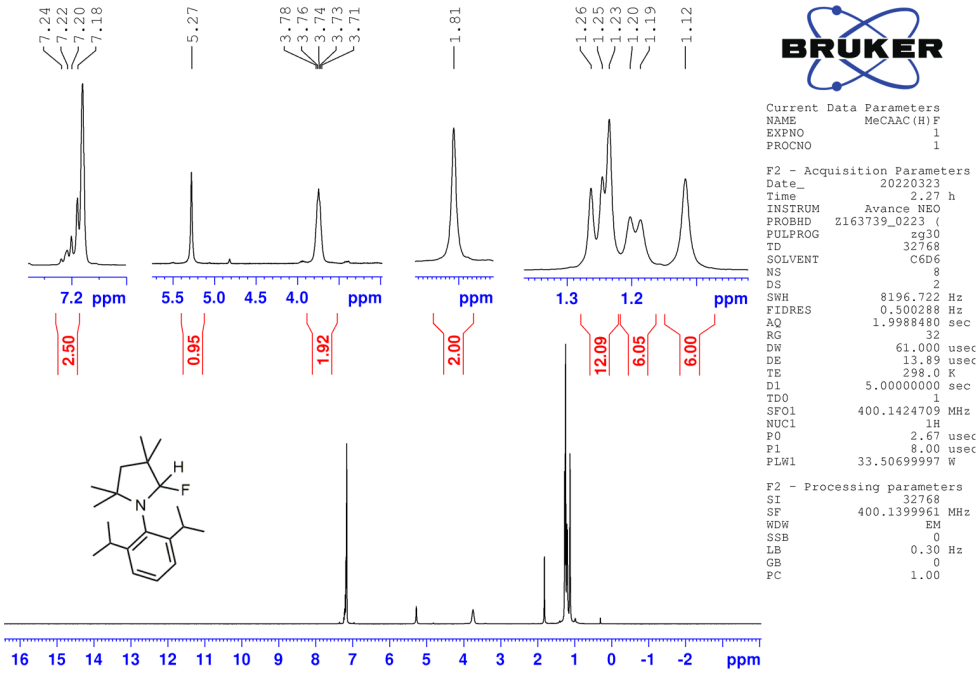


Figure S1. ^{1}H NMR spectrum of ^{Me}CAAC(H)F (**1**) in C_6D_6 solution.

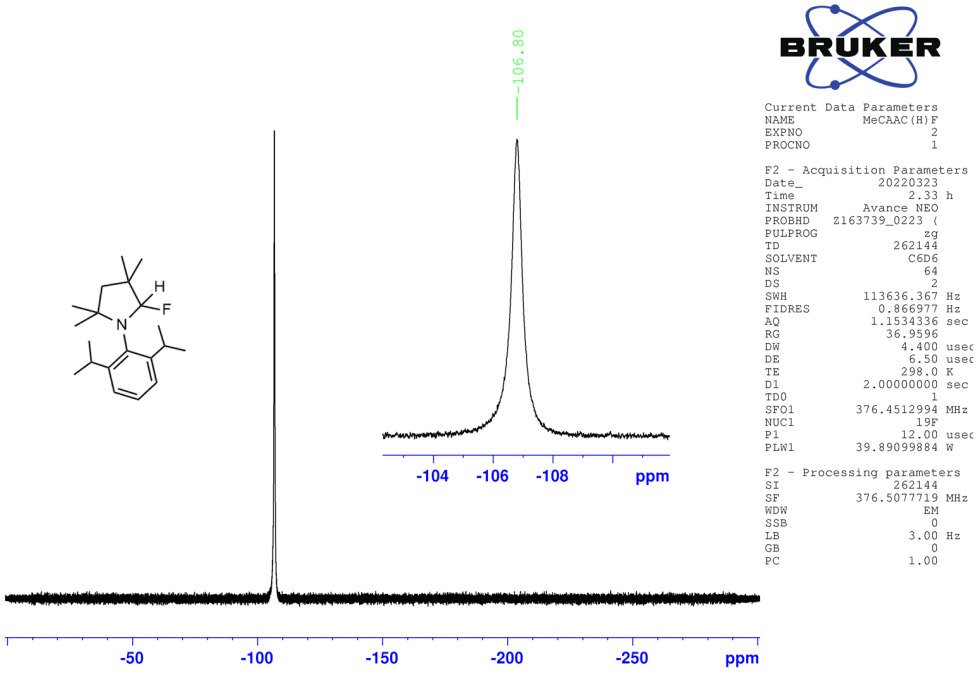


Figure S2. ^{19}F NMR spectrum ^{Me}CAAC(H)F (**1**) in C_6D_6 solution.

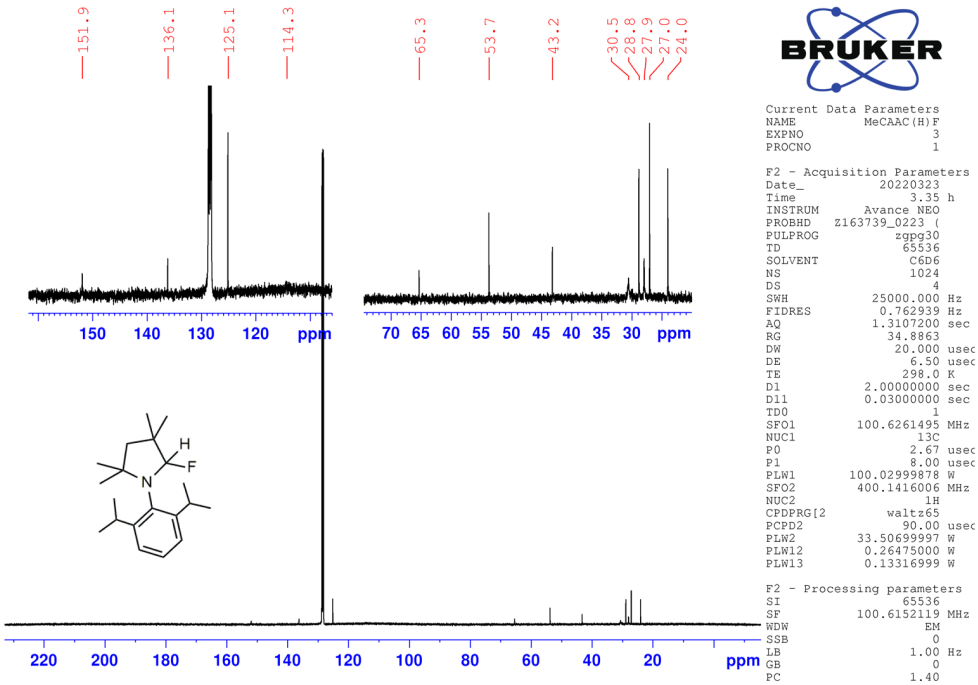


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum ^{Me}CAAC(H)F (**1**) in C_6D_6 solution.

*S1.1.2 Temperature dependence of ^{Me}CAAC(H)F (**1**) in toluene solution*

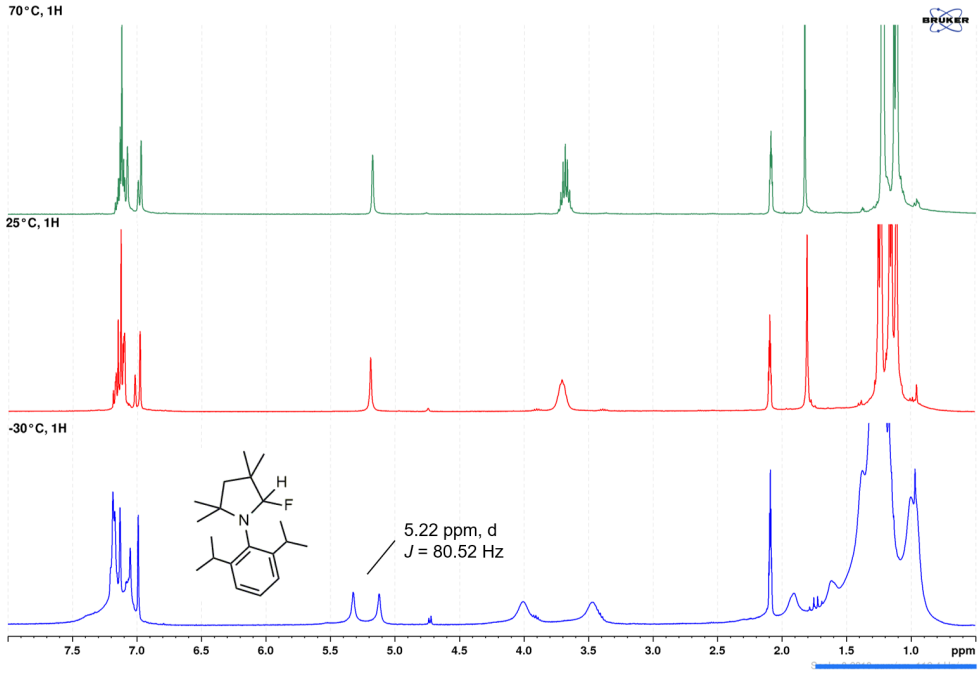


Figure S4. Comparison of ^{1}H NMR spectra of ^{Me}CAAC(H)F (**1**) in toluene solution measured at −30 °C, 25 °C and 70 °C.

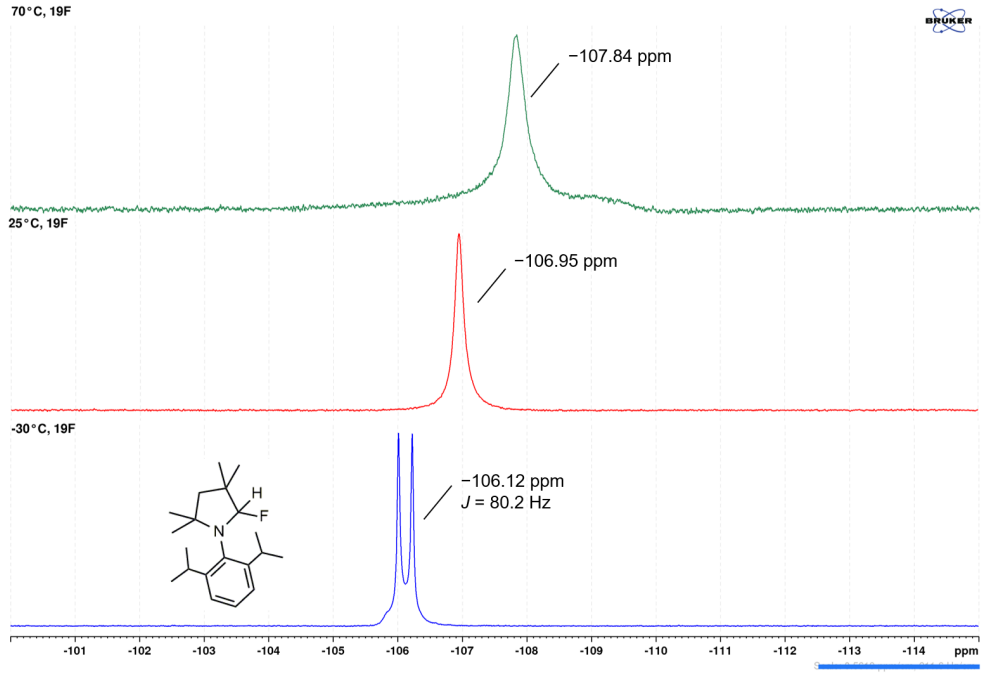


Figure S5. Comparison of ^{19}F NMR spectra of ^{Me}CAAC(H)F (**1**) in toluene solution measured at −30 °C, 25 °C and 70 °C.

*S1.1.3 [^{Me}CAACH][F(HF)] (**2**)*

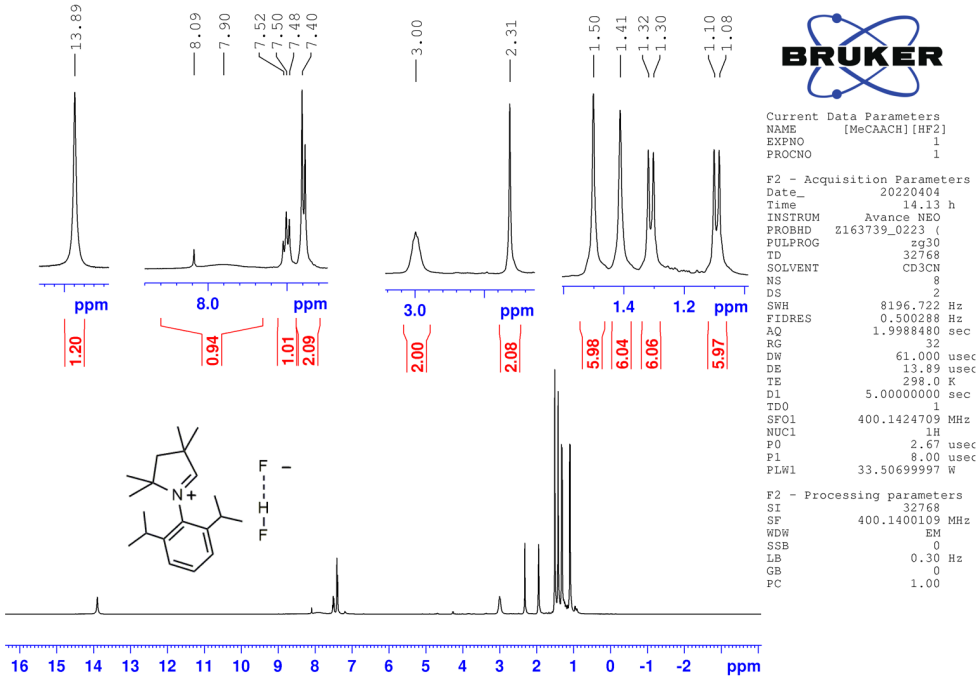


Figure S6. ^{1}H NMR spectrum of [^{Me}CAACH][F(HF)] (**2**) in acetonitrile solution.

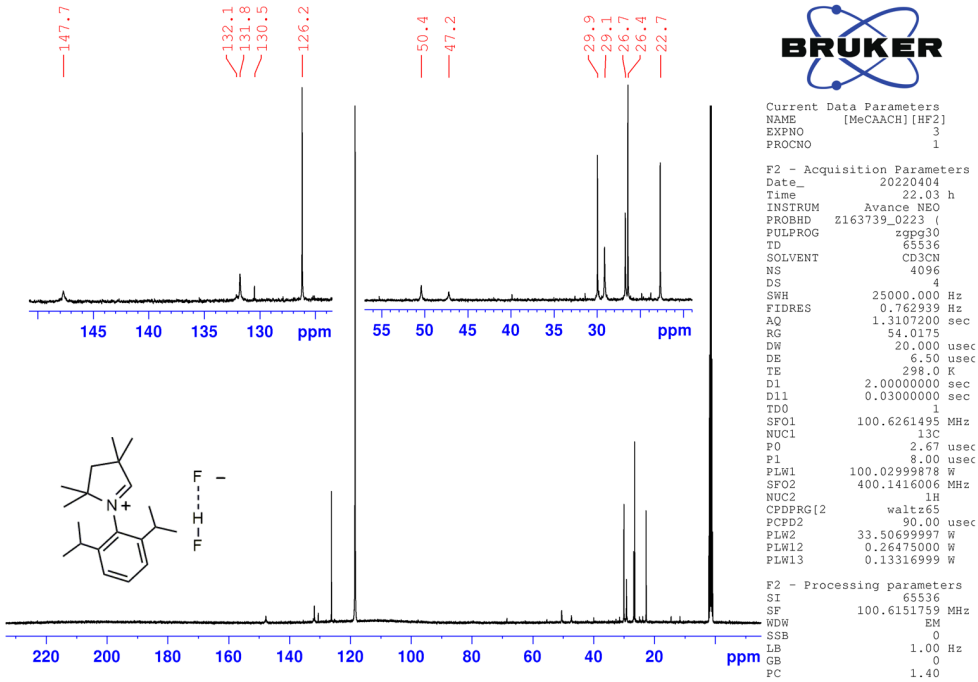


Figure S7. ^{13}C{^{1}H} NMR spectrum of [^{Me}CAACH][F(HF)] (**2**) in acetonitrile solution.

*S1.1.4 Temperature dependence of [^{Me}CAACH][F(HF)] (**2**) in acetonitrile solution*

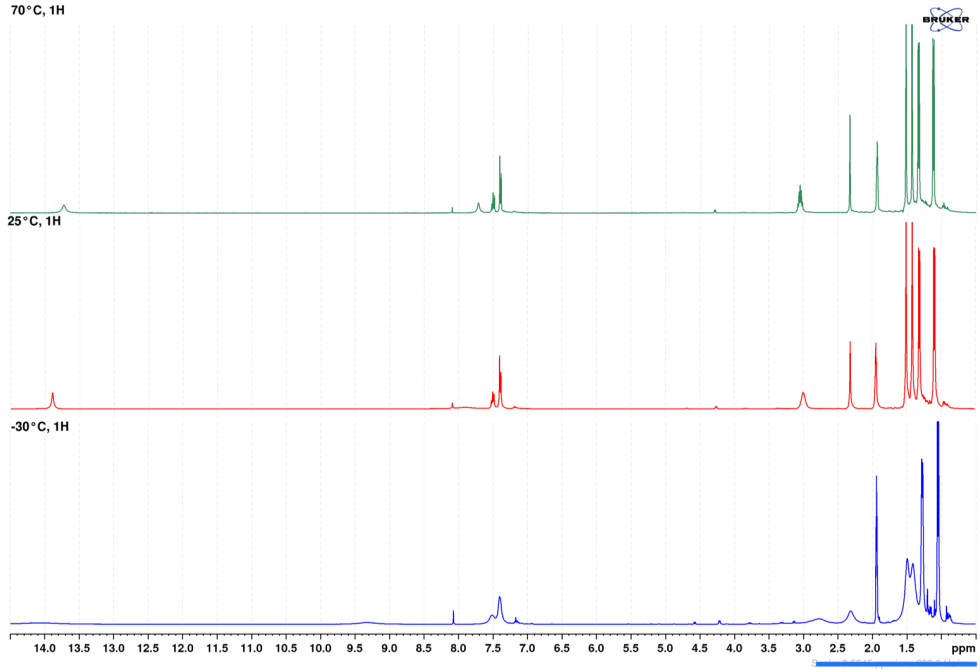


Figure S8. Comparison of ^{1}H NMR spectra of [^{Me}CAACH][F(HF)] (**2**) in acetonitrile solution measured at −30 °C, 25 °C and 70 °C.

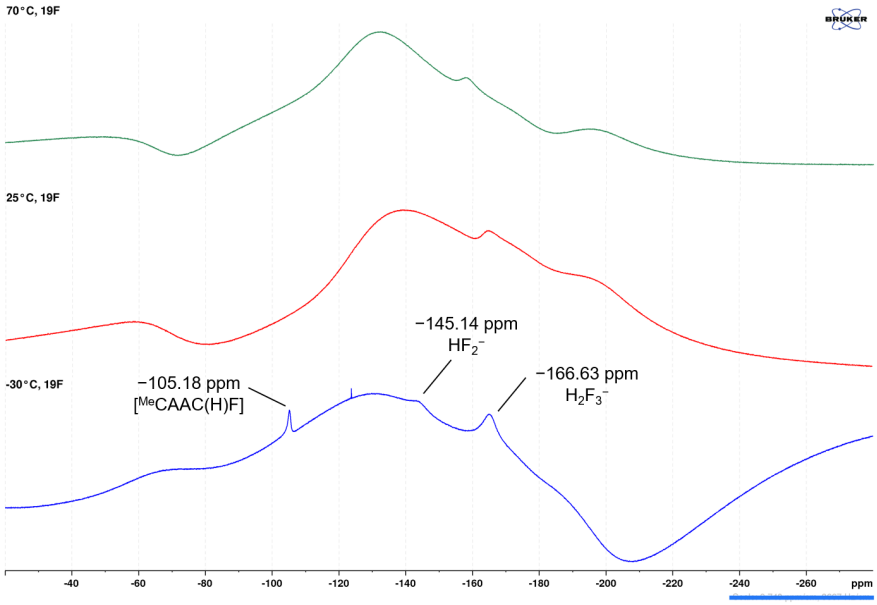


Figure S9. Comparison of ^{19}F NMR spectra of [^{Me}CAACH][F(HF)] (**2**) in acetonitrile solution measured at −30 °C, 25 °C and 70 °C.

S1.1.5 [^{Me}CAACH][F(HF)$_2$] (3)

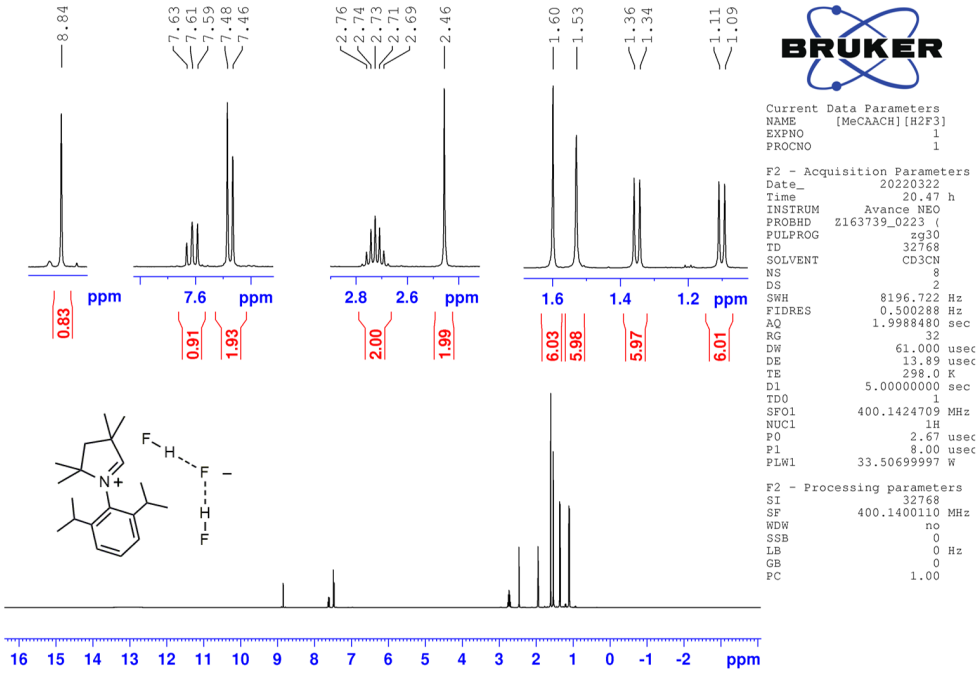


Figure S10. ^{1}H NMR spectrum of [^{Me}CAACH][F(HF)$_2$] (**3**) in acetonitrile solution.

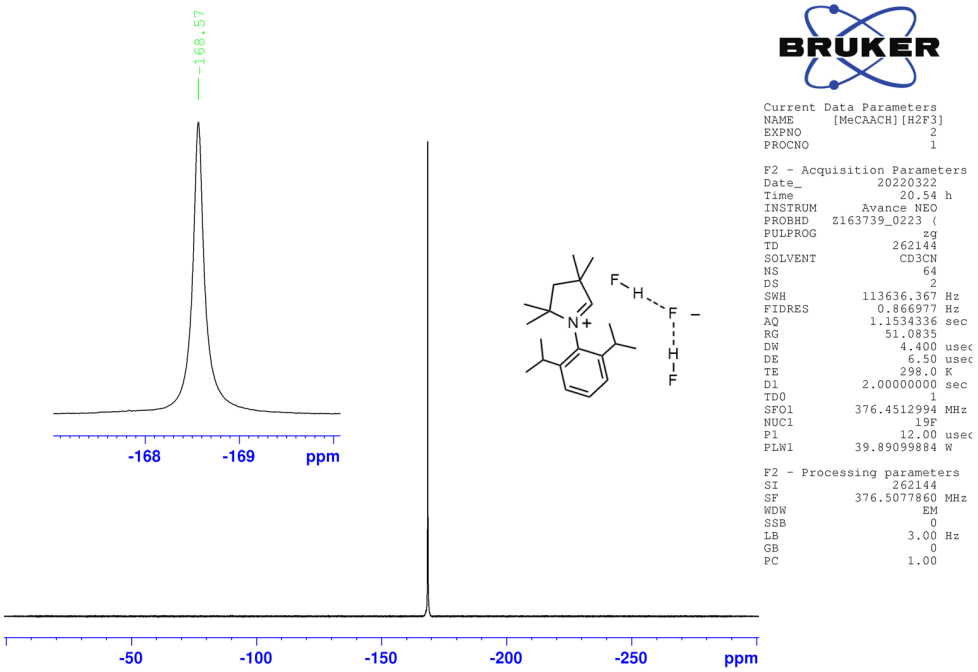


Figure S11. ^{19}F NMR spectrum [^{Me}CAACH][F(HF)$_2$] (**3**) in acetonitrile solution.

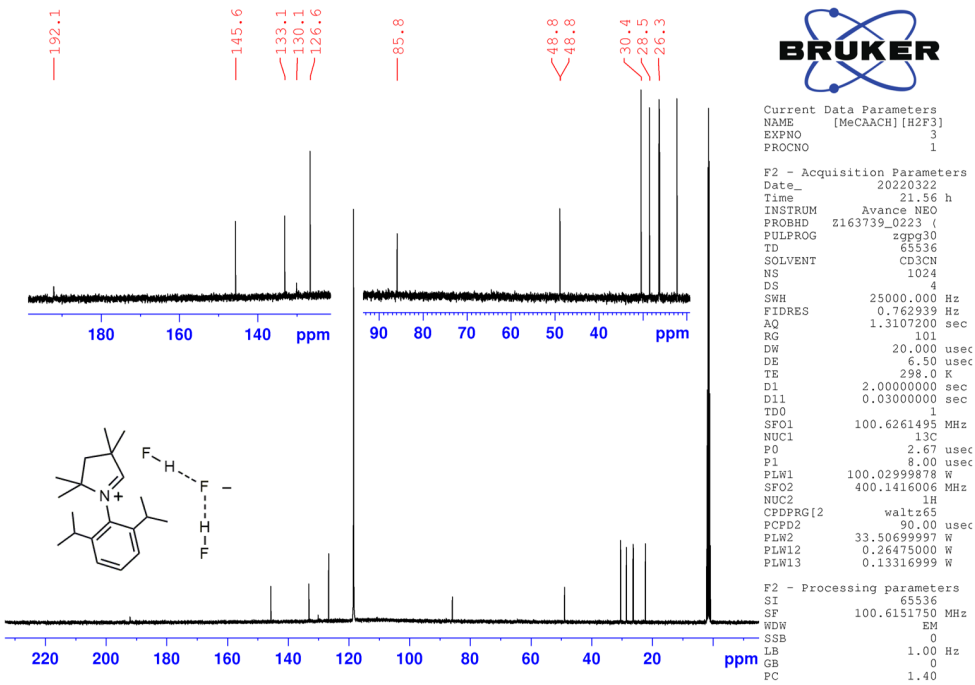


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of [^{Me}CAACH][F(HF)$_2$] (**3**) in acetonitrile solution.

*S1.1.6 [^{Me}CAACH][F(HF)$_3$] (**4**)*

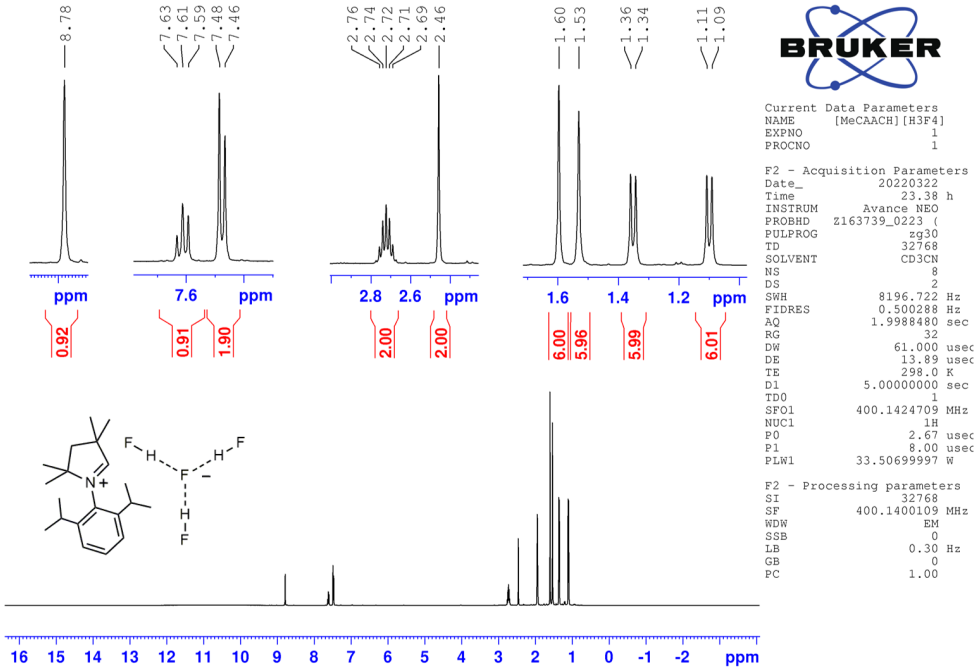


Figure S13. ^{1}H NMR spectrum of [^{Me}CAACH][F(HF)$_3$] (**4**) in acetonitrile solution.

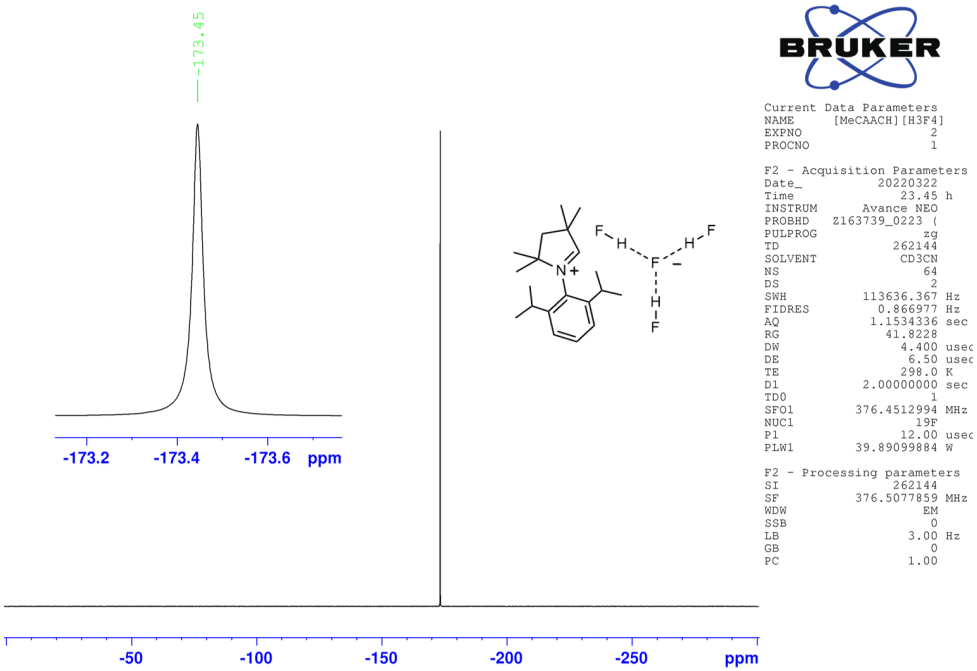


Figure S14. ^{19}F NMR spectrum [^{Me}CAACH][F(HF)$_3$] (**4**) in acetonitrile solution.

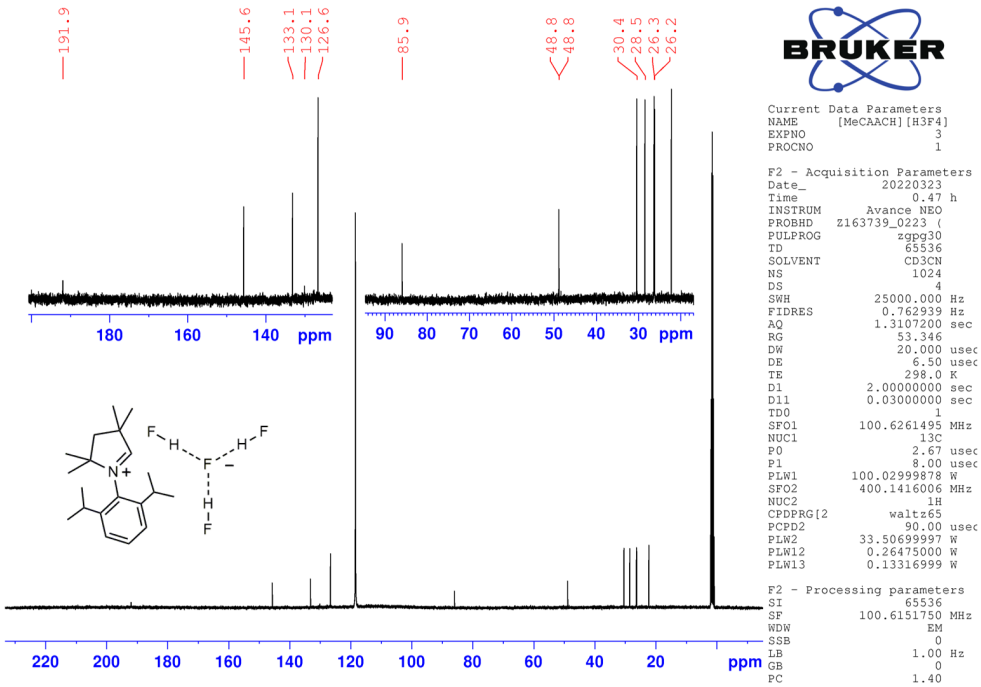


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of [^{Me}CAACH][F(HF)$_3$] (**4**) in acetonitrile solution.

*S1.1.7 [^{Me}CAACH][Br] obtained from **3***

[^{Me}CAACH][Br] was isolated with precipitation with hexane after completion of reactions between bromide substrates and reagent **3**. In ^{1}H NMR spectrum residual peaks of dimethylformamide (DMF) and water are visible.

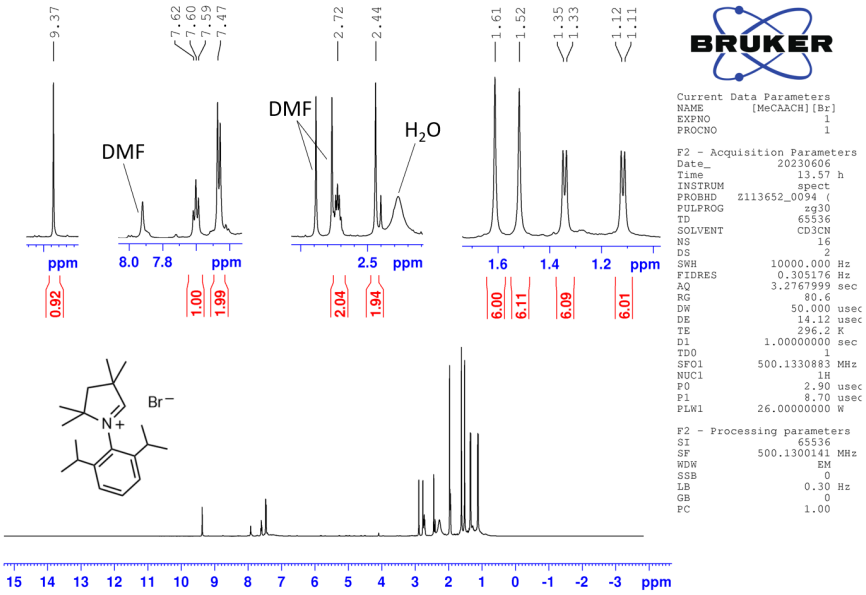


Figure S16. ^{1}H NMR spectrum of [^{Me}CAACH][Br] in acetonitrile solution.

*S1.1.8 [^{Me}CAACH][H_3F_4] (**4**) regenerated from [^{Me}CAACH][Br]*

[^{Me}CAACH][Br] reacted with anhydrous HF to form a mixture of poly(hydrogen fluoride) salts. After the removal of excess HF under reduced pressure of 10^{-2}–10^{-3} bar compound **4** was obtained. The reaction is in agreement with the reaction described in experimental section for the chloride salt.

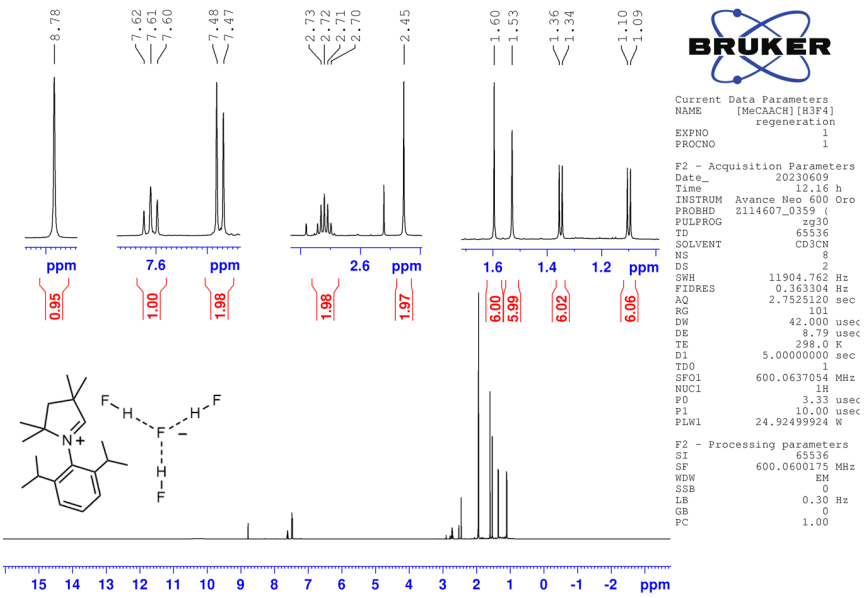


Figure S17. ^{1}H NMR spectrum of [^{Me}CAACH][$F(HF)_3$] obtained after regeneration of [^{Me}CAACH][Br] in acetonitrile solution.

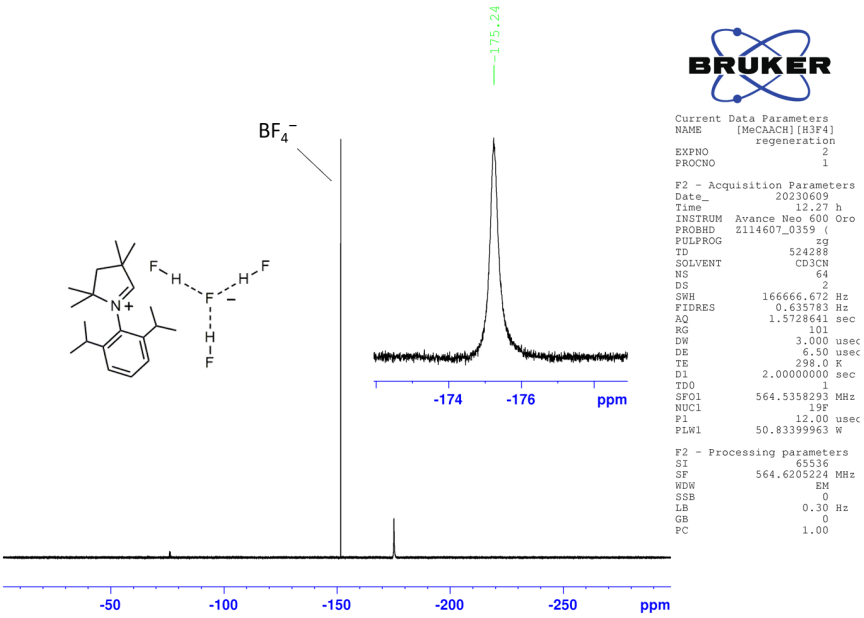


Figure S18. ^{19}F NMR spectrum of [^{Me}CAACH][$F(HF)_3$] obtained after regeneration of [^{Me}CAACH][Br] in acetonitrile solution. At −151.8 ppm the signal for $[BF_4]^-$ anion is present due to the reaction of **4** with glass.

S1.2 Raman spectroscopy

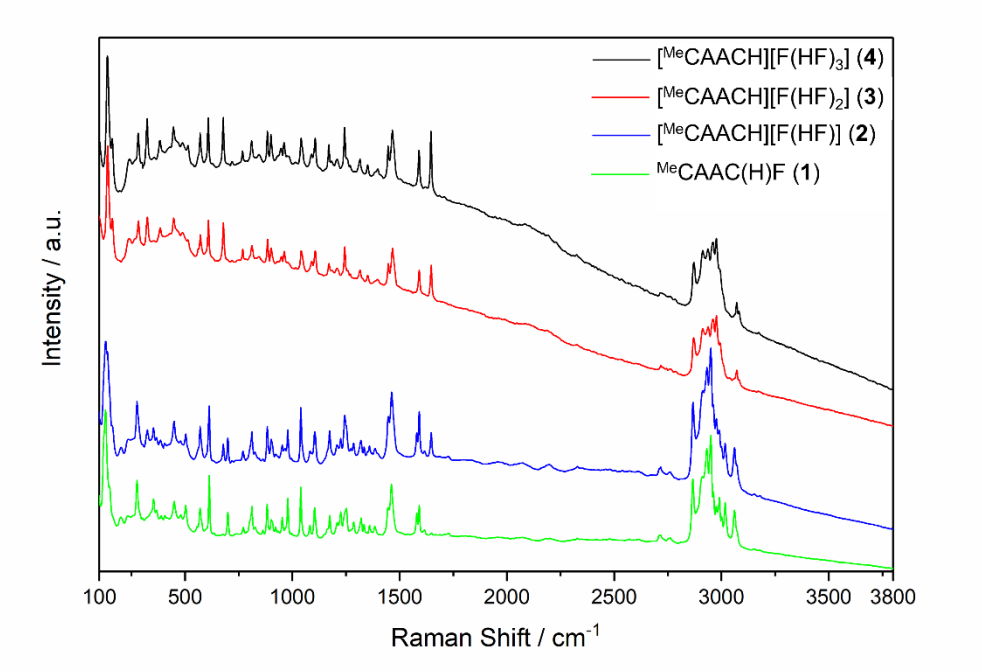


Figure S19. Raman spectra of ^{Me}CAAC(H)F (**1**), [^{Me}CAACH][F(HF)] (**2**), [^{Me}CAACH][F(HF)$_2$] (**3**) and [^{Me}CAACH][F(HF)$_3$] (**4**).

S1.3 Crystal Structure Data

Table S1. Selected crystal data for ^{Me}CAAC(H)F (**1**) and [^{Me}CAACH][F(HF)]·2^{Me}CAAC(H)F (**2a**).

	[^{Me}CAACHF] (**1**)	[^{Me}CAACH][F(HF)]·2^{Me}CAAC(H)F (**2a**)
CCDC No.	2263386	2263387
Chemical formula	$C_{20}H_{32}NF$	$2C_{20}H_{32}NF·C_{20}H_{32}N·HF_2$
F_W (g/mol)	305.46	936.40
T (K)	150	150
λ (Å)	1.54184	1.54184
Cristal size (mm)	0.34 × 0.31 × 0.23	0.35 × 0.27 × 0.12
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	$P\bar{1}$
a (Å)	12.33810(10)	9.3894(3)
b (Å)	12.42200(10)	17.6755(7)
c (Å)	12.3701(2)	17.8951(7)
α (°)	90	96.869(3)
β (°)	106.4960(10)	96.961(3)
γ (°)	90	93.453(3)
V (Å^3)	1817.85(4)	2918.4(2)
Z	4	2
ρ_{calc} (g/cm^3)	1.116	1.066
μ (mm^{-1})	0.548	0.546
F(000)	672	1028
Θ range (°)	3.5–76.3	3.3–72.1
Index ranges	$-15 \le h \le 15$ $-15 \le k \le 15$ $-14 \le l \le 15$	$-11 \le h \le 11$ $-21 \le k \le 21$ $-22 \le l \le 22$
Reflections collected	4451	11761
Independent reflections	4451	11761
Reflections with ($I > 2\sigma(I)$)	4089	8607
R_{int}	na	na
Data / restrains / parameters	4451 / 0 / 208	11761 / 0 / 702
S[a]	1.080	1.037
R_1[b], wR_2[c] ($I > 2\sigma(I)$)	0.0414, 0.1158	0.0566, 0.1491
R_1[b], wR_2[c] (all data)	0.0441, 0.1182	0.0762, 0.1600
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	−0.218, 0.369	−0.198, 0.357

[a] $S = [\Sigma(w(F_o^2-F_c^2)^2)/(N_o-N_p)]^{1/2}$.

[b] $R_1 = ||F_o|-|F_c||/\Sigma|F_o|$.

[c] $wR_2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$.

Table S2. Selected crystal data for [^{Me}CAACH][F(HF)$_2$] (**3**), [^{Me}CAACH][F(HF)$_3$] (**4**) and [^{Me}CAACH][F(HF)$_{3.5}$] (**5**).

	[^{Me}CAACH][F(HF)$_2$] (**3**)	[^{Me}CAACH][F(HF)$_3$] (**4**)	[^{Me}CAACH][F(HF)$_{3.5}$] (**5**)
CCDC No.	2263384	2263388	2263385
Chemical formula	$C_{20}H_{32}N{\cdot}H_2F_3$	$C_{20}H_{32}N{\cdot}H_3F_4$	$2C_{20}H_{32}N{\cdot}H_7F_9$
F_W (g/mol)	345.48	365.49	750.98
T (K)	150	150	150
λ (Å)	1.54184	1.54184	1.54184
Cristal size (mm)	0.46 × 0.22 × 0.20	0.61 × 0.42 × 0.27	0.34 × 0.28 × 0.22
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$
a (Å)	10.8109(4)	10.4339(3)	10.9075(2)
b (Å)	9.4778(3)	14.8964(5)	31.7144(5)
c (Å)	20.4419(7)	14.3883(5)	12.9548(2)
α (°)	90	90	90
β (°)	103.161(4)	100.056(3)	90.396(1)
γ (°)	90	90	90
V (Å^3)	2039.53(12)	2201.98(13)	4481.3(1)
Z	4	4	4
ρ_{calc} (g/cm^3)	1.125	1.102	0.756
μ (mm^{-1})	0.684	0.724	1.113
F(000)	752	792	1624
Θ range (°)	4.2–71.8	2.9–71.9	3.6–72.2
Index ranges	−13 ≤ h ≤ 13 −9 ≤ k ≤ 11 −25 ≤ l ≤ 25	−11 ≤ h ≤ 12 −18 ≤ k ≤ 17 −15 ≤ l ≤ 17	−12 ≤ h ≤ 13 −39 ≤ k ≤ 38 −15 ≤ l ≤ 14
Reflections collected	16584	16124	38097
Independent reflections	3973	4295	8757
Reflections with ($I > 2\sigma(I)$)	3211	3212	6680
R_{int}	0.0388	0.0356	0.0343
Data / restrains / parameters	3973 / 0 / 232	4295 / 0 / 243	8757 / 0 / 518
S[a]	1.056	1.044	1.038
R_1[b], wR_2[c] ($I > 2\sigma(I)$)	0.0498, 0.1289	0.0502, 0.1323	0.0607, 0.1666
R_1[b], wR_2[c] (all data)	0.0619, 0.1391	0.0671, 0.1475	0.0775, 0.1811
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	−0.163, 0.469	−0.149, 0.313	−0.292, 0.414

[a] $S = [\Sigma(w(F_o^2-F_c^2)^2)/(N_o-N_p)]^{1/2}$.

[b] $R_1 = ||F_o|-|F_c||/\Sigma|F_o|$.

[c] $wR_2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$.

S1.3.1 Crystal structures

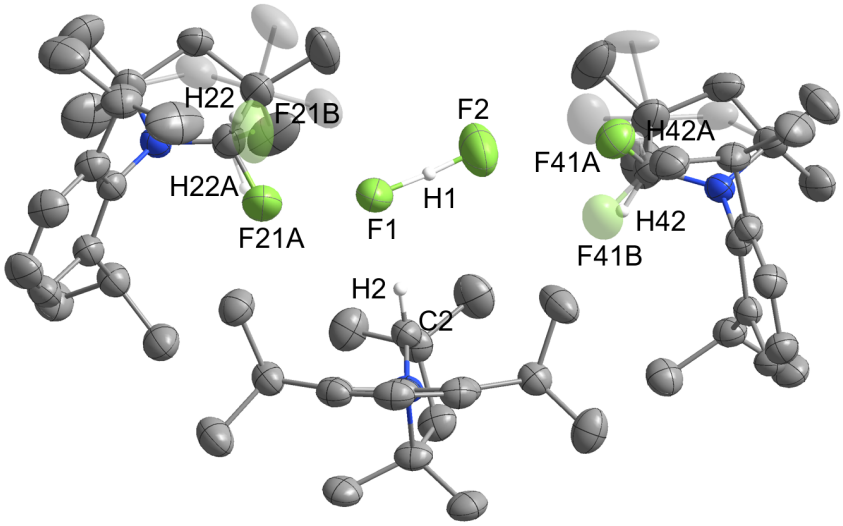


Figure S20. Crystal structure of [MeCAACH][F(HF)]·2MeCAAC(H)F (**2a**). The ellipsoids are drawn at 50% probability. The positions of disordered atoms are shown in domains A and B. For clarity, domain B is shaded and all hydrogen atoms are omitted except for the one at C2 position. Selected bond lengths (Å) and angles (°): F(1)···F(2) 2.235(2), F(1)···F(21A) 2.676(3), F(1)···F(21B) 2.672(8), F(2)···F(41A) 2.664(3), F(2)···F(41B) 2.820(5), C(2)–H(2) 0.950(2), N(1)–C(2) 1.275(3), N(1)–C(2)–H(2) 122.8(2).

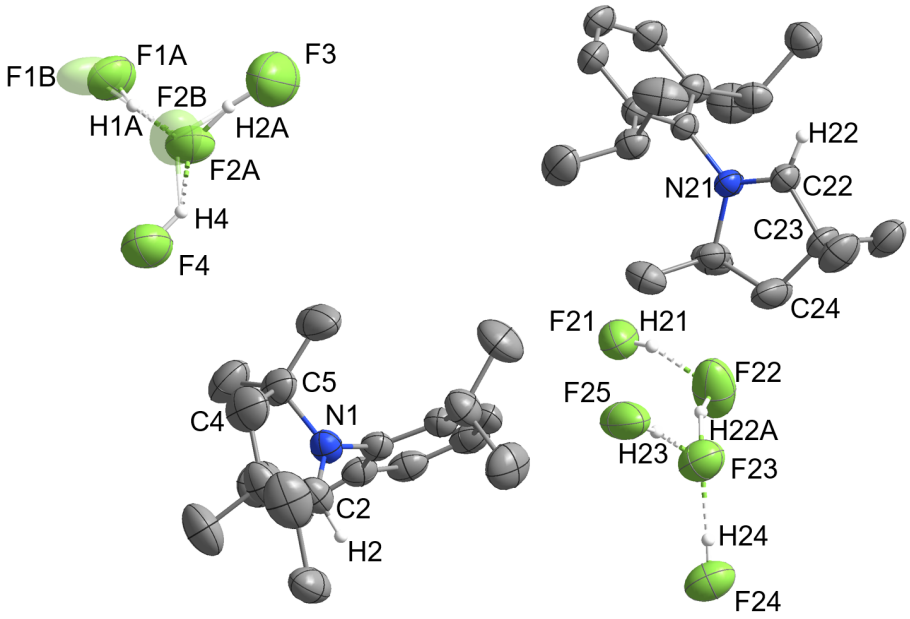


Figure S21. Crystal structure of [^{Me}CAACH][F(HF)$_{3.5}$] (**5**). The ellipsoids are drawn at 50% probability. The positions of disordered atoms are shown in domains A and B. For clarity, domain B is shaded and all hydrogen atoms are omitted except for the one at C2 position. Selected bond lengths (Å) and bond angles (°) for [^{Me}CAACH][H_3F_4] ion pair: F(1A)···F(2A) 2.26(2), F(1B)···F(2B) 2.27(2), F(2A)···F(3) 2.27(1), F(2B)···F(3) 2.29(2), F(2A)···F(4) 2.38(1), F(2B)···F(4) 2.38(1), C(2)–H(2) 0.950(2), N(1)–C(2) 1.273(3), F(1A)–F(2A)–F(3) 108.9(5), F(1B)–F(2B)–F(3) 115.4(8), F(1A)–F(2A)–F(4) 114.4(5), F(1B)–F(2B)–F(4) 113.1(5), F(3)–F(2A)–F(4) 127.3(5), F(3)–F(2B)–F(4) 131.4(8), N(1)–C(2)–H(2) 122.7(2). Selected bond lengths (Å) and bond angles (°) for [^{Me}CAACH][H_4F_5] ion pair: F(21)···F(22) 2.417(3), F(22)···F(23) 2.275(3), F(23)···F(24) 2.408(3), F(23)···F(25) 2.381(3), C(22)–H(22) 0.950(2), N(21)–C(22) 1.271(3), F(21)–F(22)–F(23) 121.8(1), F(22)–F(23)–F(24) 128.6(1), F(22)–F(23)–F(25) 112.8(1), N(21)–C(22)–H(22) 122.5(2).

S2 Computational study

S2.1 Fluoropyrrolidine 1A/dihydropyrrolium fluoride 1B system

The initial conformational search using the RI-DFT method and the double-ζ def2-SVP basis set in the simulated solvent (see Experimental for computational details) showed a strong energetical preference for **1A** over **1B** in agreement with the experimental data. The computational results are given in Table S3. Regarding the position of F^- in **1B**, two orientations were found leading to the structures **1Ba** and **1Bb**. **1Ba** (Table S3, entry 2), in which the F^- anion is coordinated to the dihydropyrrolium hydrogen, is preferred. In the second, less stable structure **1Bb** (Table S3, Entry 3), F^- is localised below the dihydropyrrolium ring. The three selected structures are shown in Figure S22.

Table S3. Comparison of stability of fluoropyrrolidine **1A** and dihydropyrrolium fluorides **1B** using various computational approaches (Gibbs free energies given).

Entry	Structure	Method	Rel. energy (kJ/mol)	Bond lengths (Å)	
				C2–F	H2···F
1	**1A**	M06L/def2-SVP	0	1.453	
2	**1Ba**	M06L/def2-SVP	68.8		1.487
3	**1Bb**	M06L/def2-SVP	98.2		4.339
4	**1A**	M06L/def2-SVPD	0	1.482	
5	**1Ba**	M06L/def2-SVPD	13.6		1.658
6	**1Bb**	M06L/def2-SVPD	35.5		5.051
7	**1A**	M06-2X/def2-TZVP	0	1.448	
8	**1Ba**	M06-2X/def2-TZVP	39.9		1.671
9	**1Bb**	M06-2X/def2-TZVP	55.1		4.580
10	**1A**	ma-M06-2X/def2-TZVP	0	1.449	
11	**1Ba**	ma-M06-2X/def2-TZVP	27.7		1.744
12	**1Bb**	ma-M06-2X/def2-TZVP	38.6		5.018
13	**1A**	M06-2X/def2-TZVPD	0	1.449	
14	**1Ba**	M06-2X/def2-TZVPD	24.4		1.736
15	**1Bb**	M06-2X/def2-TZVPD	39.2		5.009
16	**1A**	DSD-PBEP86/TZVP		1.463	
17	**1A**	DSD-PBEP86/TZVPP		1.463	
18	**1A**	**Exp**		**1.450(2)**	

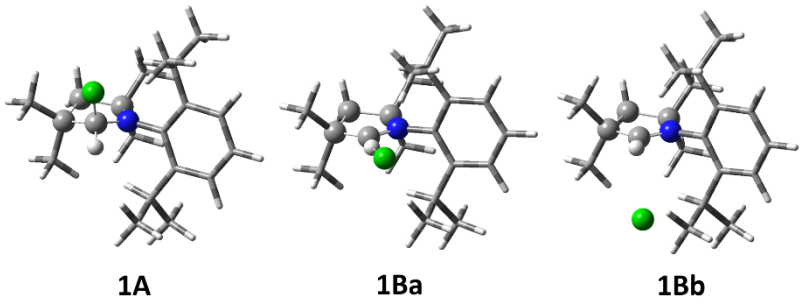


Figure 22. Selected computed structures of fluoropyrrolidine **1A** and dihydropyrrolium fluorides **1B**. For clarity, the substituents on the heterocyclic ring are drawn as tubes.

Considering that a correct description of anionic structures should include diffuse functions, we re-optimized all three structures using the same functional and the def2-SVPD basis set. Although the energetical difference between **1A** and **1B** decreased significantly, structure **1A** still remained the most stable, which is consistent with the experimental results. Aiming to obtain more quantitative results that could be more suitable for evaluating the **1** + **3** → **2** + **2** isodesmic reaction, we further switched to the more precise hybrid functional M06-2X and the more accurate triple-ζ def2-TZVP basis set, optionally supplemented by either minimally augmented (ma-def2-TZVP) or fully augmented (def2-TZVPD) basis sets (Table S3, entries 7–15). Triple-ζ basis sets were recommended instead of using diffuse functions supplemented by double-ζ basis sets, and the use of diffuse functions for larger sets was said to be unnecessary.[1] The energetical differences between **1A** and **1B** obtained using the def2-TZVPP basis set and more accurate functions were approximately between the results with double-ζ basis sets (Table S3, entries 7–9). The addition of diffuse functions reduced this difference somewhat, less for minimally augmented (Table S3, entries 10–12) and more for fully augmented (Table S3, entries 13–15) basis sets. The C2–F bond became longer when diffuse functions were added to the double-ζ basis set (from 1.453 Å to 1.482 Å), but surprisingly became shorter and almost constant (from 1.448 Å to 1.449 Å) for all triple-ζ calculations. On the other hand, the distance between H2 of the dihydropyrrolium salt and the coordinated F^- anion gradually increased from 1.487 Å to 1.744 Å as the quality of the calculations increased. Finally, to obtain even better energetics for the global minimum **1A**, we optimised it with the recently recommended Martin's „DSD"-double scale hybrid functional,[2] which combines the DFT method with spin-component-scaled MP2 mixing and TZVP or TZVPP basis sets (Table S3, entries 16 and 17). Both calculations resulted in a C–F distance of 1.463 Å, which is slightly longer than the crystal bond length of 1.450 Å (Table S3, entry 18).

S2.2 Fluoropyrrolidine·HF 2A/dihydropyrrolium hydrogen difluoride 2B system

Initial tentative calculations were again performed using a pure functional and a simple def2-SVP basis set. Seven significant geometries were found in the conformational space. The 3 selected structures are shown in Figure S23. The computational data are given in Table S4. Surprisingly, the most stable structure turned out to be a fluoropyrrolidine with HF coordinated to the fluorine assigned to **2A** (Table S4, entry 1). In fact, two stable conformers with different orientations were found, of which only the more stable one is shown.

Table S4. Comparison of stability of fluoropyrrolidine·HF **2A** and dihydropyrrolium hydrogen difluorides **2B** using various computational approaches (Gibbs free energies given).

Entry	Structure	Method	Rel. energy (kJ/mol)	Bond lengths (Å)			
				C2–F	H2···F	F–(HF)	F···F
1	**2A**	M06L/def2-SVP	0	1.571		0.952/1.569	2.521
2	**2Ba**	M06L/def2-SVP	3.6		1.772	1.032/1.288	2.318
3	**2Bb**	M06L/def2-SVP	13.1		4.607	1.067/1.232	2.300
4	**2A**	M06L/def2-SVPD	NA				
5	**2Ba**	M06L/def2-SVPD	1.5		1.888	1.040/1.281	2.321
6	**2Bb**	M06L/def2-SVPD	0		4.493	1.135/1.150	2.285
7	**2A**	M06-2X/def2-TZVP	39.9	1.532		0.951/1.563	2.514
8	**2Ba**	M06-2X/def2-TZVP	0		2.127	1.116/1.148	2.264
9	**2Bb**	M06-2X/def2-TZVP	9.8		4.810	1.123/1.144	2.269
10	**2A**	ma-M06-2X/def2-TZVP	48.5	1.539		0.952/1.555	2.507
11	**2Ba'**	ma-M06-2X/def2-TZVP	0		1.960	1.105/1.162	2.267
12	**2Bb**	ma-M06-2X/def2-TZVP	10.6		4.849	1.128/1.138	2.267
13	**2A**	M06-2X/def2-TZVPD	47.0	1.537		0.953/1.552	2.504
14	**2Ba'**	M06-2X/def2-TZVPD	0		1.953	1.106/1.162	2.270
15	**2Bb**	M06-2X/def2-TZVPD	9.8		4.858	1.101/1.139	2.268
16	**2Ba**	DSD-PBEP86/TZVP			1.918	1.094/1.176	2.270
17	**2Ba**	DSD-PBEP86/TZVPP			4.858	1.082/1.190	2.272
18	**2Ba**	**Exp**			**2.043(2)**	**1.19(3)/1.06(3)**	**2.235(2)**

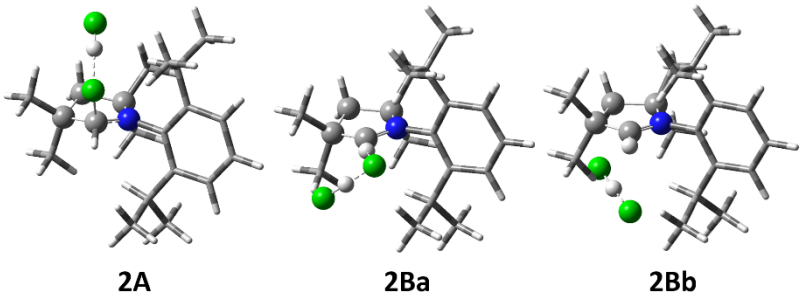
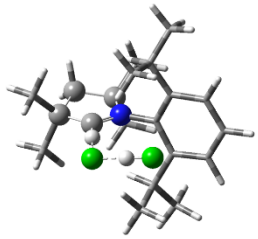


Figure 23. Selected computed structures of fluoropyrrolidine **2A** and dihydropyrrolium dihydrogen difluorides **2B** at the ma-M06L/def2-TZVP level. For clarity, the substituents on the heterocyclic ring are drawn as tubes.

Almost identical stability was shown by the ionic structure with the $[F(HF)]^-$ anion coordinated to the dihydropyrrolium C2–H hydrogen (**2Ba**, Table S4, entry 2). Other structures with the $[F(HF)]^-$ anion oriented below or above the dihydropyrrolium ring were more than 20 kJ/mol less stable. Structure **2Bb** (Table S4, entry 3) is shown as a typical example. After adding diffusion functions to the def2-SVP basis set, the results of optimisations changed significantly. Structure **2A** was no longer a minimum on the PES of the system and only **2B** structures in different conformations were found to be stable structures. Among the six calculated structures with quite similar Gibbs free energy, structure **2Ba** (Table S4, entry 5) and structure **2Bb** (Table S4, entry 6) were the most stable due to coordination energy and favourable entropy, respectively. Computations at the higher level as before (M06-2X/def2-TZVP) again revealed **2A** as a stable structure (Table S4, entry 7), but with a much higher energy (almost 40 kJ/mol) than the salts **2B**, which is in contrast to the double-ζ basis set calculation. Structure **2Ba** (Table S4, entry 8) was found to be almost 10 kJ/mol more stable than structure **2Bb** (Table S4, entry 9) and other similar structures where the anion is coordinated below or above the heterocyclic ring. The use of a minimally (ma-def2-TZVP) or fully (def2-TZVPD) augmented triple-ζ basis set by diffuse functions gave analogous results, further increasing the difference between structures **2A** and **2B** (Table S4, entries 10–15). For the last two basis sets, the **2Ba'** structure with different orientation of the $[F(HF)]^-$ anion became the most stable structure (Figure S24).



2Ba'

Figure 24. Preferred orientation of the $[F(HF)]^-$ anion in the **2Ba'** structure computed at the triple-ζ basis set level. For clarity, the substituents on the heterocyclic ring are drawn as tubes.

In computations, compound 2 appears to be the most sensitive to the quality of the calculations, with the simple double-ζ basis set underestimating the stability of the $[F(HF)]^-$ anion and the double-ζ basis set including diffuse functions overestimating it. Again, all triple-ζ basis sets gave analogous results. The higher stability of the $[F(HF)]^-$ anion**,** observed in the higher quality calculations**,** is reflected in the fact that the C2–H···$[F(HF)]^-$ distance increases from 1.772 Å to 1.918 Å. The $[F(HF)]^-$ anion becomes increasingly symmetrical as more diffuse functions are added. On the other hand, the $[F(HF)]^-$ anion becomes slightly dissymmetric when calculated at the DSD level. The computed orientation of the $[F(HF)]^-$ anion agrees well with that observed in the crystal structure. The computed structure of the $[F(HF)]^-$ anion is quite close to that of the crystal, with F···F distance decreasing from 2.321 Å for the simple SVPD basis set to 2.264 Å for the TZVP basis set. The best DSD calculation including the TZVPP basis set gave a length of 2.272 Å, which is slightly larger than the crystal value of 2.235**(2)** Å, probably due to the inclusion of the implicit solvent in the calculation. As for the geometry of the $[F(HF)]^-$ anion, the computations gave a linear structure in contrast to the slightly bent structure in the crystal (168°), which is probably caused by the intermolecular interactions in the crystal.

S2.3 Fluoropyrrolidine·2HF 3A/dihydropyrrolium dihydrogen trifluoride 3B system

No **3A** structures were found on the PES of the system, even with the simple double-ζ basis set. Among the multiple minimae found, the structures **3Ba**, **3Bb** and **3Bc** showed the lowest energy, which in all cases involved different coordinations of the $[F(HF)_2]^-$ anion to the C2–H hydrogen (see Figure S25 and Table S5).

Table S5. Relative stability and structural parameters of dihydropyrrolium dihydrogen trifluorides **3B** using various computational approaches (Gibbs free energies given).

Entry	Structure	Method	Rel. energy (kJ/mol)	Angles (°)	Bond lengths (Å)		
				$F^1\cdots F^2\cdots F^3$	$F^1\cdots F^2$	$F^2\cdots F^3$	H2$\cdots$F[a]
1	**3Ba**	M06L/def2-SVP	0	155	2.375	2.383	2.169 (F^1)
2	**3Bb**	M06L/def2-SVP	0.4	95	2.384	2.367	2.137 (F^2)
3	**3Bc**	M06L/def2-SVP	2.5	120	2.353	2.356	2.225 (F^1)
4	**3Ba**	M06L/def2-SVPD	3.3	122	2.379	2.379	2.433 (F^1)
5	**3Bc**	M06L/def2-SVPD	0	122	2.397	2.389	2.006 (F^2)
6	**3Bc'**	M06L/def2-SVPD	4.4	111	2.391	2.394	2.066 (F^2)
7	**3Ba**	M06-2X/def2-TZVP	7.2	121	2.319	2.318	2.370 (F^1)
8	**3Bc**	M06-2X/def2-TZVP	0	131	2.330	2.331	2.051 (F^2)
9	**3Bc'**	M06-2X/def2-TZVP	10.9	112	2.329	2.331	2.133 (F^2)
10	**3Ba**	ma-M06-2X/def2-TZVP	7.5	122	2.320	2.319	2.409 (F^1)
11	**3Bc**	ma-M06-2X/def2-TZVP	0	131	2.330	2.331	2.051 (F^2)
12	**3Bc'**	ma-M06-2X/def2-TZVP	6.7	115	2.330	2.330	2.103 (F^2)
13	**3Ba**	M06-2X/def2-TZVPD	6.9	121	2.321	2.318	2.409 (F^1)
14	**3Bb**	M06-2X/def2-TZVPD	8.2	141	2.314	2.331	2.220 (F^2)
15	**3Bc**	M06-2X/def2-TZVPD	0	115	2.330	2.329	2.056 (F^2)
16	**3Bc**	DSD-PBEP86/TZVP		125	2.354	2.355	2.017 (F^2)
17	**3Bc**	DSD-PBEP86/TZVPP		124	2.351	2.353	2.000 (F^2)
18	**3Bc'**	**Exp**		**108.54(8)**	**2.263(2)**	**2.320(2)**	**2.343(2) (F^1)**

[a] distance to the closest F atom

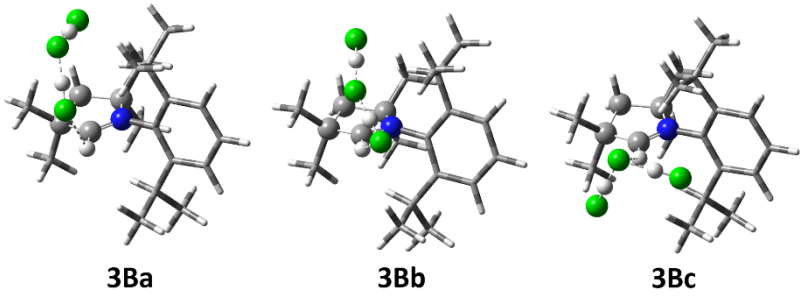
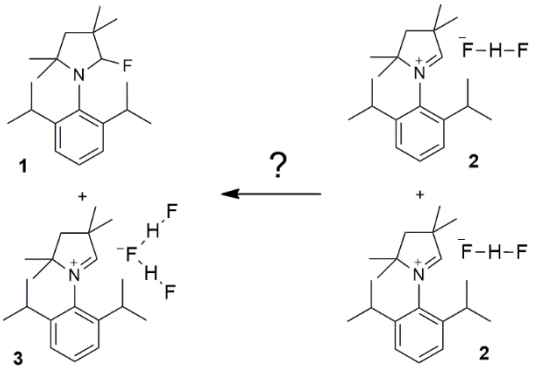


Figure 25. Selected computed structures of dihydropyrrolium dihydrogen trifluorides **3B** at the M06L/def2-SVP level. For clarity, the substituents on the heterocyclic ring are drawn as tubes.

The $[F(HF)_2]^-$ anion corresponds in all cases to an F^- anion coordinated to two HF molecules. The angle varies greatly between 90 and 160° for different structures. Analogous structures were obtained with previously used computational methods (M05L/def2-SVPD, M06-2X/def2-TZVP, M06-2X/ma-def2-TZVP, M06-2X/def2-TZVPD) with different geometries, and the results are listed in the Supporting Information, Table S5. The three main geometries are listed, with the most stable structure at higher levels being **3Bc**, where the $[F(HF)_2]^-$ anion is coordinated to the C2–H hydrogen by the central F atom. This agrees well with the coordination of the $[F(HF)_2]^-$ anion in the crystal structure. The slightly different orientation is probably due to the crystal packing. The observed F···F···F angle of 109° is not far from the calculated value of 124° for the best calculation used. The F···F lengths are about 5% longer than the observed crystal values, again probably as a result off tighter crystal packing compared to the isolated calculated structure in the simulated solvent (Table S5, entries 17 and 18).

S2.4 Isodesmic reaction 1 + 3 → 2 + 2

According to the experimental data, we were able to synthesise and isolate the crystal structures of both the fluoropyrrolidine ^{Me}CAAC(H)F (**1**) and the dihydropyrrolium salt $[^{Me}CAACH][F(HF)_2]$ (**3**), however, the salt $[^{Me}CAACH][F(HF)]$ (**2**) proved to be unstable and disproportionate to **1** and **3**. As mentioned earlier, this was the trigger for us to start the computational study and find all the critical structures. Assuming that the disproportionation was indeed caused by the lower thermodynamic stability of **2**, the isodesmic reaction **1** + **3** → **2** + **2** should be endergonic (Scheme S1).



Scheme 1. Isodesmic reaction of ^{Me}CAAC(H)F (**1**) + $[^{Me}CAACH][H_2F_3]$ (**3**) → $[^{Me}CAACH][HF_2]$ (**2**) + $[^{Me}CAACH][HF_2]$ (**2**).

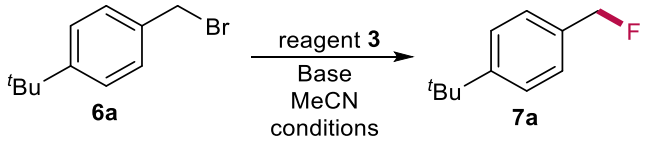
Indeed, the sum of the energies of **1** + **3** calculated with the preliminary double-ζ basis set was 26.4 kJ/mol lower than the sum of the energies **2** + **2** (Table S6, entry 1). However, extending the basis set with diffuse functions gave opposite results and showed that the reaction in Scheme 4 is exergonic with ΔG = −13.9 kJ/mol (Table S6, entry 2). We then tried to improve the quality of our calculations by using a triple-ζ basis set with optional minimal or full augmentation with diffuse functions. The isodesmic reaction was still exergonic even at this level, with the exergonicity increasing with the addition of diffuse functions (Table S6, entries 3–5). Finally, we decided to use the calculation recently recommended spin-component scaled double hybrid functionals blending DFT and perturbation theory, and performed optimisations using the DSD-PBEP86 functional[2] with the triple-ζ def2-TZVP basis set (Table S6, entry 6) or the def2-TZVPP basis with additional polarisation functions (Table S6, entry 7). The energy difference finally obtained, ΔG = −12.5 kJ/mol, is probably the best estimate of the isodesmic equilibrium between the isolated structures **1**, **2** and **3**. The discrepancy between the observed and the calculated results is unclear to us, is probably related to the crystal packing and will be further studied.

Table S6. Results of the isodesmic reaction ^{Me}CAAC(H)F (**1**) + [^{Me}CAACH][H_2F_3] (**3**) → [^{Me}CAACH][HF_2] (**2**) + [^{Me}CAACH][HF_2] (**2**) at various levels of theory.

Entry	Method	ΔG (kJ/mol)
1	M06L/def2-SVP	26.4
2	M06L/def2-SVPD	−13.9
3	M06-2X/def2-TZVP	−10.2
4	M06-2X/ma-def2-TZVP	−22.4
5	M06-2X/def2-TZVPD	−22.3
6	DSDPBEP86/def2-TZVP	−18.4
7	DSDPBEP86/def2-TZVPP	−12.5

S3 Reactivity analysis

Table S7. Model reaction for fluorination of benzyl bromide **4a**. Additional data.



Entry	Reagent **3** [eq.]	Base (eq.)	**6a**	Conversion[a]	Yield of **7a**[a]
1	0.7	DIPEA 1.8	0	100	65
2	1.1	DIPEA 1.8	0	100	60
3	0	DIPEA 4	34	56	0
4	0.7	DIPEA 0.5	32	70	60
5	1	DBU 2	0	100	22
6	1	di-^{t}BuPy[b] 1	49	51	49
7	1	$NaHCO_3$ 1	30	72	64
8	1	$NaHCO_3$ 2	34	70	59
9	1	$NaHCO_3$ 4	92	8	6
10	1	K_2CO_3 1	14	86	78
11	1	Na_2CO_3 1	20	80	74
12	1	Cs_2CO_3 1.2	0	100	98
13	1	Cs_2CO_3 0.5	0	100	99

[a] Conversions and yields were determined with qNMR with naphthalene as an internal standard.

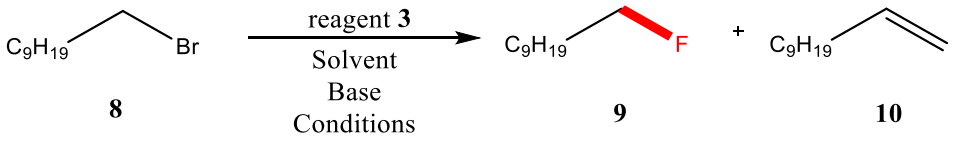
[b] 2,6-di-*tert*-butylpyridine.

Table S8. Conversion of **6a** to **7a** depending on the amount of reagent **3** used.

Entry	Reagent **3**[eq.]	**6a**	**7a**	Conversion [a]	Yield of **7a** [a]
9	0.9	0	100	100	99
10	0.8	0	100	100	99
11	0.7	0	100	100	99
12	0.6	7	93	94	91
13	0.5	10	89	11	83
24	0.4	15	83	17	75

[a] Conversions and yields were determined with qNMR with naphthalene as an internal standard.

Table S9. Fluorination of primary bromide **8**.

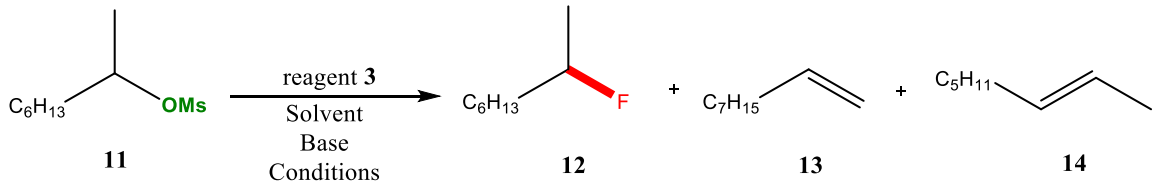


8 **9** **10**

Entry	Reagent **3** [eq.]	Base (eq)	Solvent	Conditions	t [h]	**8**	**9**	**10**	Conversion[a]	NMR yield[a]
1	0.7	Cs_2CO_3 0.5	MeCN	140 °C	1	78	22	0	22	22
2	0.7	Cs_2CO_3 0.5	MeCN	140 °C	5	40	60	0	60	60
3	0.7	Cs_2CO_3 0.5	DMSO	140 °C	5	0	76	24	100	60
4	0.7	Cs_2CO_3 0.5	DMF	140 °C	5	0	100	0	100	35
5	0.7	Cs_2CO_3 0.5	MeCN	140 °C	21	11	83	6	89	83
6	0.7	Cs_2CO_3 0.5	MeCN	140 °C	30	7	91	2	93	91
7	0.7	Cs_2CO_3 0.5	acetone	140 °C	1	99	1	0	99	1

[a] Conversions and yields were determined with qNMR with naphthalene as an internal standard.

Table S10. Optimization of reaction conditions for fluorination of secondary mesylate **11**.



11 **12** **13** **14**

Entry	Reagent **3** (eq.)	Base (eq)	Solvent	Conditions	t [h]	**11**	**12**	**13**	**14**	Conversion[a]	NMR yield[a]
1	1	Cs_2CO_3 1	MeCN	140 °C	2	31	20	15	34	69	22
2	1	Cs_2CO_3 1	MeCN	140 °C	5	23	20	19	38	77	22
3	1	Cs_2CO_3 1	MeCN	140 °C	6	33	11	9	47	67	30
4	1	Cs_2CO_3 1	^{t}BuOH	140 °C	2	0	30	8	46	100	50
5	1	Cs_2CO_3 1	^{t}BuOH	140 °C	6	0	31	11	31	100	30
6	1	Cs_2CO_3 1	^{t}BuOH	130 °C	24	0	23	6	30	100	18
7	1.5	Cs_2CO_3 1.5	^{t}BuOH	140 °C	3	0	47	11	24	100	42
8	1.1	Cs_2CO_3 1.5	^{t}BuOH	140 °C	3	0	56	6	19	100	58

[a] Conversions and yields were determined with qNMR with naphthalene as an internal standard.

Table S11. Characterisation of products obtained by the fluorination of substituted benzyl bromides (additional information to **Table 6**).

6	Substituent	δ ^{1}H (ppm)	δ ^{19}F (ppm)	Ref.
6a	4-^{t}Bu	7.43 (d, J = 7.9 Hz, 2H), 7.34–7.31 (m, 2H), 5.35 (d, J = 48.1 Hz, 2H), 1.33 (s, 10H)	−204.24 (t, J = 48.2 Hz)	3
6b	4-NO_2	8.25 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 7.8 Hz, 2H), 5.49 (d, J = 46.8 Hz, 2H)	−215.68 (t, J = 46.9 Hz)	3
6c	3-OMe	6.98–6.88 (m, 1H), 5.36 (d, J = 47.7 Hz, 1H), 3.83 (s, 1H)	−207.77 (t, J = 47.7 Hz)	3
6d	3-Br	7.36 (d, J = 7.9 Hz, 2H), 7.28 (d, J = 7.8 Hz, 1H), 5.36 (d, J = 47.4 Hz, 2H)	−209.71 (t, J = 47.5 Hz)	4
6e	4-Br	7.47 (dd, J = 7.7, 3.8 Hz, 1H), 7.31 (d, J = 7.8 Hz, 1H), 5.28 (d, J = 47.6 Hz, 1H)	−208.01 (t, J = 47.7 Hz)	5
6f	3,5-CF_3	7.88 (s, 1H), 7.84 (s, 2H), 5.53 (d, J = 46.8 Hz, 2H)	−62.97, −214.29 (t, J = 46.8 Hz)	6
6g	3-Cl	7.35 (s, 1H), 7.32 (d, J = 5.2 Hz, 2H), 7.24 (d, J = 4.4 Hz, 1H), 5.35 (d, J = 47.5 Hz, 2H)	−209.78 (t, J = 47.6 Hz)	7
6h	4-Me	7.28 (dd, J = 8.1, 2.1 Hz, 2H), 7.21 (d, J = 7.7 Hz, 2H), 5.33 (d, J = 48.2 Hz, 2H), 2.37 (d, J = 2.4 Hz, 3H)	−206.35 (t, J = 47.6 Hz)	8
6i	H	7.41–7.38 (m, 3H), 7.36 (d, J = 7.8 Hz, 2H), 5.39 (d, J = 47.9 Hz, 2H)	−206.54 (t, J = 47.8 Hz)	3
6j	4-F	7.36 (d, J = 7.8 Hz, 2H), 7.11–7.06 (m, 2H), 5.34 (d, J = 48.0 Hz, 2H)	(−112.85)–(−112.93) (m), −203.87 (t, J = 48.3 Hz)	NA
6k	2-Ph	7.56 (t, J = 5.7 Hz, 1H), 7.46–7.34 (m, 8H), 5.29 (d, J = 48.1 Hz, 2H)	−199.62 (t, J = 48.0 Hz)	9

Table S12. Characterisation of products obtained by the fluorination of alkyl bromides, alkyl mesylates and other substrates.

Product	**δ ^{19}F (ppm)**	**Ref.**
4-Nitrofluorobenzene	(−102.30)–(−102.36) (m)	10
4-Nitrobenzoyl fluoride	21.23 (s)	11
t-Bu(fluoro)dimethyl silane	(−170.99)–(−171.08) (m)	12
4-Nitrobenzenesulfonyl fluoride	66.00 (s)	13
Phenacyl fluoride	(−199.07)–(−199.26) (m)	14
1,5-Difluoropentane	–218.65 (m)	NA
1-Fluorodecane (**9**)[a]	–217.94 (m)	15
2-Fluorooctane (**12**)	(−171.81)–(−172.13) (m)	15

[a] ^{1}H NMR δ (ppm): 4.43 (dt, J = 47.4, 6.2 Hz, 2H), 1.71–1.65 (m, 2H), 1.28–1.25 (m, 10H), 0.88 (t, J = 6.9 Hz, 3H).

S4 List of computed structures (energies in kJ/mol)

Method M06L/def2-SVP

1A: ΔG = -2454347.8 kJ/mol

C	1.11616	0.49328	1.46002
C	2.46730	1.08094	1.01893
C	2.71719	0.63240	-0.43053
N	0.47886	0.21547	0.13856
H	2.40800	2.18059	1.04538
H	3.28435	0.78854	1.69571
C	0.32380	1.49312	2.29431
H	-0.68397	1.11405	2.52372
H	0.83101	1.66370	3.25536
H	0.22472	2.46705	1.79708
C	1.25963	-0.78474	2.28563
H	1.65969	-0.54821	3.28228
H	0.28068	-1.26601	2.43487
H	1.93417	-1.52081	1.82980
C	3.55398	1.64099	-1.20406
H	4.57056	1.69003	-0.78600
H	3.64858	1.35739	-2.26324
H	3.12566	2.65041	-1.16416
C	3.40118	-0.73071	-0.51063
H	3.50797	-1.05826	-1.55624
H	4.41014	-0.67858	-0.07587
H	2.85837	-1.51971	0.02514
C	-0.85040	-0.28797	-0.00508
C	-1.06424	-1.68753	-0.10693
C	-1.95651	0.59840	-0.06801
C	-2.37395	-2.17280	-0.20363
C	-3.24882	0.06313	-0.15701
C	-3.46400	-1.30923	-0.21058
H	-2.53784	-3.25153	-0.28517
H	-4.10373	0.74444	-0.20405
H	-4.48072	-1.70517	-0.27937
C	-1.80554	2.10511	-0.13612
H	-0.74416	2.33639	0.01729
C	0.07934	-2.67546	-0.19869
H	0.99820	-2.12806	0.04398
C	-2.62297	2.83372	0.92308
H	-2.40083	2.48145	1.94059
H	-2.41853	3.91474	0.89610
H	-3.70546	2.71070	0.76247
C	-2.17391	2.60607	-1.53037
H	-1.58137	2.10951	-2.31116
H	-3.23829	2.43096	-1.75468
H	-1.99619	3.68897	-1.61776
C	-0.04984	-3.83150	0.78390
H	0.84506	-4.47101	0.75169
H	-0.17027	-3.48312	1.82019

H	-0.91134	-4.47647	0.55113
C	0.22688	-3.19231	-1.62732
H	-0.65705	-3.77107	-1.93986
H	0.35510	-2.37261	-2.34989
H	1.10132	-3.85490	-1.71834
C	1.28176	0.51956	-0.95807
H	1.15731	-0.18944	-1.79490
F	0.90826	1.78788	-1.56166

1Ba: ΔG = -2454278.9 kJ/mol

C	-1.30907	-0.17973	1.59958
C	-2.71333	-0.57651	1.12165
C	-2.79599	-0.25230	-0.38565
N	-0.58151	-0.09005	0.25340
H	-2.85886	-1.65625	1.27284
H	-3.49198	-0.06249	1.70140
C	-0.66593	-1.22031	2.49654
H	0.38051	-0.97482	2.72888
H	-1.21315	-1.24274	3.44884
H	-0.71055	-2.23069	2.07204
C	-1.26249	1.17871	2.28216
H	-1.75007	1.09593	3.26291
H	-0.22789	1.50779	2.45809
H	-1.79054	1.95553	1.71432
C	-3.45773	-1.36543	-1.19358
H	-4.49768	-1.50279	-0.86403
H	-3.47187	-1.12680	-2.26647
H	-2.93486	-2.32454	-1.06496
C	-3.48377	1.08716	-0.67725
H	-3.42633	1.34008	-1.74573
H	-4.54613	1.02381	-0.40124
H	-3.03534	1.91439	-0.10949
C	0.85201	0.05586	0.17161
C	1.40970	1.34768	0.13193
C	1.63686	-1.11319	0.13344
C	2.80633	1.44473	0.16994
C	3.02674	-0.95724	0.17182
C	3.60638	0.30769	0.21854
H	3.27217	2.43300	0.13625
H	3.66493	-1.84395	0.14101
H	4.69398	0.40768	0.25561
C	1.02623	-2.47652	-0.11957
H	-0.03982	-2.43492	0.15046
C	0.57262	2.58522	-0.11974
H	-0.47763	2.34328	0.09676
C	1.66103	-3.59300	0.69314
H	1.63823	-3.38379	1.77306
H	1.12817	-4.54041	0.52683
H	2.71034	-3.76541	0.41054
C	1.08843	-2.75448	-1.62224

H	0.68110	-1.90822	-2.20029
H	2.13072	-2.90566	-1.94697
H	0.52757	-3.66646	-1.87819
C	0.95677	3.77081	0.75119
H	0.27449	4.61493	0.57408
H	0.91382	3.52884	1.82356
H	1.97293	4.13256	0.53335
C	0.64860	2.92125	-1.60968
H	1.66305	3.25265	-1.88492
H	0.40379	2.03973	-2.22571
H	-0.04448	3.73818	-1.86331
C	-1.36371	-0.11729	-0.77383
H	-0.89198	-0.03646	-1.83478
F	-0.00157	0.03885	-3.02319

1Bb: ΔG = -2454249.6 kJ/mol

C	-0.74958	-1.00051	1.39753
C	-1.56136	-2.21105	0.90257
C	-1.71791	-2.09558	-0.63137
N	-0.19288	-0.47116	0.06284
H	-1.02855	-3.14000	1.15133
H	-2.53676	-2.25547	1.40434
C	0.38531	-1.38154	2.32810
H	1.04259	-0.52720	2.54602
H	-0.05212	-1.70399	3.28271
H	0.99027	-2.21527	1.95063
C	-1.61101	0.08135	2.02607
H	-2.00795	-0.32013	2.96993
H	-1.00344	0.96227	2.28576
H	-2.46064	0.39466	1.38185
C	-1.33447	-3.38457	-1.35874
H	-2.02272	-4.18906	-1.06324
H	-1.40345	-3.26564	-2.44914
H	-0.31230	-3.70700	-1.11064
C	-3.10799	-1.61825	-1.06945
H	-3.14697	-1.49860	-2.16296
H	-3.84394	-2.38951	-0.79650
H	-3.39052	-0.65420	-0.59554
C	0.82139	0.55452	-0.03185
C	0.42776	1.90340	-0.12249
C	2.16959	0.14452	-0.06276
C	1.44790	2.86273	-0.15832
C	3.14278	1.14905	-0.10372
C	2.78869	2.49467	-0.13040
H	1.17621	3.91938	-0.22837
H	4.19789	0.86546	-0.13304
H	3.56632	3.26196	-0.15673
C	2.58675	-1.30953	-0.16786
H	1.71809	-1.94066	0.07129
C	-1.01206	2.32972	-0.28586

H	-1.69774	1.49761	-0.06921
C	3.69992	-1.67623	0.80301
H	3.43893	-1.42758	1.84190
H	3.90821	-2.75499	0.76048
H	4.64083	-1.15839	0.56411
C	2.97818	-1.63030	-1.60826
H	2.15820	-1.41947	-2.31096
H	3.84901	-1.03735	-1.92821
H	3.24348	-2.69266	-1.71346
C	-1.41171	3.45917	0.65403
H	-2.50213	3.59653	0.61419
H	-1.14833	3.23991	1.69958
H	-0.94397	4.42021	0.38854
C	-1.28884	2.70958	-1.73866
H	-0.72184	3.60103	-2.05213
H	-1.03199	1.89325	-2.43124
H	-2.35981	2.92684	-1.87030
C	-0.73597	-1.03459	-0.95577
H	-0.46190	-0.72292	-1.97018
F	-3.77854	1.07330	0.17494

TS **1A** → **1Ba**: ΔG = -2454260.3 kJ/mol

C	-1.13976	-0.38418	1.60605
C	-2.47464	-1.02044	1.19224
C	-2.69740	-0.70083	-0.30116
N	-0.49981	-0.17461	0.23294
H	-2.41430	-2.11073	1.32469
H	-3.29958	-0.66305	1.82360
C	-0.29338	-1.29198	2.47532
H	0.70429	-0.86674	2.65760
H	-0.78418	-1.39689	3.45261
H	-0.18454	-2.29834	2.05357
C	-1.29753	0.96401	2.29425
H	-1.70455	0.80072	3.30121
H	-0.32921	1.47239	2.41107
H	-1.98653	1.63491	1.76587
C	-3.23771	-1.89163	-1.08365
H	-4.22708	-2.17526	-0.69527
H	-3.33969	-1.65277	-2.15039
H	-2.56991	-2.75951	-1.00477
C	-3.60143	0.51928	-0.52494
H	-3.65018	0.78664	-1.59056
H	-4.62222	0.28806	-0.18806
H	-3.25660	1.40372	0.02916
C	0.84751	0.30823	0.05402
C	1.04457	1.69583	-0.12030
C	1.91512	-0.61259	0.02933
C	2.36181	2.15376	-0.23739
C	3.21109	-0.09474	-0.09072
C	3.43738	1.27237	-0.20316

H	2.54256	3.22297	-0.37533
H	4.05743	-0.78646	-0.11599
H	4.45821	1.65207	-0.29191
C	1.72714	-2.11778	0.02540
H	0.65938	-2.33120	0.19083
C	-0.09682	2.68028	-0.28721
H	-1.03162	2.18476	0.00854
C	2.53350	-2.80775	1.11886
H	2.34445	-2.38631	2.11640
H	2.29045	-3.87975	1.15884
H	3.61554	-2.73286	0.93042
C	2.07220	-2.68414	-1.35033
H	1.37218	-2.29606	-2.10597
H	3.10809	-2.44435	-1.63771
H	1.98150	-3.78145	-1.34225
C	0.05523	3.91859	0.58517
H	-0.83409	4.56001	0.50082
H	0.18100	3.66278	1.64732
H	0.91977	4.53048	0.28668
C	-0.24595	3.05748	-1.75904
H	0.65108	3.57452	-2.13412
H	-0.40704	2.17248	-2.39212
H	-1.10215	3.73312	-1.90430
C	-1.32703	-0.32987	-0.75345
H	-0.99435	-0.31161	-1.81201
F	-0.60141	-1.70971	-2.61831

2A: ΔG = -2717843.7 kJ/mol

C	0.82811	-0.69500	1.49924
C	2.08713	-1.46559	1.06945
C	1.87569	-1.93231	-0.38122
N	0.24587	-0.33487	0.16094
H	2.94884	-0.78154	1.09461
H	2.31163	-2.29962	1.75032
C	1.18223	0.53114	2.32927
H	0.29511	1.15092	2.52912
H	1.57904	0.21146	3.30364
H	1.94902	1.15262	1.84958
C	-0.15467	-1.54022	2.30511
H	0.25473	-1.73226	3.30695
H	-1.11019	-1.01078	2.44062
H	-0.36594	-2.51460	1.84721
C	3.18617	-2.02843	-1.15040
H	3.79247	-2.85375	-0.74909
H	3.01333	-2.23572	-2.21676
H	3.78392	-1.11192	-1.07594
C	1.16686	-3.28474	-0.47058
H	0.96606	-3.55606	-1.51814
H	1.80298	-4.07125	-0.03991
H	0.20986	-3.31217	0.06529

C	-0.94485	0.44857	-0.00353
C	-2.19754	-0.20058	-0.13788
C	-0.86690	1.86261	-0.05609
C	-3.35262	0.58054	-0.26593
C	-2.05240	2.59864	-0.17838
C	-3.28870	1.96955	-0.27032
H	-4.32095	0.08345	-0.37478
H	-1.99636	3.69049	-0.21921
H	-4.20239	2.56208	-0.36528
C	0.44859	2.61061	-0.07295
H	1.23984	1.88200	0.12640
C	-2.33088	-1.70603	-0.22870
H	-1.35804	-2.13754	0.03513
C	0.53334	3.70248	0.98518
H	0.31749	3.32606	1.99537
H	1.54306	4.14038	1.00497
H	-0.16917	4.52624	0.78401
C	0.72064	3.18861	-1.45898
H	0.66105	2.41920	-2.24062
H	0.00370	3.98522	-1.71426
H	1.73005	3.62646	-1.50307
C	-3.36400	-2.27012	0.73747
H	-3.35918	-3.37007	0.71137
H	-3.17096	-1.96265	1.77564
H	-4.38581	-1.94924	0.48273
C	-2.63709	-2.13228	-1.66190
H	-3.61568	-1.75152	-1.99508
H	-1.88204	-1.76292	-2.37165
H	-2.66515	-3.22928	-1.74810
C	0.93411	-0.84937	-0.89878
H	0.32567	-1.09640	-1.77938
F	1.82751	0.25220	-1.57393
H	2.91245	0.97250	-0.69851
F	3.57261	1.41733	-0.17721

2Ba: -2717840.0 kJ/mol

C	0.61848	-0.88233	-1.93472
C	1.94409	-1.60342	-1.63588
C	2.45293	-1.09605	-0.26961
N	0.26347	-0.37416	-0.53148
H	1.76516	-2.68700	-1.57958
H	2.67597	-1.43695	-2.43746
C	-0.46321	-1.80987	-2.45341
H	-1.43688	-1.30438	-2.52936
H	-0.18504	-2.13250	-3.46581
H	-0.57315	-2.71354	-1.84178
C	0.76523	0.30652	-2.87186
H	0.95653	-0.07072	-3.88525
H	-0.15630	0.90529	-2.91321
H	1.60246	0.96163	-2.60025

C	2.98397	-2.20166	0.63740
H	3.86892	-2.66908	0.18319
H	3.27612	-1.79197	1.61449
H	2.23206	-2.98684	0.80293
C	3.49075	0.03029	-0.38332
H	3.68663	0.47139	0.60357
H	4.43053	-0.37999	-0.77964
H	3.15755	0.82998	-1.05952
C	-0.99143	0.26250	-0.20931
C	-1.07167	1.66727	-0.28164
C	-2.06611	-0.54523	0.20697
C	-2.32226	2.24699	-0.03747
C	-3.29132	0.08951	0.44001
C	-3.42624	1.46659	0.29251
H	-2.42354	3.33406	-0.08551
H	-4.14669	-0.50705	0.76726
H	-4.39364	1.94152	0.47309
C	-1.88999	-2.00871	0.55702
H	-0.93858	-2.35654	0.12807
C	0.15166	2.54375	-0.46253
H	0.96047	1.92962	-0.88196
C	-2.99542	-2.89781	0.00927
H	-3.10778	-2.79395	-1.07989
H	-2.78057	-3.95492	0.22236
H	-3.97033	-2.67218	0.46681
C	-1.75977	-2.13886	2.07445
H	-0.96305	-1.49103	2.47164
H	-2.69751	-1.85305	2.57676
H	-1.53524	-3.17744	2.36004
C	-0.07291	3.70652	-1.41633
H	0.86502	4.25758	-1.57630
H	-0.43289	3.37035	-2.39992
H	-0.80361	4.42941	-1.02365
C	0.63269	3.02231	0.90753
H	-0.10695	3.69278	1.37353
H	0.79837	2.18342	1.59991
H	1.57536	3.58288	0.81447
C	1.22672	-0.49751	0.31275
H	1.07965	-0.15709	1.36215
F	0.55857	0.32220	2.98633
H	1.82575	0.54952	2.94352
F	2.83629	0.71681	2.81419

2Bb: ΔG = -2717830.5 kJ/mol

C	-0.63994	-0.96257	1.26308
C	-1.63718	-1.98484	0.68071
C	-1.50405	-1.97460	-0.86107
N	0.05396	-0.45752	-0.01361
H	-1.42960	-2.98679	1.07944
H	-2.65923	-1.70873	0.97210

C	0.39400	-1.58382	2.18309
H	1.18217	-0.86796	2.45867
H	-0.11070	-1.88691	3.11023
H	0.85665	-2.48144	1.75309
C	-1.33439	0.19947	1.94934
H	-1.76635	-0.17301	2.88860
H	-0.63067	1.00438	2.20781
H	-2.15963	0.59426	1.34316
C	-1.08882	-3.32829	-1.43948
H	-1.88045	-4.06521	-1.24449
H	-0.93921	-3.27288	-2.52699
H	-0.16053	-3.70018	-0.98182
C	-2.76442	-1.45002	-1.55706
H	-2.61120	-1.34970	-2.64134
H	-3.58527	-2.16359	-1.39478
H	-3.07457	-0.48057	-1.14063
C	1.11953	0.52163	-0.01167
C	0.78035	1.88593	-0.11165
C	2.45132	0.06623	0.05140
C	1.82986	2.81045	-0.05687
C	3.45705	1.03875	0.10190
C	3.15162	2.39539	0.06887
H	1.60061	3.87649	-0.13351
H	4.50131	0.71942	0.14895
H	3.95413	3.13560	0.11363
C	2.83218	-1.39734	-0.05028
H	1.92505	-2.00356	0.08068
C	-0.63057	2.35918	-0.38267
H	-1.33271	1.53881	-0.19289
C	3.82715	-1.82600	1.01855
H	3.46710	-1.59907	2.03233
H	4.00740	-2.90929	0.96370
H	4.80252	-1.33242	0.89356
C	3.36121	-1.69544	-1.45107
H	2.62778	-1.43612	-2.22903
H	4.28129	-1.12857	-1.66164
H	3.59882	-2.76404	-1.55883
C	-1.05958	3.51348	0.51136
H	-2.13052	3.71552	0.36844
H	-0.90623	3.28839	1.57718
H	-0.51596	4.44391	0.28641
C	-0.79336	2.71656	-1.85762
H	-0.16638	3.57617	-2.14301
H	-0.52238	1.87636	-2.51500
H	-1.84080	2.97844	-2.06990
C	-0.41320	-0.99819	-1.08045
H	-0.00696	-0.72394	-2.06075
F	-3.63505	1.39457	-0.16986
H	-4.07780	0.45245	0.48985
F	-4.44361	-0.37227	1.06003

2Bc: ΔG = -2717837.4 kJ/mol

C	-0.95053	0.16572	1.79668
C	-2.44842	-0.11520	1.56115
C	-2.72296	0.05469	0.05597
N	-0.40804	0.04936	0.39748
H	-2.67396	-1.15253	1.85156
H	-3.08584	0.53634	2.17651
C	-0.32938	-0.86470	2.72922
H	0.76035	-0.73115	2.80742
H	-0.74514	-0.74610	3.74022
H	-0.53431	-1.89424	2.40730
C	-0.68171	1.55287	2.37103
H	-0.99607	1.58331	3.42375
H	0.39234	1.79229	2.34548
H	-1.22454	2.35019	1.84771
C	-3.83225	-0.85386	-0.45503
H	-4.80580	-0.51536	-0.07144
H	-3.88436	-0.83361	-1.55444
H	-3.69046	-1.89610	-0.14645
C	-3.07342	1.49751	-0.31254
H	-3.13454	1.62558	-1.40391
H	-4.05438	1.76128	0.10797
H	-2.35211	2.23109	0.06857
C	0.98049	0.21553	0.06896
C	1.45125	1.49873	-0.30771
C	1.86830	-0.88728	0.10462
C	2.81385	1.66558	-0.58093
C	3.22380	-0.66535	-0.17450
C	3.70137	0.59828	-0.49970
H	3.18085	2.65266	-0.87580
H	3.91451	-1.51315	-0.15150
H	4.76330	0.74791	-0.71139
C	1.41474	-2.31480	0.33025
H	0.36386	-2.28768	0.63791
C	0.52103	2.67459	-0.51587
H	-0.44147	2.41145	-0.06402
C	2.21442	-3.03075	1.41051
H	2.20965	-2.48287	2.36413
H	1.79635	-4.03031	1.60231
H	3.26649	-3.17635	1.12053
C	1.46721	-3.08689	-0.98616
H	0.86442	-2.60225	-1.76662
H	2.49887	-3.17504	-1.36264
H	1.07735	-4.10824	-0.85633
C	1.00770	3.95380	0.14996
H	0.24845	4.74557	0.06603
H	1.21722	3.80823	1.21999
H	1.92547	4.34291	-0.31686
C	0.26718	2.89181	-2.00509

H	1.19179	3.17095	-2.53499
H	-0.12846	1.98616	-2.48844
H	-0.46233	3.70024	-2.16633
C	-1.35388	-0.27960	-0.51492
H	-1.13665	0.00925	-1.55180
F	-1.38725	-1.87632	-0.73699
H	-1.43127	-2.03744	-2.27244
F	-1.42009	-1.97287	-3.22187

2Bd: ΔG = -2717820.5 kJ/mol

C	0.24684	1.19275	1.33054
C	0.46515	2.63967	0.85945
C	0.52448	2.63725	-0.68479
N	-0.22444	0.54130	0.01646
H	-0.37489	3.26549	1.19341
H	1.37744	3.06108	1.30116
C	-0.81270	1.05857	2.40495
H	-1.04582	0.00640	2.62257
H	-0.41613	1.49995	3.32918
H	-1.73962	1.59176	2.16228
C	1.53010	0.51272	1.77031
H	1.86841	0.99106	2.69996
H	1.36711	-0.55162	1.99474
H	2.33636	0.59636	1.03068
C	-0.36154	3.71858	-1.30446
H	0.01074	4.70890	-1.00654
H	-0.34716	3.66881	-2.40213
H	-1.40516	3.63533	-0.96824
C	1.94644	2.73068	-1.25001
H	1.93044	2.68393	-2.34877
H	2.37624	3.70188	-0.96541
H	2.60615	1.92700	-0.88603
C	-0.83944	-0.76525	-0.05875
C	-0.03420	-1.90249	-0.26169
C	-2.24451	-0.82609	0.04249
C	-0.68260	-3.14385	-0.28178
C	-2.83330	-2.09490	0.01216
C	-2.06109	-3.24364	-0.12902
H	-0.08882	-4.04757	-0.44055
H	-3.92063	-2.17872	0.08265
H	-2.54208	-4.22458	-0.14598
C	-3.12430	0.40900	0.06647
H	-2.49653	1.28361	0.29295
C	1.44505	-1.82314	-0.56563
H	1.83048	-0.83050	-0.30256
C	-4.21049	0.34154	1.13057
H	-3.79709	0.14064	2.12952
H	-4.75798	1.29365	1.18113
H	-4.95167	-0.44207	0.91408
C	-3.71969	0.64312	-1.31980

H	-2.93974	0.74548	-2.08897
H	-4.37225	-0.19125	-1.62034
H	-4.32611	1.56079	-1.33441
C	2.27170	-2.83331	0.21715
H	3.34125	-2.63299	0.07149
H	2.07884	-2.77290	1.29872
H	2.07735	-3.86958	-0.09977
C	1.68161	-1.97185	-2.06651
H	1.38559	-2.96803	-2.43233
H	1.11778	-1.22549	-2.64660
H	2.74802	-1.82943	-2.29454
C	-0.03187	1.29974	-1.00266
H	-0.28246	0.94643	-2.00920
F	3.80115	0.23830	-0.58163
H	4.14144	-0.29994	0.51871
F	4.40416	-0.73913	1.42607

2Be: ΔG = -2717822.9 kJ/mol

C	-0.09537	-1.27478	1.41508
C	-0.71251	-2.59183	0.91939
C	-1.12486	-2.39935	-0.55745
N	0.18716	-0.57651	0.07285
H	0.03238	-3.39691	0.99327
H	-1.56628	-2.88333	1.54493
C	1.17706	-1.47237	2.21318
H	1.68914	-0.52048	2.41470
H	0.90192	-1.90219	3.18577
H	1.87864	-2.16827	1.73799
C	-1.06204	-0.39461	2.18849
H	-1.27392	-0.88493	3.14894
H	-0.60413	0.57877	2.42012
H	-2.02131	-0.22825	1.67365
C	-0.63882	-3.53475	-1.45877
H	-1.10939	-4.47655	-1.14346
H	-0.91066	-3.35625	-2.50844
H	0.45146	-3.66598	-1.40145
C	-2.63012	-2.18560	-0.74316
H	-2.86985	-1.93694	-1.78645
H	-3.14977	-3.12124	-0.49090
H	-3.02449	-1.38155	-0.10570
C	0.94292	0.64897	-0.02038
C	0.25923	1.88069	-0.01043
C	2.34580	0.55047	-0.11750
C	1.04616	3.03997	0.01278
C	3.07529	1.74337	-0.10043
C	2.43465	2.97555	-0.00734
H	0.54951	4.01382	0.02320
H	4.16454	1.70231	-0.17998
H	3.02347	3.89566	0.01556
C	3.05567	-0.76537	-0.36930

H	2.35657	-1.58567	-0.14962
C	-1.24204	2.01467	-0.16157
H	-1.72648	1.03055	-0.07058
C	4.28535	-0.95679	0.50591
H	4.05337	-0.84602	1.57497
H	4.70992	-1.96025	0.35880
H	5.07907	-0.23506	0.26207
C	3.40805	-0.87771	-1.85100
H	2.51628	-0.79782	-2.49044
H	4.10712	-0.08416	-2.15721
H	3.88798	-1.84392	-2.06562
C	-1.87806	2.91075	0.89167
H	-2.97062	2.90333	0.77442
H	-1.65689	2.57208	1.91422
H	-1.54160	3.95541	0.80549
C	-1.55278	2.53084	-1.56554
H	-1.14023	3.53984	-1.72317
H	-1.13101	1.87561	-2.34287
H	-2.63840	2.56517	-1.71968
C	-0.40696	-1.14979	-0.91108
H	-0.35567	-0.71675	-1.91657
F	-3.90452	0.27760	0.98866
H	-3.95838	0.51168	-0.22120
F	-4.00462	0.69240	-1.26866

3Ba: ΔG = -2981366.0 kJ/mol

C	0.62091	0.90704	-1.74610
C	1.76776	1.84804	-1.35050
C	1.58742	2.20625	0.13710
N	0.16634	0.42043	-0.36129
H	2.72383	1.32123	-1.47662
H	1.79211	2.73815	-1.99333
C	1.08468	-0.24713	-2.60779
H	0.26785	-0.95263	-2.81468
H	1.41502	0.15735	-3.57439
H	1.93253	-0.78245	-2.16350
C	-0.54849	1.60948	-2.41977
H	-0.24075	1.90443	-3.43182
H	-1.41545	0.94096	-2.52313
H	-0.86519	2.51976	-1.89560
C	2.90942	2.28243	0.89106
H	3.48322	3.14539	0.52390
H	2.74861	2.41863	1.96937
H	3.50637	1.37688	0.74368
C	0.81329	3.51767	0.35559
H	0.57459	3.66614	1.41871
H	1.44053	4.35899	0.02929
H	-0.12451	3.56037	-0.21377
C	-0.91796	-0.52340	-0.18324
C	-2.21412	-0.01082	0.04961

C	-0.66241	-1.90844	-0.26044
C	-3.26861	-0.92802	0.12504
C	-1.75873	-2.77563	-0.18512
C	-3.05138	-2.29450	-0.01352
H	-4.28043	-0.55758	0.30816
H	-1.58278	-3.85344	-0.23842
H	-3.89252	-2.98983	0.04090
C	0.73373	-2.48993	-0.28118
H	1.44301	-1.65783	-0.36257
C	-2.49911	1.45465	0.30970
H	-1.61563	2.03953	0.02190
C	0.97796	-3.45785	-1.43091
H	0.74694	-3.02542	-2.41382
H	2.03336	-3.76902	-1.44644
H	0.37493	-4.37286	-1.32436
C	1.02129	-3.17500	1.05334
H	0.78582	-2.51776	1.89785
H	0.43389	-4.10025	1.16403
H	2.08601	-3.44476	1.12391
C	-3.66836	1.98813	-0.50629
H	-3.77418	3.07283	-0.35962
H	-3.53549	1.80928	-1.58309
H	-4.62375	1.53111	-0.20836
C	-2.71657	1.68333	1.80366
H	-3.61751	1.16009	2.16000
H	-1.86818	1.32012	2.40216
H	-2.84812	2.75400	2.02028
C	0.69728	1.10381	0.59809
H	0.36892	0.94680	1.62786
F	3.57593	-0.87517	-0.12247
H	3.02956	-0.73078	0.68534
F	2.26187	-0.44199	1.81763
H	1.14833	-0.57170	2.64205
F	0.31071	-0.58277	3.16520

3Bb: ΔG = -2981365.6 kJ/mol

C	0.69688	-0.35319	-2.22685
C	2.09403	-0.96449	-2.03017
C	2.56020	-0.61488	-0.59966
N	0.28671	-0.14409	-0.76006
H	2.03111	-2.05729	-2.13591
H	2.79616	-0.60313	-2.79294
C	-0.27450	-1.27791	-2.93350
H	-1.30104	-0.88421	-2.91722
H	0.02820	-1.35086	-3.98661
H	-0.27154	-2.29460	-2.52402
C	0.71480	0.99435	-2.93155
H	0.96621	0.82785	-3.98740
H	-0.27122	1.47988	-2.90149
H	1.46386	1.68100	-2.51835

C	3.20953	-1.78327	0.13810
H	4.13616	-2.08102	-0.37211
H	3.45632	-1.49594	1.16900
H	2.54415	-2.65836	0.17641
C	3.47675	0.61517	-0.54041
H	3.67582	0.89796	0.50111
H	4.43225	0.37376	-1.02706
H	3.04189	1.48125	-1.05806
C	-1.04342	0.21146	-0.32431
C	-1.34595	1.57100	-0.12006
C	-1.94708	-0.82862	-0.03887
C	-2.64486	1.87683	0.30231
C	-3.23043	-0.46133	0.38051
C	-3.58322	0.87575	0.53145
H	-2.91486	2.92139	0.47634
H	-3.95689	-1.24324	0.61638
H	-4.59143	1.13938	0.86003
C	-1.54600	-2.29060	-0.03780
H	-0.57664	-2.38793	-0.54831
C	-0.30574	2.66991	-0.21141
H	0.55757	2.28548	-0.77099
C	-2.54464	-3.17424	-0.77135
H	-2.73048	-2.82526	-1.79765
H	-2.17288	-4.20723	-0.83255
H	-3.51475	-3.21338	-0.25348
C	-1.32676	-2.76800	1.39618
H	-0.52994	-2.20337	1.89959
H	-2.24246	-2.65995	1.99875
H	-1.04597	-3.83180	1.40862
C	-0.81030	3.90069	-0.95079
H	0.00319	4.62797	-1.08539
H	-1.20198	3.65090	-1.94780
H	-1.61086	4.41612	-0.39927
C	0.20301	3.02821	1.18398
H	-0.61697	3.37047	1.83481
H	0.68241	2.17378	1.68283
H	0.94341	3.84011	1.12700
C	1.27405	-0.27013	0.05337
H	1.12362	-0.15419	1.13304
F	-0.64452	0.17564	2.87166
H	0.14951	-0.40061	2.97139
F	1.32274	-1.16466	3.00545
H	2.23010	-0.14207	2.84607
F	2.82434	0.63296	2.66294

3Bc: ΔG = -2981363.5 kJ/mol

C	0.13063	-1.06490	1.62069
C	1.14306	-2.15543	1.24699
C	0.98821	-2.44372	-0.26138
N	-0.16923	-0.48191	0.22989

H	2.15713	-1.77589	1.43337
H	1.00127	-3.05685	1.85779
C	0.70647	-0.00621	2.53444
H	-0.00646	0.81254	2.70899
H	0.90936	-0.47128	3.50900
H	1.65401	0.39008	2.15362
C	-1.16369	-1.60302	2.20973
H	-0.95415	-1.96032	3.22682
H	-1.92830	-0.81707	2.29120
H	-1.57845	-2.44664	1.64403
C	2.33707	-2.59457	-0.95858
H	2.85980	-3.46862	-0.54441
H	2.21791	-2.74873	-2.03951
H	2.96294	-1.70661	-0.80491
C	0.09690	-3.65520	-0.56857
H	-0.07381	-3.75946	-1.64961
H	0.59562	-4.56844	-0.21488
H	-0.88189	-3.59000	-0.07386
C	-0.99242	0.68895	0.03825
C	-2.37399	0.50516	-0.18349
C	-0.39032	1.96264	0.08470
C	-3.16805	1.65447	-0.26684
C	-1.23927	3.07326	0.00313
C	-2.61339	2.92481	-0.14888
H	-4.24141	1.54657	-0.44257
H	-0.80268	4.07507	0.03895
H	-3.25491	3.80742	-0.20625
C	1.10941	2.18314	0.09967
H	1.61552	1.20676	0.15772
C	-2.99942	-0.85235	-0.43911
H	-2.28325	-1.63145	-0.14173
C	1.57663	3.03818	1.27220
H	1.22306	2.66636	2.24301
H	2.67601	3.06468	1.30707
H	1.22988	4.07835	1.17225
C	1.54854	2.82707	-1.21421
H	1.24875	2.22766	-2.08262
H	1.12351	3.83671	-1.32578
H	2.64329	2.91858	-1.24410
C	-4.27392	-1.07984	0.36123
H	-4.64021	-2.10633	0.21587
H	-4.11697	-0.93167	1.43942
H	-5.08353	-0.40411	0.04758
C	-3.24771	-1.03163	-1.93502
H	-3.96547	-0.28785	-2.31437
H	-2.32114	-0.92490	-2.51819
H	-3.66203	-2.02892	-2.14469
C	0.26207	-1.23184	-0.72334
H	0.04156	-0.98576	-1.76382
F	1.89886	-0.01184	-2.50589

H	2.68801	0.21126	-1.92615
F	3.75901	0.48752	-1.15339
H	3.69527	0.26756	0.18372
F	3.65497	0.09106	1.16685

3Bd: ΔG = -2981358.5 kJ/mol

C	-0.55587	-0.23032	2.17561
C	-1.94187	-0.89419	2.13529
C	-2.50320	-0.72194	0.70946
N	-0.25267	-0.11750	0.67422
H	-1.84000	-1.96582	2.35826
H	-2.60800	-0.46632	2.89624
C	0.48994	-1.08454	2.85932
H	1.48922	-0.63023	2.79925
H	0.23147	-1.16384	3.92397
H	0.52713	-2.10214	2.45083
C	-0.56424	1.16339	2.78342
H	-0.70980	1.06705	3.86760
H	0.39282	1.68139	2.62611
H	-1.37672	1.79190	2.39759
C	-3.21079	-1.96487	0.18282
H	-4.12906	-2.13407	0.76279
H	-3.49141	-1.84028	-0.87232
H	-2.57886	-2.85699	0.26293
C	-3.43922	0.49070	0.56528
H	-3.69111	0.66955	-0.48955
H	-4.37183	0.28922	1.11081
H	-3.00085	1.41113	0.97428
C	0.98686	0.43523	0.17187
C	1.01858	1.81398	-0.13334
C	2.11172	-0.39872	0.01703
C	2.25123	2.36286	-0.50320
C	3.31878	0.21049	-0.34761
C	3.39708	1.57814	-0.58178
H	2.30660	3.42651	-0.74690
H	4.20720	-0.41353	-0.47625
H	4.35106	2.03138	-0.86169
C	2.04268	-1.91161	0.06246
H	1.03092	-2.20354	0.38366
C	-0.22549	2.67833	-0.18450
H	-1.02540	2.17547	0.37570
C	3.05743	-2.53657	1.00998
H	2.96641	-2.16143	2.03858
H	2.93109	-3.62860	1.04199
H	4.08925	-2.34359	0.67907
C	2.23114	-2.44744	-1.35686
H	1.54714	-1.96042	-2.06350
H	3.26130	-2.27798	-1.70755
H	2.04170	-3.53030	-1.39350
C	-0.03171	4.04671	0.45237

H	-0.98567	4.59255	0.48255
H	0.34207	3.97240	1.48409
H	0.67464	4.67192	-0.11384
C	-0.70432	2.80206	-1.63006
H	0.04493	3.31520	-2.25298
H	-0.90311	1.82318	-2.09003
H	-1.63491	3.38731	-1.68175
C	-1.27549	-0.39295	-0.05852
H	-1.20947	-0.29973	-1.14634
F	-0.80638	-2.70099	-1.48612
H	-0.60346	-1.97441	-2.12925
F	-0.37202	-0.85625	-2.92893
H	-1.64320	-0.29818	-3.02974
F	-2.55303	0.08784	-2.97993

3Be: ΔG = -2981350.3 kJ/mol

C	-0.09961	1.15312	1.28648
C	-0.29860	2.59583	0.78664
C	0.45464	2.74053	-0.54975
N	0.37371	0.46605	-0.01212
H	-1.36777	2.77355	0.61427
H	0.04817	3.32274	1.53334
C	-1.38722	0.53347	1.78753
H	-1.27181	-0.53663	2.01399
H	-1.66249	1.03345	2.72650
H	-2.21769	0.66996	1.08876
C	0.98719	1.00393	2.33945
H	0.61808	1.43684	3.27852
H	1.21699	-0.05351	2.53501
H	1.91604	1.52710	2.08146
C	-0.27389	3.58121	-1.59242
H	-0.36980	4.61134	-1.22188
H	0.29456	3.61983	-2.53254
H	-1.27512	3.19115	-1.79990
C	1.87663	3.30749	-0.37489
H	2.46352	3.21778	-1.30036
H	1.79655	4.37566	-0.12871
H	2.43454	2.81998	0.43489
C	0.75155	-0.93353	-0.09946
C	2.12045	-1.25662	0.04157
C	-0.23131	-1.91365	-0.34554
C	2.47241	-2.61038	-0.01014
C	0.18436	-3.24951	-0.38687
C	1.51723	-3.60032	-0.20755
H	3.52475	-2.88617	0.09454
H	-0.55812	-4.02664	-0.58377
H	1.81701	-4.65037	-0.24307
C	-1.66584	-1.57554	-0.67548
H	-1.85777	-0.54210	-0.37586
C	3.22402	-0.22565	0.16729

H	2.76812	0.75136	0.36867
C	-2.67063	-2.46036	0.04647
H	-2.49268	-2.48461	1.13151
H	-3.68387	-2.06876	-0.10870
H	-2.64946	-3.49850	-0.31903
C	-1.88192	-1.61208	-2.18575
H	-1.18828	-0.94043	-2.71364
H	-1.74092	-2.62560	-2.59392
H	-2.90483	-1.28938	-2.43028
C	4.17335	-0.51729	1.32151
H	4.89318	0.30524	1.44200
H	3.63873	-0.63473	2.27510
H	4.75894	-1.43333	1.15288
C	3.97962	-0.09801	-1.15235
H	4.48920	-1.03803	-1.41493
H	3.30855	0.15805	-1.98550
H	4.74702	0.68766	-1.08737
C	0.61099	1.31816	-0.94846
H	0.99149	0.97664	-1.91828
F	-4.32616	-0.43625	1.99668
H	-4.27013	-0.12193	1.06736
F	-4.21464	0.31410	-0.27227
H	-3.20424	0.96859	-0.81945
F	-2.42442	1.45956	-1.24290

3Bf: ΔG = -2981336.5 kJ/mol

C	-2.32932	-0.14265	1.05458
C	-3.35863	-0.43460	-0.04978
C	-2.72029	-0.05091	-1.40382
N	-1.04830	-0.05824	0.21120
H	-3.59679	-1.50810	-0.05192
H	-4.29764	0.10521	0.13035
C	-2.22045	-1.24157	2.09404
H	-1.36030	-1.08636	2.76138
H	-3.12377	-1.21446	2.71793
H	-2.15927	-2.24397	1.65533
C	-2.56194	1.18609	1.75678
H	-3.46005	1.08954	2.38113
H	-1.72560	1.44562	2.42109
H	-2.73535	2.01272	1.05675
C	-2.97648	-1.08785	-2.49391
H	-4.05548	-1.15933	-2.69042
H	-2.47904	-0.81188	-3.43403
H	-2.62088	-2.08488	-2.19636
C	-3.12702	1.34469	-1.89553
H	-2.56869	1.62661	-2.79937
H	-4.19743	1.34327	-2.14464
H	-2.95577	2.11783	-1.13390
C	0.30234	-0.02100	0.72735
C	0.92075	1.22778	0.92067

C	0.98007	-1.24626	0.87007
C	2.25910	1.21798	1.32988
C	2.31446	-1.19243	1.28391
C	2.94725	0.02416	1.51757
H	2.77645	2.17033	1.47414
H	2.87681	-2.12434	1.38600
H	3.99527	0.04246	1.82661
C	0.36227	-2.57904	0.49336
H	-0.71265	-2.42611	0.32190
C	0.23770	2.54680	0.61931
H	-0.82700	2.34846	0.44293
C	0.50660	-3.61662	1.59782
H	0.09462	-3.26261	2.55415
H	-0.02170	-4.54333	1.33011
H	1.55980	-3.88519	1.77013
C	0.93459	-3.08835	-0.82567
H	0.80894	-2.35206	-1.63184
H	2.01071	-3.29783	-0.74682
H	0.43008	-4.01845	-1.12750
C	0.33296	3.52474	1.78242
H	-0.24550	4.43589	1.57052
H	-0.05341	3.09457	2.71809
H	1.37134	3.83917	1.96727
C	0.77746	3.16466	-0.66591
H	1.84154	3.42485	-0.57528
H	0.68669	2.47694	-1.51805
H	0.22524	4.08520	-0.90800
C	-1.27794	-0.00624	-1.05420
H	-0.41407	0.07257	-1.74050
F	3.25264	1.69728	-1.86827
H	2.49751	1.08095	-1.96095
F	1.50343	0.06068	-2.10291
H	2.58721	-0.85690	-1.87040
F	3.39564	-1.39186	-1.73859

Method M06L/def2-SVPD

1A: ΔG = -2455050.2 kJ/mol

C	-1.07730	-0.57334	1.45366
C	-2.41438	-1.19842	1.02211
C	-2.69604	-0.73513	-0.41857
N	-0.46109	-0.26134	0.12870
H	-2.32056	-2.29341	1.03367
H	-3.22966	-0.93917	1.70982
C	-0.24226	-1.55507	2.26717
H	0.74394	-1.13531	2.50650
H	-0.74435	-1.76407	3.22061
H	-0.10441	-2.51047	1.74979
C	-1.25016	0.69238	2.29425
H	-1.62719	0.42753	3.29032
H	-0.28648	1.19994	2.43769

H	-1.95420	1.40857	1.85892
C	-3.49787	-1.76621	-1.20144
H	-4.50751	-1.85378	-0.77789
H	-3.60764	-1.47486	-2.25483
H	-3.03560	-2.75860	-1.17297
C	-3.44709	0.59721	-0.46345
H	-3.57784	0.94040	-1.49889
H	-4.44702	0.48096	-0.02562
H	-2.94494	1.39852	0.08772
C	0.83973	0.31711	-0.01024
C	0.97597	1.72525	-0.10298
C	1.98918	-0.50880	-0.07222
C	2.25730	2.28098	-0.18750
C	3.25120	0.09523	-0.14583
C	3.39150	1.47686	-0.18888
H	2.36320	3.36521	-0.26185
H	4.13972	-0.53784	-0.19038
H	4.38461	1.92704	-0.24579
C	1.92120	-2.02113	-0.15678
H	0.87124	-2.31039	-0.04688
C	-0.22110	2.64788	-0.19475
H	-1.10755	2.04651	0.02446
C	2.73924	-2.71496	0.92752
H	2.46444	-2.38508	1.93679
H	2.59393	-3.80300	0.88244
H	3.81542	-2.53021	0.80116
C	2.37673	-2.48804	-1.53902
H	1.81712	-1.99638	-2.34420
H	3.44418	-2.27711	-1.69833
H	2.23784	-3.57249	-1.64959
C	-0.17178	3.79174	0.81093
H	-1.10165	4.37576	0.77613
H	-0.04451	3.43080	1.83968
H	0.65197	4.48723	0.59870
C	-0.37695	3.18124	-1.61771
H	0.46974	3.82438	-1.89804
H	-0.43343	2.37011	-2.35567
H	-1.29201	3.78249	-1.71204
C	-1.27472	-0.53334	-0.95928
H	-1.18792	0.20168	-1.77240
F	-0.84995	-1.77381	-1.65020

1Ba: ΔG = -2455036.6 kJ/mol

C	-1.07730	-0.57334	1.45366
C	-2.41438	-1.19842	1.02211
C	-2.69604	-0.73513	-0.41857
N	-0.46109	-0.26134	0.12870
H	-2.32056	-2.29341	1.03367
H	-3.22966	-0.93917	1.70982
C	-0.24226	-1.55507	2.26717

H	0.74394	-1.13531	2.50650
H	-0.74435	-1.76407	3.22061
H	-0.10441	-2.51047	1.74979
C	-1.25016	0.69238	2.29425
H	-1.62719	0.42753	3.29032
H	-0.28648	1.19994	2.43769
H	-1.95420	1.40857	1.85892
C	-3.49787	-1.76621	-1.20144
H	-4.50751	-1.85378	-0.77789
H	-3.60764	-1.47486	-2.25483
H	-3.03560	-2.75860	-1.17297
C	-3.44709	0.59721	-0.46345
H	-3.57784	0.94040	-1.49889
H	-4.44702	0.48096	-0.02562
H	-2.94494	1.39852	0.08772
C	0.83973	0.31711	-0.01024
C	0.97597	1.72525	-0.10298
C	1.98918	-0.50880	-0.07222
C	2.25730	2.28098	-0.18750
C	3.25120	0.09523	-0.14583
C	3.39150	1.47686	-0.18888
H	2.36320	3.36521	-0.26185
H	4.13972	-0.53784	-0.19038
H	4.38461	1.92704	-0.24579
C	1.92120	-2.02113	-0.15678
H	0.87124	-2.31039	-0.04688
C	-0.22110	2.64788	-0.19475
H	-1.10755	2.04651	0.02446
C	2.73924	-2.71496	0.92752
H	2.46444	-2.38508	1.93679
H	2.59393	-3.80300	0.88244
H	3.81542	-2.53021	0.80116
C	2.37673	-2.48804	-1.53902
H	1.81712	-1.99638	-2.34420
H	3.44418	-2.27711	-1.69833
H	2.23784	-3.57249	-1.64959
C	-0.17178	3.79174	0.81093
H	-1.10165	4.37576	0.77613
H	-0.04451	3.43080	1.83968
H	0.65197	4.48723	0.59870
C	-0.37695	3.18124	-1.61771
H	0.46974	3.82438	-1.89804
H	-0.43343	2.37011	-2.35567
H	-1.29201	3.78249	-1.71204
C	-1.27472	-0.53334	-0.95928
H	-1.18792	0.20168	-1.77240
F	-0.84995	-1.77381	-1.65020

1Bb: ΔG = -2455014.6 kJ/mol

C	-0.63272	-1.10788	1.34716

C	-1.34325	-2.36623	0.82010
C	-1.56666	-2.17662	-0.69760
N	-0.10289	-0.51684	0.02811
H	-0.70573	-3.24305	0.98822
H	-2.28470	-2.53926	1.35270
C	0.51449	-1.41261	2.29039
H	1.09539	-0.51309	2.53082
H	0.08976	-1.78438	3.22994
H	1.18371	-2.18764	1.90621
C	-1.58009	-0.10543	1.98778
H	-1.92326	-0.53171	2.93802
H	-1.06832	0.83633	2.22331
H	-2.46704	0.10611	1.37641
C	-1.22893	-3.42744	-1.50537
H	-1.89684	-4.24525	-1.20780
H	-1.36231	-3.25716	-2.58098
H	-0.19578	-3.75524	-1.33188
C	-2.97588	-1.67377	-1.04438
H	-3.06213	-1.44790	-2.11520
H	-3.70030	-2.46447	-0.81026
H	-3.25641	-0.77505	-0.47607
C	0.82829	0.58801	-0.03771
C	0.32428	1.89805	-0.13871
C	2.20385	0.29128	-0.03730
C	1.26037	2.93836	-0.15815
C	3.09034	1.37281	-0.05694
C	2.62575	2.68296	-0.09775
H	0.90616	3.96684	-0.23931
H	4.16377	1.17807	-0.06003
H	3.33530	3.51193	-0.10956
C	2.74444	-1.12215	-0.13399
H	1.91867	-1.82488	0.03113
C	-1.14671	2.20754	-0.33274
H	-1.72643	1.30238	-0.12151
C	3.81802	-1.41212	0.90739
H	3.47121	-1.19903	1.92654
H	4.11516	-2.46805	0.86720
H	4.72314	-0.81541	0.73160
C	3.25997	-1.38010	-1.54915
H	2.47994	-1.21153	-2.30334
H	4.10504	-0.72053	-1.79100
H	3.60686	-2.41690	-1.65149
C	-1.64716	3.29823	0.60577
H	-2.72675	3.44602	0.47717
H	-1.46743	3.04697	1.65906
H	-1.16231	4.26316	0.40510
C	-1.41386	2.56890	-1.79302
H	-0.89156	3.49259	-2.07938
H	-1.08344	1.77509	-2.47606
H	-2.48814	2.72702	-1.95836

C	-0.61427	-1.08138	-1.00444
H	-0.35837	-0.73530	-2.00854
F	-4.41870	0.95764	0.47250

2Ba: ΔG = -2718719.8 kJ/mol

C	0.23700	-1.23119	-1.82469
C	1.43796	-2.14857	-1.54074
C	2.17191	-1.58122	-0.30502
N	0.12058	-0.50540	-0.47573
H	1.07847	-3.16092	-1.31851
H	2.09673	-2.22052	-2.41321
C	-1.03850	-1.98920	-2.13634
H	-1.90533	-1.31939	-2.20073
H	-0.92083	-2.46288	-3.11780
H	-1.24236	-2.78319	-1.41247
C	0.49786	-0.20511	-2.91812
H	0.51803	-0.73066	-3.87962
H	-0.30391	0.54215	-2.97099
H	1.45819	0.30662	-2.80152
C	2.59010	-2.65953	0.69120
H	3.30695	-3.34268	0.21898
H	3.07203	-2.21924	1.57345
H	1.72939	-3.25144	1.02798
C	3.37606	-0.70129	-0.67524
H	3.81948	-0.23530	0.21250
H	4.14278	-1.32653	-1.14959
H	3.10315	0.09328	-1.37986
C	-0.96693	0.38956	-0.14866
C	-0.79919	1.76469	-0.40078
C	-2.12774	-0.14616	0.43734
C	-1.88580	2.60085	-0.12231
C	-3.18053	0.73879	0.69431
C	-3.07075	2.09320	0.39973
H	-1.78985	3.67250	-0.30196
H	-4.09346	0.35663	1.15351
H	-3.90609	2.76443	0.60564
C	-2.23569	-1.58729	0.89588
H	-1.35890	-2.13600	0.52987
C	0.52119	2.36761	-0.83873
H	1.17673	1.55944	-1.18115
C	-3.48469	-2.27907	0.36261
H	-3.55806	-2.21804	-0.73039
H	-3.48219	-3.34113	0.64028
H	-4.39867	-1.83780	0.78264
C	-2.18382	-1.64970	2.42156
H	-1.27008	-1.18856	2.81670
H	-3.04125	-1.12913	2.87039
H	-2.21025	-2.69192	2.76630
C	0.37309	3.35037	-1.99255
H	1.35998	3.69473	-2.32811

H	-0.13358	2.89770	-2.85469
H	-0.19626	4.24290	-1.70066
C	1.21285	3.01042	0.36251
H	0.63308	3.86103	0.74745
H	1.33937	2.29556	1.18576
H	2.20699	3.38407	0.08219
C	1.13695	-0.69464	0.28798
H	1.19845	-0.21052	1.28034
F	1.26855	0.47695	3.03687
H	2.48971	0.82744	2.87516
F	3.48139	1.09972	2.71897

2Bb: ΔG = -2718721.3 kJ/mol

C	-0.69448	-0.84762	1.27655
C	-1.79663	-1.74630	0.69002
C	-1.41402	-2.06726	-0.77183
N	0.01062	-0.38782	-0.01158
H	-1.91948	-2.65664	1.28659
H	-2.75217	-1.20924	0.70604
C	0.30878	-1.59453	2.14226
H	1.17160	-0.96619	2.39656
H	-0.18832	-1.86146	3.08169
H	0.66218	-2.52166	1.68042
C	-1.24205	0.34655	2.03436
H	-1.70554	-0.02428	2.95607
H	-0.44691	1.04386	2.32760
H	-2.01276	0.87969	1.46944
C	-0.72098	-3.43151	-0.92405
H	-1.45091	-4.22274	-0.71289
H	-0.34631	-3.58071	-1.94456
H	0.11698	-3.54904	-0.22659
C	-2.59418	-1.96691	-1.73417
H	-2.28162	-2.14991	-2.76996
H	-3.34265	-2.72444	-1.47018
H	-3.07510	-0.98326	-1.67979
C	1.10533	0.55888	-0.01775
C	0.81079	1.93132	-0.10381
C	2.42078	0.05853	0.03790
C	1.88745	2.82202	-0.04396
C	3.45632	0.99788	0.09538
C	3.19479	2.36347	0.07589
H	1.69212	3.89326	-0.11309
H	4.48776	0.64558	0.13870
H	4.01988	3.07584	0.12629
C	2.75590	-1.41635	-0.06889
H	1.83496	-1.99551	0.05973
C	-0.58389	2.44910	-0.38295
H	-1.29602	1.62709	-0.25897
C	3.73653	-1.87973	1.00087
H	3.37990	-1.64891	2.01273

H	3.88360	-2.96575	0.93790
H	4.72331	-1.41347	0.87945
C	3.27729	-1.72642	-1.47138
H	2.56135	-1.42619	-2.24792
H	4.22194	-1.20130	-1.67019
H	3.46455	-2.80254	-1.58531
C	-1.00406	3.56881	0.55965
H	-2.04842	3.85115	0.37303
H	-0.92111	3.27215	1.61303
H	-0.39441	4.47180	0.41841
C	-0.68543	2.88679	-1.84348
H	-0.01063	3.72735	-2.05877
H	-0.42860	2.06857	-2.52983
H	-1.70816	3.21090	-2.07795
C	-0.38942	-1.02951	-1.04914
H	0.05348	-0.82777	-2.02751
F	-3.64182	1.20109	-0.47343
H	-4.26625	0.52145	0.21342
F	-4.88323	-0.14621	0.89217

2Bc: ΔG = -2718719.5 kJ/mol

C	-0.64519	0.72701	1.95528
C	-2.17360	0.86556	1.86269
C	-2.54638	0.90459	0.36439
N	-0.31833	0.27084	0.52597
H	-2.64889	-0.00377	2.33352
H	-2.52404	1.75629	2.39566
C	-0.19953	-0.32194	2.95496
H	0.88451	-0.48807	2.91684
H	-0.43814	0.04196	3.96103
H	-0.72032	-1.27410	2.81856
C	0.07017	2.03986	2.23501
H	-0.11807	2.31622	3.27878
H	1.15621	1.94146	2.11464
H	-0.28831	2.86064	1.60652
C	-3.76994	0.05552	0.03371
H	-4.64324	0.44696	0.57011
H	-3.99403	0.07896	-1.03975
H	-3.62829	-0.99001	0.33446
C	-2.73336	2.33409	-0.17003
H	-2.87924	2.33734	-1.25776
H	-3.62561	2.77462	0.29226
H	-1.87656	2.97755	0.06444
C	1.01561	-0.10795	0.11620
C	1.85317	0.88434	-0.42938
C	1.41570	-1.44759	0.26755
C	3.16505	0.51114	-0.74101
C	2.73983	-1.76077	-0.05878
C	3.61248	-0.78961	-0.53660
H	3.84024	1.25410	-1.16749

H	3.08073	-2.79193	0.04500
H	4.64236	-1.05517	-0.78074
C	0.45593	-2.56215	0.63407
H	-0.50135	-2.11501	0.93171
C	1.36222	2.27336	-0.78844
H	0.39187	2.43610	-0.30660
C	0.95855	-3.42152	1.78783
H	1.19663	-2.82615	2.67796
H	0.19941	-4.16186	2.07205
H	1.86293	-3.97881	1.50854
C	0.18028	-3.41488	-0.60403
H	-0.17015	-2.80584	-1.44579
H	1.08778	-3.94322	-0.92829
H	-0.58709	-4.17094	-0.39154
C	2.29757	3.37758	-0.31301
H	1.85570	4.36228	-0.51330
H	2.49600	3.31370	0.76458
H	3.26411	3.34744	-0.83342
C	1.12155	2.35862	-2.29507
H	2.05688	2.22315	-2.85576
H	0.41626	1.59042	-2.63695
H	0.70911	3.33970	-2.56646
C	-1.31854	0.36350	-0.27638
H	-1.22456	0.08293	-1.34265
F	-2.73345	-2.31592	-2.43008
H	-2.08413	-1.56593	-2.72913
F	-1.28097	-0.61957	-3.07733

2Bd: ΔG = -2718717.8 kJ/mol

C	0.24855	1.22068	1.25288
C	0.56071	2.63808	0.74442
C	0.61899	2.57998	-0.79902
N	-0.29601	0.57866	-0.03583
H	-0.24006	3.32132	1.05297
H	1.49516	3.01385	1.17496
C	-0.80006	1.18646	2.34694
H	-1.10665	0.16052	2.58709
H	-0.35639	1.61282	3.25392
H	-1.68306	1.78393	2.10357
C	1.48812	0.45951	1.69545
H	1.84748	0.91217	2.62702
H	1.26606	-0.59305	1.91048
H	2.30213	0.51425	0.96522
C	-0.11030	3.74673	-1.46118
H	0.37924	4.68802	-1.18245
H	-0.08622	3.66474	-2.55492
H	-1.15850	3.80350	-1.14085
C	2.04851	2.45771	-1.34782
H	2.04555	2.31237	-2.43554
H	2.59248	3.38633	-1.13386

H	2.60030	1.62670	-0.89065
C	-0.94292	-0.71452	-0.07589
C	-0.16406	-1.85748	-0.33534
C	-2.33779	-0.75883	0.10389
C	-0.82505	-3.09099	-0.32778
C	-2.94157	-2.02047	0.10169
C	-2.19278	-3.17598	-0.09265
H	-0.25444	-3.99842	-0.52948
H	-4.02203	-2.09112	0.23496
H	-2.68416	-4.15026	-0.08779
C	-3.20338	0.48412	0.17865
H	-2.55268	1.35958	0.29401
C	1.29962	-1.79109	-0.72376
H	1.67429	-0.78582	-0.50282
C	-4.16411	0.45858	1.36087
H	-3.64167	0.29744	2.31242
H	-4.70822	1.40920	1.43268
H	-4.91493	-0.33580	1.25430
C	-3.95208	0.66875	-1.14056
H	-3.26365	0.72479	-1.99418
H	-4.64444	-0.16449	-1.32503
H	-4.54216	1.59463	-1.12432
C	2.16017	-2.78029	0.05169
H	3.21751	-2.65326	-0.21081
H	2.06535	-2.64492	1.13659
H	1.89380	-3.82037	-0.17958
C	1.44712	-1.99280	-2.23126
H	1.11876	-2.99678	-2.53478
H	0.85508	-1.26361	-2.80016
H	2.49725	-1.87974	-2.53288
C	-0.07842	1.29908	-1.07510
H	-0.37973	0.94760	-2.06457
F	4.33917	0.05376	-0.31528
H	4.50593	-0.44688	0.78401
F	4.66071	-0.88303	1.75913

2Be: ΔG = -2718717.2 kJ/mol

C	-0.06082	-1.28125	1.36494
C	-0.65651	-2.60078	0.84535
C	-1.00804	-2.40023	-0.64648
N	0.28438	-0.58803	0.03596
H	0.08766	-3.40077	0.94153
H	-1.53193	-2.89632	1.43383
C	1.18549	-1.47382	2.20640
H	1.67558	-0.51896	2.43494
H	0.88267	-1.91882	3.16124
H	1.90695	-2.15335	1.74367
C	-1.05823	-0.40981	2.11118
H	-1.27158	-0.88916	3.07369
H	-0.63850	0.58051	2.32823

H	-2.00959	-0.29296	1.58160
C	-0.57788	-3.57394	-1.52252
H	-1.11497	-4.47839	-1.21158
H	-0.80960	-3.39000	-2.57905
H	0.49801	-3.77154	-1.43306
C	-2.49134	-2.07133	-0.87161
H	-2.68700	-1.79365	-1.91504
H	-3.09133	-2.96046	-0.64038
H	-2.83381	-1.25488	-0.22464
C	1.01563	0.65584	-0.03144
C	0.29440	1.86438	-0.05752
C	2.42003	0.59667	-0.08682
C	1.04244	3.04739	-0.04144
C	3.11215	1.81165	-0.07253
C	2.43249	3.02434	-0.02587
H	0.51845	4.00389	-0.06265
H	4.20208	1.80237	-0.11895
H	2.99172	3.96118	-0.00867
C	3.17892	-0.70024	-0.28761
H	2.48750	-1.53756	-0.13220
C	-1.21127	1.93890	-0.23129
H	-1.63827	0.93773	-0.08899
C	4.33894	-0.86383	0.68590
H	4.01583	-0.77235	1.73064
H	4.80485	-1.85010	0.56333
H	5.12195	-0.11364	0.51209
C	3.65340	-0.79246	-1.73757
H	2.81612	-0.71513	-2.44382
H	4.36522	0.01047	-1.97493
H	4.15867	-1.75020	-1.91945
C	-1.88197	2.86691	0.77321
H	-2.96909	2.86452	0.62448
H	-1.68577	2.56277	1.80917
H	-1.54250	3.90500	0.65887
C	-1.52699	2.36154	-1.66633
H	-1.13497	3.36603	-1.87849
H	-1.08670	1.67273	-2.39939
H	-2.61087	2.38524	-1.83453
C	-0.22898	-1.18141	-0.97874
H	-0.10317	-0.77027	-1.98313
F	-4.28194	0.20215	1.18861
H	-4.51490	0.45530	0.03078
F	-4.72700	0.67851	-1.01153

2Bf: ΔG = -2718708.3 kJ/mol

C	0.54643	-0.89897	1.58712
C	1.61187	-1.94466	1.22423
C	1.41794	-2.30849	-0.26195
N	0.14292	-0.40698	0.18947
H	2.60982	-1.50960	1.36053

H	1.54621	-2.82322	1.87582
C	1.10022	0.24076	2.41643
H	0.33604	1.00222	2.61417
H	1.41392	-0.16359	3.38611
H	1.97531	0.70701	1.95380
C	-0.67456	-1.48344	2.28428
H	-0.38928	-1.74481	3.30978
H	-1.48992	-0.75215	2.35069
H	-1.04927	-2.39421	1.80761
C	2.73375	-2.55841	-0.98671
H	3.19462	-3.46889	-0.58265
H	2.57554	-2.71218	-2.06114
H	3.43349	-1.72877	-0.85850
C	0.50841	-3.53705	-0.46241
H	0.28416	-3.69682	-1.52472
H	1.03497	-4.42543	-0.09245
H	-0.43954	-3.46262	0.08102
C	-0.85995	0.62122	-0.00785
C	-2.19720	0.21242	-0.20244
C	-0.48527	1.97913	0.01033
C	-3.17108	1.21100	-0.30557
C	-1.50561	2.93272	-0.08680
C	-2.83591	2.55774	-0.22592
H	-4.21098	0.92108	-0.46148
H	-1.23948	3.99091	-0.07511
H	-3.61419	3.31924	-0.29879
C	0.95352	2.45124	0.00808
H	1.60140	1.57160	0.08417
C	-2.60804	-1.23470	-0.39001
H	-1.77407	-1.87486	-0.08775
C	1.27694	3.40432	1.15402
H	1.02653	2.99087	2.13751
H	2.34927	3.64285	1.15588
H	0.73632	4.35509	1.04788
C	1.26949	3.12095	-1.32950
H	1.01148	2.47941	-2.17939
H	0.71927	4.06662	-1.43679
H	2.34102	3.35173	-1.39915
C	-3.80531	-1.62785	0.46634
H	-4.00477	-2.70315	0.36961
H	-3.63608	-1.41395	1.52950
H	-4.71971	-1.10259	0.16040
C	-2.86699	-1.51601	-1.86912
H	-3.71550	-0.92633	-2.24342
H	-1.99441	-1.27141	-2.48907
H	-3.10413	-2.57684	-2.02649
C	0.64337	-1.13059	-0.75583
H	0.35951	-0.95803	-1.79193
F	2.38327	0.22167	-1.92888
H	3.19823	0.51329	-1.01422

F	3.87468	0.74483	-0.24090

3Ba: ΔG = -2982375.4 kJ/mol

C	-0.00339	-1.05119	1.67018
C	0.96313	-2.20481	1.35896
C	0.90086	-2.47075	-0.16093
N	-0.21157	-0.46801	0.26214
H	1.98322	-1.91222	1.63452
H	0.71093	-3.09863	1.93976
C	0.59893	-0.00129	2.58034
H	-0.08507	0.84227	2.73513
H	0.77491	-0.46181	3.55952
H	1.56109	0.36212	2.20866
C	-1.34297	-1.51000	2.22606
H	-1.18352	-1.83720	3.25987
H	-2.07256	-0.69110	2.25353
H	-1.76945	-2.35472	1.67613
C	2.27570	-2.72700	-0.76836
H	2.70807	-3.62243	-0.30467
H	2.21255	-2.90464	-1.84845
H	2.95912	-1.88907	-0.59257
C	-0.05585	-3.61778	-0.52925
H	-0.17967	-3.70239	-1.61616
H	0.36804	-4.56118	-0.16340
H	-1.04719	-3.49519	-0.07752
C	-1.01585	0.71266	0.02675
C	-2.38587	0.53026	-0.25331
C	-0.41387	1.98267	0.09048
C	-3.17272	1.67957	-0.37777
C	-1.25500	3.09476	-0.03330
C	-2.62081	2.94883	-0.24302
H	-4.23566	1.57259	-0.59784
H	-0.81801	4.09337	0.01549
H	-3.25612	3.83151	-0.33240
C	1.08477	2.20144	0.16081
H	1.57674	1.22333	0.25362
C	-3.00057	-0.82862	-0.52669
H	-2.30604	-1.60233	-0.18233
C	1.50264	3.07212	1.34149
H	1.13142	2.69461	2.30101
H	2.59735	3.13004	1.40305
H	1.13092	4.09947	1.22459
C	1.56605	2.82973	-1.14768
H	1.28670	2.22834	-2.02027
H	1.13814	3.83332	-1.27899
H	2.65827	2.93820	-1.14523
C	-4.31756	-1.04622	0.20664
H	-4.67387	-2.07276	0.05106
H	-4.21619	-0.88800	1.28798
H	-5.10568	-0.37400	-0.15746

C	-3.16391	-1.02419	-2.03346
H	-3.86825	-0.29368	-2.45519
H	-2.20955	-0.90907	-2.56428
H	-3.55224	-2.02753	-2.25397
C	0.27761	-1.21640	-0.66111
H	0.16668	-0.94287	-1.71150
F	2.24845	-0.11123	-2.65721
H	3.00142	0.08096	-2.03713
F	4.06544	0.34256	-1.18974
H	3.94140	0.24108	0.18707
F	3.86669	0.17121	1.17500

3Bb: ΔG = -2982364.7 kJ/mol

C	-0.33501	-1.06202	-1.79116
C	-1.25749	-2.23363	-1.42256
C	-1.05870	-2.52480	0.07941
N	-0.06478	-0.46551	-0.39799
H	-2.30120	-1.94581	-1.60074
H	-1.04910	-3.11153	-2.04401
C	-0.99721	-0.05176	-2.70157
H	-0.33485	0.79691	-2.90862
H	-1.20156	-0.54371	-3.65976
H	-1.95178	0.30823	-2.30598
C	0.99457	-1.49358	-2.39479
H	0.80534	-1.85255	-3.41279
H	1.69411	-0.65170	-2.47062
H	1.47427	-2.30770	-1.84369
C	-2.35806	-2.87084	0.79833
H	-2.74028	-3.82097	0.40472
H	-2.19631	-2.99471	1.87612
H	-3.12398	-2.10452	0.65031
C	-0.03126	-3.64118	0.34609
H	0.19662	-3.72552	1.41620
H	-0.46116	-4.59513	0.01678
H	0.90912	-3.49438	-0.19608
C	0.78680	0.69028	-0.19275
C	2.14352	0.45470	0.11964
C	0.25478	1.98939	-0.30850
C	2.98085	1.56889	0.23647
C	1.14488	3.06293	-0.19032
C	2.49566	2.85946	0.06189
H	4.03285	1.41468	0.48018
H	0.75650	4.07890	-0.27664
H	3.17029	3.71272	0.14940
C	-1.22531	2.28763	-0.43296
H	-1.76240	1.33495	-0.50298
C	2.71571	-0.91925	0.40875
H	1.98295	-1.67688	0.11349
C	-1.56239	3.13602	-1.65540
H	-1.19006	2.70752	-2.59238

H	-2.65069	3.25028	-1.74940
H	-1.13952	4.14600	-1.56303
C	-1.72039	2.99234	0.83074
H	-1.47836	2.43027	1.73832
H	-1.27213	3.99141	0.92361
H	-2.80991	3.12437	0.79416
C	3.98943	-1.20374	-0.37806
H	4.31538	-2.23888	-0.21190
H	3.84303	-1.06824	-1.45729
H	4.81634	-0.55161	-0.06749
C	2.94089	-1.08628	1.91043
H	3.69272	-0.37568	2.28084
H	2.01795	-0.92024	2.48146
H	3.30014	-2.09904	2.13710
C	-0.44552	-1.25184	0.54919
H	-0.21560	-1.01092	1.58739
F	-3.82757	0.26398	0.07871
H	-3.24509	0.18309	0.87104
F	-2.43670	-0.00069	2.00633
H	-1.32050	0.42048	2.72580
F	-0.49621	0.65140	3.22220

3Bc: ΔG = -2982378.6 kJ/mol

C	-0.62455	-1.95003	1.30474
C	-1.89613	-2.48817	0.62730
C	-2.43301	-1.37665	-0.30384
N	-0.29268	-0.77440	0.37323
H	-1.64386	-3.37350	0.03074
H	-2.63997	-2.79636	1.37002
C	0.51523	-2.95022	1.33074
H	1.44935	-2.49512	1.68375
H	0.25318	-3.74512	2.03838
H	0.68327	-3.42151	0.35836
C	-0.86323	-1.41194	2.70845
H	-1.03901	-2.26452	3.37419
H	0.01363	-0.87443	3.09104
H	-1.73936	-0.75904	2.76951
C	-2.85824	-1.89896	-1.67434
H	-3.68898	-2.60605	-1.55898
H	-3.19639	-1.08165	-2.32405
H	-2.03548	-2.42190	-2.17850
C	-3.56660	-0.55746	0.33030
H	-3.86020	0.28333	-0.30913
H	-4.44295	-1.20411	0.46214
H	-3.28810	-0.16079	1.31364
C	0.93336	-0.01503	0.46864
C	0.94232	1.14874	1.25984
C	2.05114	-0.45693	-0.26029
C	2.16073	1.82508	1.38251
C	3.24058	0.26222	-0.10218

C	3.30272	1.37633	0.72759
H	2.20539	2.73338	1.98457
H	4.12622	-0.04880	-0.65817
H	4.24217	1.92010	0.83897
C	1.97608	-1.57440	-1.28204
H	1.02286	-2.10151	-1.15302
C	-0.32106	1.74699	1.84594
H	-1.10171	0.97867	1.84827
C	3.09768	-2.59279	-1.12559
H	3.14039	-3.00469	-0.10911
H	2.95456	-3.42980	-1.82108
H	4.07878	-2.15272	-1.34885
C	1.95497	-0.97823	-2.68896
H	1.11364	-0.28668	-2.82235
H	2.87932	-0.42264	-2.90017
H	1.86195	-1.77123	-3.44289
C	-0.15248	2.22081	3.28252
H	-1.11358	2.56728	3.68378
H	0.21277	1.41884	3.93711
H	0.54875	3.06233	3.35940
C	-0.81633	2.86891	0.93357
H	-0.09837	3.70017	0.89865
H	-0.96210	2.51726	-0.09565
H	-1.77418	3.26737	1.29428
C	-1.24857	-0.49002	-0.43589
H	-1.15751	0.34846	-1.14163
F	-3.03443	2.63349	-2.02832
H	-2.16371	2.24671	-2.29033
F	-0.94633	1.65394	-2.65061
H	0.28486	2.24343	-2.29103
F	1.15357	2.63547	-2.04091

3Bc': ΔG = -2982374.2 kJ/mol

C	-0.00640	0.22123	2.31758
C	-1.42323	-0.25774	2.67175
C	-2.26340	-0.21875	1.37654
N	-0.02924	0.05107	0.79003
H	-1.37742	-1.28873	3.04339
H	-1.86328	0.35629	3.46506
C	1.08380	-0.63848	2.92466
H	2.07981	-0.34308	2.57165
H	1.06672	-0.49270	4.01082
H	0.92758	-1.70417	2.73355
C	0.24707	1.68428	2.65208
H	0.34327	1.77169	3.74032
H	1.18585	2.04390	2.21243
H	-0.57099	2.34074	2.34005
C	-3.17149	-1.43402	1.21753
H	-3.90114	-1.45375	2.03650
H	-3.72680	-1.39573	0.27200

H	-2.60204	-2.37091	1.24917
C	-3.08403	1.07442	1.23672
H	-3.58467	1.12939	0.26285
H	-3.85648	1.08734	2.01572
H	-2.46648	1.97224	1.35813
C	1.13762	0.27299	-0.03527
C	1.33003	1.55964	-0.57598
C	2.02208	-0.79514	-0.26828
C	2.50664	1.77848	-1.29955
C	3.18460	-0.51415	-0.99518
C	3.43658	0.76128	-1.48709
H	2.68535	2.76168	-1.73650
H	3.89114	-1.32096	-1.19550
H	4.35157	0.95760	-2.04843
C	1.71148	-2.23026	0.10781
H	0.79562	-2.24319	0.71333
C	0.27519	2.64608	-0.50627
H	-0.45052	2.37880	0.26916
C	2.82657	-2.88781	0.91236
H	3.08645	-2.31759	1.81234
H	2.52691	-3.89570	1.22780
H	3.74018	-2.99614	0.31220
C	1.41638	-3.02853	-1.16194
H	0.63882	-2.55199	-1.77001
H	2.31667	-3.12258	-1.78508
H	1.07737	-4.04264	-0.91265
C	0.84238	4.01035	-0.13940
H	0.03076	4.74012	-0.02282
H	1.40264	3.98079	0.80407
H	1.51441	4.39894	-0.91598
C	-0.49289	2.69177	-1.82656
H	0.16048	2.99405	-2.65682
H	-0.91699	1.71198	-2.08076
H	-1.31883	3.41348	-1.77054
C	-1.20687	-0.18190	0.33128
H	-1.36867	-0.30082	-0.74831
F	-2.05957	-3.06269	-1.75725
H	-1.84061	-2.18928	-2.16268
F	-1.53476	-0.92970	-2.70923
H	-2.65588	-0.08702	-2.70302
F	-3.44442	0.50772	-2.66556

3Bd: ΔG = -2982371.7 kJ/mol

C	-0.15021	1.13398	1.17100
C	-0.59868	2.49827	0.61933
C	0.18240	2.75478	-0.68933
N	0.51489	0.53184	-0.07947
H	-1.67359	2.46855	0.40309
H	-0.43514	3.29368	1.35439
C	-1.30572	0.26741	1.63116

H	-0.98158	-0.74914	1.88797
H	-1.72029	0.71649	2.54101
H	-2.11274	0.21934	0.89553
C	0.89063	1.23410	2.27560
H	0.39130	1.59951	3.18001
H	1.32140	0.25376	2.51469
H	1.69703	1.93442	2.03764
C	-0.69386	3.30881	-1.80932
H	-1.10434	4.27942	-1.50503
H	-0.11643	3.46013	-2.72985
H	-1.53454	2.64096	-2.03254
C	1.41842	3.64559	-0.48633
H	2.01922	3.71059	-1.40212
H	1.08770	4.65863	-0.22590
H	2.06141	3.27942	0.32305
C	1.01313	-0.82462	-0.14351
C	2.36535	-1.05771	0.17120
C	0.13406	-1.84180	-0.55556
C	2.80382	-2.38616	0.14375
C	0.62934	-3.14981	-0.56426
C	1.94311	-3.42329	-0.19950
H	3.84638	-2.60401	0.37942
H	-0.02661	-3.96195	-0.88161
H	2.30787	-4.45165	-0.20916
C	-1.25509	-1.55647	-1.08600
H	-1.49591	-0.50773	-0.88253
C	3.36213	0.05711	0.42101
H	2.81069	0.99132	0.57445
C	-2.32524	-2.41740	-0.42687
H	-2.27678	-2.36621	0.66754
H	-3.32547	-2.08785	-0.73590
H	-2.22710	-3.47307	-0.71459
C	-1.27340	-1.71440	-2.60543
H	-0.53944	-1.05705	-3.09057
H	-1.04486	-2.74733	-2.90326
H	-2.26446	-1.46384	-3.00674
C	4.21219	-0.17739	1.66295
H	4.85897	0.68931	1.85109
H	3.59648	-0.33565	2.55756
H	4.86839	-1.05063	1.54999
C	4.23194	0.25906	-0.81890
H	4.83912	-0.63234	-1.02955
H	3.62663	0.46616	-1.71144
H	4.91908	1.10377	-0.67622
C	0.67314	1.39311	-1.01751
H	1.16885	1.11064	-1.94935
F	-4.26532	-1.17853	2.45808
H	-4.51131	-0.60957	1.68447
F	-4.89450	0.19514	0.61595
H	-4.13868	0.57408	-0.48015

F	-3.62242	0.86184	-1.27847

Method M06-2X/def2-TZVP

1A: ΔG = -2456241.1 kJ/mol

C	1.11587	0.49390	1.46002
C	2.46730	1.08116	1.01911
C	2.71704	0.63291	-0.43053
N	0.47877	0.21573	0.13859
H	2.40885	2.18087	1.04605
H	3.28417	0.78794	1.69574
C	0.32353	1.49418	2.29381
H	-0.68438	1.11541	2.52310
H	0.83054	1.66501	3.25493
H	0.22472	2.46796	1.79623
C	1.25906	-0.78387	2.28607
H	1.65882	-0.54704	3.28277
H	0.28010	-1.26516	2.43514
H	1.93380	-1.52001	1.83064
C	3.55388	1.64153	-1.20393
H	4.57043	1.69063	-0.78579
H	3.64860	1.35794	-2.26311
H	3.12554	2.65093	-1.16410
C	3.40093	-0.73025	-0.51084
H	3.50659	-1.05822	-1.55642
H	4.41035	-0.67790	-0.07718
H	2.85876	-1.51901	0.02592
C	-0.85032	-0.28823	-0.00507
C	-1.06361	-1.68790	-0.10690
C	-1.95685	0.59763	-0.06802
C	-2.37310	-2.17372	-0.20370
C	-3.24894	0.06179	-0.15700
C	-3.46354	-1.31064	-0.21063
H	-2.53650	-3.25252	-0.28533
H	-4.10413	0.74275	-0.20401
H	-4.48008	-1.70703	-0.27946
C	-1.80659	2.10441	-0.13634
H	-0.74533	2.33618	0.01706
C	0.08040	-2.67533	-0.19846
H	0.99887	-2.12758	0.04480
C	-2.62437	2.83289	0.92265
H	-2.40198	2.48110	1.94026
H	-2.42054	3.91402	0.89532
H	-3.70679	2.70922	0.76213
C	-2.17505	2.60491	-1.53076
H	-1.58226	2.10841	-2.31139
H	-3.23933	2.42936	-1.75513
H	-1.99770	3.68786	-1.61837
C	-0.04873	-3.83165	0.78381
H	0.84655	-4.47066	0.75205
H	-0.16999	-3.48351	1.82008

H	-0.90972	-4.47708	0.55042
C	0.22890	-3.19174	-1.62715
H	-0.65475	-3.77051	-1.94045
H	0.35750	-2.37179	-2.34937
H	1.10349	-3.85418	-1.71782
C	1.28156	0.52034	-0.95797
H	1.15700	-0.18823	-1.79512
F	0.90813	1.78897	-1.56099

1Ba: ΔG = -2456208.7 kJ/mol

C	-1.30907	-0.17973	1.59958
C	-2.71333	-0.57651	1.12165
C	-2.79599	-0.25230	-0.38565
N	-0.58151	-0.09005	0.25340
H	-2.85886	-1.65625	1.27284
H	-3.49198	-0.06249	1.70140
C	-0.66593	-1.22031	2.49654
H	0.38051	-0.97482	2.72888
H	-1.21315	-1.24274	3.44884
H	-0.71055	-2.23069	2.07204
C	-1.26249	1.17871	2.28216
H	-1.75007	1.09593	3.26291
H	-0.22789	1.50779	2.45809
H	-1.79054	1.95553	1.71432
C	-3.45773	-1.36543	-1.19358
H	-4.49768	-1.50279	-0.86403
H	-3.47187	-1.12680	-2.26647
H	-2.93486	-2.32454	-1.06496
C	-3.48377	1.08716	-0.67725
H	-3.42633	1.34008	-1.74573
H	-4.54613	1.02381	-0.40124
H	-3.03534	1.91439	-0.10949
C	0.85201	0.05586	0.17161
C	1.40970	1.34768	0.13193
C	1.63686	-1.11319	0.13344
C	2.80633	1.44473	0.16994
C	3.02674	-0.95724	0.17182
C	3.60638	0.30769	0.21854
H	3.27217	2.43300	0.13625
H	3.66493	-1.84395	0.14101
H	4.69398	0.40768	0.25561
C	1.02623	-2.47652	-0.11957
H	-0.03982	-2.43492	0.15046
C	0.57262	2.58522	-0.11974
H	-0.47763	2.34328	0.09676
C	1.66103	-3.59300	0.69314
H	1.63823	-3.38379	1.77306
H	1.12817	-4.54041	0.52683
H	2.71034	-3.76541	0.41054
C	1.08843	-2.75448	-1.62224

H	0.68110	-1.90822	-2.20029
H	2.13072	-2.90566	-1.94697
H	0.52757	-3.66646	-1.87819
C	0.95677	3.77081	0.75119
H	0.27449	4.61493	0.57408
H	0.91382	3.52884	1.82356
H	1.97293	4.13256	0.53335
C	0.64860	2.92125	-1.60968
H	1.66305	3.25265	-1.88492
H	0.40379	2.03973	-2.22571
H	-0.04448	3.73818	-1.86331
C	-1.36371	-0.11729	-0.77383
H	-0.89198	-0.03646	-1.83478
F	-0.00157	0.03885	-3.02319

1Bb: ΔG = -2456186.0 kJ/mol

C	-0.74958	-1.00051	1.39753
C	-1.56136	-2.21105	0.90257
C	-1.71791	-2.09558	-0.63137
N	-0.19288	-0.47116	0.06284
H	-1.02855	-3.14000	1.15133
H	-2.53676	-2.25547	1.40434
C	0.38531	-1.38154	2.32810
H	1.04259	-0.52720	2.54602
H	-0.05212	-1.70399	3.28271
H	0.99027	-2.21527	1.95063
C	-1.61101	0.08135	2.02607
H	-2.00795	-0.32013	2.96993
H	-1.00344	0.96227	2.28576
H	-2.46064	0.39466	1.38185
C	-1.33447	-3.38457	-1.35874
H	-2.02272	-4.18906	-1.06324
H	-1.40345	-3.26564	-2.44914
H	-0.31230	-3.70700	-1.11064
C	-3.10799	-1.61825	-1.06945
H	-3.14697	-1.49860	-2.16296
H	-3.84394	-2.38951	-0.79650
H	-3.39052	-0.65420	-0.59554
C	0.82139	0.55452	-0.03185
C	0.42776	1.90340	-0.12249
C	2.16959	0.14452	-0.06276
C	1.44790	2.86273	-0.15832
C	3.14278	1.14905	-0.10372
C	2.78869	2.49467	-0.13040
H	1.17621	3.91938	-0.22837
H	4.19789	0.86546	-0.13304
H	3.56632	3.26196	-0.15673
C	2.58675	-1.30953	-0.16786
H	1.71809	-1.94066	0.07129
C	-1.01206	2.32972	-0.28586

H	-1.69774	1.49761	-0.06921
C	3.69992	-1.67623	0.80301
H	3.43893	-1.42758	1.84190
H	3.90821	-2.75499	0.76048
H	4.64083	-1.15839	0.56411
C	2.97818	-1.63030	-1.60826
H	2.15820	-1.41947	-2.31096
H	3.84901	-1.03735	-1.92821
H	3.24348	-2.69266	-1.71346
C	-1.41171	3.45917	0.65403
H	-2.50213	3.59653	0.61419
H	-1.14833	3.23991	1.69958
H	-0.94397	4.42021	0.38854
C	-1.28884	2.70958	-1.73866
H	-0.72184	3.60103	-2.05213
H	-1.03199	1.89325	-2.43124
H	-2.35981	2.92684	-1.87030
C	-0.73597	-1.03459	-0.95577
H	-0.46190	-0.72292	-1.97018
F	-3.77854	1.07330	0.17494

2A: ΔG = -2720006.5 kJ/mol

C	0.82811	-0.69500	1.49924
C	2.08713	-1.46559	1.06945
C	1.87569	-1.93231	-0.38122
N	0.24587	-0.33487	0.16094
H	2.94884	-0.78154	1.09461
H	2.31163	-2.29962	1.75032
C	1.18223	0.53114	2.32927
H	0.29511	1.15092	2.52912
H	1.57904	0.21146	3.30364
H	1.94902	1.15262	1.84958
C	-0.15467	-1.54022	2.30511
H	0.25473	-1.73226	3.30695
H	-1.11019	-1.01078	2.44062
H	-0.36594	-2.51460	1.84721
C	3.18617	-2.02843	-1.15040
H	3.79247	-2.85375	-0.74909
H	3.01333	-2.23572	-2.21676
H	3.78392	-1.11192	-1.07594
C	1.16686	-3.28474	-0.47058
H	0.96606	-3.55606	-1.51814
H	1.80298	-4.07125	-0.03991
H	0.20986	-3.31217	0.06529
C	-0.94485	0.44857	-0.00353
C	-2.19754	-0.20058	-0.13788
C	-0.86690	1.86261	-0.05609
C	-3.35262	0.58054	-0.26593
C	-2.05240	2.59864	-0.17838
C	-3.28870	1.96955	-0.27032

H	-4.32095	0.08345	-0.37478
H	-1.99636	3.69049	-0.21921
H	-4.20239	2.56208	-0.36528
C	0.44859	2.61061	-0.07295
H	1.23984	1.88200	0.12640
C	-2.33088	-1.70603	-0.22870
H	-1.35804	-2.13754	0.03513
C	0.53334	3.70248	0.98518
H	0.31749	3.32606	1.99537
H	1.54306	4.14038	1.00497
H	-0.16917	4.52624	0.78401
C	0.72064	3.18861	-1.45898
H	0.66105	2.41920	-2.24062
H	0.00370	3.98522	-1.71426
H	1.73005	3.62646	-1.50307
C	-3.36400	-2.27012	0.73747
H	-3.35918	-3.37007	0.71137
H	-3.17096	-1.96265	1.77564
H	-4.38581	-1.94924	0.48273
C	-2.63709	-2.13228	-1.66190
H	-3.61568	-1.75152	-1.99508
H	-1.88204	-1.76292	-2.37165
H	-2.66515	-3.22928	-1.74810
C	0.93411	-0.84937	-0.89878
H	0.32567	-1.09640	-1.77938
F	1.82751	0.25220	-1.57393
H	2.91245	0.97250	-0.69851
F	3.57261	1.41733	-0.17721

2Ba: ΔG = -2720046.5 kJ/mol

C	0.61848	-0.88233	-1.93472
C	1.94409	-1.60342	-1.63588
C	2.45293	-1.09605	-0.26961
N	0.26347	-0.37416	-0.53148
H	1.76516	-2.68700	-1.57958
H	2.67597	-1.43695	-2.43746
C	-0.46321	-1.80987	-2.45341
H	-1.43688	-1.30438	-2.52936
H	-0.18504	-2.13250	-3.46581
H	-0.57315	-2.71354	-1.84178
C	0.76523	0.30652	-2.87186
H	0.95653	-0.07072	-3.88525
H	-0.15630	0.90529	-2.91321
H	1.60246	0.96163	-2.60025
C	2.98397	-2.20166	0.63740
H	3.86892	-2.66908	0.18319
H	3.27612	-1.79197	1.61449
H	2.23206	-2.98684	0.80293
C	3.49075	0.03029	-0.38332
H	3.68663	0.47139	0.60357

H	4.43053	-0.37999	-0.77964
H	3.15755	0.82998	-1.05952
C	-0.99143	0.26250	-0.20931
C	-1.07167	1.66727	-0.28164
C	-2.06611	-0.54523	0.20697
C	-2.32226	2.24699	-0.03747
C	-3.29132	0.08951	0.44001
C	-3.42624	1.46659	0.29251
H	-2.42354	3.33406	-0.08551
H	-4.14669	-0.50705	0.76726
H	-4.39364	1.94152	0.47309
C	-1.88999	-2.00871	0.55702
H	-0.93858	-2.35654	0.12807
C	0.15166	2.54375	-0.46253
H	0.96047	1.92962	-0.88196
C	-2.99542	-2.89781	0.00927
H	-3.10778	-2.79395	-1.07989
H	-2.78057	-3.95492	0.22236
H	-3.97033	-2.67218	0.46681
C	-1.75977	-2.13886	2.07445
H	-0.96305	-1.49103	2.47164
H	-2.69751	-1.85305	2.57676
H	-1.53524	-3.17744	2.36004
C	-0.07291	3.70652	-1.41633
H	0.86502	4.25758	-1.57630
H	-0.43289	3.37035	-2.39992
H	-0.80361	4.42941	-1.02365
C	0.63269	3.02231	0.90753
H	-0.10695	3.69278	1.37353
H	0.79837	2.18342	1.59991
H	1.57536	3.58288	0.81447
C	1.22672	-0.49751	0.31275
H	1.07965	-0.15709	1.36215
F	0.55857	0.32220	2.98633
H	1.82575	0.54952	2.94352
F	2.83629	0.71681	2.81419

2Bb: ΔG = -2720036.7 kJ/mol

C	-0.63994	-0.96257	1.26308
C	-1.63718	-1.98484	0.68071
C	-1.50405	-1.97460	-0.86107
N	0.05396	-0.45752	-0.01361
H	-1.42960	-2.98679	1.07944
H	-2.65923	-1.70873	0.97210
C	0.39400	-1.58382	2.18309
H	1.18217	-0.86796	2.45867
H	-0.11070	-1.88691	3.11023
H	0.85665	-2.48144	1.75309
C	-1.33439	0.19947	1.94934
H	-1.76635	-0.17301	2.88860

H	-0.63067	1.00438	2.20781
H	-2.15963	0.59426	1.34316
C	-1.08882	-3.32829	-1.43948
H	-1.88045	-4.06521	-1.24449
H	-0.93921	-3.27288	-2.52699
H	-0.16053	-3.70018	-0.98182
C	-2.76442	-1.45002	-1.55706
H	-2.61120	-1.34970	-2.64134
H	-3.58527	-2.16359	-1.39478
H	-3.07457	-0.48057	-1.14063
C	1.11953	0.52163	-0.01167
C	0.78035	1.88593	-0.11165
C	2.45132	0.06623	0.05140
C	1.82986	2.81045	-0.05687
C	3.45705	1.03875	0.10190
C	3.15162	2.39539	0.06887
H	1.60061	3.87649	-0.13351
H	4.50131	0.71942	0.14895
H	3.95413	3.13560	0.11363
C	2.83218	-1.39734	-0.05028
H	1.92505	-2.00356	0.08068
C	-0.63057	2.35918	-0.38267
H	-1.33271	1.53881	-0.19289
C	3.82715	-1.82600	1.01855
H	3.46710	-1.59907	2.03233
H	4.00740	-2.90929	0.96370
H	4.80252	-1.33242	0.89356
C	3.36121	-1.69544	-1.45107
H	2.62778	-1.43612	-2.22903
H	4.28129	-1.12857	-1.66164
H	3.59882	-2.76404	-1.55883
C	-1.05958	3.51348	0.51136
H	-2.13052	3.71552	0.36844
H	-0.90623	3.28839	1.57718
H	-0.51596	4.44391	0.28641
C	-0.79336	2.71656	-1.85762
H	-0.16638	3.57617	-2.14301
H	-0.52238	1.87636	-2.51500
H	-1.84080	2.97844	-2.06990
C	-0.41320	-0.99819	-1.08045
H	-0.00696	-0.72394	-2.06075
F	-3.63505	1.39457	-0.16986
H	-4.07780	0.45245	0.48985
F	-4.44361	-0.37227	1.06003

2Aa: ΔG = -2720005.5 kJ/mol

C	-0.95053	0.16572	1.79668
C	-2.44842	-0.11520	1.56115
C	-2.72296	0.05469	0.05597
N	-0.40804	0.04936	0.39748

H	-2.67396	-1.15253	1.85156
H	-3.08584	0.53634	2.17651
C	-0.32938	-0.86470	2.72922
H	0.76035	-0.73115	2.80742
H	-0.74514	-0.74610	3.74022
H	-0.53431	-1.89424	2.40730
C	-0.68171	1.55287	2.37103
H	-0.99607	1.58331	3.42375
H	0.39234	1.79229	2.34548
H	-1.22454	2.35019	1.84771
C	-3.83225	-0.85386	-0.45503
H	-4.80580	-0.51536	-0.07144
H	-3.88436	-0.83361	-1.55444
H	-3.69046	-1.89610	-0.14645
C	-3.07342	1.49751	-0.31254
H	-3.13454	1.62558	-1.40391
H	-4.05438	1.76128	0.10797
H	-2.35211	2.23109	0.06857
C	0.98049	0.21553	0.06896
C	1.45125	1.49873	-0.30771
C	1.86830	-0.88728	0.10462
C	2.81385	1.66558	-0.58093
C	3.22380	-0.66535	-0.17450
C	3.70137	0.59828	-0.49970
H	3.18085	2.65266	-0.87580
H	3.91451	-1.51315	-0.15150
H	4.76330	0.74791	-0.71139
C	1.41474	-2.31480	0.33025
H	0.36386	-2.28768	0.63791
C	0.52103	2.67459	-0.51587
H	-0.44147	2.41145	-0.06402
C	2.21442	-3.03075	1.41051
H	2.20965	-2.48287	2.36413
H	1.79635	-4.03031	1.60231
H	3.26649	-3.17635	1.12053
C	1.46721	-3.08689	-0.98616
H	0.86442	-2.60225	-1.76662
H	2.49887	-3.17504	-1.36264
H	1.07735	-4.10824	-0.85633
C	1.00770	3.95380	0.14996
H	0.24845	4.74557	0.06603
H	1.21722	3.80823	1.21999
H	1.92547	4.34291	-0.31686
C	0.26718	2.89181	-2.00509
H	1.19179	3.17095	-2.53499
H	-0.12846	1.98616	-2.48844
H	-0.46233	3.70024	-2.16633
C	-1.35388	-0.27960	-0.51492
H	-1.13665	0.00925	-1.55180
F	-1.38725	-1.87632	-0.73699

H	-1.43127	-2.03744	-2.27244
F	-1.42009	-1.97287	-3.22187

2Ba': ΔG = -2720044.8 kJ/mol

C	1.63025	-0.12724	-1.60520
C	2.96886	-0.47187	-0.93126
C	2.82649	-0.15369	0.57285
N	0.71392	-0.06262	-0.37779
H	3.17806	-1.54380	-1.06069
H	3.79941	0.07698	-1.39477
C	1.15148	-1.18892	-2.57669
H	0.12874	-0.99135	-2.92902
H	1.80726	-1.17258	-3.45755
H	1.19616	-2.20088	-2.15632
C	1.63688	1.22891	-2.29381
H	2.26297	1.15799	-3.19328
H	0.62887	1.52581	-2.61829
H	2.05681	2.02107	-1.66095
C	3.39555	-1.24737	1.47377
H	4.48073	-1.33265	1.32055
H	3.21865	-1.01908	2.53449
H	2.94594	-2.22704	1.25585
C	3.40836	1.20884	0.96969
H	3.17161	1.45048	2.01589
H	4.50238	1.18457	0.86576
H	3.02542	2.02245	0.33771
C	-0.72508	0.01538	-0.47453
C	-1.34260	1.27950	-0.50090
C	-1.45145	-1.19104	-0.50006
C	-2.72980	1.30887	-0.69076
C	-2.83446	-1.10133	-0.68789
C	-3.46405	0.13417	-0.81173
H	-3.24356	2.27307	-0.71634
H	-3.43176	-2.01592	-0.71214
H	-4.54514	0.18092	-0.96394
C	-0.80691	-2.52145	-0.16758
H	0.27177	-2.44617	-0.37157
C	-0.59470	2.55608	-0.17676
H	0.48089	2.36815	-0.29825
C	-1.34255	-3.68180	-0.99041
H	-1.26394	-3.49102	-2.07097
H	-0.77707	-4.59909	-0.77252
H	-2.39748	-3.89945	-0.76646
C	-0.95230	-2.77771	1.33165
H	-0.54563	-1.95046	1.93020
H	-2.01208	-2.88353	1.61318
H	-0.43333	-3.70320	1.62278
C	-0.95832	3.71801	-1.08762
H	-0.33193	4.59320	-0.86266
H	-0.81407	3.47008	-2.14965

H	-2.00439	4.03440	-0.95952
C	-0.81425	2.90243	1.29562
H	-1.87833	3.09759	1.50385
H	-0.49629	2.08510	1.95986
H	-0.25031	3.80708	1.56942
C	1.35167	-0.07638	0.74124
H	0.81124	-0.00509	1.72929
F	0.04363	0.14192	3.18294
H	-1.23794	0.08129	2.82397
F	-2.20136	0.03687	2.52138

2Bc: ΔG = -2720038.4 kJ/mol

C	0.24684	1.19275	1.33054
C	0.46515	2.63967	0.85945
C	0.52448	2.63725	-0.68479
N	-0.22444	0.54130	0.01646
H	-0.37489	3.26549	1.19341
H	1.37744	3.06108	1.30116
C	-0.81270	1.05857	2.40495
H	-1.04582	0.00640	2.62257
H	-0.41613	1.49995	3.32918
H	-1.73962	1.59176	2.16228
C	1.53010	0.51272	1.77031
H	1.86841	0.99106	2.69996
H	1.36711	-0.55162	1.99474
H	2.33636	0.59636	1.03068
C	-0.36154	3.71858	-1.30446
H	0.01074	4.70890	-1.00654
H	-0.34716	3.66881	-2.40213
H	-1.40516	3.63533	-0.96824
C	1.94644	2.73068	-1.25001
H	1.93044	2.68393	-2.34877
H	2.37624	3.70188	-0.96541
H	2.60615	1.92700	-0.88603
C	-0.83944	-0.76525	-0.05875
C	-0.03420	-1.90249	-0.26169
C	-2.24451	-0.82609	0.04249
C	-0.68260	-3.14385	-0.28178
C	-2.83330	-2.09490	0.01216
C	-2.06109	-3.24364	-0.12902
H	-0.08882	-4.04757	-0.44055
H	-3.92063	-2.17872	0.08265
H	-2.54208	-4.22458	-0.14598
C	-3.12430	0.40900	0.06647
H	-2.49653	1.28361	0.29295
C	1.44505	-1.82314	-0.56563
H	1.83048	-0.83050	-0.30256
C	-4.21049	0.34154	1.13057
H	-3.79709	0.14064	2.12952
H	-4.75798	1.29365	1.18113

H	-4.95167	-0.44207	0.91408
C	-3.71969	0.64312	-1.31980
H	-2.93974	0.74548	-2.08897
H	-4.37225	-0.19125	-1.62034
H	-4.32611	1.56079	-1.33441
C	2.27170	-2.83331	0.21715
H	3.34125	-2.63299	0.07149
H	2.07884	-2.77290	1.29872
H	2.07735	-3.86958	-0.09977
C	1.68161	-1.97185	-2.06651
H	1.38559	-2.96803	-2.43233
H	1.11778	-1.22549	-2.64660
H	2.74802	-1.82943	-2.29454
C	-0.03187	1.29974	-1.00266
H	-0.28246	0.94643	-2.00920
F	3.80115	0.23830	-0.58163
H	4.14144	-0.29994	0.51871
F	4.40416	-0.73913	1.42607

2Bd: ΔG = -2720036.1 kJ/mol

C	-0.09537	-1.27478	1.41508
C	-0.71251	-2.59183	0.91939
C	-1.12486	-2.39935	-0.55745
N	0.18716	-0.57651	0.07285
H	0.03238	-3.39691	0.99327
H	-1.56628	-2.88333	1.54493
C	1.17706	-1.47237	2.21318
H	1.68914	-0.52048	2.41470
H	0.90192	-1.90219	3.18577
H	1.87864	-2.16827	1.73799
C	-1.06204	-0.39461	2.18849
H	-1.27392	-0.88493	3.14894
H	-0.60413	0.57877	2.42012
H	-2.02131	-0.22825	1.67365
C	-0.63882	-3.53475	-1.45877
H	-1.10939	-4.47655	-1.14346
H	-0.91066	-3.35625	-2.50844
H	0.45146	-3.66598	-1.40145
C	-2.63012	-2.18560	-0.74316
H	-2.86985	-1.93694	-1.78645
H	-3.14977	-3.12124	-0.49090
H	-3.02449	-1.38155	-0.10570
C	0.94292	0.64897	-0.02038
C	0.25923	1.88069	-0.01043
C	2.34580	0.55047	-0.11750
C	1.04616	3.03997	0.01278
C	3.07529	1.74337	-0.10043
C	2.43465	2.97555	-0.00734
H	0.54951	4.01382	0.02320
H	4.16454	1.70231	-0.17998

H	3.02347	3.89566	0.01556
C	3.05567	-0.76537	-0.36930
H	2.35657	-1.58567	-0.14962
C	-1.24204	2.01467	-0.16157
H	-1.72648	1.03055	-0.07058
C	4.28535	-0.95679	0.50591
H	4.05337	-0.84602	1.57497
H	4.70992	-1.96025	0.35880
H	5.07907	-0.23506	0.26207
C	3.40805	-0.87771	-1.85100
H	2.51628	-0.79782	-2.49044
H	4.10712	-0.08416	-2.15721
H	3.88798	-1.84392	-2.06562
C	-1.87806	2.91075	0.89167
H	-2.97062	2.90333	0.77442
H	-1.65689	2.57208	1.91422
H	-1.54160	3.95541	0.80549
C	-1.55278	2.53084	-1.56554
H	-1.14023	3.53984	-1.72317
H	-1.13101	1.87561	-2.34287
H	-2.63840	2.56517	-1.71968
C	-0.40696	-1.14979	-0.91108
H	-0.35567	-0.71675	-1.91657
F	-3.90452	0.27760	0.98866
H	-3.95838	0.51168	-0.22120
F	-4.00462	0.69240	-1.26866

3Bb: ΔG = -2983831.6 kJ/mol

C	0.62142	-0.90599	1.74629
C	1.76961	-1.84559	1.35108
C	1.59034	-2.20373	-0.13669
N	0.16680	-0.41986	0.36136
H	2.72500	-1.31771	1.47775
H	1.79462	-2.73579	1.99376
C	1.08341	0.24897	2.60791
H	0.26546	0.95322	2.81471
H	1.41439	-0.15487	3.57456
H	1.93036	0.78552	2.16342
C	-0.54719	-1.60997	2.41972
H	-0.23956	-1.90355	3.43221
H	-1.41545	-0.94300	2.52199
H	-0.86181	-2.52129	1.89609
C	2.91266	-2.27880	-0.89013
H	3.48680	-3.14169	-0.52335
H	2.75237	-2.41438	-1.96860
H	3.50920	-1.37311	-0.74191
C	0.81729	-3.51576	-0.35573
H	0.57983	-3.66459	-1.41907
H	1.44482	-4.35656	-0.02864
H	-0.12110	-3.55899	0.21264

C	-0.91882	0.52240	0.18298
C	-2.21418	0.00779	-0.04982
C	-0.66537	1.90783	0.26000
C	-3.27009	0.92334	-0.12536
C	-1.76305	2.77331	0.18458
C	-3.05496	2.29017	0.01305
H	-4.28133	0.55133	-0.30847
H	-1.58880	3.85139	0.23775
H	-3.89715	2.98421	-0.04145
C	0.72985	2.49161	0.28064
H	1.44060	1.66077	0.36225
C	-2.49670	-1.45816	-0.30986
H	-1.61259	-2.04156	-0.02103
C	0.97231	3.46017	1.43022
H	0.74217	3.02739	2.41318
H	2.02708	3.77345	1.44568
H	0.36744	4.37397	1.32361
C	1.01611	3.17686	-1.05406
H	0.78222	2.51879	-1.89836
H	0.42666	4.10075	-1.16515
H	2.08023	3.44900	-1.12460
C	-3.66586	-1.99343	0.50509
H	-3.76961	-3.07835	0.35858
H	-3.53435	-1.81410	1.58198
H	-4.62177	-1.53819	0.20608
C	-2.71228	-1.68753	-1.80399
H	-3.61376	-1.16588	-2.16132
H	-1.86393	-1.32298	-2.40173
H	-2.84178	-2.75846	-2.02054
C	0.69932	-1.10215	-0.59792
H	0.37185	-0.94483	-1.62793
F	3.57357	0.87686	0.12638
H	3.02884	0.73304	-0.68264
F	2.26356	0.44672	-1.81732
H	1.15043	0.57270	-2.64271
F	0.31311	0.58144	-3.16642

3Bc: ΔG = -2983841.6

C	-2.32932	-0.14265	1.05458
C	-3.35863	-0.43460	-0.04978
C	-2.72029	-0.05091	-1.40382
N	-1.04830	-0.05824	0.21120
H	-3.59679	-1.50810	-0.05192
H	-4.29764	0.10521	0.13035
C	-2.22045	-1.24157	2.09404
H	-1.36030	-1.08636	2.76138
H	-3.12377	-1.21446	2.71793
H	-2.15927	-2.24397	1.65533
C	-2.56194	1.18609	1.75678
H	-3.46005	1.08954	2.38113

H	-1.72560	1.44562	2.42109
H	-2.73535	2.01272	1.05675
C	-2.97648	-1.08785	-2.49391
H	-4.05548	-1.15933	-2.69042
H	-2.47904	-0.81188	-3.43403
H	-2.62088	-2.08488	-2.19636
C	-3.12702	1.34469	-1.89553
H	-2.56869	1.62661	-2.79937
H	-4.19743	1.34327	-2.14464
H	-2.95577	2.11783	-1.13390
C	0.30234	-0.02100	0.72735
C	0.92075	1.22778	0.92067
C	0.98007	-1.24626	0.87007
C	2.25910	1.21798	1.32988
C	2.31446	-1.19243	1.28391
C	2.94725	0.02416	1.51757
H	2.77645	2.17033	1.47414
H	2.87681	-2.12434	1.38600
H	3.99527	0.04246	1.82661
C	0.36227	-2.57904	0.49336
H	-0.71265	-2.42611	0.32190
C	0.23770	2.54680	0.61931
H	-0.82700	2.34846	0.44293
C	0.50660	-3.61662	1.59782
H	0.09462	-3.26261	2.55415
H	-0.02170	-4.54333	1.33011
H	1.55980	-3.88519	1.77013
C	0.93459	-3.08835	-0.82567
H	0.80894	-2.35206	-1.63184
H	2.01071	-3.29783	-0.74682
H	0.43008	-4.01845	-1.12750
C	0.33296	3.52474	1.78242
H	-0.24550	4.43589	1.57052
H	-0.05341	3.09457	2.71809
H	1.37134	3.83917	1.96727
C	0.77746	3.16466	-0.66591
H	1.84154	3.42485	-0.57528
H	0.68669	2.47694	-1.51805
H	0.22524	4.08520	-0.90800
C	-1.27794	-0.00624	-1.05420
H	-0.41407	0.07257	-1.74050
F	3.25264	1.69728	-1.86827
H	2.49751	1.08095	-1.96095
F	1.50343	0.06068	-2.10291
H	2.58721	-0.85690	-1.87040
F	3.39564	-1.39186	-1.73859

3Bc': ΔG = -2983830.7 kJ/mol

C	-0.55587	-0.23032	2.17561
C	-1.94187	-0.89419	2.13529

C	-2.50320	-0.72194	0.70946
N	-0.25267	-0.11750	0.67422
H	-1.84000	-1.96582	2.35826
H	-2.60800	-0.46632	2.89624
C	0.48994	-1.08454	2.85932
H	1.48922	-0.63023	2.79925
H	0.23147	-1.16384	3.92397
H	0.52713	-2.10214	2.45083
C	-0.56424	1.16339	2.78342
H	-0.70980	1.06705	3.86760
H	0.39282	1.68139	2.62611
H	-1.37672	1.79190	2.39759
C	-3.21079	-1.96487	0.18282
H	-4.12906	-2.13407	0.76279
H	-3.49141	-1.84028	-0.87232
H	-2.57886	-2.85699	0.26293
C	-3.43922	0.49070	0.56528
H	-3.69111	0.66955	-0.48955
H	-4.37183	0.28922	1.11081
H	-3.00085	1.41113	0.97428
C	0.98686	0.43523	0.17187
C	1.01858	1.81398	-0.13334
C	2.11172	-0.39872	0.01703
C	2.25123	2.36286	-0.50320
C	3.31878	0.21049	-0.34761
C	3.39708	1.57814	-0.58178
H	2.30660	3.42651	-0.74690
H	4.20720	-0.41353	-0.47625
H	4.35106	2.03138	-0.86169
C	2.04268	-1.91161	0.06246
H	1.03092	-2.20354	0.38366
C	-0.22549	2.67833	-0.18450
H	-1.02540	2.17547	0.37570
C	3.05743	-2.53657	1.00998
H	2.96641	-2.16143	2.03858
H	2.93109	-3.62860	1.04199
H	4.08925	-2.34359	0.67907
C	2.23114	-2.44744	-1.35686
H	1.54714	-1.96042	-2.06350
H	3.26130	-2.27798	-1.70755
H	2.04170	-3.53030	-1.39350
C	-0.03171	4.04671	0.45237
H	-0.98567	4.59255	0.48255
H	0.34207	3.97240	1.48409
H	0.67464	4.67192	-0.11384
C	-0.70432	2.80206	-1.63006
H	0.04493	3.31520	-2.25298
H	-0.90311	1.82318	-2.09003
H	-1.63491	3.38731	-1.68175
C	-1.27549	-0.39295	-0.05852

H	-1.20947	-0.29973	-1.14634
F	-0.80638	-2.70099	-1.48612
H	-0.60346	-1.97441	-2.12925
F	-0.37202	-0.85625	-2.92893
H	-1.64320	-0.29818	-3.02974
F	-2.55303	0.08784	-2.97993

3Bd: ΔG = -2983834.4 kJ/mol

C	0.13063	-1.06490	1.62069
C	1.14306	-2.15543	1.24699
C	0.98821	-2.44372	-0.26138
N	-0.16923	-0.48191	0.22989
H	2.15713	-1.77589	1.43337
H	1.00127	-3.05685	1.85779
C	0.70647	-0.00621	2.53444
H	-0.00646	0.81254	2.70899
H	0.90936	-0.47128	3.50900
H	1.65401	0.39008	2.15362
C	-1.16369	-1.60302	2.20973
H	-0.95415	-1.96032	3.22682
H	-1.92830	-0.81707	2.29120
H	-1.57845	-2.44664	1.64403
C	2.33707	-2.59457	-0.95858
H	2.85980	-3.46862	-0.54441
H	2.21791	-2.74873	-2.03951
H	2.96294	-1.70661	-0.80491
C	0.09690	-3.65520	-0.56857
H	-0.07381	-3.75946	-1.64961
H	0.59562	-4.56844	-0.21488
H	-0.88189	-3.59000	-0.07386
C	-0.99242	0.68895	0.03825
C	-2.37399	0.50516	-0.18349
C	-0.39032	1.96264	0.08470
C	-3.16805	1.65447	-0.26684
C	-1.23927	3.07326	0.00313
C	-2.61339	2.92481	-0.14888
H	-4.24141	1.54657	-0.44257
H	-0.80268	4.07507	0.03895
H	-3.25491	3.80742	-0.20625
C	1.10941	2.18314	0.09967
H	1.61552	1.20676	0.15772
C	-2.99942	-0.85235	-0.43911
H	-2.28325	-1.63145	-0.14173
C	1.57663	3.03818	1.27220
H	1.22306	2.66636	2.24301
H	2.67601	3.06468	1.30707
H	1.22988	4.07835	1.17225
C	1.54854	2.82707	-1.21421
H	1.24875	2.22766	-2.08262
H	1.12351	3.83671	-1.32578

H	2.64329	2.91858	-1.24410
C	-4.27392	-1.07984	0.36123
H	-4.64021	-2.10633	0.21587
H	-4.11697	-0.93167	1.43942
H	-5.08353	-0.40411	0.04758
C	-3.24771	-1.03163	-1.93502
H	-3.96547	-0.28785	-2.31437
H	-2.32114	-0.92490	-2.51819
H	-3.66203	-2.02892	-2.14469
C	0.26207	-1.23184	-0.72334
H	0.04156	-0.98576	-1.76382
F	1.89886	-0.01184	-2.50589
H	2.68801	0.21126	-1.92615
F	3.75901	0.48752	-1.15339
H	3.69527	0.26756	0.18372
F	3.65497	0.09106	1.16685

3Be: ΔG = -2983825.5 kJ/mol

C	-0.09961	1.15312	1.28648
C	-0.29860	2.59583	0.78664
C	0.45464	2.74053	-0.54975
N	0.37371	0.46605	-0.01212
H	-1.36777	2.77355	0.61427
H	0.04817	3.32274	1.53334
C	-1.38722	0.53347	1.78753
H	-1.27181	-0.53663	2.01399
H	-1.66249	1.03345	2.72650
H	-2.21769	0.66996	1.08876
C	0.98719	1.00393	2.33945
H	0.61808	1.43684	3.27852
H	1.21699	-0.05351	2.53501
H	1.91604	1.52710	2.08146
C	-0.27389	3.58121	-1.59242
H	-0.36980	4.61134	-1.22188
H	0.29456	3.61983	-2.53254
H	-1.27512	3.19115	-1.79990
C	1.87663	3.30749	-0.37489
H	2.46352	3.21778	-1.30036
H	1.79655	4.37566	-0.12871
H	2.43454	2.81998	0.43489
C	0.75155	-0.93353	-0.09946
C	2.12045	-1.25662	0.04157
C	-0.23131	-1.91365	-0.34554
C	2.47241	-2.61038	-0.01014
C	0.18436	-3.24951	-0.38687
C	1.51723	-3.60032	-0.20755
H	3.52475	-2.88617	0.09454
H	-0.55812	-4.02664	-0.58377
H	1.81701	-4.65037	-0.24307
C	-1.66584	-1.57554	-0.67548

H	-1.85777	-0.54210	-0.37586
C	3.22402	-0.22565	0.16729
H	2.76812	0.75136	0.36867
C	-2.67063	-2.46036	0.04647
H	-2.49268	-2.48461	1.13151
H	-3.68387	-2.06876	-0.10870
H	-2.64946	-3.49850	-0.31903
C	-1.88192	-1.61208	-2.18575
H	-1.18828	-0.94043	-2.71364
H	-1.74092	-2.62560	-2.59392
H	-2.90483	-1.28938	-2.43028
C	4.17335	-0.51729	1.32151
H	4.89318	0.30524	1.44200
H	3.63873	-0.63473	2.27510
H	4.75894	-1.43333	1.15288
C	3.97962	-0.09801	-1.15235
H	4.48920	-1.03803	-1.41493
H	3.30855	0.15805	-1.98550
H	4.74702	0.68766	-1.08737
C	0.61099	1.31816	-0.94846
H	0.99149	0.97664	-1.91828
F	-4.32616	-0.43625	1.99668
H	-4.27013	-0.12193	1.06736
F	-4.21464	0.31410	-0.27227
H	-3.20424	0.96859	-0.81945
F	-2.42442	1.45956	-1.24290

Method M06-2X/ma-def2-TZVP

1A: ΔG = -2456248.6 kJ/mol

C	1.11587	0.49390	1.46002
C	2.46730	1.08116	1.01911
C	2.71704	0.63291	-0.43053
N	0.47877	0.21573	0.13859
H	2.40885	2.18087	1.04605
H	3.28417	0.78794	1.69574
C	0.32353	1.49418	2.29381
H	-0.68438	1.11541	2.52310
H	0.83054	1.66501	3.25493
H	0.22472	2.46796	1.79623
C	1.25906	-0.78387	2.28607
H	1.65882	-0.54704	3.28277
H	0.28010	-1.26516	2.43514
H	1.93380	-1.52001	1.83064
C	3.55388	1.64153	-1.20393
H	4.57043	1.69063	-0.78579
H	3.64860	1.35794	-2.26311
H	3.12554	2.65093	-1.16410
C	3.40093	-0.73025	-0.51084
H	3.50659	-1.05822	-1.55642
H	4.41035	-0.67790	-0.07718

H	2.85876	-1.51901	0.02592
C	-0.85032	-0.28823	-0.00507
C	-1.06361	-1.68790	-0.10690
C	-1.95685	0.59763	-0.06802
C	-2.37310	-2.17372	-0.20370
C	-3.24894	0.06179	-0.15700
C	-3.46354	-1.31064	-0.21063
H	-2.53650	-3.25252	-0.28533
H	-4.10413	0.74275	-0.20401
H	-4.48008	-1.70703	-0.27946
C	-1.80659	2.10441	-0.13634
H	-0.74533	2.33618	0.01706
C	0.08040	-2.67533	-0.19846
H	0.99887	-2.12758	0.04480
C	-2.62437	2.83289	0.92265
H	-2.40198	2.48110	1.94026
H	-2.42054	3.91402	0.89532
H	-3.70679	2.70922	0.76213
C	-2.17505	2.60491	-1.53076
H	-1.58226	2.10841	-2.31139
H	-3.23933	2.42936	-1.75513
H	-1.99770	3.68786	-1.61837
C	-0.04873	-3.83165	0.78381
H	0.84655	-4.47066	0.75205
H	-0.16999	-3.48351	1.82008
H	-0.90972	-4.47708	0.55042
C	0.22890	-3.19174	-1.62715
H	-0.65475	-3.77051	-1.94045
H	0.35750	-2.37179	-2.34937
H	1.10349	-3.85418	-1.71782
C	1.28156	0.52034	-0.95797
H	1.15700	-0.18823	-1.79512
F	0.90813	1.78897	-1.56099

1Ba: ΔG = -2456216.3 kJ/mol

C	-1.30907	-0.17973	1.59958
C	-2.71333	-0.57651	1.12165
C	-2.79599	-0.25230	-0.38565
N	-0.58151	-0.09005	0.25340
H	-2.85886	-1.65625	1.27284
H	-3.49198	-0.06249	1.70140
C	-0.66593	-1.22031	2.49654
H	0.38051	-0.97482	2.72888
H	-1.21315	-1.24274	3.44884
H	-0.71055	-2.23069	2.07204
C	-1.26249	1.17871	2.28216
H	-1.75007	1.09593	3.26291
H	-0.22789	1.50779	2.45809
H	-1.79054	1.95553	1.71432
C	-3.45773	-1.36543	-1.19358

H	-4.49768	-1.50279	-0.86403
H	-3.47187	-1.12680	-2.26647
H	-2.93486	-2.32454	-1.06496
C	-3.48377	1.08716	-0.67725
H	-3.42633	1.34008	-1.74573
H	-4.54613	1.02381	-0.40124
H	-3.03534	1.91439	-0.10949
C	0.85201	0.05586	0.17161
C	1.40970	1.34768	0.13193
C	1.63686	-1.11319	0.13344
C	2.80633	1.44473	0.16994
C	3.02674	-0.95724	0.17182
C	3.60638	0.30769	0.21854
H	3.27217	2.43300	0.13625
H	3.66493	-1.84395	0.14101
H	4.69398	0.40768	0.25561
C	1.02623	-2.47652	-0.11957
H	-0.03982	-2.43492	0.15046
C	0.57262	2.58522	-0.11974
H	-0.47763	2.34328	0.09676
C	1.66103	-3.59300	0.69314
H	1.63823	-3.38379	1.77306
H	1.12817	-4.54041	0.52683
H	2.71034	-3.76541	0.41054
C	1.08843	-2.75448	-1.62224
H	0.68110	-1.90822	-2.20029
H	2.13072	-2.90566	-1.94697
H	0.52757	-3.66646	-1.87819
C	0.95677	3.77081	0.75119
H	0.27449	4.61493	0.57408
H	0.91382	3.52884	1.82356
H	1.97293	4.13256	0.53335
C	0.64860	2.92125	-1.60968
H	1.66305	3.25265	-1.88492
H	0.40379	2.03973	-2.22571
H	-0.04448	3.73818	-1.86331
C	-1.36371	-0.11729	-0.77383
H	-0.89198	-0.03646	-1.83478
F	-0.00157	0.03885	-3.02319

1Bb: ΔG = -2456205.4 kJ/mol

C	-0.74958	-1.00051	1.39753
C	-1.56136	-2.21105	0.90257
C	-1.71791	-2.09558	-0.63137
N	-0.19288	-0.47116	0.06284
H	-1.02855	-3.14000	1.15133
H	-2.53676	-2.25547	1.40434
C	0.38531	-1.38154	2.32810
H	1.04259	-0.52720	2.54602
H	-0.05212	-1.70399	3.28271

H	0.99027	-2.21527	1.95063
C	-1.61101	0.08135	2.02607
H	-2.00795	-0.32013	2.96993
H	-1.00344	0.96227	2.28576
H	-2.46064	0.39466	1.38185
C	-1.33447	-3.38457	-1.35874
H	-2.02272	-4.18906	-1.06324
H	-1.40345	-3.26564	-2.44914
H	-0.31230	-3.70700	-1.11064
C	-3.10799	-1.61825	-1.06945
H	-3.14697	-1.49860	-2.16296
H	-3.84394	-2.38951	-0.79650
H	-3.39052	-0.65420	-0.59554
C	0.82139	0.55452	-0.03185
C	0.42776	1.90340	-0.12249
C	2.16959	0.14452	-0.06276
C	1.44790	2.86273	-0.15832
C	3.14278	1.14905	-0.10372
C	2.78869	2.49467	-0.13040
H	1.17621	3.91938	-0.22837
H	4.19789	0.86546	-0.13304
H	3.56632	3.26196	-0.15673
C	2.58675	-1.30953	-0.16786
H	1.71809	-1.94066	0.07129
C	-1.01206	2.32972	-0.28586
H	-1.69774	1.49761	-0.06921
C	3.69992	-1.67623	0.80301
H	3.43893	-1.42758	1.84190
H	3.90821	-2.75499	0.76048
H	4.64083	-1.15839	0.56411
C	2.97818	-1.63030	-1.60826
H	2.15820	-1.41947	-2.31096
H	3.84901	-1.03735	-1.92821
H	3.24348	-2.69266	-1.71346
C	-1.41171	3.45917	0.65403
H	-2.50213	3.59653	0.61419
H	-1.14833	3.23991	1.69958
H	-0.94397	4.42021	0.38854
C	-1.28884	2.70958	-1.73866
H	-0.72184	3.60103	-2.05213
H	-1.03199	1.89325	-2.43124
H	-2.35981	2.92684	-1.87030
C	-0.73597	-1.03459	-0.95577
H	-0.46190	-0.72292	-1.97018
F	-3.77854	1.07330	0.17494

2A: ΔG = -2720010.5 kJ/mol

C	0.81799	-0.69239	1.50289
C	2.06841	-1.49954	1.10173
C	1.87378	-1.94826	-0.35778

N	0.25688	-0.33132	0.16702
H	2.94646	-0.85255	1.16297
H	2.22756	-2.34745	1.76923
C	1.19734	0.52982	2.33368
H	0.32017	1.14605	2.54141
H	1.60420	0.19390	3.28940
H	1.95495	1.13750	1.84007
C	-0.18613	-1.50975	2.31710
H	0.22977	-1.70353	3.30714
H	-1.11498	-0.94984	2.44830
H	-0.41914	-2.46811	1.85733
C	3.19375	-2.05127	-1.11528
H	3.78064	-2.87105	-0.69599
H	3.02184	-2.26622	-2.17215
H	3.78642	-1.14148	-1.03886
C	1.16819	-3.30531	-0.46282
H	0.94919	-3.54273	-1.50637
H	1.82811	-4.08066	-0.06964
H	0.23770	-3.35129	0.09830
C	-0.93462	0.45043	-0.00716
C	-2.17791	-0.19829	-0.14898
C	-0.86270	1.85686	-0.05151
C	-3.33143	0.57283	-0.27545
C	-2.04469	2.58691	-0.17201
C	-3.27307	1.95636	-0.26918
H	-4.28822	0.07768	-0.39168
H	-1.99472	3.66876	-0.20764
H	-4.18026	2.54083	-0.36249
C	0.44747	2.61727	-0.06833
H	1.24434	1.90701	0.11743
C	-2.30646	-1.70351	-0.25534
H	-1.33754	-2.13598	-0.03179
C	0.51975	3.70777	1.00072
H	0.30644	3.31642	1.99608
H	1.52096	4.14446	1.01532
H	-0.18831	4.51309	0.79414
C	0.68405	3.22536	-1.45381
H	0.65130	2.46272	-2.23298
H	-0.07580	3.97761	-1.67928
H	1.66146	3.71202	-1.49113
C	-3.32095	-2.28105	0.73116
H	-3.30369	-3.37205	0.68690
H	-3.10074	-1.97845	1.75609
H	-4.33567	-1.95633	0.49193
C	-2.66796	-2.10347	-1.68900
H	-3.65037	-1.71195	-1.96371
H	-1.93746	-1.71942	-2.40397
H	-2.69841	-3.19130	-1.78181
C	0.94060	-0.86126	-0.88962
H	0.33171	-1.12001	-1.75446

F	1.81934	0.21458	-1.55145
H	2.94876	0.97615	-0.80086
F	3.64935	1.46593	-0.38076

2Ba': ΔG = -2720059.0 kJ/mol

C	0.81799	-0.69239	1.50289
C	2.06841	-1.49954	1.10173
C	1.87378	-1.94826	-0.35778
N	0.25688	-0.33132	0.16702
H	2.94646	-0.85255	1.16297
H	2.22756	-2.34745	1.76923
C	1.19734	0.52982	2.33368
H	0.32017	1.14605	2.54141
H	1.60420	0.19390	3.28940
H	1.95495	1.13750	1.84007
C	-0.18613	-1.50975	2.31710
H	0.22977	-1.70353	3.30714
H	-1.11498	-0.94984	2.44830
H	-0.41914	-2.46811	1.85733
C	3.19375	-2.05127	-1.11528
H	3.78064	-2.87105	-0.69599
H	3.02184	-2.26622	-2.17215
H	3.78642	-1.14148	-1.03886
C	1.16819	-3.30531	-0.46282
H	0.94919	-3.54273	-1.50637
H	1.82811	-4.08066	-0.06964
H	0.23770	-3.35129	0.09830
C	-0.93462	0.45043	-0.00716
C	-2.17791	-0.19829	-0.14898
C	-0.86270	1.85686	-0.05151
C	-3.33143	0.57283	-0.27545
C	-2.04469	2.58691	-0.17201
C	-3.27307	1.95636	-0.26918
H	-4.28822	0.07768	-0.39168
H	-1.99472	3.66876	-0.20764
H	-4.18026	2.54083	-0.36249
C	0.44747	2.61727	-0.06833
H	1.24434	1.90701	0.11743
C	-2.30646	-1.70351	-0.25534
H	-1.33754	-2.13598	-0.03179
C	0.51975	3.70777	1.00072
H	0.30644	3.31642	1.99608
H	1.52096	4.14446	1.01532
H	-0.18831	4.51309	0.79414
C	0.68405	3.22536	-1.45381
H	0.65130	2.46272	-2.23298
H	-0.07580	3.97761	-1.67928
H	1.66146	3.71202	-1.49113
C	-3.32095	-2.28105	0.73116
H	-3.30369	-3.37205	0.68690

H	-3.10074	-1.97845	1.75609
H	-4.33567	-1.95633	0.49193
C	-2.66796	-2.10347	-1.68900
H	-3.65037	-1.71195	-1.96371
H	-1.93746	-1.71942	-2.40397
H	-2.69841	-3.19130	-1.78181
C	0.94060	-0.86126	-0.88962
H	0.33171	-1.12001	-1.75446
F	1.81934	0.21458	-1.55145
H	2.94876	0.97615	-0.80086
F	3.64935	1.46593	-0.38076

2Bb: ΔG = -2720052.4 kJ/mol

C	0.24684	1.19275	1.33054
C	0.46515	2.63967	0.85945
C	0.52448	2.63725	-0.68479
N	-0.22444	0.54130	0.01646
H	-0.37489	3.26549	1.19341
H	1.37744	3.06108	1.30116
C	-0.81270	1.05857	2.40495
H	-1.04582	0.00640	2.62257
H	-0.41613	1.49995	3.32918
H	-1.73962	1.59176	2.16228
C	1.53010	0.51272	1.77031
H	1.86841	0.99106	2.69996
H	1.36711	-0.55162	1.99474
H	2.33636	0.59636	1.03068
C	-0.36154	3.71858	-1.30446
H	0.01074	4.70890	-1.00654
H	-0.34716	3.66881	-2.40213
H	-1.40516	3.63533	-0.96824
C	1.94644	2.73068	-1.25001
H	1.93044	2.68393	-2.34877
H	2.37624	3.70188	-0.96541
H	2.60615	1.92700	-0.88603
C	-0.83944	-0.76525	-0.05875
C	-0.03420	-1.90249	-0.26169
C	-2.24451	-0.82609	0.04249
C	-0.68260	-3.14385	-0.28178
C	-2.83330	-2.09490	0.01216
C	-2.06109	-3.24364	-0.12902
H	-0.08882	-4.04757	-0.44055
H	-3.92063	-2.17872	0.08265
H	-2.54208	-4.22458	-0.14598
C	-3.12430	0.40900	0.06647
H	-2.49653	1.28361	0.29295
C	1.44505	-1.82314	-0.56563
H	1.83048	-0.83050	-0.30256
C	-4.21049	0.34154	1.13057
H	-3.79709	0.14064	2.12952

H	-4.75798	1.29365	1.18113
H	-4.95167	-0.44207	0.91408
C	-3.71969	0.64312	-1.31980
H	-2.93974	0.74548	-2.08897
H	-4.37225	-0.19125	-1.62034
H	-4.32611	1.56079	-1.33441
C	2.27170	-2.83331	0.21715
H	3.34125	-2.63299	0.07149
H	2.07884	-2.77290	1.29872
H	2.07735	-3.86958	-0.09977
C	1.68161	-1.97185	-2.06651
H	1.38559	-2.96803	-2.43233
H	1.11778	-1.22549	-2.64660
H	2.74802	-1.82943	-2.29454
C	-0.03187	1.29974	-1.00266
H	-0.28246	0.94643	-2.00920
F	3.80115	0.23830	-0.58163
H	4.14144	-0.29994	0.51871
F	4.40416	-0.73913	1.42607

2Aa: ΔG = -2720010.0 kJ/mol

C	-0.95053	0.16572	1.79668
C	-2.44842	-0.11520	1.56115
C	-2.72296	0.05469	0.05597
N	-0.40804	0.04936	0.39748
H	-2.67396	-1.15253	1.85156
H	-3.08584	0.53634	2.17651
C	-0.32938	-0.86470	2.72922
H	0.76035	-0.73115	2.80742
H	-0.74514	-0.74610	3.74022
H	-0.53431	-1.89424	2.40730
C	-0.68171	1.55287	2.37103
H	-0.99607	1.58331	3.42375
H	0.39234	1.79229	2.34548
H	-1.22454	2.35019	1.84771
C	-3.83225	-0.85386	-0.45503
H	-4.80580	-0.51536	-0.07144
H	-3.88436	-0.83361	-1.55444
H	-3.69046	-1.89610	-0.14645
C	-3.07342	1.49751	-0.31254
H	-3.13454	1.62558	-1.40391
H	-4.05438	1.76128	0.10797
H	-2.35211	2.23109	0.06857
C	0.98049	0.21553	0.06896
C	1.45125	1.49873	-0.30771
C	1.86830	-0.88728	0.10462
C	2.81385	1.66558	-0.58093
C	3.22380	-0.66535	-0.17450
C	3.70137	0.59828	-0.49970
H	3.18085	2.65266	-0.87580

H	3.91451	-1.51315	-0.15150
H	4.76330	0.74791	-0.71139
C	1.41474	-2.31480	0.33025
H	0.36386	-2.28768	0.63791
C	0.52103	2.67459	-0.51587
H	-0.44147	2.41145	-0.06402
C	2.21442	-3.03075	1.41051
H	2.20965	-2.48287	2.36413
H	1.79635	-4.03031	1.60231
H	3.26649	-3.17635	1.12053
C	1.46721	-3.08689	-0.98616
H	0.86442	-2.60225	-1.76662
H	2.49887	-3.17504	-1.36264
H	1.07735	-4.10824	-0.85633
C	1.00770	3.95380	0.14996
H	0.24845	4.74557	0.06603
H	1.21722	3.80823	1.21999
H	1.92547	4.34291	-0.31686
C	0.26718	2.89181	-2.00509
H	1.19179	3.17095	-2.53499
H	-0.12846	1.98616	-2.48844
H	-0.46233	3.70024	-2.16633
C	-1.35388	-0.27960	-0.51492
H	-1.13665	0.00925	-1.55180
F	-1.38725	-1.87632	-0.73699
H	-1.43127	-2.03744	-2.27244
F	-1.42009	-1.97287	-3.22187

2Ba: ΔG = -2720055.5 kJ/mol

C	0.61848	-0.88233	-1.93472
C	1.94409	-1.60342	-1.63588
C	2.45293	-1.09605	-0.26961
N	0.26347	-0.37416	-0.53148
H	1.76516	-2.68700	-1.57958
H	2.67597	-1.43695	-2.43746
C	-0.46321	-1.80987	-2.45341
H	-1.43688	-1.30438	-2.52936
H	-0.18504	-2.13250	-3.46581
H	-0.57315	-2.71354	-1.84178
C	0.76523	0.30652	-2.87186
H	0.95653	-0.07072	-3.88525
H	-0.15630	0.90529	-2.91321
H	1.60246	0.96163	-2.60025
C	2.98397	-2.20166	0.63740
H	3.86892	-2.66908	0.18319
H	3.27612	-1.79197	1.61449
H	2.23206	-2.98684	0.80293
C	3.49075	0.03029	-0.38332
H	3.68663	0.47139	0.60357
H	4.43053	-0.37999	-0.77964

H	3.15755	0.82998	-1.05952
C	-0.99143	0.26250	-0.20931
C	-1.07167	1.66727	-0.28164
C	-2.06611	-0.54523	0.20697
C	-2.32226	2.24699	-0.03747
C	-3.29132	0.08951	0.44001
C	-3.42624	1.46659	0.29251
H	-2.42354	3.33406	-0.08551
H	-4.14669	-0.50705	0.76726
H	-4.39364	1.94152	0.47309
C	-1.88999	-2.00871	0.55702
H	-0.93858	-2.35654	0.12807
C	0.15166	2.54375	-0.46253
H	0.96047	1.92962	-0.88196
C	-2.99542	-2.89781	0.00927
H	-3.10778	-2.79395	-1.07989
H	-2.78057	-3.95492	0.22236
H	-3.97033	-2.67218	0.46681
C	-1.75977	-2.13886	2.07445
H	-0.96305	-1.49103	2.47164
H	-2.69751	-1.85305	2.57676
H	-1.53524	-3.17744	2.36004
C	-0.07291	3.70652	-1.41633
H	0.86502	4.25758	-1.57630
H	-0.43289	3.37035	-2.39992
H	-0.80361	4.42941	-1.02365
C	0.63269	3.02231	0.90753
H	-0.10695	3.69278	1.37353
H	0.79837	2.18342	1.59991
H	1.57536	3.58288	0.81447
C	1.22672	-0.49751	0.31275
H	1.07965	-0.15709	1.36215
F	0.55857	0.32220	2.98633
H	1.82575	0.54952	2.94352
F	2.83629	0.71681	2.81419

2Bc: ΔG = -2720048.4 kJ/mol

C	-0.63994	-0.96257	1.26308
C	-1.63718	-1.98484	0.68071
C	-1.50405	-1.97460	-0.86107
N	0.05396	-0.45752	-0.01361
H	-1.42960	-2.98679	1.07944
H	-2.65923	-1.70873	0.97210
C	0.39400	-1.58382	2.18309
H	1.18217	-0.86796	2.45867
H	-0.11070	-1.88691	3.11023
H	0.85665	-2.48144	1.75309
C	-1.33439	0.19947	1.94934
H	-1.76635	-0.17301	2.88860
H	-0.63067	1.00438	2.20781

H	-2.15963	0.59426	1.34316
C	-1.08882	-3.32829	-1.43948
H	-1.88045	-4.06521	-1.24449
H	-0.93921	-3.27288	-2.52699
H	-0.16053	-3.70018	-0.98182
C	-2.76442	-1.45002	-1.55706
H	-2.61120	-1.34970	-2.64134
H	-3.58527	-2.16359	-1.39478
H	-3.07457	-0.48057	-1.14063
C	1.11953	0.52163	-0.01167
C	0.78035	1.88593	-0.11165
C	2.45132	0.06623	0.05140
C	1.82986	2.81045	-0.05687
C	3.45705	1.03875	0.10190
C	3.15162	2.39539	0.06887
H	1.60061	3.87649	-0.13351
H	4.50131	0.71942	0.14895
H	3.95413	3.13560	0.11363
C	2.83218	-1.39734	-0.05028
H	1.92505	-2.00356	0.08068
C	-0.63057	2.35918	-0.38267
H	-1.33271	1.53881	-0.19289
C	3.82715	-1.82600	1.01855
H	3.46710	-1.59907	2.03233
H	4.00740	-2.90929	0.96370
H	4.80252	-1.33242	0.89356
C	3.36121	-1.69544	-1.45107
H	2.62778	-1.43612	-2.22903
H	4.28129	-1.12857	-1.66164
H	3.59882	-2.76404	-1.55883
C	-1.05958	3.51348	0.51136
H	-2.13052	3.71552	0.36844
H	-0.90623	3.28839	1.57718
H	-0.51596	4.44391	0.28641
C	-0.79336	2.71656	-1.85762
H	-0.16638	3.57617	-2.14301
H	-0.52238	1.87636	-2.51500
H	-1.84080	2.97844	-2.06990
C	-0.41320	-0.99819	-1.08045
H	-0.00696	-0.72394	-2.06075
F	-3.63505	1.39457	-0.16986
H	-4.07780	0.45245	0.48985
F	-4.44361	-0.37227	1.06003

2Bd: ΔG = -2720050.8 kJ/mol

C	-0.63994	-0.96257	1.26308
C	-1.63718	-1.98484	0.68071
C	-1.50405	-1.97460	-0.86107
N	0.05396	-0.45752	-0.01361
H	-1.42960	-2.98679	1.07944

H	-2.65923	-1.70873	0.97210
C	0.39400	-1.58382	2.18309
H	1.18217	-0.86796	2.45867
H	-0.11070	-1.88691	3.11023
H	0.85665	-2.48144	1.75309
C	-1.33439	0.19947	1.94934
H	-1.76635	-0.17301	2.88860
H	-0.63067	1.00438	2.20781
H	-2.15963	0.59426	1.34316
C	-1.08882	-3.32829	-1.43948
H	-1.88045	-4.06521	-1.24449
H	-0.93921	-3.27288	-2.52699
H	-0.16053	-3.70018	-0.98182
C	-2.76442	-1.45002	-1.55706
H	-2.61120	-1.34970	-2.64134
H	-3.58527	-2.16359	-1.39478
H	-3.07457	-0.48057	-1.14063
C	1.11953	0.52163	-0.01167
C	0.78035	1.88593	-0.11165
C	2.45132	0.06623	0.05140
C	1.82986	2.81045	-0.05687
C	3.45705	1.03875	0.10190
C	3.15162	2.39539	0.06887
H	1.60061	3.87649	-0.13351
H	4.50131	0.71942	0.14895
H	3.95413	3.13560	0.11363
C	2.83218	-1.39734	-0.05028
H	1.92505	-2.00356	0.08068
C	-0.63057	2.35918	-0.38267
H	-1.33271	1.53881	-0.19289
C	3.82715	-1.82600	1.01855
H	3.46710	-1.59907	2.03233
H	4.00740	-2.90929	0.96370
H	4.80252	-1.33242	0.89356
C	3.36121	-1.69544	-1.45107
H	2.62778	-1.43612	-2.22903
H	4.28129	-1.12857	-1.66164
H	3.59882	-2.76404	-1.55883
C	-1.05958	3.51348	0.51136
H	-2.13052	3.71552	0.36844
H	-0.90623	3.28839	1.57718
H	-0.51596	4.44391	0.28641
C	-0.79336	2.71656	-1.85762
H	-0.16638	3.57617	-2.14301
H	-0.52238	1.87636	-2.51500
H	-1.84080	2.97844	-2.06990
C	-0.41320	-0.99819	-1.08045
H	-0.00696	-0.72394	-2.06075
F	-3.63505	1.39457	-0.16986
H	-4.07780	0.45245	0.48985

F	-4.44361	-0.37227	1.06003

3Ba: ΔG = -2983843.8 kJ/mol

C	0.13063	-1.06490	1.62069
C	1.14306	-2.15543	1.24699
C	0.98821	-2.44372	-0.26138
N	-0.16923	-0.48191	0.22989
H	2.15713	-1.77589	1.43337
H	1.00127	-3.05685	1.85779
C	0.70647	-0.00621	2.53444
H	-0.00646	0.81254	2.70899
H	0.90936	-0.47128	3.50900
H	1.65401	0.39008	2.15362
C	-1.16369	-1.60302	2.20973
H	-0.95415	-1.96032	3.22682
H	-1.92830	-0.81707	2.29120
H	-1.57845	-2.44664	1.64403
C	2.33707	-2.59457	-0.95858
H	2.85980	-3.46862	-0.54441
H	2.21791	-2.74873	-2.03951
H	2.96294	-1.70661	-0.80491
C	0.09690	-3.65520	-0.56857
H	-0.07381	-3.75946	-1.64961
H	0.59562	-4.56844	-0.21488
H	-0.88189	-3.59000	-0.07386
C	-0.99242	0.68895	0.03825
C	-2.37399	0.50516	-0.18349
C	-0.39032	1.96264	0.08470
C	-3.16805	1.65447	-0.26684
C	-1.23927	3.07326	0.00313
C	-2.61339	2.92481	-0.14888
H	-4.24141	1.54657	-0.44257
H	-0.80268	4.07507	0.03895
H	-3.25491	3.80742	-0.20625
C	1.10941	2.18314	0.09967
H	1.61552	1.20676	0.15772
C	-2.99942	-0.85235	-0.43911
H	-2.28325	-1.63145	-0.14173
C	1.57663	3.03818	1.27220
H	1.22306	2.66636	2.24301
H	2.67601	3.06468	1.30707
H	1.22988	4.07835	1.17225
C	1.54854	2.82707	-1.21421
H	1.24875	2.22766	-2.08262
H	1.12351	3.83671	-1.32578
H	2.64329	2.91858	-1.24410
C	-4.27392	-1.07984	0.36123
H	-4.64021	-2.10633	0.21587
H	-4.11697	-0.93167	1.43942
H	-5.08353	-0.40411	0.04758

C	-3.24771	-1.03163	-1.93502
H	-3.96547	-0.28785	-2.31437
H	-2.32114	-0.92490	-2.51819
H	-3.66203	-2.02892	-2.14469
C	0.26207	-1.23184	-0.72334
H	0.04156	-0.98576	-1.76382
F	1.89886	-0.01184	-2.50589
H	2.68801	0.21126	-1.92615
F	3.75901	0.48752	-1.15339
H	3.69527	0.26756	0.18372
F	3.65497	0.09106	1.16685

3Bc: ΔG = -2983858.1 kJ/mol

C	0.69688	-0.35319	-2.22685
C	2.09403	-0.96449	-2.03017
C	2.56020	-0.61488	-0.59966
N	0.28671	-0.14409	-0.76006
H	2.03111	-2.05729	-2.13591
H	2.79616	-0.60313	-2.79294
C	-0.27450	-1.27791	-2.93350
H	-1.30104	-0.88421	-2.91722
H	0.02820	-1.35086	-3.98661
H	-0.27154	-2.29460	-2.52402
C	0.71480	0.99435	-2.93155
H	0.96621	0.82785	-3.98740
H	-0.27122	1.47988	-2.90149
H	1.46386	1.68100	-2.51835
C	3.20953	-1.78327	0.13810
H	4.13616	-2.08102	-0.37211
H	3.45632	-1.49594	1.16900
H	2.54415	-2.65836	0.17641
C	3.47675	0.61517	-0.54041
H	3.67582	0.89796	0.50111
H	4.43225	0.37376	-1.02706
H	3.04189	1.48125	-1.05806
C	-1.04342	0.21146	-0.32431
C	-1.34595	1.57100	-0.12006
C	-1.94708	-0.82862	-0.03887
C	-2.64486	1.87683	0.30231
C	-3.23043	-0.46133	0.38051
C	-3.58322	0.87575	0.53145
H	-2.91486	2.92139	0.47634
H	-3.95689	-1.24324	0.61638
H	-4.59143	1.13938	0.86003
C	-1.54600	-2.29060	-0.03780
H	-0.57664	-2.38793	-0.54831
C	-0.30574	2.66991	-0.21141
H	0.55757	2.28548	-0.77099
C	-2.54464	-3.17424	-0.77135
H	-2.73048	-2.82526	-1.79765

H	-2.17288	-4.20723	-0.83255
H	-3.51475	-3.21338	-0.25348
C	-1.32676	-2.76800	1.39618
H	-0.52994	-2.20337	1.89959
H	-2.24246	-2.65995	1.99875
H	-1.04597	-3.83180	1.40862
C	-0.81030	3.90069	-0.95079
H	0.00319	4.62797	-1.08539
H	-1.20198	3.65090	-1.94780
H	-1.61086	4.41612	-0.39927
C	0.20301	3.02821	1.18398
H	-0.61697	3.37047	1.83481
H	0.68241	2.17378	1.68283
H	0.94341	3.84011	1.12700
C	1.27405	-0.27013	0.05337
H	1.12362	-0.15419	1.13304
F	-0.64452	0.17564	2.87166
H	0.14951	-0.40061	2.97139
F	1.32274	-1.16466	3.00545
H	2.23010	-0.14207	2.84607
F	2.82434	0.63296	2.66294

3Bc': ΔG = -2983844.9 kJ/mol

C	-0.55587	-0.23032	2.17561
C	-1.94187	-0.89419	2.13529
C	-2.50320	-0.72194	0.70946
N	-0.25267	-0.11750	0.67422
H	-1.84000	-1.96582	2.35826
H	-2.60800	-0.46632	2.89624
C	0.48994	-1.08454	2.85932
H	1.48922	-0.63023	2.79925
H	0.23147	-1.16384	3.92397
H	0.52713	-2.10214	2.45083
C	-0.56424	1.16339	2.78342
H	-0.70980	1.06705	3.86760
H	0.39282	1.68139	2.62611
H	-1.37672	1.79190	2.39759
C	-3.21079	-1.96487	0.18282
H	-4.12906	-2.13407	0.76279
H	-3.49141	-1.84028	-0.87232
H	-2.57886	-2.85699	0.26293
C	-3.43922	0.49070	0.56528
H	-3.69111	0.66955	-0.48955
H	-4.37183	0.28922	1.11081
H	-3.00085	1.41113	0.97428
C	0.98686	0.43523	0.17187
C	1.01858	1.81398	-0.13334
C	2.11172	-0.39872	0.01703
C	2.25123	2.36286	-0.50320
C	3.31878	0.21049	-0.34761

C	3.39708	1.57814	-0.58178
H	2.30660	3.42651	-0.74690
H	4.20720	-0.41353	-0.47625
H	4.35106	2.03138	-0.86169
C	2.04268	-1.91161	0.06246
H	1.03092	-2.20354	0.38366
C	-0.22549	2.67833	-0.18450
H	-1.02540	2.17547	0.37570
C	3.05743	-2.53657	1.00998
H	2.96641	-2.16143	2.03858
H	2.93109	-3.62860	1.04199
H	4.08925	-2.34359	0.67907
C	2.23114	-2.44744	-1.35686
H	1.54714	-1.96042	-2.06350
H	3.26130	-2.27798	-1.70755
H	2.04170	-3.53030	-1.39350
C	-0.03171	4.04671	0.45237
H	-0.98567	4.59255	0.48255
H	0.34207	3.97240	1.48409
H	0.67464	4.67192	-0.11384
C	-0.70432	2.80206	-1.63006
H	0.04493	3.31520	-2.25298
H	-0.90311	1.82318	-2.09003
H	-1.63491	3.38731	-1.68175
C	-1.27549	-0.39295	-0.05852
H	-1.20947	-0.29973	-1.14634
F	-0.80638	-2.70099	-1.48612
H	-0.60346	-1.97441	-2.12925
F	-0.37202	-0.85625	-2.92893
H	-1.64320	-0.29818	-3.02974
F	-2.55303	0.08784	-2.97993

3Bb: ΔG = -2983840.3 kJ/mol

C	0.62142	-0.90599	1.74629
C	1.76961	-1.84559	1.35108
C	1.59034	-2.20373	-0.13669
N	0.16680	-0.41986	0.36136
H	2.72500	-1.31771	1.47775
H	1.79462	-2.73579	1.99376
C	1.08341	0.24897	2.60791
H	0.26546	0.95322	2.81471
H	1.41439	-0.15487	3.57456
H	1.93036	0.78552	2.16342
C	-0.54719	-1.60997	2.41972
H	-0.23956	-1.90355	3.43221
H	-1.41545	-0.94300	2.52199
H	-0.86181	-2.52129	1.89609
C	2.91266	-2.27880	-0.89013
H	3.48680	-3.14169	-0.52335
H	2.75237	-2.41438	-1.96860

H	3.50920	-1.37311	-0.74191
C	0.81729	-3.51576	-0.35573
H	0.57983	-3.66459	-1.41907
H	1.44482	-4.35656	-0.02864
H	-0.12110	-3.55899	0.21264
C	-0.91882	0.52240	0.18298
C	-2.21418	0.00779	-0.04982
C	-0.66537	1.90783	0.26000
C	-3.27009	0.92334	-0.12536
C	-1.76305	2.77331	0.18458
C	-3.05496	2.29017	0.01305
H	-4.28133	0.55133	-0.30847
H	-1.58880	3.85139	0.23775
H	-3.89715	2.98421	-0.04145
C	0.72985	2.49161	0.28064
H	1.44060	1.66077	0.36225
C	-2.49670	-1.45816	-0.30986
H	-1.61259	-2.04156	-0.02103
C	0.97231	3.46017	1.43022
H	0.74217	3.02739	2.41318
H	2.02708	3.77345	1.44568
H	0.36744	4.37397	1.32361
C	1.01611	3.17686	-1.05406
H	0.78222	2.51879	-1.89836
H	0.42666	4.10075	-1.16515
H	2.08023	3.44900	-1.12460
C	-3.66586	-1.99343	0.50509
H	-3.76961	-3.07835	0.35858
H	-3.53435	-1.81410	1.58198
H	-4.62177	-1.53819	0.20608
C	-2.71228	-1.68753	-1.80399
H	-3.61376	-1.16588	-2.16132
H	-1.86393	-1.32298	-2.40173
H	-2.84178	-2.75846	-2.02054
C	0.69932	-1.10215	-0.59792
H	0.37185	-0.94483	-1.62793
F	3.57357	0.87686	0.12638
H	3.02884	0.73304	-0.68264
F	2.26356	0.44672	-1.81732
H	1.15043	0.57270	-2.64271
F	0.31311	0.58144	-3.16642

3Bd: ΔG = -2983847.3 kJ/mol

C	0.62142	-0.90599	1.74629
C	1.76961	-1.84559	1.35108
C	1.59034	-2.20373	-0.13669
N	0.16680	-0.41986	0.36136
H	2.72500	-1.31771	1.47775
H	1.79462	-2.73579	1.99376
C	1.08341	0.24897	2.60791

H	0.26546	0.95322	2.81471
H	1.41439	-0.15487	3.57456
H	1.93036	0.78552	2.16342
C	-0.54719	-1.60997	2.41972
H	-0.23956	-1.90355	3.43221
H	-1.41545	-0.94300	2.52199
H	-0.86181	-2.52129	1.89609
C	2.91266	-2.27880	-0.89013
H	3.48680	-3.14169	-0.52335
H	2.75237	-2.41438	-1.96860
H	3.50920	-1.37311	-0.74191
C	0.81729	-3.51576	-0.35573
H	0.57983	-3.66459	-1.41907
H	1.44482	-4.35656	-0.02864
H	-0.12110	-3.55899	0.21264
C	-0.91882	0.52240	0.18298
C	-2.21418	0.00779	-0.04982
C	-0.66537	1.90783	0.26000
C	-3.27009	0.92334	-0.12536
C	-1.76305	2.77331	0.18458
C	-3.05496	2.29017	0.01305
H	-4.28133	0.55133	-0.30847
H	-1.58880	3.85139	0.23775
H	-3.89715	2.98421	-0.04145
C	0.72985	2.49161	0.28064
H	1.44060	1.66077	0.36225
C	-2.49670	-1.45816	-0.30986
H	-1.61259	-2.04156	-0.02103
C	0.97231	3.46017	1.43022
H	0.74217	3.02739	2.41318
H	2.02708	3.77345	1.44568
H	0.36744	4.37397	1.32361
C	1.01611	3.17686	-1.05406
H	0.78222	2.51879	-1.89836
H	0.42666	4.10075	-1.16515
H	2.08023	3.44900	-1.12460
C	-3.66586	-1.99343	0.50509
H	-3.76961	-3.07835	0.35858
H	-3.53435	-1.81410	1.58198
H	-4.62177	-1.53819	0.20608
C	-2.71228	-1.68753	-1.80399
H	-3.61376	-1.16588	-2.16132
H	-1.86393	-1.32298	-2.40173
H	-2.84178	-2.75846	-2.02054
C	0.69932	-1.10215	-0.59792
H	0.37185	-0.94483	-1.62793
F	3.57357	0.87686	0.12638
H	3.02884	0.73304	-0.68264
F	2.26356	0.44672	-1.81732
H	1.15043	0.57270	-2.64271

F	0.31311	0.58144	-3.16642

Method M06-2X/ def2-TZVPD

1A: ΔG = -2456241.1 kJ/mol

C	1.11587	0.49390	1.46002
C	2.46730	1.08116	1.01911
C	2.71704	0.63291	-0.43053
N	0.47877	0.21573	0.13859
H	2.40885	2.18087	1.04605
H	3.28417	0.78794	1.69574
C	0.32353	1.49418	2.29381
H	-0.68438	1.11541	2.52310
H	0.83054	1.66501	3.25493
H	0.22472	2.46796	1.79623
C	1.25906	-0.78387	2.28607
H	1.65882	-0.54704	3.28277
H	0.28010	-1.26516	2.43514
H	1.93380	-1.52001	1.83064
C	3.55388	1.64153	-1.20393
H	4.57043	1.69063	-0.78579
H	3.64860	1.35794	-2.26311
H	3.12554	2.65093	-1.16410
C	3.40093	-0.73025	-0.51084
H	3.50659	-1.05822	-1.55642
H	4.41035	-0.67790	-0.07718
H	2.85876	-1.51901	0.02592
C	-0.85032	-0.28823	-0.00507
C	-1.06361	-1.68790	-0.10690
C	-1.95685	0.59763	-0.06802
C	-2.37310	-2.17372	-0.20370
C	-3.24894	0.06179	-0.15700
C	-3.46354	-1.31064	-0.21063
H	-2.53650	-3.25252	-0.28533
H	-4.10413	0.74275	-0.20401
H	-4.48008	-1.70703	-0.27946
C	-1.80659	2.10441	-0.13634
H	-0.74533	2.33618	0.01706
C	0.08040	-2.67533	-0.19846
H	0.99887	-2.12758	0.04480
C	-2.62437	2.83289	0.92265
H	-2.40198	2.48110	1.94026
H	-2.42054	3.91402	0.89532
H	-3.70679	2.70922	0.76213
C	-2.17505	2.60491	-1.53076
H	-1.58226	2.10841	-2.31139
H	-3.23933	2.42936	-1.75513
H	-1.99770	3.68786	-1.61837
C	-0.04873	-3.83165	0.78381
H	0.84655	-4.47066	0.75205
H	-0.16999	-3.48351	1.82008

H	-0.90972	-4.47708	0.55042
C	0.22890	-3.19174	-1.62715
H	-0.65475	-3.77051	-1.94045
H	0.35750	-2.37179	-2.34937
H	1.10349	-3.85418	-1.71782
C	1.28156	0.52034	-0.95797
H	1.15700	-0.18823	-1.79512
F	0.90813	1.78897	-1.56099

1Ba: ΔG = -2456224.3 kJ/mol

C	-1.30907	-0.17973	1.59958
C	-2.71333	-0.57651	1.12165
C	-2.79599	-0.25230	-0.38565
N	-0.58151	-0.09005	0.25340
H	-2.85886	-1.65625	1.27284
H	-3.49198	-0.06249	1.70140
C	-0.66593	-1.22031	2.49654
H	0.38051	-0.97482	2.72888
H	-1.21315	-1.24274	3.44884
H	-0.71055	-2.23069	2.07204
C	-1.26249	1.17871	2.28216
H	-1.75007	1.09593	3.26291
H	-0.22789	1.50779	2.45809
H	-1.79054	1.95553	1.71432
C	-3.45773	-1.36543	-1.19358
H	-4.49768	-1.50279	-0.86403
H	-3.47187	-1.12680	-2.26647
H	-2.93486	-2.32454	-1.06496
C	-3.48377	1.08716	-0.67725
H	-3.42633	1.34008	-1.74573
H	-4.54613	1.02381	-0.40124
H	-3.03534	1.91439	-0.10949
C	0.85201	0.05586	0.17161
C	1.40970	1.34768	0.13193
C	1.63686	-1.11319	0.13344
C	2.80633	1.44473	0.16994
C	3.02674	-0.95724	0.17182
C	3.60638	0.30769	0.21854
H	3.27217	2.43300	0.13625
H	3.66493	-1.84395	0.14101
H	4.69398	0.40768	0.25561
C	1.02623	-2.47652	-0.11957
H	-0.03982	-2.43492	0.15046
C	0.57262	2.58522	-0.11974
H	-0.47763	2.34328	0.09676
C	1.66103	-3.59300	0.69314
H	1.63823	-3.38379	1.77306
H	1.12817	-4.54041	0.52683
H	2.71034	-3.76541	0.41054
C	1.08843	-2.75448	-1.62224

H	0.68110	-1.90822	-2.20029
H	2.13072	-2.90566	-1.94697
H	0.52757	-3.66646	-1.87819
C	0.95677	3.77081	0.75119
H	0.27449	4.61493	0.57408
H	0.91382	3.52884	1.82356
H	1.97293	4.13256	0.53335
C	0.64860	2.92125	-1.60968
H	1.66305	3.25265	-1.88492
H	0.40379	2.03973	-2.22571
H	-0.04448	3.73818	-1.86331
C	-1.36371	-0.11729	-0.77383
H	-0.89198	-0.03646	-1.83478
F	-0.00157	0.03885	-3.02319

1Bb: ΔG = -2456209.5 kJ/mol

C	-0.74958	-1.00051	1.39753
C	-1.56136	-2.21105	0.90257
C	-1.71791	-2.09558	-0.63137
N	-0.19288	-0.47116	0.06284
H	-1.02855	-3.14000	1.15133
H	-2.53676	-2.25547	1.40434
C	0.38531	-1.38154	2.32810
H	1.04259	-0.52720	2.54602
H	-0.05212	-1.70399	3.28271
H	0.99027	-2.21527	1.95063
C	-1.61101	0.08135	2.02607
H	-2.00795	-0.32013	2.96993
H	-1.00344	0.96227	2.28576
H	-2.46064	0.39466	1.38185
C	-1.33447	-3.38457	-1.35874
H	-2.02272	-4.18906	-1.06324
H	-1.40345	-3.26564	-2.44914
H	-0.31230	-3.70700	-1.11064
C	-3.10799	-1.61825	-1.06945
H	-3.14697	-1.49860	-2.16296
H	-3.84394	-2.38951	-0.79650
H	-3.39052	-0.65420	-0.59554
C	0.82139	0.55452	-0.03185
C	0.42776	1.90340	-0.12249
C	2.16959	0.14452	-0.06276
C	1.44790	2.86273	-0.15832
C	3.14278	1.14905	-0.10372
C	2.78869	2.49467	-0.13040
H	1.17621	3.91938	-0.22837
H	4.19789	0.86546	-0.13304
H	3.56632	3.26196	-0.15673
C	2.58675	-1.30953	-0.16786
H	1.71809	-1.94066	0.07129
C	-1.01206	2.32972	-0.28586

H	-1.69774	1.49761	-0.06921
C	3.69992	-1.67623	0.80301
H	3.43893	-1.42758	1.84190
H	3.90821	-2.75499	0.76048
H	4.64083	-1.15839	0.56411
C	2.97818	-1.63030	-1.60826
H	2.15820	-1.41947	-2.31096
H	3.84901	-1.03735	-1.92821
H	3.24348	-2.69266	-1.71346
C	-1.41171	3.45917	0.65403
H	-2.50213	3.59653	0.61419
H	-1.14833	3.23991	1.69958
H	-0.94397	4.42021	0.38854
C	-1.28884	2.70958	-1.73866
H	-0.72184	3.60103	-2.05213
H	-1.03199	1.89325	-2.43124
H	-2.35981	2.92684	-1.87030
C	-0.73597	-1.03459	-0.95577
H	-0.46190	-0.72292	-1.97018
F	-3.77854	1.07330	0.17494

2a: ΔG = -2720017.5 kJ/mol

C	0.82811	-0.69500	1.49924
C	2.08713	-1.46559	1.06945
C	1.87569	-1.93231	-0.38122
N	0.24587	-0.33487	0.16094
H	2.94884	-0.78154	1.09461
H	2.31163	-2.29962	1.75032
C	1.18223	0.53114	2.32927
H	0.29511	1.15092	2.52912
H	1.57904	0.21146	3.30364
H	1.94902	1.15262	1.84958
C	-0.15467	-1.54022	2.30511
H	0.25473	-1.73226	3.30695
H	-1.11019	-1.01078	2.44062
H	-0.36594	-2.51460	1.84721
C	3.18617	-2.02843	-1.15040
H	3.79247	-2.85375	-0.74909
H	3.01333	-2.23572	-2.21676
H	3.78392	-1.11192	-1.07594
C	1.16686	-3.28474	-0.47058
H	0.96606	-3.55606	-1.51814
H	1.80298	-4.07125	-0.03991
H	0.20986	-3.31217	0.06529
C	-0.94485	0.44857	-0.00353
C	-2.19754	-0.20058	-0.13788
C	-0.86690	1.86261	-0.05609
C	-3.35262	0.58054	-0.26593
C	-2.05240	2.59864	-0.17838
C	-3.28870	1.96955	-0.27032

H	-4.32095	0.08345	-0.37478
H	-1.99636	3.69049	-0.21921
H	-4.20239	2.56208	-0.36528
C	0.44859	2.61061	-0.07295
H	1.23984	1.88200	0.12640
C	-2.33088	-1.70603	-0.22870
H	-1.35804	-2.13754	0.03513
C	0.53334	3.70248	0.98518
H	0.31749	3.32606	1.99537
H	1.54306	4.14038	1.00497
H	-0.16917	4.52624	0.78401
C	0.72064	3.18861	-1.45898
H	0.66105	2.41920	-2.24062
H	0.00370	3.98522	-1.71426
H	1.73005	3.62646	-1.50307
C	-3.36400	-2.27012	0.73747
H	-3.35918	-3.37007	0.71137
H	-3.17096	-1.96265	1.77564
H	-4.38581	-1.94924	0.48273
C	-2.63709	-2.13228	-1.66190
H	-3.61568	-1.75152	-1.99508
H	-1.88204	-1.76292	-2.37165
H	-2.66515	-3.22928	-1.74810
C	0.93411	-0.84937	-0.89878
H	0.32567	-1.09640	-1.77938
F	1.82751	0.25220	-1.57393
H	2.91245	0.97250	-0.69851
F	3.57261	1.41733	-0.17721

2Ba': ΔG = -2720064.5 kJ/mol

C	1.63025	-0.12724	-1.60520
C	2.96886	-0.47187	-0.93126
C	2.82649	-0.15369	0.57285
N	0.71392	-0.06262	-0.37779
H	3.17806	-1.54380	-1.06069
H	3.79941	0.07698	-1.39477
C	1.15148	-1.18892	-2.57669
H	0.12874	-0.99135	-2.92902
H	1.80726	-1.17258	-3.45755
H	1.19616	-2.20088	-2.15632
C	1.63688	1.22891	-2.29381
H	2.26297	1.15799	-3.19328
H	0.62887	1.52581	-2.61829
H	2.05681	2.02107	-1.66095
C	3.39555	-1.24737	1.47377
H	4.48073	-1.33265	1.32055
H	3.21865	-1.01908	2.53449
H	2.94594	-2.22704	1.25585
C	3.40836	1.20884	0.96969
H	3.17161	1.45048	2.01589

H	4.50238	1.18457	0.86576
H	3.02542	2.02245	0.33771
C	-0.72508	0.01538	-0.47453
C	-1.34260	1.27950	-0.50090
C	-1.45145	-1.19104	-0.50006
C	-2.72980	1.30887	-0.69076
C	-2.83446	-1.10133	-0.68789
C	-3.46405	0.13417	-0.81173
H	-3.24356	2.27307	-0.71634
H	-3.43176	-2.01592	-0.71214
H	-4.54514	0.18092	-0.96394
C	-0.80691	-2.52145	-0.16758
H	0.27177	-2.44617	-0.37157
C	-0.59470	2.55608	-0.17676
H	0.48089	2.36815	-0.29825
C	-1.34255	-3.68180	-0.99041
H	-1.26394	-3.49102	-2.07097
H	-0.77707	-4.59909	-0.77252
H	-2.39748	-3.89945	-0.76646
C	-0.95230	-2.77771	1.33165
H	-0.54563	-1.95046	1.93020
H	-2.01208	-2.88353	1.61318
H	-0.43333	-3.70320	1.62278
C	-0.95832	3.71801	-1.08762
H	-0.33193	4.59320	-0.86266
H	-0.81407	3.47008	-2.14965
H	-2.00439	4.03440	-0.95952
C	-0.81425	2.90243	1.29562
H	-1.87833	3.09759	1.50385
H	-0.49629	2.08510	1.95986
H	-0.25031	3.80708	1.56942
C	1.35167	-0.07638	0.74124
H	0.81124	-0.00509	1.72929
F	0.04363	0.14192	3.18294
H	-1.23794	0.08129	2.82397
F	-2.20136	0.03687	2.52138

2Bb: ΔG = -2720054.7 kJ/mol

C	-0.63994	-0.96257	1.26308
C	-1.63718	-1.98484	0.68071
C	-1.50405	-1.97460	-0.86107
N	0.05396	-0.45752	-0.01361
H	-1.42960	-2.98679	1.07944
H	-2.65923	-1.70873	0.97210
C	0.39400	-1.58382	2.18309
H	1.18217	-0.86796	2.45867
H	-0.11070	-1.88691	3.11023
H	0.85665	-2.48144	1.75309
C	-1.33439	0.19947	1.94934
H	-1.76635	-0.17301	2.88860

H	-0.63067	1.00438	2.20781
H	-2.15963	0.59426	1.34316
C	-1.08882	-3.32829	-1.43948
H	-1.88045	-4.06521	-1.24449
H	-0.93921	-3.27288	-2.52699
H	-0.16053	-3.70018	-0.98182
C	-2.76442	-1.45002	-1.55706
H	-2.61120	-1.34970	-2.64134
H	-3.58527	-2.16359	-1.39478
H	-3.07457	-0.48057	-1.14063
C	1.11953	0.52163	-0.01167
C	0.78035	1.88593	-0.11165
C	2.45132	0.06623	0.05140
C	1.82986	2.81045	-0.05687
C	3.45705	1.03875	0.10190
C	3.15162	2.39539	0.06887
H	1.60061	3.87649	-0.13351
H	4.50131	0.71942	0.14895
H	3.95413	3.13560	0.11363
C	2.83218	-1.39734	-0.05028
H	1.92505	-2.00356	0.08068
C	-0.63057	2.35918	-0.38267
H	-1.33271	1.53881	-0.19289
C	3.82715	-1.82600	1.01855
H	3.46710	-1.59907	2.03233
H	4.00740	-2.90929	0.96370
H	4.80252	-1.33242	0.89356
C	3.36121	-1.69544	-1.45107
H	2.62778	-1.43612	-2.22903
H	4.28129	-1.12857	-1.66164
H	3.59882	-2.76404	-1.55883
C	-1.05958	3.51348	0.51136
H	-2.13052	3.71552	0.36844
H	-0.90623	3.28839	1.57718
H	-0.51596	4.44391	0.28641
C	-0.79336	2.71656	-1.85762
H	-0.16638	3.57617	-2.14301
H	-0.52238	1.87636	-2.51500
H	-1.84080	2.97844	-2.06990
C	-0.41320	-0.99819	-1.08045
H	-0.00696	-0.72394	-2.06075
F	-3.63505	1.39457	-0.16986
H	-4.07780	0.45245	0.48985
F	-4.44361	-0.37227	1.06003

2Aa: ΔG = -2720016.1 kJ/mol

C	-0.95053	0.16572	1.79668
C	-2.44842	-0.11520	1.56115
C	-2.72296	0.05469	0.05597
N	-0.40804	0.04936	0.39748

H	-2.67396	-1.15253	1.85156
H	-3.08584	0.53634	2.17651
C	-0.32938	-0.86470	2.72922
H	0.76035	-0.73115	2.80742
H	-0.74514	-0.74610	3.74022
H	-0.53431	-1.89424	2.40730
C	-0.68171	1.55287	2.37103
H	-0.99607	1.58331	3.42375
H	0.39234	1.79229	2.34548
H	-1.22454	2.35019	1.84771
C	-3.83225	-0.85386	-0.45503
H	-4.80580	-0.51536	-0.07144
H	-3.88436	-0.83361	-1.55444
H	-3.69046	-1.89610	-0.14645
C	-3.07342	1.49751	-0.31254
H	-3.13454	1.62558	-1.40391
H	-4.05438	1.76128	0.10797
H	-2.35211	2.23109	0.06857
C	0.98049	0.21553	0.06896
C	1.45125	1.49873	-0.30771
C	1.86830	-0.88728	0.10462
C	2.81385	1.66558	-0.58093
C	3.22380	-0.66535	-0.17450
C	3.70137	0.59828	-0.49970
H	3.18085	2.65266	-0.87580
H	3.91451	-1.51315	-0.15150
H	4.76330	0.74791	-0.71139
C	1.41474	-2.31480	0.33025
H	0.36386	-2.28768	0.63791
C	0.52103	2.67459	-0.51587
H	-0.44147	2.41145	-0.06402
C	2.21442	-3.03075	1.41051
H	2.20965	-2.48287	2.36413
H	1.79635	-4.03031	1.60231
H	3.26649	-3.17635	1.12053
C	1.46721	-3.08689	-0.98616
H	0.86442	-2.60225	-1.76662
H	2.49887	-3.17504	-1.36264
H	1.07735	-4.10824	-0.85633
C	1.00770	3.95380	0.14996
H	0.24845	4.74557	0.06603
H	1.21722	3.80823	1.21999
H	1.92547	4.34291	-0.31686
C	0.26718	2.89181	-2.00509
H	1.19179	3.17095	-2.53499
H	-0.12846	1.98616	-2.48844
H	-0.46233	3.70024	-2.16633
C	-1.35388	-0.27960	-0.51492
H	-1.13665	0.00925	-1.55180
F	-1.38725	-1.87632	-0.73699

H	-1.43127	-2.03744	-2.27244
F	-1.42009	-1.97287	-3.22187

2Ba: ΔG = -2720061.4 kJ/mol

C	0.61848	-0.88233	-1.93472
C	1.94409	-1.60342	-1.63588
C	2.45293	-1.09605	-0.26961
N	0.26347	-0.37416	-0.53148
H	1.76516	-2.68700	-1.57958
H	2.67597	-1.43695	-2.43746
C	-0.46321	-1.80987	-2.45341
H	-1.43688	-1.30438	-2.52936
H	-0.18504	-2.13250	-3.46581
H	-0.57315	-2.71354	-1.84178
C	0.76523	0.30652	-2.87186
H	0.95653	-0.07072	-3.88525
H	-0.15630	0.90529	-2.91321
H	1.60246	0.96163	-2.60025
C	2.98397	-2.20166	0.63740
H	3.86892	-2.66908	0.18319
H	3.27612	-1.79197	1.61449
H	2.23206	-2.98684	0.80293
C	3.49075	0.03029	-0.38332
H	3.68663	0.47139	0.60357
H	4.43053	-0.37999	-0.77964
H	3.15755	0.82998	-1.05952
C	-0.99143	0.26250	-0.20931
C	-1.07167	1.66727	-0.28164
C	-2.06611	-0.54523	0.20697
C	-2.32226	2.24699	-0.03747
C	-3.29132	0.08951	0.44001
C	-3.42624	1.46659	0.29251
H	-2.42354	3.33406	-0.08551
H	-4.14669	-0.50705	0.76726
H	-4.39364	1.94152	0.47309
C	-1.88999	-2.00871	0.55702
H	-0.93858	-2.35654	0.12807
C	0.15166	2.54375	-0.46253
H	0.96047	1.92962	-0.88196
C	-2.99542	-2.89781	0.00927
H	-3.10778	-2.79395	-1.07989
H	-2.78057	-3.95492	0.22236
H	-3.97033	-2.67218	0.46681
C	-1.75977	-2.13886	2.07445
H	-0.96305	-1.49103	2.47164
H	-2.69751	-1.85305	2.57676
H	-1.53524	-3.17744	2.36004
C	-0.07291	3.70652	-1.41633
H	0.86502	4.25758	-1.57630
H	-0.43289	3.37035	-2.39992

H	-0.80361	4.42941	-1.02365
C	0.63269	3.02231	0.90753
H	-0.10695	3.69278	1.37353
H	0.79837	2.18342	1.59991
H	1.57536	3.58288	0.81447
C	1.22672	-0.49751	0.31275
H	1.07965	-0.15709	1.36215
F	0.55857	0.32220	2.98633
H	1.82575	0.54952	2.94352
F	2.83629	0.71681	2.81419

2Bc: ΔG = -2720057.3 kJ/mol

C	0.18331	1.20597	1.30357
C	0.46386	2.64910	0.84381
C	0.57399	2.62325	-0.69672
N	-0.28131	0.57713	-0.00618
H	-0.36875	3.28987	1.13634
H	1.37241	3.03161	1.30641
C	-0.89871	1.11543	2.36542
H	-1.16308	0.07783	2.57634
H	-0.49697	1.55352	3.27988
H	-1.79183	1.67261	2.09083
C	1.43582	0.48322	1.78214
H	1.73524	0.93125	2.73016
H	1.23932	-0.57671	1.95331
H	2.26151	0.58897	1.08004
C	-0.19975	3.75881	-1.36710
H	0.23595	4.71151	-1.06218
H	-0.13773	3.68164	-2.45359
H	-1.24995	3.74878	-1.07126
C	2.02264	2.59777	-1.20775
H	2.04674	2.45336	-2.28927
H	2.48637	3.55782	-0.97583
H	2.60715	1.80597	-0.73700
C	-0.88364	-0.73735	-0.09740
C	-0.06064	-1.84448	-0.33506
C	-2.27573	-0.83003	0.02311
C	-0.67486	-3.09480	-0.37116
C	-2.83438	-2.10485	-0.02002
C	-2.04237	-3.22758	-0.19641
H	-0.07146	-3.97389	-0.55878
H	-3.90832	-2.21415	0.06668
H	-2.49696	-4.20993	-0.22502
C	-3.18927	0.37841	0.09031
H	-2.58609	1.27587	0.21709
C	1.41618	-1.73249	-0.65756
H	1.75947	-0.72547	-0.43261
C	-4.17216	0.29768	1.25764
H	-3.65834	0.13067	2.20541
H	-4.73590	1.22917	1.33235

H	-4.88822	-0.51313	1.11190
C	-3.93870	0.52783	-1.23729
H	-3.24401	0.63230	-2.07309
H	-4.56949	-0.34383	-1.42436
H	-4.57791	1.41219	-1.20885
C	2.26810	-2.70472	0.15611
H	3.32454	-2.52796	-0.05076
H	2.10445	-2.58438	1.22844
H	2.04820	-3.74080	-0.10794
C	1.63188	-1.95365	-2.15784
H	1.32340	-2.96019	-2.44940
H	1.06034	-1.23591	-2.74986
H	2.68934	-1.83593	-2.40309
C	-0.05364	1.31537	-1.01929
H	-0.29923	0.96986	-2.01934
F	4.32448	0.02962	-0.38301
H	4.45840	-0.25440	0.71095
F	4.60231	-0.52433	1.79750

2Bd: ΔG = -2720053.8 kJ/mol

C	-0.09938	-1.27116	1.39170
C	-0.69639	-2.60103	0.89351
C	-1.07584	-2.40462	-0.59068
N	0.20122	-0.57900	0.06616
H	0.05460	-3.38719	0.97675
H	-1.55965	-2.88500	1.49363
C	1.16261	-1.46019	2.21622
H	1.63981	-0.50489	2.44072
H	0.86699	-1.91851	3.16092
H	1.87694	-2.12290	1.73251
C	-1.09039	-0.41378	2.16748
H	-1.28285	-0.90957	3.11971
H	-0.66471	0.56900	2.37936
H	-2.03970	-0.29362	1.64591
C	-0.59788	-3.55005	-1.48507
H	-1.09058	-4.47186	-1.17245
H	-0.85223	-3.35786	-2.52857
H	0.48134	-3.68972	-1.40447
C	-2.57484	-2.15774	-0.80899
H	-2.77029	-1.82497	-1.82992
H	-3.10424	-3.09831	-0.64681
H	-2.97529	-1.41797	-0.11430
C	0.96575	0.64676	-0.03275
C	0.28757	1.87140	-0.02792
C	2.35742	0.54191	-0.15141
C	1.06921	3.02564	-0.04768
C	3.08609	1.72767	-0.17117
C	2.45147	2.95720	-0.09556
H	0.58312	3.99309	-0.04913
H	4.16393	1.68503	-0.26652

H	3.03650	3.86823	-0.10677
C	3.07404	-0.77642	-0.37161
H	2.37452	-1.59417	-0.20614
C	-1.22123	2.00041	-0.13592
H	-1.67968	1.02146	0.00512
C	4.25749	-0.96339	0.57622
H	3.96006	-0.84576	1.61912
H	4.67814	-1.96251	0.45001
H	5.04859	-0.24179	0.36463
C	3.52991	-0.86943	-1.83116
H	2.68311	-0.78516	-2.51524
H	4.23880	-0.07233	-2.06537
H	4.02145	-1.82759	-2.00981
C	-1.80885	2.94820	0.90842
H	-2.89546	2.97258	0.81054
H	-1.56487	2.63265	1.92393
H	-1.44105	3.96631	0.76914
C	-1.57686	2.47667	-1.54857
H	-1.12968	3.45325	-1.74679
H	-1.21768	1.77563	-2.30471
H	-2.65863	2.57195	-1.65272
C	-0.33365	-1.16302	-0.93157
H	-0.23823	-0.74673	-1.93041
F	-4.18501	0.40857	1.13948
H	-4.39791	0.56875	0.03299
F	-4.61070	0.72342	-1.06382

3Ba: ΔG = -2983851.2 kJ/mol

C	-1.30907	-0.17973	1.59958
C	-2.71333	-0.57651	1.12165
C	-2.79599	-0.25230	-0.38565
N	-0.58151	-0.09005	0.25340
H	-2.85886	-1.65625	1.27284
H	-3.49198	-0.06249	1.70140
C	-0.66593	-1.22031	2.49654
H	0.38051	-0.97482	2.72888
H	-1.21315	-1.24274	3.44884
H	-0.71055	-2.23069	2.07204
C	-1.26249	1.17871	2.28216
H	-1.75007	1.09593	3.26291
H	-0.22789	1.50779	2.45809
H	-1.79054	1.95553	1.71432
C	-3.45773	-1.36543	-1.19358
H	-4.49768	-1.50279	-0.86403
H	-3.47187	-1.12680	-2.26647
H	-2.93486	-2.32454	-1.06496
C	-3.48377	1.08716	-0.67725
H	-3.42633	1.34008	-1.74573
H	-4.54613	1.02381	-0.40124
H	-3.03534	1.91439	-0.10949

C	0.85201	0.05586	0.17161
C	1.40970	1.34768	0.13193
C	1.63686	-1.11319	0.13344
C	2.80633	1.44473	0.16994
C	3.02674	-0.95724	0.17182
C	3.60638	0.30769	0.21854
H	3.27217	2.43300	0.13625
H	3.66493	-1.84395	0.14101
H	4.69398	0.40768	0.25561
C	1.02623	-2.47652	-0.11957
H	-0.03982	-2.43492	0.15046
C	0.57262	2.58522	-0.11974
H	-0.47763	2.34328	0.09676
C	1.66103	-3.59300	0.69314
H	1.63823	-3.38379	1.77306
H	1.12817	-4.54041	0.52683
H	2.71034	-3.76541	0.41054
C	1.08843	-2.75448	-1.62224
H	0.68110	-1.90822	-2.20029
H	2.13072	-2.90566	-1.94697
H	0.52757	-3.66646	-1.87819
C	0.95677	3.77081	0.75119
H	0.27449	4.61493	0.57408
H	0.91382	3.52884	1.82356
H	1.97293	4.13256	0.53335
C	0.64860	2.92125	-1.60968
H	1.66305	3.25265	-1.88492
H	0.40379	2.03973	-2.22571
H	-0.04448	3.73818	-1.86331
C	-1.36371	-0.11729	-0.77383
H	-0.89198	-0.03646	-1.83478
F	-0.00157	0.03885	-3.02319

3Bb: ΔG = -2983849.9 kJ/mol

C	0.62142	-0.90599	1.74629
C	1.76961	-1.84559	1.35108
C	1.59034	-2.20373	-0.13669
N	0.16680	-0.41986	0.36136
H	2.72500	-1.31771	1.47775
H	1.79462	-2.73579	1.99376
C	1.08341	0.24897	2.60791
H	0.26546	0.95322	2.81471
H	1.41439	-0.15487	3.57456
H	1.93036	0.78552	2.16342
C	-0.54719	-1.60997	2.41972
H	-0.23956	-1.90355	3.43221
H	-1.41545	-0.94300	2.52199
H	-0.86181	-2.52129	1.89609
C	2.91266	-2.27880	-0.89013
H	3.48680	-3.14169	-0.52335

H	2.75237	-2.41438	-1.96860
H	3.50920	-1.37311	-0.74191
C	0.81729	-3.51576	-0.35573
H	0.57983	-3.66459	-1.41907
H	1.44482	-4.35656	-0.02864
H	-0.12110	-3.55899	0.21264
C	-0.91882	0.52240	0.18298
C	-2.21418	0.00779	-0.04982
C	-0.66537	1.90783	0.26000
C	-3.27009	0.92334	-0.12536
C	-1.76305	2.77331	0.18458
C	-3.05496	2.29017	0.01305
H	-4.28133	0.55133	-0.30847
H	-1.58880	3.85139	0.23775
H	-3.89715	2.98421	-0.04145
C	0.72985	2.49161	0.28064
H	1.44060	1.66077	0.36225
C	-2.49670	-1.45816	-0.30986
H	-1.61259	-2.04156	-0.02103
C	0.97231	3.46017	1.43022
H	0.74217	3.02739	2.41318
H	2.02708	3.77345	1.44568
H	0.36744	4.37397	1.32361
C	1.01611	3.17686	-1.05406
H	0.78222	2.51879	-1.89836
H	0.42666	4.10075	-1.16515
H	2.08023	3.44900	-1.12460
C	-3.66586	-1.99343	0.50509
H	-3.76961	-3.07835	0.35858
H	-3.53435	-1.81410	1.58198
H	-4.62177	-1.53819	0.20608
C	-2.71228	-1.68753	-1.80399
H	-3.61376	-1.16588	-2.16132
H	-1.86393	-1.32298	-2.40173
H	-2.84178	-2.75846	-2.02054
C	0.69932	-1.10215	-0.59792
H	0.37185	-0.94483	-1.62793
F	3.57357	0.87686	0.12638
H	3.02884	0.73304	-0.68264
F	2.26356	0.44672	-1.81732
H	1.15043	0.57270	-2.64271
F	0.31311	0.58144	-3.16642

3Bc: ΔG = -2983858.1 kJ/mol

C	0.62142	-0.90599	1.74629
C	1.76961	-1.84559	1.35108
C	1.59034	-2.20373	-0.13669
N	0.16680	-0.41986	0.36136
H	2.72500	-1.31771	1.47775
H	1.79462	-2.73579	1.99376

C	1.08341	0.24897	2.60791
H	0.26546	0.95322	2.81471
H	1.41439	-0.15487	3.57456
H	1.93036	0.78552	2.16342
C	-0.54719	-1.60997	2.41972
H	-0.23956	-1.90355	3.43221
H	-1.41545	-0.94300	2.52199
H	-0.86181	-2.52129	1.89609
C	2.91266	-2.27880	-0.89013
H	3.48680	-3.14169	-0.52335
H	2.75237	-2.41438	-1.96860
H	3.50920	-1.37311	-0.74191
C	0.81729	-3.51576	-0.35573
H	0.57983	-3.66459	-1.41907
H	1.44482	-4.35656	-0.02864
H	-0.12110	-3.55899	0.21264
C	-0.91882	0.52240	0.18298
C	-2.21418	0.00779	-0.04982
C	-0.66537	1.90783	0.26000
C	-3.27009	0.92334	-0.12536
C	-1.76305	2.77331	0.18458
C	-3.05496	2.29017	0.01305
H	-4.28133	0.55133	-0.30847
H	-1.58880	3.85139	0.23775
H	-3.89715	2.98421	-0.04145
C	0.72985	2.49161	0.28064
H	1.44060	1.66077	0.36225
C	-2.49670	-1.45816	-0.30986
H	-1.61259	-2.04156	-0.02103
C	0.97231	3.46017	1.43022
H	0.74217	3.02739	2.41318
H	2.02708	3.77345	1.44568
H	0.36744	4.37397	1.32361
C	1.01611	3.17686	-1.05406
H	0.78222	2.51879	-1.89836
H	0.42666	4.10075	-1.16515
H	2.08023	3.44900	-1.12460
C	-3.66586	-1.99343	0.50509
H	-3.76961	-3.07835	0.35858
H	-3.53435	-1.81410	1.58198
H	-4.62177	-1.53819	0.20608
C	-2.71228	-1.68753	-1.80399
H	-3.61376	-1.16588	-2.16132
H	-1.86393	-1.32298	-2.40173
H	-2.84178	-2.75846	-2.02054
C	0.69932	-1.10215	-0.59792
H	0.37185	-0.94483	-1.62793
F	3.57357	0.87686	0.12638
H	3.02884	0.73304	-0.68264
F	2.26356	0.44672	-1.81732

H	1.15043	0.57270	-2.64271
F	0.31311	0.58144	-3.16642

3Bd: ΔG = -2983848.8 kJ/mol

C	-0.55587	-0.23032	2.17561
C	-1.94187	-0.89419	2.13529
C	-2.50320	-0.72194	0.70946
N	-0.25267	-0.11750	0.67422
H	-1.84000	-1.96582	2.35826
H	-2.60800	-0.46632	2.89624
C	0.48994	-1.08454	2.85932
H	1.48922	-0.63023	2.79925
H	0.23147	-1.16384	3.92397
H	0.52713	-2.10214	2.45083
C	-0.56424	1.16339	2.78342
H	-0.70980	1.06705	3.86760
H	0.39282	1.68139	2.62611
H	-1.37672	1.79190	2.39759
C	-3.21079	-1.96487	0.18282
H	-4.12906	-2.13407	0.76279
H	-3.49141	-1.84028	-0.87232
H	-2.57886	-2.85699	0.26293
C	-3.43922	0.49070	0.56528
H	-3.69111	0.66955	-0.48955
H	-4.37183	0.28922	1.11081
H	-3.00085	1.41113	0.97428
C	0.98686	0.43523	0.17187
C	1.01858	1.81398	-0.13334
C	2.11172	-0.39872	0.01703
C	2.25123	2.36286	-0.50320
C	3.31878	0.21049	-0.34761
C	3.39708	1.57814	-0.58178
H	2.30660	3.42651	-0.74690
H	4.20720	-0.41353	-0.47625
H	4.35106	2.03138	-0.86169
C	2.04268	-1.91161	0.06246
H	1.03092	-2.20354	0.38366
C	-0.22549	2.67833	-0.18450
H	-1.02540	2.17547	0.37570
C	3.05743	-2.53657	1.00998
H	2.96641	-2.16143	2.03858
H	2.93109	-3.62860	1.04199
H	4.08925	-2.34359	0.67907
C	2.23114	-2.44744	-1.35686
H	1.54714	-1.96042	-2.06350
H	3.26130	-2.27798	-1.70755
H	2.04170	-3.53030	-1.39350
C	-0.03171	4.04671	0.45237
H	-0.98567	4.59255	0.48255
H	0.34207	3.97240	1.48409

H	0.67464	4.67192	-0.11384
C	-0.70432	2.80206	-1.63006
H	0.04493	3.31520	-2.25298
H	-0.90311	1.82318	-2.09003
H	-1.63491	3.38731	-1.68175
C	-1.27549	-0.39295	-0.05852
H	-1.20947	-0.29973	-1.14634
F	-0.80638	-2.70099	-1.48612
H	-0.60346	-1.97441	-2.12925
F	-0.37202	-0.85625	-2.92893
H	-1.64320	-0.29818	-3.02974
F	-2.55303	0.08784	-2.97993

3Be: ΔG = -2983847.6 kJ/mol

C	-0.00107	1.13028	1.30514
C	-0.25924	2.57394	0.82879
C	0.45456	2.74254	-0.52930
N	0.46655	0.47769	0.00530
H	-1.33028	2.72564	0.69427
H	0.10282	3.29184	1.56365
C	-1.25392	0.45722	1.84180
H	-1.08808	-0.60522	2.02679
H	-1.49233	0.93215	2.79478
H	-2.10744	0.59595	1.18009
C	1.11426	1.01909	2.33837
H	0.74534	1.44769	3.27035
H	1.37117	-0.02520	2.52412
H	2.00912	1.56511	2.04525
C	-0.37984	3.48503	-1.57216
H	-0.55980	4.50164	-1.21852
H	0.15608	3.54360	-2.52108
H	-1.33986	2.99635	-1.73176
C	1.83270	3.41721	-0.40686
H	2.37138	3.36974	-1.35487
H	1.67517	4.46530	-0.14805
H	2.44610	2.95837	0.36820
C	0.82215	-0.92576	-0.10698
C	2.17216	-1.27519	0.04818
C	-0.17436	-1.86566	-0.39502
C	2.49376	-2.62882	-0.01681
C	0.20628	-3.20459	-0.45227
C	1.52111	-3.58695	-0.24740
H	3.52739	-2.93049	0.09747
H	-0.53957	-3.95536	-0.68059
H	1.79328	-4.63399	-0.29347
C	-1.59841	-1.48912	-0.74699
H	-1.75121	-0.43546	-0.52907
C	3.29585	-0.26564	0.18932
H	2.87201	0.72316	0.34229
C	-2.62362	-2.30307	0.04065

H	-2.45649	-2.23035	1.11671
H	-3.62979	-1.94143	-0.17321
H	-2.58192	-3.35840	-0.23595
C	-1.81998	-1.65785	-2.25332
H	-1.12739	-1.03894	-2.82762
H	-1.67723	-2.69906	-2.55159
H	-2.83918	-1.36401	-2.51366
C	4.20340	-0.56234	1.38230
H	4.93576	0.23906	1.49458
H	3.63318	-0.63801	2.30927
H	4.75234	-1.49509	1.24110
C	4.10654	-0.21290	-1.10903
H	4.57714	-1.17800	-1.30934
H	3.47278	0.04047	-1.96132
H	4.89290	0.54018	-1.02970
C	0.68592	1.32659	-0.92202
H	1.06920	0.99998	-1.88466
F	-4.73255	-0.23762	1.93739
H	-4.72273	-0.01705	0.95331
F	-4.72970	0.27870	-0.33261
H	-3.73588	0.97914	-0.77312
F	-2.96415	1.53837	-1.13185

Method DSD-PBEP86/TZVP

1A: ΔG = -2452673.6 kJ/mol

C	1.10611	0.48869	1.46126
C	2.46767	1.07095	1.03754
C	2.72222	0.63277	-0.41577
N	0.47640	0.22043	0.14381
H	2.41691	2.16145	1.07797
H	3.26747	0.74796	1.70592
C	0.31971	1.49224	2.30263
H	-0.67623	1.10787	2.53365
H	0.84221	1.65449	3.24763
H	0.22191	2.45450	1.80184
C	1.23642	-0.79214	2.29036
H	1.65849	-0.55141	3.26776
H	0.25158	-1.23680	2.45244
H	1.87777	-1.53566	1.82046
C	3.52934	1.67005	-1.18942
H	4.53152	1.74096	-0.76078
H	3.63177	1.38376	-2.23869
H	3.06898	2.65592	-1.14451
C	3.46013	-0.70594	-0.49800
H	3.56461	-1.02120	-1.53881
H	4.46078	-0.59651	-0.07517
H	2.95711	-1.50287	0.04623
C	-0.85135	-0.28564	-0.00932
C	-1.06264	-1.67576	-0.12407

C	-1.94890	0.59785	-0.07347
C	-2.36562	-2.15929	-0.22147
C	-3.23644	0.06854	-0.16233
C	-3.45062	-1.29813	-0.22007
H	-2.52958	-3.22692	-0.31075
H	-4.08298	0.74365	-0.20684
H	-4.45822	-1.68990	-0.28852
C	-1.79293	2.10472	-0.14242
H	-0.74166	2.33754	-0.00383
C	0.08122	-2.66336	-0.22689
H	1.00143	-2.12037	-0.03578
C	-2.60632	2.83411	0.92735
H	-2.38295	2.46660	1.92953
H	-2.38400	3.90309	0.90029
H	-3.67864	2.71650	0.75598
C	-2.19154	2.60687	-1.53371
H	-1.61440	2.10851	-2.31364
H	-3.25230	2.42528	-1.72307
H	-2.01457	3.68199	-1.61196
C	-0.02496	-3.79899	0.79043
H	0.86758	-4.42665	0.74470
H	-0.12253	-3.42008	1.80884
H	-0.88735	-4.43584	0.58216
C	0.16459	-3.23096	-1.64713
H	-0.73325	-3.80590	-1.88698
H	0.26515	-2.43544	-2.38818
H	1.02641	-3.89560	-1.73977
C	1.29511	0.46611	-0.95461
H	1.19724	-0.28206	-1.74544
F	0.89760	1.68219	-1.63201

2Ba: ΔG = -2716234.6 kJ/mol

C	0.61902	-0.87037	-1.91327
C	1.94501	-1.61146	-1.65433
C	2.47735	-1.13146	-0.28638
N	0.29898	-0.36591	-0.51243
H	1.75553	-2.68457	-1.61276
H	2.65779	-1.41946	-2.45497
C	-0.48058	-1.78324	-2.42856
H	-1.43725	-1.26083	-2.48279
H	-0.20670	-2.08957	-3.43895
H	-0.58650	-2.68119	-1.82348
C	0.76448	0.32294	-2.84994
H	0.95153	-0.06177	-3.85274
H	-0.15495	0.91031	-2.87860
H	1.59718	0.96675	-2.57081
C	2.96039	-2.27526	0.60503
H	3.81224	-2.76343	0.12918
H	3.27627	-1.89665	1.57865
H	2.17411	-3.01729	0.75294

C	3.56755	-0.05503	-0.39744
H	3.81576	0.33928	0.58884
H	4.45986	-0.50835	-0.83181
H	3.25163	0.77119	-1.03547
C	-0.95192	0.26905	-0.15286
C	-1.03652	1.66547	-0.21641
C	-2.00691	-0.54086	0.28332
C	-2.26881	2.24136	0.08477
C	-3.21487	0.08847	0.57358
C	-3.35263	1.46199	0.45501
H	-2.37071	3.31876	0.04902
H	-4.05141	-0.50721	0.91741
H	-4.30183	1.93074	0.68261
C	-1.85743	-2.02485	0.55781
H	-0.88736	-2.35762	0.19278
C	0.15942	2.56181	-0.47375
H	0.99344	1.95451	-0.81881
C	-2.93794	-2.85655	-0.13130
H	-2.97848	-2.65647	-1.20285
H	-2.73416	-3.91932	0.01112
H	-3.92264	-2.64794	0.29128
C	-1.87035	-2.26734	2.07027
H	-1.07587	-1.70628	2.56631
H	-2.82549	-1.96134	2.50265
H	-1.72539	-3.32875	2.28026
C	-0.11800	3.62143	-1.53826
H	0.79633	4.17782	-1.75186
H	-0.46990	3.17329	-2.46878
H	-0.86901	4.33711	-1.19886
C	0.59455	3.21312	0.84303
H	-0.20001	3.85025	1.23827
H	0.83305	2.45859	1.59571
H	1.47983	3.83124	0.68092
C	1.26948	-0.49813	0.30345
H	1.17638	-0.13914	1.32636
F	0.52453	0.48555	3.25230
H	1.64076	0.69490	3.08178
F	2.72050	0.87057	2.85939

3Bc: ΔG = -2979777.2 kJ/mol

C	-2.26757	-0.14722	1.00956
C	-3.28468	-0.34696	-0.13134
C	-2.56373	0.00229	-1.45145
N	-0.96336	-0.11023	0.22331
H	-3.59812	-1.39118	-0.15613
H	-4.16629	0.27340	0.02308
C	-2.26010	-1.29624	2.00497
H	-1.45457	-1.18761	2.73323
H	-3.20801	-1.26889	2.54388
H	-2.18117	-2.26415	1.51396

C	-2.44828	1.16825	1.75703
H	-3.36141	1.09037	2.34767
H	-1.61721	1.34750	2.44152
H	-2.55137	2.01559	1.08132
C	-2.82450	-1.00707	-2.56843
H	-3.88637	-0.99663	-2.81906
H	-2.25507	-0.74648	-3.46245
H	-2.55173	-2.01717	-2.25908
C	-2.86216	1.42576	-1.94801
H	-2.23656	1.67352	-2.80672
H	-3.90823	1.47431	-2.25415
H	-2.69310	2.16753	-1.16670
C	0.34021	-0.10691	0.85330
C	0.93620	1.12431	1.15117
C	0.95374	-1.33671	1.11534
C	2.15180	1.09303	1.83105
C	2.16961	-1.30939	1.79418
C	2.75056	-0.10929	2.17139
H	2.64594	2.02486	2.07544
H	2.67625	-2.24163	2.01028
H	3.69394	-0.11038	2.70294
C	0.42062	-2.65322	0.58565
H	-0.59235	-2.50453	0.21614
C	0.39041	2.44669	0.64954
H	-0.63230	2.30295	0.30841
C	0.37590	-3.74271	1.65460
H	-0.18975	-3.41912	2.53017
H	-0.10100	-4.63738	1.25057
H	1.37988	-4.02048	1.98034
C	1.27078	-3.08984	-0.61190
H	1.24711	-2.33796	-1.40414
H	2.31103	-3.23830	-0.31325
H	0.89253	-4.02976	-1.01840
C	0.37427	3.53154	1.72332
H	-0.10952	4.42842	1.33264
H	-0.17225	3.20801	2.61085
H	1.38557	3.80761	2.02677
C	1.20768	2.88864	-0.56883
H	2.25176	3.05521	-0.29318
H	1.17879	2.12957	-1.35352
H	0.80581	3.81906	-0.97513
C	-1.13656	-0.04103	-1.03776
H	-0.28057	-0.00929	-1.71199
F	0.35556	1.85488	-3.96488
H	0.81738	1.09025	-3.51077
F	1.38463	0.04968	-2.90796
H	2.39382	0.02269	-2.04726
F	3.15483	-0.02455	-1.39490

Method DSD-PBEP86/TZVPP

1A: ΔG = -2452683.6 kJ/mol

C	1.10611	0.48869	1.46126
C	2.46767	1.07095	1.03754
C	2.72222	0.63277	-0.41577
N	0.47640	0.22043	0.14381
H	2.41691	2.16145	1.07797
H	3.26747	0.74796	1.70592
C	0.31971	1.49224	2.30263
H	-0.67623	1.10787	2.53365
H	0.84221	1.65449	3.24763
H	0.22191	2.45450	1.80184
C	1.23642	-0.79214	2.29036
H	1.65849	-0.55141	3.26776
H	0.25158	-1.23680	2.45244
H	1.87777	-1.53566	1.82046
C	3.52934	1.67005	-1.18942
H	4.53152	1.74096	-0.76078
H	3.63177	1.38376	-2.23869
H	3.06898	2.65592	-1.14451
C	3.46013	-0.70594	-0.49800
H	3.56461	-1.02120	-1.53881
H	4.46078	-0.59651	-0.07517
H	2.95711	-1.50287	0.04623
C	-0.85135	-0.28564	-0.00932
C	-1.06264	-1.67576	-0.12407
C	-1.94890	0.59785	-0.07347
C	-2.36562	-2.15929	-0.22147
C	-3.23644	0.06854	-0.16233
C	-3.45062	-1.29813	-0.22007
H	-2.52958	-3.22692	-0.31075
H	-4.08298	0.74365	-0.20684
H	-4.45822	-1.68990	-0.28852
C	-1.79293	2.10472	-0.14242
H	-0.74166	2.33754	-0.00383
C	0.08122	-2.66336	-0.22689
H	1.00143	-2.12037	-0.03578
C	-2.60632	2.83411	0.92735
H	-2.38295	2.46660	1.92953
H	-2.38400	3.90309	0.90029
H	-3.67864	2.71650	0.75598
C	-2.19154	2.60687	-1.53371
H	-1.61440	2.10851	-2.31364
H	-3.25230	2.42528	-1.72307
H	-2.01457	3.68199	-1.61196
C	-0.02496	-3.79899	0.79043
H	0.86758	-4.42665	0.74470
H	-0.12253	-3.42008	1.80884
H	-0.88735	-4.43584	0.58216
C	0.16459	-3.23096	-1.64713

H	-0.73325	-3.80590	-1.88698
H	0.26515	-2.43544	-2.38818
H	1.02641	-3.89560	-1.73977
C	1.29511	0.46611	-0.95461
H	1.19724	-0.28206	-1.74544
F	0.89760	1.68219	-1.63201

2Ba: ΔG = -2717388.9 kJ/mol

C	0.61902	-0.87037	-1.91327
C	1.94501	-1.61146	-1.65433
C	2.47735	-1.13146	-0.28638
N	0.29898	-0.36591	-0.51243
H	1.75553	-2.68457	-1.61276
H	2.65779	-1.41946	-2.45497
C	-0.48058	-1.78324	-2.42856
H	-1.43725	-1.26083	-2.48279
H	-0.20670	-2.08957	-3.43895
H	-0.58650	-2.68119	-1.82348
C	0.76448	0.32294	-2.84994
H	0.95153	-0.06177	-3.85274
H	-0.15495	0.91031	-2.87860
H	1.59718	0.96675	-2.57081
C	2.96039	-2.27526	0.60503
H	3.81224	-2.76343	0.12918
H	3.27627	-1.89665	1.57865
H	2.17411	-3.01729	0.75294
C	3.56755	-0.05503	-0.39744
H	3.81576	0.33928	0.58884
H	4.45986	-0.50835	-0.83181
H	3.25163	0.77119	-1.03547
C	-0.95192	0.26905	-0.15286
C	-1.03652	1.66547	-0.21641
C	-2.00691	-0.54086	0.28332
C	-2.26881	2.24136	0.08477
C	-3.21487	0.08847	0.57358
C	-3.35263	1.46199	0.45501
H	-2.37071	3.31876	0.04902
H	-4.05141	-0.50721	0.91741
H	-4.30183	1.93074	0.68261
C	-1.85743	-2.02485	0.55781
H	-0.88736	-2.35762	0.19278
C	0.15942	2.56181	-0.47375
H	0.99344	1.95451	-0.81881
C	-2.93794	-2.85655	-0.13130
H	-2.97848	-2.65647	-1.20285
H	-2.73416	-3.91932	0.01112
H	-3.92264	-2.64794	0.29128
C	-1.87035	-2.26734	2.07027
H	-1.07587	-1.70628	2.56631
H	-2.82549	-1.96134	2.50265

H	-1.72539	-3.32875	2.28026
C	-0.11800	3.62143	-1.53826
H	0.79633	4.17782	-1.75186
H	-0.46990	3.17329	-2.46878
H	-0.86901	4.33711	-1.19886
C	0.59455	3.21312	0.84303
H	-0.20001	3.85025	1.23827
H	0.83305	2.45859	1.59571
H	1.47983	3.83124	0.68092
C	1.26948	-0.49813	0.30345
H	1.17638	-0.13914	1.32636
F	0.52453	0.48555	3.25230
H	1.64076	0.69490	3.08178
F	2.72050	0.87057	2.85939

3Bc: ΔG = -2980961.5 kJ/mol

C	-2.26757	-0.14722	1.00956
C	-3.28468	-0.34696	-0.13134
C	-2.56373	0.00229	-1.45145
N	-0.96336	-0.11023	0.22331
H	-3.59812	-1.39118	-0.15613
H	-4.16629	0.27340	0.02308
C	-2.26010	-1.29624	2.00497
H	-1.45457	-1.18761	2.73323
H	-3.20801	-1.26889	2.54388
H	-2.18117	-2.26415	1.51396
C	-2.44828	1.16825	1.75703
H	-3.36141	1.09037	2.34767
H	-1.61721	1.34750	2.44152
H	-2.55137	2.01559	1.08132
C	-2.82450	-1.00707	-2.56843
H	-3.88637	-0.99663	-2.81906
H	-2.25507	-0.74648	-3.46245
H	-2.55173	-2.01717	-2.25908
C	-2.86216	1.42576	-1.94801
H	-2.23656	1.67352	-2.80672
H	-3.90823	1.47431	-2.25415
H	-2.69310	2.16753	-1.16670
C	0.34021	-0.10691	0.85330
C	0.93620	1.12431	1.15117
C	0.95374	-1.33671	1.11534
C	2.15180	1.09303	1.83105
C	2.16961	-1.30939	1.79418
C	2.75056	-0.10929	2.17139
H	2.64594	2.02486	2.07544
H	2.67625	-2.24163	2.01028
H	3.69394	-0.11038	2.70294
C	0.42062	-2.65322	0.58565
H	-0.59235	-2.50453	0.21614
C	0.39041	2.44669	0.64954

H	-0.63230	2.30295	0.30841
C	0.37590	-3.74271	1.65460
H	-0.18975	-3.41912	2.53017
H	-0.10100	-4.63738	1.25057
H	1.37988	-4.02048	1.98034
C	1.27078	-3.08984	-0.61190
H	1.24711	-2.33796	-1.40414
H	2.31103	-3.23830	-0.31325
H	0.89253	-4.02976	-1.01840
C	0.37427	3.53154	1.72332
H	-0.10952	4.42842	1.33264
H	-0.17225	3.20801	2.61085
H	1.38557	3.80761	2.02677
C	1.20768	2.88864	-0.56883
H	2.25176	3.05521	-0.29318
H	1.17879	2.12957	-1.35352
H	0.80581	3.81906	-0.97513
C	-1.13656	-0.04103	-1.03776
H	-0.28057	-0.00929	-1.71199
F	0.35556	1.85488	-3.96488
H	0.81738	1.09025	-3.51077
F	1.38463	0.04968	-2.90796
H	2.39382	0.02269	-2.04726
F	3.15483	-0.02455	-1.39490

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