How Cinchona Alkaloid-Derived Primary Amines Control Asymmetric Electrophilic Fluorination of Cyclic Ketones

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Supporting Information

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A. Computational methods

All of the geometries were fully optimized at the B3LYP[1-4]/6-31G(d) level of theory, in conjunction with the IEF-PCM implicit solvation model[5] to account for the solvation effects of tetrahydrofuran, the solvent used experimentally. All of the optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition structures (a single imaginary frequency). Single-point energy calculations on the optimized geometries were then evaluated using the dispersion-corrected density functional method B3LYP-D3[6] (with a Becke–Johnson (BJ) damping function[7-9]) and the triple-zeta valence quality def2-TZVPP basis set of Weigend and Ahlrichs,[10] within the IEF-PCM model (THF). The thermal corrections evaluated from the unscaled vibrational frequencies at the B3LYP/6-31G(d) level on the optimized geometries were then added to the B3LYP-D3(BJ)/def2-TZVPP electronic energies to obtain the free energies. The free energy corrections were calculated using Truhlar's quasiharmonic approximation.[11,12] This uses the same usual harmonic oscillator approximation in the calculations of the vibrational partition functions, except that all of the real vibrational frequencies that are lower than 100 cm^{-1} are set equal to 100 cm^{-1}, as a way to correct for the spurious overestimation of vibrational entropies introduced by treating low-frequency vibrational modes as harmonic oscillators.[13] Additionally, single-point energies were calculated within the IEF-PCM model by using B3LYP/def2-TZVPP, M06-2X[14]/def2-TZVPP and ωB97XD[15]/def2-TZVPP on B3LYP/6-31G(d) geometries to check for robustness of our conclusions regarding the origin of stereoselectivity across different theoretical methods.

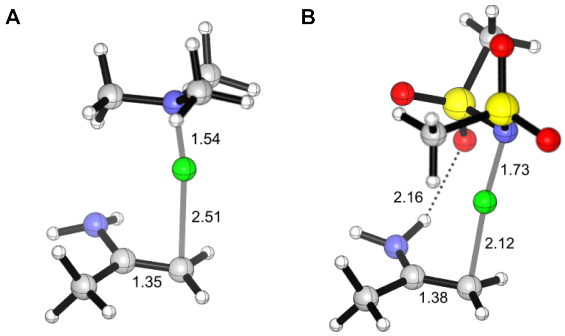
Additional CBS-QB3[16] and UB3LYP/6-31G(d) calculations were performed on model fluorine transfer transition structures to validate the DFT method used.

All of the quantum chemical computations were performed using *Gaussian 09*. All of the structural representations were generated with *CYLview*.[17]

B. Additional computational data

1. Fluorine transfer from *N*-fluorotrimethylammonium and *N*-fluoromethanesulfonimide

CBS-QB3 calculations were performed for the fluorine transfers from the N–F species to the enamine derived from acetone and ammonia, using methyl groups to replace the quinuclidine cage of the cinchona organocatalyst and the phenyl groups of NFSI due to the large sizes of the full systems. As shown in Figure S1, the free energy of activation ($\Delta G^{\ddagger}$) for the bimolecular fluorine transfer from *N*-fluorotrimethylammonium ion (Me_3NF^+) to the enamine (**TS-13a**) is 6.6 kcal/mol relative to infinitely separated reactants (8.6 kcal/mol relative to the reactant complex). The value of $\Delta G^{\ddagger}$ for the corresponding fluorine transfer from *N*-fluoromethanesulfonimide ($(MeSO_2)_2NF$) (**TS-13b**) is 21.3 kcal/mol relative to infinitely separated reactants (18.2 kcal/mol relative to the reactant complex). Density functional methods including B3LYP, M06-2X and wB97XD also give large differences (> 14.3 kcal/mol) in activation barriers between the fluorination by Me_3NF^+ and by $(MeSO_2)_2NF$, although B3LYP/def2-TZVPP//B3LYP/6-31G(d) gives the closest agreement in $\Delta G^{\ddagger}$ values compared with CBS-QB3 results. For the fluorinations of **1**–**5** under experimental conditions, the fluorine transfer from the *N*-fluoroquinuclidinium moiety of the organocatalyst **I** to the enamine moiety is intramolecular and should thus have an even greater kinetic advantage compared with an intermolecular fluorine transfer involving NFSI.



	TS-13a	TS-13b
CBS-QB3	$\Delta G^{\ddagger}$ = 6.6 (8.6)	$\Delta G^{\ddagger}$ = 21.3 (18.2)
B3LYP/def2-TZVPP// B3LYP/6-31G(d)	$\Delta G^{\ddagger}$ = 6.5	$\Delta G^{\ddagger}$ = 23.2
B3LYP-D3/def2-TZVPP// B3LYP/6-31G(d)	$\Delta G^{\ddagger}$ = 3.4	$\Delta G^{\ddagger}$ = 17.7
M06-2X/def2-TZVPP// B3LYP/6-31G(d)	$\Delta G^{\ddagger}$ = 11.0	$\Delta G^{\ddagger}$ = 33.0
wB97XD/def2-TZVPP// B3LYP/6-31G(d)	$\Delta G^{\ddagger}$ = 9.4	$\Delta G^{\ddagger}$ = 29.3

Figure S1. Transition structures for the bimolecular fluorine transfer from *N*-fluorotrimethylammonium ion (**TS-13a**; A) and *N*-fluoromethanesulfonimide (**TS-13b**; B) to the enamine formed from acetone and ammonia. The geometries shown are obtained by using CBS-QB3 calculations. Results obtained by geometry optimizations and single-point energy evaluations with other density functional methods are also shown. All of the free energies of activation ($\Delta G^{\ddagger}$) are reported in kcal/mol relative to infinitely separated reactants, except the values in parentheses, which are reported relative to the reactant complex.

For **TS-13a,** the energy was also calculated using UB3LYP/6-31G(d) on the optimized B3LYP/6-31G(d) geometry with the *Gaussian 09* keywords: "stable=opt" and "guess=(mix,always)". In other words, the stability of the RB3LYP SCF solution was tested and, if any instability was found, reoptimized to a lower-energy solution, mixing the HOMO and LUMO to destroy spin and spatial symmetries and generating a new initial guess at each point of the wavefunction optimization. The UB3LYP/6-31G(d) SCF solution is identical to the RB3LYP/6-31G(d) solution. Thus, spin-restricted, closed-shell DFT calculations are appropriate for modeling the fluorine transfer in our work.

2. Complete set of TSs for fluorination of cyclohexanone (1)

As shown in Figure S2, **TS-6a** and **TS-6b** correspond to axial attack of fluorine on the half-chair cyclohexene ring, while the corresponding boat-like TSs (**TS-6c** and **TS-6d**) are higher in energy by 1.1 kcal/mol.

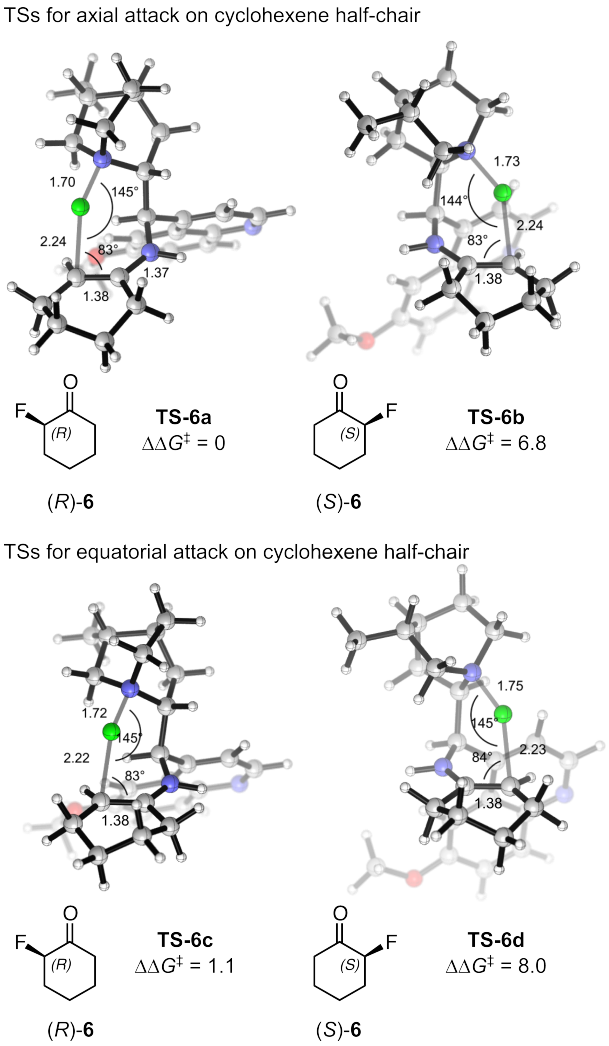


Figure S2. Fluorination transition structures **TS-6a–6d** for fluorination of **1** (B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM (THF)//B3LYP/6-31G(d)–IEF-PCM (THF)). The resulting enantiomer of **6** for each TS is also shown. The differences in free energy of activation ($\Delta\Delta G^{\ddagger}$) are reported, relative to **TS-6a**, in kcal/mol.

3. TSs for fluorination of 4,4-dimethylcyclohexanone (2)

TS-7a and **TS-7b** correspond to axial attack of fluorine on the half-chair cyclohexene ring, giving rise to (*R*)-**7** and (*S*)-**7**, respectively. **TS-7a** is 7.2 kcal/mol lower in energy than **TS-7b**. This is consistent with the high (98% ee) *R*-enantioselectivity observed.

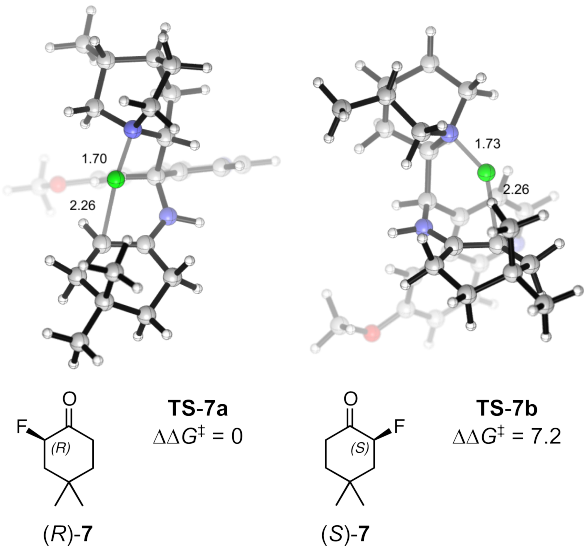


Figure S3. Fluorination transition structures **TS-7a–7b** for fluorination of **2** (B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM (THF)//B3LYP/6-31G(d)–IEF-PCM (THF)). The resulting enantiomer of **7** for each TS is also shown. The difference in free energy of activation ($\Delta\Delta G^{\ddagger}$) is reported, relative to **TS-7a**, in kcal/mol.

4. TSs for fluorination of 4-oxacyclohexanone (3)

TS-8a and **TS-8b** correspond to axial attack of fluorine on the half-chair cyclohexene ring, giving rise to (*R*)-**8** and (*S*)-**8**, respectively. **TS-8a** is 7.1 kcal/mol more stable than **TS-8b**. This is consistent with the high (98% ee) *R*-enantioselectivity observed.

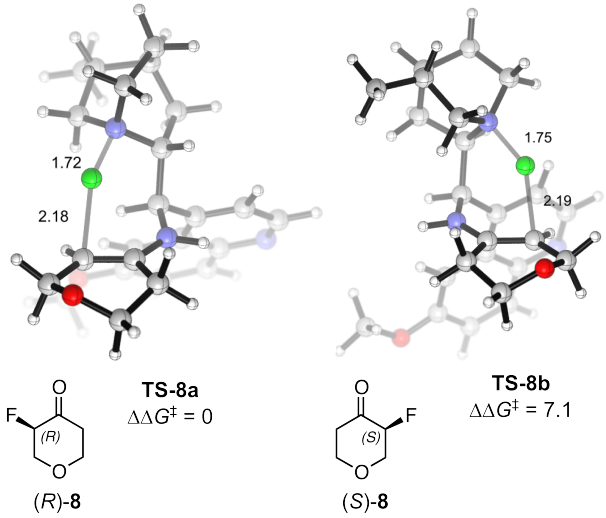


Figure S4. Fluorination transition structures **TS-8a–8b** for fluorination of **3** (B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM (THF)//B3LYP/6-31G(d)–IEF-PCM (THF)). The resulting enantiomer of **8** for each TS is also shown. The difference in free energy of activation ($\Delta\Delta G^{\ddagger}$) is reported, relative to **TS-8a**, in kcal/mol.

5. Computational results by other density functionals

5.1 TS-6a and TS-6b fully optimized at B3LYP-D3(BJ)/TZVP–IEF-PCM (THF)

TS-6a and **TS-6b** were also *fully optimized* at the B3LYP-D3(BJ)/TZVP–IEF-PCM (THF) level of theory. Single-point electronic energies were then evaluated by B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM. As shown in Figure S5, the $\Delta\Delta G^{\ddagger}$ values of **TS-6a** and **TS-6b** are 0 and 6.5 kcal/mol. The geometries of **TS-6a** and **TS-6b** are closely analogous to the geometries optimized at B3LYP/6-31G(d)–IEF-PCM (THF) level of theory, shown in Figure 1 of the Main Text and Figure S2 of Supporting Information. These results show that using B3LYP with the double-zeta 6-31G(d) basis set in geometry optimization does not significantly affect the fluorination TS geometries in accuracy compared with the dispersion-corrected B3LYP-D3(BJ) method in conjunction with the triple-zeta quality TZVP basis set.

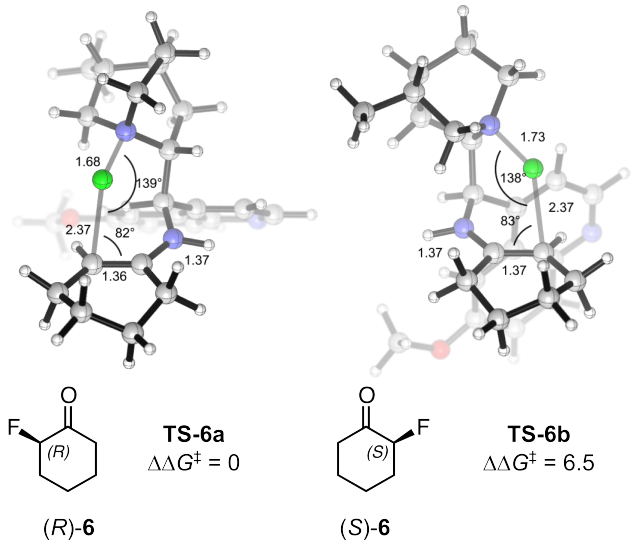


Figure S5. Fluorination transition structures **TS-6a–6b** for fluorination of **1** (B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM (THF)//B3LYP-D3(BJ)/TZVP–IEF-PCM (THF)) featuring axial attack of fluorine on the cyclohexene half-chair. The resulting enantiomer of **6** for each TS is also shown. The difference in free energy of activation ($\Delta\Delta G^{\ddagger}$) is reported, relative to **TS-6a**, in kcal/mol.

5.2. Additional single-point energies using other density functionals

To study the extent to which the stereoselectivities depend on dispersion interactions, single-point energies of the fluorination transition structures were computed using M06-2X/def2-TZVPP and ωB97XD/def2-TZVPP, in addition to the B3LYP-D3(BJ)/def2-TZVPP results discussed in the Main Text. The results are listed in Table S1. Results using the plain B3LYP functional, in conjunction with the 6-31G(d) and the larger def2-TZVPP basis sets are also listed. Only the energetically important transition structures are included. B3LYP/6-31G(d)–IEF-PCM (THF) geometries and thermal corrections were used.

Table S1. Selectivity Data ($\Delta\Delta G^{\ddagger}$) Predicted for Fluorination Using Different Density Functionals [a]

TS	Product	B3LYP/ 6-31G(d)	B3LYP/ def2-TZVPP	B3LYP-D3(BJ)/ def2-TZVPP	M06-2X/ def2-TZVPP	wB97XD/ def2-TZVPP
TS-6a	(*R*)-**6**	**0**	**0**	**0**	**0**	**0**
TS-6b	(*S*)-**6**	**8.3**	**9.0**	**6.8**	**7.8**	**7.3**
TS-6c	(*R*)-**6**	1.1	1.1	1.1	2.0	1.6
TS-6d	(*S*)-**6**	9.5	10.1	8.0	9.8	8.9
TS-7a	(*R*)-**7**	**0**	**0**	**0**	**0**	**0**
TS-7b	(*S*)-**7**	**9.1**	**9.6**	**7.2**	**8.6**	**7.8**
TS-8a	(*R*)-**8**	**0**	**0**	**0**	**0**	**0**
TS-8b	(*S*)-**8**	**8.6**	**9.3**	**7.1**	**7.7**	**7.4**
TS-9a	(2*R*,4*S*)-**9**	**0**	**0**	**0**	**0**	**0**
TS-9b	(2*S*,4*R*)-**9**	**8.6**	**9.3**	**7.1**	**8.4**	**7.8**
TS-9c	(2*R*,4*R*)-**9**	**1.1**	**3.1**	**0.8**	**0.2**	**0.5**
TS-9d	(2*S*,4*S*)-**9**	**9.2**	**11.8**	**6.9**	**8.1**	**7.4**
TS-10a	(3a*S*,4*R*,7a*S*)-**10**	**0**	**0**	**0**	**0**	**0**
TS-10b	(3a*S*,6*R*,7a*S*)-**10**	**3.1**	**2.4**	**2.8**	**2.8**	**3.0**
TS-10c	(2*R*,3a*S*,7a*S*)-**10**	**2.8**	**3.6**	**1.9**	**2.4**	**1.6**
TS-11a	(*R*)-**6**	**0**	**0**	**0**	**0**	**0**
TS-11b	(*S*)-**6**	**5.0**	**4.8**	**4.1**	**5.5**	**4.6**
TS-12a	(*R*)-**6**	**6.4**	**7.7**	**7.6**	**6.4**	**6.8**
TS-12b	(*S*)-**6**	**0**	**0**	**0**	**0**	**0**

a Single-point energies calculated by the specified method within the IEF-PCM (THF) model, using B3LYP/6-31G(d)–IEF-PCM (THF) geometries and thermal corrections. All of the differences in free energies are in kcal/mol. Values for the selectivity-determining transition structures are shown in boldface.

The data in Table S1 show that all of the density functional methods give the same trends in relative energy of the transition structures. In general, the differences in free energy of activation calculated by the dispersion-inclusive density functional methods are

smaller than those calculated by plain B3LYP. However, for the fluorinations modeled by **TS-6**, **TS-7** and **TS-8**, as well as the model systems **TS-11** and **TS-12**, the transition structure leading to the minor enantiomer is still high in energy after taking dispersion effects into account and does not contribute to the formation of the minor enantiomer under the experimental conditions. For example, using the def2-TZVPP basis set, the energy difference between **TS-6a** and **TS-6b** is 9.0 kcal/mol with B3LYP, and 6.8 kcal/mol with B3LYP-D3(BJ).

For the desymmetrizing fluorination of **4** (**TS-9a–d**), the plain B3LYP functional seriously overestimates the anti/syn selectivity, with the energy difference between **TS-9a** and **TS-9c** calculated as 3.1 kcal/mol using the def2-TZVPP basis set. On the other hand, the dispersion-inclusive density functionals B3LYP-D3(BJ), M06-2X and wB97XD bring the predicted level of anti/syn selectivity into better agreement with experiment. In particular, the $\Delta\Delta G^{\ddagger}$ values of **TS-9a** and **TS-9c** computed by B3LYP-D3(BJ)/def2-TZVPP//B3LYP/6-31G(d) are 0 and 0.8 kcal/mol, in close agreement to the experimental anti/syn selectivity of 4:1, which corresponds to $\Delta\Delta G^{\ddagger} = 0.7$ kcal/mol.

The high chemo- and regioselectivity of the fluorination of **5** (**TS-10a–c**) is also reproduced by the different methods, although, again, the energy differences are smaller with the use of dispersion-inclusive functionals. Thus, using B3LYP-D3(BJ)/def2-TZVPP, the difference in free energy between the most favorable transition structure **TS-10a** and the next higher-energy transition structure **TS-10c** is 1.9 kcal/mol, giving the product ratio of (3a*S*,4*R*,7a*S*)-**10** versus (2*R*,3a*S*,7a*S*)-**10** as 1:0.02 under the experimental conditions, in good agreement with the experimental result that (3a*S*,4*R*,7a*S*)-**10** was the sole product.

To summarize, comparison of the differences in free energy of activation computed by dispersion-corrected and dispersion-uncorrected functionals shows that differential dispersion interactions do not play a significant role in influencing the experimentally observed *enantiofacial* control, but the inclusion of dispersion interactions is essential for reproducing the experimental diastereoselectivity of the fluorination of **4** and the carbonyl selectivity in the fluorination of **5**.

C. Cartesian coordinates and energies

Unless stated otherwise, all of the cartesian coordinates correspond to B3LYP/6-31G(d)–IEF-PCM (THF)-optimized geometries.

N-Fluorinated enamine formed from 1 and N-fluorinated II C25H33F1N3O1(1+)
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C,-3.3276220869,-0.6479586308,-0.6403653361
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C,-5.8306412805,-0.6738112513,-0.2343765114
C,-5.4776651838,-1.1658110289,1.1730861104
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Enthalpy = -1311.021976
Free energy = -1311.105320
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B3LYP/def2-TZVPP SCF = -1312.0930435
M062X/def2-TZVPP SCF = -1311.5504217
wB97XD/def2-TZVPP SCF = -1311.6981123

TS-6a C25H33F1N3O1(1+)
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C,-3.4135710143,-2.4113666993,-2.0106375227
C,-4.5973928588,-2.8671626408,-1.1486904179
C,-4.0928066827,-3.5287163424,0.1375353949
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C,3.4877947182,-1.3924070524,-1.2335246509
H,1.4553655216,-0.8411703345,-1.3834705589
C,4.4864850248,-1.4186991771,0.9663884338
N,3.23322312,-0.8383596592,2.905590523
H,2.0848607962,-0.3243334674,4.5281983143

H,-2.0334244834,3.9114760022,2.0245755586
H,-2.3248985514,4.9663267259,0.6380323066
H,-1.067704985,4.5729321887,-1.4195127527
C,0.9678585417,3.9577758306,-1.6606082291
C,4.6086522092,-1.6117770894,-0.3901150654
O,3.5114544868,-1.5622255791,-2.5821415621
H,5.3292744799,-1.5847986267,1.6297430355
H,0.9160961596,3.8796248471,-2.7522017297
H,1.366988145,4.9472898594,-1.4144752506
H,1.6821955978,3.2058564796,-1.307099062
H,5.5571386953,-1.9320682575,-0.8042411302
C,4.7237870856,-1.9880994322,-3.205266206
H,4.4988394891,-2.0517992466,-4.2705068489
H,5.0367348701,-2.9731452452,-2.8404117867
H,5.5307775713,-1.2633970412,-3.0472085702
H,-1.3520529405,-1.3262934029,1.8942932079
F,-2.577184262,0.4903655431,-0.8268977844
Electronic energy = -1311.5869176
Zero-point electronic energy = -1311.037110
Thermal energy = -1311.010790
Enthalpy = -1311.009846
Free energy = -1311.093214
Free energy (quasiharmonic approximation) = -1311.087938
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.223832
B3LYP/def2-TZVPP SCF = -1312.0798408
M062X/def2-TZVPP SCF = -1311.5104504
wB97XD/def2-TZVPP SCF = -1311.6649428

TS-6b C25H33F1N3O1(1+)
C,-0.1984261026,1.9439454163,0.3310040381
C,-0.0380387779,2.2697030026,-1.0001533091
C,-0.1323411093,3.6834051053,-1.507579105
C,-0.7905387651,4.649296945,-0.5161219221
C,-0.2198868571,4.429613209,0.8875823032
C,-0.518745405,3.0038855844,1.3679192758
H,0.8848717021,4.0338228461,-1.7481432697
H,0.3584231975,1.5404215312,-1.6886485394
H,0.0352665617,2.7881723811,2.2914700553
H,-1.5864463411,2.919214982,1.6252015325
H,-0.6700357853,3.6825837564,-2.4647477358
N,-0.1841412069,0.6744076338,0.8521374328
C,-0.1097669804,-0.6433701502,0.2370556514
C,-1.4891775631,-1.3456009509,-0.1777365968
H,0.2310467698,-1.2948685132,1.0476276843
H,-1.2425249921,-1.9743212918,-1.0324852094
C,-2.0999950868,-2.2662620186,0.9189754009
N,-2.5939011043,-0.4924048688,-0.6349102745
C,-3.626328478,-2.3502140487,0.6705900021
H,-1.8931285371,-1.8813455386,1.9235534678
H,-1.620785753,-3.247313694,0.8443535989
C,-3.4442396221,-1.2221213066,-1.5936576417
C,-3.4033981261,0.1105929308,0.4452089788
C,-3.8953191779,-2.5272648289,-0.8440099736
H,-4.0601565689,-3.1840664754,1.2299302039
C,-4.2690385966,-1.0109849468,1.1021802719
H,-2.8614851733,-1.4373126092,-2.4903238091
H,-4.2818829712,-0.5751808901,-1.8583926618
H,-2.7129548719,0.5610725686,1.1592152332
H,-4.007758323,0.898367419,-0.0064838698
H,-3.3469217213,-3.3887829704,-1.2374062895
H,-4.9595882788,-2.6981376338,-1.0294287991
H,-5.2735454077,-0.9629252328,0.6649865314
H,-0.2757989363,0.6450712183,1.8605077104
F,-1.789052674,0.8960027401,-1.2732250733
H,-0.6337363956,5.6834061187,-0.841723841

H,-1.8757955556,4.4796847607,-0.499018385
H,0.8656748307,4.5936828131,0.8731256235
H,-0.6416112022,5.1449347823,1.6018624752
C,0.9673443068,-0.759541914,-0.8491377331
C,2.3459582769,-0.8181889624,-0.4611483594
C,0.6738033908,-0.8506581645,-2.1952172822
C,2.8003686315,-0.7113478451,0.8832262294
C,3.3127632397,-1.0015021966,-1.5058500146
C,1.7088564965,-1.0179966322,-3.1414300462
H,-0.3436471399,-0.7553976363,-2.5543152895
C,4.1496784255,-0.7968182843,1.1768981944
H,2.0895666629,-0.539397734,1.6794959451
C,4.6919840615,-1.086036404,-1.1625405224
N,2.9857999001,-1.1019229932,-2.8241137218
H,1.4590881336,-1.0864804563,-4.1988029405
C,5.1040352521,-0.9885903775,0.1387328104
O,4.6839960583,-0.7082294777,2.4216225887
H,5.4028067057,-1.2285332362,-1.970092717
H,6.1529884246,-1.0506599513,0.4103835321
C,3.8064737884,-0.5241869581,3.5299566243
H,4.4450015917,-0.4970601793,4.4134238929
H,3.0967923985,-1.3558069503,3.6157211812
H,3.2566324383,0.4209873984,3.4473651012
C,-4.4063329968,-0.8071128402,2.6127360943
H,-4.846382557,0.1717644325,2.8331279278
H,-5.0616542348,-1.5725465867,3.0414023212
H,-3.4408218687,-0.861145827,3.1281050179
Electronic energy = -1311.5739801
Zero-point electronic energy = -1311.023970
Thermal energy = -1310.997804
Enthalpy = -1310.996860
Free energy = -1311.079664
Free energy (quasiharmonic approximation) = -1311.074667
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.2132581
B3LYP/def2-TZVPP SCF = -1312.065839
M062X/def2-TZVPP SCF = -1311.4983994
wB97XD/def2-TZVPP SCF = -1311.6537022

TS-6c C25H33F1N3O1(1+)
C,-2.253162052,-1.7717436834,0.1855834024
C,-2.3370988389,-1.7369405668,-1.1909274324
C,-3.3845474291,-2.4896514772,-1.9718163726
C,-4.1557930757,-3.5176344902,-1.130909828
C,-4.5066712893,-2.9388307264,0.2424366876
C,-3.231047258,-2.5812119079,1.0161351763
H,-4.088546339,-1.7640432266,-2.4070480212
H,-1.5305138814,-1.3019225778,-1.7669301227
H,-3.4809538779,-2.0268718649,1.9296146451
H,-2.7274886201,-3.5034699689,1.34139035
H,-2.9055737419,-2.979623383,-2.8295385163
N,-1.31992391,-1.1022551158,0.9231161405
C,-0.3692539404,-0.0711065974,0.5402907826
C,-0.9551560824,1.3910740291,0.787053682
H,-0.1659881533,-0.170385732,-0.5224430301
C,0.912439196,-0.2945768834,1.3407361555
H,-1.6145119507,1.3164557727,1.6547897722
C,0.0874716937,2.5355129712,1.018727145
N,-1.8011790175,1.8768061623,-0.3105184819
C,2.1281825538,-0.7368962621,0.7214360665
C,0.9106521852,-0.1153610256,2.7093421942
C,-0.4748726919,3.8447448813,0.4155189931
H,1.0492015259,2.2833368216,0.562550114
H,0.2605449405,2.6379210149,2.0920868022
C,-2.7848576392,2.8626557666,0.1695364359
C,-1.0667588256,2.3670786611,-1.4930342024

C,2.2860104877,-0.9740603623,-0.6640279882
C,3.2594314102,-0.9476288262,1.5855470404
C,2.0815151926,-0.3629431527,3.4644170255
H,0.0222495221,0.225584647,3.234765475
C,-1.9521434287,4.0092023698,0.8396011374
H,0.1152437489,4.69841039,0.7616667977
C,-0.4348872048,3.7500403081,-1.1291269943
H,-3.4573506091,2.3616270803,0.8672620153
H,-3.3571726694,3.2054995375,-0.6938232399
H,-0.3054437358,1.6296018291,-1.7520961599
H,-1.7795002464,2.4300489901,-2.316232851
C,3.4990920224,-1.3913642643,-1.1895845861
H,1.4663235541,-0.8477791745,-1.3612854952
C,4.4854647162,-1.3744839802,1.015966013
N,3.2202102085,-0.7607881894,2.9369481324
H,2.0622523865,-0.2174481954,4.5431503671
H,-2.0508370333,3.9592329471,1.9284549466
H,-2.3441214297,4.9773055244,0.5150484164
H,-1.0848916089,4.5363354522,-1.5304601864
C,0.9519852906,3.918802379,-1.7550278664
C,4.6157165359,-1.5922629152,-0.3360243644
O,3.5311063372,-1.5850673463,-2.5347949478
H,5.3250904575,-1.5254945948,1.6868931646
H,0.9014540304,3.8140026345,-2.844461475
H,1.3498386396,4.9144798199,-1.5326725713
H,1.6669377115,3.1765917361,-1.3826641248
H,5.5674265789,-1.9172471291,-0.7389320474
C,4.7486304134,-2.0172189416,-3.143319877
H,4.5304674032,-2.0994500416,-4.2086972574
H,5.0625043651,-2.9949926311,-2.7601559831
H,5.5522723031,-1.2873029568,-2.9924398201
H,-1.3596102884,-1.2758210545,1.9207455659
F,-2.5852162971,0.4433735235,-0.8416857
H,-3.5410205923,-4.41778677,-0.9962566675
H,-5.0616049223,-3.8284105285,-1.6633049621
H,-5.1242072885,-2.0394077484,0.1180844454
H,-5.0949894416,-3.6531309571,0.8285960851
Electronic energy = -1311.5853407
Zero-point electronic energy = -1311.035293
Thermal energy = -1311.008998
Enthalpy = -1311.008054
Free energy = -1311.091325
Free energy (quasiharmonic approximation) = -1311.086170
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.2222616
B3LYP/def2-TZVPP SCF = -1312.0783083
M062X/def2-TZVPP SCF = -1311.5074639
wB97XD/def2-TZVPP SCF = -1311.6625868

TS-6d C25H33F1N3O1(1+)
C,-0.1593955059,1.9442726256,0.309882991
C,-0.0029823163,2.2536180102,-1.0284888659
C,-0.0310796094,3.668794364,-1.5488556941
C,0.0813612719,4.7362719058,-0.4511762528
C,-0.7969595865,4.368274748,0.7462223733
C,-0.346902235,3.0322171671,1.3515196164
H,0.7714294784,3.7909996565,-2.2873326275
H,0.3301865075,1.4967192211,-1.7190963388
H,0.6089064701,3.171149648,1.8780008356
H,-1.0679363803,2.6980330352,2.10892336
H,-0.9674946153,3.8148633478,-2.1089380513
N,-0.1963723779,0.6814402033,0.8393261107
C,-0.1393570274,-0.644081249,0.2385262101
C,-1.5283372625,-1.3268624372,-0.1792354279
H,0.1843882151,-1.2921561299,1.0588107625
H,-1.2852713771,-1.9640690842,-1.0287120431

C,-2.1570184136,-2.2345354377,0.9185960136
N,-2.6167959965,-0.46092993,-0.6473133594
C,-3.6832409803,-2.2961246734,0.6635726627
H,-1.9494378984,-1.8495626919,1.9228819166
H,-1.6927085459,-3.2232184372,0.8498550154
C,-3.4718037627,-1.1841969677,-1.6057834555
C,-3.4234494858,0.1600354059,0.4235796869
C,-3.9482430603,-2.477666375,-0.851117423
H,-4.1321585173,-3.1202390037,1.2256027413
C,-4.3077168507,-0.9449050039,1.0848819205
H,-2.8878249069,-1.4148546428,-2.4979245749
H,-4.298230088,-0.5269940249,-1.8806748877
H,-2.7320313182,0.6074828861,1.1382085224
H,-4.0152293676,0.9527450098,-0.0361516103
H,-3.4123664043,-3.3506241116,-1.236636536
H,-5.0144497112,-2.6322080709,-1.040211152
H,-5.3101375274,-0.8853213673,0.6441325467
H,-0.2955372257,0.6640596033,1.8473641562
F,-1.7720071889,0.9272409778,-1.2832649351
C,0.9437425972,-0.7866806104,-0.8377298827
C,2.3185595836,-0.857196977,-0.4385619562
C,0.6591687025,-0.888623736,-2.1849182212
C,2.7635396526,-0.7447288864,0.9085216077
C,3.2913133258,-1.0592546809,-1.4741690348
C,1.6994876745,-1.076088281,-3.1216248431
H,-0.354722464,-0.7867730892,-2.5523858855
C,4.1097595,-0.839987152,1.2132308103
H,2.0477292369,-0.5634963245,1.6982691088
C,4.6670549626,-1.1535727795,-1.1196295717
N,2.9731555415,-1.1688681665,-2.7938921458
H,1.4569164175,-1.1527218633,-4.1801062807
C,5.0701358928,-1.0485723013,0.1838745925
O,4.6354791394,-0.7466036388,2.4612257159
H,5.3826214146,-1.3098064974,-1.9204134026
H,6.1163833267,-1.1178755753,0.464066842
C,3.7516525027,-0.5444445666,3.5613488905
H,4.3840663152,-0.5140413563,4.4490928815
H,3.0344466653,-1.3692350245,3.6501524736
H,3.2104162849,0.4044552327,3.4656033169
H,-0.7528315558,5.1445178849,1.5178715003
H,-1.8449884357,4.2925225439,0.4274978341
H,-0.2026403591,5.7148744273,-0.8536242994
H,1.1260075041,4.817691384,-0.1222066711
C,-4.447393687,-0.7307965356,2.5938862266
H,-4.8727451354,0.256086538,2.8074766169
H,-5.1163393289,-1.4834141491,3.0243246224
H,-3.4848516742,-0.7973639962,3.1136049484
Electronic energy = -1311.5724276
Zero-point electronic energy = -1311.022060
Thermal energy = -1310.995965
Enthalpy = -1310.995020
Free energy = -1311.077277
Free energy (quasiharmonic approximation) = -1311.072808
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.2117182
B3LYP/def2-TZVPP SCF = -1312.0644329
M062X/def2-TZVPP SCF = -1311.4955102
wB97XD/def2-TZVPP SCF = -1311.6514785

TS-7a C27H37F1N3O1(1+)
C,0.0929340502,0.1611113757,0.618428886
C,-0.1677725831,1.7300812808,0.7289055484
C,1.3766348137,-0.2252030582,1.3507583254
C,1.0998176693,2.6494512769,0.7149829166
N,-1.0203692932,2.2663138968,-0.3427694634
H,-0.7254323983,1.8902472317,1.6545244448

N,-0.9944008215,-0.617133799,1.1862063025
H,0.1779644908,-0.0863234756,-0.4363567483
C,2.4305580413,-0.9561521594,0.7098623993
C,1.5257296852,0.0915943216,2.685874712
C,0.7395922322,3.9798747625,0.0111641358
H,1.4150997109,2.8216806321,1.7461967405
H,1.9307867653,2.1533329687,0.2052836512
C,-1.7314518235,3.479999715,0.1002650068
C,-0.3385171291,2.4682855678,-1.6385484788
C,-2.1147759501,-1.1388046315,0.5983468782
H,-0.9716555299,-0.6837867615,2.1969052888
C,2.4185203093,-1.3645657344,-0.6442309499
C,3.5733687438,-1.2917527879,1.5173742353
C,2.6926513329,-0.295814012,3.3862555799
H,0.7613054586,0.6464577566,3.2241922534
C,-0.6177380728,4.4864761465,0.5484610614
C,0.5809602517,3.7245494451,-1.5072000538
H,1.5208185304,4.723234561,0.1950207757
H,-2.4059345896,3.2026623212,0.9115760538
H,-2.318743186,3.8470537124,-0.7428766484
H,-1.1121618255,2.5836815715,-2.3984266005
H,0.2344272249,1.5672534042,-1.8631735651
C,-3.1923831266,-1.5458895512,1.5802197433
C,-2.3120455779,-1.2416638191,-0.7582065763
C,3.4795118374,-2.0686321804,-1.1926197359
H,1.5793295441,-1.1539572166,-1.2966348605
C,4.6421850216,-2.0101672076,0.9248227443
N,3.6880843027,-0.958809119,2.8359842652
H,2.7948146819,-0.0369983791,4.4387697286
H,-0.8483463356,5.4783783006,0.1500782765
H,-0.5970632022,4.5630123181,1.6397558431
C,1.8913405506,3.5468976277,-2.2789776659
H,0.0494225282,4.5805123766,-1.93956006
C,-4.2894175581,-2.4088162303,0.9445240151
H,-2.7338916931,-2.0835190371,2.4212193906
H,-3.6256677743,-0.6304956998,2.0076591812
C,-3.5582447166,-1.8251509324,-1.3658548876
H,-1.4858683371,-1.0675514503,-1.4375787704
C,4.6085374146,-2.3942742913,-0.3956622063
O,3.355491023,-2.4083232021,-2.5031876713
H,5.4941294749,-2.2510514261,1.5525813011
H,1.6938046917,3.3373188205,-3.3361087176
H,2.4972527937,2.7239438075,-1.8838743711
H,2.4884903259,4.4631189081,-2.2255799068
C,-4.7761502645,-1.8611402823,-0.4148644455
H,-5.1313562358,-2.4884756285,1.6429015439
H,-3.9055888272,-3.4270051258,0.7956463438
H,-3.8090481485,-1.2664319658,-2.2783701587
H,-3.3325221874,-2.8492872066,-1.7074439984
H,5.44207678,-2.9436130971,-0.8165413152
C,4.401418971,-3.1540498655,-3.1272216499
C,-5.3702429371,-0.4449145545,-0.2662368561
C,-5.8489867026,-2.8012547751,-0.9882052559
H,4.5428029609,-4.1266276605,-2.6420272965
H,5.3464827799,-2.5989180969,-3.122690111
H,4.0774078525,-3.3074480043,-4.1572019982
H,-4.6067254759,0.2940774201,-0.0038556492
H,-6.1525936469,-0.4256181993,0.5022918624
H,-5.823737654,-0.1232249176,-1.2115970591
H,-6.7390767697,-2.8155693337,-0.3476226339
H,-6.161627906,-2.4766207352,-1.9881605072
H,-5.4756458826,-3.8294493649,-1.0691876087
F,-2.1181776829,1.0054034483,-0.6318219537
Electronic energy = -1390.215648
Zero-point electronic energy = -1389.609746

Thermal energy = -1389.580733
Enthalpy = -1389.579788
Free energy = -1389.668154
Free energy (quasiharmonic approximation) = -1389.662630
B3LYP-D3(BJ)/def2-TZVPP SCF = -1390.8955835
B3LYP/def2-TZVPP SCF = -1390.7367461
M062X/def2-TZVPP SCF = -1390.1318173
wB97XD/def2-TZVPP SCF = -1390.3038258

TS-7b C27H37F1N3O1(1+)
C,0.2060964097,-0.9911483019,0.1673989218
C,-1.0048308921,-1.9161597961,-0.3347962717
C,1.2596364053,-0.7506425521,-0.9207251838
C,-1.3582848985,-3.0859745594,0.6303384027
N,-2.2832094041,-1.2725728655,-0.6620219209
H,-0.6613410276,-2.3560123566,-1.2701075943
N,-0.1314109669,0.1990426227,0.9345305674
H,0.693988914,-1.6453082772,0.8961078028
C,2.631806953,-0.5878511056,-0.5399082973
C,0.9577898032,-0.7260851446,-2.2678674559
C,-2.8421340059,-3.4602116372,0.398926227
H,-0.6892763823,-3.9228328755,0.407368806
H,-1.1881048729,-2.8070059573,1.6757120262
C,-2.9971438441,-2.0403705408,-1.6983581235
C,-3.1574818158,-0.9994251202,0.49617626
C,-0.4234730276,1.4889186845,0.5679926349
H,-0.2136028778,0.026934149,1.9295203809
C,3.0882706612,-0.5618326229,0.8080700887
C,3.5920729299,-0.4536271703,-1.5982811092
C,1.9835636662,-0.5696910571,-3.2257991435
H,-0.0677425592,-0.7870129704,-2.6119496495
C,-3.7311258654,-2.3563826296,1.0183312962
C,-3.1330369986,-3.4952115111,-1.1214445598
H,-3.0660924414,-4.4323602687,0.8474197216
H,-2.4173909333,-2.0111728733,-2.6220199225
H,-3.9618673678,-1.5590789782,-1.8658538381
H,-2.5513293778,-0.4978785485,1.2509757019
H,-3.9388074249,-0.3172048338,0.1584287992
C,-0.9588309507,2.3245764608,1.7118011796
C,-0.3547929373,2.0001698677,-0.7111072688
C,4.4364958775,-0.4301140059,1.0895896632
H,2.3768688694,-0.6213112297,1.620530984
C,4.9704046012,-0.3204573457,-1.2668513218
N,3.2601638344,-0.4483605375,-2.9190585731
H,1.727595583,-0.5503106153,-4.2837141595
C,-3.8336099782,-2.3734065375,2.5454147139
H,-4.7432035846,-2.4731909787,0.6133914785
H,-4.1444925468,-3.8643590329,-1.3129983076
H,-2.4320904339,-4.1615689047,-1.6331467908
C,-1.0212438273,3.8233641905,1.3926793431
H,-0.3411945621,2.1598596275,2.6047290212
H,-1.9624328692,1.9518234364,1.96723772
C,-0.7298953421,3.4187645627,-1.0438200221
H,0.1637204095,1.4545084192,-1.48320145
C,5.3865454827,-0.3113138756,0.0366698676
O,4.9728323185,-0.3975977122,2.3361358904
H,5.6769324644,-0.2258242045,-2.0851381046
H,-4.4676558292,-1.5528354683,2.8992409203
H,-2.8555148177,-2.2688888663,3.0287124736
H,-4.2816611034,-3.3125906904,2.8865091051
C,-1.6258106124,4.1160328302,0.002413975
H,-1.6013867414,4.3296326942,2.1736989513
H,-0.0069296053,4.2424885141,1.4301362919
H,-1.2158877059,3.4346846857,-2.0292418621
H,0.2001225247,3.9974499889,-1.1730652728

H,6.4347615607,-0.2108854769,0.2995144047
C,4.1006013754,-0.5168089217,3.457437671
C,-1.62656584,5.6333595727,-0.2444714513
C,-3.0691666111,3.5825180959,-0.1030164834
H,3.5621779504,-1.4721074422,3.4410532875
H,3.3812651467,0.3102064079,3.4883851353
H,4.7415043066,-0.4746751162,4.3385784132
H,-0.6194488022,6.0548063603,-0.1392958399
H,-1.9857711691,5.8660804787,-1.2542764526
H,-2.2824840718,6.1452364004,0.4700889951
H,-3.100435011,2.4883880841,-0.0945080605
H,-3.5276394332,3.9134579723,-1.0425157938
H,-3.6890307388,3.9560398808,0.7211760903
F,-1.8160659392,0.3276575286,-1.1358829286
Electronic energy = -1390.2024486
Zero-point electronic energy = -1389.595473
Thermal energy = -1389.566837
Enthalpy = -1389.565893
Free energy = -1389.652553
Free energy (quasiharmonic approximation) = -1389.648081
B3LYP-D3(BJ)/def2-TZVPP SCF = -1390.8854706
B3LYP/def2-TZVPP SCF = -1390.7229321
M062X/def2-TZVPP SCF = -1390.1194905
wB97XD/def2-TZVPP SCF = -1390.2927091

TS-8a C24H31F1N3O2(1+)
C,-0.3737366644,-0.0972967488,0.5341255319
C,-0.9541032081,1.3588255508,0.8258954159
C,0.9063102728,-0.3539168308,1.3268023345
C,0.0928297261,2.4881230623,1.1070776801
N,-1.7867894814,1.8877869477,-0.2620713902
H,-1.6214232646,1.2587666472,1.6847443423
N,-1.3290905976,-1.1390818602,0.883314811
H,-0.1721014736,-0.1646403749,-0.5313485227
C,2.1207747722,-0.7775526913,0.6923626939
C,0.9042866114,-0.2213282045,2.7007213766
C,-0.4608570789,3.8216645044,0.5506015027
H,0.2597663662,2.5487862159,2.1844703382
H,1.056151959,2.2489932648,0.6472915897
C,-2.7719874912,2.8583475377,0.2457126441
C,-1.0391098828,2.4199271108,-1.417936665
C,-2.272467159,-1.7615968193,0.1261302721
H,-1.3585655819,-1.3605214421,1.8720471472
C,2.2769681815,-0.9722012352,-0.6998430854
C,3.2529600921,-1.0147422338,1.5484432414
C,2.0754666411,-0.4942370774,3.446612631
H,0.016343191,0.1025519839,3.2377225615
C,-1.941350071,3.9740789943,0.9684574556
C,-0.4080157496,3.7868025095,-0.9961784733
H,0.1288808074,4.6590343339,0.9348658354
H,-3.4537344193,2.3338246982,0.9166834626
H,-3.3343189799,3.236991731,-0.6090842828
H,-1.7429105642,2.515432742,-2.2457771872
H,-0.2761201698,1.691357435,-1.696695421
C,-3.2916241583,-2.563351113,0.9061267845
C,-2.3855662788,-1.6631225176,-1.2441027804
C,3.4904199206,-1.3699964184,-1.2396119456
H,1.4556864167,-0.828369226,-1.391846864
C,4.4793162427,-1.4207160007,0.9643803148
N,3.2142010278,-0.8726132834,2.9051370582
H,2.0566658334,-0.3853796919,4.5296073882
H,-2.3277087242,4.9556660828,0.6798329528
H,-2.0496947515,3.8805252576,2.0535577098
C,0.9837508608,3.9765651487,-1.604961726
H,-1.0533854289,4.5891487339,-1.3724203199

C,-4.0449100204,-3.5221950461,-0.0176148118
H,-2.7961273673,-3.1246443744,1.7089737561
H,-4.001064647,-1.874648946,1.3837749716
C,-3.4860342615,-2.372403362,-1.9859293765
H,-1.5728959347,-1.2883103872,-1.8531616811
C,4.6086378551,-1.594731389,-0.3939576527
O,3.5210947745,-1.5218057917,-2.5899464429
H,5.3198042353,-1.5916341357,1.6293908185
H,0.9405010251,3.9138835392,-2.6979623267
H,1.694933597,3.2192057825,-1.2566326717
H,1.3817461647,4.9621993915,-1.3418685759
O,-4.5409661201,-2.8208883745,-1.1515361459
H,-4.9118942321,-3.949649845,0.4912300607
H,-3.3875973264,-4.3466438496,-0.3348134412
H,-3.9396055935,-1.7010585912,-2.723650372
H,-3.0549402577,-3.221893582,-2.5479739292
H,5.5605832442,-1.9046877726,-0.8079955633
C,4.7397295056,-1.929051495,-3.2136863464
H,5.0585739548,-2.9169091289,-2.8619184691
H,5.5400757669,-1.2004112823,-3.0409553777
H,4.5201095793,-1.9786011503,-4.2807607891
F,-2.5672216856,0.4703330677,-0.8522220462
Electronic energy = -1347.4753196
Zero-point electronic energy = -1346.949763
Thermal energy = -1346.923708
Enthalpy = -1346.922763
Free energy = -1347.005623
Free energy (quasiharmonic approximation) = -1347.000487
B3LYP-D3(BJ)/def2-TZVPP SCF = -1348.1274796
B3LYP/def2-TZVPP SCF = -1347.9879198
M062X/def2-TZVPP SCF = -1347.4135362
wB97XD/def2-TZVPP SCF = -1347.5586577

TS-8b C24H31F1N3O2(1+)
C,-0.1168747029,-0.6463139071,0.2383976485
C,-1.4975881137,-1.3393952376,-0.1856548566
C,0.9569699352,-0.7358098441,-0.8534985281
C,-2.1148523114,-2.267536331,0.9012003766
N,-2.5975457859,-0.4826573567,-0.6454602631
H,-1.2445379631,-1.9630311684,-1.0424140804
N,-0.1887182455,0.6612892638,0.8793738764
H,0.2265824712,-1.3123233365,1.0356207502
C,2.3371704669,-0.8042772447,-0.47246474
C,0.6576155521,-0.7922494785,-2.20028706
C,-3.6393300258,-2.3494860681,0.6406417894
H,-1.6350181914,-3.248066915,0.8231073572
H,-1.9152888638,-1.8896526903,1.9098488182
C,-3.4396942116,-1.2065289846,-1.6155131879
C,-3.4164982252,0.1126097559,0.4310447047
C,-0.2014417855,1.9302926815,0.374278576
H,-0.2820541647,0.6178739368,1.8878205143
C,2.7973661476,-0.7374344174,0.8723119481
C,3.3000670411,-0.954311652,-1.5262719569
C,1.6890862048,-0.9318388077,-3.1549632591
H,-0.3613824733,-0.689814515,-2.5523355992
C,-4.2855404233,-1.0134518998,1.0764845028
C,-3.8971204075,-2.5166278656,-0.8769739649
H,-4.0769993071,-3.187277038,1.1911036452
H,-2.8507695463,-1.4179201431,-2.5091644021
H,-4.2755911016,-0.5586843779,-1.8834660394
H,-2.7337045638,0.5614758012,1.1531311983
H,-4.0188154434,0.9021329242,-0.020341564
C,-0.4971999121,3.0020025643,1.4017976592
C,-0.0691295795,2.2819250666,-0.9541800012
C,4.1484029734,-0.8255316262,1.1574919074

H,2.089529972,-0.5984366608,1.6773836637
C,4.6812199068,-1.0431041097,-1.1917329564
N,2.9676620955,-1.0190039563,-2.8452092311
H,1.4350043357,-0.9731396089,-4.2126630533
C,-4.4321876674,-0.8191524671,2.587470327
H,-5.2874500739,-0.9633724209,0.6335814132
H,-4.9601263943,-2.685685778,-1.0712732479
H,-3.3463063327,-3.3759817524,-1.2718552894
C,-0.1718173646,4.3922717556,0.8527207087
H,0.0762772303,2.8166784616,2.3194748478
H,-1.5617546369,2.955860917,1.6724000249
C,-0.1905278853,3.7167511268,-1.3897928626
H,0.3511885445,1.6035818408,-1.6794873428
C,5.0989090934,-0.9817086802,0.1098474226
O,4.6876806759,-0.7722363801,2.4017483332
H,5.3887519473,-1.1593483243,-2.0063201945
H,-4.8731722519,0.1585012634,2.8113709553
H,-3.4699901278,-0.8771126349,3.1087071478
H,-5.0905370277,-1.586971815,3.0071863192
O,-0.7794864325,4.5672116845,-0.4204695644
H,-0.5764892143,5.1691268602,1.505367655
H,0.9177564292,4.5329100492,0.7805451206
H,-0.8188653504,3.7840379407,-2.2847709589
H,0.8100321321,4.0941539257,-1.6720879688
H,6.1493238075,-1.0471915128,0.3748740302
C,3.8147909264,-0.6210570371,3.5187916395
H,3.1085092999,-1.457201358,3.5855551824
H,3.2614153824,0.3240931732,3.4637816695
H,4.4574311931,-0.6152892139,4.3996221248
F,-1.7693976563,0.9306336228,-1.2495116847
Electronic energy = -1347.4626432
Zero-point electronic energy = -1346.936395
Thermal energy = -1346.910619
Enthalpy = -1346.909675
Free energy = -1346.991548
Free energy (quasiharmonic approximation) = -1346.986822
B3LYP-D3(BJ)/def2-TZVPP SCF = -1348.1170879
B3LYP/def2-TZVPP SCF = -1347.9741259
M062X/def2-TZVPP SCF = -1347.4023119
wB97XD/def2-TZVPP SCF = -1347.5478134

TS-9a C31H37F1N3O1(1+)
C,1.0572195408,0.3496296288,0.6846182071
C,1.297394634,1.9242324082,0.6700454369
C,2.2329727998,-0.3772665122,1.3353307828
C,2.7763888823,2.4020722592,0.4811181734
N,0.5451280934,2.6240781383,-0.381248686
H,0.906281786,2.308233543,1.6150564268
N,-0.1473061561,-0.0119969623,1.4143378086
H,0.943712272,0.0246948499,-0.3460794842
C,2.9320006472,-1.4409054199,0.6746957814
C,2.617989188,-0.0467860333,2.618972581
C,2.7699590675,3.7231889834,-0.323661288
H,3.2242227339,2.5442041261,1.4669212662
H,3.3691071011,1.6383778239,-0.0304208356
C,0.2849087757,4.0256846932,-0.0071728129
C,1.1204197052,2.5155148521,-1.7363984392
C,-1.4273407428,-0.1997054698,0.9753747339
H,-0.0323821664,-0.0248471444,2.4210181902
C,2.6540971466,-1.8956105251,-0.6355394398
C,3.989348194,-2.0806084813,1.4123270204
C,3.6722323622,-0.7472928053,3.2515313394
H,2.1306290912,0.7553736222,3.1676830023
C,1.6905159073,4.6644606981,0.2582103217
C,2.3929326422,3.4218382477,-1.7952391458

H,3.7541782884,4.1976915252,-0.2704208771
H,-0.3578101179,4.0300031513,0.8744420933
H,-0.2440914278,4.4970300008,-0.8368656568
H,0.3472578903,2.8205220686,-2.4426580378
H,1.3605039665,1.4669790981,-1.9199865363
C,-2.4629180885,-0.2227688561,2.0808708452
C,-1.7914054967,-0.3051196656,-0.3480700717
C,3.376702562,-2.9321486862,-1.2059560653
H,1.8650542947,-1.4591917919,-1.2365058268
C,4.70890708,-3.1370804269,0.7993285059
N,4.3420502356,-1.72757821,2.682658295
H,3.9633145507,-0.4741262822,4.2643529533
H,1.7346688092,5.6485678074,-0.216651902
H,1.840669172,4.8065490255,1.3328780612
C,3.500928333,2.7813290063,-2.6354018793
H,2.1135478031,4.3689853585,-2.2718047411
C,-3.8148844151,-0.7848936161,1.625519993
H,-2.0771996878,-0.8068410646,2.9268659352
H,-2.591463431,0.8045747504,2.4518511678
C,-3.2135942202,-0.4968299124,-0.7943403124
H,-1.0316309725,-0.4510612444,-1.1063737286
C,4.4197834225,-3.5615268341,-0.476821521
O,3.0193014736,-3.2823644363,-2.4699130154
H,5.501481816,-3.6046840781,1.3746810306
H,3.1483091464,2.5810754641,-3.6532885664
H,3.8468826409,1.8321009863,-2.2112695387
H,4.3612032293,3.4550827354,-2.7061107669
C,-4.2522829897,-0.1484787435,0.29125595
H,-4.5640670214,-0.5976221628,2.4020243914
H,-3.7418797764,-1.8736159209,1.5085704837
H,-3.396574479,0.1042395057,-1.6946713861
H,-3.3468678367,-1.5428938066,-1.113334236
H,4.9889088105,-4.3726246828,-0.9150671579
C,3.7101891552,-4.353910772,-3.113354613
H,3.5914750464,-5.2937810738,-2.5622673323
H,4.7762972485,-4.1287511983,-3.23251495
H,3.2492640415,-4.4507442365,-4.096981212
F,-0.9095083361,1.7363034653,-0.4617307095
H,-4.2316450858,0.9416816512,0.4268583426
C,-5.6640080077,-0.5336112909,-0.1185044584
C,-6.6478858949,0.4511343993,-0.2800833338
C,-6.0227518447,-1.8719742023,-0.3448503163
C,-7.9505848388,0.1154611684,-0.6565825287
H,-6.390315783,1.4942428135,-0.1093665219
C,-7.3228777826,-2.212684419,-0.7206462038
H,-5.2822327973,-2.6597131888,-0.2274005171
C,-8.2928387355,-1.2193249296,-0.8785479689
H,-8.6958402577,0.8975004687,-0.7762433521
H,-7.578507824,-3.2553636112,-0.8903423335
H,-9.3050633726,-1.4843396266,-1.1715908138
Electronic energy = -1542.6380991
Zero-point electronic energy = -1542.007080
Thermal energy = -1541.976146
Enthalpy = -1541.975202
Free energy = -1542.070125
Free energy (quasiharmonic approximation) = -1542.062140
B3LYP-D3(BJ)/def2-TZVPP SCF = -1543.3858014
B3LYP/def2-TZVPP SCF = -1543.214604
M062X/def2-TZVPP SCF = -1542.5516344
wB97XD/def2-TZVPP SCF = -1542.7193531

TS-9b C31H37F1N3O1(1+)
C,-1.8116883029,0.2922117732,0.1411292081
C,-2.218663434,1.7503116705,-0.385235766
C,-1.9061281181,-0.7817928284,-0.9498576879

C,-3.2162618319,2.5057904971,0.5413967879
N,-1.1486149427,2.7098726913,-0.6821171003
H,-2.7186378737,1.5779813124,-1.3373915004
N,-0.6202543868,0.187835089,0.9724791047
H,-2.6337205421,0.0734623599,0.8294459194
C,-2.2644978311,-2.1201466278,-0.582661328
C,-1.7066417725,-0.5129593097,-2.2894003351
C,-3.0269650731,4.0235332044,0.3031707305
H,-4.2294485597,2.1785858478,0.2885054923
H,-3.0496157559,2.2530370484,1.5945992976
C,-1.5737904098,3.6419950638,-1.7424765767
C,-0.6224645922,3.4396776233,0.4895212954
C,0.7050357945,0.0060680509,0.6753957231
H,-0.8034022338,0.3252447295,1.9593173145
C,-2.4777859423,-2.5490370276,0.7572251588
C,-2.423410017,-3.0700948179,-1.6467149107
C,-1.8749858747,-1.5313548453,-3.2533812836
H,-1.3807666263,0.4660550793,-2.6195568097
C,-1.7003316989,4.4655234119,0.9642480963
C,-2.9024300861,4.2963992237,-1.2161843328
H,-3.8695667419,4.5842127272,0.7180159
H,-1.723208897,3.0824273186,-2.6671620965
H,-0.7735380792,4.3687673668,-1.8908220026
H,-0.3977297241,2.7019699512,1.2604476601
H,0.3064845539,3.9202859708,0.1795900984
C,1.6153138405,0.203039326,1.8706141418
C,1.2237599803,-0.2365921389,-0.5807663631
C,-2.850976571,-3.8537527327,1.0259992343
H,-2.3245910142,-1.8584763854,1.5745449734
C,-2.8059580021,-4.4043018274,-1.3287695969
N,-2.230163441,-2.7668721276,-2.9602541462
H,-1.7106773555,-1.3031242779,-4.3050379787
C,-1.7327614006,4.5850412892,2.4900056934
H,-1.4335071274,5.4484177439,0.5581135408
H,-2.8755364939,5.3719101696,-1.4128091522
H,-3.7590813773,3.8809138266,-1.7560154155
C,3.0375891545,-0.3205115369,1.6439704812
H,1.1716520648,-0.2801082148,2.7511798157
H,1.6514637192,1.2798253415,2.0991957088
C,2.6992398914,-0.3715186571,-0.8391337802
H,0.5732424049,-0.5465532353,-1.3829990699
C,-3.0175175098,-4.7898582862,-0.0328377174
O,-3.0833059564,-4.3576706567,2.2647315324
H,-2.9236294231,-5.102818021,-2.1509025986
H,-0.7516149953,4.8853727909,2.8741938601
H,-2.0046032481,3.6412578059,2.9764086545
H,-2.4588273089,5.3452921002,2.7965008709
C,3.5899518104,0.1756318328,0.2939481792
H,3.6794173607,0.0120323586,2.4665209868
H,3.0349011376,-1.4176316693,1.6638325141
H,2.9447134489,0.1278704952,-1.7853968351
H,2.9261221446,-1.436084247,-1.0091497579
H,-3.3107993217,-5.8039688355,0.2191957808
C,-2.9671065237,-3.4869187567,3.3876513689
H,-3.6733651937,-2.6509878455,3.3147374115
H,-1.946713127,-3.0970402072,3.483652895
H,-3.2082799038,-4.0936243317,4.2609610632
F,0.2026911025,1.6875215932,-1.0781938963
H,3.4972897175,1.2705603329,0.2852522823
C,5.0578515666,-0.1613945255,0.0908573994
C,5.5148054527,-1.4887705575,0.1044939147
C,5.9965935785,0.8592697962,-0.1107736327
C,6.8668168968,-1.7838036989,-0.0762884477
H,4.8121202631,-2.3040291853,0.2591662282
C,7.3508853334,0.5692087495,-0.2931835831

H,5.6624360392,1.8945144512,-0.1243570953
C,7.7911205461,-0.7551426411,-0.2759923797
H,7.1986422786,-2.8186698378,-0.0605622732
H,8.0596434247,1.3785081081,-0.4479022686
H,8.8437411366,-0.9849462287,-0.4167685994
Electronic energy = -1542.6250355
Zero-point electronic energy = -1541.993449
Thermal energy = -1541.962768
Enthalpy = -1541.961824
Free energy = -1542.055512
Free energy (quasiharmonic approximation) = -1542.048390
B3LYP-D3(BJ)/def2-TZVPP SCF = -1543.3751045
B3LYP/def2-TZVPP SCF = -1543.2005283
M062X/def2-TZVPP SCF = -1542.5388753
wB97XD/def2-TZVPP SCF = -1542.7076448

TS-9c C31H37F1N3O1(1+)
C,0.6926885405,-0.0288591044,0.6332555852
C,0.4089938935,1.5267482121,0.8401304305
C,1.9632046384,-0.4502264437,1.3701673162
C,1.6578497497,2.4574155122,1.0011315087
N,-0.3649347815,2.1278298859,-0.2565632152
H,-0.2257863841,1.6113126491,1.7246641547
N,-0.4096205272,-0.8441303699,1.1082807216
H,0.8085026487,-0.2077243239,-0.4321866443
C,3.1095267131,-0.9644682565,0.6786398787
C,2.022740353,-0.3606665943,2.7461928952
C,1.3490558036,3.8206802867,0.339835332
H,1.8663414471,2.5715656199,2.0672893136
H,2.5432967639,2.0031288953,0.5491481318
C,-1.1190914011,3.3089108311,0.202999442
C,0.407841493,2.411067088,-1.4828664835
C,-1.4850877217,-1.3606813582,0.4382426775
H,-0.4213885132,-0.9890449396,2.1104117932
C,3.2078883052,-1.1032516657,-0.726083208
C,4.2336307703,-1.3590361251,1.4859399329
C,3.1823587678,-0.7799091738,3.4400954709
H,1.1920129768,0.0335604555,3.3265018139
C,-0.0519699855,4.2960089335,0.7857629744
C,1.3275356686,3.6448500918,-1.1983828329
H,2.1059948093,4.5555725151,0.6288916842
H,-1.8440669742,2.979549186,0.94817847
H,-1.6498983792,3.7174363181,-0.6580237701
H,-0.3092871009,2.5910056564,-2.2845751176
H,0.9885255065,1.5210328142,-1.730627525
C,-2.5686870671,-1.916293921,1.3376931999
C,-1.6348432789,-1.3662702621,-0.9279924701
C,4.3527951034,-1.6102137253,-1.3215547261
H,2.3944923703,-0.8256355145,-1.3860589447
C,5.3883798691,-1.8750295679,0.8453419706
N,4.2537063267,-1.2635623031,2.8470506561
H,3.2114048173,-0.704909451,4.5257270117
H,-0.2563765634,5.3048484381,0.4165566601
H,-0.1219295125,4.3196613957,1.8774933827
C,2.7004090306,3.4790032674,-1.8558617849
H,0.8499548508,4.5309400282,-1.6322452742
C,-3.4621697058,-2.9250154049,0.6089873143
H,-2.1094787482,-2.3899993229,2.2151056446
H,-3.1726621562,-1.0801413837,1.7177286922
C,-2.8273318637,-1.9591950338,-1.6302050113
H,-0.7959596545,-1.1133390075,-1.5652794863
C,5.4589686151,-2.0023034712,-0.5225247004
O,4.3303789893,-1.6973697014,-2.677651529
H,6.2227409247,-2.1679318444,1.4745723762
H,2.5968180344,3.3539642562,-2.9392650281

H,3.2411698695,2.6070389158,-1.4714703124
H,3.315609909,4.3673754383,-1.6789246921
C,-4.0123054423,-2.3565356388,-0.7206344191
H,-4.2879003723,-3.2228843802,1.2638063889
H,-2.8810577112,-3.8303215291,0.3906164311
H,-3.167290457,-1.2704752616,-2.4151190341
H,-2.4843239405,-2.8568366965,-2.1679713248
H,6.3571689452,-2.3999520855,-0.9795035574
C,5.4727554179,-2.2200563339,-3.3572958418
H,5.6785446704,-3.2534541795,-3.0558799942
H,6.3603069957,-1.6011908998,-3.1821941526
H,5.2187624885,-2.1963380755,-4.417598244
F,-1.4302300759,0.890033125,-0.6905063062
H,-4.5380029857,-3.1776046218,-1.222568998
C,-5.051055154,-1.2640234415,-0.4864373923
C,-6.3829565024,-1.6450473544,-0.2548452027
C,-4.7451502348,0.1051158404,-0.4718616098
C,-7.3777343965,-0.6974867449,-0.0141372945
H,-6.6434868408,-2.7015451324,-0.2712956065
C,-5.7409109922,1.0574395936,-0.2322652821
H,-3.7264189084,0.4374919649,-0.6445199532
C,-7.0591641881,0.6628707681,-0.0018819574
H,-8.4014605621,-1.0206496899,0.1559788609
H,-5.482130888,2.1134824435,-0.2291396725
H,-7.8312161056,1.405489909,0.1806104826
Electronic energy = -1542.6377565
Zero-point electronic energy = -1542.005799
Thermal energy = -1541.975238
Enthalpy = -1541.974294
Free energy = -1542.067143
Free energy (quasiharmonic approximation) = -1542.060343
B3LYP-D3(BJ)/def2-TZVPP SCF = -1543.3860355
B3LYP/def2-TZVPP SCF = -1543.2110671
M062X/def2-TZVPP SCF = -1542.5527375
wB97XD/def2-TZVPP SCF = -1542.7200652

TS-9d C31H37F1N3O1(1+)
C,-1.1542682872,0.9912839597,0.2433023383
C,-0.3796193873,2.3316434902,-0.1742959835
C,-2.0755275514,0.4668391629,-0.8654911333
C,-0.4315607726,3.4643111682,0.89457354
N,1.0292302847,2.2233395269,-0.567158413
H,-0.8954486046,2.6963441239,-1.061109245
N,-0.3802524105,-0.0473030499,0.907824415
H,-1.8277640033,1.3611017979,1.0226640806
C,-3.2696056291,-0.2401101803,-0.505078383
C,-1.8358321555,0.6824799614,-2.2081003766
C,0.8105866921,4.3641619416,0.69100432
H,-1.3629288198,4.0203308732,0.7513590539
H,-0.4519460881,3.0560878013,1.9105550522
C,1.3809427481,3.2805541525,-1.531661205
C,1.9867912821,2.1809409607,0.5561026904
C,0.3328793861,-1.1197630152,0.4368621389
H,-0.3335671544,0.0622617444,1.9137852566
C,-3.6357876073,-0.5591699784,0.8327844449
C,-4.1410472722,-0.6381918781,-1.5741115275
C,-2.7583767236,0.2342880826,-3.1788399568
H,-0.9240625295,1.1604204635,-2.5448062635
C,2.0585547458,3.6049208743,1.1989313741
C,1.0112457446,4.6324194656,-0.8206510373
H,0.6900616663,5.3097430675,1.2276395462
H,0.8141909288,3.1247990197,-2.4508009066
H,2.4463265491,3.1930176147,-1.7484954367
H,1.6264776162,1.4327188517,1.2625212738
H,2.9473414729,1.8552018779,0.1542075734

C,1.1379111356,-1.8236864485,1.5090263999
C,0.4171306376,-1.5222621958,-0.8797477881
C,-4.8172202701,-1.2295089339,1.0962795369
H,-2.9783930397,-0.2964360275,1.6500203382
C,-5.3491226841,-1.3234890151,-1.2610709211
N,-3.8795070954,-0.3955515496,-2.8883995102
H,-2.5521939546,0.4119902132,-4.2328895903
C,2.2086245891,3.5299640471,2.7202145602
H,2.9454156443,4.1103597161,0.7989234361
H,1.8172009662,5.3540274371,-0.9812833769
H,0.1002062401,5.0457488419,-1.264564567
C,1.530441366,-3.2481668698,1.1065723977
H,0.5668625405,-1.8441960743,2.4461706509
H,2.0428146179,-1.2309120953,1.7110524254
C,1.2405182127,-2.7011822949,-1.3264062257
H,-0.2711096874,-1.129623365,-1.6111561682
C,-5.683413133,-1.6121800818,0.0340261608
O,-5.2548083219,-1.5804222941,2.3322166385
H,-5.992588995,-1.6096838014,-2.0867566093
H,3.1057474193,2.9634241305,2.993014035
H,1.350957268,3.0440864903,3.198739083
H,2.3071713942,4.5357006265,3.1420463441
C,2.2141285069,-3.2820869479,-0.2800848236
H,2.1916765464,-3.6724890228,1.8691723365
H,0.6313523897,-3.87652902,1.0720582262
H,1.778346235,-2.4366835421,-2.2462055665
H,0.5391688118,-3.4952568108,-1.6271023864
H,-6.6011847986,-2.1355136367,0.2824461777
C,-4.4513851357,-1.2455420976,3.4612359632
H,-4.315029847,-0.1604736902,3.5434306637
H,-3.4717754144,-1.7359012722,3.4093219733
H,-4.9956402323,-1.6113013092,4.3323970446
F,1.1470957324,0.6063848289,-1.1926824606
H,2.3657383685,-4.33804254,-0.5346906668
C,3.6000524547,-2.6433617049,-0.2487712348
C,3.8626862884,-1.3389908723,-0.6928717935
C,4.6713806139,-3.3962419971,0.2599987206
C,5.1556908264,-0.8086298911,-0.6268253721
H,3.0598407856,-0.7246786992,-1.0872150354
C,5.9604760039,-2.8688150729,0.3295260775
H,4.4920129321,-4.4150351335,0.5979925367
C,6.2085610222,-1.5675770995,-0.115449636
H,5.3385824533,0.2026019627,-0.9826295373
H,6.7719617583,-3.476039837,0.7220595547
H,7.2124047273,-1.1541189305,-0.0691052418
Electronic energy = -1542.6248817
Zero-point electronic energy = -1541.993026
Thermal energy = -1541.962463
Enthalpy = -1541.961519
Free energy = -1542.055223
Free energy (quasiharmonic approximation) = -1542.047429
B3LYP-D3(BJ)/def2-TZVPP SCF = -1543.3763545
B3LYP/def2-TZVPP SCF = -1543.1972632
M062X/def2-TZVPP SCF = -1542.5401865
wB97XD/def2-TZVPP SCF = -1542.7091144

TS-10a C29H37F1N3O2(1+)
N,-0.5943335671,-0.1022716016,1.3741744603
N,-0.075037279,2.5483699822,-0.4637306313
N,3.9971984823,-1.3254875933,2.8619135954
C,0.6020823233,0.353613332,0.6824230981
C,0.6869020288,1.9462313307,0.6389572447
C,1.8129519513,-0.2396817086,1.4003236859
C,2.1187751889,2.5697286332,0.517887981
C,2.6587591494,-1.2227927231,0.7880500742

C,2.0935553386,0.1402430549,2.6971778231
C,2.0213029285,3.8672491411,-0.3189231742
C,-0.4942161141,3.9220119618,-0.1352745418
C,0.5760183648,2.4736020564,-1.7861001468
C,2.4945435787,-1.7225555721,-0.5250551506
C,3.7479642826,-1.727611143,1.5818542284
C,3.1902346795,-0.4278798927,3.3874068956
C,0.8240397777,4.7072371548,0.1813489748
C,1.7565769951,3.4992239759,-1.7991662656
C,3.3580490254,-2.6739022691,-1.046320257
C,4.614120113,-2.6976548579,1.0173780491
C,2.9658769141,2.9548951122,-2.5647530657
C,4.4349979965,-3.1667687184,-0.2632178743
C,3.9391796046,-4.071003085,-2.9118415191
O,3.0997596536,-3.0799307393,-2.3175637427
F,-1.4382745656,1.5109923467,-0.5858656178
H,0.5635032571,-0.0045539654,-0.3424075779
H,0.211732653,2.3057456448,1.5543328276
H,2.8142376327,1.8630970366,0.05669446
H,2.4936360384,2.7747762662,1.5230028938
H,1.4888967614,0.8823748069,3.2126125781
H,2.9490515111,4.439683058,-0.228032761
H,-1.1753554754,3.8773657201,0.7156622766
H,-1.0278470621,4.3214241517,-0.9991221785
H,0.9233856184,1.4503188523,-1.9369321562
H,-0.1845144686,2.693080211,-2.5363744242
H,1.6860658558,-1.392380879,-1.166466083
H,3.3982124722,-0.1157975303,4.4094029289
H,0.9013263718,4.8906066027,1.2574629286
H,0.7940253238,5.6787156724,-0.3198521053
H,1.4128929516,4.4042097017,-2.3137950052
H,5.4288857927,-3.0626753481,1.6344981028
H,2.6911114355,2.7067144932,-3.5959888349
H,3.7609610693,3.706919726,-2.6031473213
H,3.3769634171,2.0493474491,-2.1044427652
H,5.1150036522,-3.909054509,-0.6635634073
H,3.5357475292,-4.2352063189,-3.9116364527
H,3.9082661349,-5.0105994442,-2.348525984
H,4.9752570731,-3.722311931,-2.9908196813
H,-0.5276646472,-0.0508437568,2.3842051355
C,-2.9226271003,-0.4049988906,1.9474468223
C,-2.1298067006,-0.5879827345,-0.4408793913
C,-3.5148288947,-0.852654441,-0.9512705916
C,-4.642220206,-0.5448894868,0.0638957956
C,-4.2205749994,-1.0604102264,1.4648058583
C,-3.7691421145,-2.3225755511,-1.4063600314
C,-5.3010419962,-2.4348595537,-1.4488658919
C,-5.0429246008,0.9361815332,0.0981239947
C,-1.8373649682,-0.3939670018,0.8921585276
C,-5.8053776336,-1.4317942201,-0.412207621
O,-6.9499342878,-1.3386781954,-0.0138194908
H,-2.5568990335,-0.929075129,2.8401368245
H,-1.3259214455,-0.7217149652,-1.1555028401
H,-4.0789402436,-2.1477540506,1.4348351259
H,-5.0247813875,-0.8683145969,2.182345621
H,-3.3526630628,-3.0222166675,-0.6733058751
H,-3.2952766821,-2.5372727395,-2.3683174758
H,-5.6971557183,-3.4363083444,-1.2559191239
H,-5.6964427758,-2.1171716103,-2.4242404171
H,-4.1791508822,1.5680130518,0.3291270133
H,-5.8236261803,1.1117090756,0.8449611261
H,-5.4307986009,1.2540280095,-0.8762130524
H,-3.6681460433,-0.2166614319,-1.8358008636
H,-3.1075221909,0.6321642788,2.2595844392
Electronic energy = -1541.649723

Zero-point electronic energy = -1541.026911
Thermal energy = -1540.995925
Enthalpy = -1540.994981
Free energy = -1541.088991
Free energy (quasiharmonic approximation) = -1541.081741
B3LYP-D3(BJ)/def2-TZVPP SCF = -1542.4008626
B3LYP/def2-TZVPP SCF = -1542.2300859
M062X/def2-TZVPP SCF = -1541.5753647
wB97XD/def2-TZVPP SCF = -1541.7525537

TS-10b C29H37F1N3O2(1+)
N,-0.6517237921,-0.4382862248,1.0559784701
N,-0.2514713416,2.5167056671,-0.2750684379
N,3.8569574508,-1.4596421288,2.8884810652
C,0.5490184313,0.2403414049,0.5944063305
C,0.4622124491,1.8189004854,0.8020450952
C,1.7357925213,-0.3477965504,1.3556391392
C,1.824432481,2.5805233646,0.932285341
C,2.7287990189,-1.1574425849,0.7116990963
C,1.8474841033,-0.1431182195,2.7161092538
C,1.6684440745,3.9815413108,0.2944776641
C,-0.8440003233,3.7763633037,0.207698676
C,0.5270468992,2.7137994069,-1.5133172615
C,2.7432081888,-1.4684803014,-0.6681653059
C,3.7770110265,-1.6848777465,1.5447946092
C,2.919141202,-0.717891785,3.439495902
C,0.346731582,4.6172659898,0.7820256661
C,1.5847951347,3.8331206166,-1.2444232207
C,3.7418432136,-2.25833874,-1.2168566031
C,4.7846434245,-2.4860913007,0.951090506
C,2.9141220516,3.5316800764,-1.9417330026
C,4.7792582218,-2.7716904593,-0.3944379498
C,4.6383105341,-3.313442576,-3.1788705706
O,3.6511976316,-2.4928047095,-2.5527313833
F,-1.4755693672,1.387532662,-0.7048293413
H,0.6596508367,0.053360238,-0.4703251788
H,-0.1347845759,1.9820692901,1.7024017435
H,2.6294457901,2.0231428553,0.4450322737
H,2.0832268595,2.654385405,1.9906255055
H,1.1265794064,0.4638295724,3.2584309723
H,2.5172288517,4.6136658819,0.5716707796
H,-1.5951119385,3.5339186292,0.9608630864
H,-1.3331376017,4.2596834455,-0.6392607522
H,0.9984921716,1.7648494918,-1.7751204064
H,-0.1781711377,2.9761664218,-2.3030285884
H,1.9726047623,-1.1130510491,-1.3420973218
H,2.9931100651,-0.54601786,4.5119301382
H,0.3040812977,4.629626053,1.8755159875
H,0.260101333,5.6507726191,0.4348279191
H,1.1956342196,4.7731801399,-1.6533819142
H,5.5663217513,-2.8711210513,1.5980941123
H,2.7687908776,3.4187091578,-3.0218075815
H,3.6207418939,4.3531762279,-1.7837352795
H,3.3761215434,2.6100595994,-1.5705981945
H,5.5651118099,-3.3866482072,-0.8164861913
H,4.3541108105,-3.3629330764,-4.230577316
H,4.6438177798,-4.3242534782,-2.7551961301
H,5.6380316737,-2.872464493,-3.0927357802
H,-0.6838671848,-0.5829640263,2.0582003297
C,-1.9303124988,-0.7470884192,-0.9842947649
C,-2.9523336382,-1.1444245195,1.2749016908
C,-4.0405105582,-2.0130543378,0.6124605705
C,-4.386278006,-1.5298469653,-0.8175459887
C,-3.1834358539,-1.1558592519,-1.6997888424
C,-5.3728795745,-1.8541494457,1.3935397158

C,-6.0120630378,-0.5711691898,0.8189526793
C,-5.241522936,-2.5832636016,-1.5714369546
C,-1.7865327463,-0.7884435126,0.3833809744
C,-5.338254289,-0.3512587814,-0.5384245446
O,-5.531223375,0.5904756728,-1.281541873
H,-1.0580522666,-0.6261566679,-1.6142887514
H,-3.3904282439,-0.2002108471,1.6316469346
H,-2.5892082523,-1.6577243353,2.1745953014
H,-3.4971211839,-0.3541080159,-2.3834564065
H,-2.929247196,-2.0055734097,-2.3504410384
H,-5.2031969407,-1.7900335554,2.4728231401
H,-6.0193288512,-2.7197211825,1.2226108469
H,-5.8242593081,0.3124411991,1.4407334691
H,-7.0984849367,-0.6332389511,0.6948475925
H,-5.4856984486,-2.2182373471,-2.5745886157
H,-6.1823957665,-2.8103694979,-1.0608965833
H,-4.6763348486,-3.5167690952,-1.6696828132
H,-3.7019833554,-3.0547486902,0.5966083106
Electronic energy = -1541.6451367
Zero-point electronic energy = -1541.022077
Thermal energy = -1540.991252
Enthalpy = -1540.990308
Free energy = -1541.083831
Free energy (quasiharmonic approximation) = -1541.076755
B3LYP-D3(BJ)/def2-TZVPP SCF = -1542.3968352
B3LYP/def2-TZVPP SCF = -1542.2266308
M062X/def2-TZVPP SCF = -1541.571236
wB97XD/def2-TZVPP SCF = -1541.7481931

TS-10c C29H37F1N3O2(1+)
C,-4.5969364492,0.0941643777,0.4069486968
C,-5.2474478173,-2.0045422246,-0.9261532661
C,-3.736110279,-2.282640138,-0.99775237
C,-2.9716905115,-1.9022882672,0.3265899802
C,-3.8181550239,-0.9474566422,1.2194377494
C,-3.0346486193,-1.517894732,-2.1581086311
C,-1.7772142432,-0.9676350332,-1.5572062366
C,-2.6033870815,-3.162393791,1.1358956184
C,-5.5583758486,-0.5561978459,-0.5777723111
C,-1.7232645296,-1.1908585076,-0.2003448579
O,-6.5093771452,0.0426405955,-1.0508185301
H,-5.1646887142,0.7751640874,1.0499048948
H,-3.8969647228,0.7143982816,-0.1707021486
H,-5.7463520075,-2.2595996261,-1.8662043249
H,-5.7046865984,-2.6312634753,-0.145355961
H,-3.1715974222,-0.4477255047,1.950342712
H,-4.5207186153,-1.5541998803,1.8040541154
H,-3.666825348,-0.7117861893,-2.5597055879
H,-2.8227575733,-2.1772021985,-3.0098754238
H,-0.9516127922,-0.6216437784,-2.1636748509
H,-2.1287514152,-2.9163618722,2.0939199047
H,-1.923992314,-3.8116307432,0.5738049253
H,-3.5093553129,-3.7336987103,1.3660689477
H,-3.6002750786,-3.3556523524,-1.1658260461
N,-0.7556787684,-0.8160379055,0.671689915
N,-0.6298318465,2.3383812891,-0.1429767365
N,3.6865952899,-1.5852207555,2.7990933314
C,0.3841684065,0.0650596652,0.4633756111
C,0.0585827139,1.5622723447,0.8977306017
C,1.5676959042,-0.4973189311,1.2471295786
C,1.2814772898,2.4515380796,1.307489152
C,2.7129611745,-1.058677204,0.5909907862
C,1.5349185311,-0.5165386615,2.6268839179
C,1.0005585862,3.9093549391,0.8726814273
C,-1.4374203105,3.4214505594,0.4452270695

C,0.2390620103,2.8270174131,-1.2314236431
C,2.8860054228,-1.1263613761,-0.8115404781
C,3.7515128505,-1.5863913528,1.435930893
C,2.6118061179,-1.0709103832,3.3587405216
C,-0.4388588913,4.2928333716,1.2823499197
C,1.095846423,4.0083575062,-0.6691709964
C,4.0283761535,-1.6799032037,-1.3693044959
C,4.907549881,-2.1430793973,0.8330947047
C,2.5177720217,3.9931532069,-1.2372121821
C,5.0549791457,-2.1934752768,-0.5335792312
C,5.2260477577,-2.254888732,-3.3706026669
O,4.082600318,-1.6904898665,-2.7272146274
F,-1.638748522,1.1601921757,-0.8958102783
H,0.6125456515,0.0716988819,-0.599034694
H,-0.6448139062,1.5010521278,1.7315113117
H,2.2016921784,2.0803263715,0.8478298489
H,1.4141416795,2.3802521805,2.3891523511
H,0.6950833312,-0.1045269377,3.180733389
H,1.7206661219,4.5843089278,1.3444163553
H,-2.221203787,2.9719312838,1.0562962176
H,-1.8982760886,3.974851008,-0.3743393051
H,0.8629274713,1.996567488,-1.5648698995
H,-0.4079340605,3.1263209752,-2.0568507789
H,2.133395501,-0.7599155582,-1.5001188293
H,2.5712729046,-1.077231475,4.4465731741
H,-0.5959425697,4.1206511601,2.3515525643
H,-0.6310105616,5.3509774328,1.0839830481
H,0.6210234484,4.9478396193,-0.97595193
H,5.6781052703,-2.5328402743,1.4904788987
H,2.498518182,4.0463559921,-2.3313266845
H,3.0811035517,4.857579012,-0.8703831879
H,3.0670450974,3.0869762527,-0.9581902389
H,5.9513292937,-2.6262869981,-0.9614564737
H,5.0405187831,-2.1521182608,-4.44031256
H,5.341011559,-3.3160915775,-3.1219085444
H,6.1414361684,-1.7128755776,-3.1068770776
H,-0.8630574172,-1.143815389,1.6242639533
Electronic energy = -1541.6465803
Zero-point electronic energy = -1541.023014
Thermal energy = -1540.992522
Enthalpy = -1540.991577
Free energy = -1541.083753
Free energy (quasiharmonic approximation) = -1541.077279
B3LYP-D3(BJ)/def2-TZVPP SCF = -1542.3992309
B3LYP/def2-TZVPP SCF = -1542.2257422
M062X/def2-TZVPP SCF = -1541.5729167
wB97XD/def2-TZVPP SCF = -1541.7513436

TS-11a C14H24F1N2(1+)
C,2.0908546037,0.7466550065,-0.2643972464
C,2.188108667,-0.4385709439,-0.9570328454
C,3.3345912935,-1.3968994541,-0.7793534183
C,4.1400486862,-1.1404365297,0.5006522457
C,4.4290082023,0.3561267376,0.6553630877
C,3.1200736876,1.1469320565,0.7739767921
H,2.9523493911,-2.4260757619,-0.7953581216
H,1.531001876,-0.6223902375,-1.7986719275
H,3.5691809908,-1.4921221169,1.3708713991
H,5.0727978958,-1.7147435214,0.476348334
H,5.048283814,0.5476629151,1.5384356421
H,4.9963428196,0.7113783096,-0.2153785894
H,2.6792588163,0.9912714691,1.7699776505
H,3.3149445308,2.2247786708,0.6925315362
H,3.9986544685,-1.3201385883,-1.6561909798
N,1.0635260323,1.6395599122,-0.405293232

C,-0.243792283,1.451092719,-0.9886504599
C,-1.3302732854,0.946723994,0.0236706688
H,-0.1860875858,0.7918905562,-1.8560132593
H,-1.0493001545,1.3231765854,1.0107906588
C,-2.7828131362,1.3995520672,-0.3172794943
N,-1.3954409566,-0.5133160552,0.1610170366
C,-3.7557384968,0.2711993016,0.096747472
H,-2.8777264721,1.6027870956,-1.3902973505
H,-2.9884241953,2.3332691559,0.2142137408
C,-1.97561247,-0.9027533061,1.4584452643
C,-2.0458198919,-1.2147193744,-0.964820051
C,-3.3933518733,-0.234941074,1.5122061961
H,-4.7872637136,0.6328692392,0.0774389778
C,-3.5706872853,-0.893558666,-0.8950557677
H,-1.310503261,-0.5490920832,2.2473744853
H,-2.0195390521,-1.9925817856,1.4914369632
H,-1.5901829475,-0.8615707125,-1.8896039898
H,-1.8254849542,-2.2769335082,-0.8542706248
H,-3.3914624972,0.5914811929,2.2295436796
H,-4.1246898899,-0.9713778661,1.8569944779
H,-4.1292661072,-1.7747186097,-0.565529151
H,1.1493725578,2.4794361902,0.1544033663
F,0.2444311729,-0.9359051808,0.065345163
H,-0.5877522421,2.4260503532,-1.345243441
H,-3.9303997553,-0.6240301524,-1.8922578881
Electronic energy = -757.0249822
Zero-point electronic energy = -756.651347
Thermal energy = -756.636522
Enthalpy = -756.635578
Free energy = -756.692486
Free energy (quasiharmonic approximation) = -756.691137
B3LYP-D3(BJ)/def2-TZVPP SCF = -757.3968196
B3LYP/def2-TZVPP SCF = -757.3147222
M062X/def2-TZVPP SCF = -756.9615449
wB97XD/def2-TZVPP SCF = -757.0820244

TS-11b C14H24F1N2(1+)
C,1.9223423539,-0.6955432164,-0.3465713084
C,2.2567270684,0.4739849694,-1.0009387762
C,3.4724036477,1.2844668034,-0.6430032911
C,4.0507327346,0.9323641896,0.7334662235
C,4.1338232117,-0.5883496043,0.900716548
C,2.735442955,-1.2147017148,0.8201209376
H,4.2395341907,1.1268964951,-1.4190204631
H,1.7709839678,0.728438314,-1.9353475266
H,2.8079726056,-2.3085764082,0.7552715692
H,2.1810893475,-1.0001398638,1.7467745017
H,3.2220192587,2.3518718384,-0.6967110523
N,0.8010759541,-1.4264402668,-0.6250186858
C,-0.2416829031,-1.0990309904,-1.561416932
C,-1.5558356291,-0.3806634906,-1.0511236976
H,-0.583875713,-2.0207441323,-2.0412402501
H,-1.9178158087,0.1543530773,-1.9326794291
C,-2.7043224875,-1.2983913123,-0.5418821204
N,-1.3721101026,0.6508053315,-0.0242645862
C,-3.5389864534,-0.4808947103,0.4740270536
H,-2.3142566764,-2.2052524779,-0.0643478282
H,-3.2992135978,-1.6115768092,-1.4052193381
C,-2.3962942861,1.6999692251,-0.1489669473
C,-1.2908972787,0.137333373,1.3579677866
C,-3.7759696065,0.951252552,-0.0657652668
H,-4.4957969425,-0.9723830094,0.6695875315
C,-2.7049014082,-0.3760899134,1.7633799927
H,-2.2548946986,2.2150256134,-1.1008826444
H,-2.2524169166,2.408334151,0.6687915232

H,-0.54306354,-0.6553722912,1.3637077997
H,-0.9425040755,0.9597082588,1.9837532941
H,-4.2414987351,0.9189034232,-1.0558593596
H,-4.445444894,1.5056516152,0.5981774794
H,-3.1702578194,0.3157799494,2.4721805206
H,0.7139190072,-2.311435694,-0.1401295976
F,0.2608561352,1.1735477191,-0.2976156603
H,-2.6153147675,-1.3484675738,2.2567100828
H,0.1771658155,-0.4627787289,-2.33924563
H,5.0392327527,1.3898551669,0.8505957856
H,3.4082846297,1.3504802086,1.5203557667
H,4.7723985478,-1.0101499986,0.1132029449
H,4.5924041569,-0.8540080677,1.85924405
Electronic energy = -757.0166566
Zero-point electronic energy = -756.643346
Thermal energy = -756.628435
Enthalpy = -756.627491
Free energy = -756.684660
Free energy (quasiharmonic approximation) = -756.683237
B3LYP-D3(BJ)/def2-TZVPP SCF = -757.3899414
B3LYP/def2-TZVPP SCF = -757.306608
M062X/def2-TZVPP SCF = -756.9523009
wB97XD/def2-TZVPP SCF = -757.0742812

N-Fluorinated enamine formed from 1 and N-fluorinated IV C23H29F1N3(1+)
C,-0.1293522167,-0.0851100285,-0.0061916738
C,-0.1837199718,-0.2250343474,1.3292221916
C,1.020103588,-0.0770082966,2.2312918391
C,2.1988453163,0.6132093451,1.5308385842
C,2.403158157,0.0346705705,0.1270526812
C,1.1545105775,0.2549654866,-0.7375080213
H,1.3375460994,-1.0671469656,2.5977028563
H,-1.1227466317,-0.459692322,1.8228013631
H,3.1106778143,0.5054927125,2.1301497315
H,1.9946275852,1.689730684,1.4493837621
H,3.2732507233,0.4886603447,-0.3612946966
H,2.6068175377,-1.0421687834,0.2038266846
H,1.2160117999,-0.3478805611,-1.6536917851
H,1.1076443537,1.3050768987,-1.0665749365
H,0.7353611047,0.4885437968,3.1289602104
N,-1.2143899589,-0.2735087011,-0.8958220864
C,-2.5970736615,-0.3024799234,-0.4283898801
C,-3.3537313252,-1.0019451834,-1.5988918311
H,-2.6149361684,-0.9794221267,0.4265404036
C,-3.1347413805,1.0756807531,-0.0183373072
H,-3.2750973351,-0.3729601878,-2.4882148269
C,-2.8210060457,-2.4440807736,-1.8752244228
N,-4.8657383887,-1.1587522139,-1.4251222813
C,-3.7197166456,1.3307056802,1.2639738164
C,-3.0453621953,2.1293039547,-0.9047632239
C,-3.9767356096,-3.4580691625,-1.9391926564
H,-2.1178714455,-2.714763656,-1.0838632776
H,-2.2627691879,-2.4395869183,-2.814160459
C,-5.4981983278,-1.6216395686,-2.7207838275
C,-5.2686310518,-2.0599259555,-0.2859416446
C,-3.8626034025,0.3653069345,2.3015644738
C,-4.1936183216,2.6638765719,1.5209809425
C,-3.5389473002,3.4038229592,-0.5482800254
H,-2.6025638899,2.0062272421,-1.8892580262
C,-4.9597167668,-3.0364802829,-3.0450894106
H,-3.5773108682,-4.452167688,-2.1542595231
C,-4.708353772,-3.4748431679,-0.5835545959
H,-5.2395796724,-0.8682994231,-3.4647732891
H,-6.5727615643,-1.5929186941,-2.5408746067
H,-4.8815022769,-1.6071834822,0.6247698172

H,-6.3577030145,-2.0205070313,-0.258370494
C,-4.4465409998,0.6909653357,3.5064426611
H,-3.4913716281,-0.6453416389,2.1684640688
C,-4.7916059391,2.9663903606,2.7737421757
N,-4.0999896062,3.6783134795,0.6117062288
H,-3.4658544887,4.2225746022,-1.2625470001
H,-4.4591034868,-3.023378318,-4.0164613591
H,-5.7945112159,-3.738998199,-3.1089312916
H,-5.531850587,-4.1933154792,-0.5988265744
C,-4.9202986651,2.0023640414,3.7463335385
H,-5.1371094353,3.9835813021,2.9291638197
H,-5.377799106,2.2442189847,4.7010333992
H,-1.1000610553,0.2715870279,-1.7455191478
H,-4.5371078831,-0.06448053,4.2812708179
H,-4.023252441,-3.772283893,0.2144439019
F,-5.4363579716,0.1026960365,-1.1664567359
Electronic energy = -1157.7607612
Zero-point electronic energy = -1157.269138
Thermal energy = -1157.246642
Enthalpy = -1157.245698
Free energy = -1157.321569
Free energy (quasiharmonic approximation) = -1157.316485
B3LYP-D3(BJ)/def2-TZVPP SCF = -1158.3218948
B3LYP/def2-TZVPP SCF = -1158.1910541
M062X/def2-TZVPP SCF = -1157.7093566
wB97XD/def2-TZVPP SCF = -1157.8388047

TS-12a C23H29F1N3(1+)
N,1.3224438466,1.860564596,0.3493998729
C,0.5070517325,1.4601779897,-0.806662768
C,2.4442337696,2.7121640568,-0.1052522815
C,-0.4191928023,2.677012417,-1.0941141788
C,-0.1973719941,0.0363913318,-0.8580281198
H,1.2245004477,1.3834243099,-1.6261678152
C,0.6052810555,2.5047587852,1.4769424384
C,1.7887822012,3.9053417927,-0.8833227873
H,3.0988321923,2.104193582,-0.7308136615
H,2.994388417,3.0350421084,0.7795542717
C,0.2818861564,3.9440564859,-0.5400149817
H,-0.5779638825,2.7376529824,-2.1748172704
H,-1.3992944337,2.5489534374,-0.6202262088
N,0.7389198316,-1.0231747775,-1.2490298749
H,-0.7618818145,0.1878794831,-1.7774224982
C,0.1531887693,3.9176511833,0.9930045563
H,-0.246574956,1.8864825946,1.7387019614
H,1.2965444399,2.5383487625,2.3198605391
H,2.2747662037,4.8370594016,-0.5811432284
H,1.9427262675,3.7858398015,-1.9601901613
H,-0.1798626666,4.8447872603,-0.952530666
C,1.7550009865,-1.6997213783,-0.609885039
H,0.8512188872,-1.0425386621,-2.2558315301
H,-0.8804375067,4.0855449436,1.3086004584
H,0.7735938008,4.6955227387,1.4478248978
C,2.8315445937,-2.1757855605,-1.5701868361
C,1.863089064,-1.923163401,0.7406423907
C,3.7715563112,-3.2234183377,-0.9621691837
H,2.355388137,-2.5745361011,-2.4763156979
H,3.4109727914,-1.2970044429,-1.8923152343
C,3.0242903895,-2.6512036642,1.3640866265
H,1.0145485762,-1.744389078,1.3818844152
C,4.2326029609,-2.7829356678,0.4301082865
H,4.625338887,-3.3742993823,-1.6317949906
H,3.2497911943,-4.1867828361,-0.8870669629
H,3.3078634157,-2.1440822228,2.2957308828
H,2.6834185531,-3.6534311014,1.6716734681

H,4.9515053718,-3.4971847169,0.8464564178
H,4.7483622698,-1.8157893899,0.3542582962
F,1.9460538568,0.372599741,0.8345323469
C,-1.2455703613,-0.3578344593,0.1883646856
C,-2.5611506764,-0.7485201248,-0.2480144337
C,-0.9986160172,-0.3827970347,1.5460999322
C,-2.9845109254,-0.8336290653,-1.6055099449
C,-3.5232051703,-1.0913166419,0.7662839228
C,-2.017489362,-0.748337585,2.4567396721
H,-0.0226603788,-0.1375797278,1.9402600137
C,-4.2683245588,-1.2100121607,-1.9348618186
H,-2.2963470146,-0.621436824,-2.4158599351
C,-4.8408249439,-1.4680635669,0.3936301817
H,-1.7959450598,-0.7549224417,3.5228992486
C,-5.2111479566,-1.5252975285,-0.9291357349
H,-4.5571199746,-1.2682432228,-2.9801185971
H,-5.5332620983,-1.7120015699,1.192977226
H,-6.2200088119,-1.8168418594,-1.2055778696
N,-3.2391720116,-1.0814052522,2.102383301
Electronic energy = -1157.7317632
Zero-point electronic energy = -1157.241351
Thermal energy = -1157.219411
Enthalpy = -1157.218467
Free energy = -1157.291931
Free energy (quasiharmonic approximation) = -1157.288381
B3LYP-D3(BJ)/def2-TZVPP SCF = -1158.2919855
B3LYP/def2-TZVPP SCF = -1158.1603306
M062X/def2-TZVPP SCF = -1157.6559676
wB97XD/def2-TZVPP SCF = -1157.7921972

TS-12b C23H29F1N3(1+)
C,2.0758123291,-1.4975447606,0.3361906015
C,2.2477338233,-1.7926297533,-1.0025034091
C,3.4908046016,-2.4509654476,-1.535616107
C,4.671771654,-2.398541123,-0.5587365323
C,4.2093697414,-2.778821765,0.8510612541
C,3.1563807703,-1.7843042986,1.3565553038
H,3.2532627023,-3.5002702245,-1.7759952272
H,1.4021433432,-1.758849711,-1.6793123166
H,2.6919813468,-2.1522002528,2.281062302
H,3.6432145519,-0.831777061,1.618161866
H,3.7581136086,-1.9879586796,-2.4942336307
N,0.9830078182,-0.8480676823,0.843949322
C,-0.11246815,-0.2849294623,0.0946916567
C,-0.0779398939,1.2936542225,-0.1620825958
H,-0.7394720014,1.4164485266,-1.0224431845
C,-0.5769963462,2.2516950403,0.956708602
N,1.2207880531,1.8246807259,-0.6040416059
C,0.1250043285,3.6165514594,0.7408566512
H,-0.3441929877,1.8707028605,1.9574516261
H,-1.6644639847,2.333391113,0.8818490752
C,1.0241603076,2.9460043643,-1.5382342202
C,2.1498896205,2.1900356465,0.4856908736
C,0.1340344055,3.9846654466,-0.7628104212
H,-0.3786620892,4.3980210746,1.3159817291
C,1.5831072987,3.4511529952,1.2021390586
H,0.5386801776,2.5695188707,-2.4400918629
H,2.0065956826,3.3442912311,-1.7971524944
H,2.2205018903,1.3308816367,1.1513935498
H,3.1237776129,2.3636803556,0.0269288259
H,-0.8818893359,3.9811162215,-1.169955723
H,0.5455433693,4.9873697929,-0.9091632597
H,2.1769279208,4.3333534479,0.9441267492
H,0.9570514249,-0.7581929724,1.8519317853
F,2.0281551889,0.4243465891,-1.2603412716

H,1.6414388722,3.3152658666,2.286055814
H,-0.0368380442,-0.7042294676,-0.903212225
H,5.466922014,-3.0699986617,-0.9003235891
H,5.093046964,-1.3842162774,-0.543525804
H,3.7840547962,-3.790960574,0.8385133131
H,5.0520698631,-2.7958153593,1.5503663649
C,-1.4821385431,-0.6507432368,0.6657774226
C,-2.6106632809,-0.8042791698,-0.2057782631
C,-1.6870046311,-0.8224243359,2.018350396
C,-2.5595600648,-0.6803209401,-1.6226705674
C,-3.8767755336,-1.1148967146,0.397990591
C,-2.9788746453,-1.1306183049,2.5073448399
H,-0.8839904871,-0.7324254444,2.7424982385
C,-3.6908917294,-0.8444128169,-2.3923548579
H,-1.621516511,-0.462410506,-2.1224949384
C,-5.0234216415,-1.2767860554,-0.4235850119
H,-3.1220593811,-1.2613487509,3.5787660401
C,-4.9357550485,-1.1425773059,-1.7901409816
H,-3.6248197259,-0.7486959933,-3.4720399327
H,-5.9621638,-1.510963609,0.0683517106
H,-5.8178154685,-1.2698057627,-2.4106393122
N,-4.0424227567,-1.2700950068,1.7454737829
Electronic energy = -1157.7411604
Zero-point electronic energy = -1157.251602
Thermal energy = -1157.229575
Enthalpy = -1157.228631
Free energy = -1157.302263
Free energy (quasiharmonic approximation) = -1157.298621
B3LYP-D3(BJ)/def2-TZVPP SCF = -1158.3032272
B3LYP/def2-TZVPP SCF = -1158.1717612
M062X/def2-TZVPP SCF = -1157.6652887
wB97XD/def2-TZVPP SCF = -1157.8022188

Enamine derived from acetone and ammonia C3H7N1
(CBS-QB3 geometry)
C,-1.0342927535,0.1050618211,0.0036036055
C,-0.329895447,1.2344697679,-0.1503710713
C,-0.3885749118,-1.2525955834,0.0871209026
H,-0.811731442,2.2045055628,-0.2084651221
H,-0.7595501795,-1.910320858,-0.7082842503
H,-0.6256948746,-1.7324190143,1.041987815
N,-2.4226766796,0.0764771218,0.182208139
H,-2.8849687629,-0.7283840914,-0.2184542212
H,-2.8969536259,0.934931547,-0.0621211629
H,0.7501331634,1.2129524368,-0.1908580362
H,0.6939788433,-1.1805301202,-0.0111197181
CBS-QB3 (0 K) = -172.927377
CBS-QB3 Energy = -172.922239
CBS-QB3 Enthalpy = -172.921295
CBS-QB3 Free energy = -172.954356

(B3LYP/6-31G(d) geometry)
C,-1.0349810073,0.1030684303,0.0075192612
C,-0.3324851329,1.235662782,-0.1532342673
C,-0.3877681258,-1.255579812,0.0892294453
H,-0.814911798,2.2083407065,-0.2101876151
H,-0.7569280765,-1.9177444353,-0.7072830114
H,-0.6217473572,-1.7403696998,1.0452400436
N,-2.4269208518,0.0752005772,0.1955865013
H,-2.888501602,-0.7189521431,-0.2357664966
H,-2.8938137546,0.9387005363,-0.0599985167
H,0.7502633738,1.2185493716,-0.1954281243
H,0.6975676621,-1.1827277237,-0.01043034
Electronic energy = -173.2633856
Zero-point electronic energy = -173.165758

Thermal energy = -173.160688
Enthalpy = -173.159744
Free energy = -173.192709
Free energy (quasiharmonic approximation) = -173.192709
B3LYP-D3(BJ)/def2-TZVPP SCF = -173.3576781
B3LYP/def2-TZVPP SCF = -173.3458615
M062X/def2-TZVPP SCF = -173.2508499
wB97XD/def2-TZVPP SCF = -173.2817932

N-Fluorotrimethylammonium ion C3H9F1N1(1+)
(CBS-QB3 geometry)
C,0.4848721041,1.4334159695,-0.1743247674
H,0.8919383868,1.9989216085,0.6605451731
N,0.8796883167,-0.0002684416,-0.0000619362
C,0.4847147744,-0.5665124048,1.3285366273
C,0.4848208881,-0.8677421706,-1.1549817013
H,0.8977032753,0.0745024453,2.1037634096
H,0.890744838,-1.5727406735,1.3998594248
H,0.8953126954,-0.4290137938,-2.0613357942
H,0.8930463244,-1.8612390219,-0.9854715959
F,2.292178492,-0.0003520057,0.0002536914
H,0.8965973359,1.78347007,-1.1179147614
H,-0.6040531389,-0.8946924949,-1.1930273919
H,-0.6039863176,1.479591272,-0.18279035
H,-0.6041601446,-0.5808785682,1.3731136422
CBS-QB3 (0 K) = -273.554950
CBS-QB3 Energy = -273.548651
CBS-QB3 Enthalpy = -273.547707
CBS-QB3 Free energy = -273.583779

(B3LYP/6-31G(d) geometry)
C,0.4850515373,1.435081957,-0.174430881
H,0.896267721,1.9994334717,0.6621482232
N,0.8762417827,-0.0003937144,-0.0002341592
C,0.4836558989,-0.5670150369,1.3297064958
C,0.4840936333,-0.868670398,-1.1562241135
H,0.8976878508,0.0773003716,2.104861708
H,0.8942170437,-1.5739291339,1.4005280048
H,0.8957679095,-0.4269375964,-2.0633358848
H,0.8972476107,-1.8624226719,-0.9853383451
F,2.2888381172,-0.0011571037,0.0001233609
H,0.8992295102,1.7839802854,-1.1200336162
H,-0.6064715345,-0.9001696449,-1.1965677345
H,-0.6054736998,1.4864070892,-0.1824057597
H,-0.6069355511,-0.5850460848,1.3773663713
Electronic energy = -274.0071558
Zero-point electronic energy = -273.880346
Thermal energy = -273.874147
Enthalpy = -273.873203
Free energy = -273.909085
Free energy (quasiharmonic approximation) = -273.909085
B3LYP-D3(BJ)/def2-TZVPP SCF = -274.1390568
B3LYP/def2-TZVPP SCF = -274.1227994
M062X/def2-TZVPP SCF = -273.9906067
wB97XD/def2-TZVPP SCF = -274.0388099

N-Fluoromethanesulfonimide C2H6F1N1O4S2
(CBS-QB3 geometry)
S,-0.8503354084,-0.3122574746,-1.2265617612
O,-1.1139300468,-1.3078045286,-2.224319635
O,-0.0641923526,0.8589310287,-1.523811839
N,-0.1150764645,-1.2488567674,0.1371238738
S,0.844594224,-0.3867248489,1.3340939214
O,-0.0343364951,0.6906289011,1.711511713
O,1.2749370159,-1.3881394382,2.264050151

F,0.7289223446,-2.2103178321,-0.4540314661
C,-2.3532064762,0.1667495259,-0.3988631756
H,-2.8899647932,-0.737570192,-0.1213633235
H,-2.0890777559,0.7682866374,0.4682884225
H,-2.9112000198,0.7504580439,-1.132506103
C,2.2682218816,0.2318076107,0.4526207639
H,1.9314603818,0.9500097923,-0.2905935891
H,2.9026041962,0.6956062574,1.2086124289
H,2.7725622382,-0.6201570856,-0.000341672
CBS-QB3 (0 K) = -1330.052852
CBS-QB3 Energy = -1330.041211
CBS-QB3 Enthalpy = -1330.040267
CBS-QB3 Free energy = -1330.090162

(B3LYP/6-31G(d) geometry)
S,-0.8543796883,-0.3235887335,-1.2347483146
O,-1.1261336953,-1.3342649067,-2.2461430788
O,-0.0503479246,0.8605040537,-1.5453627902
N,-0.1248615655,-1.2689424426,0.143653879
S,0.8478913401,-0.3941383531,1.3528999297
O,-0.0452791448,0.696700791,1.7420371926
O,1.2912488637,-1.4070875682,2.2978489696
F,0.7574488304,-2.1818956237,-0.4745032417
C,-2.3663240585,0.1746599916,-0.403606666
H,-2.9157938881,-0.7245853285,-0.1237132598
H,-2.0972008288,0.7714725092,0.4687994732
H,-2.9259309667,0.7671150801,-1.1318583383
C,2.2770567569,0.2318102461,0.4540106007
H,1.9317887431,0.9430364546,-0.2961475246
H,2.9158969986,0.7086924827,1.2010273118
H,2.7869026977,-0.6188390225,-0.0002854326
Electronic energy = -1331.4669237
Zero-point electronic energy = -1331.363660
Thermal energy = -1331.352090
Enthalpy = -1331.351145
Free energy = -1331.400906
Free energy (quasiharmonic approximation) = -1331.400433
B3LYP-D3(BJ)/def2-TZVPP SCF = -1331.8896846
B3LYP/def2-TZVPP SCF = -1331.8561051
M062X/def2-TZVPP SCF = -1331.571772
wB97XD/def2-TZVPP SCF = -1331.654987

Reactant complex formed from Acetone–Ammonia Enamine and Me3NF+ C6H16F1N2(1+)
(CBS-QB3 geometry)
C,2.3704560176,-0.0738866348,0.0757704162
C,2.4698006506,-1.2522936764,0.7073966611
C,2.5210977252,0.083495911,-1.412133924
H,2.4100227135,-1.3305009007,1.7881273508
H,3.3705702333,0.7346546095,-1.6448427644
H,1.631438279,0.5447384394,-1.8541236839
N,2.0411221444,1.1231101816,0.7535922467
C,-1.1829405795,-1.2913207558,0.5049405301
H,-1.5177046734,-2.0832593677,-0.1610725867
N,-1.7788485194,-0.0046728712,0.0260167892
C,-3.2638167173,-0.0640783554,-0.1362274532
C,-1.3098944411,1.1890081071,0.7988110475
H,-3.5009119608,-0.9038009341,-0.7850883655
H,-3.5939938299,0.8730949267,-0.5777003591
H,-1.7361988758,2.073815772,0.3313714273
H,2.4315838753,1.9500182894,0.3160798429
F,-1.2765008837,0.1759705512,-1.2858105558
H,2.2961224078,1.109677065,1.734942463
H,-0.0954220825,-1.1936580372,0.4889998961
H,2.6903725904,-2.1564352811,0.1570728672
H,2.6926126621,-0.8772712261,-1.8951483069

H,-3.6995288634,-0.202038767,0.8529718818
H,-1.6796809504,1.0773647215,1.8184873828
H,-0.2144802565,1.208516284,0.7731582612
H,-1.5459706656,-1.4597010508,1.5188969356
CBS-QB3 (0 K)= -446.501151
CBS-QB3 Energy = -446.488150
CBS-QB3 Enthalpy = -446.487205
CBS-QB3 Free Energy = -446.541345

Reactant complex formed from Acetone–Ammonia Enamine and (MeSO2)2NF
C5H13F1N2O4S2
(CBS-QB3 geometry)
N,1.13593,0.05735,-0.82595
O,1.87963,-2.37265,-0.90136
O,2.67219,-0.83077,0.92654
O,-0.14283,2.28147,-0.8443
O,0.216,1.23886,1.40306
S,1.62869,-1.37173,0.09243
S,0.68562,1.54981,0.07565
F,0.01985,-0.30322,-1.60526
N,-3.01375,0.56956,-1.04998
C,-3.27635,-0.31706,-0.01095
C,-3.3373,-1.65203,-0.16828
C,-3.55972,0.35507,1.30722
H,-3.14791,-2.12129,-1.1279
H,-4.38378,1.06738,1.20128
H,-2.68365,0.91512,1.65258
H,-2.52187,1.41599,-0.79797
H,-2.62689,0.15473,-1.88572
C,2.31311,2.26675,0.16846
H,2.66304,2.44682,-0.84541
H,2.18778,3.19959,0.71992
H,2.95634,1.57204,0.70525
C,0.21188,-1.84912,1.06301
H,-0.66719,-1.87646,0.41539
H,0.44239,-2.8463,1.43985
H,0.08933,-1.1287,1.86697
H,-3.65534,-2.29033,0.64458
H,-3.82485,-0.37428,2.07227
CBS-QB3 (0 K)= -1502.990867
CBS-QB3 Energy = -1502.972069
CBS-QB3 Enthalpy = -1502.971125
CBS-QB3 Free Energy = -1503.039661

TS-13a C6H16F1N2(1+)
(CBS-QB3 geometry)
C,-2.4630808934,1.018666303,0.0605256558
C,-2.4283277142,0.8802916024,-1.2835236773
C,-3.1060886818,0.0070921064,0.9658648613
H,-2.0101253435,1.6459434577,-1.9258347157
H,-3.9351213508,0.4590107779,1.5208184724
H,-2.3913532872,-0.3694754713,1.7055336735
N,-1.8282174192,2.0692621643,0.7173108068
C,2.0790154203,1.0626413171,-1.1433117172
H,1.945461275,0.8503275098,-2.2013000936
N,1.381942646,0.0161249416,-0.3615171048
C,1.7919858761,-1.3673938131,-0.6888461344
C,1.268110168,0.3182366126,1.0822760844
H,1.7472883687,-1.4976556875,-1.7675325272
H,1.1091141413,-2.0537616556,-0.1941724265
H,0.8604797345,-0.55221852,1.5905827318
H,-2.2083079753,2.3062128701,1.6245480151
F,-0.0802006653,0.106560511,-0.8461987327
H,-1.6689036823,2.8953821647,0.1551860575
H,1.6456787999,2.0268108126,-0.8885030289

H,-2.9046461921,0.0363653809,-1.7609012996
H,-3.4989944278,-0.835618348,0.3998366812
H,2.8118479817,-1.5178305214,-0.3269044413
H,2.2608467058,0.55751939,1.4673882254
H,0.5858527591,1.166541587,1.1877242719
H,3.1387073064,1.0400789374,-0.8798440679
CBS-QB3 (0 K) = -446.488578
CBS-QB3 Energy = -446.475764
CBS-QB3 Enthalpy = -446.474820
CBS-QB3 Free energy = -446.527566

(B3LYP/6-31G(d) geometry)
C,-2.4638450017,1.0297143026,0.0536665078
C,-2.3740485027,0.8464861135,-1.2884444229
C,-3.0877350358,0.0148032513,0.9723864845
H,-1.9801168611,1.61486708,-1.9468877647
H,-3.9721594637,0.4344013238,1.4691096025
H,-2.3872846465,-0.2854897742,1.7623408962
N,-1.904989435,2.1298117071,0.6930228914
C,2.0695672533,1.0711868758,-1.1258543272
H,1.911890682,0.8747387162,-2.1860887357
N,1.384926341,0.0156875263,-0.3463768041
C,1.7563807002,-1.3659979935,-0.7216347354
C,1.3212725771,0.2825167466,1.1072804022
H,1.6585770749,-1.4698009584,-1.8021547435
H,1.0825659598,-2.0534029274,-0.2109438092
H,0.8578305602,-0.5727739874,1.5985697592
H,-2.3149738584,2.3717791825,1.5885513538
F,-0.0964568335,0.1447127516,-0.7803201764
H,-1.770229598,2.9511754493,0.1129662031
H,1.6409602639,2.0336599433,-0.8471550731
H,-2.8003520172,-0.0335416498,-1.7534744865
H,-3.4006286227,-0.8763661411,0.4254132194
H,2.7908285849,-1.546269795,-0.4128581292
H,2.3367582929,0.4356197392,1.4831357354
H,0.7071816537,1.1758237393,1.252157431
H,3.1370434823,1.0457732082,-0.8872017086
Electronic energy = -447.2839131
Zero-point electronic energy = -447.059824
Thermal energy = -447.047152
Enthalpy = -447.046208
Free energy = -447.098792
Free energy (quasiharmonic approximation) = -447.096950
B3LYP-D3(BJ)/def2-TZVPP SCF = -447.5096036
B3LYP/def2-TZVPP SCF = -447.4764444
M062X/def2-TZVPP SCF = -447.2421218
wB97XD/def2-TZVPP SCF = -447.3237596

TS-13b C5H13F1N2O4S2
(CBS-QB3 geometry)
N,0.8676976758,0.0176800114,-0.7611196711
O,1.7324469931,-2.3231920973,-1.0251779971
O,2.9822816621,-0.6786462916,0.3983818008
O,-0.3728903862,2.20880583,-0.6444756371
O,0.4867604768,1.2985558654,1.5121029992
S,1.7368968991,-1.2678783844,-0.0513842543
S,0.653616633,1.4942769718,0.086423716
F,-0.7701901342,-0.5316845277,-0.8524638973
N,-3.0996654894,1.0946329804,0.1680405573
C,-3.2150191439,-0.22678866,-0.1028221915
C,-2.8226625926,-0.7540990903,-1.3122683106
C,-3.7818594499,-1.0832809409,0.994025969
H,-2.5887485573,-0.1142138887,-2.1494971079
H,-4.7739771642,-0.7217144319,1.2827102679
H,-3.145222937,-1.0407915222,1.8841160675

H,-3.1878127063,1.39323207,1.1273469239
H,-2.4323632386,1.6342193431,-0.3736924566
C,2.2224380715,2.2891807293,-0.2259899648
H,2.346938778,2.3732936819,-1.3033989796
H,2.1491409477,3.2726234209,0.2408827791
H,3.0078358197,1.6861064136,0.2234497088
C,0.8000075872,-1.8051761086,1.3718167316
H,-0.1697391976,-2.1450300895,1.0177106006
H,1.3720371112,-2.6258466423,1.805733477
H,0.7100015416,-0.9696068672,2.0615625415
H,-2.9538784338,-1.8077065419,-1.5076317735
H,-3.872849766,-2.1212882332,0.6788561013
CBS-QB3 (0 K) = -1502.964443
CBS-QB3 Energy = -1502.946573
CBS-QB3 Enthalpy = -1502.945629
CBS-QB3 Free energy = -1503.010629

(B3LYP/6-31G(d) geometry)
N,0.7761243224,-0.4503066834,0.8684110864
O,0.0794688279,1.0340084917,2.8088590538
O,1.8096533363,1.8654475667,1.1370336167
O,1.1272442781,-2.1646156909,-0.9838116503
O,0.830386764,0.2387693981,-1.7106460568
S,0.5518279354,1.1636689295,1.4358682678
S,1.3546924117,-0.7321467334,-0.7368476115
F,-0.8283275248,-1.0767618703,0.6793903724
N,-1.7535724137,-2.3656611311,-1.8553698089
C,-2.6164670479,-1.9255442724,-0.9073659868
C,-2.4821012957,-2.2927854529,0.4177540838
C,-3.7114564867,-1.0063377584,-1.3761302178
H,-1.8290447996,-3.1055347512,0.7068704121
H,-4.3011059401,-1.4870609598,-2.1667052682
H,-3.2910427957,-0.0837036453,-1.7967755056
H,-1.7428186034,-1.8821980047,-2.7443359722
H,-0.8283641896,-2.6642923687,-1.5490816829
C,3.121089959,-0.4675720627,-0.5237659502
H,3.4827652888,-1.172928657,0.2252498861
H,3.5777505189,-0.6625837599,-1.4975299997
H,3.2763156646,0.5636118809,-0.2052688478
C,-0.7669576062,1.8831374067,0.4417952962
H,-1.6606268061,1.2773070217,0.5837459355
H,-0.9121750203,2.8963071651,0.8234005135
H,-0.4497412244,1.889873504,-0.6009178608
H,-3.2142586957,-1.9622241752,1.1432789082
H,-4.3856509772,-0.7410371072,-0.5596307032
Electronic energy = -1504.7200755
Zero-point electronic energy = -1504.518421
Thermal energy = -1504.500812
Enthalpy = -1504.499867
Free energy = -1504.564235
Free energy (quasiharmonic approximation) = -1504.561560
B3LYP-D3(BJ)/def2-TZVPP SCF = -1505.2405327
B3LYP/def2-TZVPP SCF = -1505.1863752
M062X/def2-TZVPP SCF = -1504.7913891
wB97XD/def2-TZVPP SCF = -1504.9113619

TS-6a   C25H33F1N3O1(1+)
(B3LYP-D3(BJ)/TZVP geometry)
C,-2.1520178041,-2.0890423783,0.518458456
C,-2.1766524157,-2.2647169376,-0.8328665018
C,-3.1075843933,-3.2179345058,-1.5189601646
C,-4.2598811988,-3.6759220319,-0.6255491473
C,-3.7364067481,-4.0451976115,0.76005005
C,-3.1004464651,-2.8289864004,1.4310045332
H,-3.4897053127,-2.7535105466,-2.4324566361

H,-1.4216352572,-1.8023090602,-1.4514177074
H,-4.993565388,-2.8690095604,-0.5318226922
H,-4.7721592478,-4.5236894909,-1.083857614
H,-4.5386425206,-4.4298113272,1.391953613
H,-2.991703872,-4.8413487166,0.665974459
H,-3.880060255,-2.1282856509,1.7506837084
H,-2.5648474494,-3.1294196652,2.3362436335
H,-2.532331365,-4.0916519648,-1.8548838612
N,-1.3172405241,-1.2294471198,1.1761440746
C,-0.4584784506,-0.203759856,0.6404004426
C,-1.1355989535,1.2249376172,0.7016733128
H,-0.2674868636,-0.4351359891,-0.399350407
C,0.8518063739,-0.1834489978,1.406747995
H,-1.7980034631,1.2256929988,1.5650595638
C,-0.1580290785,2.4380054156,0.7893546075
N,-1.9883811839,1.5142123837,-0.4541158536
C,2.1073345798,-0.3160981864,0.7445349974
C,0.8493239955,-0.0128196349,2.7687121693
C,-0.7537793553,3.6127742103,-0.0018926667
H,0.8229106307,2.171843129,0.4014142177
H,-0.0285751174,2.6906280649,1.8390541968
C,-3.0142482981,2.5147486253,-0.1254876083
C,-1.2544458828,1.8566307345,-1.682437399
C,2.2614832832,-0.4846492611,-0.6465941099
C,3.2827090181,-0.2475477449,1.5621440592
C,2.0641629943,0.0251468228,3.4818316376
H,-0.0721590356,0.1125310395,3.3233714834
C,-2.2353876135,3.7722585114,0.376016076
H,-0.2067662764,4.5282771245,0.2198758121
C,-0.6727871274,3.2927105774,-1.5063400639
H,-3.6650039373,2.0942641908,0.6360646876
H,-3.5886906824,2.7074803843,-1.0272993883
H,-0.4666505055,1.12205714,-1.8197224541
H,-1.9495686594,1.7837707274,-2.5136517651
C,3.5130260587,-0.5813385496,-1.2187613865
H,1.41134974,-0.5558423077,-1.3085666622
C,4.548251447,-0.3526836808,0.9444075238
N,3.2411974525,-0.0824915668,2.9121319209
H,2.048776551,0.158209102,4.5582745291
H,-2.3465585247,3.8691811689,1.4556198799
H,-2.6616795143,4.6608103586,-0.0870470985
H,-1.3245912035,3.9893886216,-2.0369702435
C,0.7245047596,3.3896026969,-2.1085569686
C,4.6727686436,-0.5118823958,-0.4107132681
O,3.5474960551,-0.7398225983,-2.566688775
H,5.4236893473,-0.3008402452,1.5777560395
H,0.7071513795,3.1260181623,-3.1675866515
H,1.103000569,4.4090360854,-2.0223890067
H,1.4295129039,2.7200592197,-1.6128441195
H,5.6555351309,-0.5870993334,-0.8513956285
C,4.8160042693,-0.8551454031,-3.2169059583
H,4.5931033956,-0.9768549882,-4.2730740583
H,5.3650195639,-1.7282224672,-2.8580510963
H,5.4165835681,0.0455611907,-3.0733591182
H,-1.3539686359,-1.2774967207,2.1829081787
F,-2.7302231307,0.0432965911,-0.7944797782
Electronic energy = -1312.1631331
Zero-point electronic energy = -1311.615977
Thermal energy = -1311.590367
Enthalpy = -1311.589423
Free energy = -1311.670453
Free energy (quasiharmonic approximation) = -1311.666047
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.2270671

TS-6b C25H33F1N3O1(1+)

(B3LYP-D3(BJ)/TZVP geometry)
C,-0.1460986459,1.7565072632,0.3561926793
C,0.1513737496,2.0758996888,-0.9398373821
C,0.1983521011,3.4881524869,-1.4370707927
C,-0.4688587551,4.489967576,-0.4971150621
C,-0.0416248047,4.2198112538,0.9426678618
C,-0.4842353012,2.8221402762,1.3708166988
H,1.2509577001,3.7654394845,-1.5862579676
H,0.4994515136,1.3182730246,-1.6173541957
H,-0.0384144934,2.5593784072,2.3344766548
H,-1.5712581585,2.8108817436,1.521708321
H,-0.2540849862,3.5285858557,-2.4316193171
N,-0.2436872672,0.4896976388,0.8668503402
C,-0.1711464169,-0.8092463541,0.2349577405
C,-1.5552959244,-1.4617432834,-0.1712158537
H,0.1719427201,-1.4851492016,1.0213337199
H,-1.3349216176,-2.1357041209,-0.9920871542
C,-2.2102027487,-2.2985036406,0.9583782194
N,-2.6075007516,-0.5743485255,-0.6647328502
C,-3.7301125169,-2.3101624937,0.7126756069
H,-1.979794365,-1.8859474165,1.9413451468
H,-1.7845694352,-3.3008307993,0.9183529397
C,-3.4917334948,-1.2899368221,-1.5917895076
C,-3.375581683,0.1170022354,0.380725372
C,-4.0057250298,-2.5344683762,-0.7871500857
H,-4.2081037676,-3.0904473916,1.3033702402
C,-4.2928314612,-0.9272107772,1.0869404671
H,-2.9260908625,-1.5776318523,-2.4737833391
H,-4.2939776444,-0.6151347599,-1.876731163
H,-2.664091253,0.5552849086,1.0726427818
H,-3.9442732956,0.9066137167,-0.1017544142
H,-3.5003134076,-3.4322997331,-1.1422643299
H,-5.072705725,-2.6551845276,-0.9682895104
H,-5.2923674878,-0.8418168869,0.6558829721
H,-0.3804735907,0.4558881766,1.865926136
F,-1.7559902676,0.74949508,-1.3871434518
H,-0.2107817031,5.5081510732,-0.7928240086
H,-1.5568253343,4.398608298,-0.5743559374
H,1.0465645089,4.2998920846,1.02206812
H,-0.4681113758,4.9578110545,1.6238793758
C,0.8885375355,-0.8986640323,-0.8561027182
C,2.2604296812,-0.7702533766,-0.4869395493
C,0.5966054838,-1.1183710061,-2.1794427669
C,2.7004241659,-0.5428218549,0.8409841508
C,3.231577594,-0.8693150081,-1.5299848106
C,1.6310484867,-1.2029287959,-3.1295004248
H,-0.4207572942,-1.1797677636,-2.5318889091
C,4.0432954406,-0.4228976734,1.1191641817
H,1.978230802,-0.448674803,1.6335196337
C,4.606085563,-0.741179244,-1.2024254406
N,2.9047200639,-1.083481257,-2.8306648937
H,1.3843469565,-1.3677637133,-4.1728443063
C,5.0054635445,-0.5232119358,0.0824425932
O,4.5586290091,-0.2030401633,2.3539351043
H,5.3251101971,-0.8212095916,-2.0065949439
H,6.0514631476,-0.4231469155,0.3400477407
C,3.6566666404,-0.0800573741,3.4529735184
H,4.277046313,0.0840082321,4.3293467036
H,3.071404761,-0.9935110848,3.5844807181
H,2.9856190473,0.771485719,3.3152562012
C,-4.3922133744,-0.6499341462,2.5813278516
H,-4.7709180178,0.3576596628,2.7623628706
H,-5.0775596235,-1.3555987902,3.0528917331
H,-3.4234548446,-0.7348394483,3.0763706913
Electronic energy = -1312.1534704

```
Zero-point electronic energy = -1311.605649
Thermal energy = -1311.579548
Enthalpy = -1311.578604
Free energy = -1311.660682
Free energy (quasiharmonic approximation) = -1311.656242
B3LYP-D3(BJ)/def2-TZVPP SCF = -1312.21679099
```

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