

Supporting Information for

**Theoretical Study on Mechanism of Selective Fluorination of
Aromatic Compounds with Selectfluor**

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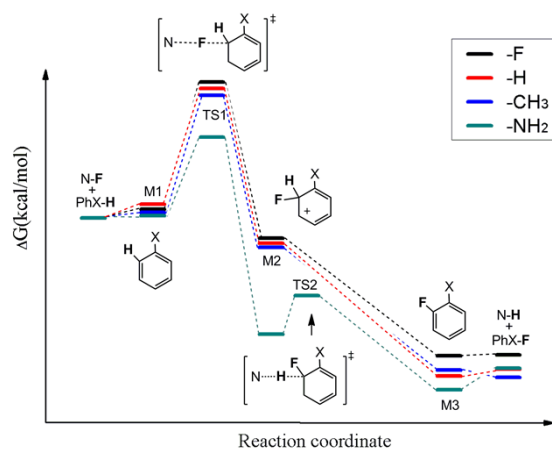


Fig. S1 DFT computed energy surfaces for the fluorination of various aromatic compounds PhX (X= F, H, CH₃, NH₂) with Selectfluor of S_N2 mechanism.

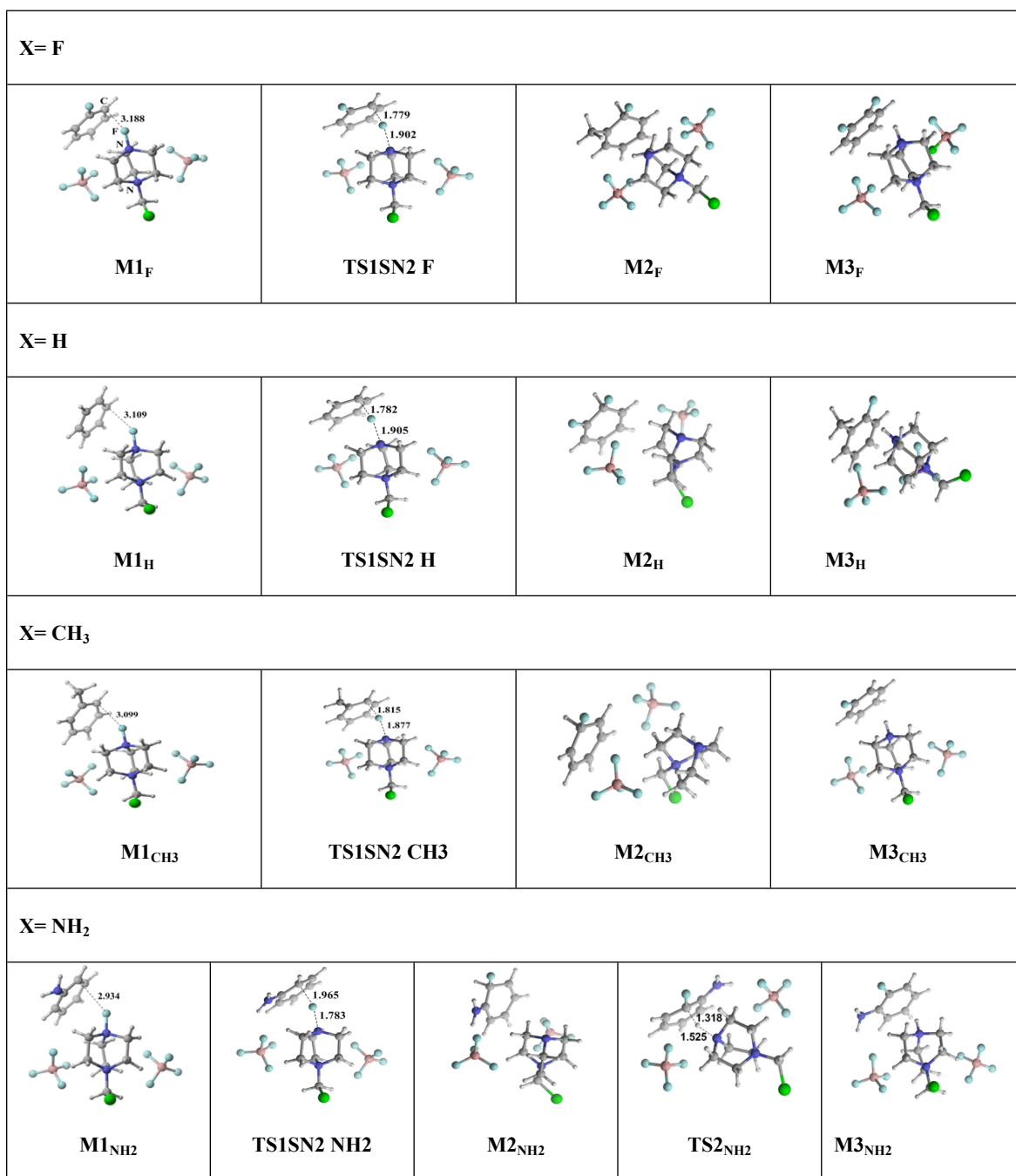
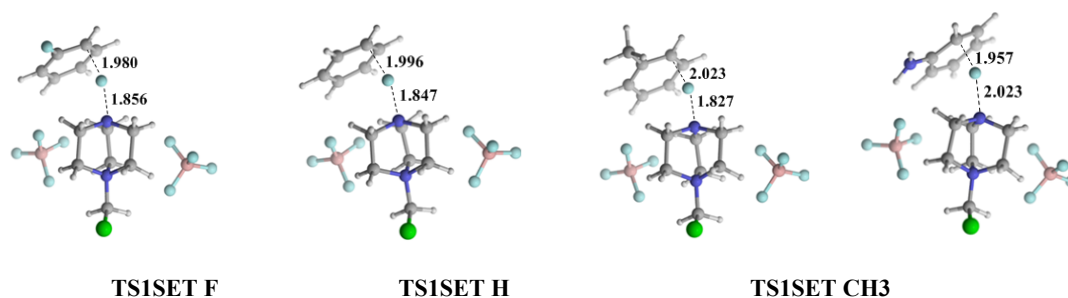


Fig. S2 The optimized structure in the S_N2 mechanism of PhX/Selectfluor (X= F, H, CH₃, NH₂).



TS1SET NH2

Fig. S3 The optimized structures of transition state in the fluorine transfer mechanism (SET) of PhX/Selectfluor (X= F, H, CH₃, NH₂).

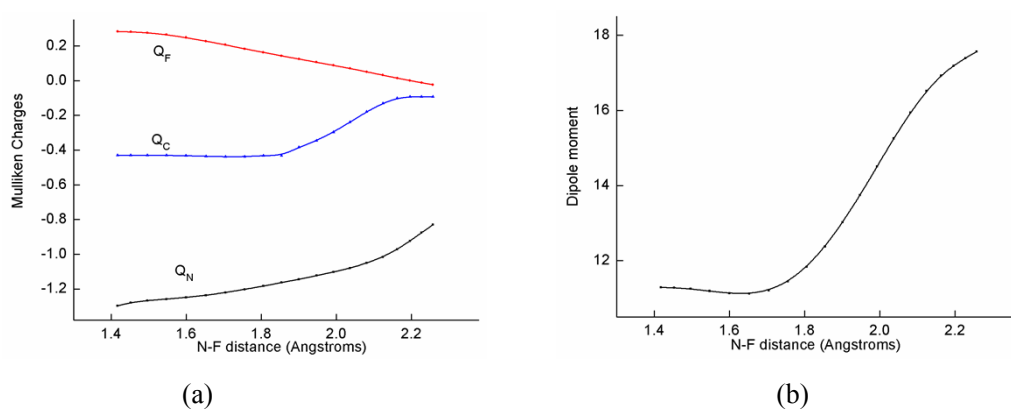


Fig. S4. The evolution of charge distribution as well as the dipole moment along the fluorine transfer process. The PhNH₂ molecule is selected as a typical model.

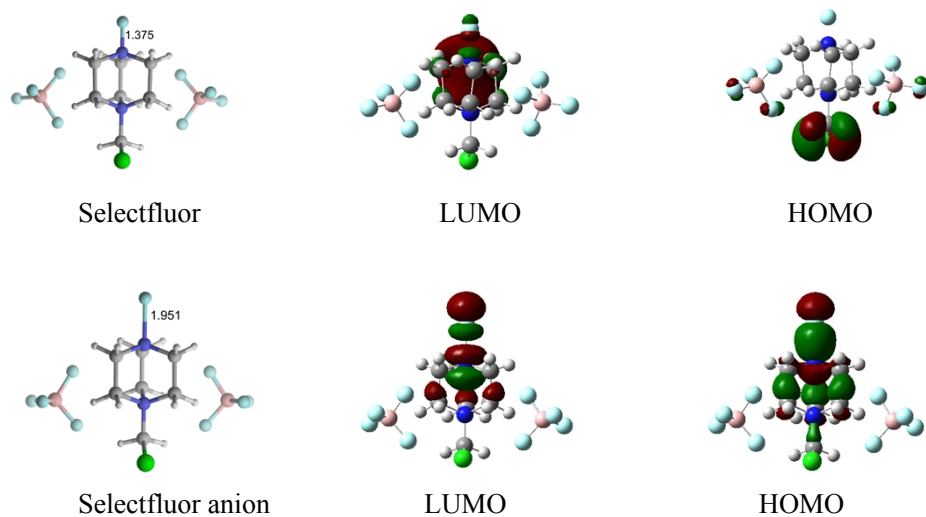


Fig. S5 The optimized structure of Selectfluor and its radical anion, the related HOMO and LUMO orbitals are also given.

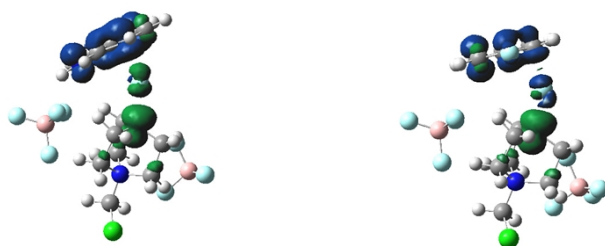


Fig. S6. Spin density distribution of π complexes at the transition state of SET mechanism, for PhNH₂ (left) and PhF (right) complexed with Selectfluor.

Table S1 The bond distances (X-ray experimental values in parentheses, MP2/cc-pVDZ structures, M06-2X/6-311++g** structures) of Selectfluor (a), radical anion (b). Bond distances in Å.

(a)

	X-ray experimental values in parentheses	MP2/cc-pVDZ	M06-2X/6-311++g**
N1-F	1.37	1.390	1.375
N1-CH ₂	1.48	1.498	1.498
CH ₂ -CH ₂	1.50	1.546	1.541
N1-N2	-	2.508	2.488
N2-CH ₂	1.50	1.518	1.503
N2-CH ₂ Cl	1.53	1.535	1.506
CH ₂ -Cl	-	1.747	1.766

(b)

	MP2/cc-pVDZ	M06-2X/6-311++g**
N1-F	1.968	1.951
N1-CH ₂	1.458	1.453
CH ₂ -CH ₂	1.552	1.477
N1-N2	2.522	2.488
N2-CH ₂	1.521	1.509
N2-CH ₂ Cl	1.509	1.493
CH ₂ -Cl	1.758	1.781

Table S2 The second-order perturbation stabilization energy (E(2), kcal/mol) due to the $\pi \rightarrow \sigma^*$ (N1-F) and $\pi \rightarrow \sigma^*$ (C-H) in the complexes at the M06-2X/6-311++G** level.

	-F	-H	-CH3	-NH2
E(2) F/ π	0.08	0.47	0.52	1.21
E(2) H1/ π	0.23	1.75	3.00	2.13
E(2) H2/ π	1.25	2.48	1.86	1.74

Table S3 The orbital energies on LUMO and HOMO of Seleclfluor and substituted benzene, and their different energy gaps between Seleclfluor and substituted benzene (energies in eV, isovalue = 0.02)

	LUMO	HOMO	HOMO \rightarrow LUMO
N-F	-1.39	-11.79	
-F	-0.05	-8.43	8.38
-H	0.00	-8.42	8.42
-CH3	-0.03	-8.06	8.03
-NH2	-0.13	-6.88	6.75

Table S4 Relative Gibbs free energies (ΔG , kcal/mol) for the fluorination of aromatic compounds with Selectfluor in the gas phase ($\Delta G_{\text{rel gas}}$) and acetonitrile solvent ($\Delta G_{\text{rel sol}}$) condition.

		$\Delta G_{\text{rel gas}}$	$\Delta G_{\text{rel sol}}$
X= F	PhXH + N-F	0.0	0.0
	M1_F	2.85	13.43
	TS1S_N2 F	44.13	48.51
	TS1SET F	38.31	44.20
	M2_F	-5.20	2.18
	M3_F	-45.75	-43.66
X= H	PhXH + N-F	0.0	0.0
	M1_H	3.50	6.80
	TS1S_N2 H	43.77	47.50
	TS1SET H	38.46	43.01
	M2_H	-8.38	-0.76
	M3_H	-52.58	-51.27
X= CH₃	PhXH + N-F	0.0	0.0
	M1_{CH3}	2.73	6.40
	TS1S_N2 CH3	40.69	44.29
	TS1SET CH3	35.67	40.73
	M2_{CH3}	-8.84	-2.46
	M3_{CH3}	-50.63	-48.68
X= NH₂	PhXH + N-F	0.0	0.0
	M1_{NH2}	0.81	5.67
	TS1S_N2 NH2	26.86	32.58
	TS1SET NH2	17.89	23.15
	M2_{NH2}	-38.62	-27.89
	TS2_{NH2}	-25.79	-20.08
	M3_{NH2}	-57.14	-52.19

Table S5 The critical geometric parameters as well as Mulliken charge of the transition state in S_N2 and SET mechanism.

Complex	d(N1-F)		d(C-F)		Charge	
	S _N 2	SET	S _N 2	SET	S _N 2	SET
N1-F/PhF	1.902	1.856	1.779	1.980	0.356	0.208
N1-F/PhH	1.905	1.847	1.782	1.996	0.339	0.197
N1-F/PhCH ₃	1.877	1.827	1.815	2.023	0.379	0.237
N1-F/PhNH ₂	1.783	2.023	1.965	1.957	0.413	0.033

Cartesian coordinates of the optimized structures

N-F			
Num. Imaginary Frequencies: 0			
H	1.23978400	-1.08706000	2.72357400
C	1.24679300	-0.97475300	1.64057400
C	1.21003900	0.50058100	1.19551300
H	2.09349200	-1.49457300	1.19168700
N	-0.00058600	-1.63514500	1.13732800
H	2.09990100	0.75817900	0.63082500
H	1.11336300	1.16687500	2.04969300
N	0.00014600	0.71867400	0.32979500
C	-1.24795200	-0.97419200	1.63990700
C	-0.00022400	-1.69944500	-0.35259400
C	-1.20984500	0.50132100	1.19558300
C	0.00055500	2.09131300	-0.29015200
C	-0.00011800	-0.24422300	-0.84862400
H	-1.24187400	-1.08695900	2.72286300
H	-2.09467700	-1.49324200	1.19018500
H	-0.90918400	-2.21761400	-0.64757600
H	0.90884100	-2.21766100	-0.64714900
H	-2.09958100	0.75997600	0.63115500
H	-1.11236300	1.16713100	2.05005100
Cl	0.00072500	3.36567000	0.93291200
H	0.91155200	2.16480100	-0.88310300
H	-0.91029100	2.16523600	-0.88327800
H	-0.90721400	-0.03664100	-1.41472300
H	0.90690100	-0.03685000	-1.41492900
F	-4.00520300	-0.04276000	0.43332600
F	-2.75853900	-1.35300300	-0.94213700
F	-2.83686300	0.90074700	-1.29781700
F	-4.70162800	-0.39071000	-1.74403000
B	-3.64070200	-0.22308900	-0.91480000
F	-0.00099100	-2.92439700	1.61604900
F	2.83681600	0.89973700	-1.29857500
F	4.00627300	-0.04168100	0.43293000
F	4.70114900	-0.39245700	-1.74447800
F	2.75852300	-1.35354400	-0.93999700
B	3.64085700	-0.22365100	-0.91466800

PhF

Num. Imaginary Frequencies: 0			
C	1.13020000	-1.20440900	0.00000200
C	1.82723300	-0.00000100	0.00000200
C	1.13020700	1.20440500	-0.00000100
C	-0.26078100	1.21356000	-0.00000100
C	-0.92508100	0.00000400	0.00000100
C	-0.26078100	-1.21355800	0.00000100
H	1.66921000	-2.14407500	0.00000400
H	2.90992900	-0.00000600	0.00000300
H	1.66921200	2.14407300	-0.00000200
H	-0.83093700	2.13380300	-0.00000300
H	-0.83095100	-2.13379300	0.00000100
F	-2.27027200	-0.00000100	-0.00000400

M1F

Num. Imaginary Frequencies: 0			
H	0.05317900	0.38235100	3.13602400
C	0.28938100	0.56795400	2.08878900
C	-0.60237800	1.64677500	1.44166300
H	1.34373000	0.80933100	1.95316900
N	0.04667600	-0.71756200	1.36776600
H	-0.00740100	2.36448700	0.88286100
H	-1.20745500	2.15144500	2.19231600
N	-1.54591000	0.97882800	0.48013500
C	-1.34561900	-1.22571300	1.57986200
C	0.34185100	-0.56518400	-0.09172800
C	-2.30710900	-0.07389900	1.24307400
C	-2.46390600	1.96680800	-0.18375800
C	-0.76464000	0.33887000	-0.65722900
H	-1.41615400	-1.52445400	2.62444200
H	-1.48477000	-2.07902700	0.91737700
H	0.28762400	-1.56036600	-0.53101600
H	1.33595900	-0.12495100	-0.18254900
H	-3.12869500	-0.43509400	0.62886800
H	-2.69396200	0.40603800	2.14011500
Cl	-3.53317000	2.75593600	0.98205000
H	-1.83076600	2.71584700	-0.65792900
H	-3.06733600	1.40085300	-0.89276000
H	-1.48260500	-0.23666500	-1.23598200

H	-0.32692800	1.14046400	-1.24738300
F	-3.60679600	-2.49372200	0.18818800
F	-1.78294100	-2.38487200	-1.17432700
F	-3.47068800	-0.85676300	-1.40410900
F	-3.81860100	-3.04982500	-2.04551200
B	-3.20640900	-2.24212600	-1.14207400
F	0.90511900	-1.64903800	1.89644000
F	0.40527000	3.22462500	-0.94114100
F	1.97870300	2.04685400	0.22496400
F	2.65768200	3.54879500	-1.38355300
F	1.61113400	1.58582800	-1.98401100
B	1.70172100	2.63485500	-1.05604800
C	3.13514300	-2.27006700	-1.38097900
C	3.43883100	-0.97331700	-1.78869900
C	3.85947600	-0.03127600	-0.85486300
C	3.96957000	-0.37522900	0.48984100
C	3.65352500	-1.66930400	0.86511500
C	3.23919300	-2.63124200	-0.04017800
H	3.33592900	-0.68824300	-2.82774500
H	4.29010900	0.34232600	1.23522700
H	3.00977100	-3.63119000	0.30679400
H	2.80946100	-3.00652300	-2.10630600
H	4.07645200	0.98318300	-1.16529600
F	3.73510900	-2.00346800	2.17025700

H	1.06866300	-0.11170400	-0.70608300
H	-3.14195500	-0.45811600	0.88315200
H	-2.41825600	0.24671800	2.35554400
Cl	-3.42505700	2.70015600	1.61434100
H	-2.09946800	2.80325100	-0.33293000
H	-3.36501500	1.50628600	-0.42183100
H	-1.85329200	-0.00598200	-1.28180400
H	-0.65247500	1.34075900	-1.28722800
F	-3.84262000	-2.40279400	0.26861300
F	-2.26573600	-2.16005800	-1.36169900
F	-3.90011700	-0.57650700	-1.11220900
F	-4.44213500	-2.66062700	-1.94731900
B	-3.64986100	-1.98907600	-1.06347900
F	1.65471200	-1.85379700	1.04161700
F	0.58047900	3.13277000	-1.16027900
F	2.20355500	1.93627800	-0.07819200
F	2.79460100	3.30337400	-1.82651700
F	1.61145700	1.37257900	-2.21221300
B	1.81471700	2.47280200	-1.34945800
C	3.12069000	-2.66883200	-0.72627500
C	3.31094800	-1.60870000	-1.56682500
C	3.77294500	-0.37338800	-1.05196500
C	4.12499600	-0.21864200	0.29006800
C	3.92971700	-1.28794000	1.12210200
C	3.27907700	-2.48788500	0.69020100
H	3.09924700	-1.69097300	-2.62489800
H	4.49171700	0.72470700	0.67177700
H	3.29946000	-3.34223200	1.35491600
H	2.74465400	-3.61749200	-1.08881100
H	3.85602100	0.47994700	-1.71595400
F	4.19712400	-1.18804900	2.41301100

TS1S_N2 F

Num. Imaginary Frequencies: 1

H	0.37603700	0.13110700	2.82703200
C	0.46765900	0.38271500	1.77032500
C	-0.46569600	1.55632300	1.37149600
H	1.49512700	0.64545500	1.52650300
N	0.07985800	-0.78790400	0.99102600
H	0.04948400	2.27952700	0.73910200
H	-0.89128400	2.04553100	2.24587000
N	-1.60143000	0.97878300	0.56930200
C	-1.20229900	-1.33521900	1.41834300
C	0.09831400	-0.52762200	-0.43962300
C	-2.21509100	-0.15488700	1.36400000
C	-2.62050900	2.00715600	0.19585500
C	-1.03559000	0.47397700	-0.75025100
H	-1.11870700	-1.71682800	2.43544400
H	-1.50766300	-2.12647600	0.73625200
H	-0.09244900	-1.46176900	-0.96548000

TS1SET F

Num. Imaginary Frequencies: 1

H	0.41073200	0.09050500	2.81189600
C	0.49344400	0.37148800	1.76255400
C	-0.45723400	1.53655300	1.38348400
H	1.51810100	0.63635100	1.51061100
N	0.09435400	-0.77719000	0.95555800
H	0.04736000	2.27521300	0.76143800
H	-0.88495900	2.00502800	2.26788700
N	-1.59074500	0.95753300	0.57646400
C	-1.16838900	-1.36677900	1.38291800

F -4.84959300 0.31446900 0.55214400

C 3.11940700 0.37714800 1.17540600

C 3.07899800 -1.00440200 1.05926600

H 3.59074300 -1.26612100 -2.25334600

H 3.33089400 2.26482200 0.20327000

H 3.17659500 -2.68647600 -0.24407100

H 3.68339400 1.20216300 -2.03230900

H 0.84932300 0.81486200 1.81285800

N -0.03474800 0.51257700 1.38976000

F 2.82675300 0.92329300 2.38426000

M3_F

Num. Imaginary Frequencies: 0

H -1.11462000 1.65226200 2.77799700

C -1.07469500 1.54821800 1.69412000

C -2.42780800 1.07636300 1.13009700

H -0.75572300 2.48002200 1.23556900

H -2.84029300 1.84311600 0.47451900

H -3.13645700 0.82183400 1.91609100

N -2.20319300 -0.16329700 0.30929100

C -0.45176200 -0.79930800 1.96998100

C 0.18922200 0.34144800 -0.09250400

C -1.71352000 -1.26390300 1.21911500

C -3.42429700 -0.60156800 -0.43785300

C -1.17092600 0.17230800 -0.75919100

H -0.63412400 -0.64684200 3.03348800

H 0.35432500 -1.51660700 1.82075100

H 0.80436300 -0.54652700 -0.22602300

H 0.69517600 1.22385400 -0.47062900

H -1.50093100 -2.12781500 0.59448100

H -2.52552800 -1.48599900 1.90958600

Cl -4.81227900 -0.86954900 0.62585500

H -3.67529400 0.18988800 -1.14082800

H -3.16750900 -1.53272200 -0.94207200

H -1.14061300 -0.64851800 -1.47259400

H -1.49821800 1.10124800 -1.22667800

F 0.47651900 -2.80052800 0.02275200

F 0.57451800 -1.92619000 -2.08494400

F -1.37756100 -2.84634700 -1.32256400

F 0.42971200 -4.20976600 -1.79967200

B 0.05049400 -2.98593900 -1.33270700

F 2.80006900 -1.72808000 2.15578500

F -1.50020400 3.23423900 -0.64028500

F 0.67899300 3.32941700 0.06478100

F -0.08718500 4.85229700 -1.48975600

F 0.18478000 2.62903500 -2.05624600

B -0.16708300 3.55861000 -1.06887200

C 3.26133400 -1.60986100 -0.16855800

C 3.48504100 -0.80326800 -1.28100700

C 3.53249100 0.58212800 -1.15819000

C 3.34722100 1.18823800 0.08230800

N-H

Num. Imaginary Frequencies: 0

H 1.25671400 -0.37585500 3.02544200

C 1.24394500 -0.59152400 1.95763100

C 1.21142600 0.69685900 1.11740000

H 2.10474100 -1.19861000 1.67719200

N -0.00068400 -1.38629900 1.67059500

H 2.09691700 0.78232800 0.49609200

H 1.12248900 1.58057400 1.74592900

N 0.00017500 0.67142500 0.22933800

C -1.24520800 -0.59103000 1.95680200

C -0.00031000 -1.83378400 0.23570400

C -1.21129500 0.69763200 1.11709200

C 0.00065300 1.81966800 -0.74161700

C -0.00009600 -0.57632100 -0.64117700

H -1.25885800 -0.37571000 3.02467000

H -2.10606200 -1.19758700 1.67539500

H -0.90449600 -2.41467800 0.07303000

H 0.90394200 -2.41470500 0.07350300

H -2.09655300 0.78405500 0.49556400

H -1.12171500 1.58104500 1.74595100

Cl 0.00081400 3.38457300 0.08147200

H 0.91115100 1.73082000 -1.33319000

H -0.90963600 1.73123200 -1.33357300

H -0.90616700 -0.52806700 -1.24386600

H 0.90598100 -0.52842100 -1.24388000

F -4.02344900 -0.03730400 0.54411400

F -2.77275800 -1.67217800 -0.42094100

F -2.86894000 0.39353200 -1.38909700

F -4.72541700 -0.98211800 -1.44597800

B -3.66011100 -0.58176700 -0.70265900

F 2.86885300 0.39266500 -1.38951400

F 4.02437600 -0.03663100 0.54340200

F	4.72470600	-0.98385500	-1.44613200
F	2.77238600	-1.67198800	-0.41916500
B	3.66007700	-0.58221600	-0.70253700
H	-0.00105200	-2.21825100	2.26196000

Ph(F)F

Num. Imaginary Frequencies: 0

C	1.85938700	-0.69530000	0.00000300
C	1.85918500	0.69508400	0.00000200
C	0.65706900	1.39650900	0.00000000
C	-0.53270200	0.69384200	-0.00000100
C	-0.53247200	-0.69379600	-0.00000100
C	0.65714900	-1.39641300	0.00000200
H	2.79474200	-1.24000500	0.00000500
H	2.79441700	1.24017300	0.00000300
H	0.62258300	2.47856200	0.00000000
H	0.62189100	-2.47853800	0.00000200
F	-1.70232100	-1.33950700	-0.00000200
F	-1.70204900	1.33953500	-0.00000300

PhH

Num. Imaginary Frequencies: 0

C	-1.39009000	0.06727100	0.00000000
C	-0.63671600	1.23756600	-0.00001000
C	0.75326500	1.17008900	-0.00000100
C	1.39008600	-0.06733100	-0.00000200
C	0.63677000	-1.23753800	-0.00000200
C	-0.75331500	-1.17005700	0.00000600
H	-2.47247900	0.11910600	0.00000600
H	-1.13288900	2.20097800	0.00001900
H	1.33987800	2.08134500	0.00002100
H	2.47248200	-0.11902500	0.00001300
H	1.13282200	-2.20101200	-0.00001000
H	-1.33981200	-2.08138700	0.00000100

M1H

Num. Imaginary Frequencies: 0

H	-0.64618100	-0.12552000	-2.75897300
C	-0.70819900	0.21767700	-1.72663100
C	0.23351500	1.39719800	-1.41535800
H	-1.73536900	0.45538200	-1.44748100
N	-0.28551700	-0.93473400	-0.87572800
H	-0.27582800	2.16418800	-0.83773300

H	0.64364100	1.81653900	-2.33215400
N	1.38804600	0.88997800	-0.59555200
C	1.05295500	-1.46244200	-1.28609000
C	-0.28578800	-0.54813700	0.56847800
C	2.01171900	-0.26056400	-1.34409500
C	2.38335000	1.97347900	-0.29365800
C	0.88653000	0.42161300	0.76148000
H	0.92461500	-1.92734400	-2.26217400
H	1.36197100	-2.19353800	-0.54026600
H	-0.12686500	-1.46173900	1.14049200
H	-1.24960700	-0.08754800	0.77794100
H	2.96191400	-0.51483300	-0.88011300
H	2.17188200	0.08193600	-2.36483400
Cl	3.15654800	2.58444600	-1.76137100
H	1.83416200	2.78111000	0.18857000
H	3.14252800	1.52806100	0.34857000
H	1.72674300	-0.06259900	1.25147600
H	0.55180900	1.29983900	1.30940600
F	3.60672100	-2.48261500	-0.25003300
F	2.10518400	-2.18154100	1.43828600
F	3.73437500	-0.61702900	1.06795300
F	4.30507000	-2.67792500	1.94539700
B	3.48270700	-2.03001700	1.08134100
F	-1.20476800	-1.93843700	-1.05417000
F	-0.39389000	3.17814400	0.94254900
F	-2.17231800	2.01023900	0.09972000
F	-2.52470800	3.60962500	1.72506100
F	-1.47066900	1.61790100	2.23086700
B	-1.67538600	2.64142200	1.28798800
C	-3.63576300	-1.89822900	1.10043400
C	-3.89720700	-2.89972700	0.16786200
C	-4.28502900	-2.56219500	-1.12560100
C	-4.41467000	-1.22258500	-1.48607800
C	-4.14839900	-0.22129700	-0.55540100
C	-3.75742800	-0.55890700	0.73954300
H	-3.34463700	-2.16148400	2.11131000
H	-3.80468500	-3.94179600	0.45120000
H	-4.49590800	-3.34185800	-1.84858500
H	-4.73591100	-0.96066500	-2.48818100
H	-4.24875100	0.82507100	-0.82099900
H	-3.54964800	0.22692700	1.45816300

TS1S_N2 H

Num. Imaginary Frequencies: 1

H	-0.36719800	0.18552700	-2.90774800
C	-0.53401100	0.37949500	-1.84806000
C	0.30261200	1.58478800	-1.34237200
H	-1.58824200	0.56656500	-1.65099000
N	-0.12032600	-0.80232600	-1.10140100
H	-0.28812200	2.23962600	-0.70233400
H	0.73933200	2.14396900	-2.16802500
N	1.43136400	1.03506800	-0.51007000
C	1.21261000	-1.25578400	-1.47852600
C	-0.23232900	-0.60317600	0.33547200
C	2.14996400	-0.02235300	-1.32142500
C	2.36862500	2.09980300	-0.03986000
C	0.83435500	0.43228400	0.75288900
H	1.20605700	-1.59664300	-2.51346200
H	1.52816500	-2.05729500	-0.81336900
H	-0.03111800	-1.54925200	0.83531100
H	-1.23318400	-0.23748500	0.55845600
H	3.06873300	-0.29403000	-0.80747300
H	2.37635900	0.43462900	-2.28377700
Cl	3.19685000	2.90439300	-1.38372200
H	1.77701400	2.83893600	0.49742400
H	3.11137600	1.61268300	0.59093200
H	1.65128200	-0.03627800	1.29619800
H	0.38307600	1.24816800	1.31645800
F	3.84486700	-2.23425700	-0.24837600
F	2.17914300	-2.14851200	1.30855600
F	3.73927000	-0.47532700	1.21470600
F	4.34776800	-2.56768400	1.98092500
B	3.56538800	-1.89435700	1.08927600
F	-1.62679500	-1.95189400	-1.29989200
F	-0.94789700	2.97194800	1.18496900
F	-2.45243300	1.77246500	-0.05524700
F	-3.20278700	3.03499600	1.71213300
F	-1.97646600	1.12744200	2.08434900
B	-2.16660600	2.25946000	1.26226200
C	-3.46532500	-1.80468700	1.15825200
C	-3.14802500	-2.84573600	0.32561900
C	-3.24411000	-2.67149800	-1.09813200
C	-3.96417400	-1.53285600	-1.60132000
C	-4.27014500	-0.49811200	-0.75896100
C	-3.97863600	-0.61279000	0.61380400
H	-3.30446400	-1.87360400	2.22660200
H	-2.71775800	-3.76198400	0.71238000

H	-3.13725800	-3.54110000	-1.73443000
H	-4.15113300	-1.46324400	-2.66646000
H	-4.70863200	0.41915500	-1.12975900
H	-4.16241400	0.23341100	1.26655500

TS1SET H**Num. Imaginary Frequencies: 1**

H	-0.40283900	0.13685100	-2.89161000
C	-0.55997000	0.35851400	-1.83654500
C	0.28889500	1.56282800	-1.35267000
H	-1.61266800	0.53985200	-1.62725000
N	-0.12772000	-0.80082000	-1.06370700
H	-0.29404900	2.23246300	-0.72162400
H	0.72567800	2.10401500	-2.18993300
N	1.41943700	1.01881900	-0.51668000
C	1.19213800	-1.28630900	-1.44664600
C	-0.25124700	-0.59563900	0.37261000
C	2.12979300	-0.05181800	-1.31958600
C	2.36281800	2.08932000	-0.06772500
C	0.83094800	0.43508700	0.76136300
H	1.16126900	-1.64672500	-2.47379900
H	1.50106700	-2.07701700	-0.76582900
H	-0.06008300	-1.54191200	0.87552000
H	-1.24941100	-0.21874200	0.58287200
H	3.05315300	-0.31875300	-0.81174100
H	2.34618900	0.38923700	-2.29138700
Cl	3.18890600	2.86402500	-1.42899600
H	1.77413600	2.83928000	0.45796400
H	3.10531200	1.60995900	0.56939000
H	1.65036600	-0.03236800	1.30139400
H	0.38927300	1.25986800	1.31914900
F	3.81465300	-2.25188200	-0.24029900
F	2.16313300	-2.14024400	1.32908100
F	3.72918000	-0.47550400	1.20197100
F	4.33602200	-2.56121900	1.98876200
B	3.54983300	-1.89619400	1.09663500
F	-1.51789300	-1.98745400	-1.32911100
F	-0.88739900	3.00377100	1.14535200
F	-2.42326500	1.80331600	-0.05446500
F	-3.13407800	3.11120200	1.69829900
F	-1.92960700	1.19156600	2.09027700
B	-2.11893100	2.31000200	1.25167500
C	-3.48091500	-1.77710400	1.17119200
C	-3.19702400	-2.84609600	0.35677400
C	-3.35400100	-2.71914700	-1.05343900

C	-3.98556100	-1.55845800	-1.58724600
C	-4.25716100	-0.49384500	-0.76555600
C	-3.97953700	-0.58740300	0.61110700
H	-3.30683000	-1.82862600	2.23869100
H	-2.78538700	-3.76308800	0.76047900
H	-3.20512900	-3.58495800	-1.68563600
H	-4.17395700	-1.50535000	-2.65266000
H	-4.66490900	0.42865000	-1.15882600
H	-4.15088900	0.27235100	1.24832000

F	2.18250900	-0.94951000	-0.92420500
F	3.33025400	-2.49840900	0.31445500
F	1.37898700	-1.59308500	1.12757000
B	2.06591900	-2.06048800	-0.04061700
C	1.76550900	1.63379500	0.94897000
C	2.24397100	1.81399000	-0.31797300
C	3.58779500	1.32960500	-0.65199200
C	4.17629300	0.31316300	0.22527800
C	3.68958300	0.16509700	1.49012300
C	2.48674300	0.80929800	1.83095300
H	0.80754300	2.05874600	1.23129300
H	1.69623000	2.40213200	-1.04880000
H	4.17634000	2.23290500	-0.31964500
H	5.03038600	-0.24396200	-0.14426800
H	4.13396800	-0.54733200	2.17120800
H	2.07010900	0.62297700	2.81583700

M2_H

Num. Imaginary Frequencies: 0

H	-2.31819100	-3.36672900	-2.01834300
C	-1.71910200	-2.50327100	-1.72555300
C	-1.70807700	-2.37537900	-0.18243300
H	-0.70069100	-2.65316600	-2.08688900
N	-2.26822000	-1.29620100	-2.34621600
H	-0.76429300	-2.70878300	0.25016100
H	-2.54049200	-2.89646800	0.28945600
N	-1.87307500	-0.91359600	0.14779300
C	-3.52242500	-0.94257400	-1.68411200
C	-1.31973400	-0.19654100	-2.15737000
C	-3.26346300	-0.47176800	-0.23080500
C	-1.56509800	-0.61165300	1.57419200
C	-0.87196100	-0.13195300	-0.68466900
H	-4.17693100	-1.81659700	-1.69946800
H	-4.01122500	-0.14062300	-2.23854400
H	-1.79915200	0.74108000	-2.44340400
H	-0.44598500	-0.35647500	-2.79073500
H	-3.27359500	0.61484000	-0.13776600
H	-3.95422900	-0.91769000	0.48357800
Cl	-2.55789500	-1.56641400	2.69787600
H	-0.52197400	-0.87268200	1.73803900
H	-1.76317500	0.44539200	1.74035900
H	-0.85670200	0.88470900	-0.30539100
H	0.09152900	-0.60712500	-0.52258300
F	-2.50083100	2.52041900	-0.66455100
F	-0.28188300	3.08691200	-0.65295900
F	-1.30074900	2.45529600	1.28633800
F	-1.82678400	4.48927600	0.33119700
B	-1.50199400	3.18836900	0.07018900
F	3.82739400	1.15052800	-1.97309300
F	1.29043200	-3.04006800	-0.64414400

M3_H

Num. Imaginary Frequencies: 0

H	0.93300000	-0.15560100	2.50675700
C	0.89627500	0.27692700	1.50603400
C	-0.11129900	1.43120400	1.39093500
H	1.88081000	0.62430600	1.20437800
N	0.47380300	-0.81688800	0.57335500
H	0.29655900	2.25563600	0.80757500
H	-0.42683900	1.77749100	2.37355100
N	-1.33273900	0.92778400	0.67051500
C	-0.78871400	-1.45383200	1.07075900
C	0.25317700	-0.27997500	-0.81124200
C	-1.79618300	-0.33091500	1.36204900
C	-2.41526800	1.96066400	0.60424000
C	-0.97155600	0.63450000	-0.77672700
H	-0.55528200	-2.01307800	1.97605600
H	-1.15885800	-2.12477800	0.29778600
H	0.06606000	-1.12974000	-1.46641600
H	1.14964800	0.25810500	-1.10295100
H	-2.78363900	-0.59488800	0.99088100
H	-1.84909000	-0.09460600	2.42370700
Cl	-3.04170200	2.37503500	2.20608200
H	-1.98064600	2.85092500	0.15188700
H	-3.22175800	1.53315200	0.00949300
H	-1.84223600	0.16217100	-1.22450600
H	-0.73997600	1.58628200	-1.25306700

F	-3.41276400	-2.53295900	0.21495400
F	-2.13596800	-1.97707000	-1.59235100
F	-3.79341700	-0.56330600	-0.88669200
F	-4.34845400	-2.56631300	-1.89664300
B	-3.46586900	-1.94623300	-1.06763800
F	0.47015100	3.36455300	-0.85935700
F	2.26632300	2.02215100	-0.37860800
F	2.52439400	3.80867600	-1.81582500
F	1.30936400	1.94978500	-2.44983800
B	1.66993500	2.82653200	-1.41394700
C	3.17743400	-2.81022700	1.17642100
C	2.74015700	-3.34602700	-0.03616000
C	2.81626300	-2.59223700	-1.20676000
C	3.33563300	-1.29840700	-1.16923800
C	3.77723400	-0.74762500	0.03093100
H	2.34618200	-4.35488300	-0.06312000
H	3.38212700	-0.69933700	-2.07173500
H	3.14418200	-3.37507300	2.10007200
H	2.47356500	-3.01256600	-2.14430400
C	3.68800700	-1.52038800	1.17865100
F	4.07691000	-0.98713500	2.34818900
H	1.21861400	-1.52208900	0.52538800
H	4.15292300	0.26780100	0.08220200

M1_{CH3}

Num. Imaginary Frequencies: 0

H	1.08716400	0.04061700	2.25790200
C	0.74275000	0.32672700	1.26514500
C	-0.41753700	1.33817700	1.30269900
H	1.57186100	0.69565100	0.66080100
N	0.24544000	-0.92292600	0.60766600
H	-0.12476900	2.27785900	0.84424600
H	-0.75844000	1.51496200	2.32054000
N	-1.58355300	0.76897100	0.54375200
C	-0.95084800	-1.50699700	1.29127700
C	-0.04099000	-0.66436500	-0.83166400
C	-2.06059900	-0.43771400	1.30273000
C	-2.68115400	1.78248600	0.36435500
C	-1.16556500	0.38512300	-0.86895500
H	-0.62820900	-1.78805200	2.29252400
H	-1.25892000	-2.37901800	0.71429500
H	-0.36424700	-1.60714600	-1.26615000
H	0.88057300	-0.28466200	-1.26796200
H	-2.96766200	-0.81206600	0.83941100
H	-2.27819800	-0.10906000	2.31656400
Cl	-3.30746800	2.35616300	1.91353200
H	-2.24534400	2.62168400	-0.17636300
H	-3.48141200	1.28322900	-0.18026500
H	-2.05152200	-0.02571300	-1.35021500
H	-0.81482000	1.29962000	-1.34501500
F	-3.80520700	-2.66042000	0.39194500
F	-2.32037400	-2.30799700	-1.29285400
F	-4.01746800	-0.81899600	-0.95590500
F	-4.49142700	-2.91642300	-1.80220200
B	-3.70649500	-2.21899500	-0.94062300
F	1.25434400	-1.85288300	0.68176500
F	-0.13679200	3.35319400	-0.90332100
F	1.78784100	3.02644000	0.30365400
F	1.90147500	3.99198800	-1.79038200
F	1.36913000	1.76028900	-1.53895500
B	1.26318600	3.08132100	-1.00834600
C	3.63626400	-1.82522700	-1.51526700
C	3.49916100	-0.43985400	-1.50483700
C	3.82682800	0.27386100	-0.35412800
C	4.28787400	-0.39921200	0.77442900
C	4.42952000	-1.78880000	0.77666600
C	4.09349500	-2.49156200	-0.38218500
H	3.14382300	0.09266000	-2.37926500

Ph(CH₃)H

Num. Imaginary Frequencies: 0

C	1.19405300	-1.20270100	0.00199800
C	1.89708000	-0.00190600	0.00756600
C	1.19839400	1.20024900	0.00199300
C	-0.19298000	1.19948200	-0.00815400
C	-0.90937700	0.00260200	-0.01044000
C	-0.19623100	-1.19742900	-0.00821400
H	1.72964100	-2.14498400	0.00162400
H	2.98043300	-0.00376500	0.01248100
H	1.73666900	2.14099200	0.00161500
H	-0.73201200	2.14128100	-0.01653300
H	-0.73876200	-2.13742400	-0.01649400
C	-2.41640900	0.00086600	0.00860000
H	-2.81656600	-0.82439300	-0.58304500
H	-2.78962400	-0.11281900	1.03021600
H	-2.81696800	0.93413800	-0.38995300

H	4.55402600	0.16458700	1.66388300
H	4.19807100	-3.57191600	-0.39785000
H	3.39034200	-2.38905600	-2.40830900
H	3.71363400	1.35295000	-0.34036300
C	4.96989800	-2.51061900	1.98425400
H	6.05230300	-2.64125400	1.89944100
H	4.77755900	-1.95076800	2.90102400
H	4.52620400	-3.50269700	2.08518300

F	2.69412000	3.40607300	-1.83531800
F	1.52620900	1.46805500	-2.24492900
B	1.74468200	2.54250400	-1.35664800
C	3.12376800	-2.69766700	-0.78955100
C	3.26864800	-1.63819900	-1.64335800
C	3.71200300	-0.39768200	-1.13723400
C	4.09503700	-0.24764100	0.19959500
C	3.95861000	-1.29603700	1.08432100
C	3.32466400	-2.50311600	0.61572900
H	3.03268200	-1.73093300	-2.69580300
H	4.45806900	0.71488100	0.53861600
H	3.32925000	-3.37079400	1.26556100
H	2.75971200	-3.65610500	-1.13972800
H	3.75831800	0.46046000	-1.79903900
C	4.26677600	-1.16461300	2.53895400
H	4.89991100	-1.98648900	2.88232900
H	4.75977000	-0.21872400	2.75911000
H	3.33338700	-1.21595600	3.11153700

TS1S_N2 CH3

Num. Imaginary Frequencies: 1

H	0.44868100	0.07950900	2.79257200
C	0.51598200	0.35124400	1.73851600
C	-0.43132300	1.52694800	1.38351100
H	1.53723800	0.62077800	1.47357700
N	0.11577000	-0.80693300	0.94781000
H	0.06821900	2.26829000	0.76018800
H	-0.84593100	1.99232800	2.27601400
N	-1.57754000	0.96021300	0.58878600
C	-1.15697000	-1.36601900	1.38882700
C	0.10976500	-0.52234500	-0.47837000
C	-2.17416700	-0.18854800	1.37401900
C	-2.60347600	1.99297000	0.24867900
C	-1.03482300	0.47754700	-0.74946000
H	-1.05261400	-1.76610800	2.39693600
H	-1.47118000	-2.14635000	0.69820300
H	-0.08521400	-1.44885900	-1.01618200
H	1.07467500	-0.09766300	-0.75318900
H	-3.10905100	-0.48560600	0.90514000
H	-2.36082700	0.19498400	2.37596200
Cl	-3.38860800	2.65920900	1.69108700
H	-2.09061100	2.79882800	-0.27337200
H	-3.35658100	1.50166500	-0.36623300
H	-1.86137300	0.00032100	-1.26963800
H	-0.66931700	1.35400300	-1.28239200
F	-3.81310400	-2.42677900	0.28167300
F	-2.27428700	-2.15269600	-1.37995000
F	-3.90798600	-0.57947600	-1.06911400
F	-4.46155200	-2.65271900	-1.92382300
B	-3.65129500	-1.99153300	-1.04829900
F	1.66289800	-1.86933100	0.97733000
F	0.50547300	3.18141400	-1.11052300
F	2.17574000	1.97458300	-0.11369700

TS1SET CH3

Num. Imaginary Frequencies: 1

H	0.46784700	0.04889500	2.78441200
C	0.53126300	0.34517300	1.73752700
C	-0.43036600	1.51141300	1.39491000
H	1.55127900	0.61540200	1.46941400
N	0.12474300	-0.79581000	0.92301200
H	0.06036600	2.26368200	0.77873600
H	-0.84722200	1.96176700	2.29386100
N	-1.57433400	0.94158400	0.59649600
C	-1.13288600	-1.39151200	1.36028100
C	0.13156900	-0.50070000	-0.50306600
C	-2.15703800	-0.22175500	1.37168200
C	-2.61042700	1.97089000	0.27287800
C	-1.03819500	0.47547500	-0.75132600
H	-1.00728700	-1.80897100	2.35823500
H	-1.43448000	-2.16183800	0.65319100
H	-0.03845200	-1.42757100	-1.04823900
H	1.08830600	-0.05010200	-0.76022600
H	-3.09281100	-0.52170500	0.90647000
H	-2.33810200	0.14546000	2.38061800
Cl	-3.39827300	2.60648900	1.72649200
H	-2.10354400	2.78783500	-0.23800900
H	-3.35957400	1.48154600	-0.34848700

H	-1.86196500	-0.01475900	-1.26307000	C	0.79346600	-0.38816500	-0.33283200
H	-0.69493200	1.36012500	-1.28508500	H	1.91382000	-0.70591000	3.35966700
F	-3.76000400	-2.46988900	0.27096700	H	1.35245300	0.88590100	2.81911600
F	-2.24090800	-2.15936600	-1.40196100	H	-0.12862100	1.00237700	1.03923000
F	-3.89170800	-0.61081900	-1.05945600	H	-1.15160000	-0.41007700	0.58317900
F	-4.42700100	-2.68220700	-1.93098200	H	2.70981000	0.86153700	0.92257200
B	-3.61771500	-2.02041700	-1.05702200	H	3.54322400	-0.53685400	1.65519600
F	1.57934400	-1.89675600	1.02449600	Cl	4.51898600	-1.93857300	-0.44535000
F	0.41887000	3.20544400	-1.06910400	H	2.54127600	-1.65554900	-1.68682100
F	2.12442800	2.02070200	-0.10638700	H	3.26449400	-0.07803800	-1.18760200
F	2.59501100	3.50539700	-1.79865600	H	1.08412400	0.50505700	-0.88458000
F	1.47749600	1.54293900	-2.24351800	H	0.36838400	-1.12975300	-1.00741000
B	1.67590600	2.60396200	-1.33620600	F	1.24746500	2.66656900	0.56964500
C	3.28701300	-1.57588300	-1.66768300	F	0.75895400	2.67927700	-1.65789200
C	3.17820100	-2.66756700	-0.84407900	F	2.83620100	2.01390500	-0.94689800
C	3.44025700	-2.52554500	0.54359800	F	2.22480200	4.23577500	-0.80469800
C	3.98444900	-1.30597500	1.05961100	B	1.78872900	2.94094900	-0.72146300
C	4.08038500	-0.22185800	0.20975200	F	-2.03211900	2.10583800	2.08334600
C	3.71032800	-0.34091100	-1.13316300	F	-0.75151900	-3.15384100	-0.89859400
H	3.03576100	-1.64292100	-2.71889300	F	-2.47456600	-2.10699000	0.19871000
H	2.83135700	-3.62171600	-1.22138900	F	-2.90237300	-3.23573000	-1.75316100
H	3.41848600	-3.40025700	1.18338900	F	-1.69901600	-1.27937000	-1.79927400
H	4.41070200	0.74062100	0.58163800	B	-1.97357600	-2.48184800	-1.07813800
H	3.73821400	0.53537700	-1.77106400	C	-1.73999000	2.40493700	-0.26456000
C	4.31557700	-1.21936500	2.51543000	C	-1.99696600	1.92331500	-1.50731600
H	3.42843400	-1.46049200	3.10920500	C	-2.98644200	0.92107700	-1.66185800
H	5.08907700	-1.94521900	2.78084500	C	-3.68982600	0.35526600	-0.59152400
H	4.66484300	-0.22389100	2.78697000	C	-3.40532900	0.75041000	0.69076400

M2_{CH3}

Num. Imaginary Frequencies: 0

H	0.69720300	-2.68763600	2.71543500
C	0.49510600	-2.16275300	1.78042600
C	1.68470300	-2.36003300	0.80441100
H	-0.41498200	-2.56626400	1.33805400
N	0.28382900	-0.74469800	2.06615300
H	1.40958200	-2.99818000	-0.03604800
H	2.57667500	-2.74819400	1.29477200
N	2.05396600	-1.00864700	0.24235600
C	1.54051100	-0.14098400	2.50315900
C	-0.14883000	-0.06860500	0.84403100
C	2.57856500	-0.12999900	1.35390800
C	3.02054400	-1.09533400	-0.88721300

M3_{CH3}

Num. Imaginary Frequencies: 0

H	-0.18323600	1.91852300	2.68161300
C	-0.25901600	1.77857000	1.60352000

C	-1.71728700	1.91169900	1.12556100
H	0.39321600	2.47433500	1.08210200
H	-1.80607300	2.76113100	0.44865900
H	-2.41695800	2.00607100	1.95394000
N	-2.08927900	0.67007800	0.36432200
C	-0.66490500	-0.60552100	1.96669700
C	0.26391500	0.10380200	-0.17511000
C	-2.05339200	-0.50593000	1.31034100
C	-3.42671600	0.76901300	-0.30074500
C	-1.08244400	0.50528900	-0.76813600
H	-0.68779800	-0.37352300	3.03115200
H	-0.24499600	-1.59634000	1.79838600
H	0.44566100	-0.96398600	-0.28845900
H	1.07012400	0.68094200	-0.61791300
H	-2.27821300	-1.39563300	0.72740600
H	-2.83086300	-0.33501200	2.05291000
Cl	-4.72862800	1.13601200	0.84036100
H	-3.36800200	1.57500500	-1.02899400
H	-3.61629000	-0.19617600	-0.76899200
H	-1.44532900	-0.27062300	-1.43958800
H	-1.01931800	1.47161700	-1.26930500
F	-0.82828600	-2.88827600	0.12923900
F	-0.46165800	-2.19182000	-2.01472100
F	-2.58104300	-2.15757200	-1.15249000
F	-1.56677500	-4.18017800	-1.63028100
B	-1.35441200	-2.90282400	-1.20264300
F	2.48085300	-1.21604200	2.70556300
F	-0.10556100	3.46291100	-0.76286300
F	1.96156400	2.63605500	-0.22137800
F	1.77627300	4.29762100	-1.81056200
F	1.02614900	2.15840700	-2.25504400
B	1.19290900	3.17371600	-1.30477500
C	2.21867100	-2.60352900	0.81518700
C	2.37049200	-2.78353400	-0.55622900
C	3.01277000	-1.80952500	-1.31394500
C	3.50866400	-0.65909000	-0.70788100
C	3.37309400	-0.44464600	0.66586000
C	2.71803600	-1.44386200	1.37697200
H	1.95341600	-3.66348100	-1.02889200
H	3.98666200	0.10875900	-1.30639200
H	1.69995200	-3.32816300	1.43070200
H	3.10536700	-1.93532600	-2.38526000
C	3.89262600	0.79193600	1.35087500
H	4.72673200	0.54386500	2.01147200

H	4.21752200	1.52373100	0.61381300
H	3.13171700	1.27756900	1.97031600
H	1.17860400	0.28981300	1.66118900
N	0.22379100	0.39310100	1.30369500

Ph(CH₃)F

Num. Imaginary Frequencies: 0

C	-1.78997600	-0.93758500	-0.00002200
C	-1.99529100	0.43721800	0.00003400
C	-0.90456200	1.30122800	0.00006600
C	0.36556000	0.75817100	0.00002100
C	0.61744300	-0.60871400	-0.00002800
C	-0.49502500	-1.44847400	-0.00008000
H	-2.63630400	-1.61330400	-0.00005900
H	-3.00026000	0.84087500	0.00009600
H	-1.02207800	2.37751400	0.00011400
H	-0.33705900	-2.52159600	-0.00014200
C	2.03190700	-1.11768700	0.00008400
H	2.04585300	-2.20736900	0.00022700
H	2.57428200	-0.76247100	-0.87878400
H	2.57402900	-0.76218500	0.87900600
F	1.42457800	1.59373300	-0.00010100

Ph(NH₂)H

Num. Imaginary Frequencies: 0

C	1.16749100	-1.19853900	0.00365800
C	1.87439500	0.00000000	0.00881400
C	1.16752200	1.19852700	0.00364800
C	-0.22086700	1.20379000	-0.00601600
C	-0.93303700	0.00001300	-0.00876600
C	-0.22087100	-1.20379300	-0.00602000
H	2.95682300	-0.00004700	0.01665400
H	-0.76319000	2.14344700	-0.01650500
H	-0.76325100	-2.14341700	-0.01651300
H	1.70085400	-2.14214900	0.00714100
H	1.70083900	2.14216200	0.00713100
N	-2.32790500	0.00000600	-0.07405300
H	-2.77226200	-0.83609900	0.27424700
H	-2.77227100	0.83607900	0.27431200

M1_{NH2}**Num. Imaginary Frequencies: 0**

H	0.70037500	-0.20064500	2.63131600
C	0.68561300	0.18546700	1.61274300
C	-0.30508300	1.34926800	1.40376700
H	1.68937800	0.45997500	1.28758300
N	0.24357800	-0.94240300	0.73786600
H	0.14571200	2.15211800	0.82622100
H	-0.66871600	1.72225500	2.35940900
N	-1.49427900	0.83985100	0.63547000
C	-1.05387200	-1.52567700	1.20065000
C	0.15174400	-0.49246300	-0.68455500
C	-2.03696300	-0.35664500	1.37501600
C	-2.53730300	1.90211900	0.44029600
C	-1.06752800	0.43436200	-0.76692800
H	-0.85420100	-2.03212000	2.14339800
H	-1.38799900	-2.22966700	0.44003400
H	-0.00371600	-1.38535600	-1.28947200
H	1.08592100	0.01490000	-0.92418200
H	-3.00967900	-0.61955100	0.96576500
H	-2.13551500	-0.06202000	2.41831500
Cl	-3.23916700	2.42265200	1.97707300
H	-2.04311600	2.74688100	-0.03753200
H	-3.32012400	1.45933600	-0.17464200
H	-1.92034400	-0.06848000	-1.21517400
H	-0.80599700	1.34033400	-1.30775300
F	-3.64920000	-2.57569700	0.30112800
F	-2.27084900	-2.17882000	-1.47134300
F	-3.90835900	-0.67080300	-0.93900800
F	-4.48715100	-2.71551800	-1.84845700
B	-3.62377900	-2.07475800	-1.01875400
F	1.19361100	-1.92950600	0.81842400
F	0.03953400	3.26699200	-0.93965600
F	1.91795900	2.13747000	-0.29015800
F	2.08508800	3.81494800	-1.86580500
F	1.06678700	1.80621700	-2.37713700
B	1.30747800	2.79550800	-1.40932200
C	3.89188300	-2.78732200	-0.55065100
C	3.66341600	-1.84784200	-1.55347500
C	3.66124000	-0.49443200	-1.22655300
C	3.87206400	-0.08565700	0.08572700
C	4.07938700	-1.02922800	1.09515100
C	4.09694900	-2.38738800	0.76420700
H	3.50413000	-2.16545100	-2.57633900

H	3.86043500	0.97336000	0.32199600
H	4.26333100	-3.12809500	1.53998600
H	3.90953000	-3.84398300	-0.79214900
H	3.48629700	0.25803600	-1.98847100
N	4.17051100	-0.61036900	2.43445100
H	4.62629800	-1.27881800	3.04082800
H	4.59061100	0.30368000	2.54224300

TS1S_N2 NH2**Num. Imaginary Frequencies: 1**

H	-0.12066700	0.56742800	-2.91044000
C	-0.31619100	0.73803100	-1.85140400
C	0.65202800	1.77968600	-1.23928000
H	-1.34778800	1.05713400	-1.69573600
N	-0.10918100	-0.52004100	-1.14894300
H	0.13601700	2.45775400	-0.56033300
H	1.17902700	2.33539100	-2.01311400
N	1.67844400	1.02532100	-0.43224000
C	1.15371600	-1.15632700	-1.51587600
C	-0.23440100	-0.37189200	0.29853400
C	2.25028600	-0.07681300	-1.30160800
C	2.74996500	1.91512800	0.10897200
C	0.98511000	0.43143700	0.78715300
H	1.11640700	-1.46246000	-2.56085200
H	1.32664500	-2.01502600	-0.87021300
H	-0.23612200	-1.36619900	0.74761100
H	-1.16344400	0.14932500	0.51097400
H	3.12191600	-0.49915600	-0.80721700
H	2.54077700	0.39637000	-2.23860200
Cl	3.72199600	2.65154700	-1.17579600
H	2.26039200	2.70731100	0.67266200
H	3.39610600	1.29310400	0.72713600
H	1.71524700	-0.19767300	1.28908700
H	0.66175000	1.26407700	1.41187600
F	3.57655600	-2.56232800	-0.35666500
F	1.94448600	-2.33242200	1.22170000
F	3.72648000	-0.89448900	1.20494100
F	4.03371700	-3.09307700	1.84464300
B	3.35150200	-2.26620300	1.00252300
F	-1.61430500	-1.42042200	-1.46873200
F	-0.54720400	3.12663300	1.22720600
F	-2.23964500	2.18128100	-0.00324500
F	-2.75024000	3.55966600	1.76800800

F	-1.84373100	1.47212500	2.13417800
B	-1.86469300	2.61806800	1.32650500
C	-3.36741300	-3.17881300	-0.64763600
C	-3.29487400	-3.11964800	0.71520300
C	-3.43562000	-1.86637700	1.37211500
C	-3.67465200	-0.70724900	0.68147400
C	-3.74403000	-0.74277000	-0.72911700
C	-3.49597300	-1.98443000	-1.40443400
H	-3.13663800	-4.01644200	1.29986300
H	-3.77129100	0.24048600	1.19810000
H	-3.65043500	-2.03640800	-2.47574200
H	-3.26383800	-4.12052000	-1.17182400
H	-3.36033300	-1.82391500	2.45290000
N	-3.89850100	0.39188200	-1.42770000
H	-3.96709900	0.37571200	-2.43201300
H	-3.78266800	1.28546700	-0.96142800

F	3.58800800	-2.63649200	-0.33139000
F	1.88116400	-2.42884500	1.17112200
F	3.66308800	-0.99234000	1.25996300
F	3.93828500	-3.19996500	1.88075000
B	3.29573900	-2.35983000	1.01815400
F	-1.80230700	-1.47479800	-1.68284600
F	-0.39453700	3.17336300	1.20802900
F	-2.10546700	2.26387500	-0.02341700
F	-2.59086300	3.60273400	1.78267800
F	-1.69138400	1.50499300	2.09188000
B	-1.70691400	2.67214400	1.31336700
C	-3.68755800	-3.04300600	-0.63799500
C	-3.57774900	-3.03832100	0.72456600
C	-3.53443400	-1.80746100	1.45034200
C	-3.64287200	-0.60352400	0.81988100
C	-3.77574600	-0.57967800	-0.59511400
C	-3.69864200	-1.81691900	-1.34051100
H	-3.52494900	-3.97172100	1.27109800
H	-3.59702800	0.33063600	1.36801800
H	-3.92607600	-1.79750300	-2.39887900
H	-3.71185600	-3.96905600	-1.19628900
H	-3.41845900	-1.83355300	2.52726900
N	-3.87064100	0.57277700	-1.24928700
H	-3.90147900	0.57951600	-2.25815900
H	-3.64748600	1.44448500	-0.77040800

TS1SET NH2

Num. Imaginary Frequencies: 1

H	-0.02589200	0.57648900	-3.01094400
C	-0.23737200	0.72153500	-1.95154200
C	0.72813900	1.74310500	-1.29665000
H	-1.26664800	1.04689800	-1.81126800
N	-0.05193400	-0.54722900	-1.27055100
H	0.20220800	2.42821100	-0.63342600
H	1.29681900	2.29550400	-2.04265400
N	1.70919500	0.96666900	-0.45532500
C	1.21532100	-1.18456600	-1.60197600
C	-0.24529100	-0.43422900	0.16693900
C	2.31443400	-0.12383400	-1.31686200
C	2.75770200	1.84033300	0.15135700
C	0.95992200	0.35366700	0.72200700
H	1.21800300	-1.46854200	-2.65371000
H	1.35654200	-2.06094100	-0.97237500
H	-0.27265300	-1.43373500	0.60006000
H	-1.17389700	0.09641500	0.35370900
H	3.15730000	-0.56219900	-0.78776500
H	2.65496700	0.36383300	-2.22940200
Cl	3.78757800	2.60249400	-1.07349700
H	2.24604600	2.62202100	0.70999200
H	3.37582700	1.20342700	0.78276300
H	1.66539100	-0.29084000	1.23941300
H	0.62502100	1.17584500	1.35339100

M2_{NH2}

Num. Imaginary Frequencies: 0

H	-2.24539400	2.05630400	2.99644500
C	-1.62439500	1.92840300	2.10816900
C	-2.51931500	1.82746300	0.84058400
H	-0.96482100	2.79063400	2.01084700
N	-0.80687600	0.73186100	2.28033600
H	-2.27731600	2.60152400	0.11331200
H	-3.58259400	1.84945600	1.07444900
N	-2.24164200	0.50083700	0.18403800
C	-1.66005300	-0.44735600	2.39767600
C	0.06520200	0.57953200	1.11899100
C	-2.57631400	-0.60410900	1.15722400
C	-2.97796700	0.33131300	-1.10093400
C	-0.76619700	0.44069100	-0.17688100
H	-2.26373300	-0.35359200	3.30182900
H	-1.02852300	-1.33066800	2.48589600

H	0.66787700	-0.32061100	1.25696700	H	1.45982900	-0.48437200	0.45306900
H	0.71176000	1.45673500	1.05472100	H	4.73570800	-1.05320400	-1.34335900
H	-2.42688000	-1.55179400	0.64282000	H	3.13994100	-2.12721800	-2.92387400
H	-3.63171300	-0.48905800	1.40025600	H	1.01868700	-3.09736600	-2.15067300
Cl	-4.73923400	0.40482800	-0.90203300	H	1.22168400	2.38209700	0.33084900
H	-2.68007100	1.14282800	-1.76084900	C	0.40678800	1.90198200	0.86239400
H	-2.71156300	-0.64489500	-1.50308400	C	-0.91523800	2.64725700	0.54658700
H	-0.61503000	-0.51884000	-0.66441100	H	0.64065500	1.92054200	1.92627200
H	-0.58326700	1.26445700	-0.86459900	N	0.28791000	0.49173100	0.44171500
F	-2.05450200	-3.75778800	0.18350300	H	-1.24219900	3.28347800	1.37089900
F	-0.18854500	-2.47173100	0.52456700	H	-0.83473300	3.25044700	-0.35635400
F	-1.30348700	-2.35086500	-1.46595100	N	-1.99560500	1.62615500	0.29749400
F	-0.08664800	-4.22719400	-0.94504100	C	-0.20603400	0.44708400	-0.94896200
B	-0.92420300	-3.24816700	-0.42349700	C	-0.68472500	-0.18694000	1.31977600
F	4.70475900	-0.57950300	1.40544400	C	-1.67379800	0.90751900	-0.99695700
F	-0.28396100	3.45187100	-0.26511000	C	-3.37404800	2.19096900	0.25944200
F	1.91780200	3.47054700	0.40007800	C	-1.96122900	0.64924600	1.45466200
F	1.26567200	4.65094500	-1.47091800	H	0.45555300	1.07258900	-1.54554500
F	1.32555400	2.34195400	-1.47243300	H	-0.15548100	-0.57884800	-1.31336300
B	1.04389800	3.54391200	-0.70632000	H	-0.93741700	-1.14371700	0.87610900
C	3.53497200	-2.46655600	0.50003400	H	-0.23192500	-0.34866300	2.29821800
C	2.49994300	-2.85476100	-0.24768600	H	-2.36818400	0.07318400	-1.07289400
C	1.89890200	-1.93012300	-1.20657200	H	-1.84966800	1.61987100	-1.80188100
C	2.24580000	-0.62253300	-1.29332600	Cl	-3.53403000	3.52693200	-0.88812100
C	3.22847200	-0.12770400	-0.37547600	H	-3.60937800	2.56677000	1.25309100
C	4.14639700	-1.12305800	0.27039700	H	-4.04293000	1.38191600	-0.03231800
H	2.05175600	-3.83534000	-0.15683400	H	-2.84840100	0.01920400	1.40281000
H	1.71975500	0.08404000	-1.92416200	H	-1.97492300	1.25933400	2.35960600
H	4.96246500	-1.25884500	-0.46094400	B	-3.08668600	-2.34503800	-0.13862200
H	4.03136200	-3.11006200	1.21605500	F	-3.81535600	-1.12315700	-0.12116000
H	1.09546700	-2.31219600	-1.82817900	F	-1.96797100	-2.15552200	-1.01472400
N	3.37888000	1.12756200	-0.10615900	F	-3.85828600	-3.38945700	-0.55645400
H	4.02258700	1.42673100	0.61788500	F	-2.55352100	-2.55747300	1.15213400
H	2.76138800	1.82923400	-0.53275900	B	3.48844100	1.77736500	-0.07191900

TS_{2NH2}

Num. Imaginary Frequencies: 1

C	1.31331100	-2.49299400	-0.09850800	F	1.86426800	-1.74500400	2.07192300
C	2.10175800	-1.60318900	0.72413000	H	4.09064100	-0.79104400	1.04008000
C	3.44488500	-1.27747200	0.32141500	N	0.28301000	-3.15554100	0.41750900
C	3.78802000	-1.42980700	-0.98526800	H	-0.47646200	-3.46453500	-0.17761000
C	2.86757400	-2.03616700	-1.87809100	H	0.07583800	-3.08353000	1.40308800
C	1.66353300	-2.55485900	-1.46931600				

M2_{NH2}**Num. Imaginary Frequencies: 0**

H	-2.24539400	2.05630400	2.99644500
C	-1.62439500	1.92840300	2.10816900
C	-2.51931500	1.82746300	0.84058400
H	-0.96482100	2.79063400	2.01084700
N	-0.80687600	0.73186100	2.28033600
H	-2.27731600	2.60152400	0.11331200
H	-3.58259400	1.84945600	1.07444900
N	-2.24164200	0.50083700	0.18403800
C	-1.66005300	-0.44735600	2.39767600
C	0.06520200	0.57953200	1.11899100
C	-2.57631400	-0.60410900	1.15722400
C	-2.97796700	0.33131300	-1.10093400
C	-0.76619700	0.44069100	-0.17688100
H	-2.26373300	-0.35359200	3.30182900
H	-1.02852300	-1.33066800	2.48589600
H	0.66787700	-0.32061100	1.25696700
H	0.71176000	1.45673500	1.05472100
H	-2.42688000	-1.55179400	0.64282000
H	-3.63171300	-0.48905800	1.40025600
Cl	-4.73923400	0.40482800	-0.90203300
H	-2.68007100	1.14282800	-1.76084900
H	-2.71156300	-0.64489500	-1.50308400
H	-0.61503000	-0.51884000	-0.66441100
H	-0.58326700	1.26445700	-0.86459900
F	-2.05450200	-3.75778800	0.18350300
F	-0.18854500	-2.47173100	0.52456700
F	-1.30348700	-2.35086500	-1.46595100
F	-0.08664800	-4.22719400	-0.94504100
B	-0.92420300	-3.24816700	-0.42349700
F	4.70475900	-0.57950300	1.40544400
F	-0.28396100	3.45187100	-0.26511000
F	1.91780200	3.47054700	0.40007800
F	1.26567200	4.65094500	-1.47091800
F	1.32555400	2.34195400	-1.47243300
B	1.04389800	3.54391200	-0.70632000
C	3.53497200	-2.46655600	0.50003400
C	2.49994300	-2.85476100	-0.24768600
C	1.89890200	-1.93012300	-1.20657200
C	2.24580000	-0.62253300	-1.29332600
C	3.22847200	-0.12770400	-0.37547600
C	4.14639700	-1.12305800	0.27039700

H	2.05175600	-3.83534000	-0.15683400
H	1.71975500	0.08404000	-1.92416200
H	4.96246500	-1.25884500	-0.46094400
H	4.03136200	-3.11006200	1.21605500
H	1.09546700	-2.31219600	-1.82817900
N	3.37888000	1.12756200	-0.10615900
H	4.02258700	1.42673100	0.61788500
H	2.76138800	1.82923400	-0.53275900

M3_{NH2}**Num. Imaginary Frequencies: 0**

H	0.88339700	-0.30608700	2.38469700
C	0.80815600	0.17599600	1.40898200
C	-0.18019500	1.35254100	1.39806100
H	1.78460900	0.52158600	1.07898200
N	0.32224800	-0.86233000	0.44585700
H	0.21525000	2.19776800	0.83584700
H	-0.44195700	1.65692500	2.40997300
N	-1.44329300	0.90691900	0.71508900
C	-0.92805300	-1.50217900	0.96706200
C	0.04875300	-0.25258400	-0.89743700
C	-1.89734400	-0.37829500	1.36402500
C	-2.51073900	1.95713900	0.75345900
C	-1.15141500	0.68519100	-0.75970800
H	-0.66446100	-2.11415300	1.82902000
H	-1.34620400	-2.12452800	0.17752300
H	-0.18824200	-1.06453200	-1.58371900
H	0.94305400	0.27882300	-1.20837600
H	-2.90731700	-0.60400100	1.03027900
H	-1.89318100	-0.19610800	2.43769600
Cl	-3.05086200	2.29983200	2.40264400
H	-2.08495200	2.86332800	0.32553800
H	-3.35205100	1.57147000	0.17839800
H	-2.05130600	0.25825000	-1.19445400
H	-0.91692800	1.65725700	-1.19265500
F	-3.61138200	-2.47536900	0.17154400
F	-2.42302200	-1.83207300	-1.66656400
F	-4.00376400	-0.43138100	-0.78169400
F	-4.66385700	-2.35392000	-1.88082100
B	-3.72004400	-1.80833500	-1.06715800
F	0.38800600	3.39669300	-0.77130300
F	2.18650300	2.01080800	-0.43845700
F	2.40087600	3.85204500	-1.80709000
F	1.12346100	2.04223400	-2.45989300

B	1.54241900	2.87038700	-1.41179800	H	-2.10375900	2.14392800	0.00000500
C	2.86748000	-3.08356600	0.82798400	H	-3.34583500	0.00000000	0.00000400
C	2.40552700	-3.32184500	-0.46980500	H	-2.10375900	-2.14392800	0.00000000
C	2.58880600	-2.34078400	-1.44457400	H	0.38055700	-2.14037300	-0.00000300
C	3.21518900	-1.13614700	-1.14033800	H	0.38055800	2.14037200	0.00000200
C	3.69073000	-0.87622400	0.15361500	Cl	2.24945300	0.00000000	-0.00000300
H	1.92829900	-4.26212000	-0.71265300				
H	3.34339800	-0.37257000	-1.90037000				
H	2.75992300	-3.81568600	1.61949700				
H	2.23961000	-2.51300900	-2.45580800				
N	4.32792000	0.29260400	0.48564600				
H	4.53158100	0.44333200	1.46126400				
H	4.04929300	1.12006500	-0.02799400				
C	3.48817500	-1.88310400	1.10817500				
F	3.90911800	-1.62689800	2.36628000				
H	1.04897300	-1.57986100	0.32598700				

Ph(NH₂)F

Num. Imaginary Frequencies: 0

C	-1.82071600	0.83338400	0.00447400
C	-1.95060200	-0.55090000	0.00611500
C	-0.80504100	-1.34339700	0.00210600
C	0.42904200	-0.73187500	-0.00438300
C	0.59609400	0.65265900	-0.00861900
C	-0.56491000	1.42932400	-0.00451300
H	-2.92871700	-1.01364100	0.01147500
H	-0.47122400	2.50978600	-0.01559600
H	-2.70423100	1.46018400	0.00799700
H	-0.85242300	-2.42522000	0.00715800
N	1.87189200	1.20007800	-0.07473100
H	1.96249700	2.12748900	0.31056500
H	2.61656500	0.58116700	0.20993700
F	1.55234400	-1.48616500	0.00227800

Chlorobenzene

Num. Imaginary Frequencies: 0

C	-1.56582500	1.20358200	0.00000300
C	-2.26281100	0.00000000	0.00000300
C	-1.56582600	-1.20358200	0.00000000
C	-0.17501800	-1.21151500	-0.00000100
C	0.50308700	0.00000000	0.00000000
C	-0.17501800	1.21151500	0.00000200

TS1SN2 chlorobenzene

Num. Imaginary Frequencies: 1

H	0.43742900	0.00842000	2.70196700
C	0.44580700	0.32096700	1.65745900
C	-0.54039700	1.48997700	1.39154700
H	1.44798800	0.62359200	1.35783100
N	0.02756600	-0.81232000	0.84164400
H	-0.08800600	2.25870000	0.76544500
H	-0.91223200	1.91924100	2.32036300
N	-1.71880900	0.92699900	0.64161600
C	-1.20639800	-1.41838000	1.32668300
C	-0.06123700	-0.47233200	-0.56877900
C	-2.24658400	-0.26250600	1.41585900
C	-2.78397600	1.94724400	0.39889900
C	-1.24596500	0.50105200	-0.74097500
H	-1.04071000	-1.85642700	2.31047200
H	-1.54297100	-2.17537100	0.62107000
H	-0.25741300	-1.38191500	-1.13458900
H	0.87310800	-0.00397900	-0.87492900
H	-3.20075500	-0.56408400	0.99039800
H	-2.38172800	0.07807700	2.44141600
Cl	-3.50505000	2.53686400	1.90539400
H	-2.31758900	2.78469800	-0.11702900
H	-3.55770400	1.46214200	-0.19489800
H	-2.08943600	0.01627000	-1.22542400
H	-0.93635100	1.40211300	-1.26845900
F	-3.88512700	-2.50671100	0.33100600
F	-2.45248500	-2.13600500	-1.40578500
F	-4.10219200	-0.61673700	-0.94435600
F	-4.65512900	-2.67271800	-1.84044900
B	-3.81164600	-2.02157200	-0.98947700
F	1.62250300	-1.83509100	0.71860200
F	0.22359800	3.23593100	-1.11945100
F	1.96984600	2.04250000	-0.24526800
F	2.36630600	3.53556600	-1.94623400
F	1.22666700	1.58179400	-2.35568000

B	1.46104100	2.63715600	-1.44632400	F	-4.62800000	-2.69851600	-1.83544700
C	3.00781400	-2.54681700	-1.13848200	B	-3.78420700	-2.04566000	-0.98853500
C	3.07894400	-1.47752400	-1.98808300	F	1.54673400	-1.87254300	0.76399600
C	3.50056800	-0.22240500	-1.49829400	F	0.12905700	3.24405400	-1.08302300
C	3.94243200	-0.05553300	-0.18158300	F	1.91856100	2.09096100	-0.24442000
C	3.87292500	-1.12812200	0.67257000	F	2.25165800	3.63612900	-1.91617200
C	3.25390400	-2.35953400	0.26419900	F	1.17802400	1.64861500	-2.35773500
H	2.79792800	-1.57310600	-3.02893200	B	1.38787400	2.69283500	-1.43238900
H	4.28208100	0.91231500	0.16157300	C	3.12590300	-1.48433100	-2.00209700
H	3.35782400	-3.22269500	0.90922200	C	3.08489100	-2.55791800	-1.14959200
H	2.66036100	-3.51506900	-1.47745500	C	3.36759200	-2.37474800	0.23226600
H	3.48099400	0.64203300	-2.15316400	C	3.87980000	-1.11459700	0.65969000
Cl	4.30775700	-0.96327100	2.32364800	C	3.91785600	-0.03603800	-0.19291400
				C	3.51131000	-0.21726500	-1.51806300
				H	2.84972300	-1.59347000	-3.04313700
				H	2.76960100	-3.53567500	-1.49141900
				H	3.43461900	-3.22420600	0.89895100
				H	4.21622800	0.94255100	0.15830300
				H	3.48299000	0.64230000	-2.17798000
				Cl	4.29664200	-0.93199800	2.32008100

TS1SET chlorobenzene

Num. Imaginary Frequencies: 1

H	0.47782800	-0.01580600	2.68045700
C	0.47287000	0.31682000	1.64290500
C	-0.52917100	1.47461600	1.39237900
H	1.46975000	0.62063700	1.32852100
N	0.03812500	-0.80076300	0.81180800
H	-0.08704000	2.25426500	0.77371000
H	-0.90115300	1.88800800	2.32807000
N	-1.70626900	0.90788400	0.64094700
C	-1.17777600	-1.44041400	1.29926200
C	-0.03935900	-0.46031400	-0.60090900
C	-2.22159200	-0.29083100	1.41019800
C	-2.77819200	1.92649400	0.41256600
C	-1.24389700	0.49265100	-0.75009800
H	-0.98772700	-1.88790600	2.27369500
H	-1.50613200	-2.19033100	0.58251400
H	-0.21819800	-1.37258000	-1.16772200
H	0.89021400	0.02413700	-0.89244800
H	-3.17712300	-0.59682100	0.99121200
H	-2.34838200	0.03824000	2.44037500
Cl	-3.49789000	2.49028700	1.92829100
H	-2.31463900	2.77156600	-0.09401800
H	-3.55006500	1.44421000	-0.18597700
H	-2.08630800	-0.00395600	-1.22383900
H	-0.95398100	1.39858200	-1.27946500
F	-3.84106300	-2.53695100	0.33089500
F	-2.42601000	-2.14508000	-1.41482000
F	-4.08470600	-0.64279500	-0.93220000

Mesitylene

Num. Imaginary Frequencies: 0

C	1.27470700	-0.58721600	0.01076300
C	1.12774800	0.80262700	0.00732900
C	-0.12865800	1.39725800	-0.00616400
C	-1.25930000	0.57522200	-0.01716200
C	-1.14603200	-0.81015900	-0.00841800
C	0.13134700	-1.37790200	0.00476100
H	2.01458900	1.43035500	0.01070800
H	-2.24605700	1.02989900	-0.03262900
H	0.23121800	-2.45973400	0.00745900
C	-2.36779500	-1.69242200	0.00659700
H	-2.24789400	-2.53979400	-0.67226700
H	-2.54385300	-2.09415700	1.00877300
H	-3.25858200	-1.13804100	-0.29291000
C	-0.28150400	2.89685500	0.00525400
H	-0.97501800	3.22698300	-0.77122200
H	-0.67609000	3.23797700	0.96608900
H	0.67611700	3.39226800	-0.15928800
C	2.64970000	-1.20468100	-0.00625900
H	2.60785100	-2.26923900	0.22674500
H	3.11051000	-1.09387500	-0.99155800

H	3.30592400	-0.72013400	0.71989100
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C	4.11796200	-0.37239500	0.97007700
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C	3.73409500	-1.60177200	1.44812800
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C	3.11462100	-2.52170900	0.54058400
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H	3.40569700	-0.73890400	-2.34561600
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H	4.53040400	0.36846700	1.64764700
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H	2.93609700	-3.53893500	0.87421800
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C	3.82379200	-1.96785600	2.89668100
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H	2.81829900	-2.12172900	3.30168800
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H	4.37122800	-2.90436800	3.02906400
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H	4.31805500	-1.18841700	3.47559600
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C	4.43108300	1.29936700	-0.87922500
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H	4.06142000	2.08778900	-0.22004400
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H	5.52645700	1.33868500	-0.86592900
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H	4.07604900	1.50643600	-1.88652500
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C	2.49971300	-3.26340400	-1.78867000
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H	2.59836300	-2.96316800	-2.83104300
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H	2.96614200	-4.24225500	-1.65446700
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H	1.43388900	-3.37900600	-1.56092600
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TS1SET mesitylene

Num. Imaginary Frequencies: 1

H	0.12507200	0.21361200	2.86069100
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C	0.20310600	0.51101300	1.81503300
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C	-0.82918200	1.60260600	1.43471300
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H	1.21175300	0.84892400	1.57960200
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N	-0.09077100	-0.65968400	0.99506700
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H	-0.37573600	2.38953200	0.83452200
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H	-1.30929800	2.02002400	2.31787100
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N	-1.89953700	0.95076800	0.59672300
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C	-1.32168600	-1.33774100	1.39079000
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C	-0.05487600	-0.36432500	-0.43379600
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C	-2.42877500	-0.24822500	1.35432100
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C	-2.99047600	1.90470300	0.22839000
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C	-1.28790500	0.51341000	-0.72872600
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H	-1.20113200	-1.73878000	2.39610400
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H	-1.53808500	-2.13309700	0.68055300
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H	-0.13239400	-1.30377500	-0.97896800
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H	0.87584000	0.15515200	-0.65512000
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H	-3.31950100	-0.61626600	0.85103200
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H	-2.67918000	0.10681800	2.35272600
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Cl	-3.87527800	2.49010400	1.64643700
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H	-2.52125300	2.75237500	-0.26866900
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H	-3.67974000	1.36285700	-0.41811900
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TS1SN2 mesitylene

Num. Imaginary Frequencies: 1

H	0.68488000	0.19574900	2.38113000
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C	0.43548900	0.40084900	1.33964500
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C	-0.63371100	1.51688900	1.22467800
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H	1.33533400	0.67611100	0.78807700
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N	-0.10846500	-0.81778500	0.75455500
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H	-0.26650300	2.37262200	0.66370600
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H	-0.98681500	1.83890500	2.20224400
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N	-1.81897500	0.94493200	0.49295500
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C	-1.29971200	-1.30592700	1.43912200
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C	-0.33014400	-0.68582800	-0.67926800
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C	-2.37654100	-0.18608400	1.32361300
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C	-2.85722600	1.98475700	0.20377700
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C	-1.36285100	0.44650900	-0.87418200
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H	-1.05102800	-1.50883100	2.48046800
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H	-1.65524400	-2.20774600	0.94268300
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H	-0.72708100	-1.62537100	-1.05529200
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H	0.61612600	-0.41989800	-1.14551100
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H	-3.28271600	-0.55218200	0.85103400
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H	-2.61654200	0.23702900	2.29732900
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Cl	-3.49311400	2.73042900	1.67940300
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H	-2.37608800	2.75755400	-0.39367400
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H	-3.67132500	1.48596800	-0.31952700
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H	-2.25155800	0.08266800	-1.38720900
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H	-0.91091400	1.30444800	-1.37302200
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F	-4.46884600	-2.21733500	0.42187000
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F	-2.79096400	-2.16334900	-1.11849300
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F	-4.32491500	-0.47278500	-1.05619600
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F	-4.95776300	-2.56336700	-1.80971300
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B	-4.17936900	-1.89217700	-0.91253700
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F	1.38254100	-1.85965700	0.79495000
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F	0.17196000	3.26443400	-1.19063100
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F	1.87905500	2.86444600	0.28927600
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F	2.37334500	3.54145400	-1.85554800
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F	1.52724800	1.44174500	-1.45989900
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B	1.50883200	2.81596500	-1.07649500
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C	3.09654200	-2.24941900	-0.86662400
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C	3.48839100	-1.00305800	-1.29711400
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C	3.98851800	-0.04228100	-0.39687600
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H	-2.05698200	-0.04529100	-1.25626700
H	-1.00189200	1.41536500	-1.26622600
F	-3.78480000	-2.64436900	0.22369000
F	-2.23834500	-2.22298900	-1.39955200
F	-4.03113100	-0.82172500	-1.14052200
F	-4.34958700	-2.94321200	-1.99656300
B	-3.63479400	-2.19962500	-1.10532300
F	1.36183200	-1.65838900	1.16531800
F	-0.05776100	3.36762400	-0.98805900
F	1.69036500	2.23853300	-0.03440100
F	2.11045000	3.79197700	-1.67660500
F	1.08939600	1.79236900	-2.19417200
B	1.22948000	2.83177600	-1.25401500
C	3.33253700	-1.14746500	-1.29376400
C	3.08608500	-2.30525100	-0.59020400
C	3.29043900	-2.29543400	0.81910600
C	3.83961100	-1.15754200	1.47517900
C	4.06341600	-0.01923200	0.73389300
C	3.82048700	0.01054900	-0.65435500
H	3.14466800	-1.11213600	-2.36204200
H	3.17858200	-3.22198700	1.37319800
H	4.43859000	0.87816100	1.21460300
C	4.06282000	-1.20865800	2.95633100
H	3.10876100	-1.36850800	3.46788000
H	4.71801200	-2.04124100	3.22392700
H	4.50643900	-0.28426200	3.32510900
C	4.12970800	1.23503500	-1.45254500
H	4.09171900	2.13434000	-0.83966800
H	5.13868600	1.13757400	-1.87066000
H	3.43018600	1.35265700	-2.28045700
C	2.50618800	-3.52673200	-1.23453000
H	3.08790100	-4.41714800	-0.98457100
H	1.48814700	-3.68786900	-0.86502400
H	2.46651000	-3.42576700	-2.31851400

Anisole

Num. Imaginary Frequencies: 0

C	1.32267300	1.34809100	-0.00001400
C	2.27043200	0.33626800	-0.00003200
C	1.84614000	-0.99305800	-0.00003800
C	0.49650300	-1.30096500	0.00004200
C	-0.45377900	-0.27622300	0.00007200
C	-0.04156600	1.05505000	0.00004900

H	1.63709600	2.38541900	0.00002800
H	3.32681400	0.57390200	-0.00009500
H	2.57426900	-1.79575700	-0.00005300
H	0.14626100	-2.32588100	0.00007900
H	-0.75946700	1.86390200	0.00016100
O	-1.75317400	-0.67440900	-0.00000800
C	-2.74752100	0.32711500	-0.00005100
H	-3.70163700	-0.19516400	-0.00028500
H	-2.67775800	0.95548300	0.89366900
H	-2.67747700	0.95569500	-0.89360600

TS1SN2 anisole

Num. Imaginary Frequencies: 1

H	-0.09266100	0.63446100	-2.88069200
C	-0.26613600	0.74949600	-1.81072000
C	0.64641700	1.83537000	-1.18428400
H	-1.30909300	0.98928600	-1.61672600
N	0.05669900	-0.51898100	-1.16550000
H	0.10286600	2.44286000	-0.46084100
H	1.10580100	2.46070900	-1.94810100
N	1.74898700	1.12801500	-0.43847700
C	1.34877600	-1.04072500	-1.60221600
C	-0.02194800	-0.44643700	0.28597400
C	2.37283000	0.10615500	-1.36604300
C	2.76859100	2.07169100	0.11084800
C	1.13652700	0.44080500	0.77470300
H	1.30219900	-1.29928100	-2.65952500
H	1.60858200	-1.91271000	-1.00539400
H	0.08817300	-1.45452800	0.68832700
H	-0.98382200	-0.02237200	0.55758500
H	3.28324200	-0.27476500	-0.90903500
H	2.60682300	0.63549000	-2.28867400
Cl	3.64890500	2.92895500	-1.16445500
H	2.23944500	2.80216900	0.72029600
H	3.47501600	1.47443100	0.68617000
H	1.92739300	-0.14165700	1.23918900
H	0.76439100	1.22466100	1.43411600
F	3.90834700	-2.31697700	-0.53929900
F	2.29867000	-2.26362600	1.07733800
F	3.97171300	-0.69970600	1.08007800
F	4.44986100	-2.89157500	1.63183900
B	3.69238100	-2.08594300	0.83316800
F	-1.43000100	-1.54361400	-1.40961400

F	-0.56496400	2.98737600	1.46392200	H	2.27925200	2.78307400	0.68975100
F	-2.11119400	1.91252400	0.16316700	H	3.48895500	1.43061900	0.67236500
F	-2.81683600	3.12031300	1.98512600	H	1.91638500	-0.15837300	1.23550300
F	-1.66932100	1.14620800	2.27233700	H	0.78509700	1.23455600	1.42993500
B	-1.81063400	2.32058600	1.51214300	F	3.83869400	-2.38406000	-0.53049300
C	-2.65040600	-3.33702000	-0.21362200	F	2.23660500	-2.28342300	1.09111400
C	-2.53366800	-2.99703500	1.10547900	F	3.94372500	-0.75688300	1.07610300
C	-2.95599000	-1.71462800	1.53349300	F	4.37542400	-2.95472500	1.64318300
C	-3.55332100	-0.80479400	0.67887400	B	3.63370900	-2.13896100	0.84142800
C	-3.67513000	-1.14156100	-0.66995700	F	-1.37438800	-1.53611400	-1.46619200
C	-3.10080800	-2.36681700	-1.15485100	F	-0.45972400	3.03445100	1.43443700
H	-2.11753400	-3.69139200	1.82393500	F	-2.06373600	2.01092900	0.16190700
H	-3.85736800	0.16314000	1.05222500	F	-2.69508500	3.24833300	1.99414400
H	-3.31624400	-2.64266100	-2.17910600	F	-1.61404100	1.23347800	2.26401300
H	-2.31826600	-4.30163300	-0.57665700	B	-1.72968500	2.41176900	1.50505500
H	-2.81419600	-1.42432500	2.56881100	C	-2.58965100	-2.96546900	1.16066200
O	-4.20434800	-0.36644500	-1.59931500	C	-2.75212400	-3.35281400	-0.14597200
C	-4.78957200	0.88383400	-1.20429300	C	-3.23910400	-2.42903100	-1.09191300
H	-4.03712100	1.53402600	-0.75710200	C	-3.70565800	-1.14965200	-0.65496500
H	-5.18106300	1.31670600	-2.12041900	C	-3.53749200	-0.76116800	0.67878700
H	-5.60515600	0.70193200	-0.50119500	C	-2.96432600	-1.65940400	1.55785500

TS1SET anisole

Num. Imaginary Frequencies: 1

H	-0.11216100	0.62241400	-2.88215900
C	-0.27175300	0.75677200	-1.81271500
C	0.66828000	1.82712800	-1.20218600
H	-1.30895600	1.00996400	-1.60620700
N	0.04127200	-0.50716900	-1.15142400
H	0.14088400	2.45803600	-0.48726900
H	1.14101600	2.42960200	-1.97600400
N	1.75666700	1.10461700	-0.44899400
C	1.31689900	-1.06778300	-1.58917900
C	-0.04704600	-0.42449600	0.30069700
C	2.35981600	0.06251000	-1.36910900
C	2.79490100	2.03523300	0.08966100
C	1.13566000	0.43917200	0.77304600
H	1.25067700	-1.33726400	-2.64229200
H	1.55603300	-1.93825100	-0.98180300
H	0.03702700	-1.43279800	0.70693300
H	-0.99902400	0.02764400	0.55952500
H	3.26502100	-0.33037700	-0.91194600
H	2.59962800	0.57820800	-2.29783000
Cl	3.69160700	2.85759100	-1.19647900

4-Anisaldehyde

Num. Imaginary Frequencies: 0

C	0.80342700	1.41373400	-0.00001100
C	1.46996600	0.18496600	-0.00004300
C	0.72927800	-0.99485600	-0.00007400
C	-0.65750900	-0.96111800	-0.00005600
C	-1.31373800	0.27509000	-0.00004500
C	-0.57688000	1.46490700	0.00008300
H	1.37807200	2.33492200	0.00012900
H	1.25929500	-1.94063700	0.00001900
H	-1.21520200	-1.88746800	0.00015000

H	-1.11615000	2.40361700	0.00028400
O	-2.65691200	0.41755500	-0.00001700
C	-3.45224300	-0.75293200	0.00001400
H	-4.48496300	-0.41313200	-0.00037100
H	-3.26461300	-1.35473100	-0.89404600
H	-3.26517200	-1.35433200	0.89454900
C	2.94626500	0.14506400	-0.00008500
H	3.43856800	1.13866700	-0.00047500
O	3.60425800	-0.86455900	0.00015000

F	1.69547000	-2.28924900	0.29440300
F	2.48929700	-3.22819200	2.22887300
F	1.57314100	-1.11773600	2.25489900
B	1.50933300	-2.41474700	1.72062800
C	2.88013100	2.55827900	-1.13284400
C	2.84082400	2.56106200	0.23519900
C	3.14326600	1.37031000	0.95290700
C	3.54345300	0.21479500	0.31931900
C	3.58758200	0.20097800	-1.08105800
C	3.12482500	1.34080600	-1.82993200
H	3.76429100	-0.67052200	0.89960400
H	3.30613300	1.33708200	-2.89669100
H	2.63671700	3.45182700	-1.69823700
H	3.05635600	1.39007400	2.03467200
O	3.94825200	-0.83192900	-1.81030800
C	4.44952900	-2.01093300	-1.15425300
H	3.67917600	-2.44639300	-0.51845700
H	4.71724900	-2.68880700	-1.95927900
H	5.33644300	-1.75332200	-0.57234000
C	2.49546600	3.79962800	0.98225300
H	2.22935800	4.67075400	0.35413100
O	2.50368900	3.86952200	2.18050100

TS1SN2 4-anisaldehyde

Num. Imaginary Frequencies: 1

H	-0.39659500	-1.43831600	-2.78239000
C	-0.14768400	-1.36945000	-1.72332700
C	-1.14212700	-2.16608600	-0.84004800
H	0.86503400	-1.72105800	-1.54518200
N	-0.24383000	0.03417000	-1.33442400
H	-0.62891600	-2.68542800	-0.03017100
H	-1.73321200	-2.86218400	-1.43304800
N	-2.08614300	-1.17192700	-0.21278900
C	-1.48047300	0.64255800	-1.81727000
C	-0.07773900	0.24790100	0.09708200
C	-2.62846600	-0.27433300	-1.30628300
C	-3.18676300	-1.82743400	0.55692300
C	-1.29989200	-0.36245500	0.80970000
H	-1.47488100	0.67197800	-2.90632200
H	-1.57989500	1.64508000	-1.40647200
H	-0.04527500	1.32239900	0.28176600
H	0.84320200	-0.23101800	0.41360900
H	-3.44792300	0.31520500	-0.90271700
H	-2.99239100	-0.93773000	-2.08950400
Cl	-4.25603400	-2.78425800	-0.48071300
H	-2.72494000	-2.49152600	1.28517300
H	-3.76604000	-1.03079300	1.02239700
H	-1.97084200	0.40121000	1.19426500
H	-0.97836000	-1.05539200	1.58809500
F	-3.75632700	2.45092200	-0.95570600
F	-2.06458300	2.48849900	0.57477000
F	-3.93108300	1.22252200	0.96926100
F	-4.06807400	3.52760600	1.06296300
B	-3.48281300	2.47399400	0.42657200
F	1.36305300	0.75975000	-1.83401200
F	0.21110400	-2.93047400	1.91143300

TS1SET 4-anisaldehyde

Num. Imaginary Frequencies: 1

H	-0.35294800	-1.42447800	-2.79992100
C	-0.12490400	-1.37023100	-1.73582500
C	-1.14313100	-2.15818700	-0.87210200
H	0.88335100	-1.72356700	-1.53720100
N	-0.22276500	0.02911400	-1.32965400
H	-0.64642500	-2.70087700	-0.06746400
H	-1.74292900	-2.83234400	-1.48114400
N	-2.07419900	-1.15626600	-0.23607600
C	-1.44171300	0.66563500	-1.82018300
C	-0.04379700	0.22927600	0.10345900
C	-2.60173600	-0.24137900	-1.32280200
C	-3.18559400	-1.80618500	0.52464100
C	-1.28383400	-0.36461800	0.79829300
H	-1.41798300	0.70213300	-2.90833600
H	-1.52379100	1.66592900	-1.40057900
H	0.01094000	1.30107100	0.29447200
H	0.86605500	-0.27696600	0.40935700
H	-3.41412100	0.35602700	-0.91653900

H	-2.97151500	-0.89194300	-2.11389600
Cl	-4.26346300	-2.73681800	-0.52654000
H	-2.73289600	-2.48318000	1.24681300
H	-3.75502500	-1.00649600	0.99713900
H	-1.94610700	0.40874800	1.17859100
H	-0.98153700	-1.06493900	1.57706600
F	-3.67946900	2.49647800	-0.96299200
F	-1.99224300	2.49886000	0.57261600
F	-3.88059700	1.26215200	0.95495000
F	-3.97995400	3.56904100	1.05987500
B	-3.41076500	2.50960400	0.42063000
F	1.30728100	0.77559000	-1.89921300
F	0.10650100	-2.97325500	1.87177100
F	1.66901000	-2.38390500	0.30789200
F	2.35602000	-3.34561900	2.27751600
F	1.51238400	-1.20337000	2.25848100
B	1.43063000	-2.50092700	1.72681600
C	2.82452100	2.54315300	0.31054700
C	2.92501400	2.60414300	-1.05772700
C	3.24659100	1.44142900	-1.78825200
C	3.62231000	0.25382000	-1.08153300
C	3.51552400	0.19915400	0.31693200
C	3.10216200	1.32651700	0.98927200
H	3.40953300	1.46494700	-2.85739100
H	3.70338100	-0.71567300	0.86189400
H	2.70025300	3.52266900	-1.58912600
H	2.97538200	1.29916900	2.06668100
O	4.00574400	-0.75158900	-1.84318500
C	4.43429400	-1.97304200	-1.21933100
H	3.62045500	-2.41049000	-0.64042700
H	4.72042600	-2.62498600	-2.03942600
H	5.29832000	-1.77469800	-0.58200000
C	2.43270300	3.74604700	1.09245300
H	2.18650200	4.64110200	0.49054800
O	2.38527100	3.76465000	2.29191400

Phenol

Num. Imaginary Frequencies: 0

C	-1.12752400	1.21467100	-0.00001100
C	-1.84986100	0.02758900	0.00001300
C	-1.16655700	-1.18641500	0.00001700
C	0.22072000	-1.21910200	-0.00001900
C	0.93586700	-0.02391400	0.00003000

C	0.26374500	1.19517100	-0.00000600
H	-1.64512400	2.16666600	-0.00004000
H	-2.93221500	0.04630400	-0.00000800
H	-1.71928800	-2.11853700	0.00001600
H	0.76812800	-2.15342200	-0.00006900
H	0.82572400	2.12404200	-0.00004700
O	2.29581000	-0.11048200	-0.00002600
H	2.67796000	0.77080100	0.00021200

TS1SN2 phenol

Num. Imaginary Frequencies: 1

H	0.40826600	0.10476200	2.81829900
C	0.49222200	0.37407600	1.76511100
C	-0.45694200	1.54142800	1.38859600
H	1.51644900	0.64985900	1.52034300
N	0.11270500	-0.78895200	0.96987900
H	0.04720600	2.28113900	0.76714800
H	-0.88613800	2.01047100	2.27221400
N	-1.58901400	0.96336300	0.58115000
C	-1.16261300	-1.35663600	1.39297800
C	0.12510600	-0.50721500	-0.45724900
C	-2.18779900	-0.18711900	1.36176000
C	-2.61762600	1.98743800	0.22392600
C	-1.02571100	0.47934300	-0.74801000
H	-1.07010400	-1.75403100	2.40328200
H	-1.46056400	-2.14050300	0.69918000
H	-0.05053600	-1.43739500	-0.99567500
H	1.08963200	-0.07364000	-0.71834300
H	-3.11389000	-0.49249700	0.88091700
H	-2.39073800	0.19766200	2.36002600
Cl	-3.42696800	2.65233100	1.65352000
H	-2.10368600	2.79532900	-0.29393900
H	-3.35875100	1.48891600	-0.39968300
H	-1.84145600	-0.00775600	-1.27599900
H	-0.66131000	1.35653000	-1.28063600
F	-3.78790700	-2.44842800	0.25735800
F	-2.23162600	-2.16732800	-1.38670800
F	-3.88405600	-0.60830000	-1.10319300
F	-4.40739500	-2.69046300	-1.95482500
B	-3.61411100	-2.01729800	-1.07271400
F	1.65096300	-1.84633300	1.01475900
F	0.49942900	3.18470100	-1.11232100
F	2.16015000	2.00749200	-0.06687800

F	2.70106200	3.42768000	-1.79107500
F	1.56560200	1.47232700	-2.20701200
B	1.75147500	2.55794300	-1.32393700
C	3.14249100	-2.65750200	-0.80997300
C	3.31110100	-1.56645100	-1.60854100
C	3.75852800	-0.33786300	-1.04364800
C	4.10013100	-0.22910900	0.28941600
C	3.92622700	-1.33370300	1.11510500
C	3.30911800	-2.52607200	0.60576300
H	3.10301800	-1.61273100	-2.66959600
H	4.44792700	0.70629000	0.70741100
H	3.30267000	-3.41503100	1.22753200
H	2.78729600	-3.60050500	-1.20614800
H	3.82688000	0.53928700	-1.67748100
O	4.20084700	-1.20634200	2.41085700
H	4.02544200	-2.02498200	2.88815800

F	-3.94405900	-2.30171800	0.22273400
F	-2.26483300	-2.18030000	-1.31701800
F	-3.84220000	-0.52399800	-1.21672200
F	-4.42342700	-2.61233800	-2.01529500
B	-3.65619300	-1.94370800	-1.10844400
F	1.56232200	-2.13830800	1.34150500
F	0.62674800	3.07883500	-1.13417100
F	2.14592000	1.87556500	0.07446300
F	2.88403000	3.16700900	-1.67475100
F	1.66678100	1.26399800	-2.07783500
B	1.85146900	2.38074300	-1.23084900
C	3.06872100	-2.35312400	-1.08398800
C	3.39743300	-1.17615400	-1.70138300
C	3.98831000	-0.10303500	-0.96284600
C	4.24648300	-0.21662300	0.38150700
C	3.86348300	-1.39055000	1.03375200
C	3.28086400	-2.48909700	0.30383000
H	3.21288800	-1.03340700	-2.75867300
H	4.64071800	0.60831100	0.95947800
H	3.24011000	-3.46313800	0.77423500
H	2.64132300	-3.17937800	-1.63668600
H	4.18832600	0.83348000	-1.47106500
O	3.97868800	-1.46773800	2.34862800
H	3.37313300	-2.15176500	2.67178500

TS1SET phenol

Num. Imaginary Frequencies: 1

H	0.24304300	0.10819200	2.95627900
C	0.40091400	0.33283200	1.90214700
C	-0.46519100	1.53344900	1.41989800
H	1.45105700	0.53137600	1.69798800
N	-0.02762200	-0.81157200	1.11795400
H	0.11628100	2.22224700	0.80926800
H	-0.92571300	2.05438100	2.25722300
N	-1.57256000	0.98291500	0.55682700
C	-1.33891700	-1.31809600	1.48148200
C	0.13253300	-0.61639400	-0.30972500
C	-2.29187200	-0.09439200	1.34187400
C	-2.51119900	2.05040100	0.09042400
C	-0.96046900	0.40274300	-0.71362600
H	-1.31946200	-1.68075700	2.50810100
H	-1.62873200	-2.11085100	0.79485900
H	-0.03669000	-1.56391600	-0.81755100
H	1.12815300	-0.22473400	-0.49980000
H	-3.20065600	-0.36974400	0.81269800
H	-2.53347000	0.34122700	2.31011900
Cl	-3.37155900	2.81618400	1.43556400
H	-1.91404400	2.80444400	-0.42008200
H	-3.23728300	1.56918600	-0.56389700
H	-1.76885700	-0.07483400	-1.26108600
H	-0.52633700	1.23142400	-1.27006700

Naphthaline

Num. Imaginary Frequencies: 0

C	-2.42395800	-0.70787800	0.00000100
C	-1.24135200	-1.39815000	0.00000000
C	-0.00000700	-0.71051600	-0.00000100
C	0.00000000	0.71051900	-0.00000100
C	-1.24135300	1.39814800	-0.00000100
C	-2.42395700	0.70787900	0.00000100
H	1.23610200	-2.48294900	-0.00000400
H	-3.36610200	-1.24303100	0.00000100
H	-1.23611400	-2.48294400	0.00000100
C	1.24136100	-1.39815300	-0.00000100
C	1.24136100	1.39815600	-0.00000100
H	-1.23611600	2.48294500	0.00000200
H	-3.36610300	1.24302800	0.00000200
C	2.42395300	0.70788300	0.00000100
C	2.42395300	-0.70788700	0.00000100
H	1.23611100	2.48295000	-0.00000400

H	3.36610800	1.24301800	0.00000400
H	3.36610600	-1.24302400	0.00000100

C	3.51507500	-1.59792000	-0.69266300
C	3.91452900	-0.62260900	-1.63814000
C	4.20651200	0.65697000	-1.23210900
H	3.04755500	-2.03537100	2.67217900
H	4.30655800	2.02260800	0.42785000
H	3.71185700	0.32368100	2.12456700
C	2.92799700	-2.22359000	1.61184800
C	3.13354200	-2.90151700	-1.08859700
H	3.94841100	-0.89163900	-2.68841700
H	4.44791100	1.42741600	-1.95262200
C	2.72561500	-3.86405100	-0.17290500
C	2.66164100	-3.54526100	1.17454900
H	3.16680200	-3.14861700	-2.14551400
H	2.45260000	-4.85456300	-0.51287900
H	2.33432100	-4.28152800	1.89891800

TS1SN2 naphthaline

Num. Imaginary Frequencies: 1

H	0.12461100	0.65183900	2.68530700
C	0.13906000	0.69885300	1.59637100
C	-0.85423100	1.76688400	1.06322300
H	1.14536700	0.92260800	1.24046900
N	-0.27083800	-0.60019400	1.08044700
H	-0.37480000	2.47975200	0.39646200
H	-1.34372700	2.29959300	1.87630800
N	-1.92550200	1.04982200	0.28505900
C	-1.56277400	-1.04332400	1.58837300
C	-0.21852400	-0.65646900	-0.37185100
C	-2.59420300	0.05758100	1.20839800
C	-2.91943000	1.99509000	-0.31347000
C	-1.27424200	0.34482300	-0.89874100
H	-1.50041400	-1.16018100	2.66985500
H	-1.83320400	-1.98604700	1.11475800
H	-0.47061500	-1.66615100	-0.68948900
H	0.77980800	-0.36387500	-0.68851900
H	-3.45633100	-0.36640300	0.70084500
H	-2.91576000	0.62239000	2.08155200
Cl	-3.80622000	2.91106400	0.91438200
H	-2.36475200	2.69903500	-0.93116700
H	-3.62614800	1.39409600	-0.88403700
H	-2.06937400	-0.16400000	-1.43863400
H	-0.79414400	1.12359000	-1.49137600
F	-4.23974100	-2.31354500	0.38742100
F	-2.51109800	-2.33576900	-1.09826400
F	-4.14642700	-0.74924500	-1.28519100
F	-4.62197000	-2.95026200	-1.80025000
B	-3.91654100	-2.12968900	-0.96868000
F	1.17681500	-1.67205900	1.51034000
F	0.57556000	3.73058700	-1.01781000
F	1.90126600	2.96309500	0.69104100
F	2.84385000	3.38509700	-1.36324000
F	1.40311200	1.61181500	-1.08097900
B	1.70527100	2.95976400	-0.71048300
C	4.12681000	0.99694200	0.12948900
C	3.77406300	0.04991100	1.07646500
C	3.46316700	-1.25590000	0.68288800

TS1SET naphthaline

Num. Imaginary Frequencies: 1

H	-0.81657400	0.12001900	-2.26502900
C	-0.49694700	0.27426800	-1.23482600
C	0.48738600	1.46583500	-1.10475500
H	-1.36461600	0.42089300	-0.59283200
N	0.21287300	-0.92201100	-0.78991200
H	0.07388000	2.25878800	-0.48701600
H	0.77179200	1.86406200	-2.07665100
N	1.74721300	0.96263300	-0.44925700
C	1.40022000	-1.23106100	-1.57698800
C	0.48529500	-0.90630200	0.63805600
C	2.38338400	-0.04096900	-1.37961200
C	2.68455700	2.08247900	-0.11148400
C	1.39635500	0.31776600	0.88864500
H	1.10408800	-1.34422400	-2.61881700
H	1.84546500	-2.14934500	-1.19712500
H	0.99748000	-1.82790700	0.90112600
H	-0.46172100	-0.79369200	1.16326300
H	3.32496300	-0.36767900	-0.95002200
H	2.57015500	0.47795400	-2.31771000
Cl	3.17824000	2.99724300	-1.54504100
H	2.14926100	2.75165400	0.56055200
H	3.56671000	1.63432300	0.34310300
H	2.33729200	0.01393300	1.34455600
H	0.88081700	1.08352000	1.46728400
F	4.82063100	-1.80933400	-0.68093400

F	3.11633000	-2.10978800	0.80251900
F	4.43460900	-0.25268300	0.95226300
F	5.30154600	-2.31776600	1.52144100
B	4.46807600	-1.65803800	0.66675100
F	-1.05757100	-2.19473800	-0.93769300
F	-0.24779200	3.00668100	1.52457600
F	-1.98578000	2.63860900	0.07907300
F	-2.43894600	3.03821800	2.29652000
F	-1.45220600	1.06837200	1.65311600
B	-1.55250200	2.47597700	1.41291900
C	-4.49398200	0.27283200	-2.00111000
C	-4.05150600	-1.03925500	-1.95707400
C	-3.60827800	-1.59034200	-0.74656800
C	-3.61690900	-0.79083500	0.42652800
C	-4.06586500	0.54299900	0.35882700
C	-4.49614400	1.06587400	-0.84476600
H	-3.05068200	-3.52578200	-1.56043200
H	-4.83459400	0.69372100	-2.93993400
H	-4.03929000	-1.64711900	-2.85538200
C	-3.04900000	-2.90289500	-0.67384700
C	-3.13470300	-1.34783400	1.64249000
H	-4.02535800	1.16552600	1.24631400
H	-4.80944200	2.10084200	-0.89620900
C	-2.69384400	-2.66263100	1.71200000
C	-2.66496100	-3.44679300	0.56367300
H	-3.11217300	-0.71244400	2.52131400
H	-2.35262400	-3.06870300	2.65604700
H	-2.29111700	-4.46247400	0.60208500