Supporting Information for

Isonitriles as Stereoelectronic Chameleons: The Donor-Acceptor Dichotomy in Radical Additions

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Contents:

Computational details

Calculations were carried with the *Gaussian 09* software package,[1] using the (U)M06-2X DFT functional[2] (with an ultrafine integration grid of 99,590 points) with the 6-311++G(d,p) basis set for all atoms except of Sn and Ge, for which we have used the Def2-QZVPP[3] basis set. Grimme's D3 version (zero damping) for empirical dispersion[4] was also included. Frequency calculations were carried for all structures to confirm them as either a minimum or a Transition State (TS). Intrinsic Reaction Coordinates (IRC)[5] were determined for the TS of interest. Barriers were evaluated from isolated species due to formation of complexes for some systems, but not all of them. We performed Natural Bond Orbital[6] (NBO6) analysis on key intermediates and transition states. NBO deletions were performed at the UHF/6-311G(d) level of theory unless otherwise noted. Spin density was evaluated from the NBO analysis data. The Gibbs Free energy values are reported at 298 K, unless noted otherwise. We have used *GoodVibes*[7] by Funes-Ardoiz and Paton to obtain the temperature-corrected Gibbs Free energies for the calculating temperature effects on selectivity in multifunctional substrates.
We have also evaluated B3LYP[8], B3LYP-D3 and ωB97X-D2[9] functionals with the 6-311++G(d,p) basis set and ultrafine integration grid. Choice of methodology can be supported by internal consistency of thermodynamic data. The combination of the M06-2X with the D3 empirical dispersion correction was chosen for the evaluation of radical additions in order to provide an accurate estimate of supramolecular contributions to the transition state energies.
Geometries, energies and frequencies presented in this SI were organized with ESIgen.[10]

Method evaluation

We have evaluated a combination of functionals commonly used for radical organic chemistry and found out that they all trend similarly in terms of reaction energy and activation barriers. It was evident that dispersion functions play a major role in activation energies of aryl-radical additions to PhNC, as shown by the comparison of B3LYP data with and without the dispersion corrections. We decided to use the unrestricted M06-2X with D3 dispersion functions due to this method ability to provide good results with the heavier radicals from the group IV, such as Sn.

Table S1: Comparison of different DFT methods for the addition of Me and Ph-radicals to PhNC (6-311++G(d,p) basis set)

method	Me				Ph			
	$\Delta H^{\neq}$	ΔH_{rxn}	$\Delta G^{\neq}$	ΔG_{rxn}	$\Delta H^{\neq}$	ΔH_{rxn}	$\Delta G^{\neq}$	ΔG_{rxn}
(U)M06-2X-D3	5.1	-25.6	12.6	-15.7	0.1	-38.7	9.6	-26.9
(U)wB97X-D2	3.5	-28.6	12.7	-18.8	-0.8	-41.6	8.2	-30.2
(U)B3LYP	4.8	-40.0	12.0	-16.4	6.1	-34.1	14.7	-22.7

(U)B3LYP-D3	3.0	-26.6	10.2	-17.0	-0.9	-40.1	7.9	-29.5

*TS energies are relative to dissociated reactants
Energies in kcal/mol.
Basis set: 6-311++G(d,p)

Calculated Enthalpies and Gibbs Free Energies for additions to PhNC

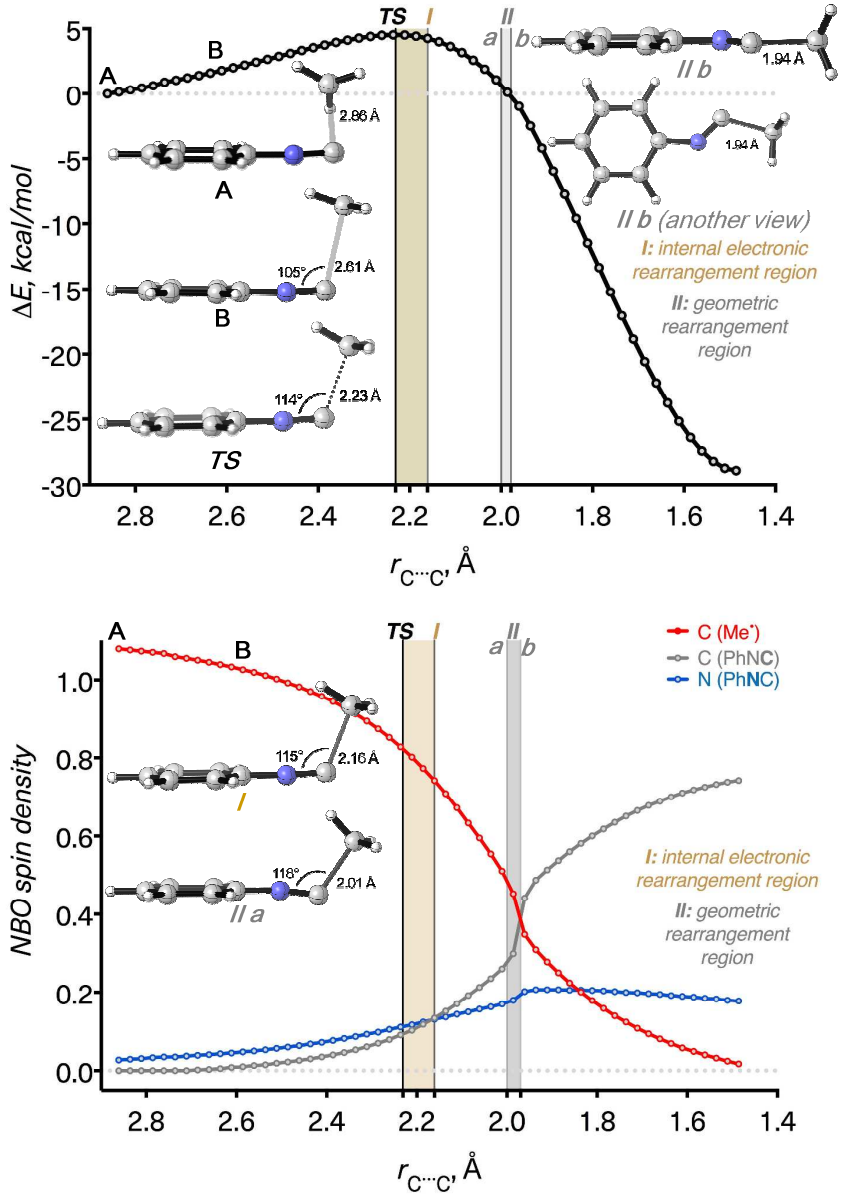
Table S2: Energies for addition of radicals to PhNC

R	$\Delta H^{\neq}$	ΔH_{rxn}	$\Delta G^{\neq}$	ΔG_{rxn}
Me	5.1	-25.6	12.6	-15.7
CF_3	0.0	-25.2	8.6	-13.5
Ph	0.1	-38.7	9.6	-26.9
Me_3Si	-1.4	-25.5	16.1	-14.6
Me_3Sn	-2.7	-13.5	6.2	-3.2
p-OMePh	-0.6	-40.8	9.3	-29.0
*per*FPh	–	-40.9	–	-29.1
*t*Bu	0.6	-21.8	11.8	-9.0
p-FPh	-0.3	-39.8	8.6	-28.4
p-CNPh	-0.8	-38.3	8.5	-26.6
OMe	5.2	-24.9	15.0	-13.8
H	2.2	-25.1	7.7	-17.9
Me_3Ge	-1.1	-15.9	7.9	-5.3
DMF	1.9	-17.3	12.3	-5.9
Et	3.4	-23.7	13.9	-12.0
H	2.2	-25.1	7.7	-17.9
$HOCH_2$	2.7	-18.8	12.7	-7.7
n-Pr	3.2	-24.4	14.6	-12.1
i-Pr	2.4	-22.7	13.2	-10.4

*TS energies are relative to dissociated reactants. UM06-2X(D3)/6-311++G(d,p), energies in kcal/mol.

Tracking addition of Me-radical to PhNC substrate with NBO scans

We have performed NBO scans on the addition of Me-radical to PhNC. NBO analysis were performed for each point of the PES shown in Figure 2 of the main text.



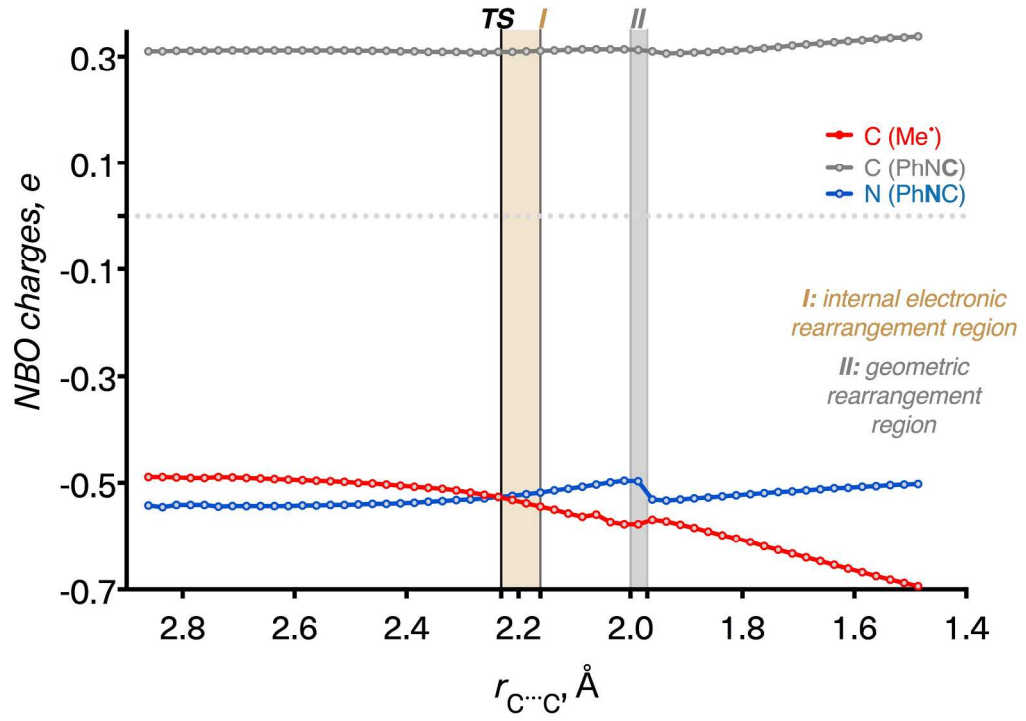


Figure S1. Potential energy profile (top), evolution of spin density (middle) and charges (bottom) for the addition of Me radical to PhNC

General correlations

We have analyzed a number of correlations throughout this project. Below we offer some of the correlations not included in the main manuscript.

Not included in the main manuscript:

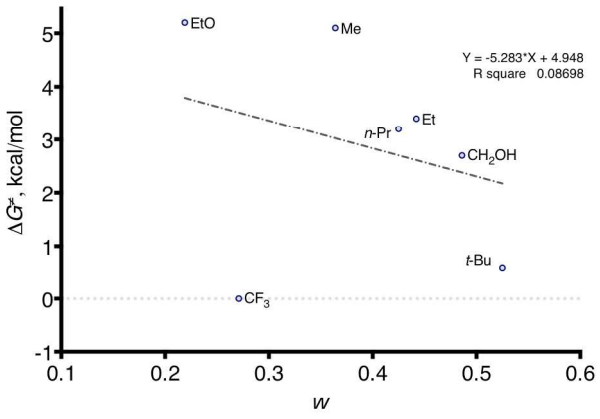


Figure S2. Activation Free energy *vs.* nucleophilicity for a few examples.

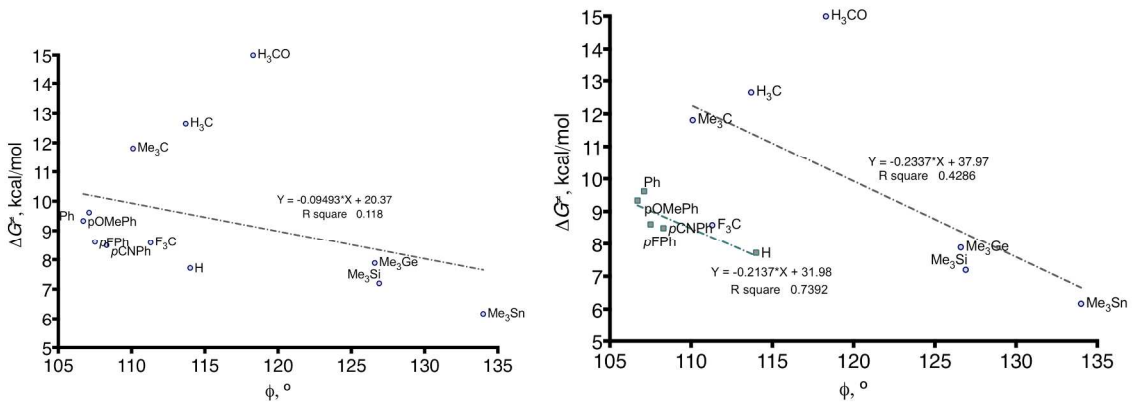


Figure S3. Activation Free energy *vs.* angle of attack for the forming bond in the TS. Left: selected examples without sorting. Right: selected examples sorted by similarities.

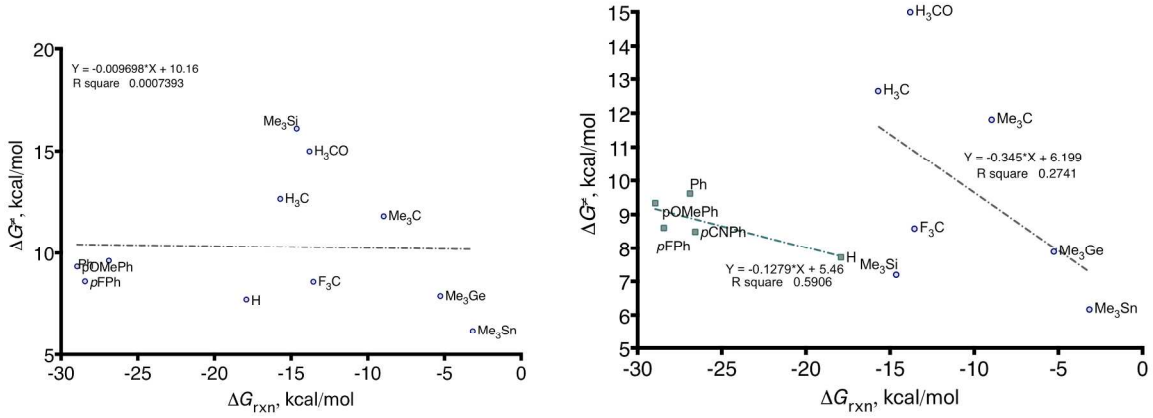


Figure S4. Activation Free energy *vs.* reaction free energy. Left: selected examples without sorting. Right: selected examples sorted by similarities.

Included in the main manuscript:

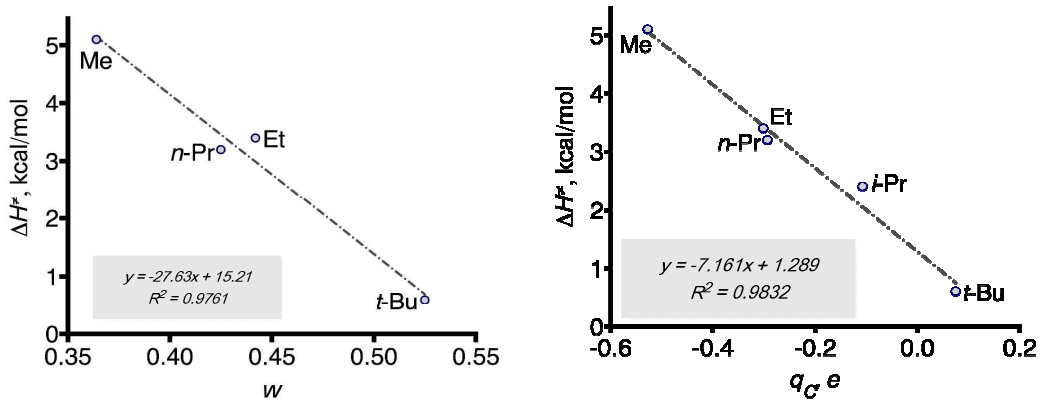


Figure S5. Activation enthalpy *vs.* nucleophilicity (left, nucleophilicity is estimated from the *w*-values) and vs. positive charge at the radical carbon (right) for Me, Et, *n*-Pr, *i*-Pr, and *t*-Bu radicals (the *w*-value for *i*-Pr radical is not available)

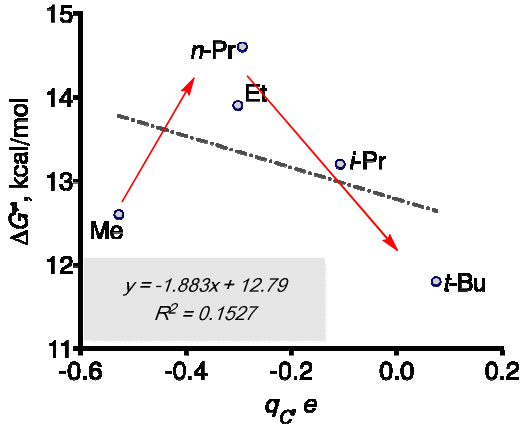
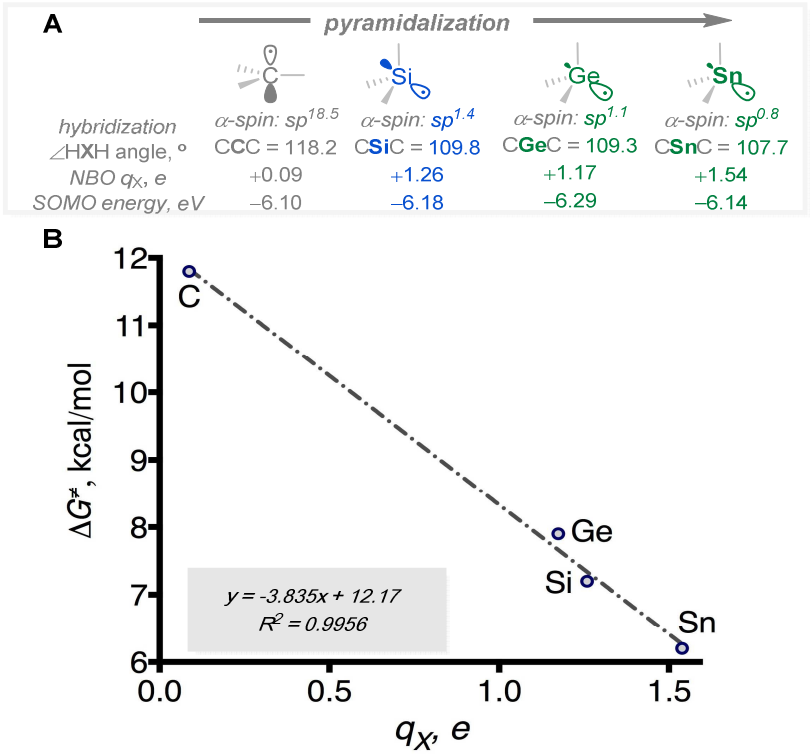
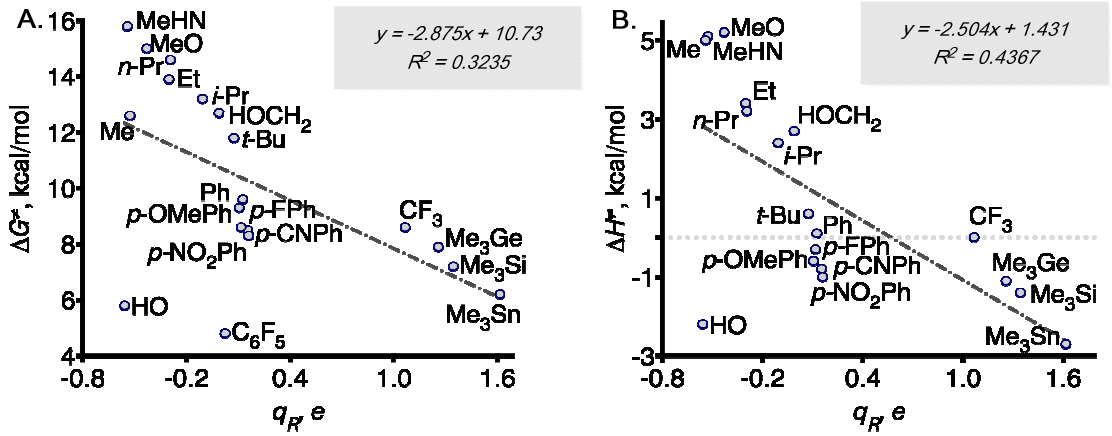


Figure S6. Correlation of the Gibbs activation barriers for alkyl radical additions to PhNC with the NBO charge at the radical carbon.



Scheme S1. A. Increase in pyramidalization of group 14 XMe_3 radicals. B: Correlation between natural charge at the radical-center for group IV elements and their free energy barriers towards addition to PhNC.



Scheme S2. Global correlations for all radicals in this work. A. Correlation between natural charge at the radical-center for all evaluated systems and their activation free energies towards addition to PhNC. B: Same but for activation enthalpies.

NBO deletions for representative radical additions (Me, *t*Bu, Ph, CF_3 and $SnMe_3$) to PhNC

We have performed NBO deletions on the addition of representative radicals to PhNC.

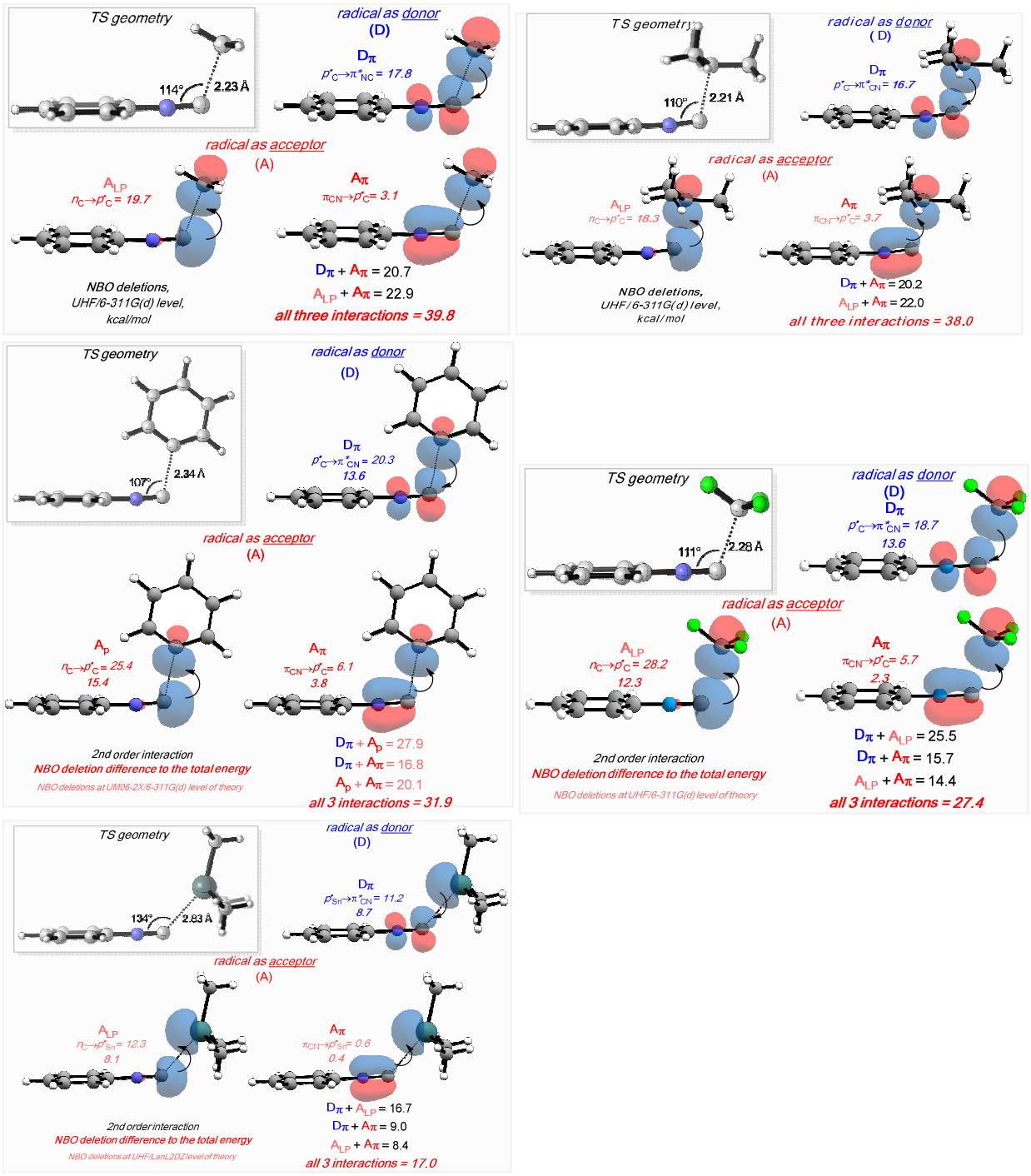
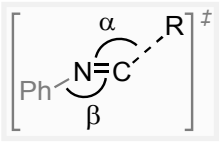


Figure S7. NBO interactions for the three odd-electron interactions identified in transition states for the addition of Me, t-Bu, Ph, CF_3 and Me_3Sn *radicals to PhNC. The deletion energies are shown for each individual interaction and for selected combinations of the three interactions. D denotes interactions where the radical is a donor, A denotes interactions where the radical is an*

acceptor; subscript π refers to interaction with the isonitrile π or π orbital, subscript LP refers to interactions with the isonitrile lone pair.*Values in kcal/mol.

Summary of geometry features for TS and products of radical addition to PhNC

Table S3. Geometry features for TS and products of radical addition to PhNC

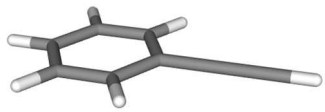


TS

R	**TS**			**Product**	
	α angle	β angle	distance	α angle	β angle
Me	113.7	176.2	2.2	129.9	127.0
CF_3	111.3	178.8	2.3	125.7	130.1
Ph	107.1	174.8	2.3	127.5	129.5
Me_3Si	126.9	177	2.7	128.1	133.1
Me_3Sn	134	178.3	2.8	127.0	128.0
p-OMePh	106.7	174.5	2.3	129.8	127.5
*t*Bu	110.1	172.7	2.2	130.3	126.9
p-FPh	107.5	175.4	2.3	129.5	127.6
p-CNPh	108.3	176.0	2.3	127.9	128.8
OMe	118.3	177.9	2.0	126.5	127.0
H	114.1	179.2	2.1	132.4	128.3
Me_3Ge	126.7	176.4	2.7	128.9	128.2
DMF	111.5	167.2	2.1	131.3	128.6
Et	110.4	174.6	2.2	130.2	126.9
HOMe	105.3	168.7	2.2	128.4	127.7
n-Pr	110.6	174.2	2.2	130.3	126.8
i-Pr	111.1	174.5	2.2	129.8	127.0

Structural, energetic and spectroscopic calculated parameters for all species

Calculated geometries (in cartesian coordinates) with their respective energies (in hartree), charge, multiplicity, stoichiometry, number of imaginary frequencies and top 10 frequencies (in cm^{-1}).



Charge	0
Multiplicity	1
Stoichiometry	C8H6
Electronic Energy (Eh)	-308.337830581
Sum of electronic and zero-point Energies (Eh)	-308.227472
Sum of electronic and thermal Energies (Eh)	-308.221097
Sum of electronic and enthalpy Energies (Eh)	-308.220153
Sum of electronic and thermal Free Energies (Eh)	-308.257866
Number of Imaginary Frequencies	0

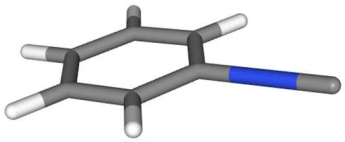
__Molecular Geometry in Cartesian Coordinates__

xyz

C	2.204126	0.000000	0.000000
C	1.507283	1.204854	0.000000
C	0.118846	1.208778	0.000000
C	-0.586138	0.000000	-0.000000
C	0.118846	-1.208778	-0.000000
C	1.507283	-1.204854	-0.000000
H	3.287543	-0.000000	0.000000
H	2.046649	2.144426	0.000000
H	-0.431527	-2.141529	-0.000000
H	2.046649	-2.144426	-0.000000
H	-0.431527	2.141529	0.000000
C	-2.020208	0.000000	-0.000000
C	-3.222028	0.000000	-0.000000
H	-4.285848	-0.000000	-0.000000

__Frequencies__ (Top 10 out of 36)

1. 142.4036 cm-1 (Symmetry: A)
2. 159.2799 cm-1 (Symmetry: A)
3. 368.1662 cm-1 (Symmetry: A)
4. 407.9600 cm-1 (Symmetry: A)
5. 471.3386 cm-1 (Symmetry: A)
6. 543.4546 cm-1 (Symmetry: A)
7. 551.9548 cm-1 (Symmetry: A)
8. 634.6191 cm-1 (Symmetry: A)
9. 693.0961 cm-1 (Symmetry: A)
10. 705.4646 cm-1 (Symmetry: A)



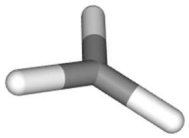
Charge	0
Multiplicity	1
Stoichiometry	C7H5N
Electronic Energy (Eh)	-324.406386185
Sum of electronic and zero-point Energies (Eh)	-324.30717
Sum of electronic and thermal Energies (Eh)	-324.300994
Sum of electronic and enthalpy Energies (Eh)	-324.30005
Sum of electronic and thermal Free Energies (Eh)	-324.337417
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	0.000000	-2.139990	0.000000
C	0.000000	-1.444482	-1.205424
C	0.000000	-0.055964	-1.213498
C	0.000000	0.628138	0.000000
C	0.000000	-0.055964	1.213498
C	0.000000	-1.444482	1.205424
H	0.000000	-3.223032	0.000000
H	0.000000	-1.983554	-2.144754
H	0.000000	0.504895	2.139279
H	0.000000	-1.983554	2.144754
H	0.000000	0.504895	-2.139279
C	0.000000	3.188172	0.000000
N	0.000000	2.018253	0.000000

__Frequencies__ (Top 10 out of 33)

1. 151.7226 cm-1 (Symmetry: A')
2. 169.5690 cm-1 (Symmetry: A")
3. 345.0788 cm-1 (Symmetry: A')
4. 414.4652 cm-1 (Symmetry: A")
5. 481.1487 cm-1 (Symmetry: A')
6. 501.5277 cm-1 (Symmetry: A")
7. 532.8006 cm-1 (Symmetry: A')
8. 632.6669 cm-1 (Symmetry: A")
9. 703.7936 cm-1 (Symmetry: A')
10. 783.3714 cm-1 (Symmetry: A')



Charge	0

Multiplicity	2
Stoichiometry	CH3
Electronic Energy (Eh)	-39.8209033598
Sum of electronic and zero-point Energies (Eh)	-39.791131
Sum of electronic and thermal Energies (Eh)	-39.788012
Sum of electronic and enthalpy Energies (Eh)	-39.787068
Sum of electronic and thermal Free Energies (Eh)	-39.809262
Number of Imaginary Frequencies	0

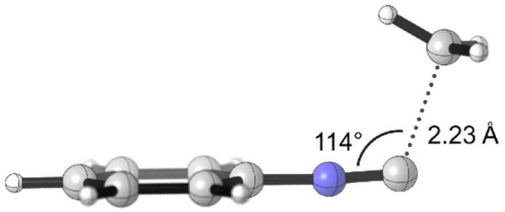
__Molecular Geometry in Cartesian Coordinates__

xyz

C	0.000000	0.000000	0.000000
H	0.000000	1.078550	0.000000
H	0.934051	-0.539275	0.000000
H	-0.934051	-0.539275	0.000000

__Frequencies__ (Top 10 out of 6)

1. 440.5996 cm-1 (Symmetry: A2")
2. 1412.6339 cm-1 (Symmetry: E')
3. 1412.6858 cm-1 (Symmetry: E')
4. 3146.7812 cm-1 (Symmetry: A1')
5. 3328.0202 cm-1 (Symmetry: E')
6. 3328.0236 cm-1 (Symmetry: E')



Charge	0
Multiplicity	2
Electronic Energy (Eh)	-364.221182617
Sum of electronic and zero-point Energies (Eh)	-364.089145
Sum of electronic and thermal Energies (Eh)	-364.079911
Sum of electronic and enthalpy Energies (Eh)	-364.078967
Sum of electronic and thermal Free Energies (Eh)	-364.12652
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

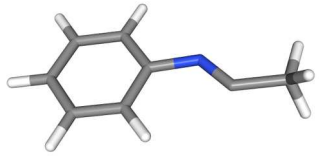
xyz

C	2.705552	-0.001403	0.363694
C	2.030699	1.203755	0.190324
C	0.686965	1.214076	-0.156875
C	0.017038	0.001031	-0.329242
C	0.685407	-1.213229	-0.159345

C	2.029157	-1.205335	0.187905
H	3.754236	-0.002350	0.633820
H	2.552811	2.143226	0.325038
H	0.144290	-2.139806	-0.302276
H	2.550058	-2.145745	0.320746
N	-1.318003	0.002183	-0.676956
C	-2.477542	0.002249	-0.898502
C	-3.742337	-0.002297	0.939303
H	0.147033	2.141632	-0.297889
H	-2.974739	-0.064144	1.699399
H	-4.234061	0.949706	0.798413
H	-4.323240	-0.890870	0.737874

__Frequencies__ (Top 10 out of 45)

1. -413.9646 cm-1 (Symmetry: A) *
2. 17.1616 cm-1 (Symmetry: A)
3. 35.8085 cm-1 (Symmetry: A)
4. 51.9496 cm-1 (Symmetry: A)
5. 174.4640 cm-1 (Symmetry: A)
6. 185.9921 cm-1 (Symmetry: A)
7. 339.2204 cm-1 (Symmetry: A)
8. 415.1699 cm-1 (Symmetry: A)
9. 467.4264 cm-1 (Symmetry: A)
10. 498.5005 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C8H8N
Electronic Energy (Eh)	-364.274508256
Sum of electronic and zero-point Energies (Eh)	-364.137125
Sum of electronic and thermal Energies (Eh)	-364.128786
Sum of electronic and enthalpy Energies (Eh)	-364.127842
Sum of electronic and thermal Free Energies (Eh)	-364.171711
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz

C	-2.749236	0.250012	-0.000067
C	-2.258302	-1.050806	-0.000061
C	-0.886748	-1.279518	0.000051
C	-0.001221	-0.205252	0.000057
C	-0.491389	1.103128	0.000059
C	-1.861151	1.324203	0.000026
H	-3.817674	0.428873	-0.000119

H	-2.942952	-1.890510	-0.000101
H	0.210037	1.929194	0.000217
H	-2.239628	2.339718	0.000069
C	2.317517	0.298843	-0.000304
C	3.783725	0.057340	0.000017
H	3.999349	-1.015008	0.000031
H	4.231654	0.523456	-0.879304
H	4.231226	0.523421	0.879574
H	-0.482204	-2.284343	0.000109
N	1.384431	-0.506071	0.000122

__Frequencies__ (Top 10 out of 45)

1. 37.7037 cm-1 (Symmetry: A)
2. 117.4953 cm-1 (Symmetry: A)
3. 130.5045 cm-1 (Symmetry: A)
4. 148.4642 cm-1 (Symmetry: A)
5. 284.5481 cm-1 (Symmetry: A)
6. 363.8318 cm-1 (Symmetry: A)
7. 415.7428 cm-1 (Symmetry: A)
8. 419.6431 cm-1 (Symmetry: A)
9. 522.7916 cm-1 (Symmetry: A)
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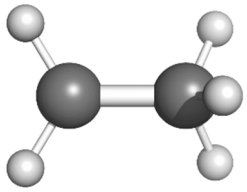


Charge	0
Multiplicity	2
Stoichiometry	C2H5
Electronic Energy (Eh)	-79.1274832889
Sum of electronic and zero-point Energies (Eh)	-79.067872
Sum of electronic and thermal Energies (Eh)	-79.063898
Sum of electronic and enthalpy Energies (Eh)	-79.062953
Sum of electronic and thermal Free Energies (Eh)	-79.091994
Number of Imaginary Frequencies	0

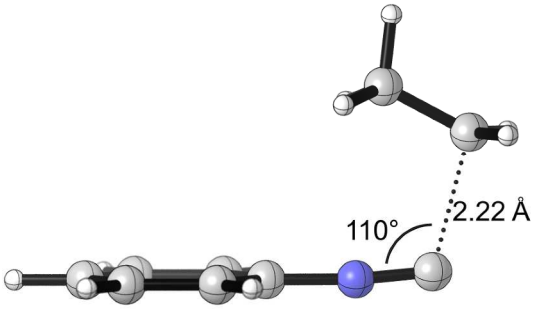
__Molecular Geometry in Cartesian Coordinates__

xyz

C	0.694069	0.000001	-0.000538
H	1.103719	0.885035	-0.492285
H	1.085667	-0.000046	1.026834
H	1.103720	-0.884991	-0.492362
C	-0.793663	0.000000	-0.023548
H	-1.347770	-0.925413	0.051165
H	-1.347774	0.925411	0.051165

__Frequencies__ (Top 10 out of 15)

1. 125.3125 cm-1 (Symmetry: A)
2. 440.2256 cm-1 (Symmetry: A)
3. 810.9625 cm-1 (Symmetry: A)
4. 982.2424 cm-1 (Symmetry: A)
5. 1080.4002 cm-1 (Symmetry: A)
6. 1193.4922 cm-1 (Symmetry: A)
7. 1405.2194 cm-1 (Symmetry: A)
8. 1471.2753 cm-1 (Symmetry: A)
9. 1489.9513 cm-1 (Symmetry: A)
10. 1491.7092 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H10N
Electronic Energy (Eh)	-403.530143155
Sum of electronic and zero-point Energies (Eh)	-403.368795
Sum of electronic and thermal Energies (Eh)	-403.358487
Sum of electronic and enthalpy Energies (Eh)	-403.357542
Sum of electronic and thermal Free Energies (Eh)	-403.407309
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

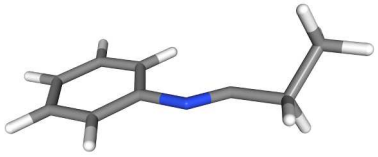
xyz

C	-2.904482	-0.000442	0.519719
C	-2.261427	-1.204582	0.246049
C	-0.983311	-1.213405	-0.294361
C	-0.343885	0.000467	-0.559001
C	-0.983385	1.213892	-0.292491
C	-2.261499	1.204154	0.247907
H	-3.901893	-0.000793	0.941340
H	-2.757732	-2.144841	0.453630
H	-0.469899	2.141435	-0.512029
H	-2.757860	2.144059	0.456951
N	0.927111	0.000915	-1.091338
C	2.056183	0.001199	-1.443652
C	3.417987	-0.000180	0.315916
H	-0.469772	-2.140577	-0.515341
H	3.946615	-0.913366	0.071880
H	3.946422	0.913534	0.073445

C	2.478272	-0.001283	1.476566
H	3.018965	-0.002439	2.431348
H	1.834484	0.881967	1.470081
H	1.834178	-0.884298	1.468141

__Frequencies__ (Top 10 out of 54)

1. -405.3073 cm-1 (Symmetry: A) *
2. 22.5219 cm-1 (Symmetry: A)
3. 41.2036 cm-1 (Symmetry: A)
4. 45.4332 cm-1 (Symmetry: A)
5. 157.0086 cm-1 (Symmetry: A)
6. 161.4716 cm-1 (Symmetry: A)
7. 194.3791 cm-1 (Symmetry: A)
8. 236.9714 cm-1 (Symmetry: A)
9. 353.4704 cm-1 (Symmetry: A)
10. 413.3752 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H10N
Electronic Energy (Eh)	-403.577589459
Sum of electronic and zero-point Energies (Eh)	-403.411254
Sum of electronic and thermal Energies (Eh)	-403.401651
Sum of electronic and enthalpy Energies (Eh)	-403.400706
Sum of electronic and thermal Free Energies (Eh)	-403.448593
Number of Imaginary Frequencies	0

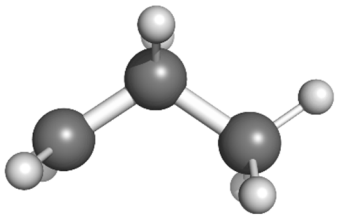
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-3.239184	0.422336	0.066140
C	-2.866302	-0.913797	0.161628
C	-1.522497	-1.268692	0.119715
C	-0.547167	-0.286070	-0.026869
C	-0.918213	1.057527	-0.120326
C	-2.260724	1.404986	-0.073225
H	-4.285800	0.699492	0.102381
H	-3.621662	-1.682601	0.272201
H	-0.146822	1.811036	-0.228086
H	-2.546730	2.447862	-0.144698
C	1.789221	-0.023896	-0.341820
C	3.236055	-0.382873	-0.375653
H	3.571952	-0.305821	-1.413628
H	3.345525	-1.427023	-0.062142
H	-1.209341	-2.302744	0.197236

N	0.805442	-0.709498	-0.058320
C	4.066925	0.551904	0.507009
H	5.123514	0.286860	0.451714
H	3.952601	1.588194	0.184925
H	3.749991	0.482678	1.548754

__Frequencies__ (Top 10 out of 54)

1. 20.7709 cm-1 (Symmetry: A)
2. 56.2311 cm-1 (Symmetry: A)
3. 82.5596 cm-1 (Symmetry: A)
4. 118.8926 cm-1 (Symmetry: A)
5. 235.9190 cm-1 (Symmetry: A)
6. 281.4424 cm-1 (Symmetry: A)
7. 350.4534 cm-1 (Symmetry: A)
8. 356.2210 cm-1 (Symmetry: A)
9. 419.1955 cm-1 (Symmetry: A)
10. 477.0157 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C3H7
Electronic Energy (Eh)	-118.430335977
Sum of electronic and zero-point Energies (Eh)	-118.341625
Sum of electronic and thermal Energies (Eh)	-118.336488
Sum of electronic and enthalpy Energies (Eh)	-118.335543
Sum of electronic and thermal Free Energies (Eh)	-118.36972
Number of Imaginary Frequencies	0

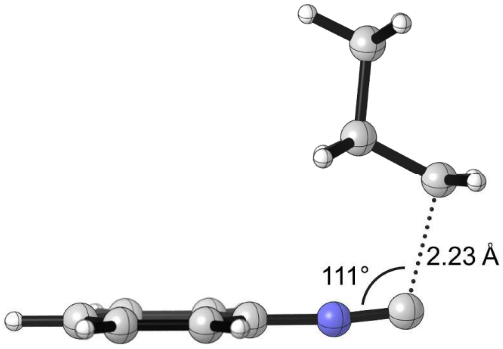
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.067052	0.579607	-0.000034
H	-0.048923	1.230852	0.878837
H	-0.048905	1.230742	-0.878989
C	-1.311431	-0.239966	0.000003
H	-1.720150	-0.622773	-0.926086
H	-1.720342	-0.622423	0.926151
C	1.206217	-0.288083	0.000025
H	2.103711	0.334880	-0.000016
H	1.234098	-0.930255	0.882824
H	1.234100	-0.930371	-0.882690

__Frequencies__ (Top 10 out of 24)

1. 22.4488 cm-1 (Symmetry: A)
2. 251.6036 cm-1 (Symmetry: A)
3. 333.6067 cm-1 (Symmetry: A)
4. 499.6403 cm-1 (Symmetry: A)
5. 748.7469 cm-1 (Symmetry: A)
6. 895.9339 cm-1 (Symmetry: A)
7. 910.9613 cm-1 (Symmetry: A)
8. 1043.1479 cm-1 (Symmetry: A)
9. 1106.1268 cm-1 (Symmetry: A)
10. 1196.5189 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H12N
Electronic Energy (Eh)	-442.833322858
Sum of electronic and zero-point Energies (Eh)	-442.643006
Sum of electronic and thermal Energies (Eh)	-442.631452
Sum of electronic and enthalpy Energies (Eh)	-442.630508
Sum of electronic and thermal Free Energies (Eh)	-442.683851
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

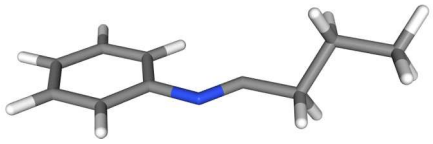
xyz

C	-3.112539	0.916855	0.000615
C	-2.545643	0.508054	1.204708
C	-1.417586	-0.300169	1.213302
C	-0.852001	-0.698166	-0.000635
C	-1.416619	-0.296931	-1.213957
C	-2.544685	0.511264	-1.204112
H	-3.992932	1.547353	0.001106
H	-2.984503	0.819198	2.144964
H	-0.963090	-0.622885	-2.141454
H	-2.982791	0.824914	-2.143887
N	0.271360	-1.496716	-0.001257
C	1.299959	-2.080279	-0.001730
C	3.009663	-0.654507	0.000129
H	-0.964807	-0.628599	2.140291
H	3.477206	-1.002244	0.914426

H	3.478168	-1.000957	-0.914163
C	2.347235	0.686103	0.000698
H	1.698004	0.778611	-0.876232
H	1.697919	0.777799	0.877661
C	3.361851	1.840006	0.001280
H	2.853204	2.807026	0.001715
H	4.003104	1.791294	0.883997
H	4.003183	1.792127	-0.881426

__Frequencies__ (Top 10 out of 63)

1. -384.8763 cm-1 (Symmetry: A) *
2. 17.7522 cm-1 (Symmetry: A)
3. 35.3858 cm-1 (Symmetry: A)
4. 40.7179 cm-1 (Symmetry: A)
5. 74.5681 cm-1 (Symmetry: A)
6. 128.9326 cm-1 (Symmetry: A)
7. 182.0073 cm-1 (Symmetry: A)
8. 203.9418 cm-1 (Symmetry: A)
9. 255.5416 cm-1 (Symmetry: A)
10. 338.4215 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H12N
Electronic Energy (Eh)	-442.881274231
Sum of electronic and zero-point Energies (Eh)	-442.686409
Sum of electronic and thermal Energies (Eh)	-442.675445
Sum of electronic and enthalpy Energies (Eh)	-442.674501
Sum of electronic and thermal Free Energies (Eh)	-442.726376
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

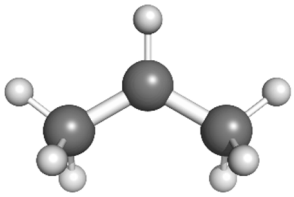
xyz

C	-3.820556	-0.387635	-0.212940
C	-2.877326	-1.387594	0.016843
C	-1.538025	-1.065101	0.182204
C	-1.134253	0.270864	0.118062
C	-2.075515	1.271546	-0.107399
C	-3.415871	0.941107	-0.274691
H	-4.864944	-0.645369	-0.340915
H	-3.188578	-2.424438	0.067659
H	-1.738640	2.300161	-0.149272
H	-4.143907	1.723738	-0.451660
C	1.197389	-0.065498	0.392177

C	2.638886	0.268257	0.564921
H	2.949980	-0.088811	1.552458
H	2.755833	1.358954	0.549938
H	-0.794074	-1.832452	0.361424
N	0.215806	0.671622	0.282733
C	3.513034	-0.389032	-0.508502
H	3.355978	-1.470720	-0.480133
H	3.182966	-0.049154	-1.493986
C	4.990110	-0.063174	-0.308711
H	5.605409	-0.534103	-1.077112
H	5.162907	1.014908	-0.354277
H	5.339182	-0.416507	0.664952

__Frequencies__ (Top 10 out of 63)

1. 12.7343 cm-1 (Symmetry: A)
2. 44.5931 cm-1 (Symmetry: A)
3. 65.5499 cm-1 (Symmetry: A)
4. 75.7564 cm-1 (Symmetry: A)
5. 150.5653 cm-1 (Symmetry: A)
6. 241.2915 cm-1 (Symmetry: A)
7. 252.5743 cm-1 (Symmetry: A)
8. 284.5116 cm-1 (Symmetry: A)
9. 337.9700 cm-1 (Symmetry: A)
10. 393.0355 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C3H7
Electronic Energy (Eh)	-118.435774429
Sum of electronic and zero-point Energies (Eh)	-118.347278
Sum of electronic and thermal Energies (Eh)	-118.342088
Sum of electronic and enthalpy Energies (Eh)	-118.341144
Sum of electronic and thermal Free Energies (Eh)	-118.37448
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

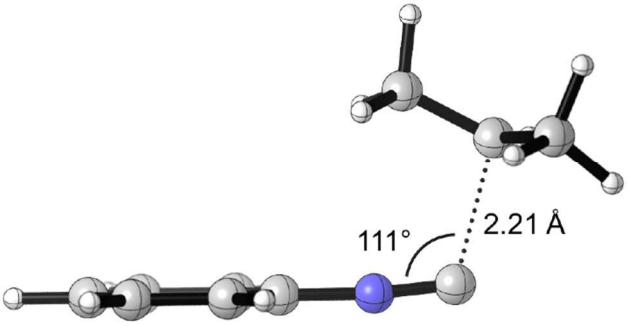
xyz

C	-1.289750	-0.200437	0.004164
H	-1.297328	-1.031032	-0.710256
H	-1.458648	-0.645214	0.996534
H	-2.143333	0.443382	-0.212524
C	0.000000	0.543113	-0.052723
H	-0.000000	1.612293	0.118864

C	1.289750	-0.200437	0.004164
H	1.297328	-1.031031	-0.710257
H	2.143333	0.443382	-0.212522
H	1.458648	-0.645215	0.996534

__Frequencies__ (Top 10 out of 24)

1. 111.5246 cm-1 (Symmetry: A)
2. 127.7835 cm-1 (Symmetry: A)
3. 331.2877 cm-1 (Symmetry: A)
4. 389.8614 cm-1 (Symmetry: A)
5. 900.9209 cm-1 (Symmetry: A)
6. 938.2266 cm-1 (Symmetry: A)
7. 946.3615 cm-1 (Symmetry: A)
8. 1027.7469 cm-1 (Symmetry: A)
9. 1156.7989 cm-1 (Symmetry: A)
10. 1182.8099 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H12N
Electronic Energy (Eh)	-442.839831017
Sum of electronic and zero-point Energies (Eh)	-442.649945
Sum of electronic and thermal Energies (Eh)	-442.638259
Sum of electronic and enthalpy Energies (Eh)	-442.637314
Sum of electronic and thermal Free Energies (Eh)	-442.69082
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

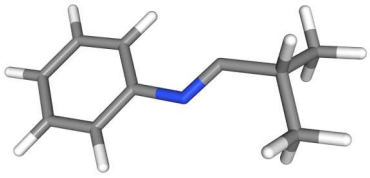
xyz

C	3.347629	0.275551	0.484678
C	2.569386	1.362069	0.094008
C	1.295494	1.167528	-0.420258
C	0.796213	-0.132525	-0.540664
C	1.572260	-1.229319	-0.155490
C	2.844162	-1.016186	0.356868
H	4.341037	0.434656	0.885150
H	2.956346	2.369422	0.189241
H	1.166946	-2.227424	-0.263549
H	3.445617	-1.865640	0.657297

N	-0.467992	-0.334273	-1.047180
C	-1.593012	-0.500215	-1.376329
C	-2.954571	-0.408985	0.366527
H	0.678230	2.001251	-0.730477
H	-3.311203	-1.429774	0.273059
C	-2.018095	-0.126939	1.496884
H	-2.560966	-0.035758	2.447499
H	-1.273945	-0.917651	1.617049
H	-1.486196	0.816710	1.338247
C	-3.899240	0.665627	-0.066175
H	-3.374774	1.617209	-0.194457
H	-4.379924	0.411482	-1.011954
H	-4.686580	0.825790	0.682854

__Frequencies__ (Top 10 out of 63)

1. -391.4675 cm-1 (Symmetry: A) *
2. 12.1798 cm-1 (Symmetry: A)
3. 31.0260 cm-1 (Symmetry: A)
4. 42.5569 cm-1 (Symmetry: A)
5. 136.9353 cm-1 (Symmetry: A)
6. 164.0401 cm-1 (Symmetry: A)
7. 184.3836 cm-1 (Symmetry: A)
8. 195.8323 cm-1 (Symmetry: A)
9. 219.5074 cm-1 (Symmetry: A)
10. 267.1037 cm-1 (Symmetry: A)



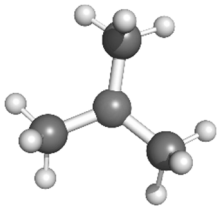
Charge	0
Multiplicity	2
Stoichiometry	C10H12N
Electronic Energy (Eh)	-442.88384463
Sum of electronic and zero-point Energies (Eh)	-442.689213
Sum of electronic and thermal Energies (Eh)	-442.678292
Sum of electronic and enthalpy Energies (Eh)	-442.677348
Sum of electronic and thermal Free Energies (Eh)	-442.728397
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz

C	3.633218	0.239007	0.064073
C	2.763624	1.322421	-0.044362
C	1.391442	1.119952	-0.088877
C	0.880936	-0.178699	-0.024541
C	1.747495	-1.261932	0.094329

C	3.121385	-1.052199	0.132440
H	4.703458	0.403003	0.098843
H	3.157951	2.330706	-0.093115
H	1.327272	-2.258638	0.152719
H	3.791785	-1.898832	0.219956
C	-1.410386	0.317727	-0.388072
C	-2.893339	0.110882	-0.403631
H	-3.209882	0.262373	-1.441796
H	0.703117	1.952798	-0.172479
N	-0.508890	-0.453077	-0.052235
C	-3.565158	1.185415	0.459839
H	-4.650654	1.080851	0.409609
H	-3.258852	1.078436	1.503278
H	-3.294874	2.187717	0.123953
C	-3.271571	-1.303643	0.045326
H	-2.787008	-2.054898	-0.579018
H	-2.951894	-1.467013	1.076626
H	-4.354083	-1.438547	-0.012073

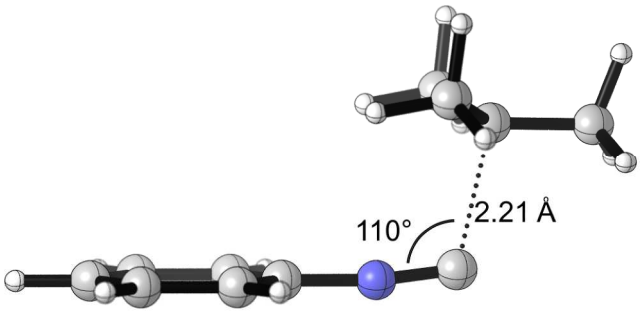
```

__Frequencies__ (Top 10 out of 63)

1. 12.9646 cm-1 (Symmetry: A)
2. 65.7103 cm-1 (Symmetry: A)
3. 74.5626 cm-1 (Symmetry: A)
4. 93.0307 cm-1 (Symmetry: A)
5. 215.4513 cm-1 (Symmetry: A)
6. 221.8845 cm-1 (Symmetry: A)
7. 263.3544 cm-1 (Symmetry: A)
8. 280.0036 cm-1 (Symmetry: A)
9. 332.3149 cm-1 (Symmetry: A)
10. 403.7317 cm-1 (Symmetry: A)



| | |
|---|---|
| Charge | 0 |
| Multiplicity | 2 |
| Stoichiometry | C4H9 |
| Electronic Energy (Eh) | -157.744991907 |
| Sum of electronic and zero-point Energies (Eh) | -157.627716 |
| Sum of electronic and thermal Energies (Eh) | -157.621372 |
| Sum of electronic and enthalpy Energies (Eh) | -157.620428 |
| Sum of electronic and thermal Free Energies (Eh) | -157.657089 |
| Number of Imaginary Frequencies | 0 |

__Molecular Geometry in Cartesian Coordinates__
```

xyz

C	-0.000007	-0.000001	-0.182727
C	0.210844	1.464940	0.019045
H	0.247837	1.721951	1.090332
H	1.154689	1.799037	-0.419573
H	-0.600479	2.051648	-0.419562
C	1.163262	-0.915064	0.019052
H	1.367255	-1.075837	1.090325
H	0.980828	-1.899413	-0.419837
H	2.077038	-0.505625	-0.419381
C	-1.374112	-0.549879	0.019050
H	-2.135336	0.100249	-0.419949
H	-1.476421	-1.546023	-0.419215
H	-1.615333	-0.645963	1.090341

__Frequencies__ (Top 10 out of 33)

1. 132.7997 cm-1 (Symmetry: A)
2. 141.8019 cm-1 (Symmetry: A)
3. 143.2372 cm-1 (Symmetry: A)
4. 258.9919 cm-1 (Symmetry: A)
5. 379.0111 cm-1 (Symmetry: A)
6. 379.9526 cm-1 (Symmetry: A)
7. 777.5295 cm-1 (Symmetry: A)
8. 934.0437 cm-1 (Symmetry: A)
9. 935.1208 cm-1 (Symmetry: A)
10. 967.9264 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H14N
Electronic Energy (Eh)	-482.151455865
Sum of electronic and zero-point Energies (Eh)	-481.933505
Sum of electronic and thermal Energies (Eh)	-481.920399
Sum of electronic and enthalpy Energies (Eh)	-481.919455
Sum of electronic and thermal Free Energies (Eh)	-481.975684
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

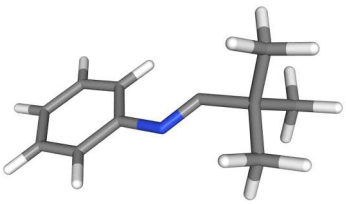
xyz

C	3.645240	0.000885	0.542859

C	3.005853	1.204784	0.258782
C	1.737144	1.213580	-0.302981
C	1.101703	-0.000720	-0.579959
C	1.738238	-1.214221	-0.301995
C	3.006932	-1.203820	0.259773
H	4.635371	0.001505	0.981232
H	3.498076	2.145258	0.475198
H	1.228270	-2.141899	-0.529647
H	3.500001	-2.143671	0.476967
N	-0.157789	-0.001507	-1.134884
C	-1.293910	-0.001924	-1.470407
H	1.226341	2.140612	-0.531396
C	-2.159078	-1.271662	0.953762
H	-2.711749	-1.443189	1.889309
H	-2.335849	-2.134028	0.305551
H	-1.095336	-1.235174	1.206638
C	-3.967389	-0.001289	-0.322796
H	-4.750000	-0.000432	0.449857
H	-4.112601	0.882133	-0.948256
H	-4.111835	-0.886766	-0.945519
C	-2.160204	1.274615	0.949807
H	-1.096691	1.239435	1.203807
H	-2.336735	2.134675	0.298468
H	-2.713863	1.449136	1.884214
C	-2.607675	0.000266	0.301116

__Frequencies__ (Top 10 out of 72)

1. -373.3129 cm-1 (Symmetry: A) *
2. 14.6765 cm-1 (Symmetry: A)
3. 34.5771 cm-1 (Symmetry: A)
4. 34.6959 cm-1 (Symmetry: A)
5. 137.5270 cm-1 (Symmetry: A)
6. 154.5348 cm-1 (Symmetry: A)
7. 181.5253 cm-1 (Symmetry: A)
8. 182.6562 cm-1 (Symmetry: A)
9. 202.8240 cm-1 (Symmetry: A)
10. 211.3117 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H14N
Electronic Energy (Eh)	-482.190960562
Sum of electronic and zero-point Energies (Eh)	-481.968373
Sum of electronic and thermal Energies (Eh)	-481.956165

Sum of electronic and enthalpy Energies (Eh)	-481.95522
Sum of electronic and thermal Free Energies (Eh)	-482.008786
Number of Imaginary Frequencies	0

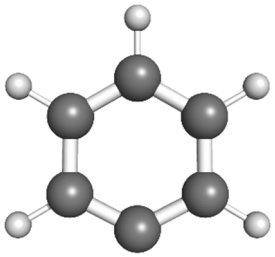
__Molecular Geometry in Cartesian Coordinates__

xyz

C	3.948536	0.276806	-0.046617
C	3.054088	1.344728	-0.006664
C	1.686405	1.114204	0.036925
C	1.205258	-0.197269	0.040414
C	2.097361	-1.265744	0.009756
C	3.466337	-1.027444	-0.038755
H	5.015201	0.462838	-0.080268
H	3.425776	2.362750	-0.008467
H	1.700428	-2.273530	0.022072
H	4.156207	-1.862414	-0.066673
N	-0.177924	-0.502139	0.093542
C	-1.115544	0.278130	-0.080596
H	0.979092	1.934673	0.068528
C	-3.167458	0.933746	1.096352
H	-4.252049	0.807518	1.148136
H	-2.741750	0.664156	2.065450
H	-2.948901	1.986245	0.903193
C	-2.892418	-1.433240	0.271597
H	-3.973170	-1.593260	0.316761
H	-2.474557	-2.069646	-0.510491
H	-2.450832	-1.733711	1.223340
C	-3.202416	0.457467	-1.368492
H	-2.983436	1.504838	-1.586962
H	-2.801043	-0.154995	-2.178942
H	-4.287318	0.326344	-1.341158
C	-2.599845	0.044144	-0.018806

__Frequencies__ (Top 10 out of 72)

1. 15.6746 cm-1 (Symmetry: A)
2. 51.5928 cm-1 (Symmetry: A)
3. 70.5547 cm-1 (Symmetry: A)
4. 82.4884 cm-1 (Symmetry: A)
5. 217.8141 cm-1 (Symmetry: A)
6. 219.7793 cm-1 (Symmetry: A)
7. 267.5438 cm-1 (Symmetry: A)
8. 282.8119 cm-1 (Symmetry: A)
9. 284.5173 cm-1 (Symmetry: A)
10. 291.2278 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C6H5
Electronic Energy (Eh)	-231.512841949
Sum of electronic and zero-point Energies (Eh)	-231.424878
Sum of electronic and thermal Energies (Eh)	-231.420519
Sum of electronic and enthalpy Energies (Eh)	-231.419575
Sum of electronic and thermal Free Energies (Eh)	-231.452909
Number of Imaginary Frequencies	0

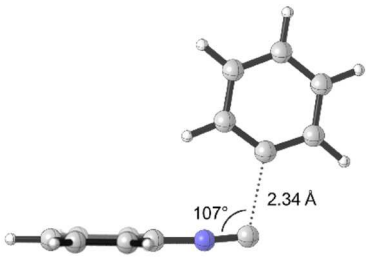
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.000000	1.320277	0.000000
C	1.209231	0.630290	-0.000000
C	1.220822	-0.767990	0.000000
C	0.000000	-1.397437	0.000000
C	-1.220822	-0.767990	0.000000
C	-1.209231	0.630290	0.000000
H	-0.000000	2.403640	0.000000
H	2.146475	1.175372	-0.000000
H	2.153738	-1.319509	0.000000
H	-2.153738	-1.319510	-0.000000
H	-2.146475	1.175372	0.000000

__Frequencies__ (Top 10 out of 27)

1. 399.4518 cm-1 (Symmetry: A)
2. 426.1630 cm-1 (Symmetry: A)
3. 599.7841 cm-1 (Symmetry: A)
4. 615.3135 cm-1 (Symmetry: A)
5. 678.9459 cm-1 (Symmetry: A)
6. 727.4992 cm-1 (Symmetry: A)
7. 838.2706 cm-1 (Symmetry: A)
8. 909.4427 cm-1 (Symmetry: A)
9. 983.8514 cm-1 (Symmetry: A)
10. 986.0415 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H10N
Electronic Energy (Eh)	-555.919820694
Sum of electronic and zero-point Energies (Eh)	-555.73232
Sum of electronic and thermal Energies (Eh)	-555.720437
Sum of electronic and enthalpy Energies (Eh)	-555.719493
Sum of electronic and thermal Free Energies (Eh)	-555.775005
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

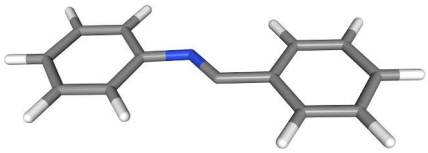
xyz

C	4.021207	-1.009826	0.014161
C	3.502585	-0.517715	1.208578
C	2.403226	0.329926	1.200790
C	1.824154	0.680289	-0.019286
C	2.336096	0.194429	-1.223013
C	3.436010	-0.652068	-1.197191
H	4.879274	-1.670408	0.027296
H	3.955626	-0.794106	2.152791
H	1.865259	0.483525	-2.153956
H	3.836909	-1.033240	-2.128409
N	0.719979	1.513625	-0.036010
C	-0.280200	2.133573	-0.050910
H	1.984141	0.722497	2.118442
C	-2.040485	0.596951	-0.005655
C	-1.651919	-0.720760	0.031803
C	-2.666370	-1.682046	0.052859
C	-4.001932	-1.286764	0.035615
C	-4.341385	0.064432	-0.002597
C	-3.340804	1.039332	-0.024165
H	-0.604705	-1.007375	0.045038
H	-2.411979	-2.735763	0.082753
H	-5.384406	0.360783	-0.015776
H	-3.577138	2.096698	-0.054220
H	-4.783926	-2.036493	0.052170

__Frequencies__ (Top 10 out of 66)

1. -241.9507 cm-1 (Symmetry: A) *
2. 17.3371 cm-1 (Symmetry: A)
3. 25.5147 cm-1 (Symmetry: A)

4. 30.4377 cm-1 (Symmetry: A)
5. 69.9650 cm-1 (Symmetry: A)
6. 85.4054 cm-1 (Symmetry: A)
7. 162.8141 cm-1 (Symmetry: A)
8. 184.1092 cm-1 (Symmetry: A)
9. 342.1671 cm-1 (Symmetry: A)
10. 402.1695 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H10N
Electronic Energy (Eh)	-555.984820363
Sum of electronic and zero-point Energies (Eh)	-555.793386
Sum of electronic and thermal Energies (Eh)	-555.782261
Sum of electronic and enthalpy Energies (Eh)	-555.781317
Sum of electronic and thermal Free Energies (Eh)	-555.833169
Number of Imaginary Frequencies	0

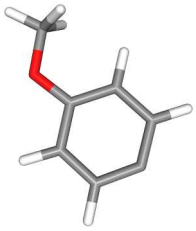
__Molecular Geometry in Cartesian Coordinates__

xyz

C	4.628062	-0.200953	-0.000051
C	3.771722	-1.300915	-0.000252
C	2.396527	-1.120471	-0.000222
C	1.867302	0.173762	0.000014
C	2.722131	1.274050	0.000209
C	4.099319	1.085183	0.000182
H	5.701244	-0.348474	-0.000077
H	4.179879	-2.304833	-0.000430
H	2.289281	2.267002	0.000378
H	4.759210	1.944432	0.000336
C	-0.437729	-0.400309	0.000183
H	1.719169	-1.966350	-0.000376
N	0.478959	0.428453	0.000033
C	-1.883574	-0.187930	0.000078
C	-2.415960	1.108503	-0.000174
C	-2.740017	-1.289854	0.000239
C	-3.790326	1.289838	-0.000247
H	-1.736426	1.952363	-0.000299
C	-4.117495	-1.102895	0.000151
H	-2.313565	-2.286375	0.000434
C	-4.642040	0.185217	-0.000092
H	-4.203091	2.291750	-0.000426
H	-4.780181	-1.959768	0.000274
H	-5.715752	0.331720	-0.000155

__Frequencies__ (Top 10 out of 66)

1. 23.6624 cm-1 (Symmetry: A)
2. 53.3246 cm-1 (Symmetry: A)
3. 66.7627 cm-1 (Symmetry: A)
4. 87.3329 cm-1 (Symmetry: A)
5. 194.0623 cm-1 (Symmetry: A)
6. 244.7038 cm-1 (Symmetry: A)
7. 292.2174 cm-1 (Symmetry: A)
8. 293.3832 cm-1 (Symmetry: A)
9. 412.4034 cm-1 (Symmetry: A)
10. 419.1887 cm-1 (Symmetry: A)



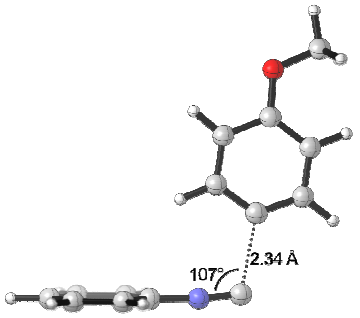
Charge	0
Multiplicity	2
Stoichiometry	C7H7O
Electronic Energy (Eh)	-346.024330907
Sum of electronic and zero-point Energies (Eh)	-345.903303
Sum of electronic and thermal Energies (Eh)	-345.896528
Sum of electronic and enthalpy Energies (Eh)	-345.895584
Sum of electronic and thermal Free Energies (Eh)	-345.934901
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-0.382653	-0.270614	-0.000125
C	0.584610	-1.282115	-0.000024
C	1.935899	-0.957126	0.000091
C	2.267514	0.380268	0.000102
C	1.359011	1.403889	-0.000009
C	-0.002981	1.071417	-0.000134
H	1.664119	2.443751	-0.000001
H	-0.740051	1.863232	-0.000262
H	0.250687	-2.312784	-0.000002
H	2.689108	-1.736148	0.000199
O	-1.674131	-0.697871	-0.000197
C	-2.690075	0.281547	0.000218
H	-2.632868	0.911821	-0.892969
H	-3.632600	-0.261045	-0.000431
H	-2.633307	0.910540	0.894330

__Frequencies__ (Top 10 out of 39)

1. 89.7890 cm-1 (Symmetry: A)
2. 226.5500 cm-1 (Symmetry: A)
3. 275.3475 cm-1 (Symmetry: A)
4. 297.5250 cm-1 (Symmetry: A)
5. 411.7538 cm-1 (Symmetry: A)
6. 453.5867 cm-1 (Symmetry: A)
7. 494.7740 cm-1 (Symmetry: A)
8. 564.1773 cm-1 (Symmetry: A)
9. 612.2141 cm-1 (Symmetry: A)
10. 682.2763 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H12NO
Electronic Energy (Eh)	-670.431448476
Sum of electronic and zero-point Energies (Eh)	-670.211003
Sum of electronic and thermal Energies (Eh)	-670.196591
Sum of electronic and enthalpy Energies (Eh)	-670.195647
Sum of electronic and thermal Free Energies (Eh)	-670.257443
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

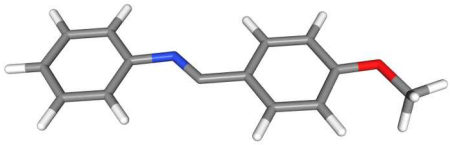
xyz

C	-4.678877	-1.411780	0.000012
C	-4.199156	-0.906633	-1.205188
C	-3.243194	0.099864	-1.214197
C	-2.768386	0.596932	0.000004
C	-3.242820	0.099517	1.214210
C	-4.198790	-0.906973	1.205209
H	-5.424586	-2.197125	0.000014
H	-4.570210	-1.297389	-2.144771
H	-2.855144	0.504368	2.140317
H	-4.569562	-1.297991	2.144795
N	-1.805015	1.589982	0.000005
C	-0.908644	2.352386	0.000040
H	-2.855825	0.504999	-2.140307
C	1.060164	1.078939	0.000097
C	0.872081	-0.286517	-0.000031
C	2.003380	-1.093899	-0.000098
C	3.277439	-0.514870	-0.000030

C	3.425495	0.872742	0.000108
C	2.285992	1.688035	0.000164
H	-0.120870	-0.725748	-0.000071
H	1.930226	-2.175042	-0.000211
H	4.405606	1.331056	0.000193
H	2.379841	2.767918	0.000265
O	4.318107	-1.393295	-0.000089
C	5.625051	-0.862506	-0.000145
H	5.807164	-0.256623	0.893273
H	6.298179	-1.716916	-0.000279
H	5.807010	-0.256454	-0.893479

__Frequencies__ (Top 10 out of 78)

1. -234.5089 cm-1 (Symmetry: A) *
2. 17.1397 cm-1 (Symmetry: A)
3. 19.2497 cm-1 (Symmetry: A)
4. 23.7001 cm-1 (Symmetry: A)
5. 45.8504 cm-1 (Symmetry: A)
6. 69.4615 cm-1 (Symmetry: A)
7. 89.5513 cm-1 (Symmetry: A)
8. 156.3860 cm-1 (Symmetry: A)
9. 184.3172 cm-1 (Symmetry: A)
10. 228.4377 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H12NO
Electronic Energy (Eh)	-670.499737631
Sum of electronic and zero-point Energies (Eh)	-670.275285
Sum of electronic and thermal Energies (Eh)	-670.261652
Sum of electronic and enthalpy Energies (Eh)	-670.260708
Sum of electronic and thermal Free Energies (Eh)	-670.318453
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

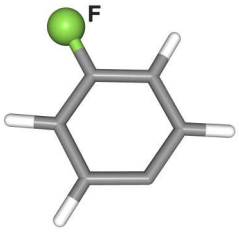
xyz

C	5.570200	-0.255346	0.000021
C	4.696049	-1.341096	-0.000258
C	3.323788	-1.138847	-0.000287
C	2.813889	0.163399	-0.000034
C	3.687266	1.249442	0.000231
C	5.061215	1.038820	0.000267
H	6.640912	-0.419802	0.000041
H	5.087989	-2.351537	-0.000454

H	3.270514	2.249282	0.000415
H	5.734391	1.887785	0.000480
C	0.499815	-0.374558	0.000116
H	2.633274	-1.974037	-0.000504
N	1.430753	0.440106	-0.000073
C	-0.937160	-0.146688	0.000057
C	-1.812148	-1.228821	0.000256
C	-1.465360	1.157206	-0.000193
C	-3.191062	-1.039901	0.000207
H	-1.404230	-2.233181	0.000450
C	-2.827973	1.357141	-0.000239
H	-0.781355	1.997491	-0.000343
C	-3.700404	0.258523	-0.000042
H	-3.846589	-1.899569	0.000361
H	-3.256912	2.351624	-0.000424
O	-5.018640	0.559875	-0.000108
C	-5.944098	-0.508968	0.000067
H	-5.828853	-1.128727	0.894224
H	-6.930570	-0.051853	-0.000036
H	-5.828819	-1.129054	-0.893858

__Frequencies__ (Top 10 out of 78)

1. 20.6822 cm-1 (Symmetry: A)
2. 37.3159 cm-1 (Symmetry: A)
3. 53.1205 cm-1 (Symmetry: A)
4. 74.3796 cm-1 (Symmetry: A)
5. 109.9837 cm-1 (Symmetry: A)
6. 173.6408 cm-1 (Symmetry: A)
7. 193.2037 cm-1 (Symmetry: A)
8. 223.1638 cm-1 (Symmetry: A)
9. 259.7019 cm-1 (Symmetry: A)
10. 280.9333 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C6H4F
Electronic Energy (Eh)	-330.75338003
Sum of electronic and zero-point Energies (Eh)	-330.673537
Sum of electronic and thermal Energies (Eh)	-330.668443
Sum of electronic and enthalpy Energies (Eh)	-330.667499
Sum of electronic and thermal Free Energies (Eh)	-330.702272
Number of Imaginary Frequencies	0

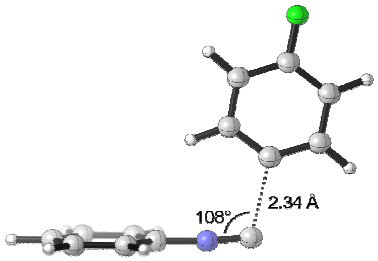
__Molecular Geometry in Cartesian Coordinates__

xyz

C	0.000000	-0.000000	0.857559
C	0.000000	1.217706	0.197441
C	-0.000000	1.219856	-1.199348
C	-0.000000	0.000000	-1.831322
C	-0.000000	-1.219856	-1.199348
C	-0.000000	-1.217706	0.197441
H	-0.000000	2.153265	-1.749129
H	0.000000	2.136501	0.770621
H	-0.000000	-2.136501	0.770621
H	-0.000000	-2.153265	-1.749129
F	0.000000	-0.000000	2.202498

__Frequencies__ (Top 10 out of 27)

1. 255.3743 cm-1 (Symmetry: B1)
2. 409.4581 cm-1 (Symmetry: B2)
3. 411.6240 cm-1 (Symmetry: A2)
4. 489.3300 cm-1 (Symmetry: B1)
5. 529.0227 cm-1 (Symmetry: A1)
6. 610.4518 cm-1 (Symmetry: B2)
7. 678.7766 cm-1 (Symmetry: B1)
8. 813.9415 cm-1 (Symmetry: A1)
9. 816.6906 cm-1 (Symmetry: A2)
10. 821.2919 cm-1 (Symmetry: B1)



Charge	0
Multiplicity	2
Stoichiometry	C13H9FN
Electronic Energy (Eh)	-655.161067713
Sum of electronic and zero-point Energies (Eh)	-654.981733
Sum of electronic and thermal Energies (Eh)	-654.969048
Sum of electronic and enthalpy Energies (Eh)	-654.968104
Sum of electronic and thermal Free Energies (Eh)	-655.025972
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

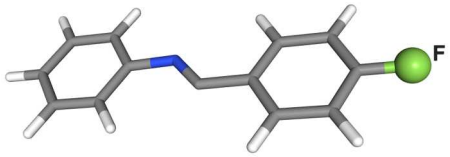
xyz

C	-4.353794	-1.226849	-0.000025
C	-3.837141	-0.759987	-1.205374

C	-2.807499	0.171052	-1.214419
C	-2.297371	0.630658	0.000012
C	-2.807481	0.170986	1.214424
C	-3.837124	-0.760053	1.205343
H	-5.157554	-1.952648	-0.000039
H	-4.237146	-1.121193	-2.144858
H	-2.391541	0.546602	2.140596
H	-4.237116	-1.121312	2.144813
N	-1.262952	1.550517	0.000030
C	-0.324272	2.259014	0.000044
H	-2.391571	0.546720	-2.140576
C	1.584190	0.901743	0.000011
C	1.344912	-0.451929	0.000019
C	2.451576	-1.304374	0.000007
C	3.717109	-0.740780	-0.000011
C	3.936718	0.627705	-0.000019
C	2.830853	1.479977	-0.000007
H	0.336546	-0.853710	0.000032
H	2.347571	-2.382509	0.000012
H	4.952405	1.003977	-0.000033
H	2.953450	2.556609	-0.000012
F	4.784618	-1.562127	-0.000020

__Frequencies__ (Top 10 out of 66)

1. -232.4129 cm-1 (Symmetry: A) *
2. 17.3261 cm-1 (Symmetry: A)
3. 21.5271 cm-1 (Symmetry: A)
4. 24.1411 cm-1 (Symmetry: A)
5. 53.2195 cm-1 (Symmetry: A)
6. 76.7794 cm-1 (Symmetry: A)
7. 159.8230 cm-1 (Symmetry: A)
8. 184.3835 cm-1 (Symmetry: A)
9. 261.8750 cm-1 (Symmetry: A)
10. 342.3687 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H9FN
Electronic Energy (Eh)	-655.227029891
Sum of electronic and zero-point Energies (Eh)	-655.043847
Sum of electronic and thermal Energies (Eh)	-655.0319
Sum of electronic and enthalpy Energies (Eh)	-655.030956
Sum of electronic and thermal Free Energies (Eh)	-655.085012
Number of Imaginary Frequencies	0

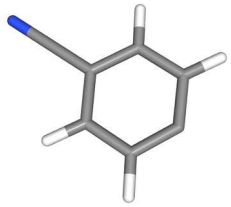
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-5.092935	0.154331	0.000059
C	-4.254348	1.267866	-0.000009
C	-2.876488	1.109396	-0.000024
C	-2.327043	-0.176261	0.000030
C	-3.163814	-1.290240	0.000097
C	-4.543846	-1.123207	0.000112
H	-6.168310	0.284730	0.000071
H	-4.678430	2.265126	-0.000051
H	-2.715528	-2.276310	0.000136
H	-5.189943	-1.992842	0.000164
C	-0.029570	0.433692	-0.000004
H	-2.212831	1.966044	-0.000078
N	-0.934618	-0.407347	0.000017
C	1.417086	0.239496	-0.000020
C	1.967122	-1.050224	-0.000022
C	2.261868	1.350917	-0.000032
C	3.340944	-1.224046	-0.000037
C	3.641258	1.189801	-0.000047
C	4.150035	-0.096744	-0.000048
F	5.480477	-0.263390	-0.000061
H	3.796040	-2.206345	-0.000039
H	4.319141	2.033372	-0.000057
H	1.826318	2.343103	-0.000029
H	1.299956	-1.903603	-0.000015

__Frequencies__ (Top 10 out of 66)

1. 19.6738 cm-1 (Symmetry: A)
2. 44.9776 cm-1 (Symmetry: A)
3. 58.5078 cm-1 (Symmetry: A)
4. 82.9276 cm-1 (Symmetry: A)
5. 179.8771 cm-1 (Symmetry: A)
6. 194.9271 cm-1 (Symmetry: A)
7. 263.4209 cm-1 (Symmetry: A)
8. 272.2353 cm-1 (Symmetry: A)
9. 383.4045 cm-1 (Symmetry: A)
10. 407.2920 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C7H4N
Electronic Energy (Eh)	-323.751369448
Sum of electronic and zero-point Energies (Eh)	-323.664635

Sum of electronic and thermal Energies (Eh)	-323.658588
Sum of electronic and enthalpy Energies (Eh)	-323.657644
Sum of electronic and thermal Free Energies (Eh)	-323.695463
Number of Imaginary Frequencies	0

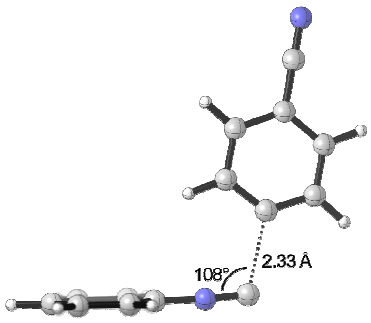
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.533323	0.000000	0.000000
C	0.154112	1.218026	0.000000
C	1.548077	1.222790	-0.000000
C	2.174031	0.000000	0.000000
C	1.548077	-1.222790	0.000000
C	0.154112	-1.218026	-0.000000
H	2.100670	2.154554	-0.000001
H	-0.402407	2.147570	0.000000
H	-0.402407	-2.147570	-0.000001
H	2.100670	-2.154554	0.000001
C	-1.970441	0.000000	0.000000
N	-3.120628	0.000000	0.000000

__Frequencies__ (Top 10 out of 30)

1. 154.2340 cm-1 (Symmetry: A)
2. 168.5061 cm-1 (Symmetry: A)
3. 395.4035 cm-1 (Symmetry: A)
4. 403.0053 cm-1 (Symmetry: A)
5. 468.2569 cm-1 (Symmetry: A)
6. 558.6803 cm-1 (Symmetry: A)
7. 569.1044 cm-1 (Symmetry: A)
8. 625.2268 cm-1 (Symmetry: A)
9. 700.7881 cm-1 (Symmetry: A)
10. 757.7602 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H9N2
Electronic Energy (Eh)	-648.15975339
Sum of electronic and zero-point Energies (Eh)	-647.973563
Sum of electronic and thermal Energies (Eh)	-647.959886
Sum of electronic and enthalpy Energies (Eh)	-647.958942

| Sum of electronic and thermal Free Energies (Eh) | -648.019346 |
| Number of Imaginary Frequencies | 1 |

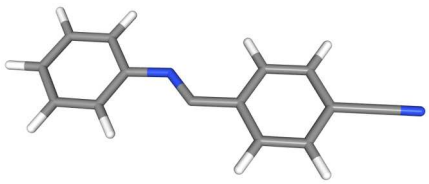
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-4.558150	-1.407609	-0.000039
C	-4.067475	-0.913961	-1.205566
C	-3.088869	0.070529	-1.214666
C	-2.604344	0.555709	0.000112
C	-3.088874	0.070347	1.214815
C	-4.067480	-0.914141	1.205565
H	-5.321951	-2.175317	-0.000098
H	-4.448122	-1.295646	-2.144938
H	-2.694395	0.468135	2.141134
H	-4.448131	-1.295966	2.144878
N	-1.618489	1.528747	0.000185
C	-0.726285	2.293782	0.000238
H	-2.694387	0.468455	-2.140924
C	1.272244	1.087340	0.000094
C	1.135193	-0.281157	-0.000038
C	2.303878	-1.039593	-0.000146
C	3.544473	-0.393053	-0.000119
C	3.632566	1.003821	0.000017
C	2.467313	1.766587	0.000126
H	0.160239	-0.757937	-0.000056
H	2.264996	-2.122433	-0.000253
H	4.607225	1.477178	0.000035
H	2.501253	2.849544	0.000232
C	4.748728	-1.177537	-0.000233
N	5.712171	-1.806233	-0.000324

__Frequencies__ (Top 10 out of 69)

1. -233.5453 cm-1 (Symmetry: A) *
2. 14.8525 cm-1 (Symmetry: A)
3. 19.5851 cm-1 (Symmetry: A)
4. 26.7444 cm-1 (Symmetry: A)
5. 42.7677 cm-1 (Symmetry: A)
6. 69.0657 cm-1 (Symmetry: A)
7. 153.3823 cm-1 (Symmetry: A)
8. 159.9799 cm-1 (Symmetry: A)
9. 177.2917 cm-1 (Symmetry: A)
10. 185.0065 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H9N2
Electronic Energy (Eh)	-648.222577924
Sum of electronic and zero-point Energies (Eh)	-648.032591
Sum of electronic and thermal Energies (Eh)	-648.019622
Sum of electronic and enthalpy Energies (Eh)	-648.018678
Sum of electronic and thermal Free Energies (Eh)	-648.075227
Number of Imaginary Frequencies	0

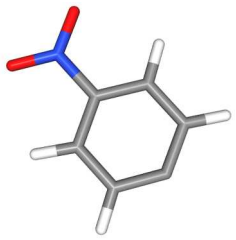
__Molecular Geometry in Cartesian Coordinates__

xyz

C	5.387413	0.097353	0.000312
C	4.571727	1.227936	0.000355
C	3.191274	1.096786	0.000267
C	2.618383	-0.178431	0.000134
C	3.431354	-1.309639	0.000091
C	4.814310	-1.169543	0.000180
H	6.465119	0.206644	0.000381
H	5.015808	2.216314	0.000457
H	2.963584	-2.286570	-0.000011
H	5.443613	-2.051265	0.000146
C	0.330824	0.473557	0.000043
H	2.544439	1.966176	0.000299
N	1.221455	-0.381211	0.000041
C	-1.120918	0.285863	-0.000049
C	-1.673810	-1.001927	-0.000143
C	-1.956874	1.403387	-0.000040
C	-3.047257	-1.165915	-0.000228
C	-3.334963	1.246160	-0.000126
C	-3.878719	-0.039559	-0.000219
H	-3.487480	-2.155264	-0.000301
H	-3.991769	2.106657	-0.000120
H	-1.515317	2.392729	0.000033
H	-1.009879	-1.857596	-0.000147
C	-5.306036	-0.209031	-0.000308
N	-6.448365	-0.344477	-0.000378

__Frequencies__ (Top 10 out of 69)

1. 21.4841 cm-1 (Symmetry: A)
2. 38.7258 cm-1 (Symmetry: A)
3. 51.2796 cm-1 (Symmetry: A)
4. 69.1276 cm-1 (Symmetry: A)
5. 136.0714 cm-1 (Symmetry: A)
6. 144.7282 cm-1 (Symmetry: A)
7. 191.6916 cm-1 (Symmetry: A)
8. 252.5970 cm-1 (Symmetry: A)
9. 281.0573 cm-1 (Symmetry: A)
10. 303.8919 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C6H4NO2
Electronic Energy (Eh)	-436.002033762
Sum of electronic and zero-point Energies (Eh)	-435.911195
Sum of electronic and thermal Energies (Eh)	-435.904422
Sum of electronic and enthalpy Energies (Eh)	-435.903478
Sum of electronic and thermal Free Energies (Eh)	-435.943816
Number of Imaginary Frequencies	0

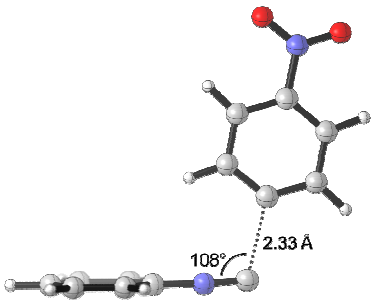
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.175282	0.000000	0.000000
C	0.484030	-1.222365	0.000000
C	1.878357	-1.224256	0.000000
C	2.503221	-0.000000	0.000000
C	1.878357	1.224256	-0.000000
C	0.484030	1.222365	-0.000000
H	2.431716	-2.155103	0.000000
H	-0.088256	-2.140498	0.000000
H	-0.088256	2.140498	-0.000000
H	2.431716	2.155103	-0.000000
N	-1.654534	-0.000000	0.000000
O	-2.213841	1.074509	0.000000
O	-2.213841	-1.074509	-0.000000

__Frequencies__ (Top 10 out of 33)

1. 46.8668 cm-1 (Symmetry: A)
2. 180.2847 cm-1 (Symmetry: A)
3. 267.1280 cm-1 (Symmetry: A)
4. 405.7001 cm-1 (Symmetry: A)
5. 407.0929 cm-1 (Symmetry: A)
6. 435.2869 cm-1 (Symmetry: A)
7. 536.0190 cm-1 (Symmetry: A)
8. 606.9005 cm-1 (Symmetry: A)
9. 651.2562 cm-1 (Symmetry: A)
10. 694.1200 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H9N2O2
Electronic Energy (Eh)	-760.41080601
Sum of electronic and zero-point Energies (Eh)	-760.220511
Sum of electronic and thermal Energies (Eh)	-760.206087
Sum of electronic and enthalpy Energies (Eh)	-760.205143
Sum of electronic and thermal Free Energies (Eh)	-760.268038
Number of Imaginary Frequencies	1

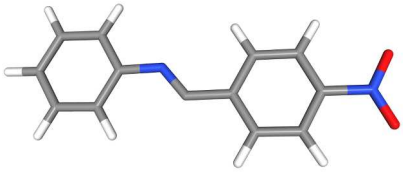
__Molecular Geometry in Cartesian Coordinates__

xyz

C	4.924494	-1.478051	0.000008
C	4.451780	-0.967443	1.205629
C	3.508644	0.051092	1.214818
C	3.041508	0.552664	-0.000018
C	3.508652	0.051068	-1.214841
C	4.451788	-0.967466	-1.205626
H	5.660386	-2.272544	0.000019
H	4.818769	-1.362405	2.144927
H	3.128565	0.462642	-2.141155
H	4.818784	-1.362447	-2.144913
N	2.089506	1.559279	-0.000031
C	1.225075	2.355186	-0.000040
H	3.128551	0.462684	2.141122
C	-0.815995	1.222862	-0.000018
C	-0.728002	-0.150407	0.000001
C	-1.921928	-0.869350	0.000017
C	-3.116946	-0.160852	0.000012
C	-3.180463	1.227610	-0.000008
C	-1.986264	1.945388	-0.000023
H	0.228957	-0.661732	0.000004
H	-1.940624	-1.951150	0.000032
H	-4.144629	1.718605	-0.000010
H	-1.981093	3.028617	-0.000039
N	-4.383611	-0.922576	0.000029
O	-4.310947	-2.132547	0.000045
O	-5.418177	-0.291577	0.000026

__Frequencies__ (Top 10 out of 72)

1. -230.9968 cm-1 (Symmetry: A) *
2. 16.4439 cm-1 (Symmetry: A)
3. 16.9603 cm-1 (Symmetry: A)
4. 21.4244 cm-1 (Symmetry: A)
5. 44.2165 cm-1 (Symmetry: A)
6. 47.5884 cm-1 (Symmetry: A)
7. 69.1725 cm-1 (Symmetry: A)
8. 155.3041 cm-1 (Symmetry: A)
9. 177.6816 cm-1 (Symmetry: A)
10. 192.6299 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H9N2O2
Electronic Energy (Eh)	-760.473229938
Sum of electronic and zero-point Energies (Eh)	-760.279242
Sum of electronic and thermal Energies (Eh)	-760.265482
Sum of electronic and enthalpy Energies (Eh)	-760.264538
Sum of electronic and thermal Free Energies (Eh)	-760.323801
Number of Imaginary Frequencies	0

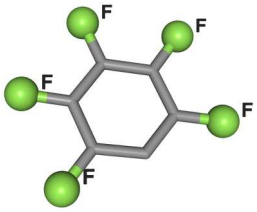
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-5.849542	0.082495	0.000065
C	-5.041946	1.218903	0.000029
C	-3.660685	1.097427	0.000016
C	-3.079387	-0.173937	0.000041
C	-3.884016	-1.311011	0.000078
C	-5.267888	-1.180482	0.000090
H	-6.927977	0.184319	0.000075
H	-5.493025	2.204077	0.000010
H	-3.409427	-2.284634	0.000097
H	-5.891153	-2.066447	0.000118
C	-0.795862	0.493206	-0.000003
H	-3.019891	1.971267	-0.000012
N	-1.681005	-0.366796	0.000031
C	0.657495	0.310622	-0.000015
C	1.213730	-0.975980	0.000010
C	1.487390	1.433030	-0.000053
C	2.588608	-1.137722	-0.000002
C	2.867487	1.284221	-0.000065
C	3.386579	-0.000332	-0.000040
H	3.049875	-2.115955	0.000016
H	3.535686	2.134245	-0.000094
H	1.041317	2.420103	-0.000072

H	0.552773	-1.833685	0.000039
N	4.857578	-0.168404	-0.000053
O	5.289914	-1.299702	-0.000029
O	5.534340	0.836010	-0.000086

__Frequencies__ (Top 10 out of 72)

1. 18.2418 cm-1 (Symmetry: A)
2. 35.5508 cm-1 (Symmetry: A)
3. 45.5307 cm-1 (Symmetry: A)
4. 48.2272 cm-1 (Symmetry: A)
5. 69.7856 cm-1 (Symmetry: A)
6. 146.2922 cm-1 (Symmetry: A)
7. 161.8421 cm-1 (Symmetry: A)
8. 222.8473 cm-1 (Symmetry: A)
9. 258.1690 cm-1 (Symmetry: A)
10. 303.5369 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C6F5
Electronic Energy (Eh)	-727.675818324
Sum of electronic and zero-point Energies (Eh)	-727.627411
Sum of electronic and thermal Energies (Eh)	-727.618889
Sum of electronic and enthalpy Energies (Eh)	-727.617945
Sum of electronic and thermal Free Energies (Eh)	-727.661872
Number of Imaginary Frequencies	0

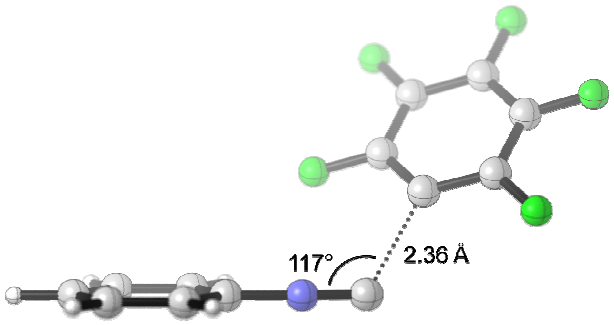
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.000000	1.071564	-0.000000
C	0.000000	0.386620	-1.207796
C	0.000000	-1.004218	-1.209139
C	-0.000000	-1.645691	0.000000
C	-0.000000	-1.004218	1.209139
C	-0.000000	0.386620	1.207796
F	-0.000000	2.395862	-0.000000
F	-0.000000	1.063074	2.347308
F	0.000000	-1.657898	2.364159
F	0.000000	-1.657898	-2.364159
F	0.000000	1.063074	-2.347308

__Frequencies__ (Top 10 out of 27)

1. 133.4031 cm-1 (Symmetry: A")
2. 163.8067 cm-1 (Symmetry: A')
3. 205.8186 cm-1 (Symmetry: A')
4. 266.9111 cm-1 (Symmetry: A')
5. 275.6983 cm-1 (Symmetry: A")
6. 300.5337 cm-1 (Symmetry: A")
7. 328.2404 cm-1 (Symmetry: A')
8. 330.2059 cm-1 (Symmetry: A')
9. 371.9046 cm-1 (Symmetry: A")
10. 434.6240 cm-1 (Symmetry: A")



Charge	0
Multiplicity	2
Stoichiometry	C13H5F5N
Electronic Energy (Eh)	-1052.093376
Sum of electronic and zero-point Energies (Eh)	-1051.94538
Sum of electronic and thermal Energies (Eh)	-1051.92927
Sum of electronic and enthalpy Energies (Eh)	-1051.928326
Sum of electronic and thermal Free Energies (Eh)	-1051.992929
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

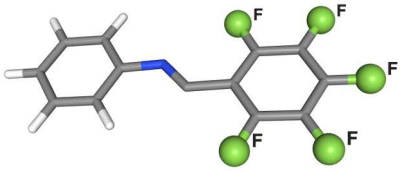
xyz

C	1.963697	-0.168184	2.297265
C	2.206788	1.082503	1.735636
C	2.699469	1.186431	0.441125
C	2.946039	0.021999	-0.285076
C	2.706100	-1.236408	0.265504
C	2.213329	-1.323334	1.561329
H	1.578538	-0.242335	3.306884
H	2.008414	1.983252	2.303547
H	2.897775	-2.121764	-0.327111
H	2.019373	-2.297763	1.992643
N	3.421864	0.117459	-1.586705
C	3.817797	0.197537	-2.685083
H	2.886022	2.149036	-0.017434
C	-0.176000	0.003701	-0.416073
C	-0.827073	-1.199054	-0.364092
C	-2.206082	-1.190339	-0.188369

C	-2.873731	0.021156	-0.064704
C	-2.181092	1.223736	-0.116162
C	-0.802096	1.214434	-0.292023
F	-4.188003	0.029733	0.103550
F	-2.889151	-2.325667	-0.134368
F	-0.191628	-2.361310	-0.474968
F	-0.142554	2.367652	-0.333018
F	-2.840447	2.367624	0.006887

__Frequencies__ (Top 10 out of 66)

1. -12.6049 cm-1 (Symmetry: A) *
2. 9.5833 cm-1 (Symmetry: A)
3. 29.7118 cm-1 (Symmetry: A)
4. 39.5882 cm-1 (Symmetry: A)
5. 61.4280 cm-1 (Symmetry: A)
6. 75.0696 cm-1 (Symmetry: A)
7. 132.8711 cm-1 (Symmetry: A)
8. 157.4149 cm-1 (Symmetry: A)
9. 164.4364 cm-1 (Symmetry: A)
10. 165.7397 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C13H5F5N
Electronic Energy (Eh)	-1052.15068871
Sum of electronic and zero-point Energies (Eh)	-1051.9997
Sum of electronic and thermal Energies (Eh)	-1051.984089
Sum of electronic and enthalpy Energies (Eh)	-1051.983145
Sum of electronic and thermal Free Energies (Eh)	-1052.045602
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

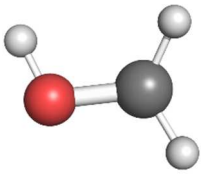
xyz

C	-5.770999	0.226261	0.000307
C	-4.915402	1.327097	0.000012
C	-3.540578	1.146445	-0.000300
C	-3.017771	-0.149790	-0.000332
C	-3.868714	-1.252286	-0.000091
C	-5.245402	-1.061236	0.000265
H	-6.844028	0.374750	0.000556
H	-5.323671	2.330731	0.000023
H	-3.434602	-2.244573	-0.000144
H	-5.906841	-1.919033	0.000489
C	-0.705402	0.411665	0.000332

H	-2.861230	1.990795	-0.000533
N	-1.629372	-0.403642	-0.000706
C	0.732532	0.183598	0.000081
C	1.312378	-1.090200	0.000052
C	1.594647	1.281834	0.000084
C	2.686320	-1.257655	0.000036
C	2.970592	1.130391	0.000020
C	3.515121	-0.144537	0.000003
F	3.768480	2.189368	-0.000012
F	1.104068	2.513398	0.000134
F	4.827477	-0.301275	-0.000041
F	3.219128	-2.472164	0.000031
F	0.557740	-2.175626	0.000083

__Frequencies__ (Top 10 out of 66)

1. 18.8950 cm-1 (Symmetry: A)
2. 37.2171 cm-1 (Symmetry: A)
3. 45.4216 cm-1 (Symmetry: A)
4. 63.0062 cm-1 (Symmetry: A)
5. 133.1232 cm-1 (Symmetry: A)
6. 153.1598 cm-1 (Symmetry: A)
7. 161.9292 cm-1 (Symmetry: A)
8. 194.0020 cm-1 (Symmetry: A)
9. 219.3454 cm-1 (Symmetry: A)
10. 220.0027 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	CH3O
Electronic Energy (Eh)	-115.042935521
Sum of electronic and zero-point Energies (Eh)	-115.005263
Sum of electronic and thermal Energies (Eh)	-115.001914
Sum of electronic and enthalpy Energies (Eh)	-115.00097
Sum of electronic and thermal Free Energies (Eh)	-115.028246
Number of Imaginary Frequencies	0

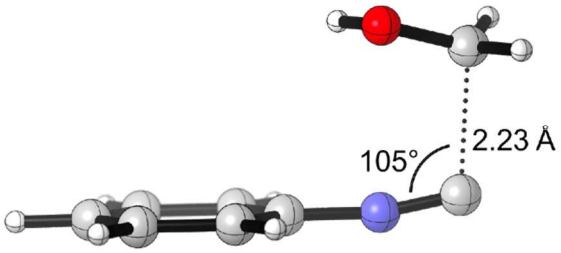
__Molecular Geometry in Cartesian Coordinates__

xyz

C	0.681725	0.028353	-0.066001
H	1.232330	-0.884514	0.099635
H	1.113990	0.991042	0.176373
O	-0.667040	-0.125308	0.023870
H	-1.100352	0.725816	-0.070964

__Frequencies__ (Top 10 out of 9)

1. 415.0229 cm-1 (Symmetry: A)
2. 591.8034 cm-1 (Symmetry: A)
3. 1062.5599 cm-1 (Symmetry: A)
4. 1237.4391 cm-1 (Symmetry: A)
5. 1356.1793 cm-1 (Symmetry: A)
6. 1496.8102 cm-1 (Symmetry: A)
7. 3159.0954 cm-1 (Symmetry: A)
8. 3302.2250 cm-1 (Symmetry: A)
9. 3915.0949 cm-1 (Symmetry: A)



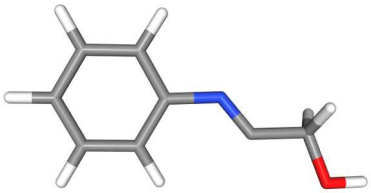
Charge	0
Multiplicity	2
Stoichiometry	C8H8NO
Electronic Energy (Eh)	-439.446327321
Sum of electronic and zero-point Energies (Eh)	-439.307453
Sum of electronic and thermal Energies (Eh)	-439.297587
Sum of electronic and enthalpy Energies (Eh)	-439.296643
Sum of electronic and thermal Free Energies (Eh)	-439.345502
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-2.813438	-0.437108	0.326327
C	-2.023215	-1.210820	-0.520887
C	-0.759197	-0.779786	-0.895790
C	-0.282606	0.443120	-0.413046
C	-1.070557	1.228893	0.433149
C	-2.332044	0.779764	0.800403
H	-3.799041	-0.780959	0.614354
H	-2.392247	-2.159690	-0.890961
H	-0.685388	2.178224	0.783680
H	-2.943066	1.387391	1.456927
N	0.973866	0.878836	-0.775541
C	2.128986	1.086058	-0.941220
C	3.180110	-0.271421	0.482913
H	-0.126419	-1.373267	-1.542954
H	3.935629	-0.693224	-0.164057
H	3.479038	0.480919	1.205634
O	2.242922	-1.181137	0.860407
H	1.602828	-0.774353	1.451820

__Frequencies__ (Top 10 out of 48)

1. -383.3243 cm-1 (Symmetry: A) *
2. 19.4784 cm-1 (Symmetry: A)
3. 38.5272 cm-1 (Symmetry: A)
4. 58.7626 cm-1 (Symmetry: A)
5. 154.6950 cm-1 (Symmetry: A)
6. 181.5987 cm-1 (Symmetry: A)
7. 244.4986 cm-1 (Symmetry: A)
8. 347.9246 cm-1 (Symmetry: A)
9. 372.0938 cm-1 (Symmetry: A)
10. 414.9613 cm-1 (Symmetry: A)



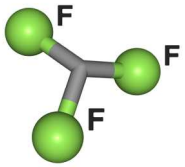
Charge	0
Multiplicity	2
Stoichiometry	C8H8NO
Electronic Energy (Eh)	-439.483889959
Sum of electronic and zero-point Energies (Eh)	-439.341277
Sum of electronic and thermal Energies (Eh)	-439.331885
Sum of electronic and enthalpy Energies (Eh)	-439.330941
Sum of electronic and thermal Free Energies (Eh)	-439.377859
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-3.241284	0.427761	-0.043569
C	-2.875556	-0.913486	-0.065461
C	-1.532786	-1.272039	-0.020556
C	-0.553377	-0.285089	0.038625
C	-0.915561	1.063568	0.064320
C	-2.257583	1.412891	0.022654
H	-4.287471	0.706950	-0.075622
H	-3.635693	-1.683844	-0.115112
H	-0.138664	1.817466	0.115715
H	-2.538821	2.459203	0.042645
C	1.806695	-0.008061	-0.017514
C	3.235315	-0.427908	0.064967
H	3.403189	-1.195701	-0.701142
H	3.393985	-0.879030	1.052891
H	-1.225548	-2.310653	-0.032152
N	0.799047	-0.704127	0.087187
O	4.058170	0.700924	-0.133779
H	4.975154	0.421281	-0.088105

__Frequencies__ (Top 10 out of 48)

1. 30.3490 cm-1 (Symmetry: A)
2. 78.7681 cm-1 (Symmetry: A)
3. 88.2877 cm-1 (Symmetry: A)
4. 142.8450 cm-1 (Symmetry: A)
5. 249.6397 cm-1 (Symmetry: A)
6. 272.4076 cm-1 (Symmetry: A)
7. 312.9507 cm-1 (Symmetry: A)
8. 341.6184 cm-1 (Symmetry: A)
9. 419.6137 cm-1 (Symmetry: A)
10. 510.6590 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	CF3
Electronic Energy (Eh)	-337.557181937
Sum of electronic and zero-point Energies (Eh)	-337.544721
Sum of electronic and thermal Energies (Eh)	-337.541313
Sum of electronic and enthalpy Energies (Eh)	-337.540368
Sum of electronic and thermal Free Energies (Eh)	-337.571395
Number of Imaginary Frequencies	0

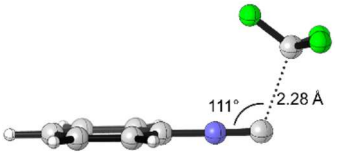
__Molecular Geometry in Cartesian Coordinates__

xyz

C	0.275633	-0.176038	0.000000
F	0.275633	0.566313	1.083714
F	0.275633	0.566313	-1.083714
F	-0.735021	-1.015268	-0.000000

__Frequencies__ (Top 10 out of 6)

1. 518.5789 cm-1 (Symmetry: A")
2. 518.8315 cm-1 (Symmetry: A')
3. 707.9754 cm-1 (Symmetry: A')
4. 1114.9371 cm-1 (Symmetry: A')
5. 1304.5404 cm-1 (Symmetry: A")
6. 1304.6487 cm-1 (Symmetry: A')



Charge	0
Multiplicity	2
Stoichiometry	C8H5F3N
Electronic Energy (Eh)	-661.963994286
Sum of electronic and zero-point Energies (Eh)	-661.852217
Sum of electronic and thermal Energies (Eh)	-661.841316
Sum of electronic and enthalpy Energies (Eh)	-661.840372
Sum of electronic and thermal Free Energies (Eh)	-661.895131
Number of Imaginary Frequencies	1

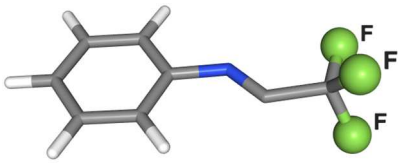
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.766120	-0.000062	-0.562610
C	-3.125397	1.205621	-0.292096
C	-1.846933	1.214862	0.248128
C	-1.216103	0.000051	0.513032
C	-1.846854	-1.214817	0.248194
C	-3.125318	-1.205689	-0.292029
H	-4.763552	-0.000106	-0.984422
H	-3.621893	2.144841	-0.502356
H	-1.330805	-2.140992	0.466136
H	-3.621753	-2.144954	-0.502235
N	0.060221	0.000105	1.052468
C	1.150869	0.000139	1.487334
C	2.707559	0.000008	-0.180584
H	-1.330944	2.141084	0.466015
F	3.450294	1.082075	-0.072108
F	3.449311	-1.082790	-0.072636
F	2.062303	0.000573	-1.335992

__Frequencies__ (Top 10 out of 45)

1. -255.3630 cm-1 (Symmetry: A) *
2. 6.1973 cm-1 (Symmetry: A)
3. 15.7065 cm-1 (Symmetry: A)
4. 28.5690 cm-1 (Symmetry: A)
5. 96.8079 cm-1 (Symmetry: A)
6. 104.8506 cm-1 (Symmetry: A)
7. 169.7574 cm-1 (Symmetry: A)
8. 189.2474 cm-1 (Symmetry: A)
9. 347.8458 cm-1 (Symmetry: A)
10. 411.9047 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2

Stoichiometry	C8H5F3N
Electronic Energy (Eh)	-662.006736732
Sum of electronic and zero-point Energies (Eh)	-661.89156
Sum of electronic and thermal Energies (Eh)	-661.881542
Sum of electronic and enthalpy Energies (Eh)	-661.880598
Sum of electronic and thermal Free Energies (Eh)	-661.930402
Number of Imaginary Frequencies	0

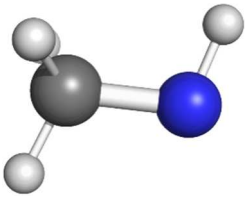
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.931850	-0.199155	-0.000067
C	-3.088630	-1.309378	-0.000005
C	-1.712124	-1.142063	0.000056
C	-1.182117	0.149618	0.000060
C	-2.017088	1.262177	0.000023
C	-3.395675	1.083756	-0.000058
H	-5.006256	-0.337221	-0.000118
H	-3.507019	-2.308606	-0.000005
H	-1.573125	2.249933	0.000057
H	-4.049406	1.947203	-0.000099
N	0.212670	0.383650	0.000145
C	1.143826	-0.407941	-0.000226
C	2.608988	-0.044622	-0.000036
H	-1.040174	-1.992144	0.000103
F	3.203598	-0.556948	-1.080526
F	2.830073	1.270662	0.000653
F	3.203586	-0.558054	1.079936

__Frequencies__ (Top 10 out of 45)

1. 18.9699 cm-1 (Symmetry: A)
2. 55.9108 cm-1 (Symmetry: A)
3. 79.4932 cm-1 (Symmetry: A)
4. 85.3805 cm-1 (Symmetry: A)
5. 212.8058 cm-1 (Symmetry: A)
6. 289.3789 cm-1 (Symmetry: A)
7. 306.6677 cm-1 (Symmetry: A)
8. 417.8630 cm-1 (Symmetry: A)
9. 430.1011 cm-1 (Symmetry: A)
10. 443.4713 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	CH4N

Electronic Energy (Eh)	-95.1664886724
Sum of electronic and zero-point Energies (Eh)	-95.117238
Sum of electronic and thermal Energies (Eh)	-95.113769
Sum of electronic and enthalpy Energies (Eh)	-95.112825
Sum of electronic and thermal Free Energies (Eh)	-95.140681
Number of Imaginary Frequencies	0

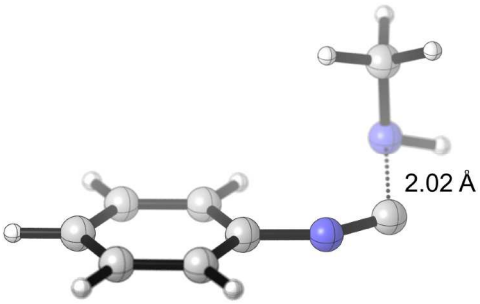
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-0.628930	0.012970	-0.000012
H	-1.124171	-0.957624	0.001244
H	-0.963631	0.582309	0.878572
H	-0.963780	0.580336	-0.879759
N	0.802407	-0.152961	-0.000020
H	1.208312	0.787890	0.000159

__Frequencies__ (Top 10 out of 12)

1. 238.8972 cm-1 (Symmetry: A)
2. 962.2170 cm-1 (Symmetry: A)
3. 1006.7095 cm-1 (Symmetry: A)
4. 1072.9854 cm-1 (Symmetry: A)
5. 1329.2570 cm-1 (Symmetry: A)
6. 1404.9951 cm-1 (Symmetry: A)
7. 1489.4872 cm-1 (Symmetry: A)
8. 1490.2047 cm-1 (Symmetry: A)
9. 2999.6824 cm-1 (Symmetry: A)
10. 3044.7053 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C8H9N2
Electronic Energy (Eh)	-419.567121424
Sum of electronic and zero-point Energies (Eh)	-419.415688
Sum of electronic and thermal Energies (Eh)	-419.405917
Sum of electronic and enthalpy Energies (Eh)	-419.404973
Sum of electronic and thermal Free Energies (Eh)	-419.45297
Number of Imaginary Frequencies	1

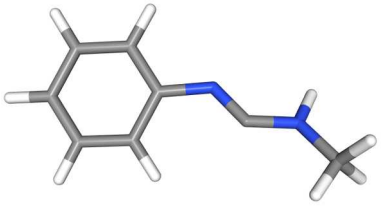
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-2.835779	0.807767	0.117858
C	-2.775821	-0.548860	0.421660
C	-1.580655	-1.244490	0.284461
C	-0.449181	-0.564984	-0.155869
C	-0.494330	0.794977	-0.465600
C	-1.696272	1.475530	-0.324991
H	-3.770430	1.344852	0.224629
H	-3.662004	-1.068820	0.764505
H	0.412938	1.280276	-0.807859
H	-1.744043	2.531292	-0.563189
N	0.763255	-1.239874	-0.292747
C	1.930330	-1.307259	-0.470791
H	-1.509661	-2.300540	0.512095
C	3.130679	0.737410	0.945238
H	3.707201	1.667139	1.030533
H	2.177693	0.886187	1.457745
H	3.692241	-0.050931	1.456120
N	2.887986	0.476087	-0.464788
H	3.763545	0.156496	-0.883635

__Frequencies__ (Top 10 out of 51)

1. -476.2773 cm-1 (Symmetry: A) *
2. 28.4408 cm-1 (Symmetry: A)
3. 50.7193 cm-1 (Symmetry: A)
4. 89.7264 cm-1 (Symmetry: A)
5. 142.1211 cm-1 (Symmetry: A)
6. 185.7468 cm-1 (Symmetry: A)
7. 235.6091 cm-1 (Symmetry: A)
8. 271.7748 cm-1 (Symmetry: A)
9. 370.9327 cm-1 (Symmetry: A)
10. 417.3860 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C8H9N2
Electronic Energy (Eh)	-419.626303335
Sum of electronic and zero-point Energies (Eh)	-419.471238
Sum of electronic and thermal Energies (Eh)	-419.461581
Sum of electronic and enthalpy Energies (Eh)	-419.460637
Sum of electronic and thermal Free Energies (Eh)	-419.508008
Number of Imaginary Frequencies	0

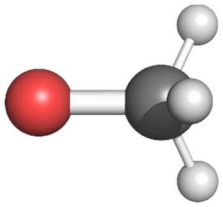
__Molecular Geometry in Cartesian Coordinates__

xyz

C	3.242853	0.433364	0.060217
C	2.873724	-0.907158	0.115631
C	1.533988	-1.270085	0.061904
C	0.543484	-0.291555	-0.046508
C	0.915938	1.056452	-0.111292
C	2.256685	1.410507	-0.052267
H	4.287896	0.714948	0.101947
H	3.632749	-1.675880	0.201680
H	0.143929	1.811454	-0.203296
H	2.534200	2.457308	-0.098912
C	-1.819083	-0.026237	0.062948
H	1.231956	-2.309468	0.104092
N	-0.789931	-0.710777	-0.114920
C	-4.208932	0.466946	0.251056
H	-4.904753	0.693805	-0.557971
H	-4.741007	-0.066100	1.042941
H	-3.825072	1.402220	0.655537
N	-3.084504	-0.302711	-0.249362
H	-3.270799	-1.167273	-0.746186

__Frequencies__ (Top 10 out of 51)

1. 43.7402 cm-1 (Symmetry: A)
2. 62.8339 cm-1 (Symmetry: A)
3. 85.9723 cm-1 (Symmetry: A)
4. 103.1881 cm-1 (Symmetry: A)
5. 219.7366 cm-1 (Symmetry: A)
6. 253.4650 cm-1 (Symmetry: A)
7. 335.6146 cm-1 (Symmetry: A)
8. 364.8639 cm-1 (Symmetry: A)
9. 419.4793 cm-1 (Symmetry: A)
10. 488.4075 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	CH3O
Electronic Energy (Eh)	-115.030455969
Sum of electronic and zero-point Energies (Eh)	-114.994098
Sum of electronic and thermal Energies (Eh)	-114.990931
Sum of electronic and enthalpy Energies (Eh)	-114.989987
Sum of electronic and thermal Free Energies (Eh)	-115.017108
Number of Imaginary Frequencies	0

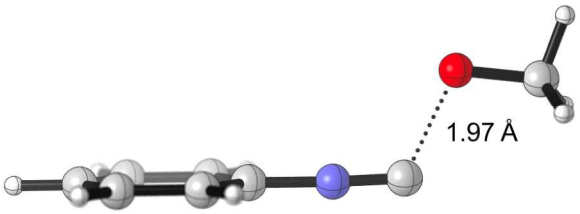
__Molecular Geometry in Cartesian Coordinates__

xyz

O	-0.791367	-0.000162	-0.007300
C	0.577126	-0.000354	-0.012176
H	0.870321	0.013978	1.052666
H	0.999711	-0.912358	-0.449795
H	0.998147	0.901798	-0.471417

__Frequencies__ (Top 10 out of 9)

1. 463.6377 cm-1 (Symmetry: A)
2. 973.3854 cm-1 (Symmetry: A)
3. 1138.6317 cm-1 (Symmetry: A)
4. 1386.7919 cm-1 (Symmetry: A)
5. 1391.0582 cm-1 (Symmetry: A)
6. 1520.6608 cm-1 (Symmetry: A)
7. 2964.4086 cm-1 (Symmetry: A)
8. 3039.7060 cm-1 (Symmetry: A)
9. 3080.8247 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C8H8NO
Electronic Energy (Eh)	-439.431524533
Sum of electronic and zero-point Energies (Eh)	-439.292479
Sum of electronic and thermal Energies (Eh)	-439.282625
Sum of electronic and enthalpy Energies (Eh)	-439.28168
Sum of electronic and thermal Free Energies (Eh)	-439.330634
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

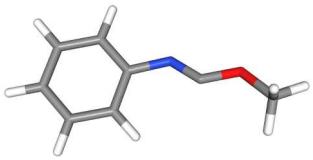
xyz

C	3.310233	-0.000196	-0.342083
C	2.631925	-1.205437	-0.185018
C	1.279907	-1.214027	0.129267
C	0.612068	0.000135	0.283900
C	1.280136	1.214132	0.128970
C	2.632153	1.205211	-0.185314
H	4.365163	-0.000327	-0.587103
H	3.156582	-2.144935	-0.307971
H	0.733482	2.140054	0.252777
H	3.156986	2.144581	-0.308497

N	-0.735426	0.000300	0.598726
C	-1.885527	0.000401	0.823262
H	0.733075	-2.139814	0.253295
O	-3.132901	-0.000369	-0.698596
C	-4.443787	-0.000025	-0.230996
H	-5.068930	-0.000478	-1.134282
H	-4.683955	-0.896343	0.349261
H	-4.683858	0.896955	0.348279

__Frequencies__ (Top 10 out of 48)

1. -430.4491 cm-1 (Symmetry: A) *
2. 23.5463 cm-1 (Symmetry: A)
3. 49.3212 cm-1 (Symmetry: A)
4. 49.8905 cm-1 (Symmetry: A)
5. 157.6275 cm-1 (Symmetry: A)
6. 183.1358 cm-1 (Symmetry: A)
7. 196.6420 cm-1 (Symmetry: A)
8. 229.6425 cm-1 (Symmetry: A)
9. 356.7283 cm-1 (Symmetry: A)
10. 415.1412 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C8H8NO
Electronic Energy (Eh)	-439.483011401
Sum of electronic and zero-point Energies (Eh)	-439.340079
Sum of electronic and thermal Energies (Eh)	-439.330727
Sum of electronic and enthalpy Energies (Eh)	-439.329783
Sum of electronic and thermal Free Energies (Eh)	-439.376516
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

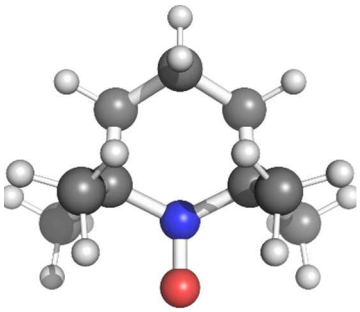
xyz

C	3.207396	0.426046	0.124341
C	2.832625	-0.912954	0.163499
C	1.495504	-1.271276	0.041947
C	0.519966	-0.286757	-0.109635
C	0.895160	1.058814	-0.159253
C	2.233236	1.407887	-0.038564
H	4.250399	0.703735	0.214927
H	3.584001	-1.684084	0.285177
H	0.131530	1.815824	-0.293308
H	2.517568	2.452993	-0.076181
C	-1.831456	-0.047735	0.013761

H	1.186837	-2.309132	0.064315
N	-0.815731	-0.704445	-0.245703
O	-3.078347	-0.415113	-0.200907
C	-4.075481	0.488336	0.286239
H	-3.960058	1.466559	-0.181730
H	-5.031075	0.051071	0.009558
H	-4.004005	0.580883	1.370408

__Frequencies__ (Top 10 out of 48)

1. 34.2424 cm-1 (Symmetry: A)
2. 80.2168 cm-1 (Symmetry: A)
3. 93.8807 cm-1 (Symmetry: A)
4. 144.0606 cm-1 (Symmetry: A)
5. 208.8545 cm-1 (Symmetry: A)
6. 251.8177 cm-1 (Symmetry: A)
7. 331.5771 cm-1 (Symmetry: A)
8. 368.1361 cm-1 (Symmetry: A)
9. 418.0194 cm-1 (Symmetry: A)
10. 482.2182 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H18NO
Electronic Energy (Eh)	-483.632462908
Sum of electronic and zero-point Energies (Eh)	-483.368355
Sum of electronic and thermal Energies (Eh)	-483.356627
Sum of electronic and enthalpy Energies (Eh)	-483.355683
Sum of electronic and thermal Free Energies (Eh)	-483.404664
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

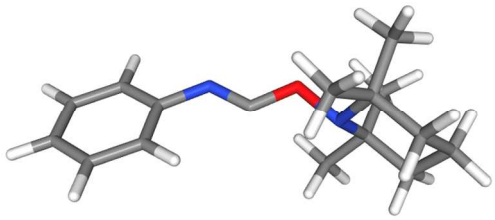
xyz

O	0.000027	-2.007575	-0.092278
C	-1.317560	-0.070945	-0.025793
C	1.317564	-0.070924	-0.025832
C	-1.240098	1.383133	-0.505074
C	1.240121	1.383040	-0.505412
C	0.000101	2.116245	-0.007203
H	-2.155330	1.890094	-0.185862
H	-1.234624	1.389660	-1.601054

H	2.155467	1.890032	-0.186582
H	1.234305	1.389330	-1.601389
H	0.000079	3.142820	-0.381281
H	0.000276	2.183574	1.084843
N	-0.000013	-0.744287	-0.224401
C	-2.344745	-0.831852	-0.864404
H	-2.469395	-1.848800	-0.495299
H	-3.303945	-0.310949	-0.814131
H	-2.023834	-0.879004	-1.907063
C	-1.710643	-0.157397	1.456142
H	-2.753053	0.148507	1.574835
H	-1.607990	-1.188662	1.798794
H	-1.096040	0.484782	2.088092
C	1.710325	-0.157092	1.456222
H	1.608083	-1.188407	1.798862
H	2.752512	0.149387	1.575299
H	1.095083	0.484667	2.087989
C	2.344972	-0.832036	-0.863995
H	2.024471	-0.879276	-1.906777
H	3.304208	-0.311228	-0.813419
H	2.469377	-1.848952	-0.494734

__Frequencies__ (Top 10 out of 81)

1. 85.6212 cm-1 (Symmetry: A)
2. 133.3641 cm-1 (Symmetry: A)
3. 198.7117 cm-1 (Symmetry: A)
4. 207.4555 cm-1 (Symmetry: A)
5. 246.7924 cm-1 (Symmetry: A)
6. 262.9127 cm-1 (Symmetry: A)
7. 282.1642 cm-1 (Symmetry: A)
8. 297.6061 cm-1 (Symmetry: A)
9. 304.2751 cm-1 (Symmetry: A)
10. 313.4584 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C16H23N2O
Electronic Energy (Eh)	-808.026871263
Sum of electronic and zero-point Energies (Eh)	-807.660903
Sum of electronic and thermal Energies (Eh)	-807.642291
Sum of electronic and enthalpy Energies (Eh)	-807.641347
Sum of electronic and thermal Free Energies (Eh)	-807.708901
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

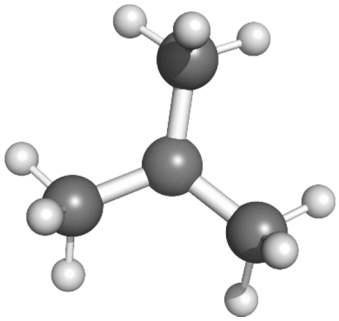
xyz

C	5.707153	0.228757	-0.656865
C	4.635152	0.855902	-1.287638
C	3.343503	0.697740	-0.805045
C	3.113222	-0.101078	0.319128
C	4.186462	-0.721230	0.956574
C	5.476826	-0.558912	0.465967
H	6.713416	0.357568	-1.036452
H	4.806682	1.475323	-2.160292
H	3.989650	-1.327614	1.832161
H	6.304690	-1.047860	0.965669
C	0.756559	-0.090839	0.282223
H	2.504128	1.185497	-1.287147
N	1.829692	-0.290754	0.867832
O	-0.443493	-0.203212	0.826393
C	-2.224047	-1.261979	-0.284174
C	-2.208158	1.250692	0.280099
C	-3.355088	-0.988869	-1.286932
C	-3.340488	1.445909	-0.739497
C	-4.219063	0.208361	-0.900136
H	-3.957190	-1.898148	-1.371815
H	-2.904414	-0.801365	-2.267503
H	-3.931686	2.310883	-0.425063
H	-2.890064	1.690983	-1.707421
H	-4.971388	0.386685	-1.672345
H	-4.768776	0.004092	0.023246
N	-1.490833	0.020143	-0.136830
C	-1.239734	-2.258439	-0.906440
H	-0.741518	-1.807982	-1.767476
H	-0.480475	-2.569191	-0.185695
H	-1.779620	-3.149963	-1.234341
C	-2.764031	-1.860027	1.025373
H	-3.016279	-2.909696	0.855674
H	-2.003650	-1.818683	1.807147
H	-3.661948	-1.360509	1.385085
C	-1.210998	2.406311	0.139560
H	-0.449542	2.370809	0.921577
H	-0.717620	2.360726	-0.833772
H	-1.739511	3.358673	0.225743
C	-2.743016	1.238591	1.721601
H	-2.979273	2.263262	2.019056
H	-3.649338	0.646312	1.835441
H	-1.985856	0.854842	2.407575

__Frequencies__ (Top 10 out of 120)

1. 13.7272 cm-1 (Symmetry: A)
2. 26.5541 cm-1 (Symmetry: A)

3. 41.3196 cm-1 (Symmetry: A)
4. 76.3561 cm-1 (Symmetry: A)
5. 93.0416 cm-1 (Symmetry: A)
6. 149.8177 cm-1 (Symmetry: A)
7. 161.7087 cm-1 (Symmetry: A)
8. 177.2682 cm-1 (Symmetry: A)
9. 209.2023 cm-1 (Symmetry: A)
10. 236.4850 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C4H9
Electronic Energy (Eh)	-157.744991907
Sum of electronic and zero-point Energies (Eh)	-157.627716
Sum of electronic and thermal Energies (Eh)	-157.621372
Sum of electronic and enthalpy Energies (Eh)	-157.620428
Sum of electronic and thermal Free Energies (Eh)	-157.657089
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

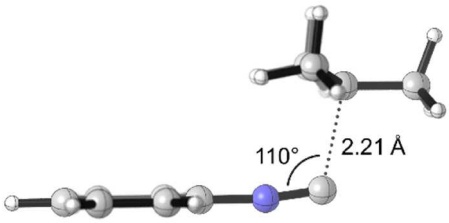
xyz

C	-0.000007	-0.000001	-0.182727
C	0.210844	1.464940	0.019045
H	0.247837	1.721951	1.090332
H	1.154689	1.799037	-0.419573
H	-0.600479	2.051648	-0.419562
C	1.163262	-0.915064	0.019052
H	1.367255	-1.075837	1.090325
H	0.980828	-1.899413	-0.419837
H	2.077038	-0.505625	-0.419381
C	-1.374112	-0.549879	0.019050
H	-2.135336	0.100249	-0.419949
H	-1.476421	-1.546023	-0.419215
H	-1.615333	-0.645963	1.090341

__Frequencies__ (Top 10 out of 33)

1. 132.7997 cm-1 (Symmetry: A)
2. 141.8019 cm-1 (Symmetry: A)
3. 143.2372 cm-1 (Symmetry: A)

4. 258.9919 cm-1 (Symmetry: A)
5. 379.0111 cm-1 (Symmetry: A)
6. 379.9526 cm-1 (Symmetry: A)
7. 777.5295 cm-1 (Symmetry: A)
8. 934.0437 cm-1 (Symmetry: A)
9. 935.1208 cm-1 (Symmetry: A)
10. 967.9264 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H14N
Electronic Energy (Eh)	-482.151455865
Sum of electronic and zero-point Energies (Eh)	-481.933505
Sum of electronic and thermal Energies (Eh)	-481.920399
Sum of electronic and enthalpy Energies (Eh)	-481.919455
Sum of electronic and thermal Free Energies (Eh)	-481.975684
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

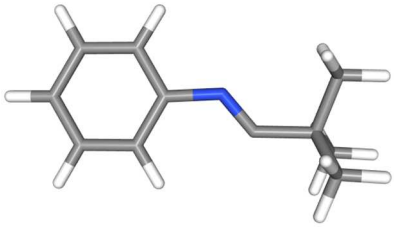
xyz

C	3.645240	0.000885	0.542859
C	3.005853	1.204784	0.258782
C	1.737144	1.213580	-0.302981
C	1.101703	-0.000720	-0.579959
C	1.738238	-1.214221	-0.301995
C	3.006932	-1.203820	0.259773
H	4.635371	0.001505	0.981232
H	3.498076	2.145258	0.475198
H	1.228270	-2.141899	-0.529647
H	3.500001	-2.143671	0.476967
N	-0.157789	-0.001507	-1.134884
C	-1.293910	-0.001924	-1.470407
H	1.226341	2.140612	-0.531396
C	-2.159078	-1.271662	0.953762
H	-2.711749	-1.443189	1.889309
H	-2.335849	-2.134028	0.305551
H	-1.095336	-1.235174	1.206638
C	-3.967389	-0.001289	-0.322796
H	-4.750000	-0.000432	0.449857
H	-4.112601	0.882133	-0.948256
H	-4.111835	-0.886766	-0.945519
C	-2.160204	1.274615	0.949807
H	-1.096691	1.239435	1.203807

H	-2.336735	2.134675	0.298468
H	-2.713863	1.449136	1.884214
C	-2.607675	0.000266	0.301116

__Frequencies__ (Top 10 out of 72)

1. -373.3129 cm-1 (Symmetry: A) *
2. 14.6765 cm-1 (Symmetry: A)
3. 34.5771 cm-1 (Symmetry: A)
4. 34.6959 cm-1 (Symmetry: A)
5. 137.5270 cm-1 (Symmetry: A)
6. 154.5348 cm-1 (Symmetry: A)
7. 181.5253 cm-1 (Symmetry: A)
8. 182.6562 cm-1 (Symmetry: A)
9. 202.8240 cm-1 (Symmetry: A)
10. 211.3117 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H14N
Electronic Energy (Eh)	-482.190960562
Sum of electronic and zero-point Energies (Eh)	-481.968373
Sum of electronic and thermal Energies (Eh)	-481.956165
Sum of electronic and enthalpy Energies (Eh)	-481.95522
Sum of electronic and thermal Free Energies (Eh)	-482.008786
Number of Imaginary Frequencies	0

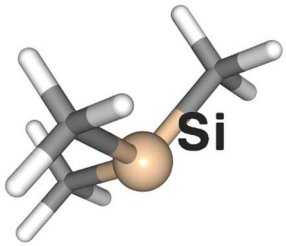
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	3.948536	0.276806	-0.046617
C	3.054088	1.344728	-0.006664
C	1.686405	1.114204	0.036925
C	1.205258	-0.197269	0.040414
C	2.097361	-1.265744	0.009756
C	3.466337	-1.027444	-0.038755
H	5.015201	0.462838	-0.080268
H	3.425776	2.362750	-0.008467
H	1.700428	-2.273530	0.022072
H	4.156207	-1.862414	-0.066673
N	-0.177924	-0.502139	0.093542
C	-1.115544	0.278130	-0.080596
H	0.979092	1.934673	0.068528
C	-3.167458	0.933746	1.096352

H	-4.252049	0.807518	1.148136
H	-2.741750	0.664156	2.065450
H	-2.948901	1.986245	0.903193
C	-2.892418	-1.433240	0.271597
H	-3.973170	-1.593260	0.316761
H	-2.474557	-2.069646	-0.510491
H	-2.450832	-1.733711	1.223340
C	-3.202416	0.457467	-1.368492
H	-2.983436	1.504838	-1.586962
H	-2.801043	-0.154995	-2.178942
H	-4.287318	0.326344	-1.341158
C	-2.599845	0.044144	-0.018806

__Frequencies__ (Top 10 out of 72)

1. 15.6746 cm-1 (Symmetry: A)
2. 51.5928 cm-1 (Symmetry: A)
3. 70.5547 cm-1 (Symmetry: A)
4. 82.4884 cm-1 (Symmetry: A)
5. 217.8141 cm-1 (Symmetry: A)
6. 219.7793 cm-1 (Symmetry: A)
7. 267.5438 cm-1 (Symmetry: A)
8. 282.8119 cm-1 (Symmetry: A)
9. 284.5173 cm-1 (Symmetry: A)
10. 291.2278 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C3H9Si
Electronic Energy (Eh)	-409.15866968
Sum of electronic and zero-point Energies (Eh)	-409.048512
Sum of electronic and thermal Energies (Eh)	-409.041088
Sum of electronic and enthalpy Energies (Eh)	-409.040144
Sum of electronic and thermal Free Energies (Eh)	-409.079571
Number of Imaginary Frequencies	0

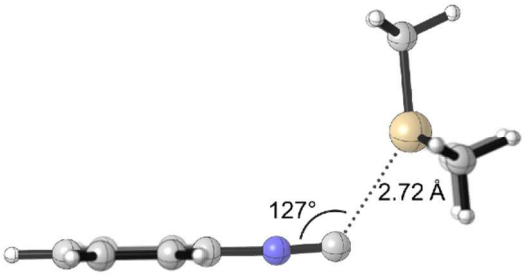
__Molecular Geometry in Cartesian Coordinates__

xyz			
Si	-0.000005	-0.000003	-0.435679
C	-0.072476	-1.780492	0.181054
C	-1.505758	0.953025	0.181047
H	-0.977132	-2.284944	-0.164547

H	0.787894	-2.356932	-0.165050
H	-0.073035	-1.801745	1.276441
C	1.578253	0.827491	0.181044
H	-2.435174	0.494824	-0.163279
H	-1.491533	1.988142	-0.166267
H	-1.522690	0.965916	1.276437
H	2.467469	0.296688	-0.165149
H	1.597204	0.836892	1.276433
H	1.646956	1.861057	-0.164389

__Frequencies__ (Top 10 out of 33)

1. 132.3464 cm-1 (Symmetry: A)
2. 147.3811 cm-1 (Symmetry: A)
3. 151.4869 cm-1 (Symmetry: A)
4. 193.4340 cm-1 (Symmetry: A)
5. 193.7330 cm-1 (Symmetry: A)
6. 220.0225 cm-1 (Symmetry: A)
7. 615.9324 cm-1 (Symmetry: A)
8. 689.0530 cm-1 (Symmetry: A)
9. 689.8768 cm-1 (Symmetry: A)
10. 690.3858 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H14NSi
Electronic Energy (Eh)	-733.567908338
Sum of electronic and zero-point Energies (Eh)	-733.358325
Sum of electronic and thermal Energies (Eh)	-733.34332
Sum of electronic and enthalpy Energies (Eh)	-733.342375
Sum of electronic and thermal Free Energies (Eh)	-733.405531
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

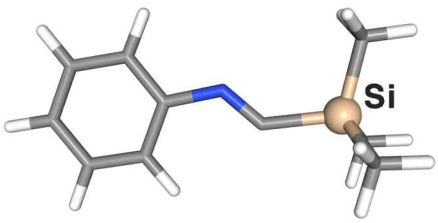
xyz

C	-3.428132	-1.542843	-0.639162
C	-3.425966	1.544400	-0.637689
H	-3.106434	-1.556861	-1.682280
H	-3.063242	-2.453087	-0.157679
H	-4.522610	-1.566122	-0.615334
C	-3.353542	-0.000534	2.027286
H	-3.104422	1.558884	-1.680849

H	-3.059651	2.453669	-0.155445
H	-4.520405	1.569281	-0.613666
H	-2.994536	-0.884418	2.558993
H	-4.448366	0.000275	2.078317
H	-2.993184	0.882272	2.559868
C	-0.538591	-0.000645	-1.310154
N	0.574735	-0.000489	-0.933707
C	1.859416	-0.000271	-0.423447
C	2.498739	-1.214197	-0.169385
C	2.498540	1.213879	-0.169955
C	3.788504	-1.204946	0.343377
H	1.979005	-2.140835	-0.376540
C	3.788306	1.205083	0.342812
H	1.978654	2.140333	-0.377552
C	4.436081	0.000182	0.600342
H	4.289066	-2.144511	0.542986
H	4.288714	2.144825	0.541975
H	5.442480	0.000357	1.000252
Si	-2.780595	-0.000092	0.223483

__Frequencies__ (Top 10 out of 72)

1. -140.3941 cm-1 (Symmetry: A) *
2. 8.1063 cm-1 (Symmetry: A)
3. 13.3606 cm-1 (Symmetry: A)
4. 23.2236 cm-1 (Symmetry: A)
5. 74.5437 cm-1 (Symmetry: A)
6. 84.3930 cm-1 (Symmetry: A)
7. 132.1874 cm-1 (Symmetry: A)
8. 144.1078 cm-1 (Symmetry: A)
9. 150.2648 cm-1 (Symmetry: A)
10. 160.3685 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H14NSi
Electronic Energy (Eh)	-733.608021231
Sum of electronic and zero-point Energies (Eh)	-733.396449
Sum of electronic and thermal Energies (Eh)	-733.381843
Sum of electronic and enthalpy Energies (Eh)	-733.380898
Sum of electronic and thermal Free Energies (Eh)	-733.440307
Number of Imaginary Frequencies	0

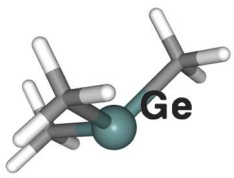
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-4.361119	-0.281207	0.000050
C	-3.462576	-1.347134	0.000009
C	-2.095406	-1.111627	-0.000037
C	-1.622261	0.202225	-0.000051
C	-2.516134	1.268702	-0.000015
C	-3.885252	1.025406	0.000041
H	-5.427681	-0.471308	0.000089
H	-3.831653	-2.366117	0.000016
H	-2.120617	2.277255	-0.000029
H	-4.579616	1.857052	0.000073
C	0.716937	-0.273252	0.000013
H	-1.381240	-1.926934	-0.000062
N	-0.233274	0.509298	-0.000099
Si	2.585554	-0.028162	0.000014
C	3.225534	-0.874066	-1.543640
H	2.816124	-0.411318	-2.444392
H	4.315437	-0.806749	-1.594450
H	2.949044	-1.930649	-1.549696
C	3.001613	1.801135	-0.000015
H	2.584832	2.290937	0.882768
H	4.083850	1.957578	-0.000059
H	2.584766	2.290904	-0.882785
C	3.225542	-0.874009	1.543696
H	2.949063	-1.930595	1.549787
H	4.315447	-0.806679	1.594491
H	2.816138	-0.411239	2.444438

__Frequencies__ (Top 10 out of 72)

1. 17.5729 cm-1 (Symmetry: A)
2. 47.1885 cm-1 (Symmetry: A)
3. 48.4214 cm-1 (Symmetry: A)
4. 69.5429 cm-1 (Symmetry: A)
5. 134.7668 cm-1 (Symmetry: A)
6. 143.1268 cm-1 (Symmetry: A)
7. 154.5366 cm-1 (Symmetry: A)
8. 155.3190 cm-1 (Symmetry: A)
9. 175.4468 cm-1 (Symmetry: A)
10. 193.4688 cm-1 (Symmetry: A)



Charge 0
Multiplicity 2
Stoichiometry C3H9Ge

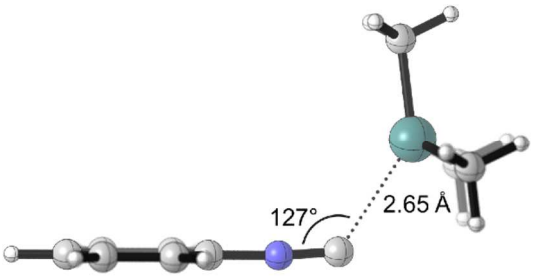
Electronic Energy (Eh) -2196.74243195
Sum of electronic and zero-point Energies (Eh) -2196.633503
Sum of electronic and thermal Energies (Eh) -2196.6256
Sum of electronic and enthalpy Energies (Eh) -2196.624656
Sum of electronic and thermal Free Energies (Eh) -2196.66619
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	1.036042	-1.545691	0.340031
H	0.599471	-2.484428	-0.002893
H	2.070450	-1.498245	-0.002271
H	1.033371	-1.542390	1.434223
C	0.820617	1.670060	0.340025
H	0.263217	2.542276	-0.003433
H	0.817778	1.666750	1.434219
H	1.852348	1.760582	-0.001684
C	-1.856629	-0.124371	0.340042
H	-1.852346	-0.124734	1.434232
H	-2.451062	0.723598	-0.002039
H	-2.333093	-1.043431	-0.003079
Ge	-0.000010	0.000001	-0.325246

Frequencies (Top 10 out of 33)

1. 114.4917 cm-1 (Symmetry: A)
2. 122.8096 cm-1 (Symmetry: A)
3. 125.6403 cm-1 (Symmetry: A)
4. 162.5968 cm-1 (Symmetry: A)
5. 163.0869 cm-1 (Symmetry: A)
6. 169.5981 cm-1 (Symmetry: A)
7. 558.8805 cm-1 (Symmetry: A)
8. 594.4450 cm-1 (Symmetry: A)
9. 594.7848 cm-1 (Symmetry: A)
10. 694.7809 cm-1 (Symmetry: A)



Charge 0
Multiplicity 2
Stoichiometry C10H14GeN
Electronic Energy (Eh) -2521.15111108
Sum of electronic and zero-point Energies (Eh) -2520.942846
Sum of electronic and thermal Energies (Eh) -2520.927338
Sum of electronic and enthalpy Energies (Eh) -2520.926394

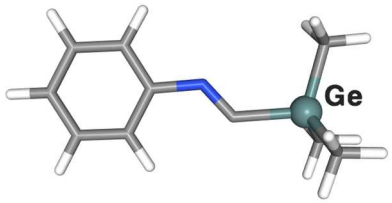
Sum of electronic and thermal Free Energies (Eh) -2520.991036
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	3.031390	1.606975	-0.715253
C	3.028499	-1.609802	-0.712031
H	2.743403	1.621756	-1.767205
H	2.661193	2.516314	-0.239144
H	4.122949	1.604502	-0.649654
C	2.814645	0.001560	2.072765
H	2.740611	-1.626128	-1.763989
H	2.656580	-2.517517	-0.234168
H	4.120054	-1.609205	-0.646321
H	2.431006	0.888111	2.579308
H	3.906053	0.000608	2.155223
H	2.429320	-0.883232	2.581101
C	0.112743	0.000414	-1.351575
N	-1.001795	0.000299	-0.974013
C	-2.279114	0.000199	-0.449947
C	-2.916124	1.214421	-0.188310
C	-2.916023	-1.214126	-0.188539
C	-4.199448	1.204994	0.339956
H	-2.399261	2.141223	-0.401849
C	-4.199346	-1.204909	0.339731
H	-2.399083	-2.140844	-0.402261
C	-4.844224	-0.000009	0.604960
H	-4.697479	2.144660	0.545445
H	-4.697299	-2.144656	0.545039
H	-5.845747	-0.000089	1.016852
Ge	2.295071	0.000128	0.155911

Frequencies (Top 10 out of 72)

1. -113.7297 cm-1 (Symmetry: A) *
2. 9.9124 cm-1 (Symmetry: A)
3. 17.6063 cm-1 (Symmetry: A)
4. 24.2623 cm-1 (Symmetry: A)
5. 68.4551 cm-1 (Symmetry: A)
6. 76.2805 cm-1 (Symmetry: A)
7. 110.9150 cm-1 (Symmetry: A)
8. 115.6016 cm-1 (Symmetry: A)
9. 120.6557 cm-1 (Symmetry: A)
10. 160.4374 cm-1 (Symmetry: A)



Charge 0
Multiplicity 2
Stoichiometry C10H14GeN
Electronic Energy (Eh) -2521.17616313
Sum of electronic and zero-point Energies (Eh) -2520.966257
Sum of electronic and thermal Energies (Eh) -2520.950944
Sum of electronic and enthalpy Energies (Eh) -2520.95
Sum of electronic and thermal Free Energies (Eh) -2521.012002
Number of Imaginary Frequencies 0

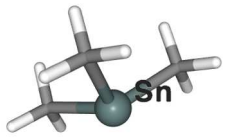
Molecular Geometry in Cartesian Coordinates

C	4.822432	-0.245624	-0.000011
C	3.952167	-1.334679	-0.000095
C	2.579133	-1.135339	-0.000100
C	2.071179	0.165539	-0.000020
C	2.936956	1.254984	0.000058
C	4.312038	1.047920	0.000066
H	5.893648	-0.407440	-0.000008
H	4.347789	-2.343671	-0.000157
H	2.515392	2.252930	0.000113
H	4.984131	1.897695	0.000129
C	-0.256788	-0.370204	0.000039
H	1.887022	-1.969326	-0.000164
N	0.674305	0.435333	-0.000027
C	-2.917221	-0.869351	1.614192
H	-2.487272	-0.416132	2.508735
H	-4.002475	-0.758590	1.658158
H	-2.676782	-1.933620	1.616682
C	-2.518233	1.920635	-0.000003
H	-2.066930	2.373070	-0.884194
H	-3.587682	2.141423	-0.000031
H	-2.066977	2.373078	0.884208
C	-2.917202	-0.869378	-1.614167
H	-2.676785	-1.933652	-1.616626
H	-4.002453	-0.758595	-1.658159
H	-2.487224	-0.416187	-2.508709
Ge	-2.208760	-0.016729	0.000014

Frequencies (Top 10 out of 72)

1. 15.7714 cm-1 (Symmetry: A)
2. 39.1563 cm-1 (Symmetry: A)
3. 50.2871 cm-1 (Symmetry: A)

4. 63.4298 cm-1 (Symmetry: A)
5. 113.9347 cm-1 (Symmetry: A)
6. 123.7099 cm-1 (Symmetry: A)
7. 125.7596 cm-1 (Symmetry: A)
8. 133.0987 cm-1 (Symmetry: A)
9. 156.5952 cm-1 (Symmetry: A)
10. 165.1241 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C3H9Sn
Electronic Energy (Eh)	-123.018977167
Sum of electronic and zero-point Energies (Eh)	-122.911855
Sum of electronic and thermal Energies (Eh)	-122.90325
Sum of electronic and enthalpy Energies (Eh)	-122.902306
Sum of electronic and thermal Free Energies (Eh)	-122.946895
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

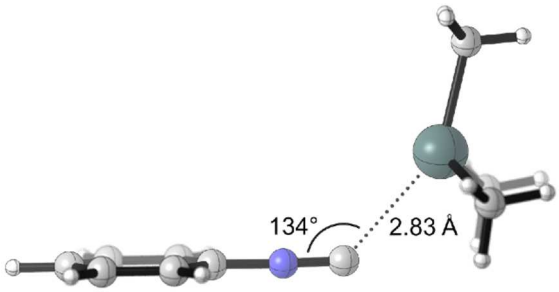
xyz

Sn	0.000004	-0.000136	-0.290148
C	-0.000493	2.011502	0.488384
H	0.885444	2.556860	0.162495
H	-0.885393	2.557293	0.160461
H	-0.001753	1.970967	1.580818
C	-1.742005	-1.005852	0.488656
H	-1.775312	-2.043796	0.156969
H	-1.703716	-0.990755	1.581067
H	-2.656840	-0.507965	0.166640
C	1.742482	-1.004997	0.488652
H	1.708035	-0.983041	1.581074
H	1.771886	-2.045073	0.163292
H	2.657533	-0.511605	0.160428

__Frequencies__ (Top 10 out of 33)

1. 64.1472 cm-1 (Symmetry: A)
2. 77.8941 cm-1 (Symmetry: A)
3. 79.3149 cm-1 (Symmetry: A)
4. 129.3453 cm-1 (Symmetry: A)
5. 129.6185 cm-1 (Symmetry: A)
6. 138.7172 cm-1 (Symmetry: A)
7. 489.5084 cm-1 (Symmetry: A)
8. 507.3741 cm-1 (Symmetry: A)
9. 507.4042 cm-1 (Symmetry: A)

10. 656.6456 cm-1 (Symmetry: A)



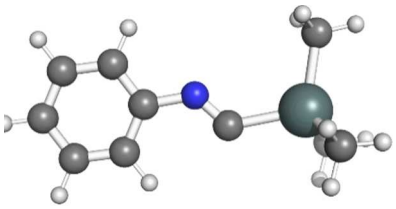
Charge	0
Multiplicity	2
Stoichiometry	C10H14NSn
Electronic Energy (Eh)	-447.430321858
Sum of electronic and zero-point Energies (Eh)	-447.223756
Sum of electronic and thermal Energies (Eh)	-447.207544
Sum of electronic and enthalpy Energies (Eh)	-447.2066
Sum of electronic and thermal Free Energies (Eh)	-447.274485
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	2.653316	1.738159	-0.989469
C	2.656064	-1.736359	-0.991342
H	2.133595	1.724903	-1.948129
H	2.395196	2.658457	-0.464053
H	3.730531	1.737101	-1.173102
C	3.311198	0.000026	1.956077
H	2.134701	-1.723970	-1.949121
H	2.401320	-2.657629	-0.465983
H	3.732957	-1.732278	-1.176807
H	3.110778	0.885519	2.559896
H	4.367803	0.000943	1.673808
H	3.112132	-0.886207	2.559255
C	-0.396651	-0.000383	-1.175283
N	-1.511384	-0.000290	-0.812011
C	-2.814418	-0.000200	-0.345369
C	-3.460096	1.214541	-0.115517
C	-3.459957	-1.214858	-0.114688
C	-4.767082	1.205400	0.351474
H	-2.932984	2.140839	-0.304666
C	-4.766942	-1.205552	0.352295
H	-2.932736	-2.141222	-0.303209
C	-5.422599	-0.000033	0.585856
H	-5.274605	2.144823	0.532844
H	-5.274356	-2.144910	0.534300
H	-6.442444	0.000032	0.950102
Sn	2.102416	-0.000177	0.151495

__Frequencies__ (Top 10 out of 72)

1. -68.4841 cm-1 (Symmetry: A) *
2. 7.6659 cm-1 (Symmetry: A)
3. 16.6946 cm-1 (Symmetry: A)
4. 23.4722 cm-1 (Symmetry: A)
5. 56.7852 cm-1 (Symmetry: A)
6. 63.5745 cm-1 (Symmetry: A)
7. 65.7624 cm-1 (Symmetry: A)
8. 80.7559 cm-1 (Symmetry: A)
9. 83.9849 cm-1 (Symmetry: A)
10. 130.3866 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H14NSn
Electronic Energy (Eh)	-447.448931465
Sum of electronic and zero-point Energies (Eh)	-447.24105
Sum of electronic and thermal Energies (Eh)	-447.224856
Sum of electronic and enthalpy Energies (Eh)	-447.223912
Sum of electronic and thermal Free Energies (Eh)	-447.289338
Number of Imaginary Frequencies	0

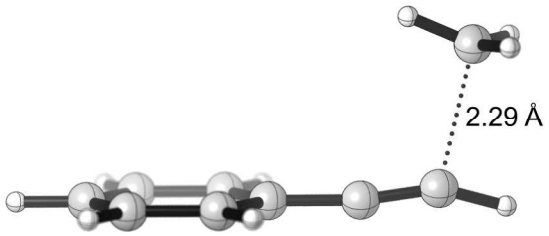
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-5.234381	-0.226757	0.000012
C	-4.379012	-1.327641	0.000051
C	-3.003411	-1.147138	0.000020
C	-2.478132	0.146662	-0.000053
C	-3.328495	1.247885	-0.000099
C	-4.706398	1.059668	-0.000061
H	-6.307716	-0.373945	0.000036
H	-4.788400	-2.331147	0.000106
H	-2.893331	2.240004	-0.000166
H	-5.366858	1.918534	-0.000095
C	-0.158495	-0.425489	0.000113
H	-2.322193	-1.990072	0.000052
N	-1.075888	0.396554	-0.000105
C	2.740616	-0.933027	-1.754070
H	2.317873	-0.476003	-2.649432
H	3.826289	-0.832869	-1.795428
H	2.491425	-1.994858	-1.759788
C	2.269002	2.101947	0.000007

H	1.811277	2.547367	0.883834
H	3.333648	2.341434	-0.000020
H	1.811233	2.547357	-0.883802
C	2.740712	-0.933035	1.754060
H	2.491533	-1.994869	1.759773
H	3.826385	-0.832862	1.795376
H	2.317998	-0.476032	2.649447
Sn	1.964200	-0.008927	0.000019

__Frequencies__ (Top 10 out of 72)

1. 17.9973 cm-1 (Symmetry: A)
2. 36.6083 cm-1 (Symmetry: A)
3. 42.5213 cm-1 (Symmetry: A)
4. 59.8388 cm-1 (Symmetry: A)
5. 66.0204 cm-1 (Symmetry: A)
6. 77.8464 cm-1 (Symmetry: A)
7. 80.2594 cm-1 (Symmetry: A)
8. 117.0406 cm-1 (Symmetry: A)
9. 128.3403 cm-1 (Symmetry: A)
10. 131.1741 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H9
Electronic Energy (Eh)	-348.150473003
Sum of electronic and zero-point Energies (Eh)	-348.007719
Sum of electronic and thermal Energies (Eh)	-347.998303
Sum of electronic and enthalpy Energies (Eh)	-347.997359
Sum of electronic and thermal Free Energies (Eh)	-348.044555
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

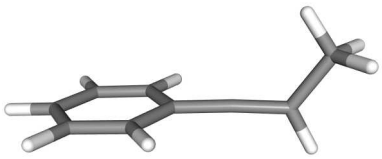
xyz

C	2.742118	0.000000	0.373514
C	2.068502	1.204882	0.188406
C	0.731220	1.210480	-0.180219
C	0.045258	-0.000000	-0.367607
C	0.731220	-1.210480	-0.180219
C	2.068503	-1.204882	0.188406
H	3.786663	0.000001	0.660569
H	2.588652	2.144596	0.331177
H	0.202153	-2.144057	-0.327160

H	2.588653	-2.144595	0.331178
C	-3.644489	0.000000	1.112110
H	-2.800978	-0.000034	1.787368
H	-4.193267	0.925732	1.002919
H	-4.193323	-0.925695	1.002894
H	0.202152	2.144056	-0.327161
C	-1.326405	-0.000000	-0.742736
C	-2.536523	-0.000000	-0.895909
H	-3.457131	0.000000	-1.436265

__Frequencies__ (Top 10 out of 48)

1. -565.1063 cm-1 (Symmetry: A) *
2. 29.5368 cm-1 (Symmetry: A)
3. 39.0195 cm-1 (Symmetry: A)
4. 60.5153 cm-1 (Symmetry: A)
5. 164.9372 cm-1 (Symmetry: A)
6. 177.3952 cm-1 (Symmetry: A)
7. 379.0407 cm-1 (Symmetry: A)
8. 408.7080 cm-1 (Symmetry: A)
9. 456.7832 cm-1 (Symmetry: A)
10. 459.8994 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H9
Electronic Energy (Eh)	-348.216677535
Sum of electronic and zero-point Energies (Eh)	-348.068586
Sum of electronic and thermal Energies (Eh)	-348.060041
Sum of electronic and enthalpy Energies (Eh)	-348.059097
Sum of electronic and thermal Free Energies (Eh)	-348.103289
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

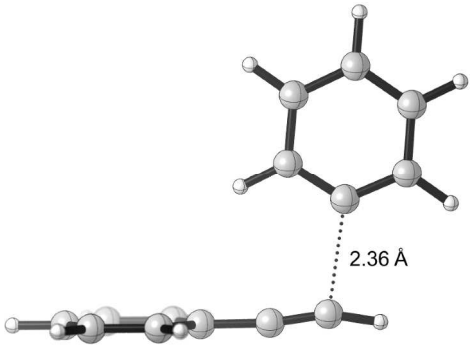
xyz

C	2.816593	-0.000020	0.167565
C	2.117106	1.208187	0.086989
C	0.746399	1.221936	-0.069754
C	0.015287	0.000016	-0.154077
C	0.746368	-1.221923	-0.069764
C	2.117075	-1.208209	0.086979
H	3.892236	-0.000034	0.291114
H	2.655206	2.147044	0.148146
H	0.204383	-2.157502	-0.131992
H	2.655152	-2.147080	0.148128

C	-2.632243	0.000004	-0.514889
C	-3.693952	-0.000013	0.561303
H	-4.332169	0.881556	0.463815
H	-4.332129	-0.881611	0.463827
H	-3.243180	0.000004	1.552964
H	0.204436	2.157529	-0.131974
C	-1.350718	0.000038	-0.303959
H	-2.995414	-0.000003	-1.546385

__Frequencies__ (Top 10 out of 48)

1. 39.5684 cm-1 (Symmetry: A)
2. 96.1207 cm-1 (Symmetry: A)
3. 152.8842 cm-1 (Symmetry: A)
4. 188.7583 cm-1 (Symmetry: A)
5. 208.9503 cm-1 (Symmetry: A)
6. 375.6612 cm-1 (Symmetry: A)
7. 408.2892 cm-1 (Symmetry: A)
8. 469.7658 cm-1 (Symmetry: A)
9. 516.5207 cm-1 (Symmetry: A)
10. 533.7473 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H11
Electronic Energy (Eh)	-539.849395431
Sum of electronic and zero-point Energies (Eh)	-539.650892
Sum of electronic and thermal Energies (Eh)	-539.638883
Sum of electronic and enthalpy Energies (Eh)	-539.637939
Sum of electronic and thermal Free Energies (Eh)	-539.693246
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

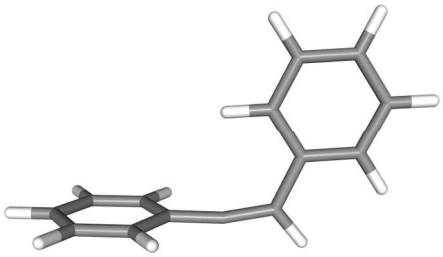
xyz

C	4.036754	-1.032871	0.000003
C	3.490864	-0.598632	1.205331
C	2.404917	0.265028	1.210903
C	1.850061	0.705268	-0.000001
C	2.404919	0.265026	-1.210903
C	3.490866	-0.598634	-1.205328

H	4.884882	-1.706851	0.000004
H	3.913128	-0.934805	2.144745
H	1.972898	0.606094	-2.143733
H	3.913132	-0.934808	-2.144740
H	1.972893	0.606098	2.143732
C	0.723293	1.577510	-0.000003
C	-0.324349	2.191197	-0.000004
H	-1.045229	2.977026	-0.000006
C	-2.055441	0.594135	0.000001
C	-3.377222	0.974805	0.000003
C	-1.616103	-0.708689	-0.000003
C	-4.336751	-0.042303	0.000003
H	-3.676531	2.017737	0.000006
C	-2.587149	-1.712018	-0.000003
H	-0.556944	-0.946228	-0.000005
C	-3.939969	-1.376736	-0.000000
H	-5.391104	0.211286	0.000005
H	-2.286827	-2.753999	-0.000006
H	-4.688438	-2.160063	-0.000000

__Frequencies__ (Top 10 out of 69)

1. -383.4326 cm-1 (Symmetry: A) *
2. 18.5582 cm-1 (Symmetry: A)
3. 27.8567 cm-1 (Symmetry: A)
4. 32.1955 cm-1 (Symmetry: A)
5. 75.8453 cm-1 (Symmetry: A)
6. 105.7922 cm-1 (Symmetry: A)
7. 163.6759 cm-1 (Symmetry: A)
8. 171.2585 cm-1 (Symmetry: A)
9. 377.4055 cm-1 (Symmetry: A)
10. 401.4960 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H11
Electronic Energy (Eh)	-539.928867247
Sum of electronic and zero-point Energies (Eh)	-539.726852
Sum of electronic and thermal Energies (Eh)	-539.715524
Sum of electronic and enthalpy Energies (Eh)	-539.71458
Sum of electronic and thermal Free Energies (Eh)	-539.76729
Number of Imaginary Frequencies	0

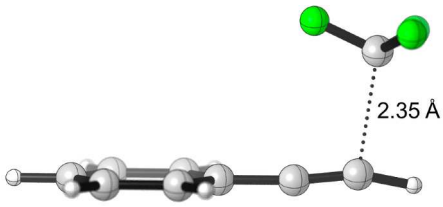
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-4.279985	0.709947	-0.000087
C	-3.650497	0.398048	1.208187
C	-2.414226	-0.216130	1.221723
C	-1.756808	-0.539034	0.000043
C	-2.414262	-0.216459	-1.221705
C	-3.650532	0.397725	-1.208294
H	-5.250458	1.190147	-0.000139
H	-4.135589	0.639391	2.146777
H	-1.925143	-0.460448	-2.156709
H	-4.135653	0.638815	-2.146934
C	0.730713	-1.506845	0.000172
H	-1.925076	-0.459864	2.156778
C	-0.527359	-1.161732	0.000119
H	0.993521	-2.566707	0.000294
C	1.877901	-0.566713	0.000100
C	3.178496	-1.073325	0.000049
C	1.691390	0.819696	0.000054
C	4.273638	-0.215404	-0.000084
H	3.330708	-2.147595	0.000101
C	2.783553	1.674634	-0.000085
H	0.683060	1.220349	0.000122
C	4.079634	1.160786	-0.000155
H	5.277550	-0.623376	-0.000125
H	2.626473	2.746899	-0.000129
H	4.930668	1.831225	-0.000255

__Frequencies__ (Top 10 out of 69)

1. 18.2532 cm-1 (Symmetry: A)
2. 33.1208 cm-1 (Symmetry: A)
3. 54.2372 cm-1 (Symmetry: A)
4. 138.1204 cm-1 (Symmetry: A)
5. 159.9890 cm-1 (Symmetry: A)
6. 249.8628 cm-1 (Symmetry: A)
7. 270.7013 cm-1 (Symmetry: A)
8. 334.2316 cm-1 (Symmetry: A)
9. 406.4790 cm-1 (Symmetry: A)
10. 413.7770 cm-1 (Symmetry: A)



Charge	0	
Multiplicity	2	
Stoichiometry	C9H6F3	

Electronic Energy (Eh)	-645.894477131
Sum of electronic and zero-point Energies (Eh)	-645.771851
Sum of electronic and thermal Energies (Eh)	-645.760778
Sum of electronic and enthalpy Energies (Eh)	-645.759834
Sum of electronic and thermal Free Energies (Eh)	-645.813454
Number of Imaginary Frequencies	1

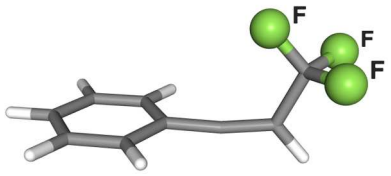
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.671176	-0.032038	-0.634920
C	-3.059296	1.188223	-0.359973
C	-1.818230	1.223170	0.258752
C	-1.175984	0.027040	0.607946
C	-1.796105	-1.198912	0.329515
C	-3.037150	-1.222844	-0.289777
H	-4.640232	-0.054987	-1.118679
H	-3.550943	2.115111	-0.629413
H	-1.294213	-2.119408	0.600877
H	-3.511400	-2.172762	-0.504641
C	2.584005	-0.007527	-0.254156
H	-1.333531	2.166980	0.475822
C	0.100441	0.057100	1.240327
C	1.236853	0.078195	1.667391
H	2.088085	0.106120	2.310073
F	3.366325	-1.074390	-0.206394
F	3.322599	1.086705	-0.348798
F	1.762419	-0.091815	-1.280882

__Frequencies__ (Top 10 out of 48)

1. -389.6297 cm-1 (Symmetry: A) *
2. 15.6163 cm-1 (Symmetry: A)
3. 25.4550 cm-1 (Symmetry: A)
4. 36.3638 cm-1 (Symmetry: A)
5. 77.9013 cm-1 (Symmetry: A)
6. 117.1327 cm-1 (Symmetry: A)
7. 162.6203 cm-1 (Symmetry: A)
8. 170.5795 cm-1 (Symmetry: A)
9. 375.4084 cm-1 (Symmetry: A)
10. 407.1121 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H6F3

Electronic Energy (Eh)	-645.961697752
Sum of electronic and zero-point Energies (Eh)	-645.836104
Sum of electronic and thermal Energies (Eh)	-645.82581
Sum of electronic and enthalpy Energies (Eh)	-645.824866
Sum of electronic and thermal Free Energies (Eh)	-645.876015
Number of Imaginary Frequencies	0

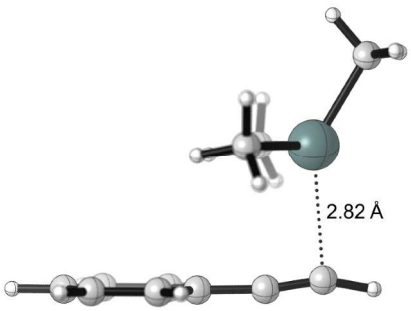
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.796951	0.000000	0.374530
C	-3.124777	-1.209100	0.176937
C	-1.801687	-1.223592	-0.214764
C	-1.104538	0.000000	-0.418299
C	-1.801687	1.223592	-0.214764
C	-3.124777	1.209100	0.176937
H	-4.835201	0.000000	0.681647
H	-3.644167	-2.147100	0.332533
H	-1.276706	2.158134	-0.367612
H	-3.644167	2.147100	0.332533
C	1.490635	-0.000000	-1.025097
C	2.481925	0.000000	0.107156
H	-1.276706	-2.158134	-0.367612
C	0.208510	0.000000	-0.827869
H	1.947628	-0.000000	-2.013909
F	3.282970	-1.076488	0.046851
F	1.897326	0.000001	1.305611
F	3.282971	1.076487	0.046851

__Frequencies__ (Top 10 out of 48)

1. 10.5865 cm-1 (Symmetry: A)
2. 28.8705 cm-1 (Symmetry: A)
3. 61.5852 cm-1 (Symmetry: A)
4. 154.7985 cm-1 (Symmetry: A)
5. 164.7574 cm-1 (Symmetry: A)
6. 289.0932 cm-1 (Symmetry: A)
7. 328.8431 cm-1 (Symmetry: A)
8. 378.6974 cm-1 (Symmetry: A)
9. 404.6288 cm-1 (Symmetry: A)
10. 472.7244 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H15Sn
Electronic Energy (Eh)	-431.362035212
Sum of electronic and zero-point Energies (Eh)	-431.144275
Sum of electronic and thermal Energies (Eh)	-431.128297
Sum of electronic and enthalpy Energies (Eh)	-431.127352
Sum of electronic and thermal Free Energies (Eh)	-431.191241
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

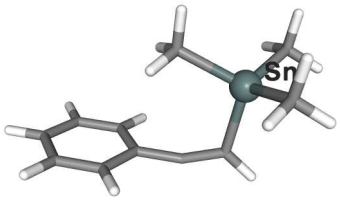
xyz

C	4.197903	-0.000394	0.997261
C	3.663837	1.205683	0.549083
C	2.600142	1.212012	-0.340814
C	2.055235	-0.000027	-0.793650
C	2.598407	-1.212256	-0.339236
C	3.662114	-1.206283	0.550665
H	5.028061	-0.000530	1.693193
H	4.077218	2.144941	0.896314
H	2.171960	-2.145364	-0.686477
H	4.074153	-2.145680	0.899115
H	2.175044	2.145280	-0.689277
C	-3.782663	0.001630	0.711427
H	-3.766262	-0.001243	1.805118
H	-4.317141	0.889648	0.372847
H	-4.319992	-0.882885	0.368239
C	-0.758244	-1.747078	0.785421
H	-1.409647	-2.250725	1.502770
H	-0.510019	-2.450774	-0.010334
H	0.166163	-1.459334	1.291224
C	-0.754504	1.743978	0.789189
H	-0.503964	2.448382	-0.005212
H	-1.405248	2.248004	1.506867
H	0.168845	1.453201	1.295194
Sn	-1.736372	0.000371	-0.012529
C	0.948264	0.000189	-1.686231
C	-0.100430	0.000502	-2.305588
H	-0.790923	0.000778	-3.118278

__Frequencies__ (Top 10 out of 75)

1. -213.3961 cm-1 (Symmetry: A) *
2. 16.7241 cm-1 (Symmetry: A)
3. 35.6116 cm-1 (Symmetry: A)
4. 59.6350 cm-1 (Symmetry: A)
5. 75.8996 cm-1 (Symmetry: A)
6. 80.0175 cm-1 (Symmetry: A)
7. 92.2163 cm-1 (Symmetry: A)
8. 104.7154 cm-1 (Symmetry: A)

9. 105.2747 cm-1 (Symmetry: A)
10. 145.7326 cm-1 (Symmetry: A)



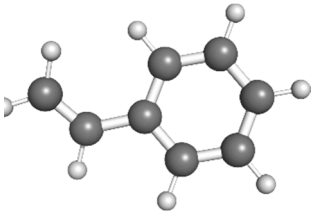
Charge	0
Multiplicity	2
Stoichiometry	C11H15Sn
Electronic Energy (Eh)	-431.393643202
Sum of electronic and zero-point Energies (Eh)	-431.175519
Sum of electronic and thermal Energies (Eh)	-431.159316
Sum of electronic and enthalpy Energies (Eh)	-431.158372
Sum of electronic and thermal Free Energies (Eh)	-431.223246
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-4.517856	-0.000049	0.645938
C	-3.908206	-1.207115	0.293632
C	-2.712201	-1.219647	-0.397458
C	-2.074616	0.000048	-0.754410
C	-2.712274	1.219693	-0.397414
C	-3.908278	1.207066	0.293673
H	-5.456421	-0.000087	1.185712
H	-4.376598	-2.146474	0.563895
H	-2.241862	2.155745	-0.673815
H	-4.376727	2.146388	0.563965
H	-2.241734	-2.155663	-0.673888
Sn	1.677315	0.000000	0.089282
C	2.903857	1.748766	0.070707
H	3.542515	1.779178	0.955274
H	3.543793	1.763739	-0.812793
H	2.285475	2.647208	0.061708
C	2.904180	-1.748534	0.070223
H	3.544239	-1.763050	-0.813197
H	3.542724	-1.779166	0.954864
H	2.285970	-2.647090	0.060799
C	0.331270	-0.000364	1.738370
H	-0.312204	0.880602	1.704225
H	-0.311970	-0.881493	1.703988
H	0.872036	-0.000421	2.686140
C	-0.873306	0.000102	-1.447261
C	0.403065	0.000104	-1.659956
H	0.821196	0.000166	-2.667237

__Frequencies__ (Top 10 out of 75)

1. 13.1894 cm-1 (Symmetry: A)
2. 29.5247 cm-1 (Symmetry: A)
3. 49.5190 cm-1 (Symmetry: A)
4. 74.7743 cm-1 (Symmetry: A)
5. 83.8530 cm-1 (Symmetry: A)
6. 88.6595 cm-1 (Symmetry: A)
7. 98.7947 cm-1 (Symmetry: A)
8. 113.6637 cm-1 (Symmetry: A)
9. 131.6080 cm-1 (Symmetry: A)
10. 131.8993 cm-1 (Symmetry: A)



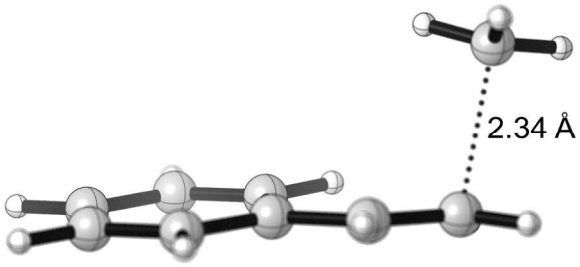
Charge	0
Multiplicity	1
Stoichiometry	C8H8
Electronic Energy (Eh)	-309.582288432
Sum of electronic and zero-point Energies (Eh)	-309.448187
Sum of electronic and thermal Energies (Eh)	-309.441442
Sum of electronic and enthalpy Energies (Eh)	-309.440497
Sum of electronic and thermal Free Energies (Eh)	-309.479534
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz			
C	2.251157	0.261528	0.047171
C	1.353032	1.324342	-0.025956
C	-0.012637	1.085359	-0.080870
C	-0.510884	-0.222588	-0.057216
C	0.401787	-1.279662	0.001948
C	1.770674	-1.042687	0.058458
H	3.317090	0.451086	0.087257
H	1.721307	2.343317	-0.048745
H	0.029522	-2.298767	0.010634
H	2.460832	-1.876553	0.108766
H	-0.697614	1.921461	-0.158972
C	-1.953861	-0.523575	-0.095775
C	-2.946358	0.335453	0.128494
H	-3.979348	0.015203	0.077816
H	-2.201361	-1.559674	-0.313834
H	-2.767885	1.374914	0.379548

__Frequencies__ (Top 10 out of 42)

1. 49.9283 cm-1 (Symmetry: A)
2. 203.0712 cm-1 (Symmetry: A)
3. 241.4458 cm-1 (Symmetry: A)
4. 410.7498 cm-1 (Symmetry: A)
5. 432.3615 cm-1 (Symmetry: A)
6. 462.7312 cm-1 (Symmetry: A)
7. 558.6518 cm-1 (Symmetry: A)
8. 631.2730 cm-1 (Symmetry: A)
9. 660.6075 cm-1 (Symmetry: A)
10. 714.4752 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H11
Electronic Energy (Eh)	-349.399026895
Sum of electronic and zero-point Energies (Eh)	-349.231907
Sum of electronic and thermal Energies (Eh)	-349.222565
Sum of electronic and enthalpy Energies (Eh)	-349.221621
Sum of electronic and thermal Free Energies (Eh)	-349.267631
Number of Imaginary Frequencies	1

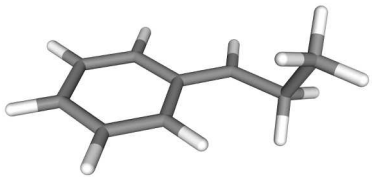
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-2.654426	0.591244	0.148080
C	-2.409546	-0.755071	0.400115
C	-1.130324	-1.271775	0.243540
C	-0.066048	-0.460818	-0.175564
C	-0.328098	0.896841	-0.417244
C	-1.605898	1.413540	-0.258966
H	-3.650699	0.998236	0.271890
H	-3.216524	-1.403205	0.721254
H	0.476021	1.556021	-0.723428
H	-1.786195	2.465210	-0.449179
C	3.270000	0.796069	0.977168
H	3.583358	-0.025092	1.605987
H	4.041242	1.351693	0.459880
H	2.374545	1.327991	1.268166
H	-0.943904	-2.322025	0.442274
C	1.264027	-1.045736	-0.328229
C	2.357896	-0.409374	-0.813569
H	3.283187	-0.953373	-0.953742
H	2.278120	0.537181	-1.334183

H 1.375356 -2.062165 0.039093

__Frequencies__ (Top 10 out of 54)

1. -507.4213 cm-1 (Symmetry: A) *
2. 44.6670 cm-1 (Symmetry: A)
3. 64.3439 cm-1 (Symmetry: A)
4. 84.8664 cm-1 (Symmetry: A)
5. 169.6078 cm-1 (Symmetry: A)
6. 247.0621 cm-1 (Symmetry: A)
7. 301.8474 cm-1 (Symmetry: A)
8. 412.5217 cm-1 (Symmetry: A)
9. 432.7329 cm-1 (Symmetry: A)
10. 462.0221 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H11
Electronic Energy (Eh)	-349.463474169
Sum of electronic and zero-point Energies (Eh)	-349.290767
Sum of electronic and thermal Energies (Eh)	-349.282299
Sum of electronic and enthalpy Energies (Eh)	-349.281355
Sum of electronic and thermal Free Energies (Eh)	-349.324731
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

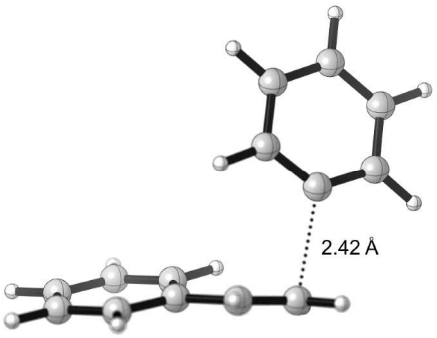
xyz

C	2.654681	0.536189	0.126506
C	1.605131	1.416046	-0.138912
C	0.309905	0.948189	-0.279849
C	0.016646	-0.433467	-0.159114
C	1.100536	-1.306885	0.111634
C	2.389777	-0.829847	0.250267
H	3.665608	0.908946	0.236059
H	1.803380	2.477347	-0.235266
H	0.900744	-2.368803	0.208566
H	3.199246	-1.520588	0.456045
C	-2.510796	-0.112858	-0.537894
C	-3.032048	0.538856	0.756067
H	-3.914690	1.150427	0.556745
H	-3.301928	-0.225042	1.487983
H	-2.264816	1.172928	1.205064
H	-0.489762	1.650455	-0.483912
C	-1.296417	-0.950010	-0.299412
H	-3.300008	-0.733522	-0.968510

H	-1.428084	-2.018653	-0.165657
H	-2.294181	0.669233	-1.272871

__Frequencies__ (Top 10 out of 54)

1. 77.1997 cm-1 (Symmetry: A)
2. 89.1885 cm-1 (Symmetry: A)
3. 189.3060 cm-1 (Symmetry: A)
4. 210.1551 cm-1 (Symmetry: A)
5. 267.0355 cm-1 (Symmetry: A)
6. 346.7200 cm-1 (Symmetry: A)
7. 412.6771 cm-1 (Symmetry: A)
8. 463.6621 cm-1 (Symmetry: A)
9. 479.4738 cm-1 (Symmetry: A)
10. 561.9364 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H13
Electronic Energy (Eh)	-541.09862968
Sum of electronic and zero-point Energies (Eh)	-540.875989
Sum of electronic and thermal Energies (Eh)	-540.863932
Sum of electronic and enthalpy Energies (Eh)	-540.862987
Sum of electronic and thermal Free Energies (Eh)	-540.917662
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

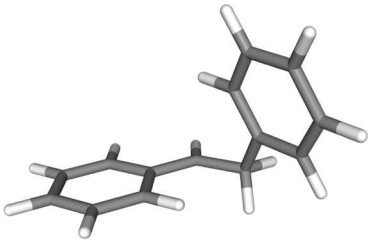
xyz

C	-3.621421	-1.366984	0.437609
C	-3.860756	-0.493456	-0.618537
C	-2.959335	0.526342	-0.896011
C	-1.807666	0.703018	-0.118268
C	-1.571416	-0.194803	0.933318
C	-2.470871	-1.214843	1.208535
H	-4.320354	-2.166073	0.653647
H	-4.749279	-0.608081	-1.228207
H	-0.663600	-0.109543	1.519890
H	-2.269224	-1.902653	2.021354
H	-3.147703	1.205944	-1.720653
C	-0.879119	1.790544	-0.437300

C	0.117454	2.224687	0.359848
H	0.744084	3.053013	0.053935
H	0.202253	1.905054	1.391794
H	-0.998544	2.243163	-1.418034
C	1.907048	0.635968	-0.005715
C	3.119016	0.805443	0.623201
C	1.565733	-0.453630	-0.771650
C	4.068566	-0.208240	0.464368
H	3.338329	1.684696	1.219505
C	2.526844	-1.456946	-0.919516
H	0.588675	-0.533658	-1.237534
C	3.770025	-1.331264	-0.303403
H	5.038412	-0.118006	0.941023
H	2.301976	-2.335464	-1.514028
H	4.510364	-2.113415	-0.421577

__Frequencies__ (Top 10 out of 75)

1. -301.4403 cm-1 (Symmetry: A) *
2. 25.8756 cm-1 (Symmetry: A)
3. 32.6582 cm-1 (Symmetry: A)
4. 39.6623 cm-1 (Symmetry: A)
5. 82.9802 cm-1 (Symmetry: A)
6. 96.3172 cm-1 (Symmetry: A)
7. 160.3171 cm-1 (Symmetry: A)
8. 233.8179 cm-1 (Symmetry: A)
9. 295.5450 cm-1 (Symmetry: A)
10. 400.2627 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C14H13
Electronic Energy (Eh)	-541.172199826
Sum of electronic and zero-point Energies (Eh)	-540.946312
Sum of electronic and thermal Energies (Eh)	-540.934823
Sum of electronic and enthalpy Energies (Eh)	-540.933878
Sum of electronic and thermal Free Energies (Eh)	-540.986422
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

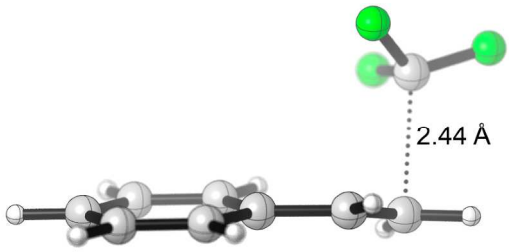
xyz

C	-3.540480	1.363043	0.274322
C	-2.334279	1.414572	0.973170

C	-1.390749	0.411793	0.827683
C	-1.630928	-0.689492	-0.030239
C	-2.861552	-0.719100	-0.731410
C	-3.795880	0.288066	-0.580101
H	-4.272966	2.152216	0.391914
H	-2.129331	2.249024	1.633712
H	-3.064151	-1.553879	-1.394202
H	-4.730719	0.241633	-1.126430
C	0.622789	-1.797856	0.517306
H	-0.452709	0.476688	1.366867
C	-0.689034	-1.737539	-0.198916
H	1.084173	-2.772975	0.337686
H	-0.947946	-2.541765	-0.877985
H	0.454204	-1.736726	1.600466
C	1.629114	-0.716474	0.141376
C	2.654701	-0.394762	1.032099
C	1.572096	-0.049005	-1.080994
C	3.606198	0.565565	0.708406
H	2.705525	-0.902311	1.990628
C	2.522835	0.913480	-1.408050
H	0.771033	-0.274104	-1.776574
C	3.543061	1.223958	-0.516114
H	4.393971	0.803090	1.413863
H	2.461249	1.425388	-2.361339
H	4.280306	1.976232	-0.769828

__Frequencies__ (Top 10 out of 75)

1. 18.3683 cm-1 (Symmetry: A)
2. 40.7284 cm-1 (Symmetry: A)
3. 60.4393 cm-1 (Symmetry: A)
4. 156.3441 cm-1 (Symmetry: A)
5. 173.8612 cm-1 (Symmetry: A)
6. 229.3038 cm-1 (Symmetry: A)
7. 274.3397 cm-1 (Symmetry: A)
8. 308.0098 cm-1 (Symmetry: A)
9. 409.3873 cm-1 (Symmetry: A)
10. 412.3218 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H8F3

Electronic Energy (Eh)	-647.14257433
Sum of electronic and zero-point Energies (Eh)	-646.995844
Sum of electronic and thermal Energies (Eh)	-646.984663
Sum of electronic and enthalpy Energies (Eh)	-646.983718
Sum of electronic and thermal Free Energies (Eh)	-647.037064
Number of Imaginary Frequencies	1

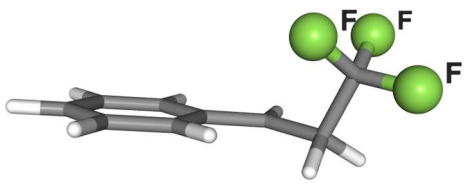
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.439124	-0.909533	-0.182816
C	-3.416195	0.414741	-0.607641
C	-2.278507	1.187102	-0.412115
C	-1.148665	0.656439	0.221510
C	-1.180169	-0.683435	0.631774
C	-2.315205	-1.455898	0.433210
H	-4.322931	-1.516489	-0.338238
H	-4.283271	0.845001	-1.094434
H	-0.305810	-1.130677	1.090669
H	-2.321710	-2.491762	0.750972
C	2.436819	-0.217525	-0.197034
H	-2.260585	2.219049	-0.746390
C	0.026687	1.508328	0.420182
C	1.076554	1.227572	1.216421
H	1.887196	1.937224	1.329158
H	1.064411	0.388965	1.903929
H	0.044025	2.428784	-0.157160
F	3.700778	0.170651	-0.188897
F	2.337310	-1.445155	0.290542
F	1.953636	-0.175144	-1.421586

__Frequencies__ (Top 10 out of 54)

1. -323.3344 cm-1 (Symmetry: A) *
2. 20.8384 cm-1 (Symmetry: A)
3. 30.0874 cm-1 (Symmetry: A)
4. 37.7108 cm-1 (Symmetry: A)
5. 82.0786 cm-1 (Symmetry: A)
6. 97.9804 cm-1 (Symmetry: A)
7. 155.5650 cm-1 (Symmetry: A)
8. 230.6397 cm-1 (Symmetry: A)
9. 294.9311 cm-1 (Symmetry: A)
10. 410.1937 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C9H8F3
Electronic Energy (Eh)	-647.215647665
Sum of electronic and zero-point Energies (Eh)	-647.065479
Sum of electronic and thermal Energies (Eh)	-647.055231
Sum of electronic and enthalpy Energies (Eh)	-647.054287
Sum of electronic and thermal Free Energies (Eh)	-647.103331
Number of Imaginary Frequencies	0

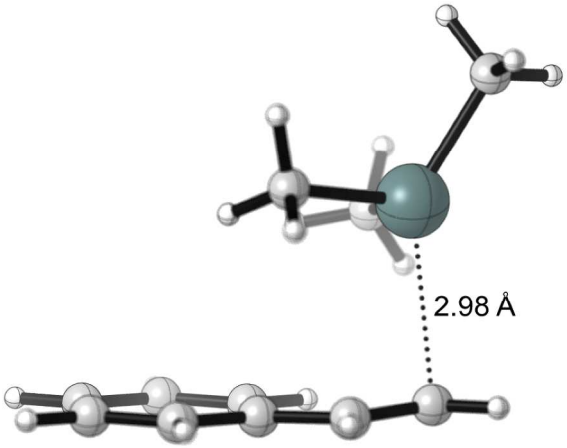
__Molecular Geometry in Cartesian Coordinates__

xyz

C	3.569961	-0.631418	-0.238831
C	2.501156	-1.447080	0.133266
C	1.255994	-0.902947	0.393690
C	1.038853	0.493093	0.290979
C	2.138324	1.300596	-0.095815
C	3.377245	0.746954	-0.353653
H	4.541332	-1.065046	-0.442088
H	2.642946	-2.518345	0.213685
H	1.991909	2.371598	-0.185090
H	4.201709	1.386180	-0.646483
C	-1.430635	0.382654	1.031089
C	-2.300333	-0.100142	-0.110213
H	0.436433	-1.560317	0.656097
C	-0.209415	1.105049	0.563455
H	-2.061067	1.039046	1.635094
H	-0.295276	2.173910	0.409748
H	-1.188946	-0.494952	1.635155
F	-1.660901	-0.981480	-0.891886
F	-2.700281	0.910463	-0.895021
F	-3.407256	-0.708165	0.346916

__Frequencies__ (Top 10 out of 54)

1. 46.0809 cm-1 (Symmetry: A)
2. 53.1192 cm-1 (Symmetry: A)
3. 68.7844 cm-1 (Symmetry: A)
4. 165.5343 cm-1 (Symmetry: A)
5. 211.4131 cm-1 (Symmetry: A)
6. 273.4671 cm-1 (Symmetry: A)
7. 309.8369 cm-1 (Symmetry: A)
8. 382.8813 cm-1 (Symmetry: A)
9. 407.4716 cm-1 (Symmetry: A)
10. 476.1603 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H17Sn
Electronic Energy (Eh)	-432.609509333
Sum of electronic and zero-point Energies (Eh)	-432.367472
Sum of electronic and thermal Energies (Eh)	-432.351479
Sum of electronic and enthalpy Energies (Eh)	-432.350535
Sum of electronic and thermal Free Energies (Eh)	-432.414145
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

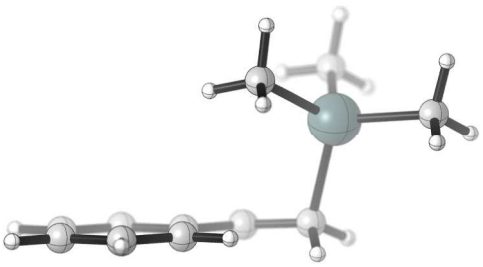
xyz

C	3.850542	-1.210024	0.433132
C	3.850445	0.023279	1.077964
C	2.965803	1.016308	0.679382
C	2.064653	0.803490	-0.372225
C	2.082897	-0.440977	-1.018599
C	2.963812	-1.435437	-0.617721
H	4.535412	-1.989336	0.744832
H	4.535787	0.208790	1.896493
H	1.401472	-0.639225	-1.837643
H	2.958613	-2.392517	-1.126467
H	2.958141	1.971548	1.194058
C	1.104167	1.853894	-0.708908
C	0.101211	1.758649	-1.606802
H	-0.559529	2.597153	-1.785862
H	0.023111	0.931610	-2.303660
H	1.171422	2.756162	-0.106678
Sn	-1.658942	-0.000748	0.033664
C	-1.142309	-1.860790	-0.944626
C	-0.444660	0.183401	1.802645
C	-3.725387	-0.167305	0.659445
H	-1.942561	-2.588497	-0.790878
H	-1.002374	-1.734742	-2.019555
H	-0.218080	-2.254879	-0.517194
H	-1.022492	-0.109807	2.681871

H	0.434554	-0.459465	1.722003
H	-0.101068	1.210337	1.938721
H	-4.384901	-0.299496	-0.198704
H	-3.826178	-1.037201	1.314624
H	-4.041250	0.720053	1.208724

__Frequencies__ (Top 10 out of 81)

1. -150.2940 cm-1 (Symmetry: A) *
2. 28.8216 cm-1 (Symmetry: A)
3. 34.9006 cm-1 (Symmetry: A)
4. 36.8092 cm-1 (Symmetry: A)
5. 60.9005 cm-1 (Symmetry: A)
6. 85.5396 cm-1 (Symmetry: A)
7. 91.5120 cm-1 (Symmetry: A)
8. 123.6188 cm-1 (Symmetry: A)
9. 138.2671 cm-1 (Symmetry: A)
10. 142.4143 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C11H17Sn
Electronic Energy (Eh)	-432.639400755
Sum of electronic and zero-point Energies (Eh)	-432.397265
Sum of electronic and thermal Energies (Eh)	-432.381069
Sum of electronic and enthalpy Energies (Eh)	-432.380125
Sum of electronic and thermal Free Energies (Eh)	-432.444275
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

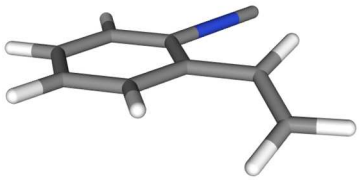
xyz

C	-4.369203	-0.726635	0.390974
C	-3.351467	-1.451896	-0.228089
C	-2.200834	-0.821135	-0.670543
C	-2.024263	0.575696	-0.504879
C	-3.073827	1.291075	0.126889
C	-4.218261	0.652428	0.562951
H	-5.266382	-1.226360	0.734557
H	-3.459658	-2.521868	-0.365146
H	-2.963540	2.361654	0.265110
H	-5.003252	1.226026	1.042207
C	0.325950	0.616084	-1.532256

H	-1.423613	-1.409461	-1.143916
C	-0.855801	1.256809	-0.935094
H	0.913565	1.322450	-2.121384
H	-0.808503	2.323838	-0.741032
H	0.084590	-0.241559	-2.163650
Sn	1.625218	-0.066092	0.085915
C	2.224079	1.691251	1.140597
C	0.520709	-1.351103	1.380084
C	3.326015	-1.074245	-0.732075
H	2.856540	1.441143	1.993921
H	2.781506	2.366455	0.489119
H	1.344778	2.220555	1.512333
H	1.101406	-1.570876	2.278091
H	-0.414543	-0.873308	1.677007
H	0.277829	-2.294772	0.889340
H	3.887928	-0.412254	-1.392804
H	3.993565	-1.407046	0.064751
H	3.018278	-1.950011	-1.305581

__Frequencies__ (Top 10 out of 81)

1. 14.3651 cm-1 (Symmetry: A)
2. 39.1613 cm-1 (Symmetry: A)
3. 58.2907 cm-1 (Symmetry: A)
4. 63.8775 cm-1 (Symmetry: A)
5. 72.9180 cm-1 (Symmetry: A)
6. 106.0271 cm-1 (Symmetry: A)
7. 110.8348 cm-1 (Symmetry: A)
8. 132.5913 cm-1 (Symmetry: A)
9. 133.7999 cm-1 (Symmetry: A)
10. 144.8387 cm-1 (Symmetry: A)



Charge	0
Multiplicity	1
Stoichiometry	C9H7N
Electronic Energy (Eh)	-401.79029794
Sum of electronic and zero-point Energies (Eh)	-401.657941
Sum of electronic and thermal Energies (Eh)	-401.649426
Sum of electronic and enthalpy Energies (Eh)	-401.648482
Sum of electronic and thermal Free Energies (Eh)	-401.691498
Number of Imaginary Frequencies	0

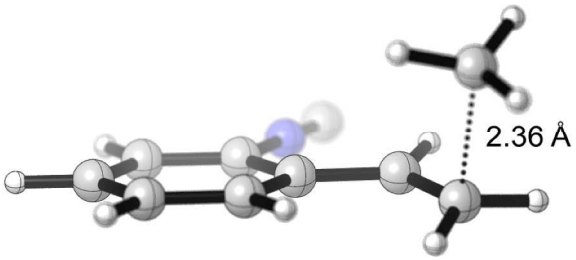
__Molecular Geometry in Cartesian Coordinates__

xyz

C	1.880707	-1.390578	-0.030434
C	0.506207	-1.553938	-0.119108
C	-0.361986	-0.457749	-0.098075
C	0.218642	0.816307	-0.007691
C	1.598084	0.993673	0.078154
C	2.430333	-0.114531	0.070198
H	2.527410	-2.259159	-0.052750
H	0.089343	-2.547605	-0.230462
H	1.993583	1.998599	0.151299
H	3.503121	0.017322	0.134072
C	-1.285758	2.887702	0.024284
N	-0.597495	1.941498	0.008859
C	-1.824633	-0.611801	-0.178575
H	-2.373783	0.237604	-0.572212
C	-2.493207	-1.693263	0.215731
H	-1.997102	-2.548904	0.660474
H	-3.570441	-1.743271	0.120668

__Frequencies__ (Top 10 out of 45)

1. 83.0818 cm-1 (Symmetry: A)
2. 126.0330 cm-1 (Symmetry: A)
3. 152.4408 cm-1 (Symmetry: A)
4. 203.1116 cm-1 (Symmetry: A)
5. 251.7339 cm-1 (Symmetry: A)
6. 351.7140 cm-1 (Symmetry: A)
7. 404.2349 cm-1 (Symmetry: A)
8. 444.8127 cm-1 (Symmetry: A)
9. 472.2569 cm-1 (Symmetry: A)
10. 547.5904 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H10N
Electronic Energy (Eh)	-441.607917168
Sum of electronic and zero-point Energies (Eh)	-441.442573
Sum of electronic and thermal Energies (Eh)	-441.431388
Sum of electronic and enthalpy Energies (Eh)	-441.430444
Sum of electronic and thermal Free Energies (Eh)	-441.480776
Number of Imaginary Frequencies	1

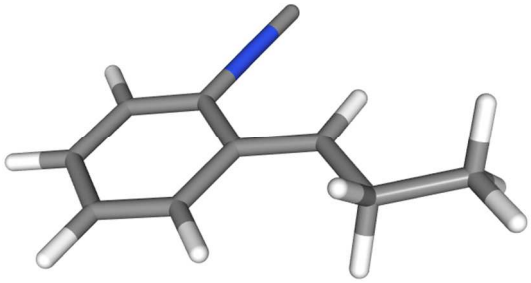
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-2.176424	-1.668233	0.155169
C	-0.931289	-2.233497	-0.115740
C	0.178110	-1.425931	-0.306615
C	0.091654	-0.026332	-0.242670
C	-1.177245	0.513588	0.041744
C	-2.298039	-0.289931	0.235882
H	-3.044644	-2.296862	0.307061
H	-0.826043	-3.310224	-0.171119
H	-3.248841	0.182490	0.447197
C	3.609776	-0.377876	1.021799
H	4.484075	-0.794034	0.539090
H	3.726973	0.554624	1.554780
H	2.856194	-1.064152	1.382778
H	1.140350	-1.884900	-0.498618
C	1.246593	0.842295	-0.436471
C	2.460188	0.426908	-0.872722
H	2.605514	-0.552189	-1.312724
H	3.243122	1.151913	-1.053676
H	1.120446	1.882896	-0.159788
N	-1.331349	1.892260	0.127298
C	-1.459608	3.053113	0.198613

__Frequencies__ (Top 10 out of 57)

1. -472.8205 cm-1 (Symmetry: A) *
2. 39.8127 cm-1 (Symmetry: A)
3. 64.4543 cm-1 (Symmetry: A)
4. 94.9306 cm-1 (Symmetry: A)
5. 127.3043 cm-1 (Symmetry: A)
6. 142.7410 cm-1 (Symmetry: A)
7. 184.7722 cm-1 (Symmetry: A)
8. 246.3328 cm-1 (Symmetry: A)
9. 297.7481 cm-1 (Symmetry: A)
10. 358.0220 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H10N
Electronic Energy (Eh)	-441.67388478
Sum of electronic and zero-point Energies (Eh)	-441.503297
Sum of electronic and thermal Energies (Eh)	-441.492863
Sum of electronic and enthalpy Energies (Eh)	-441.491919

| Sum of electronic and thermal Free Energies (Eh) | -441.540264 |
| Number of Imaginary Frequencies | 0 |

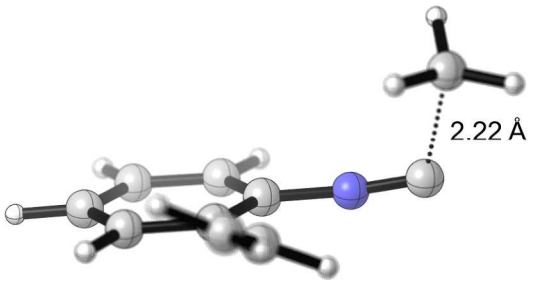
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-1.711097	-1.966285	0.000029
C	-0.380872	-1.594890	-0.000033
C	0.012343	-0.231950	-0.000055
C	-1.043374	0.724385	-0.000003
C	-2.378477	0.349074	0.000056
C	-2.719404	-0.998743	0.000073
H	-1.973348	-3.017417	0.000045
H	0.387383	-2.358273	-0.000065
H	-3.137360	1.121229	0.000087
H	-3.761542	-1.291115	0.000121
C	-0.441248	3.209538	-0.000022
C	3.865693	-0.100641	0.000219
H	4.683315	-0.822557	0.000193
H	3.972689	0.532999	-0.882767
H	3.972385	0.532594	0.883534
N	-0.727821	2.074579	-0.000014
C	1.367966	0.160490	-0.000120
H	1.595686	1.220506	-0.000156
C	2.509702	-0.803063	-0.000175
H	2.434211	-1.463537	-0.874289
H	2.433921	-1.463974	0.873581

__Frequencies__ (Top 10 out of 57)

1. 45.7554 cm-1 (Symmetry: A)
2. 117.1057 cm-1 (Symmetry: A)
3. 117.7738 cm-1 (Symmetry: A)
4. 130.8900 cm-1 (Symmetry: A)
5. 179.3093 cm-1 (Symmetry: A)
6. 221.8672 cm-1 (Symmetry: A)
7. 273.7619 cm-1 (Symmetry: A)
8. 312.8597 cm-1 (Symmetry: A)
9. 355.6386 cm-1 (Symmetry: A)
10. 380.6028 cm-1 (Symmetry: A)



| Charge | 0 |

Multiplicity	2
Stoichiometry	C10H10N
Electronic Energy (Eh)	-441.605678842
Sum of electronic and zero-point Energies (Eh)	-441.440514
Sum of electronic and thermal Energies (Eh)	-441.429013
Sum of electronic and enthalpy Energies (Eh)	-441.428069
Sum of electronic and thermal Free Energies (Eh)	-441.48022
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	38.5

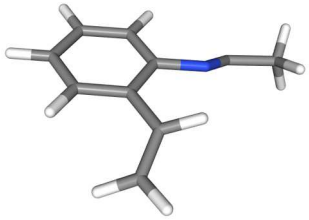
__Molecular Geometry in Cartesian Coordinates__

xyz

C	2.754389	0.026107	0.353560
C	1.793567	0.992389	0.092985
C	0.475898	0.645978	-0.219364
C	0.165078	-0.724078	-0.285585
C	1.126991	-1.703019	-0.031957
C	2.419594	-1.325249	0.293865
H	3.768296	0.324559	0.589982
H	2.065665	2.041168	0.109178
H	0.840486	-2.745114	-0.093393
H	3.167317	-2.083509	0.490681
N	-1.123163	-1.112151	-0.596086
C	-2.280083	-1.315631	-0.726497
C	-3.459012	-0.545537	0.992487
H	-2.932427	0.387860	1.145583
H	-4.444974	-0.502086	0.554006
H	-3.259336	-1.350437	1.686773
C	-0.559500	1.660671	-0.479276
H	-1.367385	1.362103	-1.140946
C	-0.571256	2.881074	0.053667
H	0.186929	3.208415	0.756819
H	-1.356433	3.585873	-0.189388

__Frequencies__ (Top 10 out of 57)

1. -428.0164 cm-1 (Symmetry: A) *
2. 26.0551 cm-1 (Symmetry: A)
3. 46.0706 cm-1 (Symmetry: A)
4. 49.1814 cm-1 (Symmetry: A)
5. 94.0615 cm-1 (Symmetry: A)
6. 146.1348 cm-1 (Symmetry: A)
7. 165.0292 cm-1 (Symmetry: A)
8. 220.8757 cm-1 (Symmetry: A)
9. 255.9707 cm-1 (Symmetry: A)
10. 343.7089 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C10H10N
Electronic Energy (Eh)	-441.658115914
Sum of electronic and zero-point Energies (Eh)	-441.487573
Sum of electronic and thermal Energies (Eh)	-441.476929
Sum of electronic and enthalpy Energies (Eh)	-441.475985
Sum of electronic and thermal Free Energies (Eh)	-441.525028
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

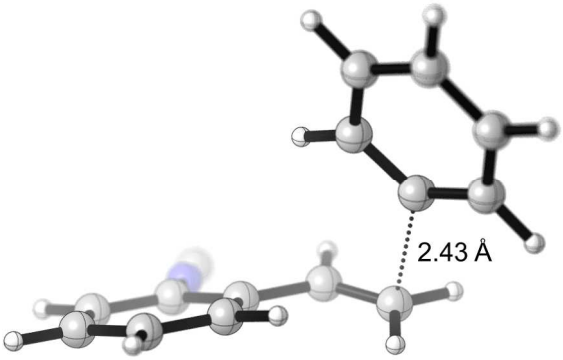
xyz

C	2.388535	-1.386260	-0.056052
C	2.175798	-0.019928	0.043604
C	0.883740	0.512257	0.121910
C	-0.199337	-0.380182	0.106468
C	0.013007	-1.757368	0.014834
C	1.301812	-2.259268	-0.069926
H	3.398937	-1.773828	-0.105025
H	3.023055	0.654211	0.089192
H	-0.847013	-2.416488	0.011614
H	1.460797	-3.328879	-0.137340
C	-2.548783	-0.340733	-0.215068
C	-3.951455	0.134261	-0.088485
H	-3.994254	1.076126	0.466041
H	-4.384059	0.269502	-1.080994
H	-4.546192	-0.622627	0.426046
N	-1.505441	0.151590	0.216593
C	0.648368	1.963704	0.222419
H	-0.281123	2.254638	0.700849
C	1.469430	2.902672	-0.244417
H	2.382421	2.657690	-0.776372
H	1.238823	3.953598	-0.121878

__Frequencies__ (Top 10 out of 57)

1. 55.5631 cm-1 (Symmetry: A)
2. 90.9234 cm-1 (Symmetry: A)
3. 103.4030 cm-1 (Symmetry: A)
4. 113.2352 cm-1 (Symmetry: A)
5. 156.2445 cm-1 (Symmetry: A)
6. 183.0692 cm-1 (Symmetry: A)
7. 235.6528 cm-1 (Symmetry: A)

8. 292.9206 cm-1 (Symmetry: A)
9. 357.4469 cm-1 (Symmetry: A)
10. 382.8307 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C15H12N
Electronic Energy (Eh)	-633.307223749
Sum of electronic and zero-point Energies (Eh)	-633.086457
Sum of electronic and thermal Energies (Eh)	-633.072502
Sum of electronic and enthalpy Energies (Eh)	-633.071557
Sum of electronic and thermal Free Energies (Eh)	-633.130916
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

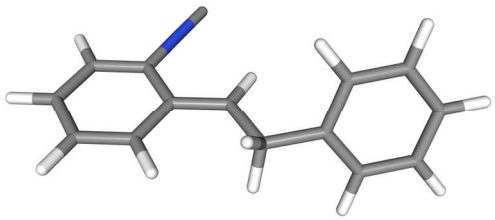
xyz

C	2.926392	-2.193801	0.197280
C	1.677573	-2.186473	0.815816
C	0.951200	-1.009747	0.913162
C	1.447862	0.200699	0.408591
C	2.703419	0.159878	-0.223118
C	3.439813	-1.017652	-0.327240
H	3.493886	-3.112384	0.116803
H	1.263656	-3.105777	1.211833
H	4.404615	-0.990024	-0.817359
H	-0.035454	-1.024550	1.361179
C	0.692700	1.450442	0.499235
C	-0.329546	1.657291	1.352510
H	-0.553191	0.965011	2.155885
H	-0.832920	2.615386	1.379421
H	0.966621	2.236220	-0.196633
N	3.239945	1.327430	-0.753247
C	3.688087	2.312812	-1.197583
C	-2.239554	0.624431	0.264731
C	-3.465338	0.628830	0.888148
C	-1.957621	-0.014641	-0.918775
C	-4.499491	-0.072339	0.260724
H	-3.633216	1.150977	1.823902
C	-3.003527	-0.710136	-1.530733

H	-0.965856	0.017795	-1.358461
C	-4.265378	-0.736374	-0.940846
H	-5.484946	-0.096839	0.712337
H	-2.830559	-1.229720	-2.466526
H	-5.071792	-1.277426	-1.421054

__Frequencies__ (Top 10 out of 78)

1. -279.4796 cm-1 (Symmetry: A) *
2. 21.3756 cm-1 (Symmetry: A)
3. 25.9626 cm-1 (Symmetry: A)
4. 31.8629 cm-1 (Symmetry: A)
5. 82.8320 cm-1 (Symmetry: A)
6. 94.0974 cm-1 (Symmetry: A)
7. 124.2573 cm-1 (Symmetry: A)
8. 132.9984 cm-1 (Symmetry: A)
9. 179.7499 cm-1 (Symmetry: A)
10. 229.9834 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C15H12N
Electronic Energy (Eh)	-633.381340581
Sum of electronic and zero-point Energies (Eh)	-633.157584
Sum of electronic and thermal Energies (Eh)	-633.144098
Sum of electronic and enthalpy Energies (Eh)	-633.143154
Sum of electronic and thermal Free Energies (Eh)	-633.200585
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

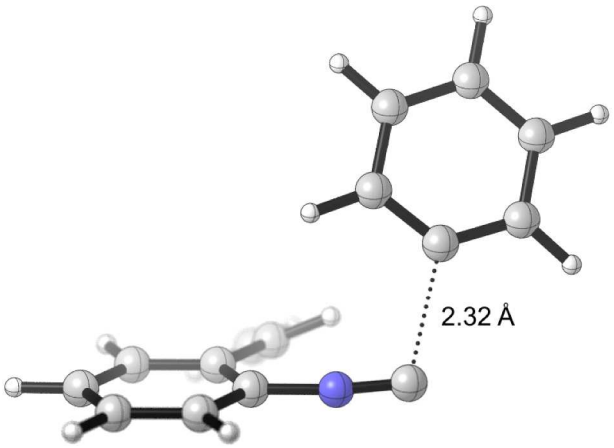
xyz

C	-3.530256	-1.784637	0.263853
C	-2.169000	-1.565475	0.181359
C	-1.634205	-0.267203	-0.018656
C	-2.581410	0.790856	-0.129738
C	-3.947715	0.568205	-0.045938
C	-4.429215	-0.721036	0.151564
H	-3.902029	-2.790720	0.415999
H	-1.488076	-2.403320	0.266722
H	-4.620035	1.411957	-0.136320
H	-5.495721	-0.893890	0.216537
C	-1.724310	3.173399	-0.485540
N	-2.125243	2.085384	-0.323887

C	-0.246079	-0.026870	-0.107808
H	0.098649	0.983243	-0.292318
C	0.782452	-1.108873	0.011393
H	0.672247	-1.823179	-0.815206
H	0.601313	-1.686904	0.927971
C	2.195388	-0.575597	0.034222
C	3.113224	-0.917562	-0.955733
C	2.598336	0.285015	1.057463
C	4.410907	-0.413106	-0.926038
H	2.810791	-1.581812	-1.758606
C	3.891676	0.790879	1.090253
H	1.888897	0.559706	1.832338
C	4.802919	0.442039	0.096584
H	5.113071	-0.687319	-1.704526
H	4.189733	1.457698	1.890719
H	5.811588	0.836654	0.120457

__Frequencies__ (Top 10 out of 78)

1. 21.5436 cm-1 (Symmetry: A)
2. 26.0459 cm-1 (Symmetry: A)
3. 56.7705 cm-1 (Symmetry: A)
4. 112.6193 cm-1 (Symmetry: A)
5. 133.3830 cm-1 (Symmetry: A)
6. 142.2312 cm-1 (Symmetry: A)
7. 174.9170 cm-1 (Symmetry: A)
8. 235.4033 cm-1 (Symmetry: A)
9. 242.9782 cm-1 (Symmetry: A)
10. 314.2042 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C15H12N
Electronic Energy (Eh)	-633.305066423
Sum of electronic and zero-point Energies (Eh)	-633.084408
Sum of electronic and thermal Energies (Eh)	-633.070239
Sum of electronic and enthalpy Energies (Eh)	-633.069295

| Sum of electronic and thermal Free Energies (Eh) | -633.129393 |
| Number of Imaginary Frequencies | 1 |

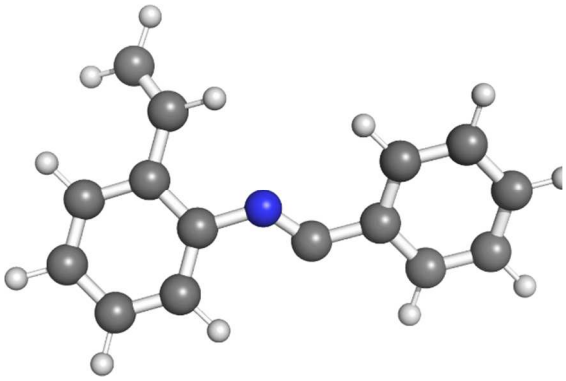
__Molecular Geometry in Cartesian Coordinates__

xyz

C	-3.861222	-0.049827	1.084772
C	-3.027034	0.938543	0.582688
C	-1.906192	0.625238	-0.192198
C	-1.646675	-0.736809	-0.423888
C	-2.477444	-1.738773	0.078231
C	-3.586947	-1.392406	0.832491
H	-4.719739	0.224937	1.685265
H	-3.227564	1.978372	0.811654
H	-2.236994	-2.772596	-0.134366
H	-4.232005	-2.167385	1.227297
C	0.460662	-1.333212	-1.745600
N	-0.542554	-1.099539	-1.175887
C	-1.010798	1.661984	-0.734880
H	0.014928	1.359892	-0.925009
C	-1.384294	2.909232	-1.013412
H	-2.406196	3.248901	-0.884134
H	-0.671673	3.626250	-1.400832
C	2.207789	-0.585729	-0.408736
C	3.484767	-0.561725	-0.915125
C	1.844135	-0.148691	0.843192
C	4.485948	-0.050602	-0.085507
H	3.702250	-0.924035	-1.913265
C	2.858904	0.358703	1.659611
H	0.815186	-0.194653	1.188456
C	4.170574	0.405808	1.193014
H	5.510617	-0.009464	-0.437993
H	2.623119	0.715608	2.656020
H	4.952910	0.800542	1.830191

__Frequencies__ (Top 10 out of 78)

1. -252.1267 cm-1 (Symmetry: A) *
2. 19.8801 cm-1 (Symmetry: A)
3. 24.4415 cm-1 (Symmetry: A)
4. 37.8422 cm-1 (Symmetry: A)
5. 67.4282 cm-1 (Symmetry: A)
6. 83.9259 cm-1 (Symmetry: A)
7. 94.7433 cm-1 (Symmetry: A)
8. 137.3787 cm-1 (Symmetry: A)
9. 169.1492 cm-1 (Symmetry: A)
10. 212.3635 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C15H12N
Electronic Energy (Eh)	-633.368250779
Sum of electronic and zero-point Energies (Eh)	-633.143822
Sum of electronic and thermal Energies (Eh)	-633.130287
Sum of electronic and enthalpy Energies (Eh)	-633.129343
Sum of electronic and thermal Free Energies (Eh)	-633.186953
Number of Imaginary Frequencies	0

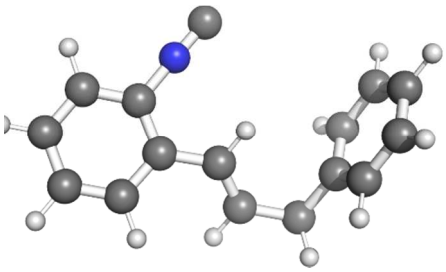
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	-4.187449	-1.179775	0.070228
C	-3.836682	0.160929	0.048089
C	-2.496286	0.563537	0.057520
C	-1.507437	-0.432845	0.104092
C	-1.860629	-1.785319	0.134419
C	-3.194100	-2.157773	0.113507
H	-5.232506	-1.465046	0.070849
H	-4.611146	0.918859	0.049449
H	-1.071173	-2.526437	0.175269
H	-3.461618	-3.207317	0.140793
C	0.843408	-0.701642	-0.125341
N	-0.158062	-0.028050	0.138417
C	-2.116646	1.987165	0.025514
H	-1.146394	2.222722	0.450103
C	-2.857676	2.962278	-0.497697
H	-3.809433	2.768216	-0.980311
H	-2.519653	3.990761	-0.474140
C	2.255921	-0.330793	-0.059565
C	3.228815	-1.265945	-0.415032
C	2.640421	0.951534	0.354686
C	4.575863	-0.927311	-0.357378
H	2.915906	-2.253075	-0.735204
C	3.984804	1.284796	0.410400
H	1.872468	1.665820	0.626944
C	4.953396	0.346143	0.054932
H	5.329262	-1.654912	-0.633659
H	4.283138	2.276070	0.730578

H 6.003256 0.610817 0.100161

__Frequencies__ (Top 10 out of 78)

1. 18.4074 cm-1 (Symmetry: A)
2. 47.7233 cm-1 (Symmetry: A)
3. 54.7289 cm-1 (Symmetry: A)
4. 78.9419 cm-1 (Symmetry: A)
5. 91.8857 cm-1 (Symmetry: A)
6. 172.8814 cm-1 (Symmetry: A)
7. 182.7358 cm-1 (Symmetry: A)
8. 207.4645 cm-1 (Symmetry: A)
9. 256.5267 cm-1 (Symmetry: A)
10. 300.2175 cm-1 (Symmetry: A)



Charge	0
Multiplicity	1
Stoichiometry	C16H13N
Electronic Energy (Eh)	-672.111260544
Sum of electronic and zero-point Energies (Eh)	-671.86866
Sum of electronic and thermal Energies (Eh)	-671.854276
Sum of electronic and enthalpy Energies (Eh)	-671.853332
Sum of electronic and thermal Free Energies (Eh)	-671.912389
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

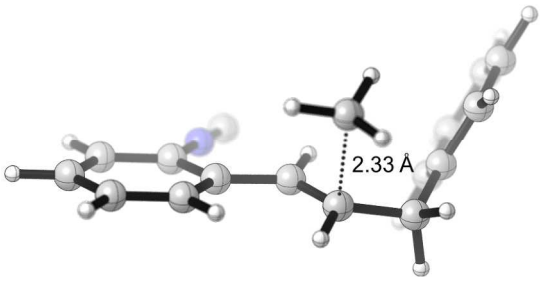
xyz

C	-4.103869	-1.166949	0.414932
C	-2.745732	-1.415211	0.275944
C	-1.833228	-0.378862	0.054865
C	-2.348646	0.925490	0.001586
C	-3.709090	1.188286	0.145437
C	-4.589358	0.136894	0.349809
H	-4.785349	-1.990787	0.589010
H	-2.371080	-2.428190	0.362916
H	-4.053758	2.213020	0.090591
H	-5.647634	0.334938	0.464649
C	-0.742297	2.873989	-0.421440
N	-1.482369	1.989955	-0.221217
C	-0.389911	-0.615037	-0.107023
H	0.270255	0.180713	0.225244
C	0.128502	-1.711310	-0.660908

H	-0.538631	-2.482548	-1.041283
C	1.600034	-1.983221	-0.849347
H	1.843986	-2.932172	-0.359247
H	1.784716	-2.143290	-1.917776
C	2.500442	-0.891752	-0.330240
C	2.717619	0.260895	-1.086715
C	3.081874	-0.985156	0.932935
C	3.497855	1.298919	-0.591169
H	2.257593	0.349100	-2.066047
C	3.868080	0.049682	1.431286
H	2.914068	-1.874127	1.532515
C	4.076551	1.194677	0.670419
H	3.649572	2.190951	-1.187048
H	4.315435	-0.038485	2.414393
H	4.684455	2.003168	1.058369

__Frequencies__ (Top 10 out of 84)

1. 23.5546 cm-1 (Symmetry: A)
2. 25.4381 cm-1 (Symmetry: A)
3. 41.6684 cm-1 (Symmetry: A)
4. 81.9529 cm-1 (Symmetry: A)
5. 98.2991 cm-1 (Symmetry: A)
6. 148.7413 cm-1 (Symmetry: A)
7. 163.4364 cm-1 (Symmetry: A)
8. 185.1886 cm-1 (Symmetry: A)
9. 212.2095 cm-1 (Symmetry: A)
10. 276.3367 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C17H16N
Electronic Energy (Eh)	-711.927746984
Sum of electronic and zero-point Energies (Eh)	-711.651628
Sum of electronic and thermal Energies (Eh)	-711.634862
Sum of electronic and enthalpy Energies (Eh)	-711.633918
Sum of electronic and thermal Free Energies (Eh)	-711.698078
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

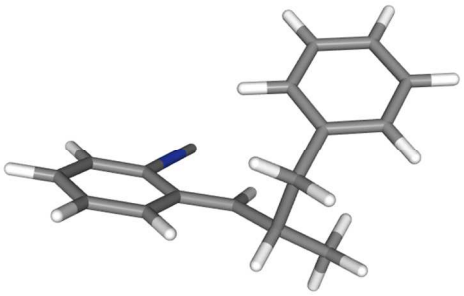
xyz

C	4.646573	0.207942	-0.311997

C	4.142863	-1.067663	-0.062847
C	2.789703	-1.255444	0.168985
C	1.883454	-0.182281	0.166364
C	2.424263	1.093680	-0.091152
C	3.782149	1.291738	-0.325660
H	5.703065	0.356560	-0.495590
H	4.810403	-1.920896	-0.055196
H	4.138325	2.296650	-0.513479
C	-0.251454	-2.689103	-1.192231
H	-0.613045	-3.642284	-0.826385
H	-0.952801	-2.051708	-1.712753
H	0.784235	-2.632115	-1.499777
H	2.419386	-2.257523	0.347730
C	0.455521	-0.341915	0.396065
C	-0.142441	-1.492865	0.803648
H	0.473973	-2.301765	1.186199
H	-0.167743	0.511952	0.157045
N	1.584268	2.201292	-0.097682
C	0.866660	3.125492	-0.089177
C	-1.600617	-1.580151	1.217809
H	-1.970611	-2.588199	1.016649
H	-1.635023	-1.452860	2.306611
C	-2.509439	-0.566697	0.568503
C	-2.567903	0.744390	1.045858
C	-3.292892	-0.911479	-0.532708
C	-3.372399	1.693158	0.425491
H	-1.968733	1.024619	1.906857
C	-4.105205	0.033002	-1.152994
H	-3.273247	-1.931846	-0.902351
C	-4.142548	1.339419	-0.678308
H	-3.395323	2.708566	0.802691
H	-4.709784	-0.252914	-2.005765
H	-4.770683	2.077382	-1.162611

__Frequencies__ (Top 10 out of 96)

1. -545.3564 cm-1 (Symmetry: A) *
2. 23.4706 cm-1 (Symmetry: A)
3. 40.8545 cm-1 (Symmetry: A)
4. 46.3011 cm-1 (Symmetry: A)
5. 65.1229 cm-1 (Symmetry: A)
6. 82.7393 cm-1 (Symmetry: A)
7. 108.4279 cm-1 (Symmetry: A)
8. 134.2649 cm-1 (Symmetry: A)
9. 155.9676 cm-1 (Symmetry: A)
10. 169.7050 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C17H16N
Electronic Energy (Eh)	-711.993809902
Sum of electronic and zero-point Energies (Eh)	-711.712556
Sum of electronic and thermal Energies (Eh)	-711.696598
Sum of electronic and enthalpy Energies (Eh)	-711.695653
Sum of electronic and thermal Free Energies (Eh)	-711.758073
Number of Imaginary Frequencies	0

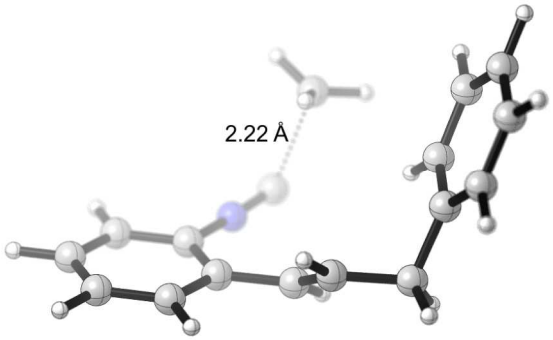
__Molecular Geometry in Cartesian Coordinates__

xyz			
C	3.460164	-1.095130	-1.322764
C	2.273830	-1.336635	-0.658325
C	1.715122	-0.392223	0.241739
C	2.449175	0.818356	0.407963
C	3.640650	1.058738	-0.260687
C	4.153154	0.102820	-1.129687
H	3.855400	-1.843136	-1.999468
H	1.756560	-2.273717	-0.821643
H	4.152434	1.997792	-0.092017
H	5.082737	0.290635	-1.651310
C	1.520797	2.609195	1.979655
C	-1.303426	-1.997880	1.936664
H	-1.956867	-2.861725	1.792103
H	-0.718232	-2.158456	2.844259
H	-1.933113	-1.117838	2.088347
N	1.955270	1.793773	1.260619
C	0.500373	-0.611882	0.929040
H	0.146484	0.166442	1.595694
C	-0.384065	-1.802863	0.730097
H	0.238128	-2.699383	0.626348
C	-1.195525	-1.679697	-0.593872
H	-0.494408	-1.615147	-1.430830
H	-1.775593	-2.598430	-0.722071
C	-2.117547	-0.486318	-0.619295
C	-1.635742	0.777044	-0.971297
C	-3.459023	-0.609457	-0.255855
C	-2.469647	1.889441	-0.947762
H	-0.597426	0.887218	-1.269168
C	-4.298226	0.500395	-0.233659

H	-3.849272	-1.586329	0.012390
C	-3.804012	1.754205	-0.576485
H	-2.077379	2.861964	-1.220809
H	-5.337799	0.384882	0.049984
H	-4.454856	2.620166	-0.558969

__Frequencies__ (Top 10 out of 96)

1. 23.8428 cm-1 (Symmetry: A)
2. 30.5938 cm-1 (Symmetry: A)
3. 40.1612 cm-1 (Symmetry: A)
4. 96.2508 cm-1 (Symmetry: A)
5. 99.6705 cm-1 (Symmetry: A)
6. 119.7052 cm-1 (Symmetry: A)
7. 131.8711 cm-1 (Symmetry: A)
8. 170.0195 cm-1 (Symmetry: A)
9. 201.7573 cm-1 (Symmetry: A)
10. 247.4945 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C17H16N
Electronic Energy (Eh)	-711.926978283
Sum of electronic and zero-point Energies (Eh)	-711.651134
Sum of electronic and thermal Energies (Eh)	-711.634062
Sum of electronic and enthalpy Energies (Eh)	-711.633118
Sum of electronic and thermal Free Energies (Eh)	-711.699223
Number of Imaginary Frequencies	1

__Molecular Geometry in Cartesian Coordinates__

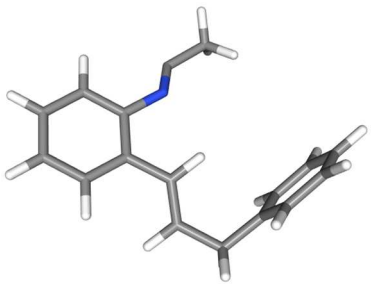
xyz

C	-3.844423	-1.714845	0.971428
C	-2.633597	-1.810488	0.297955
C	-2.042512	-0.693747	-0.297049
C	-2.724755	0.531871	-0.198653
C	-3.947000	0.635662	0.465765
C	-4.502867	-0.490232	1.053842
H	-4.282272	-2.597935	1.420321
H	-2.136581	-2.769322	0.206713
H	-4.435994	1.600164	0.516445

H	-5.451086	-0.412635	1.571144
N	-2.154257	1.661170	-0.752066
C	-1.513221	2.592711	-1.094992
C	0.050387	3.133004	0.384662
H	0.192380	2.169805	0.858954
H	0.823564	3.486152	-0.283276
H	-0.507935	3.882990	0.928155
C	-0.753520	-0.768589	-1.003954
H	-0.646672	-0.140153	-1.885504
C	0.278370	-1.513026	-0.606414
H	0.202781	-2.089245	0.313995
C	1.611781	-1.531906	-1.299687
H	1.944681	-2.562675	-1.449113
H	1.514953	-1.070241	-2.286198
C	2.646734	-0.780843	-0.483767
C	2.519999	0.600277	-0.322550
C	3.705895	-1.436210	0.138297
C	3.432796	1.312341	0.443652
H	1.690606	1.114614	-0.799116
C	4.624562	-0.725716	0.908281
H	3.815655	-2.509343	0.019662
C	4.489850	0.648549	1.063295
H	3.317429	2.383864	0.561818
H	5.444619	-1.248472	1.386545
H	5.202791	1.201366	1.663244

__Frequencies__ (Top 10 out of 96)

1. -434.3339 cm-1 (Symmetry: A) *
2. 21.7508 cm-1 (Symmetry: A)
3. 26.7747 cm-1 (Symmetry: A)
4. 31.6889 cm-1 (Symmetry: A)
5. 49.4864 cm-1 (Symmetry: A)
6. 74.5151 cm-1 (Symmetry: A)
7. 95.2702 cm-1 (Symmetry: A)
8. 101.0961 cm-1 (Symmetry: A)
9. 154.5701 cm-1 (Symmetry: A)
10. 167.6094 cm-1 (Symmetry: A)



Charge	0
Multiplicity	2
Stoichiometry	C17H16N

Electronic Energy (Eh)	-711.978666463
Sum of electronic and zero-point Energies (Eh)	-711.697829
Sum of electronic and thermal Energies (Eh)	-711.681292
Sum of electronic and enthalpy Energies (Eh)	-711.680348
Sum of electronic and thermal Free Energies (Eh)	-711.745519
Number of Imaginary Frequencies	0

__Molecular Geometry in Cartesian Coordinates__

xyz

C	3.996622	-1.661855	-0.261516
C	2.631182	-1.866129	-0.130826
C	1.737136	-0.791944	-0.056901
C	2.264076	0.507705	-0.131023
C	3.637416	0.716136	-0.271024
C	4.502615	-0.364965	-0.332086
H	4.666011	-2.511258	-0.325908
H	2.239524	-2.876487	-0.111891
H	4.004784	1.733858	-0.330072
H	5.567384	-0.198802	-0.443964
C	1.561234	2.735008	0.319752
C	0.648909	3.910158	0.325354
H	-0.336181	3.634782	-0.062712
H	0.552933	4.297161	1.340874
H	1.077833	4.705164	-0.287482
N	1.360186	1.592786	-0.092822
C	0.284718	-0.984006	0.091818
H	-0.335710	-0.174531	-0.279952
C	-0.287644	-2.040530	0.669831
H	0.335279	-2.826861	1.091349
C	-1.774508	-2.250645	0.825117
H	-2.053780	-3.177529	0.311340
H	-1.993012	-2.419269	1.885450
C	-2.612939	-1.109480	0.309249
C	-2.883113	-0.008108	1.122142
C	-3.082794	-1.104171	-1.003386
C	-3.609722	1.073338	0.636297
H	-2.511863	0.001740	2.142089
C	-3.810178	-0.024427	-1.494583
H	-2.870510	-1.951906	-1.647050
C	-4.075609	1.067792	-0.675236
H	-3.814378	1.919571	1.281904
H	-4.169878	-0.036681	-2.516814
H	-4.644136	1.908280	-1.055278

__Frequencies__ (Top 10 out of 96)

1. 16.4392 cm-1 (Symmetry: A)
2. 28.0308 cm-1 (Symmetry: A)
3. 36.1687 cm-1 (Symmetry: A)
4. 60.3748 cm-1 (Symmetry: A)

5. 81.1316 cm-1 (Symmetry: A)
6. 91.9872 cm-1 (Symmetry: A)
7. 112.0348 cm-1 (Symmetry: A)
8. 144.4888 cm-1 (Symmetry: A)
9. 155.1758 cm-1 (Symmetry: A)
10. 173.9890 cm-1 (Symmetry: A)

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