Angewandte Chemie

Supporting Information

An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes**

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Supporting Information – Table of Contents

Materials and Methods.

All computations were carried out using Spartan '06 for Mac[1] unless otherwise noted. All structures were minimized using Molecular Mechanics, and then further minimized using Density Functional Theory B3LYP/6–31G*.

Literature references for various computational methods are as follows:

B3LYP: a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785; c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200; d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623.

MP2: a) C. Møller, M. S. Plesset, *Phys. Rev.* **1934**, *46*, 618; b) M. Head-Gordon, J. A. Pople, and M. J. Frisch, *Chem. Phys. Lett.* **1988**, *153*, 503.

M06-2X: Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215.

SF-CCSD: A. I. Krylov, *Chem. Phys. Lett.* **2001**, *350*, 522.

Note: Although the use of hybrid-GGA density functionals such as B3LYP is commonplace throughout organic chemistry, reaction energies are often predicted with errors of the order of 6-8 kcal/mol.[2] Grimme and others have shown that the incorporation of dispersion corrections can partially mitigate these errors and are essential for greater quantitative accuracy with DFT calculations. In the current work, while we would expect the absolute reaction energies to alter upon the inclusion of a dispersion correction, the relative aryne stabilities would likely remain unchanged leaving our conclusions unaltered.
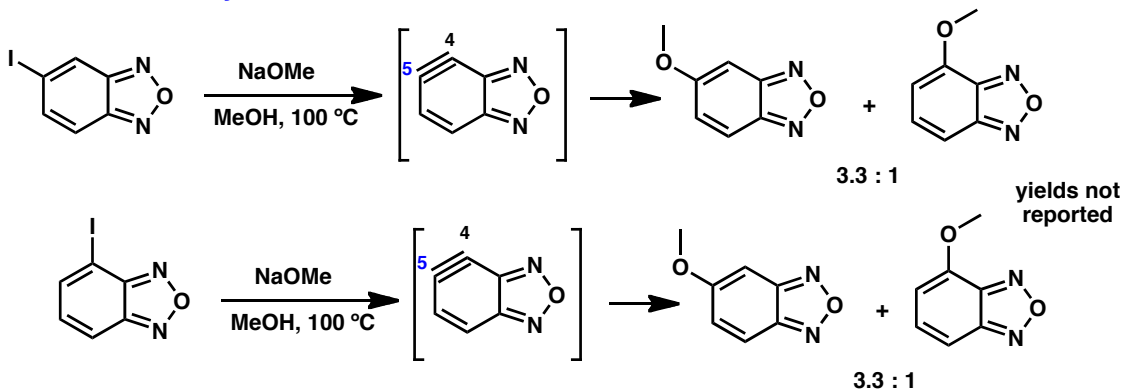
Additional Published Hetaryne Examples

2,3-pyridyne-N-oxide

75–80% yield + **trace**
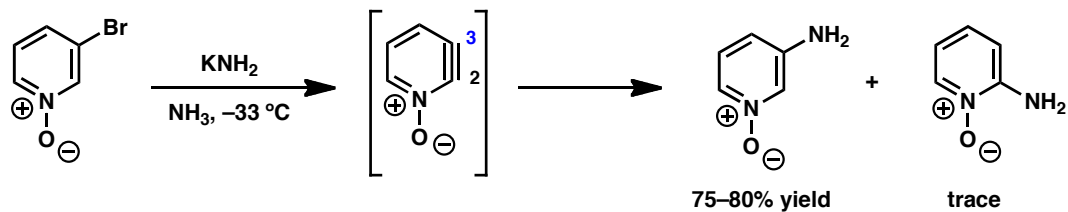
Martens, R. J.; den Hertog, H. J. *Rec. Trav. Chim. Pays–Bas* **1967**, *86*, 655–669.

4,5-benzofurazanyne

3.3 : 1   **yields not reported**

3.3 : 1

Di Nunno, L.; Florio, S.; Todesco, P. E. *J. Chem. Soc., Perkin Trans. II* **1974**, 1171–1175.

1,2-dibenzofuranyne
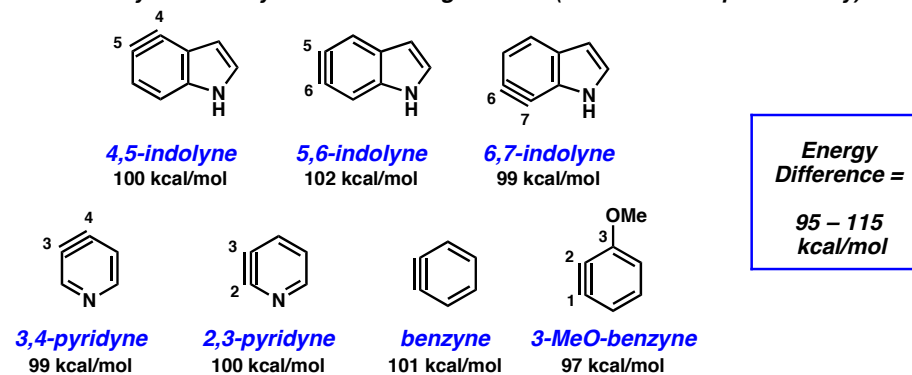

47.5% yield

(other isomer not reported)
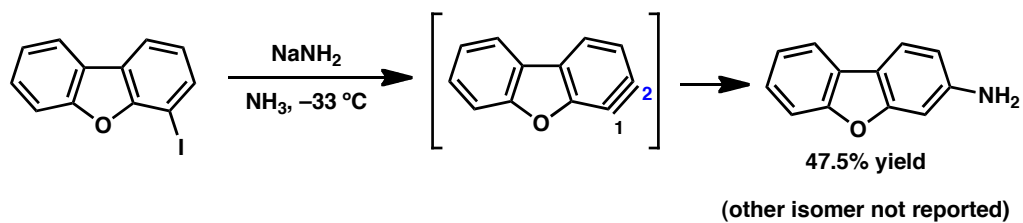
Gilman, H.; Avakian, S. *J. Am. Chem. Soc.* **1945**, *67*, 349–351.
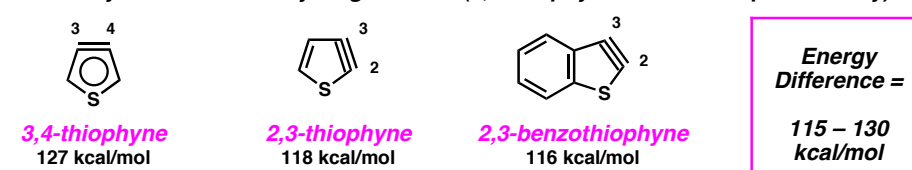
Select Energy Calculations using DFT (M06/6-311+G**)

The energies of hetarynes from Figure 2 were computed in Spartan '10³ using Density Functional Theory (M06/6-311+G**) from the previously minimized structures used throughout the manuscript. While there are small differences (typically ~ 2 kcal/mol) in the absolute energies, in all cases the hetarynes still fall into the same categories as outlined in Figure 2 in the accompanying manuscript.
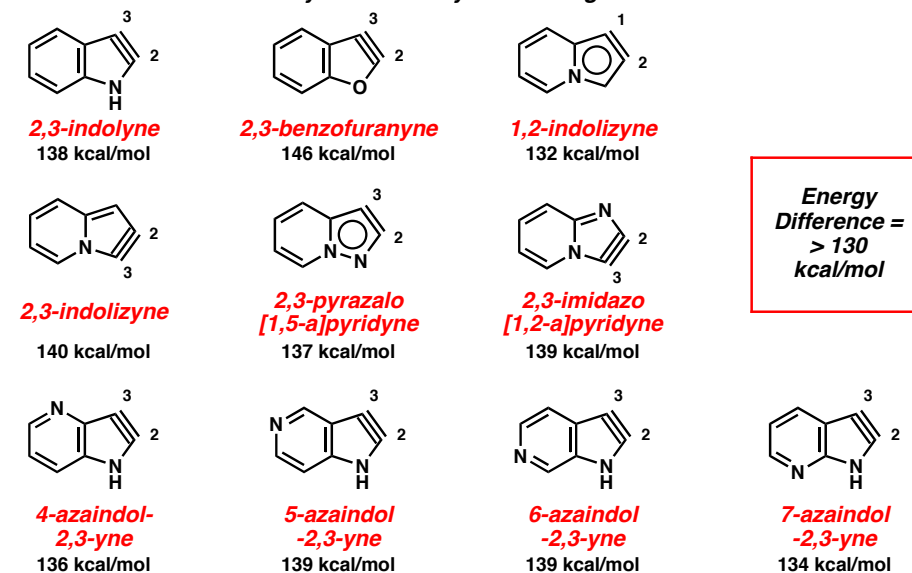
computed using DFT M06/6-311+G**

Hetarynes and arynes that can be generated (all validated experimentally)

4,5-indolyne
100 kcal/mol

5,6-indolyne
102 kcal/mol

6,7-indolyne
99 kcal/mol

Energy Difference =

95 – 115 kcal/mol

3,4-pyridyne
99 kcal/mol

2,3-pyridyne
100 kcal/mol

benzyne
101 kcal/mol

3-MeO-benzyne
97 kcal/mol

Hetarynes that can likely be generated (3,4-thiophyne validated experimentally)

3,4-thiophyne
127 kcal/mol

2,3-thiophyne
118 kcal/mol

2,3-benzothiophyne
116 kcal/mol

Energy Difference =

115 – 130 kcal/mol

Hetarynes that likely cannot be generated

2,3-indolyne
138 kcal/mol

2,3-benzofuranyne
146 kcal/mol

1,2-indolizyne
132 kcal/mol

2,3-indolizyne
140 kcal/mol

2,3-pyrazalo [1,5-a]pyridyne
137 kcal/mol

2,3-imidazo [1,2-a]pyridyne
139 kcal/mol

Energy Difference = > 130 kcal/mol

4-azaindol- 2,3-yne
136 kcal/mol

5-azaindol -2,3-yne
139 kcal/mol

6-azaindol -2,3-yne
139 kcal/mol

7-azaindol -2,3-yne
134 kcal/mol

energy difference or energy of dehydrogenation in kcal/mol	=	(energy of aryne + energy of H_2) – (energy of parent arene)

Sample Calculation Setup.

Note to user: The following section provides a simple guide for setting up hetaryne calculations. However, users should have some basic understanding of computational chemistry in order to conduct and interpret such computations.

Predicting the Preferred Site of Attack on an Aryne

1) Construct the parent arene in Spartan. Connect the two adjacent carbons using the "**make bond**" button by clicking the adjacent yellow connection points.
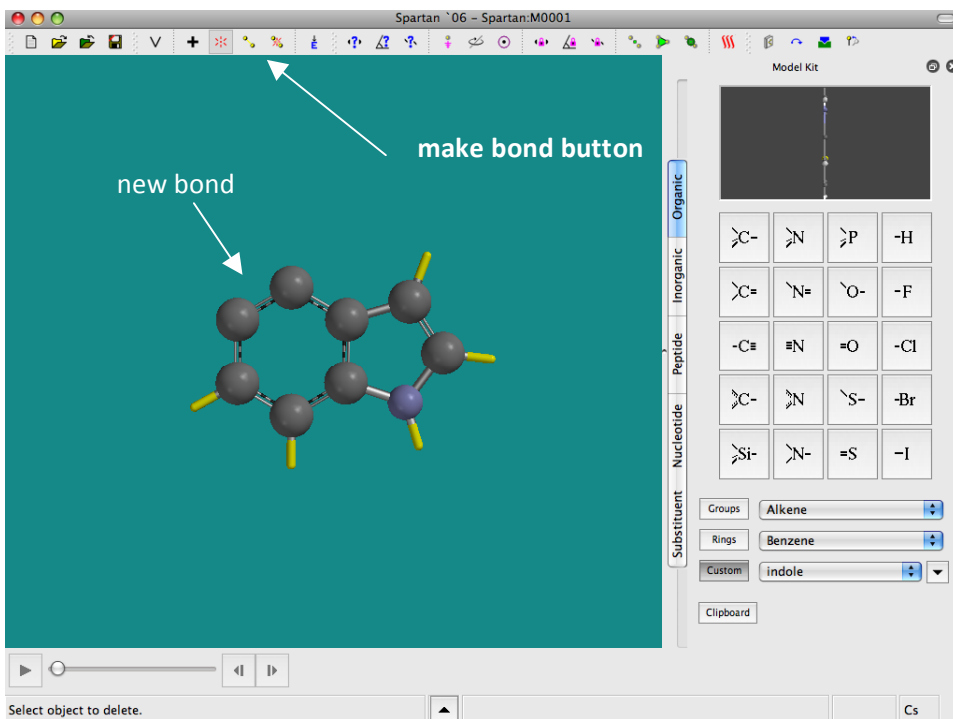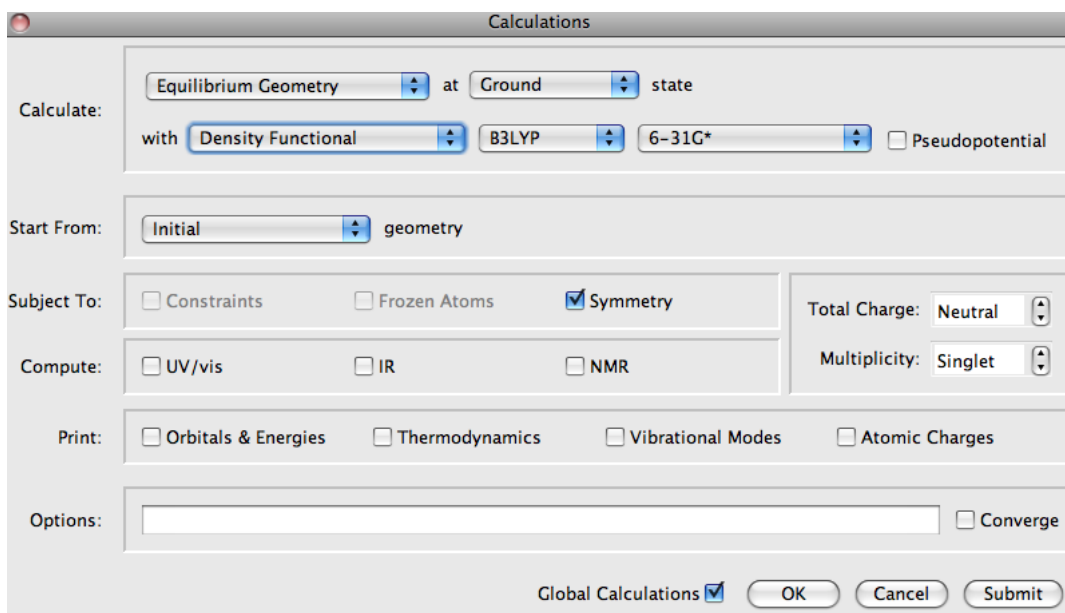

2) Perform an energy minimization by clicking the   "**minimize**" button.

3) Start the calculation by choosing "Setup" followed by "Calculations"

4) Calculate "**Equilibrium Geometry**" at "**Ground**" state with "**Density Functional/B3LYP/6-31G***". Everything else should already be setup properly.

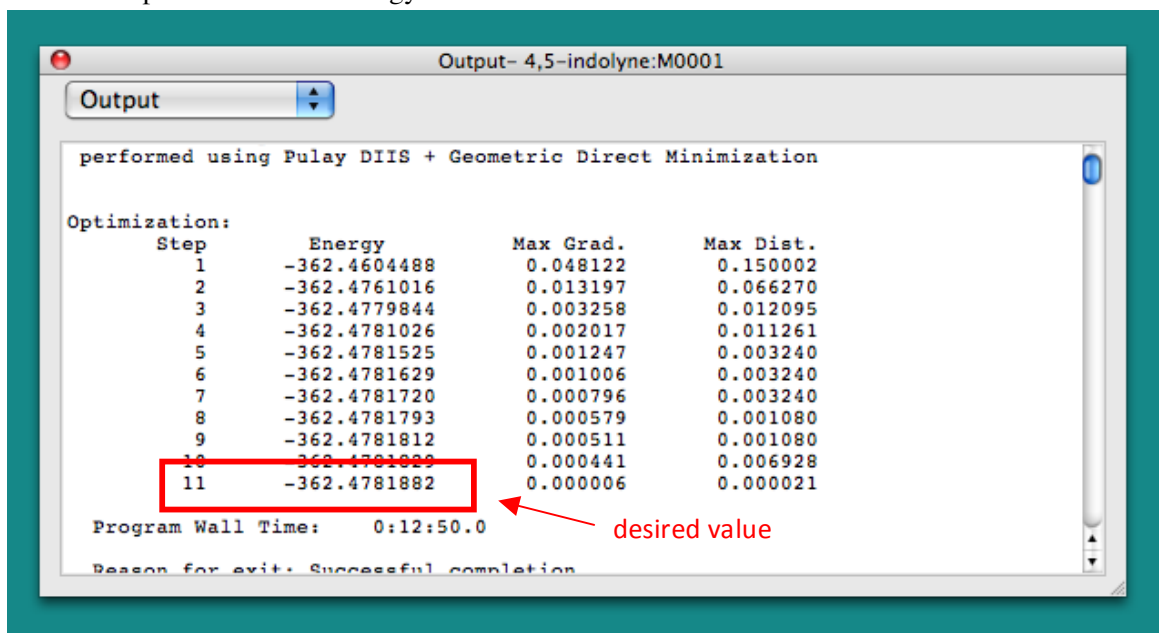5) Click "**submit**" and create a file name for the molecule.

6) After the computation has finished, measure the angles, using the "**Measure Angle**" button. Click 3 adjacent atoms in order to measure the angle of the central atom.
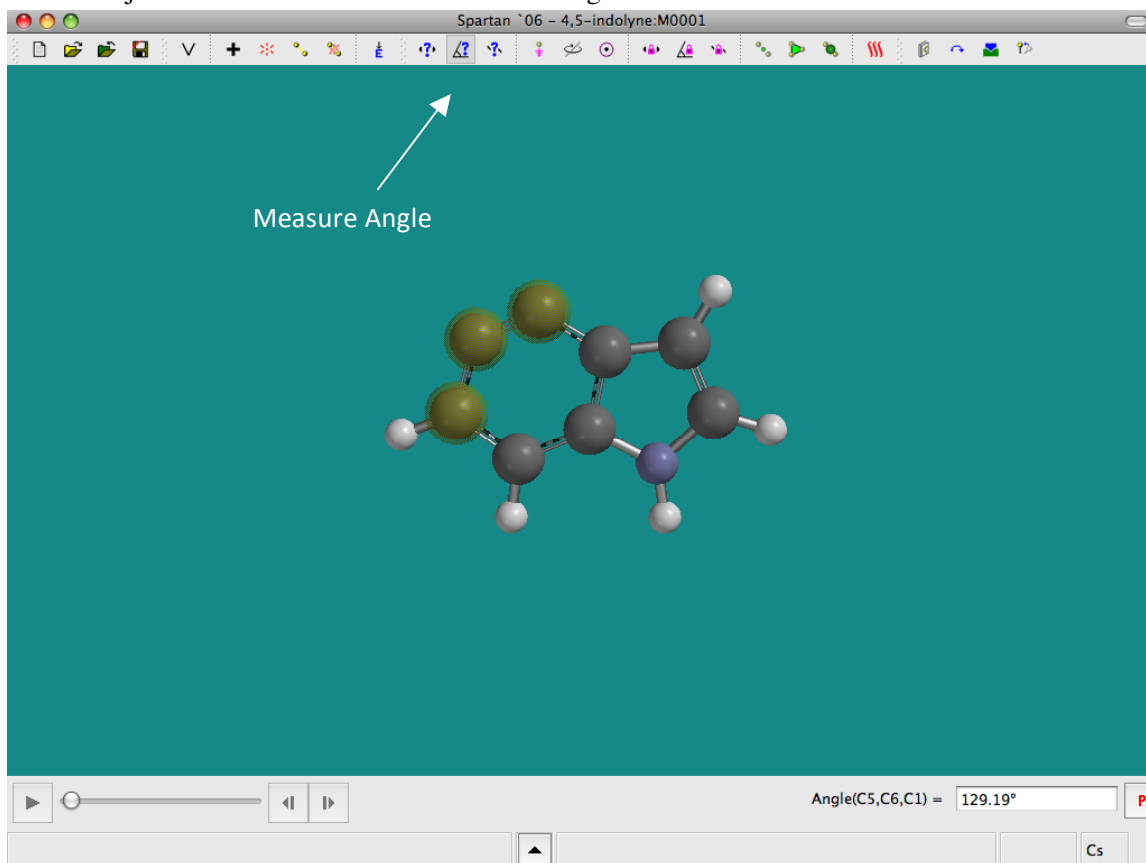
7) Compare the two termini of the aryne to find the larger angle.

Calculating the Dehydrogenation Energy of the Aryne

1) To calculate the dehydrogenation energy, you must first model the aryne in question, the parent arene (i.e. indole to correspond to 4,5-indolyne) and hydrogen (H_2).

2) After these calculations are all complete, obtain the energy of each species by choosing "**Output**" under the "**Display**" menu

3) Scroll through the output until you see a section with the heading "**Optimization**". This contains a series of "steps" as well as energies for each step. The energy that corresponds to the bottom "step" is the desired energy.

```
                                          Output– 4,5–indolyne:M0001

  Output          ⬍

   performed using Pulay DIIS + Geometric Direct Minimization


Optimization:
        Step          Energy          Max Grad.        Max Dist.
          1        -362.4604488        0.048122         0.150002
          2        -362.4761016        0.013197         0.066270
          3        -362.4779844        0.003258         0.012095
          4        -362.4781026        0.002017         0.011261
          5        -362.4781525        0.001247         0.003240
          6        -362.4781629        0.001006         0.003240
          7        -362.4781720        0.000796         0.003240
          8        -362.4781793        0.000579         0.001080
          9        -362.4781812        0.000511         0.001080
         10        -362.4781829        0.000441         0.006928
         11        -362.4781882        0.000006         0.000021

   Program Wall Time:    0:12:50.0                      desired value

   Reason for exit: Successful completion
```

4) After obtaining the value from each calculation (aryne, arene, and H_2), they must be converted from their given units (Hartrees) to kcal/mol. The conversion for this is 1 Hartree = 627.51 kcal/mol.

5) The dehydrogenation energy is calculated as (Energy of aryne + Energy of H_2) – (Energy of arene). This should give a positive value. Higher values correspond to less stable arynes.
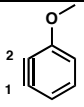
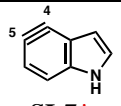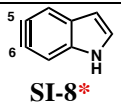**Energies and Key Angles of Calculated Structures**.

The dehydrogenation energy (kcal/mol) was obtained by calculating (energy of aryne + energy of H$_2$) – (energy of parent arene). The energy differences relative to that of *o*-benzyne are also shown as the Standardized Energy. Positive standardized energies correspond to arynes that are higher in energy compared to *o*-benzyne. Standardized energies that are negative are predicted to be lower in energy than *o*-benzyne.
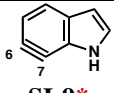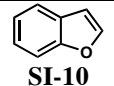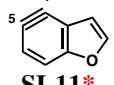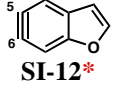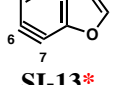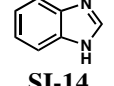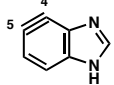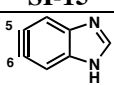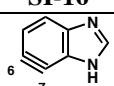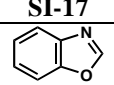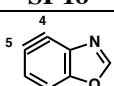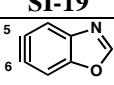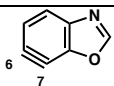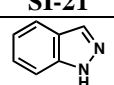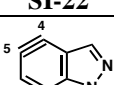
Structures marked with a (*) are included in the accompanying communication.
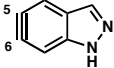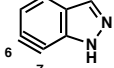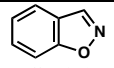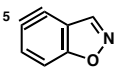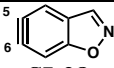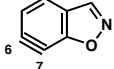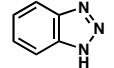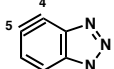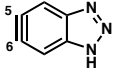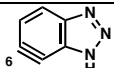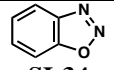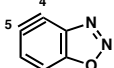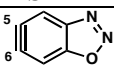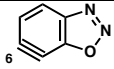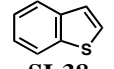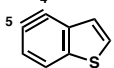
A. Benzene derived arynes
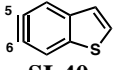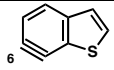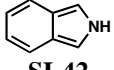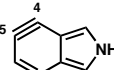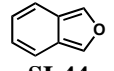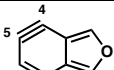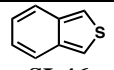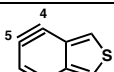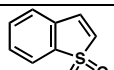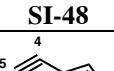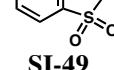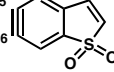
Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
H—H SI-1	-1.17548	-737.6					
SI-2	-232.2507	-145739.6					
SI-3*	-230.90996	-144898.3	103.7	0.0	127.1 (N/A)	127.1 (N/A)	0.0
SI-4	-346.7714	-217602.5					
SI-5*	-345.4388	-216766.3	98.6	-5.1	134.90 (C1)	119.2 (C2)	15.7
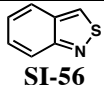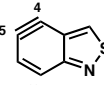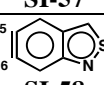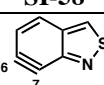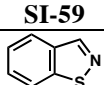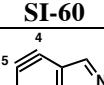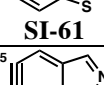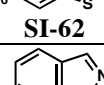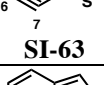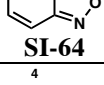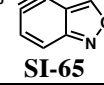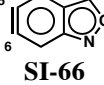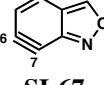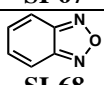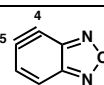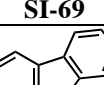
B. 6,5-bicyclic hetarynes (aryne outside of heterocycle)
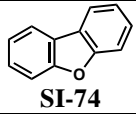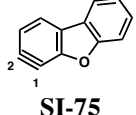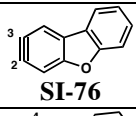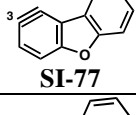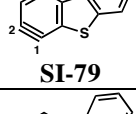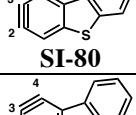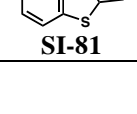
Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
SI-6	-363.8167	-228298.6					
SI-7*	-362.4782	-227458.7	102.3	-1.4	129.2 (C5)	125.1 (C4)	4.1
SI-8*	-362.4754	-227456.9	104.1	0.4	130.0 (C5)	126.8 (C6)	3.2

Structure							
SI-9*	-362.4797	-227459.6	101.4	-2.3	134.7 (C6)	117.4 (C7)	17.3
SI-10	-383.6734	-240758.9					
SI-11*	-382.3329	-239917.7	103.6	-0.1	130.6 (C5)	123.3 (C4)	7.3
SI-12*	-382.3317	-239917.0	104.3	0.6	129.7 (C5)	127.4 (C6)	2.3
SI-13*	-382.3341	-239918.5	102.8	-0.9	135.5 (C6)	115.8 (C7)	19.7
SI-14	-379.8661	-238369.8					
SI-15	-378.5264	-237529.1	103.0	-0.6	131.4 (C5)	122.1 (C4)	9.3
SI-16	-378.525	-237528.2	103.9	0.2	130.4 (C5)	127.1 (C6)	3.3
SI-17	-378.5278	-237530.0	102.2	-1.5	135.5 (C6)	116.2 (C7)	19.3
SI-18	-399.7232	-250830.3					
SI-19	-398.3816	-249988.4	104.2	0.5	132.5 (C5)	120.4 (C4)	12.1
SI-20	-398.3817	-249988.5	104.2	0.5	129.9 (C5)	127.8 (C6)	2.10
SI-21	-398.3827	-249989.1	103.6	-0.1	136.4 (C6)	114.4 (C7)	22.0
SI-22	-379.8436	-238355.7					
SI-23	-378.5034	-237514.7	103.4	-0.3	129.8 (C5)	123.7 (C4)	6.1
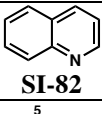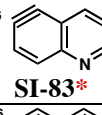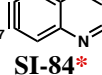
Structure							
SI-24	-378.5009	-237513.1	104.9	1.2	129.5 (C5)	128.0 (C6)	1.5
SI-25	-378.5057	-237516.1	101.9	-1.8	135.2 (C6)	116.8 (C7)	18.4
SI-26	-399.6831	-250805.1					
SI-27	-398.3405	-249962.6	104.9	1.2	131.3 (C5)	121.4 (C4)	9.9
SI-28	-398.3398	-249962.2	105.3	1.6	128.9 (C6)	128.7 (C5)	0.20
SI-29	-398.3425	-249963.9	103.6	-0.1	135.8 (C6)	115.7 (C7)	20.1
SI-30	-395.8672	-248410.6					
SI-31*	-394.5256	-247568.8	104.2	0.5	131.8 (C5)	120.9 (C4)	10.9
SI-32*	-394.5243	-247567.9	105.1	1.4	129.9 (C5)	128.3 (C6)	1.6
SI-33*	-394.5272	-247569.8	103.2	-0.5	135.7 (C6)	115.9 (C7)	19.8
SI-34	-415.7125	-260863.8					
SI-35	-414.3691	-260020.8	105.4	1.7	133.9 (C5)	117.6 (C4)	16.3
SI-36	-414.3689	-260020.6	105.5	1.8	129.9 (C6)	128.4 (C5)	1.5
SI-37	-414.3701	-260021.4	104.7	1.0	135.9 (C6)	116.3 (C7)	19.6
SI-38	-706.6536	-443432.2					
SI-39	-705.3153	-442592.4	102.2	-1.5	129.0 (C5)	125.6 (C4)	3.4
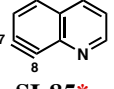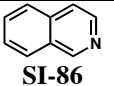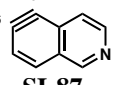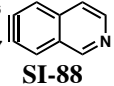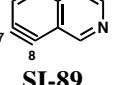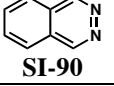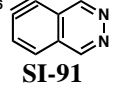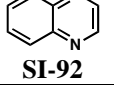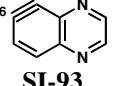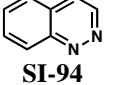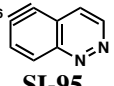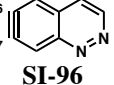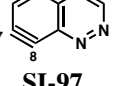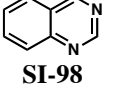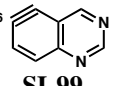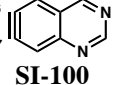
SI-40	−705.3118	−442590.2	104.4	0.7	130.0 (C5)	126.8 (C6)	3.2
SI-41	−705.3146	−442592.0	102.6	−1.1	131.7 (C6)	121.4 (C7)	10.3
SI-42	−363.8019	−228289.3					
SI-43	−362.4668	−227451.5	100.2	−3.5	129.9 (C5)	124.3 (C4)	5.6
SI-44	−383.6504	−240744.5					
SI-45	−382.3143	−239906.0	100.8	−2.9	130.7 (C5)	123.3 (C4)	7.4
SI-46	−706.6357	−443421.0					
SI-47	−705.3003	−442583.0	100.4	−3.3	130.1 (C5)	124.6 (C4)	5.5
SI-48	−857.0075	−537780.8					
SI-49	−855.6661	−536939.0	104.1	0.4	129.9 (C5)	124.3 (C4)	5.6
SI-50	−855.665	−536938.3	104.8	1.1	128.0 (C6)	127.6 (C5)	0.4
SI-51	−855.6624	−536936.7	106.4	2.7	131.1 (C6)	121.3 (C7)	9.8
SI-52	−722.6996	−453501.2					
SI-53	−721.3600	−452660.6	103.0	−0.7	131.1 (C5)	123.1 (C4)	8.0
SI-54	−721.3576	−452659.1	104.5	0.8	128.7 (C5)	128.0 (C6)	0.7
SI-55	−721.36	−452660.6	103.0	−0.7	132.6 (C6)	120.5 (C7)	12.1
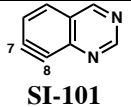
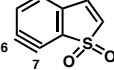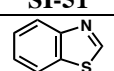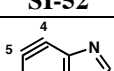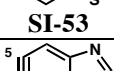| Structure							
SI-56	-722.6759	-453486.4					
SI-57	-721.3389	-452647.4	101.4	-2.3	130.4 (C5)	123.8 (C4)	6.6
SI-58	-721.3336	-452644.0	104.7	1.0	130.4 (C6)	128.6 (C5)	1.8
SI-59	-721.3395	-452647.7	101.0	-2.7	131.9 (C6)	122.7 (C7)	9.2
SI-60	-722.6891	-453494.6					
SI-61	-721.3491	-452653.8	103.2	-0.5	130.1 (C5)	123.6 (C4)	6.5
SI-62	-721.346	-452651.8	105.2	1.5	128.3 (N/A)	128.3 (N/A)	0.0
SI-63	-721.3492	-452653.8	103.2	-0.5	132.1 (C6)	121.1 (C7)	11.0
SI-64	-399.6653	-250794.0					
SI-65	-398.3266	-249953.9	102.4	-1.3	131.2 (C5)	121.9 (C4)	9.3
SI-66	-398.3221	-249951.1	105.2	1.6	130.9 (C6)	128.8 (C5)	2.1
SI-67	-398.3274	-249954.4	101.9	-1.8	132.8 (C6)	120.7 (C7)	12.1
SI-68	-415.678	-260842.1					
SI-69	-414.3375	-260000.9	103.6	-0.1	133.9 (C5)	119.5 (C4)	14.4
SI-70	-517.4707	-324718.0					
SI-71	-516.1333	-323878.8	101.6	-2.1	134.5 (C2)	118.0 (C1)	16.5

Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
SI-72	-516.1291	-323876.2	104.2	0.5	128.9 (C3)	127.4 (C2)	1.5
SI-73	-516.131	-323877.4	103.0	-0.6	129.5 (C3)	124.4 (C4)	5.1
SI-74	-537.3291	-337179.4					
SI-75	-535.9896	-336338.8	102.9	-0.8	135.3 (C2)	116.4 (C1)	18.9
SI-76	-535.9873	-336337.4	104.4	0.7	129.1 (C3)	127.7 (C2)	1.40
SI-77	-535.9881	-336337.9	103.9	0.2	130.6 (C3)	123.1 (C4)	7.5
SI-78	-860.3069	-539851.2					
SI-79	-858.9674	-539010.6	102.9	-0.8	131.6 (C2)	121.5 (C1)	10.1
SI-80	-858.9648	-539009.0	104.6	0.9	129.1 (C3)	127.7 (C2)	1.4
SI-81	-858.9687	-539011.4	102.1	-1.6	130.6	123.1	7.5
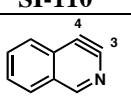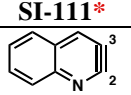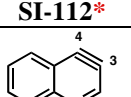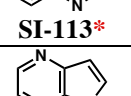
C. 6,6-bicyclic hetarynes (aryne outside of heterocycle)

Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
SI-82	-401.9308	-252215.6					
SI-83*	-400.5933	-251376.3	101.7	-2.0	128.4 (C6)	126.4 (C5)	2.0
SI-84*	-400.5898	-251374.1	103.9	0.2	128.7 (C7)	127.5 (C6)	1.2
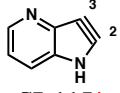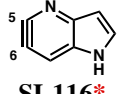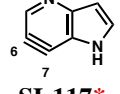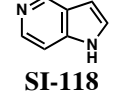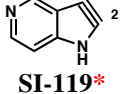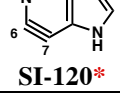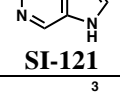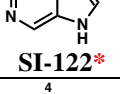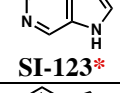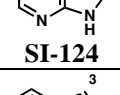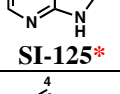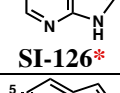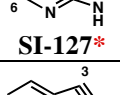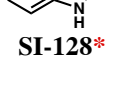
Structure							
SI-85*	-400.5932	-251376.2	101.7	-2.0	128.4 (C7)	126.8 (C8)	1.6
SI-86	-401.9291	-252214.5					
SI-87	-400.5917	-251375.3	101.6	-2.1	128.6 (C6)	126.4 (C5)	2.2
SI-88	-400.5885	-251373.3	103.6	-0.1	128.1 (N/A)	128.1 (N/A)	0.00
SI-89	-400.5906	-251374.6	102.3	-1.4	128.5 (C7)	125.8 (C8)	2.7
SI-90	-417.9343	-262258.0					
SI-91	-416.5944	-261417.2	103.2	-0.5	129.2 (C6)	124.9 (C5)	4.3
SI-92	-417.9650	-262277.2					
SI-93	-416.6269	-261437.5	102.0	-1.6	129.2 (C6)	125.7 (C5)	3.5
SI-94	-417.9321	-262256.6					
SI-95	-416.5941	-261417.0	102.0	-1.7	128.3 (C6)	126.0 (C5)	2.3
SI-96	-416.591	-261415.0	103.9	0.2	129.0 (C7)	127.8 (C6)	1.2
SI-97	-416.5922	-261415.8	103.2	-0.5	128.7 (C7)	125.9 (C8)	2.8
SI-98	-417.9701	-262280.4					
SI-99	-416.6308	-261440.0	102.8	-0.9	129.2 (C6)	124.9 (C5)	4.3
SI-100	-416.6295	-261439.2	103.6	-0.1	128.9 (C7)	127.8 (C6)	1.1
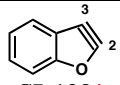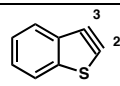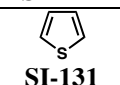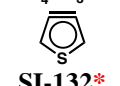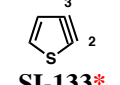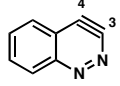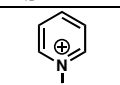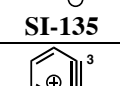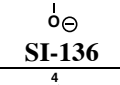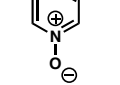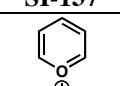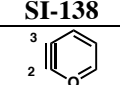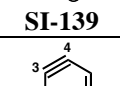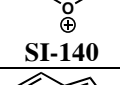
Structure							
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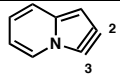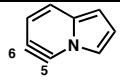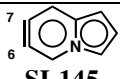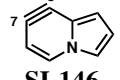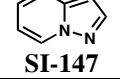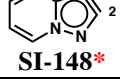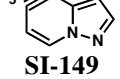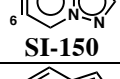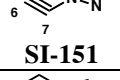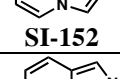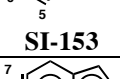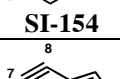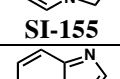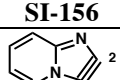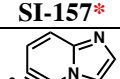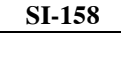
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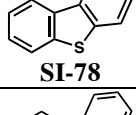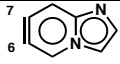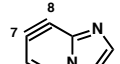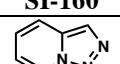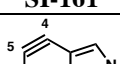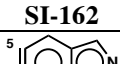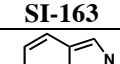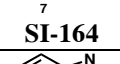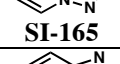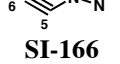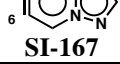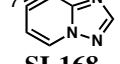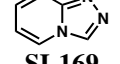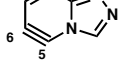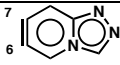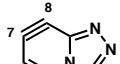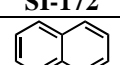| Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
SI-102	–248.285	–155801.3					
SI-103*	–246.9493	–154963.2	100.5	–3.2	125.3 (C4)	124.7 (C3)	0.6
SI-104*	–246.9413	–154958.1	105.6	1.9	151.2 (C2)	104.0 (C3)	47.2
SI-105	–264.2876	–165843.1					
SI-106*	–262.946	–165001.2	104.2	0.5	148.7 (C3)	107.0 (C4)	41.7
SI-107	–264.3237	–165865.8					
SI-108*	–262.9847	–165025.5	102.6	–1.1	147.2 (C4)	103.4 (C5)	43.8
SI-109	–280.3221	–175904.9					
SI-110*	–278.9624	–175051.7	115.6	11.9	147.7 (C5)	96.6 (C6)	51.1
SI-111*	–400.5880	–251373.0	103.9	0.2	150.8 (C3)	105.4 (C4)	45.4
SI-112*	–400.5905	–251374.5	103.4	0.7	153.0 (C2)	104.0 (C3)	49.0
SI-113*	–400.5968	–251378.5	99.5	–4.2	126.6 (C4)	124.1 (C3)	2.5
SI-114	–379.8538	–238362.1					
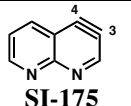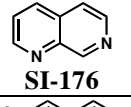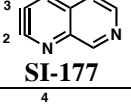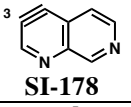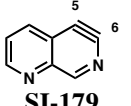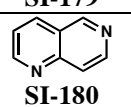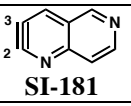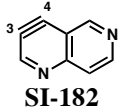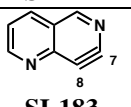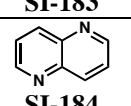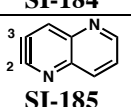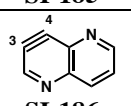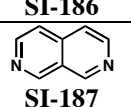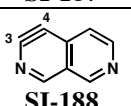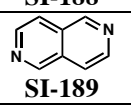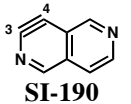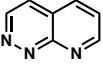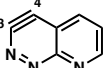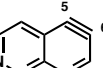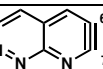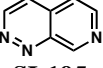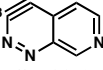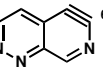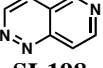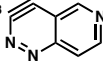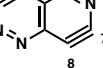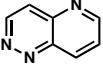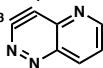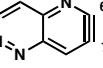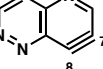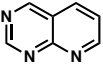
SI-115*	-378.4577	-237486.0	138.4	34.7	114.1 (C3)	110.5 (C2)	3.6
SI-116*	-378.5116	-237519.8	104.6	0.9	151.8 (C5)	106.7 (C6)	45.1
SI-117*	-378.5207	-237525.5	98.9	-4.8	130.6 (C6)	117.9 (C7)	12.7
SI-118	-379.8545	-238362.5					
SI-119*	-378.4537	-237483.5	141.4	37.7	113.7 (C3)	110.5 (C2)	3.2
SI-120*	-378.5208	-237525.6	99.3	-4.4	152.9 (C6)	100.0 (C7)	52.9
SI-121	-379.8535	-238361.9					
SI-122*	-378.4529	-237483.0	141.3	37.6	114.0 (C3)	110.7 (C2)	3.3
SI-123*	-378.5125	-237520.4	103.9	0.2	151.8 (C5)	103.5 (C4)	48.3
SI-124	-379.8608	-238366.5					
SI-125*	-378.4683	-237492.6	136.2	32.5	114.9 (C3)	110.0 (C2)	4.9
SI-126*	-378.513	-237520.7	101.3	-2.4	125.5 (C5)	125.3 (C4)	0.2
SI-127*	-378.5239	-237527.5	108.1	4.4	149.3 (C6)	108.8 (C5)	40.5
SI-128*	-362.4177	-227420.7	140.3	36.6	114.5 (C3)	110.1 (C2)	4.4
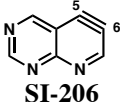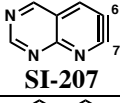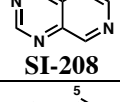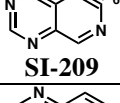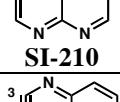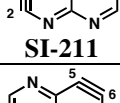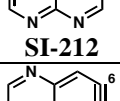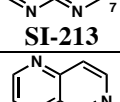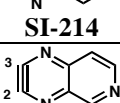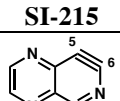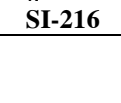
Structure						
SI-129*	-382.26	-239872.0	149.3	45.6	126.9 (C2)	100.3 (C3)	26.6
SI-130*	-705.2874	-442574.9	119.7	16.0	132.6 (C3)	102.3 (C2)	30.3
SI-131	-553.0026	-347014.7					
SI-132*	-551.621	-346147.7	129.3	25.6	118.2 (N/A)	118.2 (N/A)	0.0
SI-133*	-551.6334	-346155.5	121.6	17.9	135.6 (C3)	97.0 (C2)	38.6
SI-134	-416.5896	-261414.1	104.8	1.1	147.5 (C3)	108.3 (C4)	39.2
SI-135	-323.4472	-202966.4					
SI-136	-322.0926	-202116.3	112.4	8.7	132.1 (C3)	124.6 (C2)	7.5
SI-137	-322.1004	-202121.2	107.5	3.8	127.1 (C4)	125.4 (C3)	1.7
SI-138	-268.4764	-168471.6					
SI-139	-267.0862	-167599.3	134.7	31.0	132.2 (C2)	123.1 (C3)	9.1
SI-140	-267.1193	-167620.0	114.0	10.3	132.7 (C4)	119.5 (C3)	13.2
SI-141	-363.7988	-228287.4					
SI-142*	-362.4096	-227415.6	134.1	30.4	114.2 (C2)	110.1 (C1)	4.1

SI-143*	-362.3962	-227407.2	142.5	38.8	118.5 (C2)	106.1 (C3)	12.4
SI-144	-362.4455	-227438.2	111.6	7.9	130.1 (C6)	124.4 (C5)	5.7
SI-145	-362.4507	-227441.4	108.3	4.6	134.2 (C7)	120.9 (C6)	13.3
SI-146	-362.4601	-227447.3	102.4	-1.3	130.1 (C7)	124.1 (C8)	6.0
SI-147	-379.8340	-238349.6					
SI-148*	-378.4337	-237470.9	141.1	37.4	133.2 (C2)	94.6 (C3)	38.6
SI-149	-378.4942	-237508.9	103.1	-0.6	130.9 (C5)	122.9 (C4)	8.0
SI-150	-378.4857	-237503.6	108.4	4.7	134.4 (C5)	121.1 (C6)	13.3
SI-151	-378.4766	-237497.9	114.2	10.5	130.2 (C6)	123.4 (C7)	6.8
SI-152	-379.8431	-238355.3					
SI-153	-378.4888	-237505.5	112.2	8.5	131.1 (C6)	122.9 (C5)	8.2
SI-154	-378.4937	-237508.6	109.1	5.4	134.5 (C7)	121.3 (C6)	13.2
SI-155	-378.5035	-237514.7	103.0	-0.7	130.7 (C7)	123.1 (C8)	7.6
SI-156	-379.8496	-238359.4					
SI-157*	-378.4444	-237477.6	144.2	40.5	136.4	89.9	46.5
SI-158	-378.495	-237509.4	112.4	8.7	129.7 (C6)	124.1 (C5)	5.6

Structure							
SI-159	-378.502	-237513.8	108.0	4.3	134.7 (C7)	120.9 (C6)	13.8
SI-160	-378.5095	-237518.5	103.3	-0.4	131.4 (C7)	122.7 (C8)	8.7
SI-161	-395.8547	-248402.8					
SI-162	-394.5125	-247560.5	104.6	0.9	131.0 (C5)	122.1 (C4)	8.9
SI-163	-394.5044	-247555.5	109.7	6.0	134.1 (C5)	121.7 (C6)	12.4
SI-164	-394.4956	-247549.9	115.2	11.5	131.2 (C6)	121.9 (C7)	9.3
SI-165	-395.8872	-248423.2					
SI-166	-394.5285	-247570.6	115.0	11.3	130.4 (C6)	122.3 (C5)	8.1
SI-167	-394.5392	-247577.3	108.3	4.6	134.8 (C7)	121.2 (C6)	13.6
SI-168	-394.5457	-247581.4	104.2	0.5	132.1 (C7)	121.4 (C8)	10.7
SI-169	-395.8681	-248411.2					
SI-170	-394.5115	-247559.9	113.7	10.0	130.4 (C6)	122.7 (C5)	7.7
SI-171	-394.5187	-247564.4	109.1	5.4	135.4 (C7)	120.9 (C6)	14.5
SI-172	-394.5265	-247569.3	104.2	0.5	132.1 (C7)	121.5 (C8)	10.6
SI-173	-417.966	-262277.8					
SI-174	-416.6274	-261437.9	102.4	-1.3	153.5 (C2)	103.2 (C3)	50.3
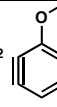
SI-175	-416.6305	-261439.8	100.4	-3.3	125.6 (C4)	124.3 (C3)	1.3
SI-176	-417.9652	-262277.3					
SI-177	-416.6239	-261435.7	104.1	0.4	152.5 (C2)	105.2 (C3)	47.3
SI-178	-416.6306	-261439.9	99.8	-3.9	125.5 (C4)	125.1 (C3)	0.3
SI-179	-416.6236	-261435.5	104.2	0.5	151.5 (C6)	104.4 (C5)	47.1
SI-180	-417.9661	-262277.9					
SI-181	-416.6250	-261436.4	103.9	0.2	152.6 (C2)	104.9 (C3)	47.7
SI-182	-416.6303	-261439.7	100.6	-3.1	125.1 (C4)	125.0 (C3)	0.1
SI-183	-416.6229	-261435.0	105.2	1.5	149.8 (C7)	107.5 (C8)	42.3
SI-184	-417.9685	-262279.4					
SI-185	-416.6255	-261436.7	105.1	1.4	152.9 (C2)	105.1 (C3)	47.8
SI-186	-416.6338	-261441.9	99.9	-3.8	125.6 (C3)	125.1 (C4)	0.5
SI-187	-417.964	-262276.6					
SI-188	-416.6224	-261434.7	104.2	0.5	151.0 (C3)	105.0 (C4)	46.0
SI-189	-417.9629	-262275.9					
SI-190	-416.6208	-261433.7	104.6	0.9	151.2 (C3)	103.8 (C4)	47.4

Structure						
SI-191	-433.9645	-272317.1				
SI-192	-432.6200	-271473.4	106.1	2.4	148.7 (C3)	106.4 (C4)	42.3
SI-193	-432.6286	-271478.8	100.7	-3.0	125.4 (C5)	124.3 (C6)	1.0
SI-194	-432.6245	-271476.2	103.2	-0.5	153.3 (C7)	104.3 (C6)	49.0
SI-195	-433.9648	-272317.3				
SI-196	-432.6216	-271474.4	105.2	1.5	147.4 (C3)	108.1 (C4)	39.3
SI-197	-432.6225	-271474.9	104.7	1.0	151.5 (C6)	104.2 (C5)	47.1
SI-198	-433.9645	-272317.1				
SI-199	-432.6206	-271473.8	105.7	2.0	148.4 (C3)	106.3 (C4)	42.1
SI-200	-432.6192	-271472.9	106.6	2.9	149.9 (C7)	106.2 (C8)	43.7
SI-201	-433.9687	-272319.7				
SI-202	-432.6252	-271476.6	105.4	1.7	146.2 (C3)	109.9 (C4)	36.3
SI-203	-432.6248	-271476.4	105.7	2.0	152.5 (C6)	106.1 (C7)	46.4
SI-204	-432.6314	-271480.5	101.5	-2.2	125.6 (C7)	124.6 (C8)	1.0
SI-205	-434.0045	-272342.2				
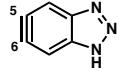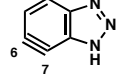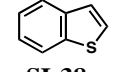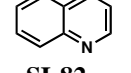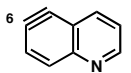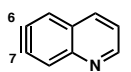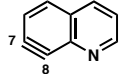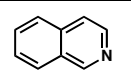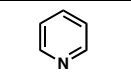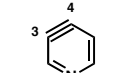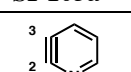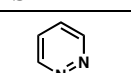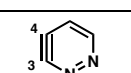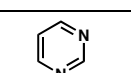
Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
SI-206	-432.6671	-271502.9	101.6	-2.1	124.9 (C6)	124.5 (C5)	0.4
SI-207	-432.6647	-271501.4	103.1	-0.6	153.0 (C7)	104.3 (C6)	48.7
SI-208	-434.0037	-272341.7					
SI-209	-432.6592	-271498.0	106.1	2.4	151.9 (C6)	102.6 (C5)	49.3
SI-210	-434.0001	-272339.4					
SI-211	-432.6304	-271479.9	121.9	18.2	154.1 (C2)	91.8 (C3)	62.3
SI-212	-432.6637	-271500.8	101.0	-2.7	125.5 (C6)	124.4 (C5)	1.1
SI-213	-432.6583	-271497.4	104.4	0.7	153.5 (C7)	104.4 (C6)	49.1
SI-214	-433.9981	-272338.1					
SI-215	-432.6244	-271476.1	124.4	20.7	131.9 (C3)	131.5 (C2)	0.4
SI-216	-432.6546	-271495.1	105.4	1.7	150.4 (C6)	106.4 (C5)	44.0

E. Selected Energies using MP2/6-311+G**
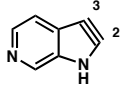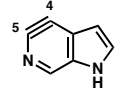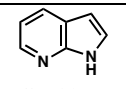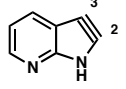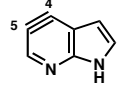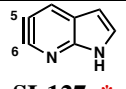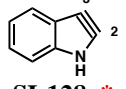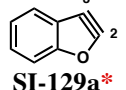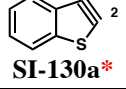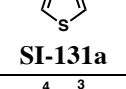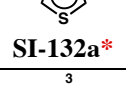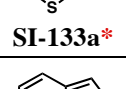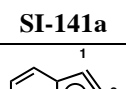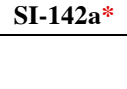
Structure	Energy (hartrees)	Energy (kcal/mol)	Dehydrogenation Energy (kcal/mol)	Standardized Energy (kcal/mol)	Larger Terminus	Smaller Terminus	Angle Difference
H—H SI-1a	-1.1602722	-728.1					
SI-2a	-231.5838779	-145321.2					
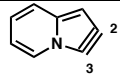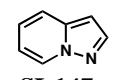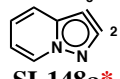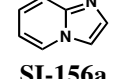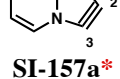
Structure							
SI-3a*	-230.2732476	-144498.8	94.4	0.0	126.8 (N/A)	126.8 (N/A)	0.0
SI-4a	-345.8429028	-217019.9					
SI-5a*	-344.5380523	-216201.1	90.7	-3.6	130.6 (C1)	122.8 (C2)	7.8
SI-6a	-362.8267529	-227677.4					
SI-7a*	-361.5173825	-226855.8	93.6	-0.8	127.4 (C5)	126.1 (C4)	1.3
SI-8a*	-361.5120066	-226852.4	96.9	2.6	128.3 (C6)	128.0 (C5)	0.3
SI-9a*	-361.5181322	-226856.2	93.1	-1.3	129.2 (C6)	122.3 (C7)	6.9
SI-10a	-382.6636787	-240125.3					
SI-11a*	-381.3515379	-239301.9	95.3	0.9	127.8 (C5)	125.2 (C4)	2.6
SI-12a*	-381.3488424	-239300.2	97.0	2.6	128.3 (N/A)	128.3 (N/A)	0.0
SI-13a*	-381.3520756	-239302.2	95.0	0.6	129.9 (C6)	120.8 (C7)	9.1
SI-30a	-394.8552468	-247775.6					
SI-31a*	-393.5423481	-246951.8	95.8	1.4	128.1 (C5)	124.0 (C4)	4.1

Structure							
SI-32a*	-393.5378788	-246949.0	98.6	4.2	129.5 (C6)	128.3 (C5)	1.2
SI-33a*	-393.5433232	-246952.4	95.2	0.8	129.7 (C6)	121.1 (C7)	8.6
SI-38a	-705.2721885	-442565.4					
SI-82a	-400.8327162	-251526.5					
SI-83a*	-399.5239462	-250705.3	93.2	-1.2	127.3 (C5)	126.8 (C6)	0.5
SI-84a*	-399.5173046	-250701.1	97.4	3.0	128.2 (C7)	127.2 (C6)	1.0
SI-85a*	-399.5236281	-250705.1	93.4	-1.0	128.7 (C7)	125.5 (C8)	3.2
SI-86a	-400.830496	-251525.1					
SI-102a	-247.6089605	-155377.1					
SI-103a*	-246.3010004	-154556.3	92.7	-1.7	126.2 (C4)	123.0 (C3)	3.2
SI-104a*	-246.2879319	-154548.1	100.9	6.5	145.9 (C2)	111.6 (C3)	34.3
SI-105a	-263.6000902	-165411.7					
SI-106a*	-262.2797103	-164583.1	100.5	6.1	140.0 (C3)	116.6 (C4)	23.4
SI-107a	-263.63605	-165434.3					

Structure							
SI-108a*	-262.3192632	-164608.0	98.2	3.9	141.9 (C4)	110.5 (C5)	31.4
SI-109a	-279.6239417	-175466.8					
SI-110a*	-278.2851891	-174626.7	112.0	17.6	132.8 (C5)	123.9 (C6)	8.9
SI-111a*	-399.5109697	-250697.1	99.9	5.6	141.5 (C3)	117.0 (C4)	24.5
SI-112a*	-399.5123645	-250698.0	100.5	6.1	151.0 (C2)	107.7 (C3)	43.3
SI-113a*	-399.5278657	-250707.7	90.7	-3.6	126.8 (C4)	123.3 (C3)	3.5
SI-114a	-378.8526836	-237733.8					
SI-115a*	-377.4848399	-236875.5	130.3	35.9	118.0 (C2)	105.2 (C3)	12.8
SI-116a*	-377.5302974	-236904.0	101.7	7.4	148.5 (C5)	112.2 (C6)	36.3
SI-117a*	-377.5473884	-236914.8	91.0	-3.3	125.1 (C6)	122.8 (C7)	2.3
SI-118a	-378.8527666	-237733.9					
SI-119a*	-377.4832556	-236874.5	131.3	36.9	116.6 (C2)	106.0 (C3)	10.6
SI-120a*	-377.5387573	-236909.3	96.5	2.1	151.7 (C6)	103.0 (C7)	48.7
SI-121	-378.8521074	-237733.5					

Structure							
SI-122a*	-377.4820657	-236873.8	131.6	37.3	117.5 (C2)	105.4 (C3)	12.1
SI-123a*	-377.5313632	-236904.7	100.7	6.3	144.3 (C5)	113.4 (C4)	30.9
SI-124a	-378.8594773	-237738.1					
SI-125a*	-377.4963563	-236882.7	127.3	32.9	116.9 (C2)	106.5 (C3)	10.4
SI-126a*	-377.5512763	-236917.2	92.8	-1.5	126.2 (C4)	123.9 (C5)	2.3
SI-127a*	-377.5343047	-236906.6	103.5	9.1	142.4 (C6)	117.2 (C5)	25.2
SI-128a*	-361.4587617	-226819.0	130.3	36.0	116.9 (C2)	106.1 (C3)	10.8
SI-129a*	-381.2835416	-239259.2	138.0	43.6	118.8 (C2)	106.4 (C3)	12.4
SI-130a*	-703.9307758	-441723.6	113.7	19.3	118.1 (C2)	114.5 (C3)	3.6
SI-131a	-552.0441704	-346413.2					
SI-132a*	-550.6874736	-345561.9	123.3	28.9	116.7 (N/A)	116.7 (N/A)	0.0
SI-133a*	-550.6969653	-345567.9	117.3	23.0	115.9 (C2)	114.7 (C3)	1.2
SI-141a	-362.8059171	-227664.3					
SI-142a*	-361.4470206	-226811.6	124.6	30.3	113.1 (C2)	110.0 (C1)	3.1

SI-143a*	-361.4325605	-226802.5	133.7	39.4	114.2 (C3)	109.2 (C2)	5.0
SI-147a	-378.8302728	-237719.8					
SI-148a*	-377.4548064	-236856.7	135.0	40.7	119.4 (C2)	106.4 (C3)	13.0
SI-156a	-378.8460432	-237729.7					
SI-157a*	-377.4509762	-236854.3	147.3	53.0	113.0 (C3)	112.2 (C2)	0.8

Coordinates of Computed Structures

A. Calculations with B3LYP/6-31G*

SI–1

H	0.000000	0.000000	0.371578
H	0.000000	0.000000	−0.371578

SI-2
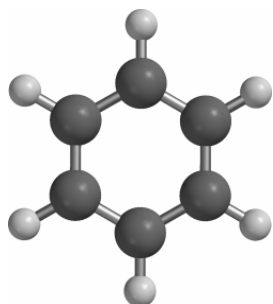
H	2.484269	0.000000	−0.000000
C	1.397048	0.000000	−0.000000
C	−1.397048	−0.000000	0.000000
C	0.698524	1.209879	0.000000
C	0.698524	−1.209879	−0.000000
C	−0.698524	−1.209879	−0.000000
C	−0.698524	1.209879	0.000000
H	1.242135	2.151440	0.000000
H	1.242135	−2.151440	−0.000000
H	−1.242135	−2.151440	−0.000000
H	−1.242135	2.151440	0.000000
H	−2.484269	−0.000000	0.000000

SI-3*
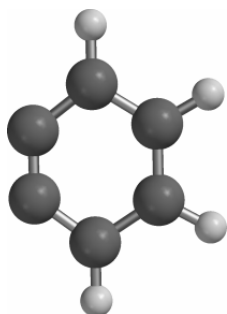
C	0.625554	0.000000	1.237609
C	−0.703547	−0.000000	−1.058538
C	−0.625554	−0.000000	1.237609
C	1.461350	0.000000	0.133663
C	0.703547	0.000000	−1.058538
C	−1.461350	−0.000000	0.133663
H	2.546616	0.000000	0.134515
H	1.229529	0.000000	−2.010917
H	−2.546616	−0.000000	0.134515
H	−1.229529	−0.000000	−2.010917

SI-4
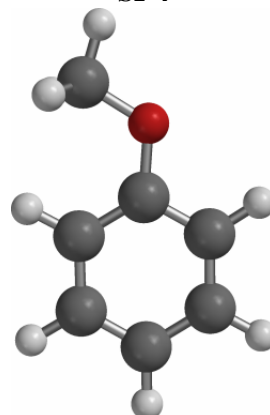
H	−0.135193	−2.330225	0.000000
C	−0.492177	−1.304778	0.000000
C	−1.343988	1.346699	0.000000
C	0.453709	−0.268524	0.000000
C	−1.849965	−1.007648	0.000000
C	−2.286811	0.321871	0.000000
C	0.025817	1.063988	0.000000
H	−2.573123	−1.819173	0.000000
H	−3.348440	0.551637	0.000000
H	0.739070	1.880156	0.000000
H	−1.667645	2.384512	0.000000
O	1.762023	−0.664345	0.000000
C	2.765670	0.336671	0.000000
H	2.705220	0.971054	−0.894707
H	3.719247	−0.194937	0.000000
H	2.705220	0.971054	0.894707

SI-5*
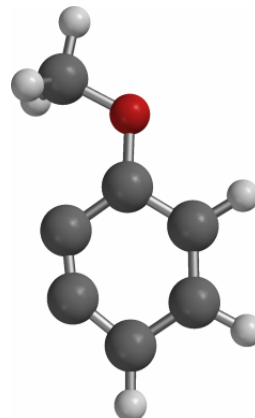
H	−0.279144	−2.243871	0.000000
C	−0.560704	−1.194627	0.000000
C	−1.220427	1.310456	0.000000
C	0.473728	−0.226055	0.000000
C	−1.912589	−0.830830	0.000000
C	−2.343404	0.520072	0.000000
C	0.014839	1.093266	0.000000
H	−2.667498	−1.614583	0.000000
H	−3.383608	0.820240	0.000000
O	1.759860	−0.642419	0.000000
C	2.744737	0.386160	0.000000
H	2.651629	1.016573	−0.892610
H	3.711716	−0.119566	0.000000

H   2.651629   1.016573   0.892610

SI-6
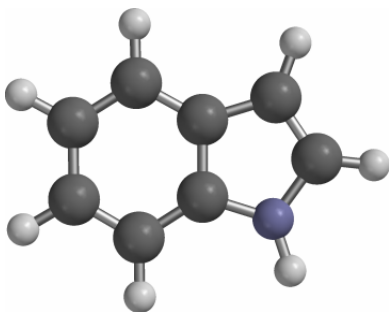
H	−1.016054	−2.513274	0.000000
C	−0.985787	−1.426483	0.000000
C	−0.934480	1.420966	0.000000
C	0.247658	−0.751135	0.000000
C	−2.161696	−0.687735	0.000000
C	−2.136209	0.722456	0.000000
C	0.247797	0.672737	0.000000
H	−3.119466	−1.201144	0.000000
H	−3.072698	1.273637	0.000000
H	−0.916247	2.508033	0.000000
C	1.622707	−1.168675	0.000000
H	1.993539	−2.184640	0.000000
C	2.388865	−0.033424	0.000000
H	3.463985	0.082184	0.000000
N	1.567169	1.079268	0.000000
H	1.883789	2.036046	0.000000

SI-8*
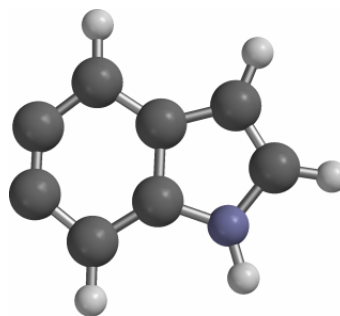
H	−1.137958	−2.575893	0.000000
C	−1.099803	−1.491332	0.000000
C	−1.059455	1.475166	−0.000000
C	0.121887	−0.760476	0.000000
C	−2.156485	−0.611040	−0.000000
C	−2.161208	0.644711	−0.000000
C	0.116248	0.682985	−0.000000
H	−1.046542	2.561466	−0.000000
C	1.501365	−1.165227	0.000000
H	1.876684	−2.179267	0.000000
C	2.262569	−0.027547	0.000000
H	3.337696	0.090979	0.000000
N	1.437982	1.082782	0.000000
H	1.753550	2.039798	−0.000000

SI-9*
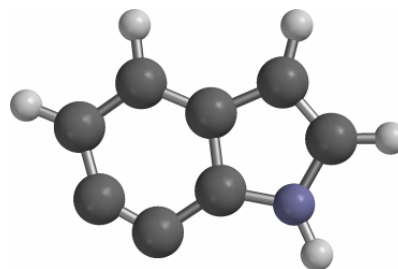
H	−1.257405	−2.341034	0.000000
C	−1.166698	−1.257261	0.000000
C	−0.934782	1.505611	0.000000
C	0.116526	−0.660828	0.000000
C	−2.340641	−0.483505	0.000000
C	−2.008758	0.864042	0.000000
C	0.250204	0.773065	0.000000
H	−3.332302	−0.919301	0.000000
C	1.456396	−1.181163	0.000000
H	1.749941	−2.222165	0.000000
C	2.314449	−0.112211	0.000000
H	3.395239	−0.089322	0.000000
N	1.591861	1.068688	0.000000
H	1.981978	1.998035	0.000000

SI-7*
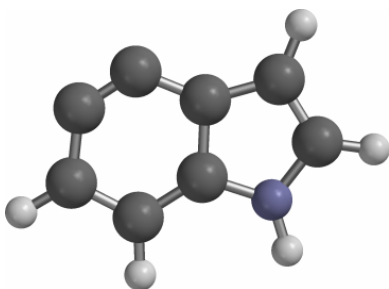
C	−0.999055	−1.465025	0.000000
C	−1.119874	1.247945	0.000000
C	0.260615	−0.864366	0.000000
C	−2.084933	−0.852996	0.000000
C	−2.322232	0.523128	0.000000
C	0.119028	0.572630	0.000000
H	−3.288928	1.014761	0.000000
H	−1.149899	2.335151	0.000000
C	1.656839	−1.161591	0.000000
H	2.117196	−2.139101	0.000000
C	2.315393	0.043591	0.000000
H	3.376305	0.251677	0.000000
N	1.403907	1.080172	0.000000
H	1.645458	2.058821	0.000000

SI-10
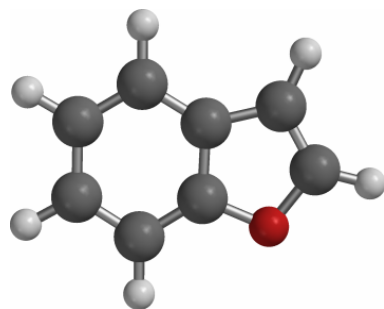
H	−0.876074	−2.499235	0.000000
C	−0.911963	−1.414616	0.000000
C	−0.964783	1.440415	0.000000
C	0.249954	−0.651998	0.000000
C	−2.115688	−0.711741	0.000000
C	−2.140674	0.695892	0.000000
C	0.260367	0.755890	0.000000
H	−3.052220	−1.262374	0.000000
H	−3.098727	1.208605	0.000000
H	−0.995211	2.526662	0.000000
C	1.655982	1.127045	0.000000
H	2.074639	2.124094	0.000000
C	2.352486	−0.035617	0.000000
H	3.410051	−0.254982	0.000000
O	1.531489	−1.137232	0.000000

SI-12*
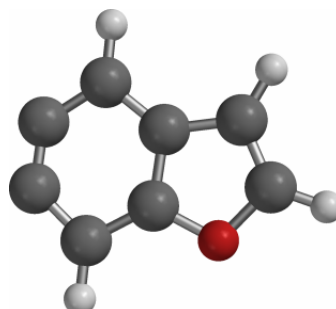
H	−1.144718	−2.576332	0.000000
C	−1.095012	−1.492582	0.000000
C	−1.024714	1.481654	0.000000
C	0.122798	−0.765101	0.000000
C	−2.147046	−0.599424	0.000000
C	−2.132468	0.654411	0.000000
C	0.121751	0.663860	0.000000
H	−0.984070	2.565320	0.000000
C	1.518551	−1.135662	0.000000
H	1.932272	−2.134492	0.000000
C	2.222251	0.022271	0.000000
H	3.281470	0.234667	0.000000
O	1.409150	1.128841	0.000000

SI-13*

H	−1.244032	−2.349703	0.000000
C	−1.146057	−1.267136	0.000000
C	−0.897150	1.507194	0.000000
C	0.132354	−0.667956	0.000000
C	−2.314896	−0.479834	0.000000
C	−1.970403	0.859538	0.000000
C	0.261696	0.750725	0.000000
H	−3.310305	−0.906649	0.000000
C	1.491013	−1.156215	0.000000
H	1.824751	−2.184811	0.000000
C	2.289830	−0.059774	0.000000
H	3.362682	0.062330	0.000000
O	1.574915	1.114169	0.000000

SI-11*

C	−0.984044	−1.484390	0.000000
C	−1.101388	1.244675	0.000000
C	0.265578	−0.865982	0.000000
C	−2.060443	−0.852761	0.000000
C	−2.306077	0.518698	0.000000
C	0.119361	0.551482	0.000000
H	−3.274453	1.006061	0.000000
H	−1.109049	2.330292	0.000000
C	1.679376	−1.120323	0.000000
H	2.182058	−2.076646	0.000000
C	2.268934	0.103456	0.000000
H	3.303505	0.413185	0.000000
O	1.360126	1.130814	0.000000

SI-14
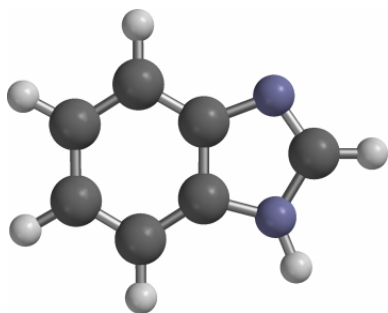
C	−0.274193	−0.720132	0.000000
C	−0.256889	0.696219	0.000000
N	−1.582746	−1.191123	0.000000
C	−2.321586	−0.112562	0.000000
H	−3.404715	−0.098727	0.000000
N	−1.593957	1.056711	0.000000
H	−1.968205	1.993733	0.000000
C	0.934003	−1.429087	0.000000
H	0.928841	−2.514731	0.000000
C	2.119952	−0.702661	0.000000
H	3.070597	−1.228630	0.000000
C	2.117529	0.707435	0.000000
H	3.064321	1.240380	0.000000
C	0.929427	1.433446	0.000000
H	0.931990	2.520063	0.000000

SI-15

C	−0.935530	−1.485329	0.000000
C	−1.103408	1.257746	0.000000
C	0.297977	−0.833243	0.000000
C	−2.016687	−0.860778	0.000000
C	−2.290806	0.503571	0.000000
C	0.137687	0.594206	0.000000
H	−3.268660	0.971694	0.000000
H	−1.155775	2.343429	0.000000
N	1.441586	1.062248	0.000000
H	1.739439	2.026739	0.000000
C	2.267467	−0.036986	0.000000
H	3.344690	0.071969	0.000000
N	1.629130	−1.182087	0.000000

SI-16

H	−1.063894	−2.574431	0.000000
C	−1.053603	−1.490434	0.000000
C	−1.040279	1.491372	0.000000
C	0.148314	−0.735075	0.000000
C	−2.113798	−0.612857	0.000000
C	−2.131938	0.641939	0.000000
C	0.132259	0.703385	0.000000
H	−1.044562	2.577203	0.000000
N	1.474061	1.046579	0.000000
H	1.854476	1.981178	0.000000
C	2.196808	−0.125230	0.000000
H	3.280265	−0.115310	0.000000
N	1.454527	−1.200682	0.000000

SI-17
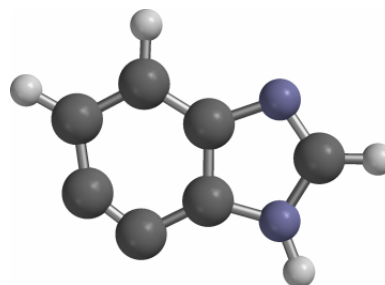
H	−1.174415	−2.358845	0.000000
C	−1.117038	−1.274398	0.000000
C	−0.921662	1.507547	0.000000
C	0.148779	−0.646299	0.000000
C	−2.297755	−0.511987	0.000000
C	−1.980782	0.839198	0.000000
C	0.262937	0.778951	0.000000
H	−3.286090	−0.955088	0.000000
N	1.620518	1.027903	0.000000
H	2.066661	1.933131	0.000000
C	2.242880	−0.201132	0.000000
H	3.322728	−0.282104	0.000000
N	1.415004	−1.215215	0.000000

SI-18
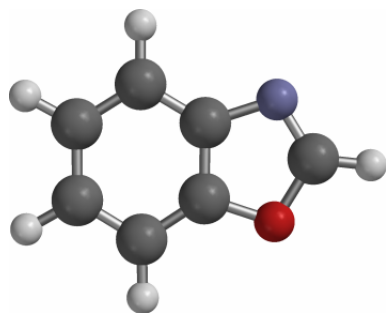
H	−0.933123	−2.522706	0.000000
C	−0.926882	−1.437477	0.000000
C	−0.896639	1.434753	0.000000
C	0.276878	−0.728234	0.000000
C	−2.106531	−0.694794	0.000000
C	−2.092383	0.712815	0.000000
C	0.262349	0.672766	0.000000
H	−3.061802	−1.211816	0.000000
H	−3.035041	1.252624	0.000000
H	−0.873782	2.519250	0.000000
O	1.570134	1.099402	0.000000
C	2.287097	−0.068213	0.000000
H	3.362444	0.044815	0.000000
N	1.607511	−1.164251	0.000000

SI-20
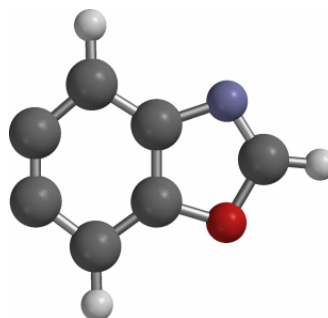
H	−1.070857	−2.579363	0.000000
C	−1.050854	−1.495750	0.000000
C	−1.015329	1.495396	0.000000
C	0.143676	−0.739305	0.000000
C	−2.109478	−0.608703	0.000000
C	−2.109099	0.644716	0.000000
C	0.130611	0.684533	0.000000
H	−0.997595	2.579320	0.000000
O	1.441851	1.094893	0.000000
C	2.155840	−0.074475	0.000000
H	3.231796	0.034897	0.000000
N	1.472395	−1.167275	0.000000

SI-19
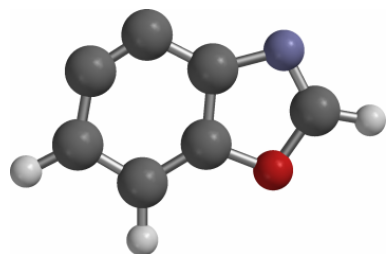
C	−0.921033	−1.489046	0.000000
C	−1.074132	1.270420	0.000000
C	0.302150	−0.824390	0.000000
C	−1.991360	−0.842926	0.000000
C	−2.266385	0.518823	0.000000
C	0.146513	0.584426	0.000000
H	−3.243735	0.987153	0.000000
H	−1.103065	2.355277	0.000000
O	1.413011	1.117992	0.000000
C	2.231781	0.019942	0.000000
H	3.292264	0.229395	0.000000
N	1.655589	−1.136273	0.000000

SI-21
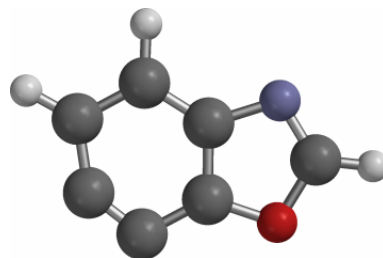
H	−1.162187	−2.364978	0.000000
C	−1.099292	−1.281145	0.000000
C	−0.891077	1.514507	0.000000
C	0.158555	−0.647048	0.000000
C	−2.276309	−0.506224	0.000000
C	−1.947769	0.837536	0.000000
C	0.268175	0.763451	0.000000
H	−3.268173	−0.940982	0.000000
O	1.602343	1.079580	0.000000
C	2.216961	−0.145380	0.000000
H	3.297846	−0.124398	0.000000
N	1.448873	−1.183301	0.000000

SI-22
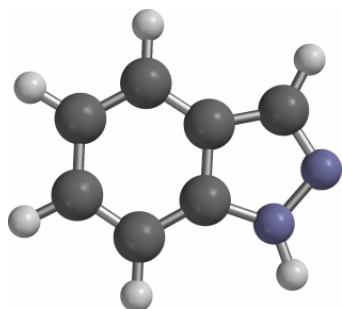

```
H    -0.999303    -2.519540     0.000000
C    -0.973118    -1.433152     0.000000
C    -0.926134     1.426835     0.000000
C     0.254464    -0.744808     0.000000
C    -2.145529    -0.695014     0.000000
C    -2.118729     0.720014     0.000000
C     0.259450     0.674257     0.000000
H    -3.104670    -1.204949     0.000000
H    -3.058300     1.265971     0.000000
H    -0.912681     2.513073     0.000000
C     1.638698    -1.101084     0.000000
H     2.081609    -2.088683     0.000000
N     2.418863    -0.034746     0.000000
N     1.578649     1.035284     0.000000
H     1.976291     1.961543     0.000000
```

SI-24
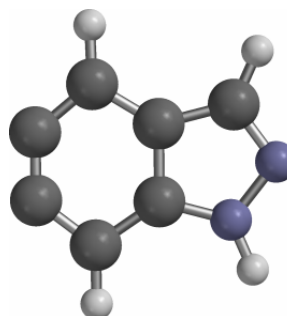

```
H    -1.139314    -2.572536     0.000000
C    -1.098367    -1.488268     0.000000
C    -1.044230     1.488055     0.000000
C     0.123362    -0.753535     0.000000
C    -2.148628    -0.604734     0.000000
C    -2.136389     0.652820     0.000000
C     0.131592     0.684109     0.000000
H    -1.031198     2.573350     0.000000
N     1.454723     1.030731     0.000000
H     1.856791     1.955007     0.000000
N     2.291588    -0.041948     0.000000
C     1.508766    -1.105906     0.000000
H     1.949766    -2.094210     0.000000
```

SI-23
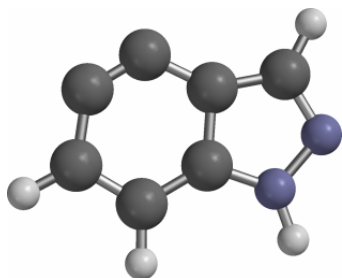

```
C    -0.975395    -1.478955     0.000000
C    -1.116485     1.252269     0.000000
C     0.273281    -0.851378     0.000000
C    -2.057795    -0.863846     0.000000
C    -2.305383     0.512689     0.000000
C     0.130562     0.580745     0.000000
H    -3.277569     0.993179     0.000000
H    -1.158872     2.338154     0.000000
C     1.675822    -1.078329     0.000000
H     2.212297    -2.017242     0.000000
N     2.346275     0.064014     0.000000
N     1.413935     1.051045     0.000000
H     1.732450     2.007862     0.000000
```

SI-25
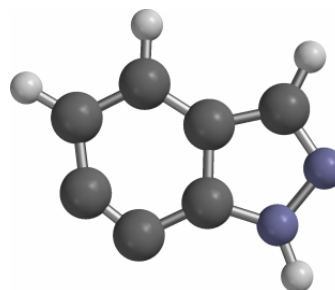

```
H    -1.249819    -2.345974     0.000000
C    -1.158061    -1.262722     0.000000
C    -0.917883     1.510424     0.000000
C     0.124125    -0.660191     0.000000
C    -2.324651    -0.485174     0.000000
C    -1.986991     0.865228     0.000000
C     0.266774     0.768369     0.000000
H    -3.318843    -0.914363     0.000000
N     1.605219     1.014635     0.000000
H     2.078659     1.904912     0.000000
N     2.344156    -0.128272     0.000000
C     1.473983    -1.125317     0.000000
H     1.838605    -2.144678     0.000000
```

SI-26
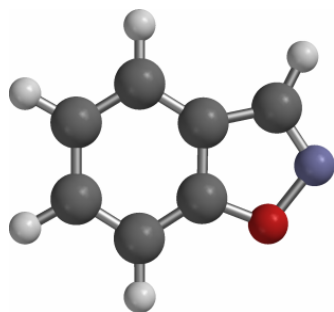
H	−0.999503	−2.531250	0.000000
C	−0.968355	−1.445592	0.000000
C	−0.897814	1.419067	0.000000
C	0.253405	−0.753862	0.000000
C	−2.136708	−0.695311	0.000000
C	−2.098263	0.716209	0.000000
C	0.265213	0.647388	0.000000
H	−3.099479	−1.197638	0.000000
H	−3.033458	1.269149	0.000000
H	−0.860841	2.502956	0.000000
O	1.542655	1.098898	0.000000
N	2.408238	−0.017411	0.000000
C	1.649712	−1.080069	0.000000
H	2.121958	−2.055212	0.000000

SI-28
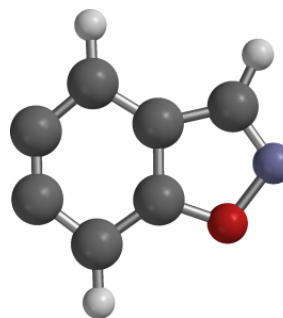
C	2.112681	−0.626035	0.000000
C	2.124611	0.629725	0.000000
C	1.063475	1.506844	0.000000
H	1.095336	2.591010	0.000000
C	−0.140308	0.753110	0.000000
C	−0.136262	−0.667031	0.000000
C	1.026059	−1.474220	0.000000
H	1.002588	−2.557618	0.000000
O	−1.411693	−1.123029	0.000000
N	−2.289029	−0.016441	0.000000
C	−1.541890	1.054319	0.000000
H	−2.027341	2.022707	0.000000

SI-27
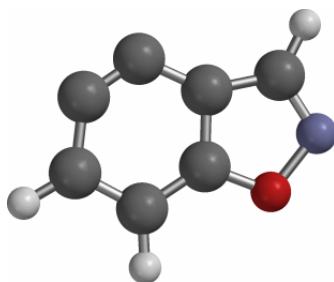
H	3.254364	−0.988418	0.000000
C	2.280028	−0.513092	0.000000
C	−0.283332	0.838389	0.000000
C	1.089275	−1.256422	0.000000
C	2.022273	0.856927	0.000000
C	0.949352	1.492414	0.000000
C	−0.143235	−0.572259	0.000000
H	1.113686	−2.341185	0.000000
O	−1.372350	−1.136815	0.000000
N	−2.342934	−0.109623	0.000000
C	−1.698993	1.028093	0.000000
H	−2.267028	1.949588	0.000000

SI-29
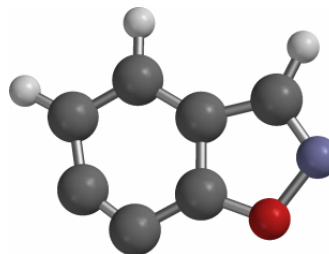
C	1.961199	−0.833422	0.000000
C	−0.145042	0.664513	0.000000
C	0.898309	−1.493065	0.000000
C	2.295087	0.513029	0.000000
C	1.122788	1.288073	0.000000
C	−0.273957	−0.747286	0.000000
H	3.287296	0.946399	0.000000
H	1.205457	2.371546	0.000000
O	−1.573944	−1.101292	0.000000
N	−2.349513	0.081139	0.000000
C	−1.513360	1.086355	0.000000
H	−1.920033	2.090693	0.000000

SI-30
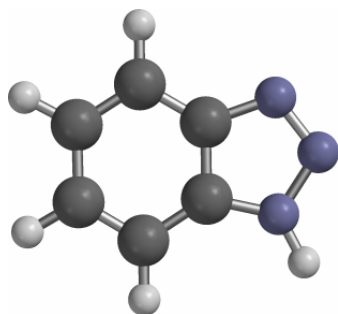
H	−0.936129	−2.514189	0.000000
C	−0.936883	−1.428955	0.000000
C	−0.911917	1.445163	0.000000
C	0.272326	−0.715167	0.000000
C	−2.111653	−0.694094	0.000000
C	−2.096085	0.722163	0.000000
C	0.273445	0.695456	0.000000
H	−3.068211	−1.208399	0.000000
H	−3.041316	1.257887	0.000000
H	−0.909411	2.530831	0.000000
N	1.580122	−1.160660	0.000000
N	2.365426	−0.135220	0.000000
N	1.604321	0.998129	0.000000
H	2.067931	1.894848	0.000000

SI-32*
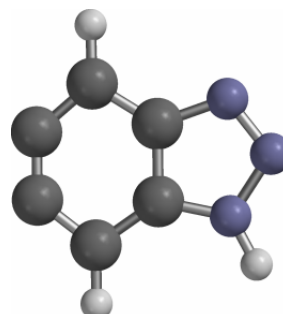
C	2.111054	−0.657535	0.000000
C	−0.140580	0.726025	0.000000
C	1.027571	−1.507014	0.000000
C	2.115777	0.600063	0.000000
C	1.065897	1.483101	0.000000
C	−0.145104	−0.705099	0.000000
H	1.026985	−2.591785	0.000000
H	1.081753	2.566853	0.000000
N	−1.479626	−0.990074	0.000000
H	−1.949564	−1.883508	0.000000
N	−2.235856	0.147012	0.000000
N	−1.444734	1.168288	0.000000

SI-31*
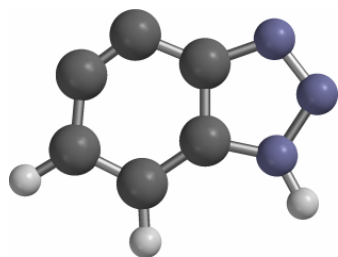
H	3.246004	−0.990687	0.000000
C	2.267555	−0.524056	0.000000
C	−0.303016	0.812434	0.000000
C	1.087424	−1.280382	0.000000
C	1.997465	0.845170	0.000000
C	0.924923	1.479359	0.000000
C	−0.157550	−0.610908	0.000000
H	1.142002	−2.365071	0.000000
N	−1.455634	−1.026632	0.000000
H	−1.841442	−1.960010	0.000000
N	−2.318159	0.030173	0.000000
N	−1.635252	1.130937	0.000000

SI-33*
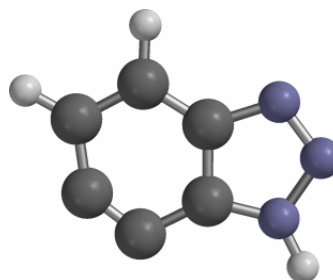
C	1.960354	−0.853015	0.000000
C	−0.152171	0.637795	0.000000
C	0.903190	−1.518541	0.000000
C	2.285749	0.501842	0.000000
C	1.115547	1.270513	0.000000
C	−0.281550	−0.780817	0.000000
H	3.277641	0.936236	0.000000
H	1.176123	2.354495	0.000000
N	−1.627314	−0.974688	0.000000
H	−2.161204	−1.831811	0.000000
N	−2.287774	0.220885	0.000000
N	−1.418394	1.180748	0.000000

SI-34
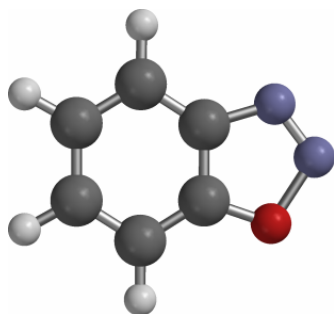
H	−0.905502	−2.525113	0.000000
C	−0.914277	−1.440423	0.000000
C	−0.893226	1.437103	0.000000
C	0.277618	−0.708839	0.000000
C	−2.093870	−0.707271	0.000000
C	−2.077047	0.705796	0.000000
C	0.288306	0.691327	0.000000
H	−3.048659	−1.223899	0.000000
H	−3.022850	1.240363	0.000000
H	−0.882883	2.521104	0.000000
N	1.605206	−1.114851	0.000000
N	2.373414	−0.134781	0.000000
O	1.559592	1.109484	0.000000

SI-36
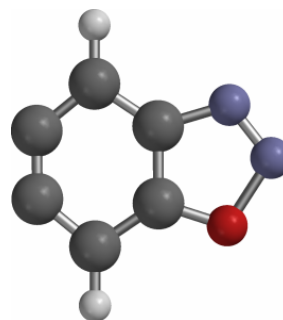
C	2.080315	−0.624393	0.000000
C	2.096422	0.631131	0.000000
C	1.028931	1.500466	0.000000
H	1.031549	2.584350	0.000000
C	−0.154132	0.720348	0.000000
C	−0.161472	−0.702672	0.000000
C	1.010689	−1.494637	0.000000
H	1.009987	−2.577787	0.000000
N	−1.478640	1.113308	0.000000
N	−2.250173	0.136266	0.000000
O	−1.433910	−1.111030	0.000000

SI-35
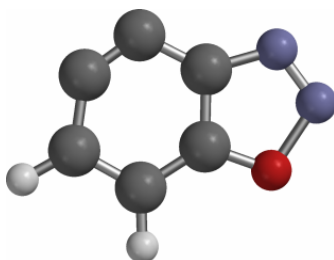
C	−0.886904	−1.518760	0.000000
C	−1.086328	1.264110	0.000000
C	0.304950	−0.800420	0.000000
C	−1.954175	−0.869713	0.000000
C	−2.256351	0.486295	0.000000
C	0.164735	0.612466	0.000000
H	−3.244213	0.932016	0.000000
H	−1.143562	2.347220	0.000000
N	1.660910	−1.069062	0.000000
N	2.329630	−0.023048	0.000000
O	1.380376	1.153982	0.000000

SI-37
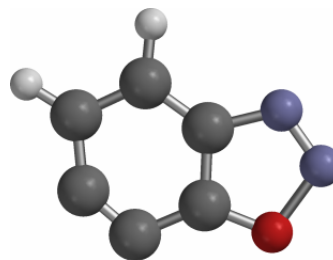
H	−1.156787	−2.354485	0.000000
C	−1.100883	−1.270490	0.000000
C	−0.876032	1.513961	0.000000
C	0.154521	−0.625707	0.000000
C	−2.271272	−0.497698	0.000000
C	−1.936153	0.851632	0.000000
C	0.307259	0.783458	0.000000
H	−3.264527	−0.928323	0.000000
N	1.436030	−1.146131	0.000000
N	2.296597	−0.247045	0.000000
O	1.600420	1.086861	0.000000

SI-38
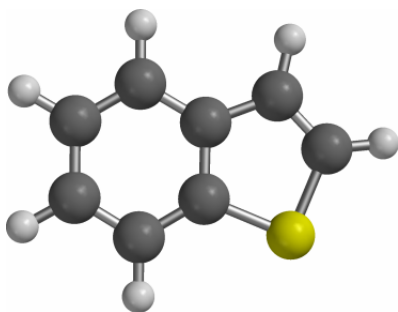
H	−0.899493	−2.505831	0.000000
C	−1.037730	−1.428432	0.000000
C	−1.403072	1.376939	0.000000
C	0.061047	−0.563518	0.000000
C	−2.313621	−0.875370	0.000000
C	−2.494585	0.519883	0.000000
C	−0.100360	0.844853	0.000000
H	−3.180588	−1.530295	0.000000
H	−3.501230	0.928780	0.000000
H	−1.546493	2.454484	0.000000
C	1.166869	1.531402	0.000000
H	1.262214	2.612224	0.000000
C	2.228432	0.685436	0.000000
H	3.279705	0.942647	0.000000
S	1.763672	−1.003957	0.000000

SI-40
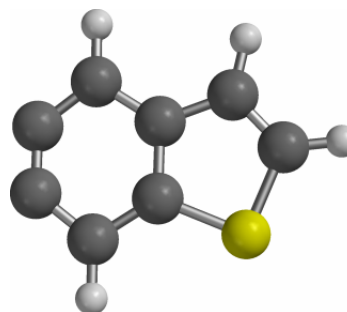
H	−1.753502	−2.450830	0.000000
C	−1.569734	−1.381101	0.000000
C	−1.097197	1.533036	0.000000
C	−0.253135	−0.835598	0.000000
C	−2.499716	−0.368148	0.000000
C	−2.305943	0.871319	0.000000
C	−0.045535	0.584193	0.000000
H	−0.927170	2.604849	0.000000
S	1.675566	0.960362	0.000000
C	2.085329	−0.743813	0.000000
H	3.128078	−1.034963	0.000000
C	0.997540	−1.554113	0.000000
H	1.058263	−2.637263	0.000000

SI-41

H	−1.792994	−2.254537	0.000000
C	−1.581148	−1.187757	0.000000
C	−1.023267	1.480767	0.000000
C	−0.231910	−0.753280	0.000000
C	−2.657970	−0.285806	0.000000
C	−2.183487	1.018397	0.000000
C	0.084472	0.648413	0.000000
H	−3.692584	−0.608409	0.000000
S	1.813658	0.926812	0.000000
C	2.107328	−0.800997	0.000000
H	3.128753	−1.158956	0.000000
C	0.971373	−1.546444	0.000000
H	0.973932	−2.631337	0.000000

SI-39
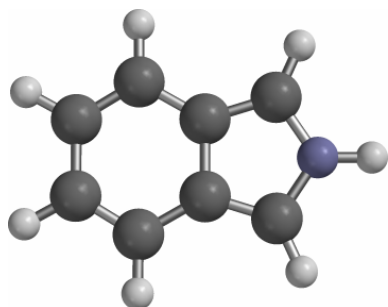
C	−1.442077	−1.403698	0.000000
C	−1.211176	1.284790	0.000000
C	−0.115006	−0.975945	0.000000
C	−2.443392	−0.661077	0.000000
C	−2.502992	0.730041	0.000000
C	−0.066122	0.461571	0.000000
H	−3.395649	1.345546	0.000000
H	−1.098656	2.366030	0.000000
S	1.608343	0.996988	0.000000
C	2.182454	−0.655847	0.000000
H	3.249219	−0.838378	0.000000
C	1.184831	−1.579812	0.000000
H	1.350836	−2.650620	0.000000

SI-42

C	0.714999	0.000000	2.153016
H	1.238782	0.000000	3.105450
C	1.430766	0.000000	0.980872
H	2.518142	0.000000	0.992527
C	-0.714999	0.000000	2.153016
H	-1.238782	0.000000	3.105450
C	-1.430766	0.000000	0.980872
H	-2.518142	0.000000	0.992527
C	0.726058	0.000000	-0.255083
C	-0.726058	0.000000	-0.255083
C	1.134924	0.000000	-1.587443
H	2.117187	0.000000	-2.036008
C	-1.134924	0.000000	-1.587443
H	-2.117187	0.000000	-2.036008
N	0.000000	0.000000	-2.354387
H	0.000000	0.000000	-3.363930

SI-44
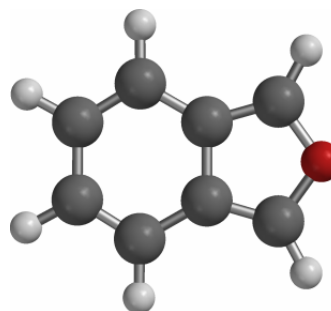
C	-1.437862	0.000000	0.981922
H	-2.524388	0.000000	0.993307
C	-0.719051	0.000000	2.146076
H	-1.238232	0.000000	3.100707
C	0.719051	0.000000	2.146076
H	1.238232	0.000000	3.100707
C	1.437862	0.000000	0.981922
H	2.524388	0.000000	0.993307
C	0.727608	0.000000	-0.258078
C	-0.727608	0.000000	-0.258078
C	-1.103412	0.000000	-1.581820
H	-2.052316	0.000000	-2.094975
C	1.103412	0.000000	-1.581820
H	2.052316	0.000000	-2.094975
O	0.000000	0.000000	-2.373275

SI-43
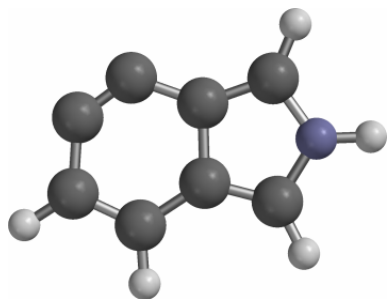
C	-0.987781	-1.455736	0.000000
C	-2.070407	-0.851822	0.000000
C	-2.333624	0.535957	0.000000
H	-3.312355	1.002831	0.000000
C	-1.158667	1.274216	0.000000
H	-1.217946	2.360398	0.000000
C	0.127893	0.644704	0.000000
C	0.271838	-0.825035	0.000000
C	1.626709	-1.116069	0.000000
H	2.160843	-2.053482	0.000000
C	1.425233	1.152611	0.000000
H	1.795303	2.167469	0.000000
N	2.285838	0.088489	0.000000
H	3.291301	0.178124	0.000000

SI-45
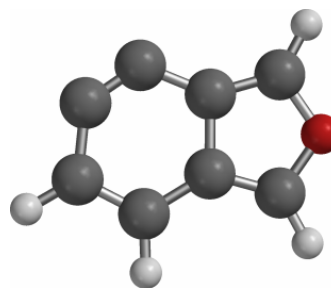
C	1.148545	-1.278632	0.000000
H	1.211275	-2.363931	0.000000
C	2.313730	-0.534985	0.000000
H	3.295453	-0.994617	0.000000
C	2.043174	0.856214	0.000000
C	0.968509	1.469001	0.000000
C	-0.290919	0.826503	0.000000
C	-0.144496	-0.647293	0.000000
C	-1.635862	1.083434	0.000000
H	-2.234415	1.979996	0.000000
C	-1.433876	-1.124356	0.000000
H	-1.869391	-2.111880	0.000000
O	-2.317760	-0.094660	0.000000

SI-46
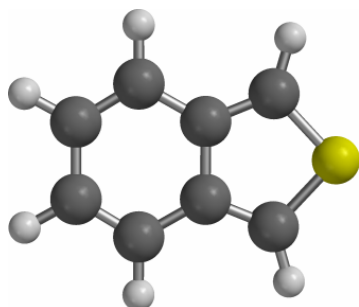
C	−1.426903	0.000000	1.306048
H	−2.513713	0.000000	1.311467
C	−0.716954	0.000000	2.475314
H	−1.241222	0.000000	3.427216
C	0.716954	0.000000	2.475314
H	1.241222	0.000000	3.427216
C	1.426903	0.000000	1.306048
H	2.513713	0.000000	1.311467
C	−0.727176	0.000000	0.056999
C	0.727176	0.000000	0.056999
C	1.248444	0.000000	−1.226762
H	2.287221	0.000000	−1.527599
C	−1.248444	0.000000	−1.226762
H	−2.287221	0.000000	−1.527599
S	0.000000	0.000000	−2.407968

SI-47

C	1.467868	1.278860	0.000000
H	1.502876	2.365699	0.000000
C	2.650536	0.565431	0.000000
H	3.622468	1.045699	0.000000
C	2.406260	−0.828826	0.000000
C	1.336829	−1.449816	0.000000
C	0.056152	−0.844600	0.000000
C	0.177322	0.632288	0.000000
C	−1.251931	−1.276419	0.000000
H	−1.624650	−2.290627	0.000000
C	−1.072572	1.225912	0.000000
H	−1.312627	2.280577	0.000000
S	−2.338359	0.060563	0.000000

SI-48

H	2.572660	−2.153310	0.000000
C	2.159369	−1.148150	0.000000
C	1.095469	1.472599	0.000000
C	0.779400	−0.951912	0.000000
C	3.004363	−0.031581	0.000000
C	2.482444	1.263916	0.000000
C	0.278474	0.356931	0.000000
H	4.080921	−0.176051	0.000000
H	3.153379	2.117899	0.000000
H	0.678631	2.475128	0.000000
C	−0.284734	−1.973525	0.000000
H	−0.050258	−3.034000	0.000000
C	−1.531543	−1.487306	0.000000
H	−2.476553	−2.014479	0.000000
S	−1.524537	0.310849	0.000000
O	−2.059964	0.825665	−1.268547
O	−2.059964	0.825665	1.268547

SI-49

C	2.181325	−1.165656	0.000000
C	1.265635	1.375674	0.000000
C	0.801104	−1.071327	0.000000
C	2.956528	−0.180711	0.000000
C	2.671926	1.169276	0.000000
C	0.395623	0.288676	0.000000
H	3.375642	1.993608	0.000000
H	0.876561	2.390250	0.000000
S	−1.412121	0.336804	0.000000
O	−1.918560	0.875503	1.269398
O	−1.918560	0.875503	−1.269398
C	−1.523451	−1.459105	0.000000
H	−2.501051	−1.923758	0.000000
C	−0.312448	−2.030016	0.000000
H	−0.142551	−3.101493	0.000000

SI-50
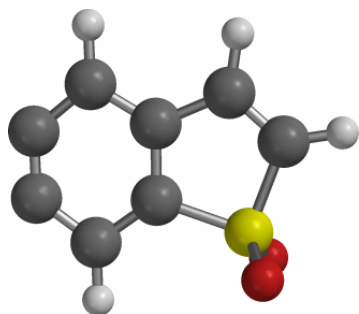

```
S    -1.433466     0.277308     0.000000
O    -1.985238     0.770032    -1.269179
O    -1.985238     0.770032     1.269179
C    -1.359252    -1.516677     0.000000
H    -2.277888    -2.089407     0.000000
C    -0.090427    -1.944448     0.000000
H     0.188155    -2.994170     0.000000
C     0.935574    -0.884484     0.000000
C     2.456916     1.288218     0.000000
C     0.372510     0.413964     0.000000
C     2.335372    -1.074424     0.000000
C     2.979924     0.152857     0.000000
C     1.105046     1.605938     0.000000
H     2.791932    -2.059096     0.000000
H     0.649663     2.590115     0.000000
```

SI-52
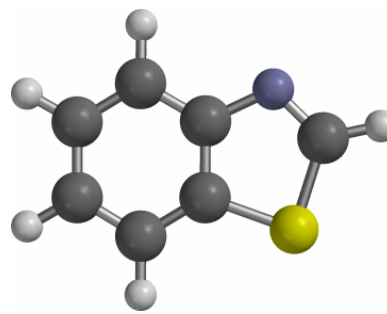

```
H    -1.489381    -2.454492     0.000000
C    -1.373124    -1.375369     0.000000
C    -1.023525     1.441413     0.000000
C    -0.082921    -0.825308     0.000000
C    -2.468176    -0.521130     0.000000
C    -2.294780     0.874581     0.000000
C     0.078276     0.581963     0.000000
H    -3.472903    -0.934073     0.000000
H    -3.166380     1.523227     0.000000
H    -0.895658     2.519553     0.000000
S     1.789875     0.965111     0.000000
C     2.118829    -0.772856     0.000000
H     3.146868    -1.119380     0.000000
N     1.096359    -1.560254     0.000000
```

SI-51
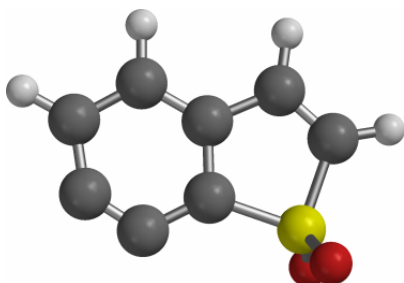

```
H     2.719526    -1.947495     0.000000
C     2.276825    -0.954543     0.000000
C     1.151898     1.519672     0.000000
C     0.879419    -0.815840     0.000000
C     3.134414     0.174593     0.000000
C     2.392648     1.334900     0.000000
C     0.274620     0.466220     0.000000
H     4.214449     0.083342     0.000000
S    -1.526524     0.306888     0.000000
O    -2.090788     0.779816     1.270506
O    -2.090788     0.779816    -1.270506
C    -1.401645    -1.487939     0.000000
H    -2.308001    -2.079622     0.000000
C    -0.126768    -1.897031     0.000000
H     0.166429    -2.942831     0.000000
```

SI-53
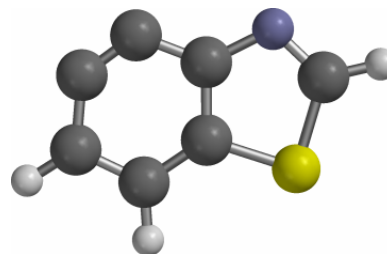

```
C    -1.373162    -1.430147     0.000000
C    -1.203575     1.290227     0.000000
C    -0.066255    -0.947902     0.000000
C    -2.374265    -0.684821     0.000000
C    -2.480613     0.699153     0.000000
C    -0.044380     0.490272     0.000000
H    -3.390888     1.287663     0.000000
H    -1.119535     2.373588     0.000000
S     1.631356     1.006437     0.000000
C     2.108835    -0.693714     0.000000
H     3.163239    -0.947552     0.000000
N     1.161034    -1.573230     0.000000
```

SI-54
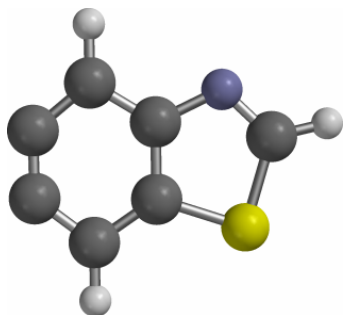

```
H    -1.652665    -2.480422     0.000000
C    -1.512542    -1.405482     0.000000
C    -1.101969     1.529547     0.000000
C    -0.216749    -0.821647     0.000000
C    -2.461639    -0.409606     0.000000
C    -2.293591     0.832776     0.000000
C    -0.034195     0.604210     0.000000
H    -0.963925     2.605446     0.000000
S     1.687474     0.949683     0.000000
C     1.989392    -0.793223     0.000000
H     3.012237    -1.155654     0.000000
N     0.954847    -1.563219     0.000000
```

SI-56
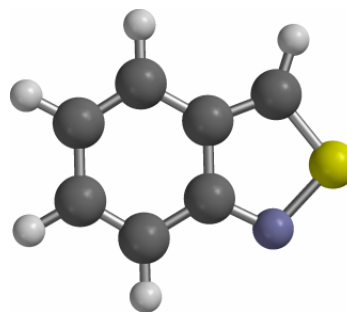

```
C     1.266471    -1.417250     0.000000
H     1.246032    -2.502213     0.000000
C     2.439502    -0.710333     0.000000
H     3.387446    -1.241723     0.000000
C     2.455180     0.722932     0.000000
H     3.412705     1.236309     0.000000
C     1.292829     1.447019     0.000000
H     1.307355     2.533396     0.000000
C     0.045558     0.750798     0.000000
C     0.030125    -0.699819     0.000000
N    -1.172303    -1.287324     0.000000
S    -2.331232    -0.097969     0.000000
C    -1.257338     1.229012     0.000000
H    -1.598580     2.256457     0.000000
```

SI-55
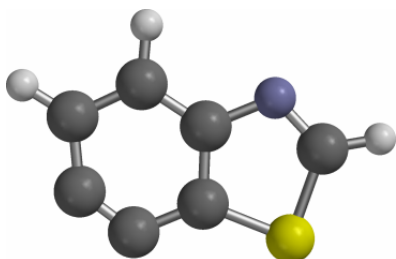

```
H    -1.709902    -2.247667     0.000000
C    -1.534154    -1.176145     0.000000
C    -1.002752     1.511027     0.000000
C    -0.195345    -0.714750     0.000000
C    -2.618245    -0.285176     0.000000
C    -2.152966     1.022423     0.000000
C     0.109509     0.687463     0.000000
H    -3.650766    -0.613799     0.000000
S     1.845531     0.918008     0.000000
C     2.007318    -0.843667     0.000000
H     2.998817    -1.283732     0.000000
N     0.918546    -1.539326     0.000000
```

SI-57
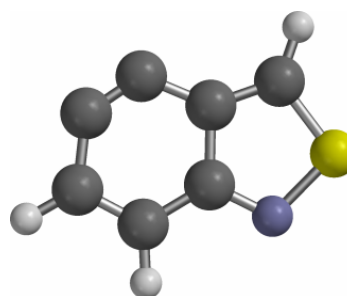

```
C     2.630099     0.514878     0.000000
H     3.608812     0.981611     0.000000
C     1.457615     1.242615     0.000000
H     1.480929     2.327943     0.000000
C     2.374224    -0.878063     0.000000
C     1.302687    -1.496916     0.000000
C     0.163402     0.599029     0.000000
C     0.035171    -0.873165     0.000000
N    -0.987898     1.271898     0.000000
C    -1.296228    -1.237919     0.000000
H    -1.724773    -2.231109     0.000000
S    -2.246535     0.184546     0.000000
```

SI-58
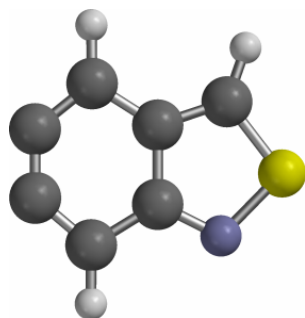
C	1.136110	−1.227667	0.000000
H	1.479949	−2.254170	0.000000
S	2.211691	0.097381	0.000000
N	1.058049	1.286591	0.000000
C	−0.170256	−0.759794	0.000000
C	−0.148462	0.714249	0.000000
C	−1.413163	−1.503676	0.000000
H	−1.444739	−2.588514	0.000000
C	−2.456852	−0.633652	0.000000
C	−2.430362	0.632052	0.000000
C	−1.380314	1.487800	0.000000
H	−1.367778	2.571568	0.000000

SI-59

C	2.634978	0.481423	0.000000
H	3.629668	0.911814	0.000000
C	1.486191	1.251144	0.000000
H	1.568129	2.335081	0.000000
C	2.316357	−0.893997	0.000000
C	1.231870	−1.491090	0.000000
C	0.176377	0.653719	0.000000
C	−0.014456	−0.814506	0.000000
C	−1.071343	1.254720	0.000000
H	−1.311717	2.310470	0.000000
N	−1.260727	−1.265828	0.000000
S	−2.283195	0.047886	0.000000

SI-60

H	−1.569175	−2.440009	0.000000
C	−1.418433	−1.363724	0.000000
C	−1.018942	1.447614	0.000000
C	−0.115571	−0.832955	0.000000
C	−2.497496	−0.493818	0.000000
C	−2.296047	0.901930	0.000000
C	0.072821	0.569082	0.000000
H	−3.510290	−0.886299	0.000000
H	−3.157464	1.564251	0.000000
H	−0.875590	2.524005	0.000000
S	1.790481	0.896219	0.000000
N	2.233064	−0.747947	0.000000
C	1.162915	−1.495627	0.000000
H	1.289931	−2.576277	0.000000

SI-61

C	2.510649	0.684893	0.000000
H	3.422828	1.270993	0.000000
C	1.239078	1.282643	0.000000
H	1.163627	2.366733	0.000000
C	2.408366	−0.703029	0.000000
C	1.398399	−1.433581	0.000000
C	0.090617	−0.944298	0.000000
C	0.069378	0.491304	0.000000
S	−1.605350	0.984083	0.000000
N	−2.220065	−0.599943	0.000000
C	−1.243273	−1.469040	0.000000
H	−1.487797	−2.527748	0.000000

SI-62
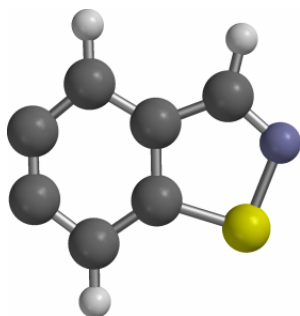
C	2.316456	−0.816487	0.000000
C	2.482104	0.428287	0.000000
C	1.525411	1.413436	0.000000
H	1.676199	2.488200	0.000000
C	0.228605	0.819782	0.000000
C	0.052314	−0.599791	0.000000
C	1.133438	−1.519931	0.000000
H	0.999975	−2.596442	0.000000
S	−1.667818	−0.933254	0.000000
N	−2.124588	0.708342	0.000000
C	−1.060289	1.463266	0.000000
H	−1.197296	2.542663	0.000000

SI-64
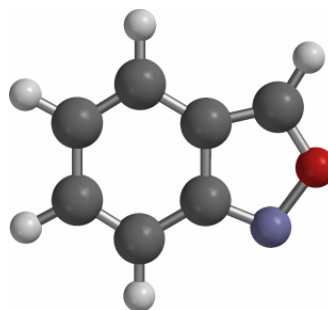
C	0.915939	−1.448130	0.000000
H	0.881874	−2.532527	0.000000
C	2.095275	−0.753723	0.000000
H	3.035763	−1.298092	0.000000
C	2.139907	0.683412	0.000000
H	3.109857	1.172239	0.000000
C	0.996852	1.436749	0.000000
H	1.035174	2.522073	0.000000
C	−0.252387	0.749948	0.000000
C	−0.295848	−0.691578	0.000000
N	−1.540988	−1.156530	0.000000
O	−2.337756	−0.009778	0.000000
C	−1.583038	1.095198	0.000000
H	−2.118116	2.033995	0.000000

SI-63
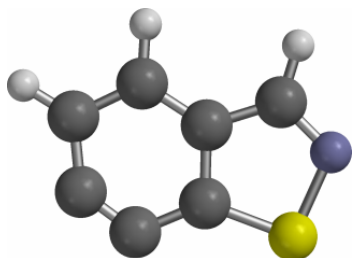
C	2.167467	1.008952	0.000000
C	1.018021	1.494558	0.000000
C	2.624966	−0.303850	0.000000
H	3.655184	−0.639263	0.000000
C	1.536715	−1.189551	0.000000
H	1.728220	−2.259920	0.000000
C	0.198203	−0.723497	0.000000
C	−0.105434	0.678266	0.000000
S	−1.833447	0.890537	0.000000
N	−2.154203	−0.780843	0.000000
C	−1.037379	−1.460180	0.000000
H	−1.102615	−2.546220	0.000000

SI-65
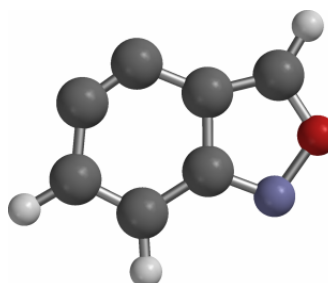
C	2.016840	0.897412	0.000000
C	0.942278	1.511429	0.000000
C	2.299192	−0.491126	0.000000
H	3.287065	−0.937731	0.000000
C	1.145825	−1.250662	0.000000
H	1.199508	−2.334726	0.000000
C	−0.299614	0.841301	0.000000
C	−0.148905	−0.615767	0.000000
C	−1.657358	1.019280	0.000000
H	−2.308206	1.880876	0.000000
N	−1.330066	−1.218184	0.000000
O	−2.261259	−0.178463	0.000000

SI-66
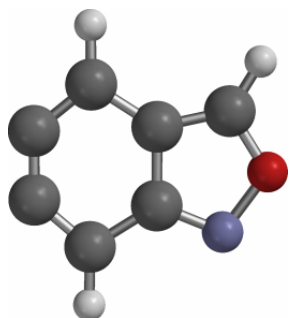
N	1.395181	−1.208174	0.000000
O	2.226340	−0.089651	0.000000
C	1.509660	1.040791	0.000000
H	2.078011	1.959680	0.000000
C	0.165816	0.749804	0.000000
C	0.163034	−0.711759	0.000000
C	−1.056417	1.526396	0.000000
H	−1.071552	2.611163	0.000000
C	−2.109296	0.668933	0.000000
C	−2.102103	−0.598928	0.000000
C	−1.072826	−1.479096	0.000000
H	−1.086124	−2.562632	0.000000

SI-68
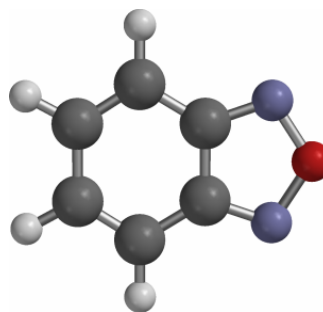
C	0.720345	0.000000	2.078185
H	1.232909	0.000000	3.035809
C	1.451187	0.000000	0.921510
H	2.535637	0.000000	0.916825
C	0.718347	0.000000	−0.302124
C	−0.718347	0.000000	−0.302124
C	−1.451187	0.000000	0.921510
H	−2.535637	0.000000	0.916825
C	−0.720345	0.000000	2.078185
H	−1.232909	0.000000	3.035809
N	1.143822	0.000000	−1.554690
N	−1.143822	0.000000	−1.554690
O	0.000000	0.000000	−2.306189

SI-67
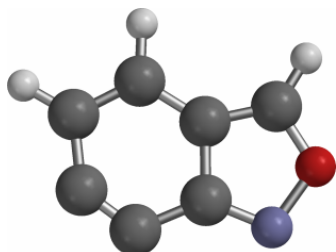
C	1.970199	0.892785	0.000000
C	0.890472	1.498075	0.000000
C	2.301380	−0.481945	0.000000
H	3.300005	−0.902086	0.000000
C	1.161444	−1.265809	0.000000
H	1.255600	−2.348317	0.000000
C	−0.335755	0.790221	0.000000
C	−0.141532	−0.663817	0.000000
N	−1.610604	1.136626	0.000000
C	−1.436710	−1.118801	0.000000
H	−1.891662	−2.099446	0.000000
O	−2.290193	−0.086468	0.000000

SI-69
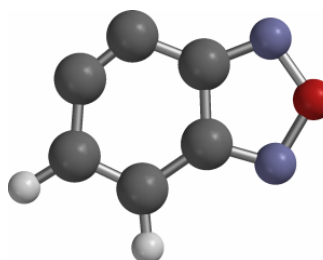
C	1.103863	−1.284942	0.000000
H	1.156735	−2.368694	0.000000
C	2.254403	−0.521853	0.000000
H	3.245348	−0.960128	0.000000
C	1.956689	0.862895	0.000000
C	0.898782	1.505208	0.000000
C	−0.333981	0.813808	0.000000
C	−0.182373	−0.638409	0.000000
N	−1.388548	−1.171286	0.000000
N	−1.614953	1.115742	0.000000
O	−2.247140	−0.101280	0.000000

SI-70
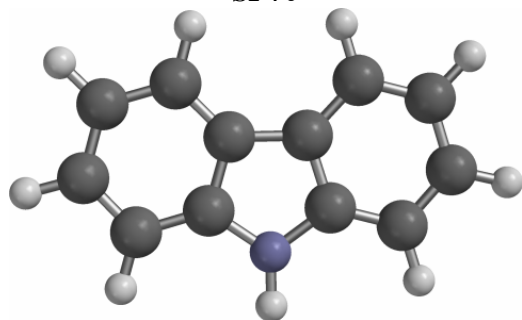
H	−1.406069	0.000000	2.558366
C	−1.698575	0.000000	1.511352
C	−2.481856	0.000000	−1.219974
C	−0.725217	0.000000	0.505213
C	−3.044395	0.000000	1.154675
C	−3.428441	0.000000	−0.197894
C	−1.133657	0.000000	−0.855344
H	−3.807626	0.000000	1.927725
H	−4.484561	0.000000	−0.454109
H	−2.785201	0.000000	−2.263745
C	0.725217	0.000000	0.505213
C	3.428441	0.000000	−0.197894
C	1.698575	0.000000	1.511352
C	1.133657	0.000000	−0.855344
C	2.481856	0.000000	−1.219974
C	3.044395	0.000000	1.154675
H	1.406069	0.000000	2.558366
H	2.785201	0.000000	−2.263745
H	3.807626	0.000000	1.927725
H	4.484561	0.000000	−0.454109
N	0.000000	0.000000	−1.653872
H	0.000000	0.000000	−2.661728

SI-72
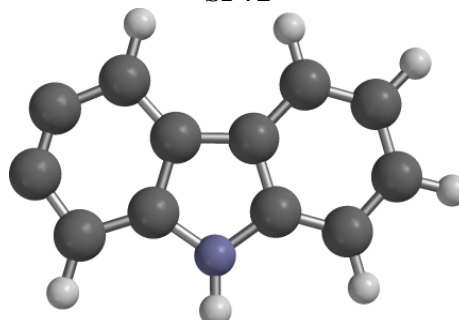
H	−1.457794	−2.662883	0.000000
C	−1.757343	−1.619762	0.000000
C	−2.626627	1.210583	0.000000
C	−0.827344	−0.551794	0.000000
C	−3.041901	−1.116348	0.000000
C	−3.419739	0.078847	0.000000
C	−1.266667	0.819828	0.000000
H	−2.949454	2.247467	0.000000
C	0.623510	−0.518045	0.000000
C	1.007362	0.848663	0.000000
N	−0.139931	1.628330	0.000000
H	−0.154330	2.636086	0.000000
C	1.615109	−1.506720	0.000000
H	1.342567	−2.559004	0.000000
H	3.730666	−1.885330	0.000000
C	2.954005	−1.125948	0.000000
H	4.364799	0.508604	0.000000
C	3.313592	0.233273	0.000000
H	2.632149	2.287180	0.000000
C	2.348555	1.237935	0.000000

SI-71
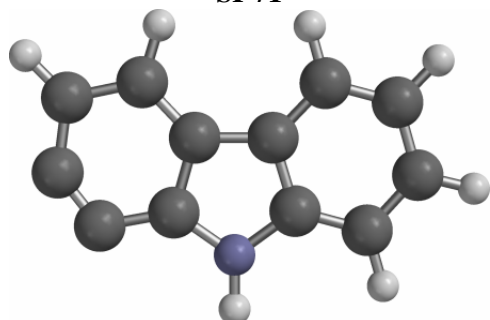
H	−1.557930	−2.466489	0.000000
C	−1.840311	−1.416133	0.000000
C	−2.549936	1.252796	0.000000
C	−0.840250	−0.423874	0.000000
C	−3.211389	−1.087978	0.000000
C	−3.350201	0.289971	0.000000
C	−1.188817	0.969856	0.000000
H	−3.996332	−1.834035	0.000000
C	0.609876	−0.466759	0.000000
C	1.066677	0.880031	0.000000
N	−0.035089	1.725298	0.000000
H	−0.003485	2.732813	0.000000
H	1.226659	−2.540637	0.000000
C	1.552342	−1.503540	0.000000
H	3.645132	−1.989347	0.000000
C	2.908410	−1.191000	0.000000
H	4.402679	0.367905	0.000000
C	3.338644	0.147665	0.000000
H	2.762297	2.233050	0.000000
C	2.426241	1.199464	0.000000

SI-73
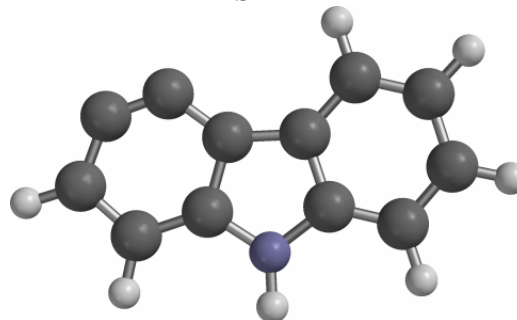
C	1.782008	−1.558426	0.000000
C	2.607360	1.030209	0.000000
C	0.734863	−0.643399	0.000000
C	2.991240	−1.247724	0.000000
C	3.580111	0.012456	0.000000
C	1.236320	0.706718	0.000000
H	4.641684	0.234671	0.000000
H	2.924430	2.070341	0.000000
C	−0.702986	−0.571544	0.000000
C	−1.033081	0.811650	0.000000
N	0.137644	1.553828	0.000000
H	0.179547	2.561023	0.000000
H	−1.485911	−2.585480	0.000000
C	−1.728541	−1.526373	0.000000
H	−3.855444	−1.825314	0.000000
C	−3.050347	−1.096146	0.000000
H	−4.400699	0.589831	0.000000
C	−3.359917	0.277364	0.000000
H	−2.607924	2.305496	0.000000
C	−2.361348	1.246959	0.000000

SI-74
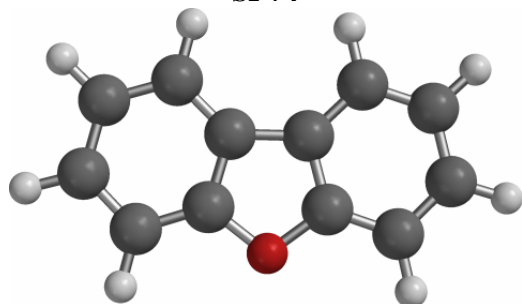
H	−1.469879	0.000000	2.570018
C	−1.726383	0.000000	1.514170
C	−2.419614	0.000000	−1.249272
C	−0.726178	0.000000	0.535458
C	−3.059550	0.000000	1.107228
C	−3.400461	0.000000	−0.255695
C	−1.099272	0.000000	−0.822026
H	−3.848369	0.000000	1.854115
H	−4.447596	0.000000	−0.545218
H	−2.668604	0.000000	−2.305273
C	0.726178	0.000000	0.535458
C	3.400461	0.000000	−0.255695
C	1.726383	0.000000	1.514170
C	1.099272	0.000000	−0.822026
C	2.419614	0.000000	−1.249272
C	3.059550	0.000000	1.107228
H	1.469879	0.000000	2.570018
H	2.668604	0.000000	−2.305273
H	3.848369	0.000000	1.854115
H	4.447596	0.000000	−0.545218
O	0.000000	0.000000	−1.651381

SI-75

H	−1.619628	−2.468636	0.000000
C	−1.863522	−1.409227	0.000000
C	−2.482899	1.296251	0.000000
C	−0.836766	−0.446060	0.000000
C	−3.222280	−1.026745	0.000000
C	−3.307626	0.351527	0.000000
C	−1.147035	0.944254	0.000000
H	−4.035031	−1.742367	0.000000
C	0.614850	−0.497341	0.000000
C	3.319637	0.193470	0.000000
C	1.579545	−1.512130	0.000000
C	1.041528	0.845664	0.000000
C	2.377046	1.222514	0.000000
C	2.926563	−1.155391	0.000000
H	1.284173	−2.557742	0.000000
H	2.664282	2.268696	0.000000
H	3.686304	−1.931795	0.000000
H	4.376916	0.442846	0.000000
O	−0.021946	1.723688	0.000000

SI-76

H	−1.528968	−2.672800	0.000000
C	−1.789690	−1.619693	0.000000
C	−2.561397	1.247240	0.000000
C	−0.831310	−0.580222	0.000000
C	−3.056896	−1.067424	0.000000
C	−3.391590	0.139586	0.000000
C	−1.231263	0.791624	0.000000
H	−2.829515	2.297744	0.000000
C	0.621216	−0.547971	0.000000
C	3.282950	0.287152	0.000000
C	1.637923	−1.510088	0.000000
C	0.973045	0.814677	0.000000
C	2.285863	1.264148	0.000000
C	2.963803	−1.081163	0.000000
H	1.399929	−2.570159	0.000000
H	2.516115	2.324346	0.000000
H	3.764358	−1.815339	0.000000
H	4.325156	0.593586	0.000000
O	−0.139349	1.627492	0.000000

SI-77

C	1.807598	−1.568551	0.000000
C	2.551130	1.057251	0.000000
C	0.740040	−0.676906	0.000000
C	3.002185	−1.202952	0.000000
C	3.557645	0.070945	0.000000
C	1.203597	0.670472	0.000000
H	4.612269	0.322350	0.000000
H	2.811419	2.111137	0.000000
C	−0.701973	−0.605442	0.000000
C	−3.325323	0.331541	0.000000
C	−1.753220	−1.530208	0.000000
C	−0.997063	0.772779	0.000000
C	−2.293134	1.270524	0.000000
C	−3.059936	−1.049408	0.000000
H	−1.548767	−2.596828	0.000000
H	−2.483794	2.338548	0.000000
H	−3.889415	−1.750694	0.000000
H	−4.355235	0.677063	0.000000
O	0.142717	1.546761	0.000000

SI-78
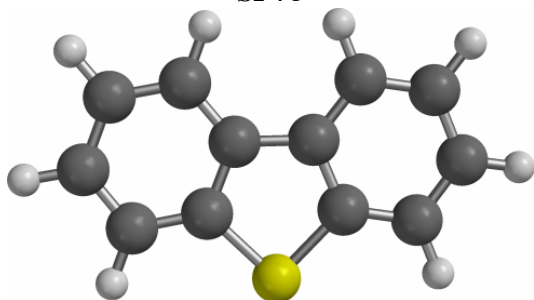
H	−1.226895	0.000000	2.670699
C	−1.613205	0.000000	1.654878
C	−2.637744	0.000000	−0.973243
C	−0.727675	0.000000	0.566358
C	−2.985508	0.000000	1.430923
C	−3.495678	0.000000	0.123581
C	−1.260639	0.000000	−0.742513
H	−3.668824	0.000000	2.275472
H	−4.570227	0.000000	−0.037067
H	−3.031679	0.000000	−1.985564
C	0.727675	0.000000	0.566358
C	3.495678	0.000000	0.123581
C	1.613205	0.000000	1.654878
C	1.260639	0.000000	−0.742513
C	2.637744	0.000000	−0.973243
C	2.985508	0.000000	1.430923
H	1.226895	0.000000	2.670699
H	3.031679	0.000000	−1.985564
H	3.668824	0.000000	2.275472
H	4.570227	0.000000	−0.037067
S	0.000000	0.000000	−1.982579

SI-80
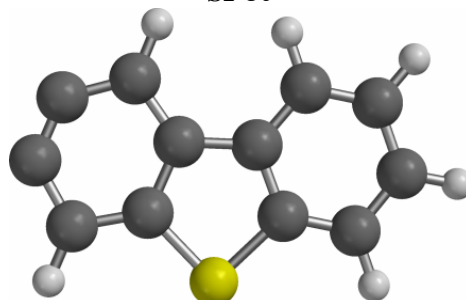
H	−1.214968	−2.797946	0.000000
C	−1.627211	−1.794139	0.000000
C	−2.782503	0.914266	0.000000
C	−0.807902	−0.633179	0.000000
C	−2.959218	−1.442144	0.000000
C	−3.454001	−0.291011	0.000000
C	−1.389083	0.673838	0.000000
H	−3.209600	1.911812	0.000000
C	0.648425	−0.577914	0.000000
C	3.401613	−0.046923	0.000000
C	1.569032	−1.637680	0.000000
C	1.140315	0.745623	0.000000
C	2.508825	1.021479	0.000000
C	2.933307	−1.369814	0.000000
H	1.217051	−2.665795	0.000000
H	2.869199	2.046274	0.000000
H	3.642969	−2.192214	0.000000
H	4.470353	0.148223	0.000000
S	−0.157962	1.947166	0.000000

SI-79
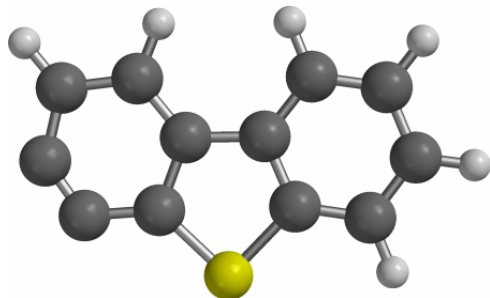
H	−1.357650	−2.601631	0.000000
C	−1.741409	−1.584285	0.000000
C	−2.687375	0.963880	0.000000
C	−0.832974	−0.501741	0.000000
C	−3.136691	−1.397331	0.000000
C	−3.427129	−0.043380	0.000000
C	−1.308636	0.849324	0.000000
H	−3.838443	−2.223007	0.000000
C	0.622496	−0.539796	0.000000
C	3.405453	−0.179173	0.000000
C	1.478083	−1.653516	0.000000
C	1.196317	0.753335	0.000000
C	2.580348	0.941713	0.000000
C	2.855798	−1.470575	0.000000
H	1.063072	−2.657769	0.000000
H	3.003397	1.942184	0.000000
H	3.513070	−2.335495	0.000000
H	4.484189	−0.050655	0.000000
S	−0.015171	2.043391	0.000000

SI-81
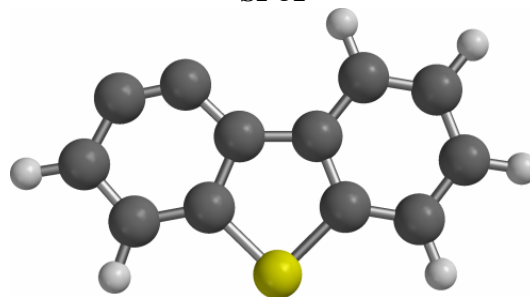
H	3.148661	−1.792929	0.000000
C	2.737324	−0.786708	0.000000
C	1.670496	1.694962	0.000000
C	1.341626	−0.602029	0.000000
C	3.617089	0.313670	0.000000
C	2.904453	1.504900	0.000000
C	0.712814	0.684565	0.000000
H	4.694582	0.193006	0.000000
C	−0.729483	0.615627	0.000000
C	−3.461715	0.035609	0.000000
C	−1.187752	−0.720822	0.000000
C	−1.662719	1.663470	0.000000
C	−3.020456	1.369466	0.000000
C	−2.552387	−1.018854	0.000000
H	−1.312584	2.692203	0.000000
H	−3.747817	2.176234	0.000000
H	−2.897880	−2.048700	0.000000
H	−4.526801	−0.179026	0.000000
S	0.135115	−1.896938	0.000000

SI-82
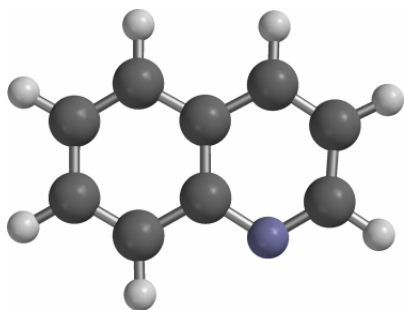
H	3.397968	−1.132760	0.000000
C	2.421728	−0.657021	0.000000
H	1.289647	−2.484344	0.000000
C	1.263204	−1.396797	0.000000
N	1.189343	1.425076	0.000000
C	0.012125	−0.729011	0.000000
C	2.325518	0.757952	0.000000
C	0.029192	0.703234	0.000000
C	−1.235014	−1.407397	0.000000
H	3.236056	1.357068	0.000000
H	−1.167263	2.490006	0.000000
C	−2.415297	−0.698458	0.000000
H	−1.242434	−2.495141	0.000000
H	−3.366133	−1.224392	0.000000
C	−2.399171	0.718935	0.000000
H	−3.339302	1.263974	0.000000
C	−1.205510	1.405089	0.000000

SI-84*
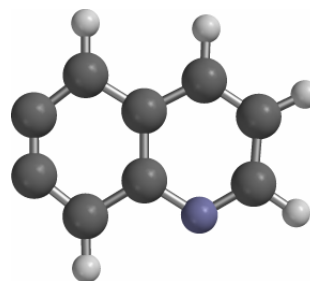
H	3.273607	−1.130427	0.000000
C	2.298311	−0.653102	0.000000
H	1.172187	−2.481141	0.000000
C	1.140894	−1.394033	0.000000
N	1.064605	1.424177	0.000000
C	−0.118224	−0.738278	0.000000
C	2.202828	0.760261	0.000000
C	−0.097861	0.712555	0.000000
C	−1.353649	−1.472098	0.000000
H	3.111151	1.362296	0.000000
H	−1.292357	2.555496	0.000000
C	−2.423259	−0.622197	0.000000
H	−1.370354	−2.558288	0.000000
C	−2.402059	0.637523	0.000000
C	−1.324895	1.472043	0.000000

SI-85*
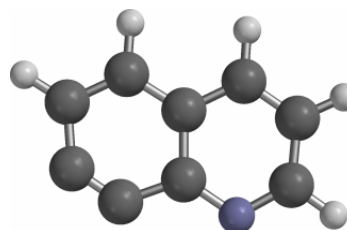
C	0.055910	−0.829680	0.000000
C	−0.112972	0.620670	0.000000
C	−1.410008	1.228747	0.000000
H	−1.463581	2.315583	0.000000
C	−2.588578	0.492763	0.000000
H	−3.569143	0.956477	0.000000
C	−2.314304	−0.883432	0.000000
C	−1.209675	−1.449707	0.000000
N	1.257633	−1.441671	0.000000
C	2.333307	−0.672745	0.000000
H	3.291819	−1.190380	0.000000
C	2.301847	0.740025	0.000000
H	3.231527	1.300861	0.000000
C	1.082229	1.381434	0.000000
H	1.026118	2.467479	0.000000

SI-83*
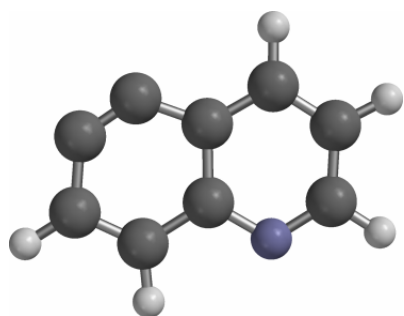
H	3.417249	−0.961824	0.000000
C	2.403627	−0.572153	0.000000
H	1.430072	−2.496043	0.000000
C	1.314497	−1.416405	0.000000
N	0.998660	1.399473	0.000000
C	0.022956	−0.850361	0.000000
C	2.188102	0.826205	0.000000
C	−0.103528	0.601221	0.000000
C	−1.248049	−1.449976	0.000000
H	3.043932	1.500474	0.000000
H	−1.400907	2.319381	0.000000
C	−2.340455	−0.860831	0.000000
C	−2.586128	0.523333	0.000000
H	−3.558922	1.003239	0.000000
C	−1.394818	1.233572	0.000000

SI-86
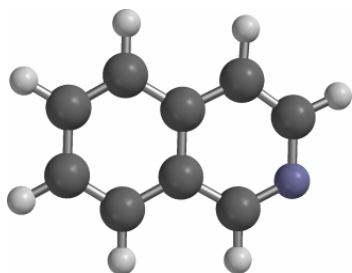
H	3.401837	−1.081834	0.000000
C	2.421846	−0.609449	0.000000
H	1.335556	−2.457244	0.000000
C	1.276440	−1.371833	0.000000
C	1.263171	1.362652	0.000000
C	0.011285	−0.729664	0.000000
N	2.430161	0.752978	0.000000
C	0.004925	0.698560	0.000000
C	−1.229482	−1.421080	0.000000
H	−1.226258	2.481035	0.000000
H	1.281951	2.453830	0.000000
C	−2.415324	−0.721022	0.000000
H	−1.228436	−2.508320	0.000000
H	−3.360750	−1.256924	0.000000
C	−2.419481	0.696898	0.000000
H	−3.366202	1.229866	0.000000
C	−1.231929	1.393511	0.000000

SI-88
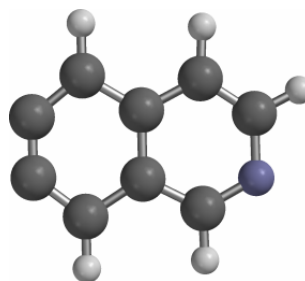
H	3.277555	−1.078799	0.000000
C	2.298317	−0.605472	0.000000
H	1.217425	−2.453808	0.000000
C	1.154243	−1.369028	0.000000
C	1.139407	1.366411	0.000000
C	−0.116526	−0.735179	0.000000
N	2.304568	0.755110	0.000000
C	−0.123853	0.706896	0.000000
C	−1.348095	−1.485332	0.000000
H	−1.355378	2.542461	0.000000
H	1.158811	2.456980	0.000000
C	−2.423556	−0.646194	0.000000
H	−1.348932	−2.570917	0.000000
C	−2.425388	0.614874	0.000000
C	−1.353123	1.456569	0.000000

SI-87
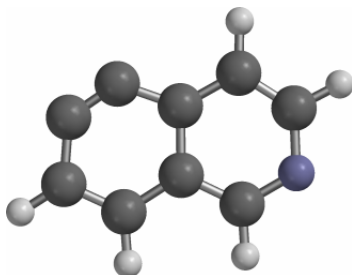
H	3.418129	−0.899305	0.000000
C	2.400143	−0.515560	0.000000
H	1.479029	−2.459477	0.000000
C	1.328803	−1.384884	0.000000
C	1.073706	1.354517	0.000000
C	0.026003	−0.847164	0.000000
N	2.287943	0.838184	0.000000
C	−0.129129	0.596922	0.000000
C	−1.238554	−1.463739	0.000000
H	−1.465314	2.303191	0.000000
H	1.011767	2.443502	0.000000
C	−2.337942	−0.887740	0.000000
C	−2.605061	0.490114	0.000000
H	−3.582128	0.960483	0.000000
C	−1.419465	1.216205	0.000000

SI-89
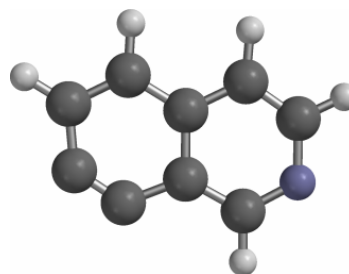
H	3.234784	−1.254043	0.000000
C	2.300314	−0.697139	0.000000
H	1.072528	−2.452058	0.000000
C	1.094174	−1.365462	0.000000
C	1.322047	1.375600	0.000000
C	−0.116936	−0.628660	0.000000
N	2.428309	0.655064	0.000000
C	0.023887	0.815896	0.000000
C	−1.410314	−1.246693	0.000000
H	1.434090	2.458868	0.000000
C	−2.594889	−0.518075	0.000000
H	−1.459113	−2.333282	0.000000
H	−3.571257	−0.990818	0.000000
C	−2.334830	0.860290	0.000000
C	−1.237819	1.439887	0.000000

SI-90
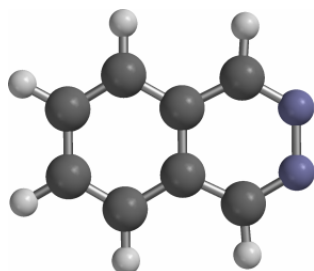
N	0.684733	0.000000	2.437193
H	2.415792	0.000000	1.368043
C	1.328591	0.000000	1.292434
C	-1.328591	0.000000	1.292434
C	0.708706	0.000000	0.010185
N	-0.684733	0.000000	2.437193
C	-0.708706	0.000000	0.010185
C	1.411033	0.000000	-1.218437
H	-2.498073	0.000000	-1.213840
H	-2.415792	0.000000	1.368043
C	0.708236	0.000000	-2.405560
H	2.498073	0.000000	-1.213840
H	1.241026	0.000000	-3.352364
C	-0.708236	0.000000	-2.405560
H	-1.241026	0.000000	-3.352364
C	-1.411033	0.000000	-1.218437

SI-92
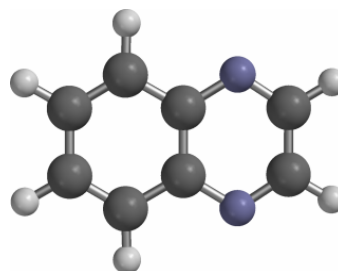
H	-1.255283	0.000000	3.262032
C	-0.710773	0.000000	2.318524
N	-1.421038	0.000000	1.210595
N	1.421038	0.000000	1.210595
C	-0.715519	0.000000	0.041912
C	0.710773	0.000000	2.318524
C	0.715519	0.000000	0.041912
C	-1.411356	0.000000	-1.194109
H	1.255283	0.000000	3.262032
H	2.496704	0.000000	-1.166927
C	-0.709419	0.000000	-2.378726
H	-2.496704	0.000000	-1.166927
H	-1.242586	0.000000	-3.325439
C	0.709419	0.000000	-2.378726
H	1.242586	0.000000	-3.325439
C	1.411356	0.000000	-1.194109

SI-91
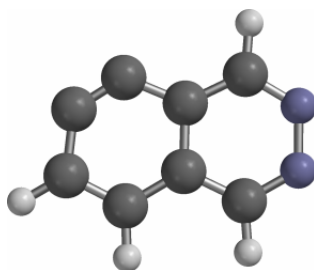
N	2.428991	0.572514	0.000000
H	1.524818	2.403585	0.000000
C	1.351013	1.329811	0.000000
C	1.104919	-1.331009	0.000000
C	0.029588	0.821632	0.000000
N	2.302373	-0.784230	0.000000
C	-0.121971	-0.608910	0.000000
C	-1.221220	1.461669	0.000000
H	-1.457889	-2.317812	0.000000
H	1.094269	-2.420321	0.000000
C	-2.317972	0.878146	0.000000
C	-2.589973	-0.495059	0.000000
H	-3.569039	-0.961497	0.000000
C	-1.406420	-1.231502	0.000000

SI-93
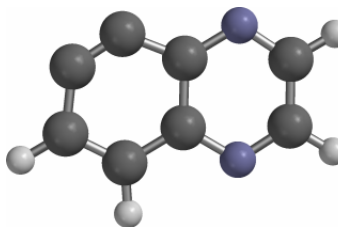
H	3.307889	-1.083631	0.000000
C	2.320531	-0.624601	0.000000
N	1.278136	-1.435032	0.000000
N	1.021570	1.395554	0.000000
C	0.066086	-0.843944	0.000000
C	2.191603	0.786220	0.000000
C	-0.085749	0.607475	0.000000
C	-1.197806	-1.462999	0.000000
H	3.080149	1.415510	0.000000
H	-1.394995	2.318250	0.000000
C	-2.291653	-0.875246	0.000000
C	-2.557850	0.504885	0.000000
H	-3.537787	0.969700	0.000000
C	-1.378059	1.232518	0.000000

SI-94
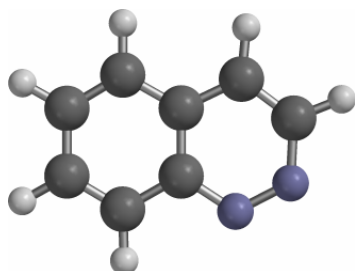
H	3.408599	−0.952523	0.000000
C	2.400512	−0.548089	0.000000
H	1.388440	−2.446626	0.000000
C	1.292219	−1.363623	0.000000
N	1.183361	1.415075	0.000000
C	0.024125	−0.748159	0.000000
N	2.342322	0.814153	0.000000
C	0.030287	0.679226	0.000000
C	−1.218420	−1.436745	0.000000
H	−1.162482	2.471520	0.000000
C	−2.396461	−0.726522	0.000000
H	−1.222203	−2.524015	0.000000
H	−3.346523	−1.253795	0.000000
C	−2.389590	0.694691	0.000000
H	−3.334133	1.231295	0.000000
C	−1.202109	1.386830	0.000000

SI-96
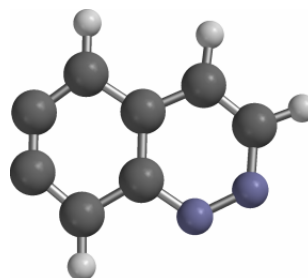
H	3.285121	−0.943776	0.000000
C	2.277642	−0.538150	0.000000
H	1.274360	−2.438638	0.000000
C	1.170842	−1.356664	0.000000
N	1.058515	1.420212	0.000000
C	−0.104557	−0.754936	0.000000
N	2.218649	0.821097	0.000000
C	−0.096810	0.689897	0.000000
C	−1.335268	−1.502452	0.000000
H	−1.295127	2.535149	0.000000
C	−2.403834	−0.654389	0.000000
H	−1.344068	−2.588241	0.000000
C	−2.389711	0.607394	0.000000
C	−1.324087	1.451646	0.000000

SI-95
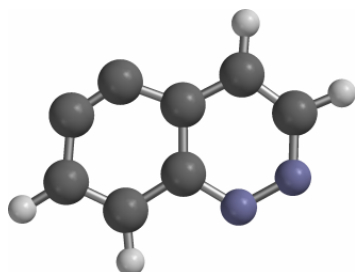
H	3.416761	−0.805337	0.000000
C	2.381642	−0.476186	0.000000
H	1.514636	−2.451921	0.000000
C	1.338912	−1.380938	0.000000
N	1.022967	1.392172	0.000000
C	0.039957	−0.855469	0.000000
N	2.223219	0.873609	0.000000
C	−0.080222	0.591533	0.000000
C	−1.233589	−1.450314	0.000000
H	−1.357451	2.327811	0.000000
C	−2.318817	−0.848537	0.000000
C	−2.556167	0.539704	0.000000
H	−3.525908	1.024959	0.000000
C	−1.362401	1.242210	0.000000

SI-97
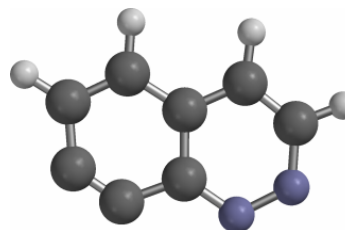
H	3.258220	−1.146578	0.000000
C	2.294345	−0.645952	0.000000
H	1.120221	−2.447307	0.000000
C	1.112918	−1.360253	0.000000
N	1.268252	1.424279	0.000000
C	−0.097158	−0.642064	0.000000
N	2.368116	0.709396	0.000000
C	0.067644	0.803406	0.000000
C	−1.393745	−1.254167	0.000000
C	−2.567033	−0.512434	0.000000
H	−1.448770	−2.340464	0.000000
H	−3.549118	−0.973019	0.000000
C	−2.292350	0.865855	0.000000
C	−1.191948	1.436991	0.000000

SI-98
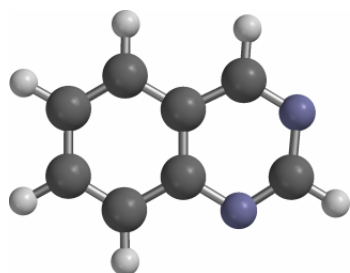
N	2.419423	0.703643	0.000000
H	1.329072	2.448766	0.000000
C	1.276642	1.358493	0.000000
N	1.232388	−1.388762	0.000000
C	0.013134	0.714328	0.000000
C	2.324563	−0.656766	0.000000
C	0.046140	−0.711585	0.000000
C	−1.230616	1.394610	0.000000
H	3.273771	−1.189211	0.000000
H	−1.134442	−2.513585	0.000000
C	−2.403720	0.674163	0.000000
H	−1.242368	2.482108	0.000000
H	−3.360644	1.188236	0.000000
C	−2.372885	−0.744430	0.000000
H	−3.310067	−1.294576	0.000000
C	−1.177286	−1.429091	0.000000

SI-99

N	2.417448	0.598340	0.000000
H	1.490093	2.442506	0.000000
C	1.341055	1.363459	0.000000
N	1.047481	−1.380239	0.000000
C	0.035619	0.827823	0.000000
C	2.201692	−0.743338	0.000000
C	−0.079018	−0.616926	0.000000
C	−1.229502	1.440536	0.000000
H	3.098095	−1.360100	0.000000
H	−1.366851	−2.346654	0.000000
C	−2.312265	0.833686	0.000000
C	−2.554131	−0.549768	0.000000
H	−3.526063	−1.031408	0.000000
C	−1.362174	−1.261047	0.000000

SI-100

N	2.292893	0.702878	0.000000
H	1.206827	2.449212	0.000000
C	1.151719	1.359659	0.000000
N	1.108530	−1.385410	0.000000
C	−0.118077	0.723609	0.000000
C	2.202615	−0.654685	0.000000
C	−0.079925	−0.720401	0.000000
C	−1.352096	1.455721	0.000000
H	3.150651	−1.188561	0.000000
H	−1.254360	−2.580608	0.000000
C	−2.409589	0.591516	0.000000
H	−1.377981	2.541560	0.000000
C	−2.377907	−0.668944	0.000000
C	−1.295247	−1.497587	0.000000

SI-101

N	2.290669	0.794314	0.000000
H	1.058326	2.440526	0.000000
C	1.093079	1.350215	0.000000
N	1.299844	−1.396501	0.000000
C	−0.112958	0.606348	0.000000
C	2.323221	−0.562729	0.000000
C	0.074261	−0.834698	0.000000
C	−1.408460	1.210654	0.000000
H	3.315732	−1.008292	0.000000
C	−2.578685	0.460378	0.000000
H	−1.470895	2.296829	0.000000
H	−3.565127	0.910657	0.000000
C	−2.284570	−0.911392	0.000000
C	−1.178931	−1.477238	0.000000

SI-102
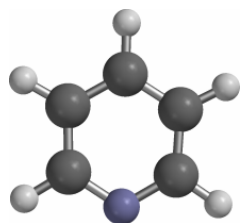
H	2.157893	0.000000	−1.180546
C	1.198748	0.000000	−0.670841
C	−1.142285	0.000000	0.724114
C	1.142285	0.000000	0.724114
C	0.000000	0.000000	−1.383231
C	−1.198748	0.000000	−0.670841
N	0.000000	0.000000	1.422944
H	2.059750	0.000000	1.311063
H	0.000000	0.000000	−2.470159
H	−2.157893	0.000000	−1.180546
H	−2.059750	0.000000	1.311063

SI-105
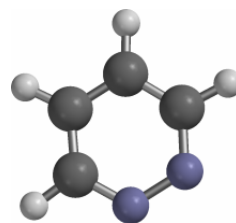
H	1.272030	0.000000	2.095067
C	0.692022	0.000000	1.176795
N	−0.668236	0.000000	−1.236408
C	1.323035	0.000000	−0.071790
C	−0.692022	0.000000	1.176795
C	−1.323035	0.000000	−0.071790
N	0.668236	0.000000	−1.236408
H	2.407245	0.000000	−0.156040
H	−1.272030	0.000000	2.095067
H	−2.407245	0.000000	−0.156040

SI-103*
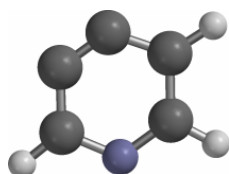
C	0.676457	−1.197022	0.000000
C	−0.662355	1.034551	−0.000000
C	1.414698	−0.020590	0.000000
C	−0.580771	−1.253776	0.000000
C	−1.426420	−0.165545	−0.000000
N	0.667732	1.100300	0.000000
H	2.494944	0.077167	0.000000
H	−2.511276	−0.152871	−0.000000
H	−1.187450	1.987886	−0.000000

SI-106*
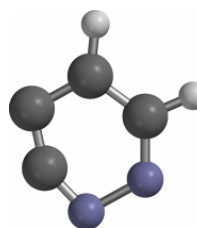
C	0.117577	−1.478973	0.000000
N	−0.299202	1.296307	0.000000
C	−0.922600	−0.732774	0.000000
C	1.229094	−0.631346	0.000000
C	0.915223	0.763998	0.000000
N	−1.418118	0.433400	0.000000
H	2.265535	−0.965902	0.000000
H	1.709610	1.506570	0.000000

SI-104*
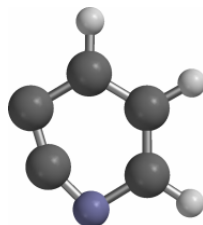
C	0.135156	−1.533551	0.000000
C	−0.345784	1.244114	0.000000
C	−0.890673	−0.774999	0.000000
C	1.233202	−0.626745	0.000000
C	0.966903	0.763711	0.000000
N	−1.419451	0.373928	0.000000
H	2.265024	−0.978229	0.000000
H	1.785211	1.477501	0.000000
H	−0.591922	2.300797	0.000000

SI-107
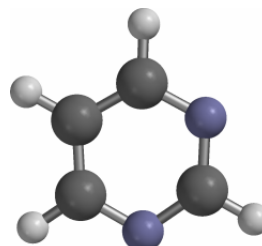
N	−1.199190	0.000000	−0.717565
C	1.184475	0.000000	0.621298
C	0.000000	0.000000	−1.310466
C	−1.184475	0.000000	0.621298
C	0.000000	0.000000	1.355217
N	1.199190	0.000000	−0.717565
H	0.000000	0.000000	−2.398906
H	−2.154491	0.000000	1.116389
H	0.000000	0.000000	2.440526
H	2.154491	0.000000	1.116389

SI-108*
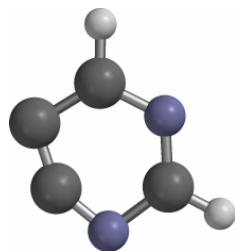
N	1.435253	−0.140692	0.000000
C	−1.284055	0.349476	0.000000
C	0.471585	−1.148780	0.000000
C	0.760700	0.927724	0.000000
C	−0.399142	1.467007	0.000000
N	−0.827504	−0.924569	0.000000
H	0.849694	−2.164927	0.000000
H	−2.365797	0.467080	0.000000

SI-109

N	0.309867	−1.351235	0.000000
N	−0.972326	−0.974817	0.000000
C	−1.242058	0.333445	0.000000
H	−2.297332	0.594740	0.000000
N	−0.359476	1.344298	0.000000
C	0.912431	0.958465	0.000000
H	1.676803	1.733967	0.000000
C	1.245564	−0.400409	0.000000
H	2.276995	−0.743015	0.000000

SI-110*

N	−0.445087	−1.139143	0.000000
N	−1.308825	−0.183672	0.000000
C	−0.986513	1.268868	0.000000
C	0.335869	1.132744	0.000000
C	0.866903	−0.934152	0.000000
H	1.571995	−1.755687	0.000000
N	1.314896	0.362946	0.000000

SI-111*

C	2.219409	0.648498	0.000000
C	1.327756	1.540945	0.000000
C	1.406472	−1.279447	0.000000
C	0.068078	0.825752	0.000000
N	2.568554	−0.588586	0.000000
C	0.136103	−0.628110	0.000000
C	−1.205972	1.446606	0.000000
H	−1.024487	−2.461973	0.000000
H	1.484683	−2.363538	0.000000
C	−2.353972	0.682779	0.000000
H	−1.249468	2.530929	0.000000
H	−3.325587	1.169880	0.000000
C	−2.289680	−0.732553	0.000000
H	−3.209651	−1.310242	0.000000
C	−1.072901	−1.375653	0.000000

SI-112*

C	2.590094	0.696050	0.000000
H	1.357111	2.504052	0.000000
C	1.385378	1.412744	0.000000
N	1.355722	−1.439809	0.000000
C	0.131146	0.699234	0.000000
C	2.219051	−0.537614	0.000000
C	0.125626	−0.741212	0.000000
C	−1.123746	1.360860	0.000000
H	−1.046941	−2.543485	0.000000
C	−2.302089	0.644159	0.000000
H	−1.140714	2.447959	0.000000
H	−3.254470	1.166586	0.000000
C	−2.282441	−0.769222	0.000000
H	−3.219672	−1.318718	0.000000
C	−1.085864	−1.459104	0.000000

SI-113*

C	2.368529	0.844729	0.000000
C	1.272111	1.439458	0.000000
N	1.369827	−1.237788	0.000000
C	0.002986	0.850930	0.000000
C	2.506137	−0.561910	0.000000
C	0.163534	−0.610496	0.000000
C	−1.287564	1.420407	0.000000
H	3.442036	−1.111603	0.000000
H	−0.908012	−2.475342	0.000000
C	−2.400429	0.604602	0.000000
H	−1.385406	2.501318	0.000000
H	−3.393269	1.045552	0.000000
C	−2.263332	−0.802357	0.000000
H	−3.154208	−1.424233	0.000000
C	−1.018731	−1.396068	0.000000

SI-114

C	0.230276	−0.696663	0.000000
C	−2.054906	0.754076	0.000000
C	0.213823	0.730457	0.000000
C	−0.965082	−1.413316	0.000000
C	−2.130521	−0.653822	0.000000
N	−0.921272	1.453814	0.000000
H	−0.991476	−2.500268	0.000000
H	−3.102720	−1.137368	0.000000
H	−2.974998	1.336866	0.000000
C	1.580445	1.168476	0.000000
H	1.927976	2.191541	0.000000
C	2.355903	0.039413	0.000000
H	3.432095	−0.065055	0.000000
N	1.550578	−1.087682	0.000000
H	1.883932	−2.039099	0.000000

SI-115*

C	0.334735	−0.637410	0.000000
C	−1.994956	0.769108	0.000000
C	0.271660	0.817973	0.000000
C	−0.844965	−1.366450	0.000000
C	−2.034777	−0.633197	0.000000
N	−0.867403	1.488266	0.000000
H	−0.849428	−2.453892	0.000000
H	−2.992862	−1.143499	0.000000
H	−2.922370	1.337676	0.000000
N	1.691303	−1.019594	0.000000
H	2.032637	−1.970029	0.000000
C	2.426746	0.137697	0.000000
C	1.670483	1.139575	0.000000

SI-116*
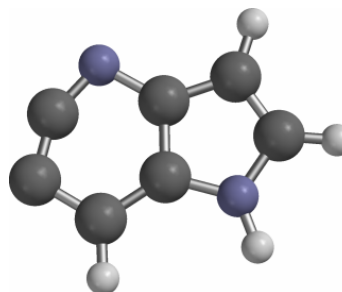
N	1.095429	−1.475247	0.000000
C	−0.105352	−0.780094	0.000000
C	−0.111323	0.659624	0.000000
H	1.047538	2.514768	0.000000
C	1.079406	1.424314	0.000000
C	2.283914	0.686258	0.000000
C	1.957563	−0.550586	0.000000
N	−1.440287	1.028483	0.000000
H	−1.781095	1.977379	0.000000
C	−2.236263	−0.097876	0.000000
H	−3.313584	−0.004158	0.000000
C	−1.455742	−1.230076	0.000000
H	−1.801501	−2.253219	0.000000

SI-117*


```
N     1.108932    -1.263614    0.000000
C    -0.081719    -0.649267    0.000000
C    -0.235139     0.795272    0.000000
C     0.958404     1.492901    0.000000
C     2.028711     0.828673    0.000000
H     3.193633    -1.069493    0.000000
C     2.242311    -0.550828    0.000000
N    -1.579309     1.066272    0.000000
H    -1.989117     1.987282    0.000000
C    -2.279855    -0.128648    0.000000
H    -3.360710    -0.121433    0.000000
C    -1.411282    -1.189111    0.000000
H    -1.678195    -2.235929    0.000000
```

SI-119*
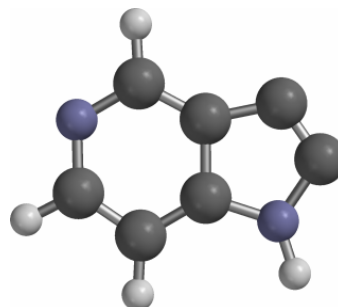

```
C     0.307605    -0.811172    0.000000
C    -2.021863     0.601077    0.000000
C    -0.939620    -1.437209    0.000000
C     0.342758     0.636521    0.000000
C    -0.848836     1.355799    0.000000
N    -2.080493    -0.745097    0.000000
H    -1.020428    -2.522678    0.000000
H    -0.879578     2.441952    0.000000
H    -2.983037     1.111210    0.000000
N     1.689597     1.037565    0.000000
H     2.019648     1.991226    0.000000
C     2.444439    -0.113987    0.000000
C     1.706425    -1.121603    0.000000
```

SI-118
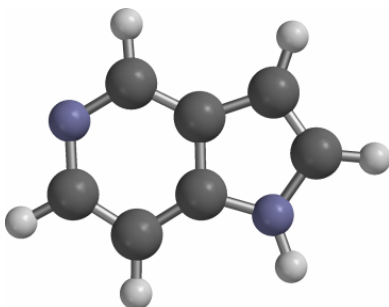

```
C     0.237122    -0.739323    0.000000
C    -2.126241     0.631638    0.000000
C    -1.010976    -1.382750    0.000000
C     0.237607     0.681812    0.000000
C    -0.964924     1.394690    0.000000
N    -2.164926    -0.719978    0.000000
H    -1.075091    -2.470782    0.000000
H    -1.003803     2.480355    0.000000
H    -3.095074     1.127398    0.000000
C     1.610533    -1.163031    0.000000
H     1.980328    -2.179039    0.000000
C     2.374305    -0.028196    0.000000
H     3.448993     0.089807    0.000000
N     1.550398     1.088577    0.000000
H     1.868315     2.045407    0.000000
```

SI-120*
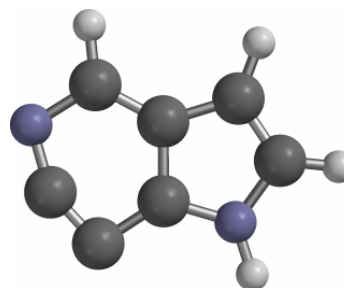

```
N     2.292795     0.527054    0.000000
H     1.309106     2.376001    0.000000
C     1.159935     1.301315    0.000000
C    -0.103849     0.687956    0.000000
C    -0.168611    -0.761129    0.000000
C     0.990732    -1.579676    0.000000
C     1.897331    -0.679947    0.000000
N    -1.499383    -1.094062    0.000000
H    -1.846775    -2.041348    0.000000
C    -2.269545     0.058273    0.000000
H    -3.348754    -0.008510    0.000000
C    -1.460438     1.161770    0.000000
H    -1.794613     2.190058    0.000000
```

SI-121
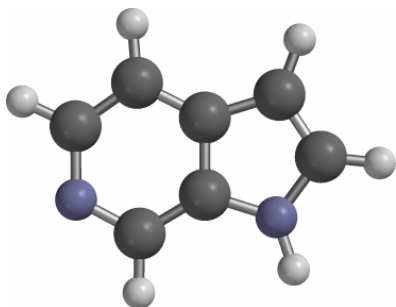
C	0.239074	−0.660636	0.000000
C	−2.151077	0.590284	0.000000
C	−0.958599	−1.381362	0.000000
C	0.233750	0.760409	0.000000
C	−1.019978	1.394896	0.000000
N	−2.136319	−0.762910	0.000000
H	−0.969844	−2.471685	0.000000
H	−1.110560	2.477540	0.000000
H	−3.140356	1.043559	0.000000
C	1.603630	1.184029	0.000000
H	1.974029	2.199795	0.000000
C	2.371201	0.046624	0.000000
H	3.447066	−0.063353	0.000000
N	1.558234	−1.068121	0.000000
H	1.879042	−2.023816	0.000000

SI-123*
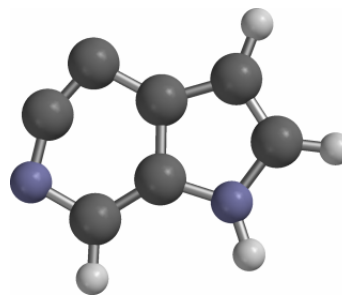
C	−1.038406	−1.566237	0.000000
C	−1.109882	1.296712	0.000000
C	0.192756	−0.836651	0.000000
C	−1.922542	−0.654279	0.000000
N	−2.272224	0.574340	0.000000
C	0.113448	0.612593	0.000000
C	1.583013	−1.170680	0.000000
H	2.008465	−2.163826	0.000000
C	2.280653	0.012360	0.000000
H	3.348595	0.184304	0.000000
N	1.410176	1.082257	0.000000
H	1.687213	2.051610	0.000000
H	−1.202753	2.378347	0.000000

SI-122*

C	0.353290	−0.616104	0.000000
C	−2.059942	0.611563	0.000000
C	−0.831773	−1.345538	0.000000
C	0.308370	0.832495	0.000000
C	−0.945058	1.446416	0.000000
N	−2.020290	−0.735924	0.000000
H	−0.833203	−2.435972	0.000000
H	−1.053480	2.526318	0.000000
H	−3.056917	1.047224	0.000000
N	1.710503	−1.011424	0.000000
H	2.048455	−1.962186	0.000000
C	2.448622	0.142584	0.000000
C	1.700598	1.146030	0.000000

SI-124

C	0.230554	−0.778267	0.000000
C	−2.026743	0.788279	0.000000
C	0.210803	0.647319	0.000000
C	−1.016858	−1.416536	0.000000
C	−2.153682	−0.613794	0.000000
N	−0.859326	1.440051	0.000000
H	−1.096418	−2.500813	0.000000
H	−3.144799	−1.057330	0.000000
H	−2.918579	1.412297	0.000000
C	1.609221	−1.175558	0.000000
H	2.000646	−2.183693	0.000000
C	2.354638	−0.024150	0.000000
H	3.427922	0.105746	0.000000
N	1.518354	1.076530	0.000000

SI-125*

C	0.312378	−0.862952	0.000000
C	−1.920405	0.750632	0.000000
C	0.328864	0.599645	0.000000
C	−0.938451	−1.472290	0.000000
C	−2.064735	−0.643167	0.000000
N	−0.729000	1.369626	0.000000
H	−1.038237	−2.553506	0.000000
H	−3.060738	−1.074774	0.000000
H	−2.795597	1.395573	0.000000
N	1.674593	1.022945	0.000000
H	1.967430	1.989524	0.000000
C	2.444261	−0.115915	0.000000
C	1.707645	−1.133365	0.000000

SI-127*
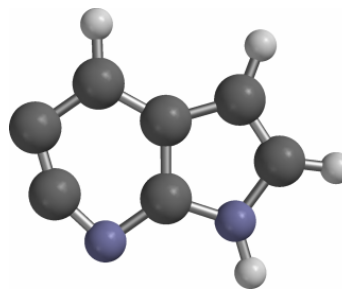
H	−1.169342	−2.513799	0.000000
C	−1.136286	−1.424670	0.000000
N	−1.017741	1.479876	0.000000
C	0.106311	−0.738579	0.000000
C	−2.296932	−0.617256	0.000000
C	−1.947303	0.603517	0.000000
C	0.106942	0.699308	0.000000
C	1.492099	−1.124699	0.000000
H	1.883025	−2.132787	0.000000
C	2.240546	0.021295	0.000000
H	3.313407	0.153575	0.000000
N	1.402852	1.129968	0.000000
H	1.687295	2.097619	0.000000

SI-126*
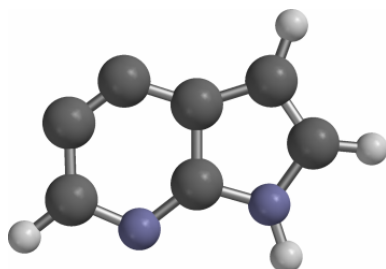
C	−1.019176	−1.452085	0.000000
N	−1.050878	1.256190	0.000000
C	0.244872	−0.887963	0.000000
C	−2.097846	−0.811925	0.000000
C	−2.214404	0.583929	0.000000
C	0.082766	0.560812	0.000000
H	−3.134990	1.156764	0.000000
C	1.644940	−1.156716	0.000000
H	2.125966	−2.124038	0.000000
C	2.280057	0.062048	0.000000
H	3.337531	0.285476	0.000000
N	1.354262	1.085585	0.000000
H	1.558631	2.073267	0.000000

SI-128*
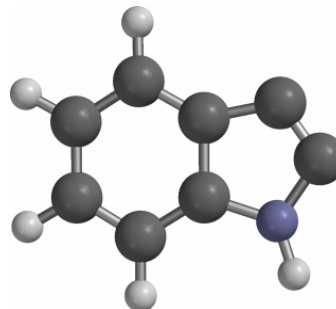
H	−0.955078	−2.566511	0.000000
C	−0.909617	−1.481663	0.000000
C	−0.815439	1.378124	0.000000
C	0.322385	−0.824155	0.000000
C	−2.073912	−0.716482	0.000000
C	−2.028162	0.688590	0.000000
C	0.357380	0.627621	0.000000
H	−3.038443	−1.216179	0.000000
H	−2.956693	1.252455	0.000000
H	−0.789165	2.465238	0.000000
C	1.722783	−1.122336	0.000000
C	2.467265	−0.117525	0.000000
N	1.711292	1.029816	0.000000
H	2.039132	1.983915	0.000000

SI-129*
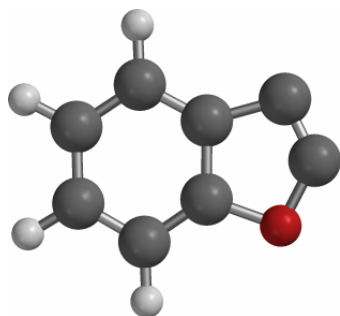

```
H    −0.724179    −2.503237     0.000000
C    −0.779898    −1.419684     0.000000
C    −0.891210     1.451392     0.000000
C     0.350708    −0.631449     0.000000
C    −2.000793    −0.731184     0.000000
C    −2.051223     0.670032     0.000000
C     0.342923     0.802267     0.000000
H    −2.925831    −1.300189     0.000000
H    −3.019246     1.163074     0.000000
H    −0.945538     2.535235     0.000000
C     1.761283     1.204392     0.000000
C     2.308303     0.091222     0.000000
O     1.704096    −1.098421     0.000000
```

SI-130*
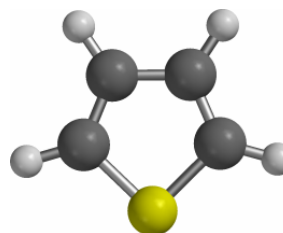

```
H    −0.781308    −2.472060     0.000000
C    −0.946336    −1.397504     0.000000
C    −1.392755     1.415172     0.000000
C     0.127610    −0.513042     0.000000
C    −2.238145    −0.870921     0.000000
C    −2.455617     0.516903     0.000000
C    −0.091589     0.902841     0.000000
H    −3.089165    −1.545876     0.000000
H    −3.472987     0.897167     0.000000
H    −1.563706     2.486914     0.000000
C     1.235789     1.399299     0.000000
C     2.349911     0.833143     0.000000
S     1.907628    −0.862472     0.000000
```

SI-131


```
C     0.714739     0.000000     1.267680
H     1.319482     0.000000     2.168299
C     1.243534     0.000000     0.006768
H     2.284636     0.000000    −0.286596
C    −0.714739     0.000000     1.267680
H    −1.319482     0.000000     2.168299
C    −1.243534     0.000000     0.006768
H    −2.284636     0.000000    −0.286596
S     0.000000     0.000000    −1.204293
```

SI-132*


```
C     0.637374     0.000000     1.363027
C     1.278310     0.000000     0.167900
H     2.319786     0.000000    −0.124165
C    −0.637374     0.000000     1.363027
C    −1.278310     0.000000     0.167900
H    −2.319786     0.000000    −0.124165
S     0.000000     0.000000    −1.069113
```

SI-133*


```
C     1.000778     0.834889     0.000000
C    −0.104263     1.438999     0.000000
C     1.410095    −0.512513     0.000000
H     2.404679    −0.933919     0.000000
C     0.204330    −1.171916     0.000000
H     0.021088    −2.241119     0.000000
S    −1.125938     0.017570     0.000000
```

SI-134
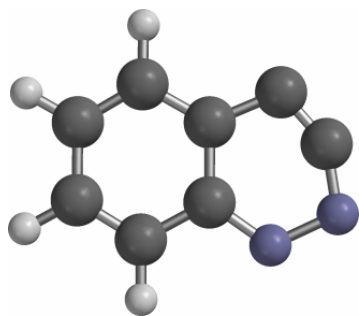
C	2.233494	0.594894	0.000000
C	1.338159	1.485057	0.000000
N	1.325421	−1.322381	0.000000
C	0.067390	0.840391	0.000000
N	2.517138	−0.669201	0.000000
C	0.160747	−0.618827	0.000000
C	−1.210548	1.453755	0.000000
H	−0.962415	−2.465514	0.000000
C	−2.343633	0.672738	0.000000
H	−1.267741	2.537312	0.000000
H	−3.322985	1.143312	0.000000
C	−2.259078	−0.746249	0.000000
H	−3.174344	−1.331248	0.000000
C	−1.043028	−1.383753	0.000000

SI-135

C	−0.280947	−1.172238	0.000000
H	−0.918779	−2.045875	0.000000
C	1.101829	−1.197442	0.000000
H	1.597909	−2.163153	0.000000
C	1.833941	−0.008525	0.000000
H	2.918331	−0.017146	0.000000
C	1.120860	1.191907	0.000000
H	1.632488	2.149465	0.000000
C	−0.262173	1.188768	0.000000
H	−0.885962	2.072490	0.000000
N	−0.975369	0.013894	0.000000
O	−2.249704	0.024046	0.000000

SI-136

C	−0.911132	−1.257399	0.000000
C	0.174736	1.076263	0.000000
C	0.334200	−1.189921	0.000000
C	−1.888359	−0.285181	0.000000
C	−1.210852	0.957630	0.000000
H	−2.964558	−0.394400	0.000000
H	−1.786513	1.880521	0.000000
H	0.697482	2.023682	0.000000
N	1.048993	−0.021130	0.000000
O	2.294319	0.125613	0.000000

SI-137

C	−1.050925	−1.271657	0.000000
C	0.032534	1.138350	0.000000
C	0.317248	−1.270615	0.000000
C	−1.775688	−0.251787	0.000000
C	−1.357905	1.068814	0.000000
H	1.048606	−2.066394	0.000000
H	−1.974435	1.960777	0.000000
H	0.589658	2.065333	0.000000
N	0.861999	0.019677	0.000000
O	2.126003	0.161617	0.000000

SI-138

H	0.000000	0.000000	2.498849
C	0.000000	0.000000	1.412619
C	1.211328	0.000000	0.707751
C	−1.211328	0.000000	0.707751
C	−1.164638	0.000000	−0.667049
C	1.164638	0.000000	−0.667049
H	2.171940	0.000000	1.210711
H	−2.171940	0.000000	1.210711
H	−2.011743	0.000000	−1.343003
H	2.011743	0.000000	−1.343003
O	0.000000	0.000000	−1.314931

SI-139

C	0.454895	−1.225561	0.000000
C	−0.785266	−1.155000	0.000000
H	−2.550219	0.192683	0.000000
C	−1.474050	0.044524	0.000000
H	−0.913948	2.157912	0.000000
C	−0.545853	1.134908	0.000000
H	1.585512	1.710206	0.000000
C	0.818547	0.944676	0.000000
O	1.377587	−0.317977	0.000000

SI-140

C	−0.937371	−0.973150	0.000000
C	−1.443687	0.302463	0.000000
C	0.234856	−1.423301	0.000000
C	1.282754	−0.558963	0.000000
C	−0.344502	1.171646	0.000000
H	−2.470079	0.651281	0.000000
H	2.358036	−0.691729	0.000000
H	−0.414822	2.255154	0.000000
O	0.917601	0.752772	0.000000

SI-141

C	0.985853	−1.410868	0.000000
H	1.002258	−2.496667	0.000000
C	2.147258	−0.681094	0.000000
H	3.111246	−1.179893	0.000000
C	2.089245	0.745491	0.000000
H	2.998524	1.336832	0.000000
C	0.885130	1.384807	0.000000
H	0.771230	2.462965	0.000000
N	−0.284342	0.656645	0.000000
C	−0.273123	−0.760583	0.000000
C	−1.602787	−1.179063	0.000000
H	−1.934435	−2.208247	0.000000
C	−2.410275	−0.022979	0.000000
H	−3.492191	0.005952	0.000000
C	−1.588084	1.092018	0.000000
H	−1.818780	2.147461	0.000000

SI-142*

N	−0.362636	−0.642801	0.000000
C	−1.683130	−1.103781	0.000000
H	−1.914526	−2.157179	0.000000
C	−2.427388	0.063740	0.000000
C	−1.733090	1.121371	0.000000
C	−0.375337	0.803022	0.000000
C	0.865621	1.471486	0.000000
H	0.862039	2.556695	0.000000
C	2.040592	0.755744	0.000000
H	2.995118	1.272019	0.000000
C	2.009946	−0.667397	0.000000
H	2.932884	−1.237467	0.000000
C	0.821487	−1.342826	0.000000
H	0.739942	−2.424111	0.000000

SI-143*

N	−0.360769	−0.733120	0.000000
C	−1.662703	−1.173881	0.000000
C	−2.381975	−0.140655	0.000000
C	−1.752135	1.114722	0.000000
H	−2.133908	2.123515	0.000000
C	−0.392903	0.712875	0.000000
C	0.845674	1.398380	0.000000
H	0.841256	2.484384	0.000000
C	2.021405	0.689426	0.000000
H	2.971623	1.214385	0.000000
C	2.010094	−0.738760	0.000000
H	2.940124	−1.296622	0.000000
C	0.830500	−1.423327	0.000000
H	0.746478	−2.503086	0.000000

SI-145
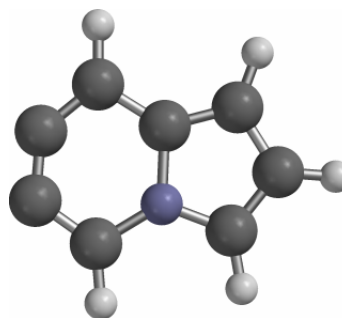
C	1.052936	−1.424746	0.000000
H	0.935602	−2.502423	0.000000
C	2.176328	−0.667379	0.000000
C	2.108449	0.598520	0.000000
C	1.091997	1.486800	0.000000
H	1.119618	2.569923	0.000000
C	−0.153563	0.762776	0.000000
N	−0.131351	−0.671248	0.000000
C	−1.492151	1.148650	0.000000
H	−1.844650	2.170732	0.000000
C	−2.274436	−0.024387	0.000000
H	−3.355872	−0.074834	0.000000
C	−1.429028	−1.122196	0.000000
H	−1.642203	−2.181203	0.000000

SI-144
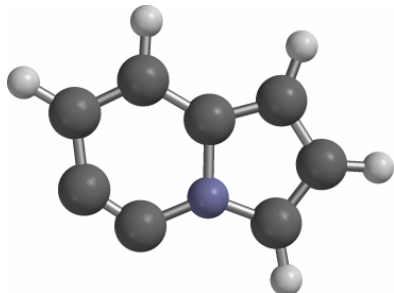
C	1.975691	−0.932453	0.000000
C	−0.131848	0.667063	0.000000
C	0.855118	−1.456005	0.000000
N	−0.311203	−0.767719	0.000000
C	−1.417847	1.205674	0.000000
H	−1.652384	2.261424	0.000000
C	−2.340495	0.138699	0.000000
H	−3.418844	0.227953	0.000000
C	−1.646621	−1.062995	0.000000
H	−1.988984	−2.086676	0.000000
C	2.342787	0.429443	0.000000
H	3.342333	0.844607	0.000000
C	1.189693	1.204036	0.000000
H	1.282330	2.287218	0.000000

SI-146
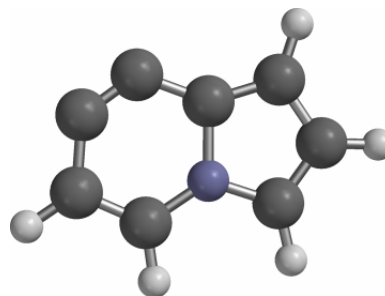
C	2.293305	0.475883	0.000000
H	3.258616	0.965470	0.000000
C	2.019226	−0.904714	0.000000
C	0.935122	−1.503578	0.000000
C	−0.314180	−0.867349	0.000000
C	1.111611	1.186789	0.000000
H	1.090726	2.271151	0.000000
N	−0.127107	0.575632	0.000000
C	−1.676278	−1.102138	0.000000
H	−2.140749	−2.077683	0.000000
C	−2.326428	0.156399	0.000000
H	−3.396127	0.319972	0.000000
C	−1.376427	1.158451	0.000000
H	−1.486269	2.233229	0.000000

SI-147
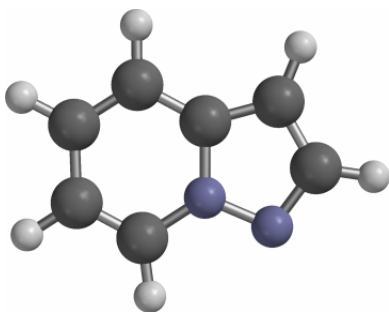
C	0.955270	−1.439384	0.000000
H	0.964631	−2.524650	0.000000
C	0.881046	1.364490	0.000000
H	0.747977	2.438904	0.000000
C	−0.292218	−0.765912	0.000000
C	−1.644662	−1.115156	0.000000
H	−2.057072	−2.113273	0.000000
C	−2.328768	0.107273	0.000000
H	−3.399015	0.271347	0.000000
N	−0.275309	0.634145	0.000000
N	−1.515576	1.174320	0.000000
C	2.081704	0.711765	0.000000
H	2.998026	1.291301	0.000000
C	2.120550	−0.712575	0.000000
H	3.079990	−1.220602	0.000000

SI-149
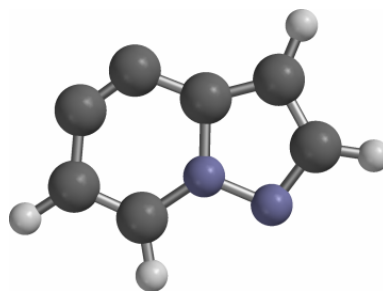
C	2.275585	0.475868	0.000000
H	3.239677	0.967358	0.000000
C	2.005155	−0.903983	0.000000
C	0.929434	−1.519544	0.000000
C	−0.316264	−0.876635	0.000000
C	1.087939	1.179469	0.000000
H	1.027863	2.260720	0.000000
N	−0.132066	0.544089	0.000000
N	−1.316505	1.199983	0.000000
C	−1.689103	−1.069572	0.000000
H	−2.210862	−2.014291	0.000000
C	−2.233930	0.226800	0.000000
H	−3.280910	0.502594	0.000000

SI-150
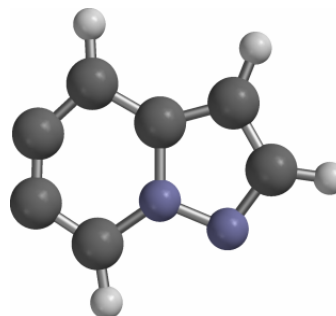
H	−1.157990	−2.568816	0.000000
C	−1.099548	−1.487303	0.000000
C	−2.094437	−0.569447	0.000000
C	−2.128015	0.695302	0.000000
C	0.154797	−0.782953	0.000000
H	1.902468	−2.147346	0.000000
C	1.503354	−1.143932	0.000000
C	−0.986664	1.430641	0.000000
H	−0.816807	2.499762	0.000000
N	0.157881	0.636670	0.000000
N	1.406336	1.146356	0.000000
H	3.277695	0.215117	0.000000
C	2.204704	0.068149	0.000000

SI-148*
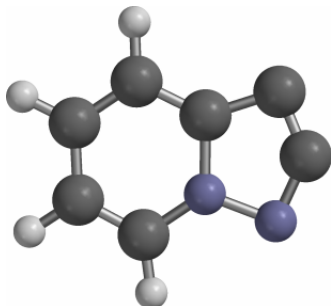
N	−0.367279	−0.644900	0.000000
N	−1.657701	−1.163738	0.000000
C	−2.225445	0.019824	0.000000
C	−1.765628	1.205971	0.000000
C	−0.405132	0.800988	0.000000
C	0.778545	−1.380589	0.000000
H	0.655044	−2.456258	0.000000
C	1.976566	−0.713141	0.000000
H	2.895760	−1.288301	0.000000
C	2.011241	0.706205	0.000000
H	2.971809	1.212306	0.000000
C	0.849465	1.448559	0.000000
H	0.866135	2.532780	0.000000

SI-151
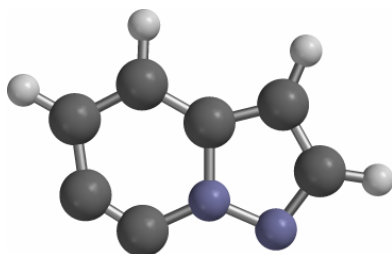
C	1.934720	−0.938155	0.000000
C	2.314615	0.414566	0.000000
H	3.320214	0.815954	0.000000
C	1.175967	1.213007	0.000000
H	1.284665	2.294112	0.000000
C	−0.147201	0.681005	0.000000
C	0.807867	−1.452730	0.000000
N	−0.333607	−0.737198	0.000000
N	−1.623579	−1.103545	0.000000
C	−1.447399	1.188949	0.000000
H	−1.737709	2.229426	0.000000
C	−2.285928	0.065376	0.000000
H	−3.368099	0.047320	0.000000

SI-153
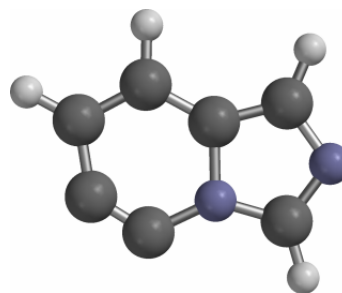
C	1.944611	0.942233	0.000000
C	0.827925	1.472035	0.000000
C	−0.138051	−0.672631	0.000000
C	−1.436359	−1.166020	0.000000
H	−1.746479	−2.202665	0.000000
N	−2.350837	−0.155463	0.000000
C	−1.673980	0.981945	0.000000
H	−2.093674	1.977671	0.000000
N	−0.329393	0.756956	0.000000
C	2.328441	−0.417530	0.000000
H	3.333391	−0.818837	0.000000
C	1.187801	−1.205048	0.000000
H	1.291218	−2.286973	0.000000

SI-152
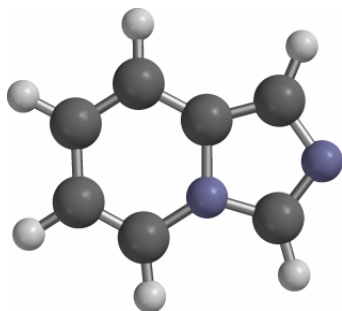
N	0.281407	−0.661682	0.000000
C	−0.896857	−1.382125	0.000000
H	−0.797350	−2.461452	0.000000
C	−2.085499	−0.719742	0.000000
H	−3.006823	−1.292105	0.000000
C	−2.120971	0.712492	0.000000
H	−3.079138	1.222143	0.000000
C	−0.953930	1.429067	0.000000
H	−0.956213	2.514605	0.000000
C	0.293047	0.751933	0.000000
C	1.641704	1.088772	0.000000
H	2.072389	2.081001	0.000000
N	2.418821	−0.030433	0.000000
C	1.592483	−1.061899	0.000000
H	1.875013	−2.105766	0.000000

SI-154
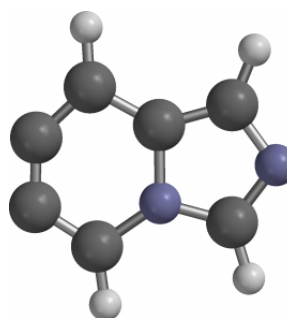
C	2.093747	0.590816	0.000000
C	1.088443	1.488209	0.000000
H	1.123106	2.570950	0.000000
C	2.155528	−0.677672	0.000000
C	1.035868	−1.435382	0.000000
H	0.913654	−2.512127	0.000000
N	−0.144879	−0.666672	0.000000
C	−0.159761	0.763085	0.000000
C	−1.509063	1.094349	0.000000
H	−1.938430	2.087085	0.000000
N	−2.285795	−0.024155	0.000000
C	−1.457653	−1.055790	0.000000
H	−1.744624	−2.098361	0.000000

SI-155
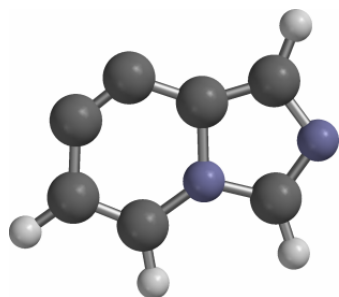
C	2.281077	0.472816	0.000000
H	3.250501	0.954086	0.000000
C	1.108408	1.192372	0.000000
H	1.090572	2.276538	0.000000
C	2.000547	−0.909577	0.000000
C	0.920951	−1.514269	0.000000
C	−0.323521	−0.862460	0.000000
C	−1.692028	−1.030864	0.000000
H	−2.239805	−1.962602	0.000000
N	−2.330125	0.179391	0.000000
C	−1.396873	1.109504	0.000000
H	−1.570575	2.177254	0.000000
N	−0.131950	0.575992	0.000000

SI-157*
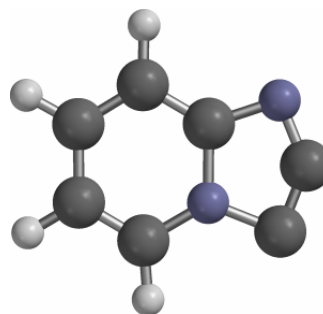
N	−0.387277	−0.718795	0.000000
C	−1.713263	−1.249666	0.000000
C	−2.192037	−0.045979	0.000000
N	−1.711198	1.148708	0.000000
C	−0.406472	0.723768	0.000000
C	0.802570	−1.400705	0.000000
H	0.720900	−2.479883	0.000000
C	1.979120	−0.698476	0.000000
H	2.913910	−1.248406	0.000000
C	1.982898	0.721730	0.000000
H	2.930281	1.251498	0.000000
C	0.802716	1.435800	0.000000
H	0.774939	2.519556	0.000000

SI-156
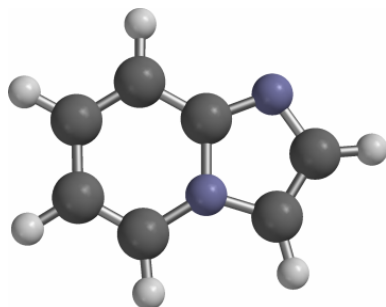
N	0.301270	−0.670655	0.000000
C	−0.859527	−1.405762	0.000000
H	−0.748805	−2.483977	0.000000
C	−2.062688	−0.758186	0.000000
H	−2.974841	−1.344854	0.000000
C	−2.115384	0.665395	0.000000
H	−3.079570	1.163992	0.000000
C	−0.955621	1.401522	0.000000
H	−0.954598	2.485917	0.000000
C	0.294799	0.740774	0.000000
C	1.626549	−1.051249	0.000000
H	1.924399	−2.088805	0.000000
N	1.534692	1.225608	0.000000
C	2.343221	0.128580	0.000000
H	3.421413	0.229373	0.000000

SI-158
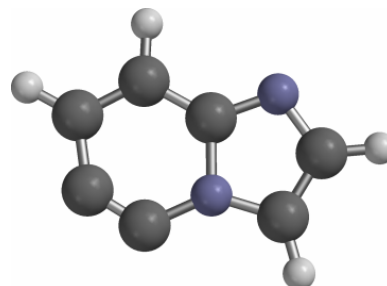
C	1.956281	0.945218	0.000000
C	0.833957	1.469360	0.000000
C	−0.153631	−0.652219	0.000000
C	−1.676252	1.018977	0.000000
H	−2.079497	2.019369	0.000000
N	−0.324416	0.776473	0.000000
N	−1.342834	−1.240959	0.000000
C	−2.261706	−0.233081	0.000000
H	−3.322210	−0.449552	0.000000
C	2.313169	−0.418311	0.000000
H	3.314028	−0.831601	0.000000
C	1.165603	−1.198824	0.000000
H	1.240345	−2.281542	0.000000

SI-159
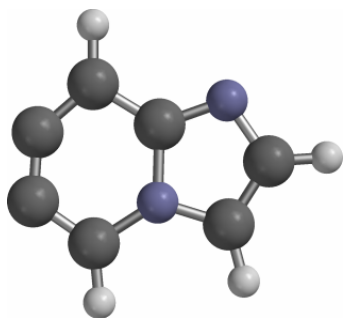
C	2.078096	0.587768	0.000000
C	1.061667	1.479712	0.000000
H	1.068533	2.562072	0.000000
C	2.153808	−0.675355	0.000000
C	1.030715	−1.442329	0.000000
H	0.923821	−2.520975	0.000000
N	−0.142533	−0.688086	0.000000
C	−0.173426	0.744543	0.000000
C	−1.461962	−1.084555	0.000000
H	−1.743680	−2.126598	0.000000
C	−2.205195	0.078945	0.000000
H	−3.285565	0.155531	0.000000
N	−1.421582	1.194032	0.000000

SI-161
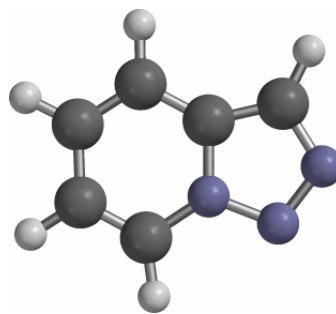
C	0.884290	−1.364703	0.000000
H	0.759331	−2.440149	0.000000
C	0.933747	1.449014	0.000000
H	0.932503	2.533992	0.000000
N	−0.274629	−0.633293	0.000000
C	−0.301904	0.755171	0.000000
C	−1.668009	1.034773	0.000000
H	−2.167270	1.992533	0.000000
N	−2.355528	−0.126783	0.000000
N	−1.533143	−1.151436	0.000000
C	2.102661	0.730107	0.000000
H	3.059057	1.243348	0.000000
C	2.075240	−0.697735	0.000000
H	2.998968	−1.265589	0.000000

SI-160
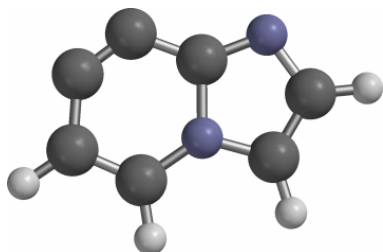
C	2.265243	0.473680	0.000000
H	3.237113	0.949901	0.000000
C	1.090481	1.201514	0.000000
H	1.079827	2.285858	0.000000
C	1.970949	−0.897483	0.000000
C	0.889313	−1.504015	0.000000
C	−0.348238	−0.845880	0.000000
C	−1.414793	1.133340	0.000000
H	−1.583078	2.199636	0.000000
N	−0.143814	0.590685	0.000000
N	−1.629629	−1.141037	0.000000
C	−2.280658	0.063444	0.000000
H	−3.362126	0.107719	0.000000

SI-162
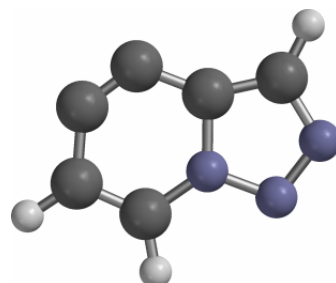
C	2.269703	0.453028	0.000000
H	3.241310	0.929689	0.000000
C	1.982415	−0.924738	0.000000
C	0.901625	−1.530288	0.000000
C	−0.328865	−0.858663	0.000000
C	1.095716	1.176782	0.000000
H	1.050098	2.258833	0.000000
N	−0.130171	0.547081	0.000000
C	−1.708347	−0.976019	0.000000
H	−2.316551	−1.867714	0.000000
N	−2.257364	0.263051	0.000000
N	−1.330590	1.188938	0.000000

SI-163
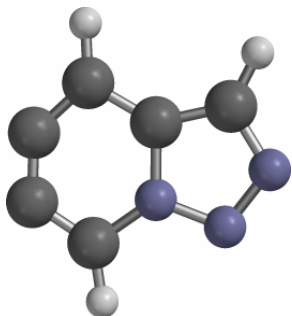
C	1.026232	−1.414449	0.000000
H	0.884907	−2.487577	0.000000
C	2.142561	−0.645165	0.000000
C	2.079622	0.619607	0.000000
C	1.062555	1.511251	0.000000
H	1.090486	2.593881	0.000000
N	−0.136135	−0.640064	0.000000
C	−0.168352	0.766107	0.000000
C	−1.536126	1.033418	0.000000
H	−2.038230	1.989639	0.000000
N	−2.220628	−0.129386	0.000000
N	−1.391536	−1.150999	0.000000

SI-165
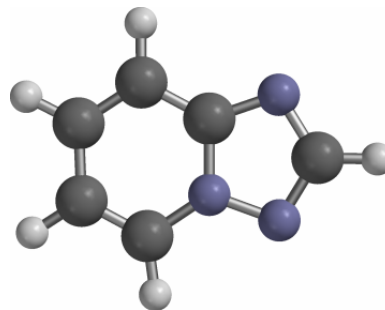
N	−0.310224	−0.636561	0.000000
N	−1.590937	−1.088647	0.000000
C	−2.275659	0.058107	0.000000
H	−3.358178	0.046425	0.000000
N	−1.558798	1.202375	0.000000
C	−0.297361	0.756648	0.000000
C	0.954012	1.411926	0.000000
H	0.973509	2.495787	0.000000
C	2.100509	0.650426	0.000000
H	3.072191	1.134560	0.000000
C	2.032534	−0.770617	0.000000
H	2.937977	−1.366898	0.000000
C	0.817748	−1.403457	0.000000
H	0.663277	−2.474905	0.000000

SI-164
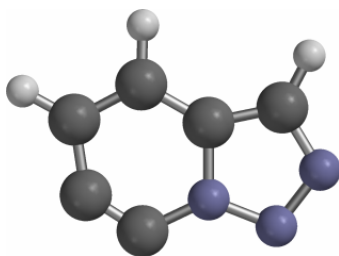
C	1.913232	−0.928176	0.000000
C	−0.157344	0.682186	0.000000
C	0.793614	−1.456871	0.000000
N	−0.342082	−0.724266	0.000000
C	−1.473339	1.134446	0.000000
H	−1.846520	2.148372	0.000000
N	−2.316625	0.077573	0.000000
N	−1.649217	−1.057234	0.000000
C	2.298290	0.424049	0.000000
H	3.304807	0.822239	0.000000
C	1.161859	1.223900	0.000000
H	1.269925	2.304823	0.000000

SI-166
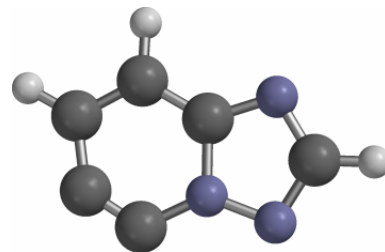
C	1.909945	−0.945109	0.000000
C	−0.169918	0.665755	0.000000
C	0.785252	−1.469555	0.000000
N	−0.345829	−0.744625	0.000000
N	−1.380563	1.222595	0.000000
C	−2.215867	0.158621	0.000000
H	−3.292524	0.265799	0.000000
N	−1.658494	−1.056289	0.000000
C	2.282746	0.407950	0.000000
H	3.289116	0.808164	0.000000
C	1.146872	1.210712	0.000000
H	1.238209	2.291854	0.000000

SI-167
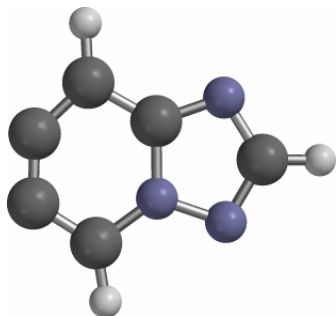
C	0.996719	−1.436848	0.000000
H	0.857413	−2.510473	0.000000
C	2.124548	−0.671518	0.000000
C	2.059041	0.589892	0.000000
C	1.048568	1.494896	0.000000
H	1.069729	2.576914	0.000000
C	−0.179894	0.756439	0.000000
N	−1.451978	1.155312	0.000000
C	−2.136042	−0.009071	0.000000
H	−3.217871	−0.050972	0.000000
N	−1.417132	−1.134627	0.000000
N	−0.149538	−0.660102	0.000000

SI-169
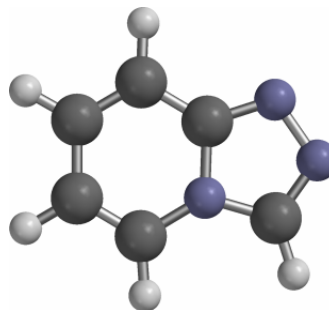
N	−0.312396	−0.663455	0.000000
N	−1.528803	1.209701	0.000000
C	−0.287842	0.737217	0.000000
C	0.971174	1.392243	0.000000
H	0.985892	2.476231	0.000000
C	2.113174	0.636345	0.000000
H	3.086378	1.116966	0.000000
C	2.041803	−0.793156	0.000000
H	2.948787	−1.387469	0.000000
C	0.835344	−1.426172	0.000000
H	0.705507	−2.501926	0.000000
N	−2.369981	0.132227	0.000000
C	−1.650290	−0.969331	0.000000
H	−2.031127	−1.980297	0.000000

SI-168
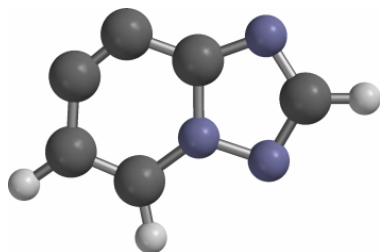
C	2.245510	0.471106	0.000000
H	3.217060	0.947429	0.000000
C	−0.351616	−0.851251	0.000000
C	1.066621	1.195283	0.000000
H	1.021002	2.277273	0.000000
N	−0.149238	0.561372	0.000000
N	−1.651043	−1.100422	0.000000
C	−2.197159	0.140810	0.000000
H	−3.267113	0.302915	0.000000
N	−1.360342	1.177018	0.000000
C	1.952491	−0.899236	0.000000
C	0.877698	−1.520328	0.000000

SI-170
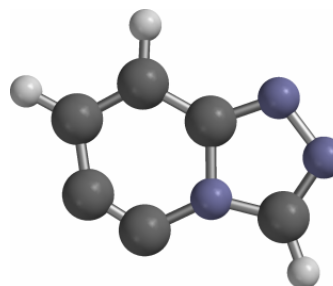
C	−0.799113	−1.488208	0.000000
C	−1.922355	−0.969747	0.000000
C	−2.303681	0.390987	0.000000
H	−3.312265	0.784635	0.000000
C	−1.175378	1.191886	0.000000
H	−1.267854	2.273016	0.000000
C	0.153101	0.654300	0.000000
N	1.340737	1.237853	0.000000
N	2.293618	0.254317	0.000000
C	1.700893	−0.922440	0.000000
H	2.189326	−1.885126	0.000000
N	0.343772	−0.759734	0.000000

SI-171
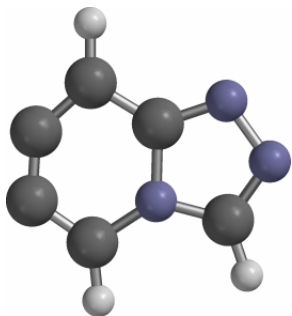
C	1.004028	−1.458906	0.000000
H	0.878496	−2.535217	0.000000
C	2.130731	−0.705787	0.000000
C	2.067297	0.561331	0.000000
C	1.074016	1.471575	0.000000
H	1.097377	2.553605	0.000000
C	−0.172013	0.741767	0.000000
N	−1.421628	1.179615	0.000000
N	−2.238466	0.083525	0.000000
C	−1.491847	−1.001379	0.000000
H	−1.855810	−2.018561	0.000000
N	−0.159721	−0.677464	0.000000

SI-173
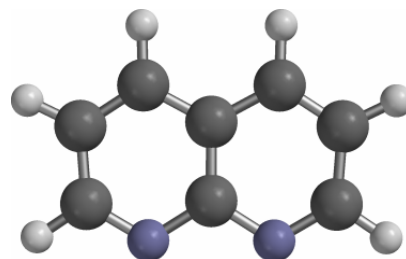
N	−1.154884	0.000000	1.426752
C	−2.292941	0.000000	0.763537
H	−3.199960	0.000000	1.368311
C	−2.403481	0.000000	−0.651109
H	−3.383432	0.000000	−1.118662
C	−1.250124	0.000000	−1.397122
H	−1.277887	0.000000	−2.484697
C	0.000000	0.000000	−0.729176
C	0.000000	0.000000	0.704072
N	1.154884	0.000000	1.426752
C	2.292941	0.000000	0.763537
H	3.199960	0.000000	1.368311
C	2.403481	0.000000	−0.651109
H	3.383432	0.000000	−1.118662
C	1.250124	0.000000	−1.397122
H	1.277887	0.000000	−2.484697

SI-172
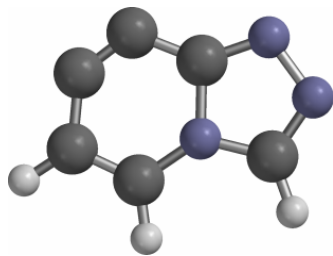
C	1.073968	−1.217013	0.000000
H	1.056947	−2.301013	0.000000
C	2.244588	−0.490724	0.000000
H	3.217280	−0.964810	0.000000
C	1.951331	0.885237	0.000000
C	0.879681	1.504838	0.000000
C	−0.356122	0.833775	0.000000
N	−1.641132	1.106344	0.000000
N	−2.313454	−0.091849	0.000000
C	−1.443138	−1.075273	0.000000
H	−1.686337	−2.128178	0.000000
N	−0.157998	−0.591533	0.000000

SI-174
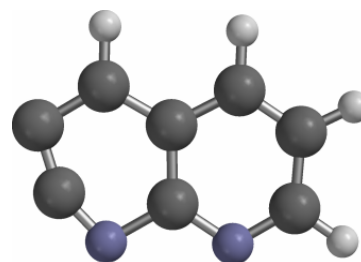
C	2.179473	−0.551313	0.000000
C	2.575007	0.678067	0.000000
C	1.372017	1.400887	0.000000
H	1.353123	2.492578	0.000000
C	0.114542	0.698772	0.000000
C	0.082499	−0.745265	0.000000
N	1.309613	−1.442627	0.000000
C	−1.142812	1.347742	0.000000
H	−1.182862	2.434363	0.000000
C	−2.295842	0.592862	0.000000
H	−3.275712	1.059831	0.000000
C	−2.188685	−0.815690	0.000000
H	−3.089837	−1.426983	0.000000
N	−1.040565	−1.476687	0.000000

SI-175
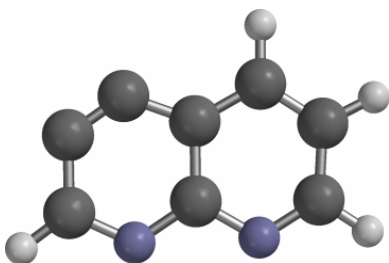
C	−0.135225	−0.614459	0.000000
C	0.005487	0.849724	0.000000
C	−1.258679	1.446855	0.000000
C	−2.348442	0.839843	0.000000
C	−2.477043	−0.570158	0.000000
H	−3.413194	−1.120024	0.000000
N	−1.343943	−1.243171	0.000000
C	1.300047	1.407052	0.000000
H	1.418896	2.485980	0.000000
C	2.383926	0.557776	0.000000
H	3.400047	0.940117	0.000000
C	2.155276	−0.838152	0.000000
H	3.006206	−1.518665	0.000000
N	0.965380	−1.408175	0.000000

SI-177
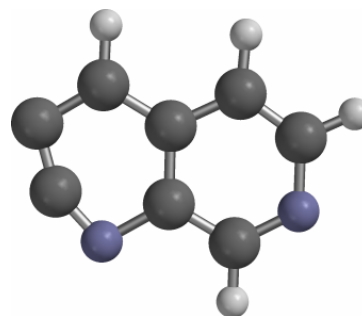
N	1.339261	1.434591	0.000000
C	0.117448	0.722607	0.000000
C	0.114503	−0.711029	0.000000
C	1.365686	−1.434724	0.000000
H	1.338453	−2.525315	0.000000
C	2.201736	0.531017	0.000000
C	2.559712	−0.707287	0.000000
C	−1.109823	1.421606	0.000000
H	−1.095363	2.509936	0.000000
N	−2.280748	0.812127	0.000000
C	−2.293911	−0.544911	0.000000
H	−3.280189	−1.002868	0.000000
C	−1.159155	−1.329640	0.000000
	−1.237216	−2.413502	0.000000

SI-176
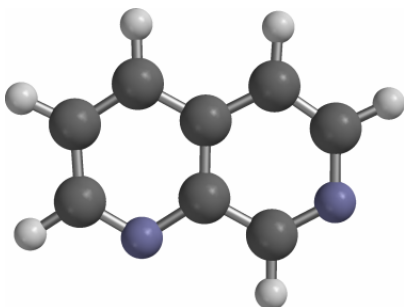
N	−1.175124	−1.412317	0.000000
C	−2.310244	−0.744550	0.000000
H	−3.222503	−1.340168	0.000000
C	−2.402088	0.673410	0.000000
H	−3.379014	1.147830	0.000000
C	−1.247427	1.418035	0.000000
H	−1.274463	2.505071	0.000000
C	0.000989	0.742794	0.000000
C	−0.023480	−0.682445	0.000000
C	1.268634	1.376671	0.000000
H	1.338537	2.461550	0.000000
C	1.225360	−1.366736	0.000000
H	1.210763	−2.455733	0.000000
N	2.395796	−0.763815	0.000000
C	2.404044	0.598474	0.000000
H	3.389750	1.058630	0.000000

SI-178
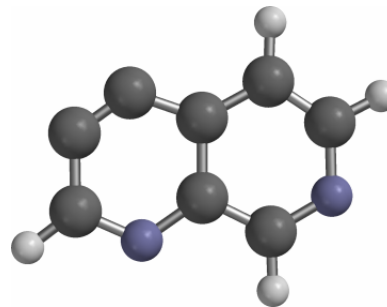
N	1.359917	−1.221453	0.000000
C	2.495572	−0.544438	0.000000
H	3.433860	−1.089257	0.000000
C	2.345574	0.861235	0.000000
C	1.255019	1.466392	0.000000
C	−0.009583	0.862474	0.000000
C	0.159898	−0.589244	0.000000
C	−1.318187	1.382769	0.000000
H	−1.481875	2.455198	0.000000
C	−2.378802	0.500092	0.000000
H	−3.400673	0.872531	0.000000
N	−2.250990	−0.851694	0.000000
C	−1.035981	−1.362409	0.000000
H	−0.943483	−2.446675	0.000000

SI-179
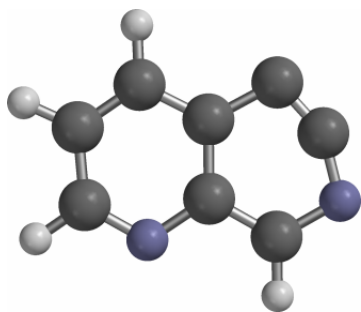

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N    -1.008693    -1.391635    0.000000
C    -2.173070    -0.776085    0.000000
H    -3.055505    -1.414734    0.000000
C    -2.333533     0.634640    0.000000
H    -3.334112     1.057552    0.000000
C    -1.220098     1.442620    0.000000
H    -1.293081     2.525718    0.000000
C     0.062907     0.838485    0.000000
C     0.110568    -0.611355    0.000000
C     1.322258     1.551503    0.000000
C     2.197871     0.640632    0.000000
N     2.538707    -0.597680    0.000000
C     1.375810    -1.282466    0.000000
H     1.419286    -2.366741    0.000000
```

SI-181
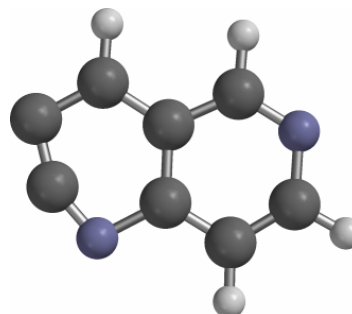

```
N     1.336936    -1.463848    0.000000
C     0.117373    -0.750891    0.000000
C     0.132589     0.684685    0.000000
C     1.382621     1.400501    0.000000
H     1.361667     2.491415    0.000000
C     2.576400     0.667756    0.000000
C     2.206974    -0.564489    0.000000
C    -1.134321     1.327858    0.000000
H    -1.172095     2.417467    0.000000
N    -2.292382     0.696347    0.000000
C    -2.270049    -0.660929    0.000000
H    -3.243992    -1.144963    0.000000
C    -1.117544    -1.422550    0.000000
H    -1.144709    -2.506749    0.000000
```

SI-180
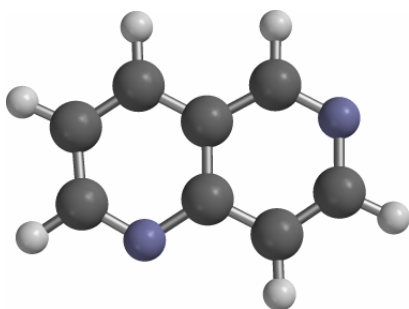

```
N    -1.171314    -1.446884    0.000000
C    -2.306763    -0.776897    0.000000
H    -3.216767    -1.376704    0.000000
C    -2.410319     0.639398    0.000000
H    -3.389701     1.107932    0.000000
C    -1.255658     1.384987    0.000000
H    -1.281894     2.472367    0.000000
C    -0.010139     0.710558    0.000000
C    -0.017733    -0.716075    0.000000
C     1.237192    -1.374213    0.000000
H     1.263061    -2.458998    0.000000
C     2.387727    -0.618649    0.000000
H     3.363965    -1.098290    0.000000
N     2.409610     0.744349    0.000000
C     1.250170     1.368037    0.000000
H     1.278605     2.458976    0.000000
```

SI-182
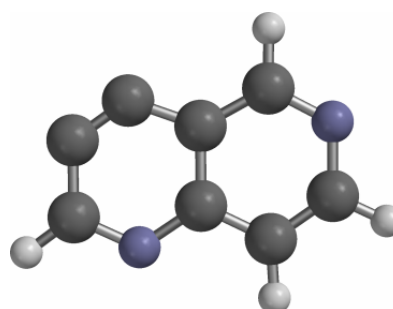

```
N     1.352727    -1.257358    0.000000
C     2.488181    -0.577518    0.000000
H     3.425158    -1.125372    0.000000
C     2.346559     0.826625    0.000000
C     1.258359     1.436726    0.000000
C    -0.003500     0.830403    0.000000
C     0.150323    -0.623935    0.000000
C    -1.308058     1.374364    0.000000
H    -1.432670     2.455927    0.000000
N    -2.404292     0.639628    0.000000
C    -2.261969    -0.711315    0.000000
H    -3.191493    -1.276147    0.000000
C    -1.052036    -1.372940    0.000000
H    -0.999305    -2.456316    0.000000
```

SI-183
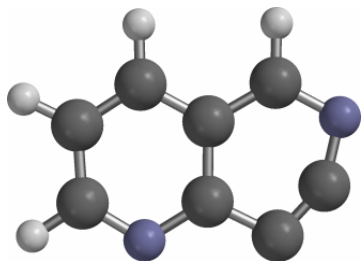
N	1.170209	−1.473559	0.000000
C	−0.023223	−0.830701	0.000000
C	−0.117177	0.625558	0.000000
C	1.094334	1.362419	0.000000
H	1.067720	2.449708	0.000000
C	2.288064	0.681068	0.000000
H	3.238671	1.205215	0.000000
C	2.265419	−0.736256	0.000000
H	3.208275	−1.282916	0.000000
C	−1.390478	1.269830	0.000000
H	−1.469945	2.354191	0.000000
N	−2.551379	0.579136	0.000000
C	−2.194239	−0.661915	0.000000
C	−1.282596	−1.527698	0.000000

SI-185
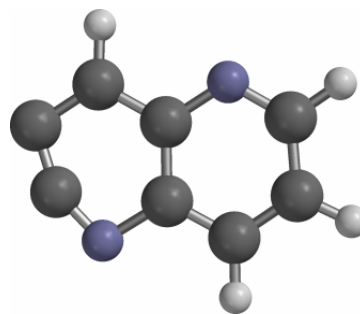
C	2.201548	−0.532924	0.000000
C	2.549619	0.704375	0.000000
C	1.347602	1.421882	0.000000
H	1.286634	2.509498	0.000000
C	0.104962	0.685789	0.000000
C	0.123538	−0.755558	0.000000
N	1.349078	−1.451484	0.000000
N	−1.065300	1.379854	0.000000
C	−2.192264	0.691896	0.000000
H	−3.111326	1.276359	0.000000
C	−2.265344	−0.721836	0.000000
H	−3.234067	−1.212154	0.000000
C	−1.098150	−1.455020	0.000000
H	−1.087522	−2.540478	0.000000

SI-184
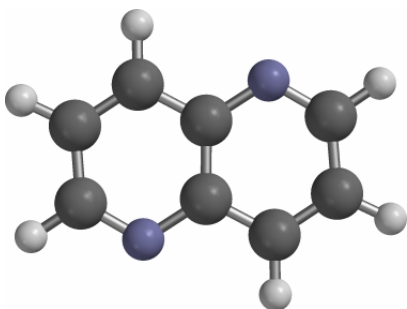
N	−1.183714	−1.425847	0.000000
C	−2.309995	−0.740590	0.000000
H	−3.229130	−1.325859	0.000000
C	−2.385144	0.676573	0.000000
H	−3.355940	1.163540	0.000000
C	−1.219162	1.404807	0.000000
H	−1.206125	2.490659	0.000000
C	0.019659	0.714465	0.000000
C	−0.019659	−0.714465	0.000000
N	1.183714	1.425847	0.000000
C	2.309995	0.740590	0.000000
H	3.229130	1.325859	0.000000
C	2.385144	−0.676573	0.000000
H	3.355940	−1.163540	0.000000
C	1.219162	−1.404807	0.000000
H	1.206125	−2.490659	0.000000

SI-186
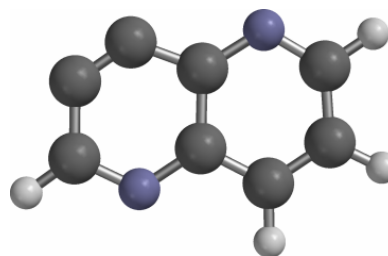
C	2.315177	0.648367	0.000000
H	3.280815	1.151720	0.000000
C	2.261448	−0.764080	0.000000
H	3.183604	−1.337287	0.000000
C	1.035665	−1.391907	0.000000
H	0.941848	−2.473065	0.000000
C	−0.147979	−0.612430	0.000000
C	0.041168	0.846229	0.000000
N	1.250912	1.432921	0.000000
N	−1.355781	−1.233148	0.000000
C	−2.482086	−0.539625	0.000000
H	−3.426552	−1.073884	0.000000
C	−2.315998	0.861270	0.000000
C	−1.222946	1.463237	0.000000

SI-187
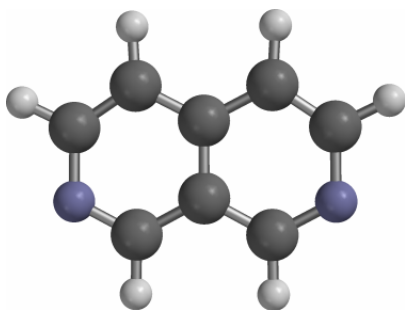

```
C    1.251535    0.000000    1.354816
H    1.270763    0.000000    2.445554
N    2.416952    0.000000    0.741446
C    2.404200    0.000000   -0.621829
H    3.384291    0.000000   -1.093889
C    1.260950    0.000000   -1.388819
H    1.320878    0.000000   -2.473699
C    0.000000    0.000000   -0.740290
C    0.000000    0.000000    0.683241
C   -1.251535    0.000000    1.354816
H   -1.270763    0.000000    2.445554
N   -2.416952    0.000000    0.741446
C   -2.404200    0.000000   -0.621829
H   -3.384291    0.000000   -1.093889
C   -1.260950    0.000000   -1.388819
H   -1.320878    0.000000   -2.473699
```

SI-189
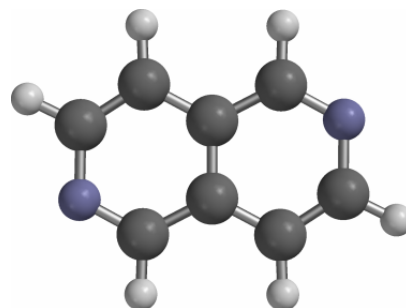

```
C    1.248628   -1.381357    0.000000
H    1.270291   -2.471874    0.000000
N    2.411206   -0.764291    0.000000
C    2.408706    0.598805    0.000000
H    3.390597    1.066165    0.000000
C    1.264399    1.363379    0.000000
H    1.319952    2.448765    0.000000
C    0.007366    0.711146    0.000000
C   -0.007366   -0.711146    0.000000
C   -1.248628    1.381357    0.000000
H   -1.270291    2.471874    0.000000
N   -2.411206    0.764291    0.000000
C   -2.408706   -0.598805    0.000000
H   -3.390597   -1.066165    0.000000
C   -1.264399   -1.363379    0.000000
H   -1.319952   -2.448765    0.000000
```

SI-188
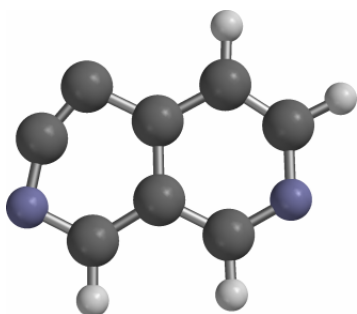

```
C    1.086644   -1.342577    0.000000
H    1.058379   -2.432924    0.000000
N    2.278091   -0.784126    0.000000
C    2.335033    0.576785    0.000000
H    3.338580    0.996847    0.000000
C    1.234938    1.408044    0.000000
H    1.343827    2.487248    0.000000
C   -0.057792    0.834470    0.000000
C   -0.135287   -0.613439    0.000000
C   -1.401921   -1.266921    0.000000
H   -1.485033   -2.350510    0.000000
N   -2.558700   -0.567760    0.000000
C   -2.203973    0.668314    0.000000
C   -1.311068    1.559767    0.000000
```

SI-190
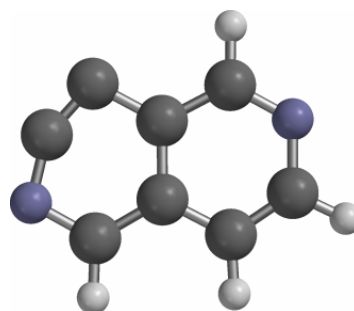

```
C    1.392920    1.298124    0.000000
H    1.480944    2.380967    0.000000
N    2.543613    0.590181    0.000000
C    2.195263   -0.643414    0.000000
C    1.306722   -1.544297    0.000000
C    0.062526   -0.801974    0.000000
C    0.122766    0.644159    0.000000
C   -1.106919    1.351918    0.000000
H   -1.117712    2.438714    0.000000
C   -2.284563    0.640064    0.000000
H   -3.241768    1.156121    0.000000
N   -2.354375   -0.719542    0.000000
C   -1.228248   -1.402142    0.000000
H   -1.294360   -2.488845    0.000000
```

SI-191
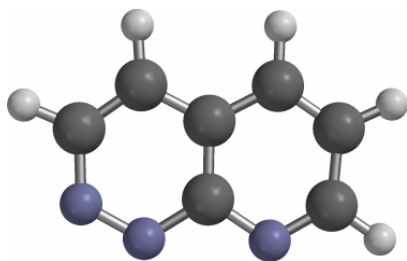
C	−0.024519	−0.672748	0.000000
N	−1.203003	−1.367333	0.000000
N	−2.336803	−0.721664	0.000000
C	−2.354504	0.641549	0.000000
H	−3.349288	1.076989	0.000000
C	−1.219570	1.418875	0.000000
H	−1.273495	2.505011	0.000000
C	0.021184	0.752292	0.000000
C	1.293780	1.382753	0.000000
H	1.359099	2.468239	0.000000
C	2.414053	0.592276	0.000000
H	3.411374	1.021606	0.000000
C	2.255856	−0.823313	0.000000
H	3.142954	−1.456141	0.000000
N	1.098506	−1.445395	0.000000

SI-193
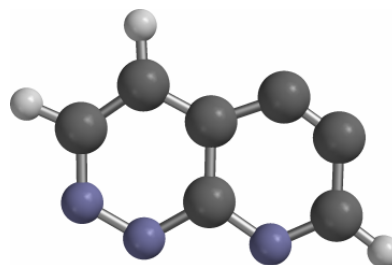
N	2.161543	0.902226	0.000000
N	0.956668	1.403049	0.000000
C	2.353641	−0.442378	0.000000
H	3.395681	−0.747926	0.000000
C	1.329566	−1.366535	0.000000
H	1.523809	−2.434012	0.000000
C	0.020899	−0.868750	0.000000
C	−0.136641	0.585932	0.000000
N	−1.344828	1.211913	0.000000
C	−2.470654	0.531983	0.000000
H	−3.411266	1.073583	0.000000
C	−1.238198	−1.481241	0.000000
C	−2.331890	−0.882233	0.000000

SI-192
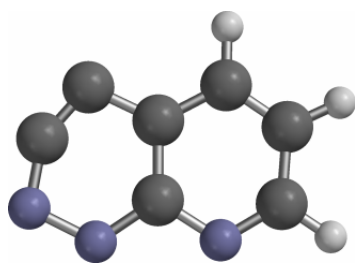
N	2.486148	0.674446	0.000000
N	1.301175	1.331486	0.000000
C	2.204103	−0.586833	0.000000
C	1.326699	−1.497657	0.000000
C	0.063375	−0.838125	0.000000
C	−1.220330	−1.443621	0.000000
H	−1.295138	−2.526422	0.000000
C	0.133740	0.619276	0.000000
C	−2.324820	−0.630018	0.000000
H	−3.329657	−1.041909	0.000000
N	−0.987812	1.398836	0.000000
C	−2.147974	0.784063	0.000000
H	−3.028003	1.426459	0.000000

SI-194
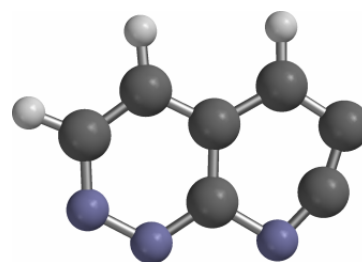
N	2.212354	0.873751	0.000000
N	1.043145	1.473533	0.000000
C	2.283430	−0.479614	0.000000
H	3.294781	−0.875015	0.000000
C	1.180703	−1.311977	0.000000
H	1.290689	−2.393319	0.000000
C	−0.091876	−0.715908	0.000000
C	−1.345008	−1.435957	0.000000
H	−1.318827	−2.526832	0.000000
C	−0.074364	0.722690	0.000000
C	−2.539065	−0.709523	0.000000
N	−1.300775	1.426121	0.000000
C	−2.160509	0.527176	0.000000

SI-195
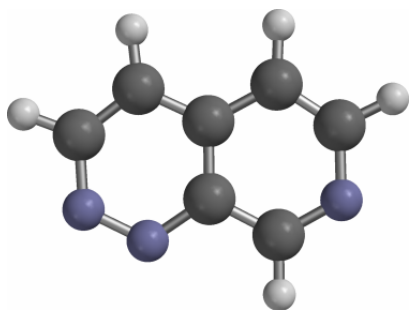
C	−0.034555	−0.660050	0.000000
N	−1.188349	−1.387747	0.000000
N	−2.339388	−0.772589	0.000000
C	−2.376351	0.592813	0.000000
H	−3.379661	1.008653	0.000000
C	−1.260783	1.398736	0.000000
H	−1.344642	2.482359	0.000000
C	−0.002809	0.760317	0.000000
C	1.268111	1.388631	0.000000
H	1.347766	2.472291	0.000000
C	2.392472	0.597107	0.000000
H	3.382734	1.046798	0.000000
N	2.376083	−0.769228	0.000000
C	1.204485	−1.364399	0.000000
H	1.177825	−2.452758	0.000000

SI-197
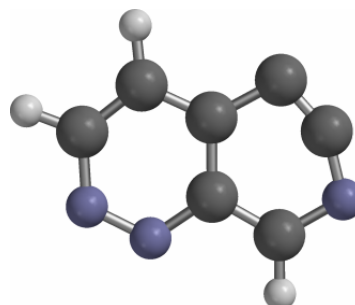
N	−0.996713	−1.384415	0.000000
N	−2.180779	−0.838646	0.000000
C	−2.303449	0.520511	0.000000
H	−3.331609	0.871119	0.000000
C	−1.244149	1.402677	0.000000
H	−1.391256	2.477864	0.000000
C	0.053305	0.855062	0.000000
C	0.113426	−0.589149	0.000000
C	1.380322	−1.261232	0.000000
H	1.428495	−2.345298	0.000000
C	1.307959	1.577803	0.000000
C	2.187194	0.672322	0.000000
N	2.533650	−0.567812	0.000000

SI-196
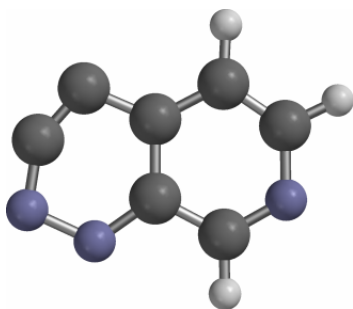
N	2.506239	0.651682	0.000000
N	1.317201	1.306824	0.000000
C	2.221128	−0.614443	0.000000
C	1.323966	−1.501649	0.000000
C	0.055520	−0.849445	0.000000
C	0.158798	0.600700	0.000000
C	−1.240482	−1.415520	0.000000
H	−1.363717	−2.493101	0.000000
C	−2.325775	−0.568471	0.000000
H	−3.335526	−0.972062	0.000000
C	−1.061241	1.351000	0.000000
H	−1.002451	2.437447	0.000000
N	−2.249381	0.795366	0.000000

SI-198
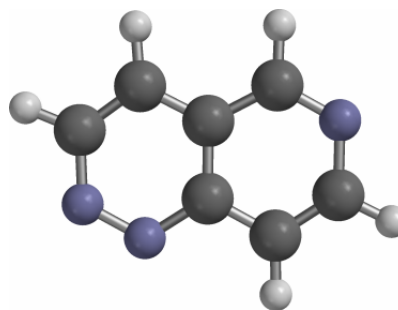
C	−0.019789	−0.691909	0.000000
N	−1.169496	−1.435825	0.000000
N	−2.325329	−0.830735	0.000000
C	−2.390879	0.532264	0.000000
H	−3.401335	0.929825	0.000000
C	−1.284902	1.352673	0.000000
H	−1.379808	2.435683	0.000000
C	−0.023381	0.729108	0.000000
C	1.235296	1.396790	0.000000
H	1.261159	2.487232	0.000000
C	1.232854	−1.355812	0.000000
H	1.257027	−2.440506	0.000000
N	2.390484	0.770842	0.000000
C	2.378261	−0.595825	0.000000
H	3.358080	−1.066666	0.000000

SI-199
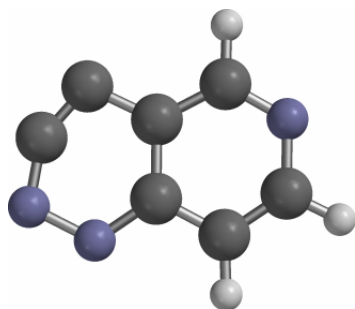
N	2.495582	0.672495	0.000000
N	1.312485	1.344372	0.000000
C	2.210597	−0.584601	0.000000
C	1.323921	−1.489449	0.000000
C	0.066455	−0.816034	0.000000
C	0.149985	0.634237	0.000000
C	−1.228790	−1.409484	0.000000
H	−1.308559	−2.495291	0.000000
C	−1.074512	1.358703	0.000000
H	−1.054277	2.443098	0.000000
C	−2.252936	0.653192	0.000000
H	−3.205689	1.176647	0.000000
N	−2.340997	−0.710355	0.000000

SI-201
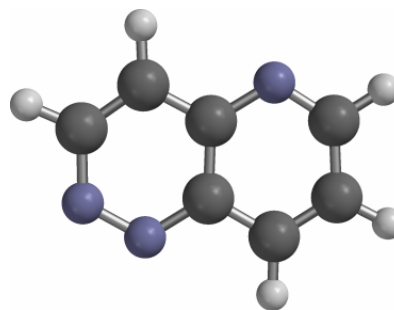
C	−0.016404	−0.694773	0.000000
N	−1.170384	−1.425694	0.000000
N	−2.323251	−0.812390	0.000000
C	−2.368361	0.550722	0.000000
H	−3.373494	0.962339	0.000000
C	−1.254682	1.361211	0.000000
H	−1.319054	2.444843	0.000000
C	0.003722	0.729107	0.000000
C	1.224844	−1.383640	0.000000
H	1.217023	−2.469431	0.000000
C	2.379690	−0.642447	0.000000
H	3.357436	−1.114483	0.000000
N	1.158724	1.457894	0.000000
C	2.287147	0.778301	0.000000
H	3.202210	1.369767	0.000000

SI-200
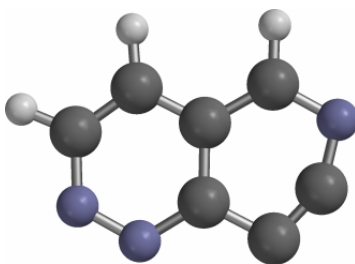
N	2.295003	0.776205	0.000000
N	1.180611	1.460557	0.000000
C	2.276251	−0.585658	0.000000
H	3.259957	−1.045381	0.000000
C	1.124240	−1.339602	0.000000
H	1.160652	−2.426287	0.000000
C	−0.101228	−0.645307	0.000000
C	−0.014860	0.803190	0.000000
C	−1.264120	1.520707	0.000000
C	−2.170585	0.647943	0.000000
C	−1.376379	−1.295069	0.000000
H	−1.460378	−2.378810	0.000000
N	−2.525818	−0.592623	0.000000

SI-202
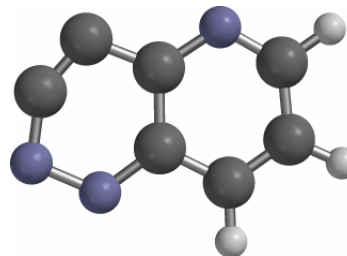
N	2.496477	0.645761	0.000000
N	1.312844	1.305287	0.000000
C	2.204561	−0.623668	0.000000
C	1.286648	−1.486662	0.000000
C	0.019176	−0.844602	0.000000
C	0.143446	0.615023	0.000000
N	−1.177959	−1.473343	0.000000
C	−2.259126	−0.719221	0.000000
H	−3.211418	−1.248319	0.000000
C	−2.257261	0.703297	0.000000
H	−3.201931	1.238126	0.000000
C	−1.061522	1.374147	0.000000
H	−0.998090	2.457477	0.000000

SI-203
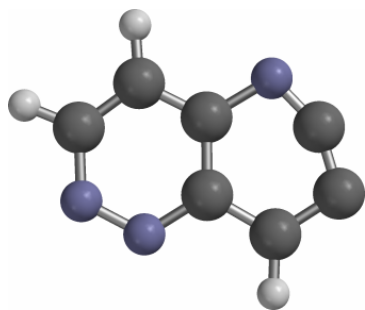
N	2.204295	0.751924	0.000000
N	1.053457	1.375117	0.000000
C	2.241861	-0.606172	0.000000
H	3.243158	-1.026795	0.000000
C	1.123405	-1.417985	0.000000
H	1.186753	-2.501141	0.000000
C	-0.115902	-0.771743	0.000000
C	-0.109707	0.665174	0.000000
N	-1.333151	-1.485203	0.000000
C	-2.192130	-0.571120	0.000000
C	-2.539909	0.666021	0.000000
C	-1.353926	1.402302	0.000000
H	-1.300528	2.489860	0.000000

SI-205
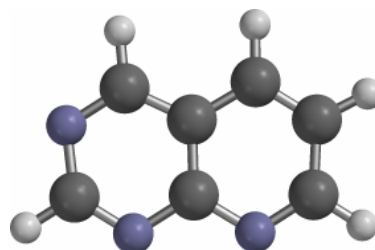
C	-0.017092	-0.712585	0.000000
N	-1.197838	-1.389985	0.000000
C	0.001694	0.713949	0.000000
C	-2.292773	-0.661773	0.000000
H	-3.239022	-1.199455	0.000000
C	1.250465	1.380447	0.000000
H	1.286304	2.467615	0.000000
C	-1.260598	1.358996	0.000000
H	-1.314421	2.449164	0.000000
N	-2.399020	0.698800	0.000000
N	1.124088	-1.453751	0.000000
C	2.266644	-0.795785	0.000000
H	3.168738	-1.407566	0.000000
C	2.394103	0.619371	0.000000
H	3.380586	1.072362	0.000000

SI-204
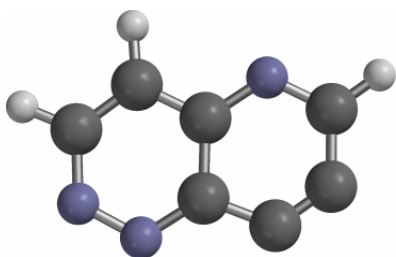
N	2.347546	0.683387	0.000000
N	1.258874	1.414255	0.000000
C	0.049692	0.818158	0.000000
C	-0.135170	-0.634536	0.000000
C	1.062930	-1.371591	0.000000
H	1.033438	-2.456247	0.000000
C	2.252516	-0.670878	0.000000
H	3.209187	-1.184939	0.000000
N	-1.342320	-1.259506	0.000000
C	-2.464461	-0.561298	0.000000
H	-3.410383	-1.093270	0.000000
C	-2.300187	0.842812	0.000000
C	-1.209316	1.445610	0.000000

SI-206
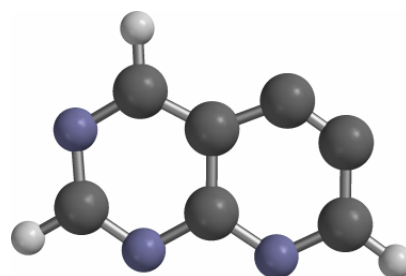
C	2.163743	0.745703	0.000000
H	3.056926	1.367009	0.000000
N	2.388204	-0.594655	0.000000
C	1.315249	-1.362554	0.000000
H	1.464841	-2.441079	0.000000
C	0.008053	-0.831614	0.000000
C	-1.253530	-1.433475	0.000000
C	-2.333631	-0.808817	0.000000
C	-0.116528	0.625140	0.000000
N	1.009416	1.381276	0.000000
N	-1.314606	1.269587	0.000000
C	-2.452457	0.600975	0.000000
H	-3.384863	1.157110	0.000000

SI-207
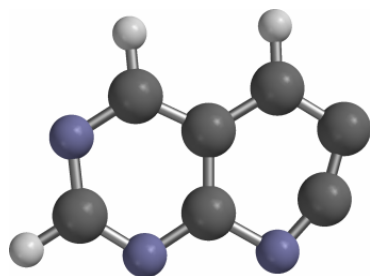
C	2.161203	−0.593089	0.000000
C	2.562147	0.632208	0.000000
C	1.378074	1.383165	0.000000
H	1.376121	2.474401	0.000000
C	0.119734	0.687278	0.000000
N	1.276290	−1.474161	0.000000
C	0.067562	−0.750289	0.000000
N	−1.084672	−1.434743	0.000000
C	−2.188186	−0.704516	0.000000
H	−3.130292	−1.247803	0.000000
N	−2.287055	0.647624	0.000000
C	−1.148460	1.316868	0.000000
H	−1.213797	2.405227	0.000000

SI-209
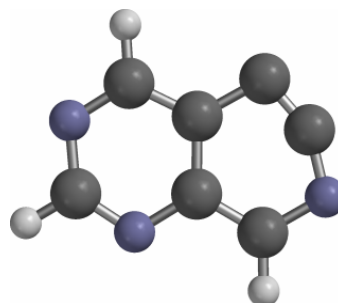
N	2.334215	−0.670705	0.000000
C	2.177901	0.684366	0.000000
H	3.101096	1.259516	0.000000
N	1.053457	1.365555	0.000000
C	1.236291	−1.396571	0.000000
H	1.336557	−2.481122	0.000000
C	−0.092334	0.626133	0.000000
C	−0.062322	−0.815897	0.000000
C	−1.309599	−1.550298	0.000000
C	−2.175289	−0.624176	0.000000
N	−2.506667	0.612562	0.000000
C	−1.350822	1.308740	0.000000
H	−1.400269	2.392482	0.000000

SI-208
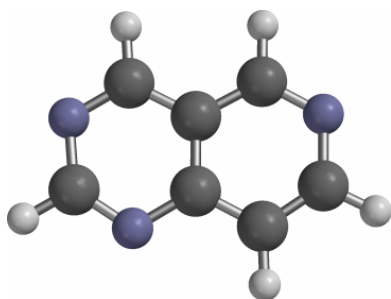
C	−0.045606	−0.719113	0.000000
N	−1.237024	−1.385815	0.000000
C	0.001391	0.701461	0.000000
C	1.187586	−1.413930	0.000000
H	1.190055	−2.498795	0.000000
C	2.353816	−0.680583	0.000000
H	3.318626	−1.182664	0.000000
C	−2.317269	−0.634608	0.000000
H	−3.274228	−1.152861	0.000000
C	1.269786	1.337826	0.000000
H	1.324738	2.427297	0.000000
N	2.412001	0.682437	0.000000
C	−1.246590	1.371134	0.000000
H	−1.284640	2.461585	0.000000
N	−2.396275	0.728194	0.000000

SI-210
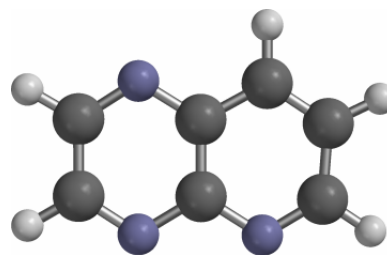
C	−0.021495	−0.716949	0.000000
N	−1.184641	−1.428949	0.000000
C	−0.012986	0.713333	0.000000
C	1.222100	−1.396537	0.000000
H	1.221279	−2.482548	0.000000
C	2.375607	−0.650280	0.000000
H	3.355078	−1.119017	0.000000
N	1.137843	1.437390	0.000000
C	2.272602	0.766666	0.000000
H	3.182701	1.366021	0.000000
N	−1.180922	1.415887	0.000000
C	−2.286760	0.703834	0.000000
H	−3.230504	1.248488	0.000000
C	−2.292256	−0.718971	0.000000
H	−3.236263	−1.261872	0.000000

SI-211
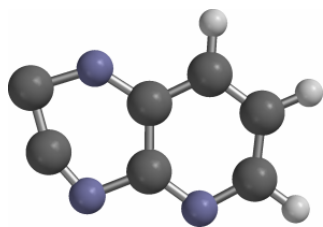

```
C     2.170855     -0.527587      0.000000
C     2.645453      0.785236      0.000000
N     1.292574     -1.382832      0.000000
N     1.343933      1.302188      0.000000
C     0.140835      0.659850      0.000000
C    -1.080953      1.373006      0.000000
H    -1.062521      2.457804      0.000000
C     0.034427     -0.774946      0.000000
N    -1.094518     -1.475546      0.000000
C    -2.215485     -0.763258      0.000000
H    -3.142843     -1.332115      0.000000
C    -2.257207      0.650291      0.000000
H    -3.218827      1.153721      0.000000
```

SI-213
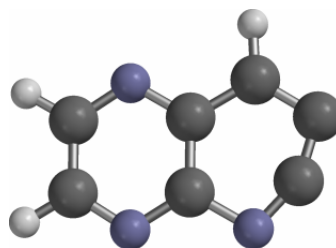

```
C     2.175521      0.773334      0.000000
H     3.109445      1.332475      0.000000
C     2.191217     -0.643674      0.000000
H     3.138890     -1.178978      0.000000
N     1.088175     -1.367296      0.000000
N     1.055269      1.475130      0.000000
C    -0.080220      0.759395      0.000000
C    -0.087692     -0.686024      0.000000
N    -1.300791      1.456093      0.000000
C    -1.332839     -1.411603      0.000000
H    -1.282850     -2.499959      0.000000
C    -2.531789     -0.685885      0.000000
C    -2.159074      0.547342      0.000000
```

SI-212
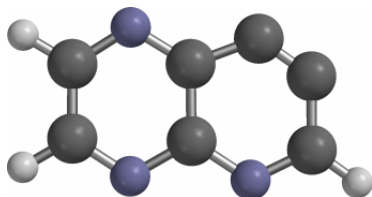

```
C     2.155625      0.806089      0.000000
H     3.037029      1.445615      0.000000
C     2.303102     -0.602695      0.000000
H     3.294173     -1.052523      0.000000
N     0.982187      1.406139      0.000000
N     1.266957     -1.419361      0.000000
C     0.050567     -0.845925      0.000000
C    -1.207974     -1.469397      0.000000
C    -0.120453      0.616594      0.000000
N    -1.330190      1.237726      0.000000
C    -2.452284      0.546114      0.000000
H    -3.397186      1.080163      0.000000
C    -2.296995     -0.860194      0.000000
```

SI-214
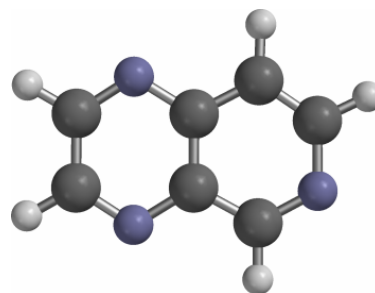

```
C    -0.029290     -0.729889      0.000000
N    -1.193756     -1.445635      0.000000
C    -0.039366      0.693574      0.000000
C     1.227256     -1.380587      0.000000
H     1.265455     -2.465184      0.000000
C     2.367931     -0.608480      0.000000
H     3.350030     -1.075685      0.000000
N    -1.201696      1.404907      0.000000
C    -2.306751      0.691454      0.000000
H    -3.253072      1.230127      0.000000
C    -2.299778     -0.733673      0.000000
H    -3.243125     -1.278434      0.000000
C     1.210692      1.372382      0.000000
H     1.206927      2.461555      0.000000
N     2.373376      0.754944      0.000000
```

SI-215
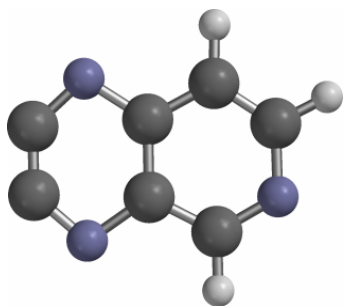

```
N    1.329486      1.479770      0.000000
C    0.157648      0.705792      0.000000
C    0.146264     -0.735339      0.000000
N    1.320199     -1.516343      0.000000
C    2.293298     -0.651336      0.000000
C    2.300133      0.610349      0.000000
C   -1.093356      1.376907      0.000000
H   -1.090188      2.465317      0.000000
N   -2.255566      0.755830      0.000000
C   -2.252367     -0.601886      0.000000
H   -3.232648     -1.072344      0.000000
C   -1.110371     -1.376065      0.000000
H   -1.151529     -2.460194      0.000000
```

SI-216
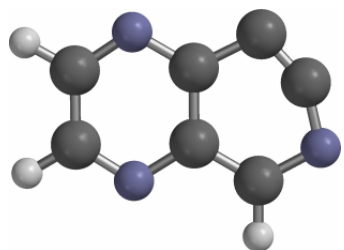

```
C    2.146228      0.818774      0.000000
H    3.036724      1.445220      0.000000
C    2.274599     -0.599302      0.000000
H    3.266628     -1.049871      0.000000
N    1.243354     -1.417859      0.000000
N    0.979278      1.425126      0.000000
C    0.014640     -0.835883      0.000000
C   -0.114569      0.612094      0.000000
C   -1.214866     -1.579020      0.000000
C   -2.144229     -0.729829      0.000000
N   -2.541638      0.498242      0.000000
C   -1.407306      1.227228      0.000000
H   -1.494904      2.309140      0.000000
```

B. Calculations using MP2/6-311+G**

SI-3a*
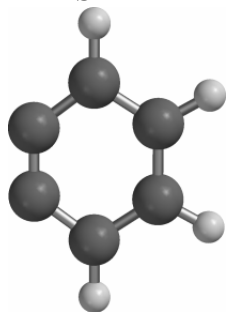
C	0.634257	0.000000	1.247993
C	-0.706963	0.000000	-1.056667
C	-0.634257	0.000000	1.247993
C	1.468416	0.000000	0.131772
C	0.706963	0.000000	-1.056667
C	-1.468416	0.000000	0.131772
H	2.553435	0.000000	0.128042
H	1.231954	0.000000	-2.009581
H	-2.553435	0.000000	0.128042
H	-1.231954	0.000000	-2.009581

SI-5a*

H	-0.284472	-2.258071	0.000000
C	-0.553949	-1.204844	0.000000
C	-1.210450	1.350307	0.000000
C	0.496125	-0.256918	0.000000
C	-1.908005	-0.821473	0.000000
C	-2.329068	0.530242	0.000000
C	0.025548	1.060671	0.000000
H	-2.668274	-1.600470	0.000000
H	-3.371352	0.825689	0.000000
O	1.779337	-0.670397	0.000000
C	2.731075	0.392597	0.000000
H	2.611454	1.013247	-0.893920
H	3.711280	-0.082381	0.000000
H	2.611454	1.013247	0.893920

SI-7a*

C	-0.998970	-1.468926	0.000000
C	-1.120255	1.248397	0.000000
C	0.268216	-0.870681	0.000000
C	-2.109773	-0.863235	0.000000
C	-2.324986	0.529152	0.000000
C	0.122092	0.566976	0.000000
H	-3.287581	1.029231	0.000000
H	-1.147794	2.336334	0.000000
C	1.660019	-1.167335	0.000000
H	2.126117	-2.142306	0.000000
C	2.320116	0.049947	0.000000
H	3.380665	0.262865	0.000000
N	1.402640	1.076605	0.000000
H	1.639316	2.057774	0.000000

SI-8a*

H	-1.145698	-2.575522	0.000000
C	-1.109618	-1.490287	0.000000
C	-1.044877	1.494882	0.000000
C	0.113510	-0.761398	0.000000
C	-2.181159	-0.610622	0.000000
C	-2.150910	0.662040	0.000000
C	0.120641	0.686439	0.000000
H	-1.023866	2.580917	0.000000
C	1.488321	-1.177700	0.000000
H	1.861004	-2.192830	0.000000
C	2.261782	-0.037237	0.000000
H	3.338493	0.072829	0.000000
N	1.444741	1.075153	0.000000
H	1.767260	2.030818	0.000000

SI-9a*
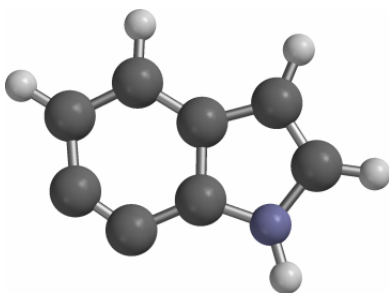
H	−1.259010	−2.337770	0.000000
C	−1.170874	−1.252946	0.000000
C	−0.936654	1.478071	0.000000
C	0.119703	−0.657609	0.000000
C	−2.345025	−0.482839	0.000000
C	−2.060416	0.893559	0.000000
C	0.266972	0.776461	0.000000
H	−3.330174	−0.935510	0.000000
C	1.455039	−1.182887	0.000000
H	1.747955	−2.224326	0.000000
C	2.324805	−0.110451	0.000000
H	3.405970	−0.090142	0.000000
N	1.602751	1.069597	0.000000
H	1.994970	1.999443	0.000000

SI-12a*
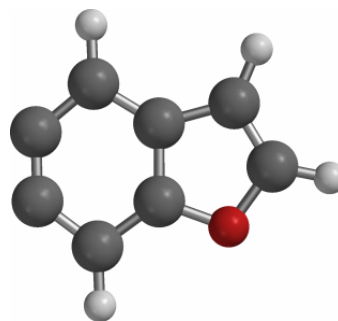
H	−0.973159	−2.574842	0.000000
C	−1.018788	−1.491162	0.000000
C	−1.095411	1.500382	0.000000
C	0.123672	−0.665019	0.000000
C	−2.129972	−0.660314	0.000000
C	−2.163302	0.611447	0.000000
C	0.119769	0.768247	0.000000
H	−1.138312	2.584851	0.000000
C	1.513766	1.140019	0.000000
H	1.936440	2.134983	0.000000
C	2.218679	−0.027614	0.000000
H	3.278937	−0.237315	0.000000
O	1.407893	−1.131095	0.000000

SI-11a*
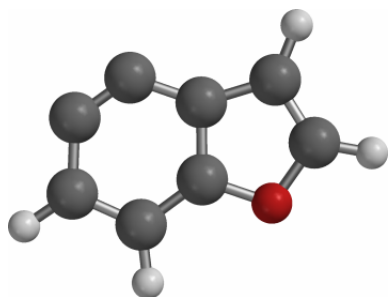
H	−1.105081	−2.329196	0.000000
C	−1.102180	−1.242791	0.000000
C	−0.986213	1.481815	0.000000
C	0.124020	−0.543814	0.000000
C	−2.307284	−0.523902	0.000000
C	−2.093011	0.867931	0.000000
C	0.273740	0.873708	0.000000
H	−3.270694	−1.021870	0.000000
C	1.683219	1.126181	0.000000
H	2.196313	2.076868	0.000000
C	2.269651	−0.111249	0.000000
H	3.303779	−0.423737	0.000000
O	1.357223	−1.128504	0.000000

SI-13a*
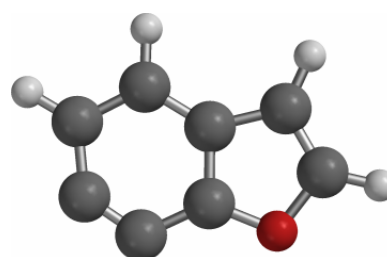
C	−0.896820	−1.478191	0.000000
C	−1.151104	1.261912	0.000000
C	0.284049	−0.751600	0.000000
C	−2.020276	−0.891836	0.000000
C	−2.318711	0.478284	0.000000
C	0.136039	0.665227	0.000000
H	−3.308171	0.921059	0.000000
H	−1.245882	2.345631	0.000000
C	1.490409	1.159138	0.000000
H	1.826877	2.186818	0.000000
C	2.299501	0.058377	0.000000
H	3.372754	−0.060738	0.000000
O	1.585734	−1.115961	0.000000

SI-31a*
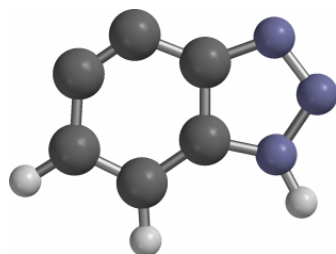

```
C    -0.913376    -1.477150     0.000000
C    -1.093507     1.268670     0.000000
C     0.324504    -0.823447     0.000000
C    -2.027782    -0.880182     0.000000
C    -2.270439     0.510391     0.000000
C     0.158275     0.601221     0.000000
H    -3.246350     0.983750     0.000000
H    -1.150680     2.354092     0.000000
N     1.451273     1.027528     0.000000
H     1.823373     1.968253     0.000000
N     2.328951    -0.003880     0.000000
N     1.648499    -1.137545     0.000000
```

SI-33a*
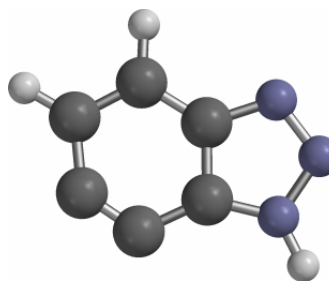

```
H    -1.201197    -2.336667     0.000000
C    -1.135608    -1.252019     0.000000
C    -0.901296     1.502667     0.000000
C     0.144137    -0.630327     0.000000
C    -2.299537    -0.477030     0.000000
C    -2.016859     0.905361     0.000000
C     0.296359     0.791082     0.000000
H    -3.287641    -0.922675     0.000000
N     1.638947     0.968889     0.000000
H     2.181486     1.822447     0.000000
N     2.291255    -0.225323     0.000000
N     1.395507    -1.191910     0.000000
```

SI-32a*
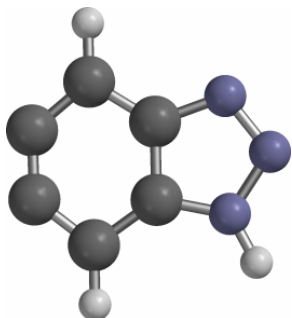

```
H    -1.073464    -2.576054     0.000000
C    -1.064525    -1.491452     0.000000
C    -1.021734     1.518893     0.000000
C     0.137880    -0.729426     0.000000
C    -2.132250    -0.612026     0.000000
C    -2.106075     0.661376     0.000000
C     0.143244     0.707793     0.000000
H    -1.019213     2.603821     0.000000
N     1.479171     0.989407     0.000000
H     1.949035     1.884334     0.000000
N     2.237014    -0.135338     0.000000
N     1.437344    -1.177655     0.000000
```

SI-83a*
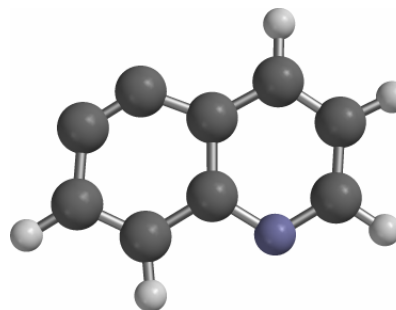

```
H     3.421433    -0.957880     0.000000
C     2.406995    -0.569440     0.000000
H     1.436229    -2.503503     0.000000
C     1.317640    -1.423601     0.000000
N     0.994543     1.407233     0.000000
C     0.027077    -0.855059     0.000000
C     2.191393     0.828622     0.000000
C    -0.103163     0.595836     0.000000
C    -1.245972    -1.453111     0.000000
H     3.044536     1.505292     0.000000
H    -1.395189     2.319465     0.000000
C    -2.365266    -0.868662     0.000000
C    -2.591561     0.526041     0.000000
H    -3.559658     1.015866     0.000000
C    -1.392749     1.232205     0.000000
```

SI-84a*
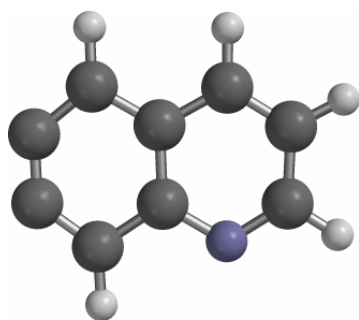

```
H    3.271940   -1.131364    0.000000
C    2.296301   -0.653846    0.000000
H    1.171091   -2.487769    0.000000
C    1.138790   -1.400146    0.000000
N    1.063535    1.436021    0.000000
C   -0.122730   -0.739851    0.000000
C    2.203460    0.763489    0.000000
C   -0.102404    0.714074    0.000000
C   -1.348082   -1.480392    0.000000
H    3.111857    1.364588    0.000000
H   -1.280325    2.562548    0.000000
C   -2.433026   -0.628221    0.000000
H   -1.358860   -2.566998    0.000000
C   -2.412234    0.644608    0.000000
C   -1.318389    1.478045    0.000000
```

SI-85a*
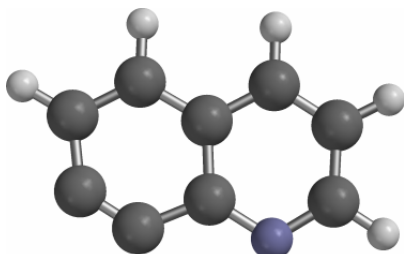

```
H    3.231628   -1.302361    0.000000
C    2.302512   -0.739726    0.000000
H    1.022397   -2.472204    0.000000
C    1.078975   -1.385641    0.000000
N    1.259351    1.451574    0.000000
C   -0.112960   -0.618255    0.000000
C    2.338649    0.673235    0.000000
C    0.057759    0.829482    0.000000
C   -1.410175   -1.233477    0.000000
H    3.296602    1.190828    0.000000
C   -2.592907   -0.496279    0.000000
H   -1.462199   -2.321059    0.000000
H   -3.571682   -0.964076    0.000000
C   -2.322568    0.883278    0.000000
C   -1.203254    1.468255    0.000000
```

SI-103a*
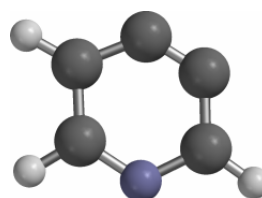

```
C    0.720372   -1.205981    0.000000
C   -0.692436    1.009838    0.000000
C    1.419443    0.009475    0.000000
C   -0.553363   -1.275485    0.000000
C   -1.430351   -0.204442    0.000000
N    0.646363    1.112700    0.000000
H    2.496415    0.135423    0.000000
H   -2.514834   -0.214756    0.000000
H   -1.241121    1.949351    0.000000
```

SI-104a*
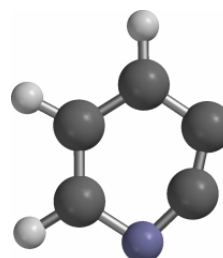

```
C    0.135020   -1.467994    0.000000
C   -0.350629    1.225328    0.000000
C   -0.936113   -0.793948    0.000000
C    1.272209   -0.633738    0.000000
C    0.972203    0.753169    0.000000
N   -1.454912    0.385054    0.000000
H    2.299871   -0.990614    0.000000
H    1.778153    1.481743    0.000000
H   -0.578136    2.287527    0.000000
```

SI-106a*
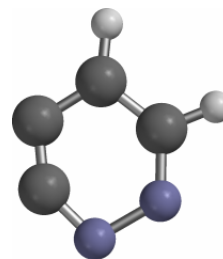

```
C    0.116289   -1.404991    0.000000
N   -0.306056    1.273672    0.000000
C   -0.985167   -0.774865    0.000000
C    1.271576   -0.636403    0.000000
C    0.925752    0.751779    0.000000
N   -1.438324    0.454903    0.000000
H    2.303124   -0.977847    0.000000
H    1.709926    1.505030    0.000000
```

SI-108a*
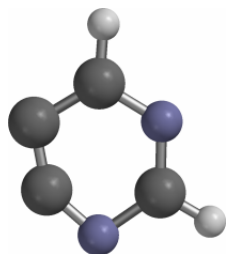
N	1.465652	−0.143376	0.000000
C	−1.319474	0.349505	0.000000
C	0.472197	−1.133533	0.000000
C	0.803134	0.955331	0.000000
C	−0.388384	1.408787	0.000000
N	−0.834596	−0.919175	0.000000
H	0.841244	−2.153556	0.000000
H	−2.399040	0.468337	0.000000

SI-110a*
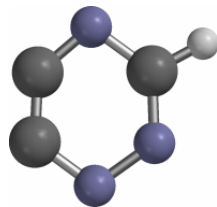
N	−0.553603	−1.111942	0.000000
N	−1.464305	−0.101897	0.000000
C	−0.791759	1.091335	0.000000
C	0.483504	1.190622	0.000000
N	1.440891	0.305620	0.000000
C	0.763208	−0.916136	0.000000
H	1.387129	−1.804126	0.000000

SI-111a*
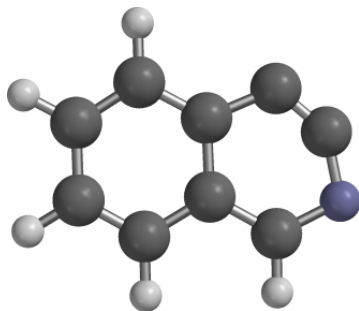
C	2.313636	0.660771	0.000000
C	1.330865	1.440043	0.000000
C	1.413085	−1.260175	0.000000
C	0.039197	0.848811	0.000000
N	2.612585	−0.626030	0.000000
C	0.137727	−0.605264	0.000000
C	−1.232564	1.467718	0.000000
H	−1.007371	−2.452983	0.000000
H	1.454495	−2.348756	0.000000
C	−2.375583	0.684366	0.000000
H	−1.292316	2.552363	0.000000
H	−3.352529	1.161111	0.000000
C	−2.292690	−0.730434	0.000000
H	−3.205492	−1.319810	0.000000
C	−1.063709	−1.366442	0.000000

SI-112a*
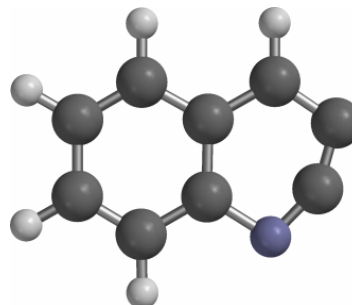
|			
C	2.559472	0.680603	0.000000
H	1.355381	2.526840	0.000000
C	1.378479	1.435928	0.000000
N	1.353781	−1.468484	0.000000
C	0.135125	0.703528	0.000000
C	2.230093	−0.557601	0.000000
C	0.135237	−0.740320	0.000000
C	−1.122501	1.367243	0.000000
H	−1.038336	−2.544504	0.000000
C	−2.303566	0.646255	0.000000
H	−1.139870	2.455055	0.000000
H	−3.255904	1.169344	0.000000
C	−2.281831	−0.769603	0.000000
H	−3.217376	−1.322625	0.000000
C	−1.079991	−1.459180	0.000000

SI-113a*
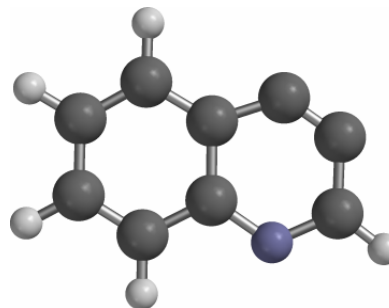
C	2.387743	0.846186	0.000000
C	1.269259	1.447167	0.000000
N	1.369392	−1.246593	0.000000
C	−0.001107	0.855399	0.000000
C	2.512557	−0.566988	0.000000
C	0.163566	−0.605221	0.000000
C	−1.291629	1.427268	0.000000
H	3.445267	−1.121979	0.000000
H	−0.901839	−2.475411	0.000000
C	−2.407064	0.603023	0.000000
H	−1.390727	2.508678	0.000000
H	−3.399898	1.045094	0.000000
C	−2.268782	−0.803997	0.000000
H	−3.156789	−1.430226	0.000000
C	−1.015740	−1.395200	0.000000

SI-115a*
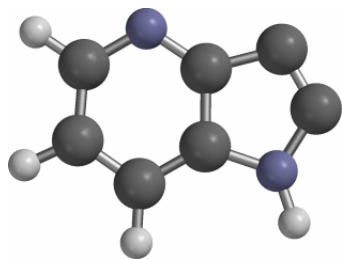
C	0.339501	−0.645280	0.000000
C	−1.975627	0.767295	0.000000
C	0.293755	0.803030	0.000000
C	−0.841026	−1.390373	0.000000
C	−2.019945	−0.643443	0.000000
N	−0.850809	1.495921	0.000000
H	−0.848762	−2.477507	0.000000
H	−2.983790	−1.144200	0.000000
H	−2.905685	1.331565	0.000000
C	1.685243	1.230281	0.000000
C	2.367229	0.149794	0.000000
N	1.688761	−1.035476	0.000000
H	2.048323	−1.978288	0.000000

SI-117a*
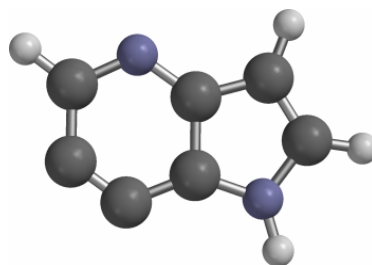
C	2.227114	0.608530	0.000000
H	3.161511	1.158031	0.000000
N	1.079066	1.297159	0.000000
C	2.096149	−0.803775	0.000000
C	0.990197	−1.437886	0.000000
C	−0.238209	−0.800630	0.000000
C	−0.101773	0.650291	0.000000
N	−1.566641	−1.096900	0.000000
H	−1.956691	−2.028009	0.000000
C	−2.295909	0.082665	0.000000
H	−3.376584	0.051842	0.000000
C	−1.438624	1.162726	0.000000
H	−1.726304	2.204595	0.000000

SI-116a*
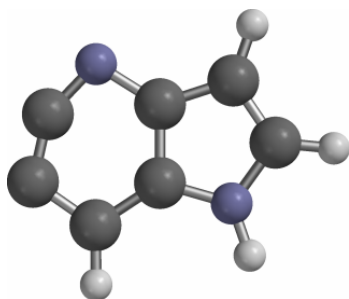
C	1.964899	0.583518	0.000000
N	1.080439	1.510583	0.000000
C	2.233267	−0.660412	0.000000
C	1.073369	−1.452255	0.000000
H	1.053328	−2.541814	0.000000
C	−0.113156	−0.669789	0.000000
C	−0.107234	0.776461	0.000000
N	−1.438175	−1.041106	0.000000
H	−1.774655	−1.992626	0.000000
C	−2.241381	0.079094	0.000000
H	−3.318948	−0.019585	0.000000
C	−1.458501	1.219590	0.000000
H	−1.809382	2.241414	0.000000

SI-119a*
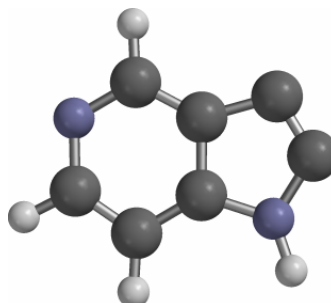
H	−0.875642	−2.457044	0.000000
C	−0.842816	−1.371005	0.000000
C	−0.929439	1.430638	0.000000
C	−2.014587	−0.614071	0.000000
C	0.349019	−0.641983	0.000000
C	0.324532	0.799123	0.000000
N	−2.074865	0.741562	0.000000
H	−2.976684	−1.121289	0.000000
H	−1.004885	2.516171	0.000000
N	1.694695	−1.045108	0.000000
H	2.043104	−1.991876	0.000000
C	1.713309	1.207976	0.000000
C	2.398679	0.126631	0.000000

SI-120a*
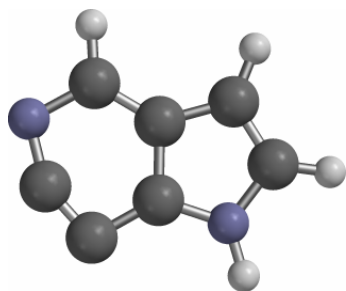

```
C    1.923626     0.652281     0.000000
C    1.012432     1.538231     0.000000
C   -0.175711     0.771799     0.000000
C   -0.114805    -0.679367     0.000000
N   -1.500685     1.116324     0.000000
H   -1.843766     2.066538     0.000000
C   -2.278940    -0.028079     0.000000
H   -3.358300     0.045164     0.000000
C   -1.471902    -1.145869     0.000000
H   -1.817990    -2.170319     0.000000
N    2.309546    -0.568439     0.000000
C    1.143764    -1.311100     0.000000
H    1.269194    -2.389815     0.000000
```

SI-123a*
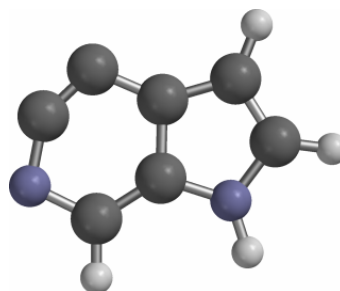

```
C    1.096523    -1.295296     0.000000
H    1.127091    -2.382711     0.000000
C   -0.116729    -0.577537     0.000000
C   -0.192119     0.873926     0.000000
N   -1.416476    -1.032021     0.000000
H   -1.701775    -2.000517     0.000000
C   -2.279985     0.039551     0.000000
H   -3.349743    -0.123899     0.000000
C   -1.569467     1.228271     0.000000
H   -1.995981     2.221253     0.000000
N    2.309556    -0.657472     0.000000
C    2.028537     0.623251     0.000000
C    1.093835     1.463752     0.000000
```

SI-122a*


```
C    0.358726    -0.619923     0.000000
C   -2.050679     0.608652     0.000000
C   -0.829110    -1.361651     0.000000
C    0.329000     0.821428     0.000000
C   -0.930480     1.438626     0.000000
N   -2.017738    -0.749083     0.000000
H   -0.830145    -2.451092     0.000000
H   -1.035486     2.519462     0.000000
H   -3.046449     1.044968     0.000000
N    1.706076    -1.023635     0.000000
H    2.058136    -1.968995     0.000000
C    2.397229     0.153588     0.000000
C    1.717989     1.236988     0.000000
```
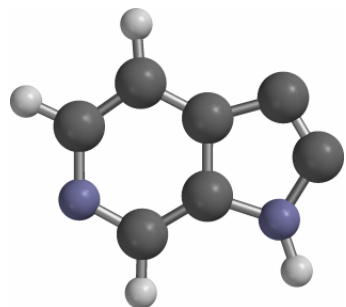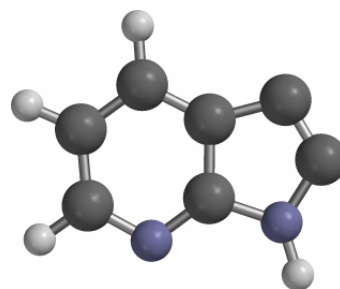
SI-125a*


```
C    0.326964    -0.849598     0.000000
C   -1.907761     0.765937     0.000000
C    0.330703     0.601813     0.000000
C   -0.929403    -1.468649     0.000000
C   -2.051332    -0.635459     0.000000
N   -0.720867     1.400043     0.000000
H   -1.025282    -2.550686     0.000000
H   -3.050213    -1.061537     0.000000
H   -2.787586     1.404781     0.000000
N    1.676493     1.029401     0.000000
H    1.987162     1.990044     0.000000
C    1.718735    -1.224950     0.000000
C    2.389949    -0.132106     0.000000
```

SI-126a*
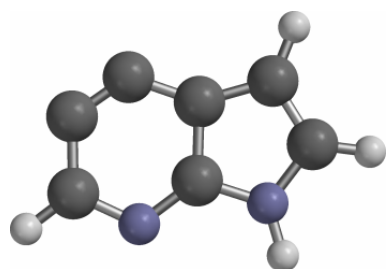
C	−0.101158	−0.556541	0.000000
C	−0.236517	0.893445	0.000000
N	−1.381237	−1.056939	0.000000
H	−1.601647	−2.042830	0.000000
C	−2.287217	−0.024904	0.000000
H	−3.349536	−0.227992	0.000000
C	−1.624114	1.193525	0.000000
H	−2.089121	2.168722	0.000000
N	1.018753	−1.289380	0.000000
C	2.198855	−0.647804	0.000000
H	3.103411	−1.245595	0.000000
C	2.135617	0.766700	0.000000
C	1.048834	1.427351	0.000000

SI-127a*

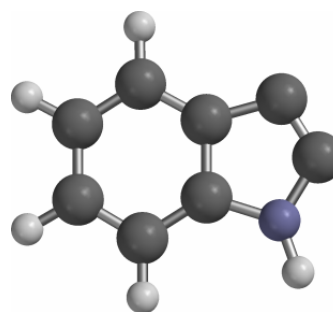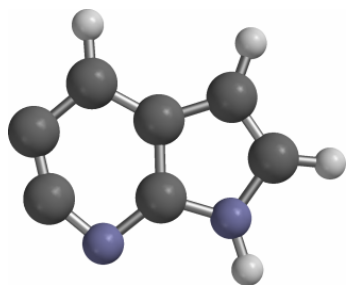|			
C	2.227482	0.595052	0.000000
C	1.128109	1.462288	0.000000
H	1.170424	2.549295	0.000000
C	−0.104181	0.749269	0.000000
C	−0.095467	−0.696466	0.000000
N	1.008040	−1.511833	0.000000
C	1.984373	−0.651225	0.000000
N	−1.394091	−1.123111	0.000000
H	−1.672748	−2.093866	0.000000
C	−1.487448	1.133359	0.000000
H	−1.884714	2.139000	0.000000
C	−2.235586	−0.025560	0.000000
H	−3.309066	−0.159572	0.000000

SI-128a*

H	−0.933889	−2.564080	0.000000
C	−0.897625	−1.478386	0.000000
C	−0.819670	1.394956	0.000000
C	0.338848	−0.810885	0.000000
C	−2.066322	−0.717527	0.000000
C	−2.027640	0.694917	0.000000
C	0.355385	0.635061	0.000000
H	−3.030038	−1.219395	0.000000
H	−2.960614	1.252197	0.000000
H	−0.798664	2.482052	0.000000
C	1.734484	−1.207420	0.000000
C	2.410577	−0.121711	0.000000
N	1.703584	1.046185	0.000000
H	2.045310	1.994945	0.000000

SI-129a*

H	−0.744388	−2.485643	0.000000
C	−0.792873	−1.400958	0.000000
C	−0.887028	1.477231	0.000000
C	0.357652	−0.623360	0.000000
C	−2.007278	−0.705190	0.000000
C	−2.051374	0.704244	0.000000
C	0.346577	0.812714	0.000000
H	−2.937243	−1.266587	0.000000
H	−3.017417	1.201214	0.000000
H	−0.930789	2.562182	0.000000
C	1.756524	1.142899	0.000000
C	2.385669	0.032249	0.000000
O	1.676489	−1.116267	0.000000

SI-130a*
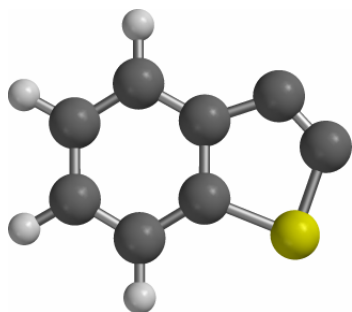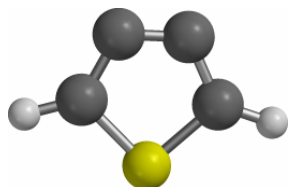


```
H    -0.701994    -2.495391     0.000000
C    -0.898957    -1.425824     0.000000
C    -1.429957     1.376086     0.000000
C     0.149530    -0.498081     0.000000
C    -2.206906    -0.938955     0.000000
C    -2.468500     0.446534     0.000000
C    -0.100437     0.917449     0.000000
H    -3.036096    -1.641210     0.000000
H    -3.497980     0.793908     0.000000
H    -1.633123     2.443190     0.000000
C     1.170505     1.598036     0.000000
C     2.178771     0.830331     0.000000
S     1.905277    -0.856389     0.000000
```

SI-132a*


```
C     0.643328     0.000000     1.410770
C     1.264269     0.000000     0.177883
H     2.302155     0.000000    -0.127276
C    -0.643328     0.000000     1.410770
C    -1.264269     0.000000     0.177883
H    -2.302155     0.000000    -0.127276
S     0.000000     0.000000    -1.014694
```

SI-133a*


```
C     1.126355     0.979625     0.000000
C    -0.113978     1.256184     0.000000
C     1.426462    -0.419338     0.000000
H     2.405041    -0.884052     0.000000
C     0.234712    -1.133671     0.000000
H     0.101862    -2.211987     0.000000
S    -1.170022    -0.072095     0.000000
```

SI-142a*


```
C     2.040303     0.767700     0.000000
H     2.991109     1.290797     0.000000
C     0.851901     1.481949     0.000000
H     0.843259     2.567895     0.000000
C     2.008893    -0.651487     0.000000
H     2.929785    -1.225743     0.000000
C     0.817353    -1.337752     0.000000
H     0.737662    -2.419914     0.000000
N    -0.369870    -0.637245     0.000000
C    -0.378858     0.807369     0.000000
C    -1.751894     1.130502     0.000000
C    -2.456193     0.054424     0.000000
C    -1.677040    -1.112596     0.000000
H    -1.892243    -2.170393     0.000000
```
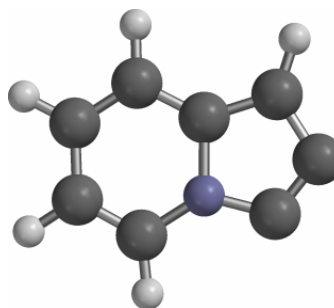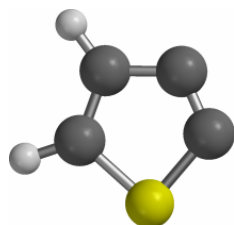
SI-143a*


```
C     2.018661     0.718914     0.000000
H     2.955915     1.266879     0.000000
C     0.820342     1.405727     0.000000
H     0.794138     2.492365     0.000000
C     2.035441    -0.706668     0.000000
H     2.973185    -1.251668     0.000000
C     0.865630    -1.422738     0.000000
H     0.805843    -2.505168     0.000000
N    -0.333289    -0.746396     0.000000
C    -0.405677     0.700345     0.000000
C    -1.782661     1.059324     0.000000
H    -2.161172     2.072665     0.000000
C    -2.482012    -0.178761     0.000000
C    -1.631025    -1.145795     0.000000
```
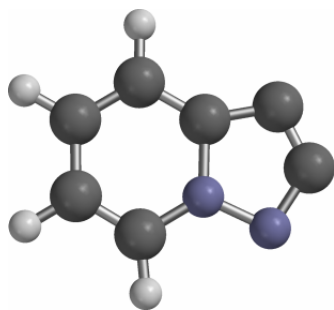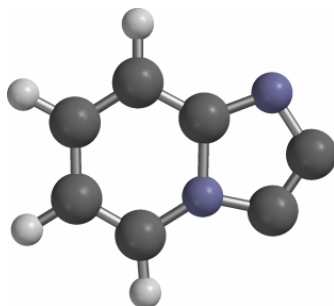
SI-148a*


```
C     2.016063      0.767368      0.000000
H     2.966859      1.291021      0.000000
C     0.832657      1.487707      0.000000
H     0.828809      2.573203      0.000000
C     1.993239     -0.651057      0.000000
H     2.918422     -1.217605      0.000000
C     0.804238     -1.344729      0.000000
H     0.698460     -2.423613      0.000000
N    -0.366232     -0.634173      0.000000
C    -0.398933      0.808236      0.000000
N    -1.616241     -1.205113      0.000000
C    -1.778426      1.071257      0.000000
C    -2.364607     -0.070192      0.000000
```

SI-157a*


```
C     1.986440      0.728046      0.000000
H     2.920064      1.282038      0.000000
C     0.784469      1.415969      0.000000
H     0.740797      2.500934      0.000000
C     2.016862     -0.691191      0.000000
H     2.961397     -1.224299      0.000000
C     0.854569     -1.427706      0.000000
H     0.809038     -2.510546      0.000000
N    -0.340564     -0.756495      0.000000
C    -0.429480      0.704732      0.000000
N    -1.722113      1.124117      0.000000
C    -2.427041     -0.062759      0.000000
C    -1.653591     -1.085462      0.000000
```

References

[1] *Spartan '06*; Wavefunction, Inc: Irvine, CA, 2006.

[2] a) S. E. Wheeler, A. Moran, S. N. Pieniazek and K. N. Houk, *J. Phys. Chem. A* **2009**, *113*, 10376. b) S. Grimme, *WIREs Comput. Mol. Sci.* **2011**, *1*, 211.

[3] *Spartan '10*; Wavefunction, Inc: Irvine, CA, 2010.