Theoretical Investigation of Tautomerism of 2- and 4-Pyridones: Origin, Substituent and Solvent Effects

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Supplementary Information

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Table S1. Comparison of calculated, BHandHLYP/6-311+G(d,p), and experimental bond lengths of 2-pyridone (**2PY**) and *syn*-2-hydroxypyridine (***syn*-2HPY**) in the gas phase.

Bond	2PY		*syn*-2HPY	
	Calc.	Exp.[a]	Calc.	Exp.[a]
N1C2	1.390	1.396	1.313	1.320
C2C3	1.446	1.471	1.392	1.410
C3C4	1.350	1.355	1.375	1.392
C4C5	1.423	1.451	1.390	1.410
C6N1	1.357	1.376	1.330	1.344
C2O	1.210	1.203	1.339	1.336
N1H	1.002	1.005	/	/
OH	/	/	0.955	0.960
[a] From ref. 6c.				

a

b

c
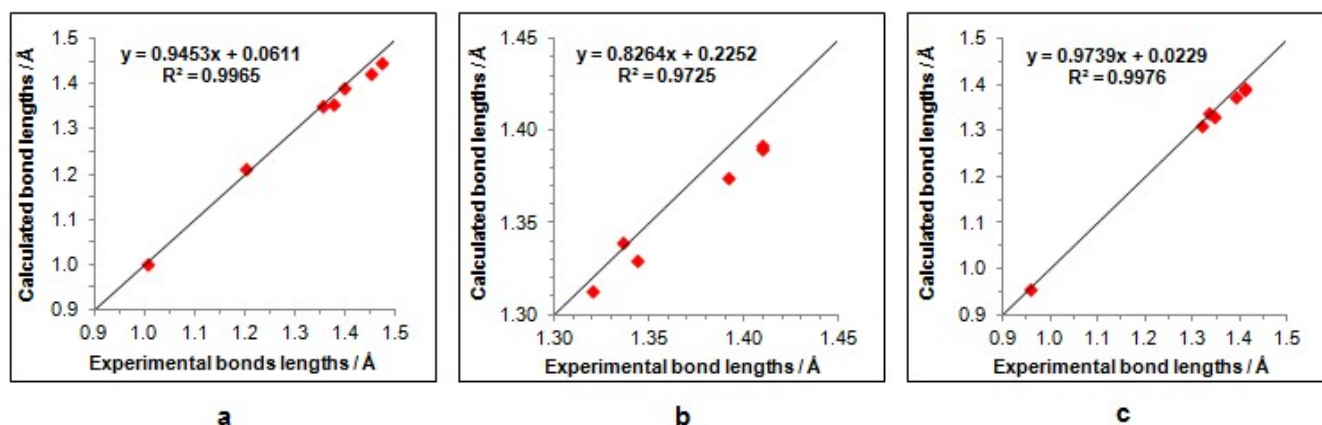
Figure S1. Correlations between calculated, BHandHLYP/6-311+G(d,p), and experimental[6c] bond lengths of 2-pyridone (**a**) and *syn*-2-hydroxypyridine (**b** - without the O–H bond, **c** - including the O–H bond) in the gas phase.

Table S2. Comparison of calculated, BHandHLYP/6-311+G(d,p), and experimental bond lengths of 4-pyridone (**4PY**) obtained by x-ray analysis.

	4PY	
Bond	Calc.	Exp.[a]
N1C2	1.363	1.354
N1C6	1.363	1.354
C2C3	1.342	1.362
C5C6	1.342	1.347
C4O	1.215	1.274
[a] Ref. 9a.		
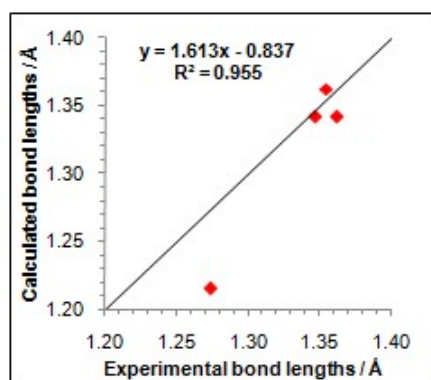
Figure S2. Correlation between calculated, BHandHLYP/6-311+G(d,p), and experimental[9a] bond lengths of 4-pyridone obtained by x-ray analysis.
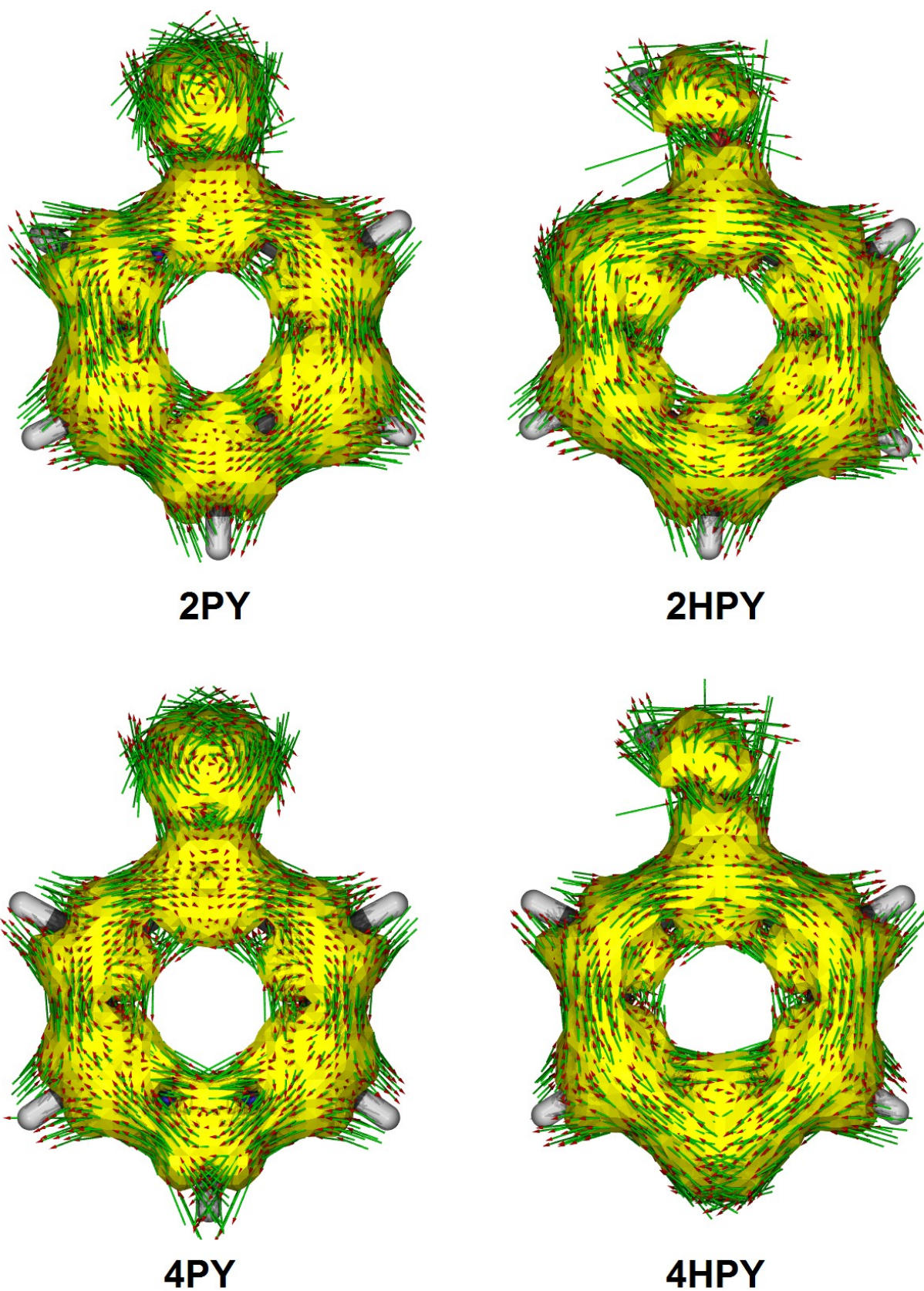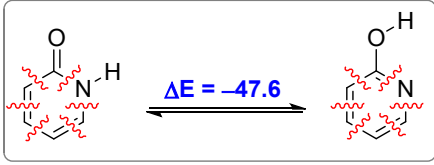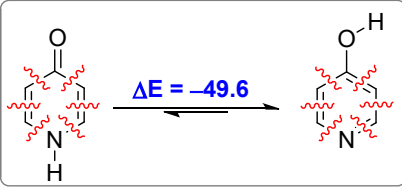
Figure S3. AICD plots of 2-pyridone (**2PY**), *syn*-2-hydroxypyridine (**2HPY**), 4-pyridone (**4PY**) and 4-hydroxypyridine (**4HPY**) at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

Table S3. Ring energy decomposition analysis of 2- and 4-pyridones. Values are in kcal/mol.[a]

4 x CH ⫻ 1 x C=O ⫻ 1 x NH⫻ for lactam
4 x CH ⫻ 1 x C-OH⫻ 1 x N ⫻ for lactim
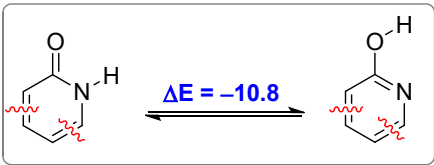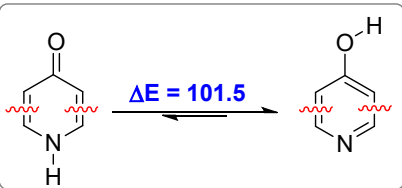
	2PY	2HPY	2PY → 2HPY	4PY	4HPY	4PY → 4HPY
ΔE_{elstat}	-981.7	-1100.7	**-119.0**	-1117.6	-1094.6	**23.0**
ΔE_{Pauli}	1690.7	1812.9	**122.2**	1881.8	1797.8	**-84.0**
ΔE_{oi}	-1332.2	-1357.1	**-24.9**	-1378.4	-1340.7	**37.8**
ΔE_{disp}	-230.0	-255.1	**-25.1**	-229.7	-254.8	**-25.0**
ΔE_{int}	-853.3	-900.0	**-46.8**	-844.0	-892.2	**-48.2**
ΔE_{def}	1.2	0.3	**-0.8**	1.6	0.2	**-1.4**
ΔE_{bond}	-852.1	-899.7	**-47.6**	-842.4	-892.0	**-49.6**

[a] ΔE_{elstat} = electrostatic energy, ΔE_{Pauli} = Pauli repulsion energy, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy, ΔE_{int} = interaction energy (the sum of the previous four energies), ΔE_{def} = deformation energy, ΔE_{bond} = bonding energy.

Table S4. Energy decomposition analysis of double bonds in 2-pyridone/2-hydroxypyridine and 4-pyridone/4-hydroxypyridine. Values are in kcal/mol.[a]

2 interacting fragments in their
quintet state for both forms

2 interacting fragments in their
quintet state for lactam
2 interacting fragments in their
quartet state for lactim

	2PY	2HPY	2PY → 2HPY	4PY	4HPY	4PY → 4HPY
ΔE_{elstat}	-373.9	-369.5	**4.4**	-359.9	-369.5	**-9.6**
ΔE_{Pauli}	551.8	548.9	**-2.8**	549.2	581.5	**32.3**
ΔE_{oi}	-474.2	-491.1	**-16.9**	-508.3	-432.2	**76.1**
ΔE_{disp}	-86.8	-84.0	**2.8**	-84.7	-68.0	**16.7**
ΔE_{int}	-383.1	-395.6	**-12.5**	-403.7	-288.2	**115.5**
ΔE_{def}	18.0	19.7	**1.7**	26.0	12.0	**-14.0**
ΔE_{bond}	-365.1	-375.9	**-10.8**	-377.7	-276.2	**101.5**

[a] Labeling of energy terms is the same as in Table S3.

Table S5. Gibbs free energy difference between *anti*- and *syn*-conformers with respect to the OH group rotation ($\Delta G_{anti\text{-}syn}$), tautomerization Gibbs free energies (ΔG_T, *syn*-lactim for **2PY** series and *anti*-lactim for **4PY** series), Gibbs free energies for proton transfer to water molecule in gas phase (ΔG_{NH} and ΔG_{OH}) and increase/decrease of acidity relative to unsubstituted pyridone ($\Delta\Delta G_{NH}$ and $\Delta\Delta G_{OH}$, *syn*-lactim for **2PY** series and *anti*-lactim for **4PY** series).

	$\Delta G_{anti\text{-}syn}$	ΔG_T	ΔG_{NH}	ΔG_{OH}	$\Delta\Delta G_{NH}$	$\Delta\Delta G_{OH}$
2PY	5.42	-0.57	184.32	184.89	/	/
3Cl-2PY	2.77	-0.30	175.91	176.20	-8.4	-8.7
4Cl-2PY	5.41	-0.51	176.11	176.61	-8.2	-8.3
5Cl-2PY	5.36	-2.16	175.54	177.70	-8.8	-7.2
6Cl-2PY	5.23	-3.62	171.11	174.72	-13.2	-10.2
3F-2PY	2.57	-0.25	177.85	178.10	-6.5	-6.8
4F-2PY	5.52	-0.34	178.02	178.36	-6.3	-6.5
5F-2PY	5.36	-2.91	178.48	181.39	-5.8	-3.5
6F-2PY	4.98	-5.58	170.72	176.30	-13.6	-8.6
3NH₂-2PY	5.35	2.28	185.72	183.44	1.4	-1.5
4NH₂-2PY	5.78	0.24	188.03	187.78	3.7	2.9
5NH₂-2PY	5.18	-2.79	184.93	187.72	0.6	2.8
6NH₂-2PY	4.60	-4.20	181.86	186.06	-2.5	1.2
3NO₂-2PY	-3.40	-0.76	163.01	163.77	-21.3	-21.1
4NO₂-2PY	5.16	-1.14	167.26	168.40	-17.1	-16.5
5NO₂-2PY	5.54	-0.32	160.20	160.53	-24.1	-24.4
6NO₂-2PY	5.43	-3.12	165.19	168.30	-19.2	-16.6
4PY	/	-3.02	172.39	175.41	/	/
2Cl-4PY	0.13	-5.59	160.96	166.54	-11.4	-8.9
3Cl-4PY	2.73	-2.41	163.83	166.24	-8.6	-9.2
2F-4PY	0.05	-7.84	160.53	168.37	-11.9	-7.0
3F-4PY	2.54	-2.88	165.65	168.53	-6.7	-6.9
2NH₂-4PY	-0.32	-7.50	170.52	178.02	-1.9	2.6
3NH₂-4PY	0.80	-0.56	173.79	174.35	1.4	-1.1
2NO₂-4PY	0.00	-5.26	154.53	159.79	-17.86	-15.62
3NO₂-4PY	9.3	-1.57	152.55	154.12	-19.85	-21.29

Table S6. Comparison of calculated, BHandHLYP/6-311+G(d,p), and experimental bond lengths of 6-chloro-2-hydroxypyridine (**6Cl-2HPY**) obtained by x-ray analysis.

	6Cl-2HPY	
Bond	Calc.	Exp.[a]
N1C2	1.313	1.341
C2C3	1.392	1.393
C3C4	1.375	1.377
C4C5	1.390	1.382
C5C6	1.377	1.362
C2O	1.339	1.321
OH	0.995	1.009
C6Cl	1.740	1.379
[a] Ref. 23a.		

a

b
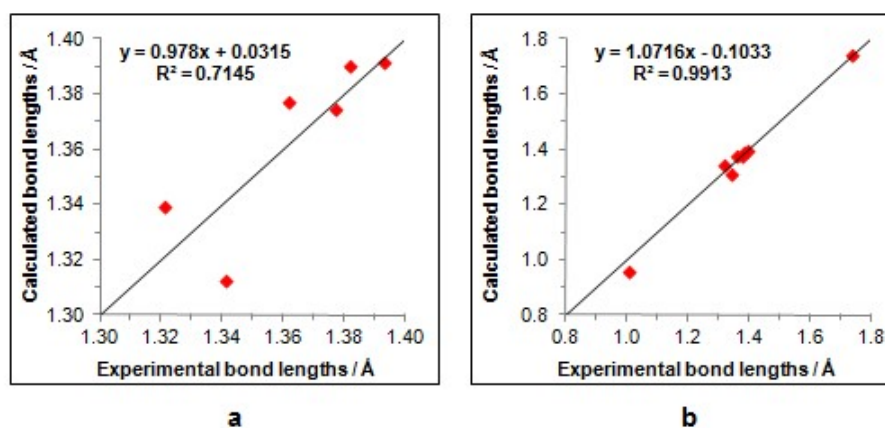
Figure S4. Correlation between calculated, BHandHLYP/6-311+G(d,p), and experimental[23a] bond lengths of 6-chloro-2-hydroxypyridine obtained by x-ray analysis (**a** - without the O–H and C–Cl bonds, **b** - including the O–H and C–Cl bonds).

Absolute energies and x, y, z coordinates of the gas-phase optimized structures at the BHandHLYP/6-311+G(d,p) level of theory
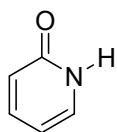
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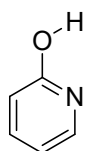
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    4          6           0       -1.218288    0.224205    0.000000
    5          6           0       -1.182029   -1.149874    0.000000
    6          1           0        0.109573   -2.877168    0.000000
    7          1           0        2.160098   -1.490282    0.000000
    8          1           0       -2.137754    0.779593    0.000000
    9          1           0       -2.100497   -1.711643    0.000000
   10          7           0        1.167612    0.296832    0.000000
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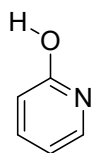
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    6           1           0        0.218879   -2.876617    0.000000
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   10           7           0        1.181959    0.331090    0.000000
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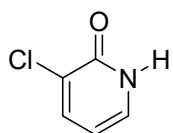

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    5           6           0        1.348654   -0.580461    0.000000
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    9           1           0        1.871735   -1.520724    0.000000
   10           7           0        0.044458    1.786581    0.000000
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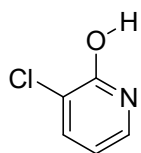
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   6          1           0       3.199093    0.493101    0.000000
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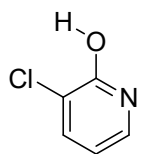

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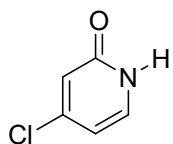
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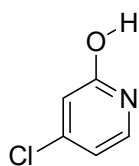
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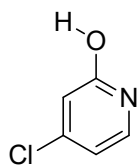
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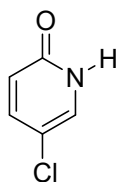
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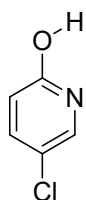
E = -783.0259329 a.u.

```
----------------------------------------------------------------
Center      Atomic      Atomic          Coordinates (Angstroms)
Number      Number      Type         X           Y           Z
----------------------------------------------------------------
   1          6           0        0.000000   -0.927088    0.000000
   2          6           0        1.155219   -0.179971    0.000000
   3          6           0       -0.016818    1.762369    0.000000
   4          6           0       -1.240550    1.099531    0.000000
   5          6           0       -1.223592   -0.273819    0.000000
   6          1           0        2.119424   -0.658752    0.000000
   7          1           0       -2.157260    1.659172    0.000000
   8          1           0       -2.139736   -0.836987    0.000000
   9          7           0        1.142055    1.147060    0.000000
  10          8           0       -0.014238    3.099877    0.000000
  11         17           0        0.079765   -2.662830    0.000000
  12          1           0        0.895545    3.390114    0.000000
----------------------------------------------------------------
```
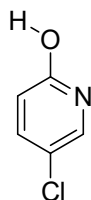

E = -783.0168101 a.u.

```
----------------------------------------------------------------
Center      Atomic      Atomic          Coordinates (Angstroms)
Number      Number      Type         X           Y           Z
----------------------------------------------------------------
   1          6           0        0.000000   -0.931154    0.000000
   2          6           0        1.164789   -0.191653    0.000000
   3          6           0        0.025643    1.764991    0.000000
   4          6           0       -1.204653    1.111188    0.000000
   5          6           0       -1.211539   -0.265586    0.000000
   6          1           0        2.122676   -0.684261    0.000000
   7          1           0       -2.128366    1.663813    0.000000
   8          1           0       -2.136965   -0.813329    0.000000
   9          7           0        1.173526    1.130890    0.000000
  10          8           0        0.118804    3.104655    0.000000
  11         17           0        0.063402   -2.667462    0.000000
  12          1           0       -0.745739    3.500441    0.000000
----------------------------------------------------------------
```
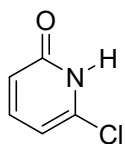
E = -783.0244539 a.u.

```
----------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
----------------------------------------------------------------
    1          6           0        1.340170   -0.691250    0.000000
    2          6           0        0.000000   -0.795846    0.000000
    3          6           0       -0.335581    1.618396    0.000000
    4          6           0        1.105589    1.724066    0.000000
    5          6           0        1.885285    0.624149    0.000000
    6          1           0        1.960118   -1.565126    0.000000
    7          1           0       -1.792952    0.191172    0.000000
    8          1           0        1.512126    2.717987    0.000000
    9          1           0        2.956813    0.731875    0.000000
   10          7           0       -0.795601    0.298745    0.000000
   11          8           0       -1.127479    2.528797    0.000000
   12         17           0       -0.824697   -2.310270    0.000000
----------------------------------------------------------------
```
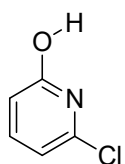

E = -783.030405 a.u.

```
----------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
----------------------------------------------------------------
    1          6           0        1.371367   -0.635844    0.000000
    2          6           0        0.000000   -0.770844    0.000000
    3          6           0       -0.352300    1.453297    0.000000
    4          6           0        1.008295    1.732878    0.000000
    5          6           0        1.869007    0.659297    0.000000
    6          1           0        2.012063   -1.496020    0.000000
    7          1           0        1.349711    2.750560    0.000000
    8          1           0        2.933049    0.822687    0.000000
    9          7           0       -0.845797    0.233043    0.000000
   10          8           0       -1.220634    2.467519    0.000000
   11         17           0       -0.699100   -2.363686    0.000000
   12          1           0       -2.102692    2.101286    0.000000
----------------------------------------------------------------
```
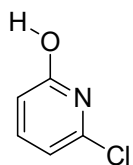
E = -783.0215614 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6          0         1.373131   -0.626114    0.000000
    2          6          0         0.000000   -0.777065    0.000000
    3          6          0        -0.394856    1.434856    0.000000
    4          6          0         0.964386    1.730212    0.000000
    5          6          0         1.848918    0.672645    0.000000
    6          1          0         2.025835   -1.477250    0.000000
    7          1          0         1.310867    2.748937    0.000000
    8          1          0         2.909297    0.857410    0.000000
    9          7          0        -0.861939    0.205998    0.000000
   10          8          0        -1.335370    2.389665    0.000000
   11         17          0        -0.667284   -2.385185    0.000000
   12          1          0        -0.935117    3.252545    0.000000
---------------------------------------------------------------------
```
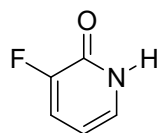

E = -422.6449526 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6          0         1.852393    0.610258    0.000000
    2          6          0         0.988524    1.640365    0.000000
    3          6          0        -0.966232    0.171957    0.000000
    4          6          0         0.000000   -0.911095    0.000000
    5          6          0         1.326726   -0.713053    0.000000
    6          1          0         2.910821    0.783378    0.000000
    7          1          0         1.292888    2.670317    0.000000
    8          1          0        -0.992619    2.185547    0.000000
    9          1          0         1.982416   -1.566546    0.000000
   10          7          0        -0.353406    1.413117    0.000000
   11          8          0        -2.165807    0.054669    0.000000
   12          9          0        -0.511296   -2.132496    0.000000
---------------------------------------------------------------------
```
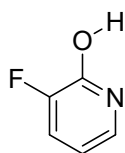
E = -422.6452294 a.u.

```
----------------------------------------------------------------
 Center      Atomic      Atomic          Coordinates (Angstroms)
 Number      Number       Type          X          Y          Z
----------------------------------------------------------------
    1          6           0        1.097363   1.629429   0.000000
    2          6           0        1.845379   0.474763   0.000000
    3          6           0        0.000000  -0.853830   0.000000
    4          6           0       -0.834844   0.260731   0.000000
    5          6           0       -0.288168   1.512066   0.000000
    6          1           0        1.572203   2.593147   0.000000
    7          1           0        2.921513   0.511861   0.000000
    8          1           0       -0.936149   2.370902   0.000000
    9          7           0        1.303773  -0.740054   0.000000
   10          8           0       -0.548228  -2.069185   0.000000
   11          1           0        0.163914  -2.705757   0.000000
   12          9           0       -2.153384   0.091639   0.000000
----------------------------------------------------------------
```
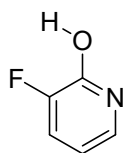
E = -422.6409337 a.u.

```
----------------------------------------------------------------
 Center      Atomic      Atomic          Coordinates (Angstroms)
 Number      Number       Type          X          Y          Z
----------------------------------------------------------------
    1          6           0       -1.893061   0.557289   0.000000
    2          6           0       -1.018863   1.623791   0.000000
    3          6           0        0.811062   0.290320   0.000000
    4          6           0        0.000000  -0.840103   0.000000
    5          6           0       -1.358964  -0.724706   0.000000
    6          1           0       -2.955673   0.715852   0.000000
    7          1           0       -1.390124   2.634952   0.000000
    8          1           0       -1.973443  -1.607632   0.000000
    9          7           0        0.302248   1.493571   0.000000
   10          8           0        2.144272   0.184125   0.000000
   11          1           0        2.398471  -0.734819   0.000000
   12          9           0        0.601090  -2.041766   0.000000
----------------------------------------------------------------
```
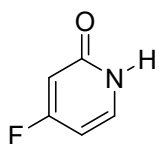
E = -422.6531069 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number       Type         X            Y            Z
--------------------------------------------------------------------
     1          6           0       -1.183104    -1.055690     0.000000
     2          6           0        0.003887    -1.691717     0.000000
     3          6           0        1.272404     0.392323     0.000000
     4          6           0        0.000000     1.071296     0.000000
     5          6           0       -1.140115     0.359868     0.000000
     6          1           0       -2.116833    -1.581993     0.000000
     7          1           0        0.088955    -2.762772     0.000000
     8          1           0        2.042708    -1.484716     0.000000
     9          1           0       -0.001472     2.144448     0.000000
    10          7           0        1.166090    -0.998889     0.000000
    11          8           0        2.361121     0.915301     0.000000
    12          9           0       -2.309266     0.988708     0.000000
--------------------------------------------------------------------
```
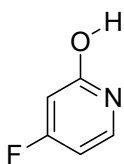
E = -422.6537432 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number       Type         X            Y            Z
--------------------------------------------------------------------
     1          6           0        1.198363    -1.058873     0.000000
     2          6           0       -0.025230    -1.689834     0.000000
     3          6           0       -1.164208     0.265225     0.000000
     4          6           0        0.000000     1.025749     0.000000
     5          6           0        1.174216     0.323623     0.000000
     6          1           0        2.125310    -1.600160     0.000000
     7          1           0       -0.079192    -2.765702     0.000000
     8          1           0       -0.025741     2.098577     0.000000
     9          7           0       -1.188657    -1.048798     0.000000
    10          8           0       -2.334991     0.907959     0.000000
    11          1           0       -3.026472     0.248954     0.000000
    12          9           0        2.323086     0.988990     0.000000
--------------------------------------------------------------------
```
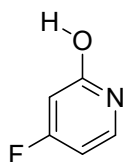
E = -422.644437 a.u.

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
 ---------------------------------------------------------------------
    1          6           0         1.187723   -1.084828    0.000000
    2          6           0        -0.046958   -1.701901    0.000000
    3          6           0        -1.176200    0.253070    0.000000
    4          6           0         0.000000    1.000073    0.000000
    5          6           0         1.174454    0.293043    0.000000
    6          1           0         2.108775   -1.636143    0.000000
    7          1           0        -0.107867   -2.777823    0.000000
    8          1           0         0.007225    2.075387    0.000000
    9          7           0        -1.204749   -1.058957    0.000000
   10          8           0        -2.379004    0.846138    0.000000
   11          1           0        -2.287306    1.792839    0.000000
   12          9           0         2.323370    0.959177    0.000000
 ---------------------------------------------------------------------
```
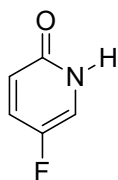

E = -422.64291 a.u.

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
 ---------------------------------------------------------------------
    1          6           0        -1.129083    0.706154    0.000000
    2          6           0        -1.170894   -0.631868    0.000000
    3          6           0         1.269451   -0.770536    0.000000
    4          6           0         1.262671    0.679440    0.000000
    5          6           0         0.112953    1.383076    0.000000
    6          1           0        -2.088191   -1.189472    0.000000
    7          1           0        -0.019858   -2.330467    0.000000
    8          1           0         2.223222    1.159902    0.000000
    9          1           0         0.114379    2.459693    0.000000
   10          7           0         0.000000   -1.328526    0.000000
   11          8           0         2.252993   -1.474598    0.000000
   12          9           0        -2.258231    1.422134    0.000000
 ---------------------------------------------------------------------
```
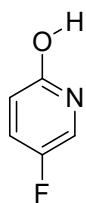
E = -422.6476105 a.u.

```
---------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number      Type         X           Y           Z
---------------------------------------------------------------
    1          6           0       -1.185358   -0.636408    0.000000
    2          6           0        0.000000   -1.323209    0.000000
    3          6           0        1.176954    0.617479    0.000000
    4          6           0        0.021988    1.394958    0.000000
    5          6           0       -1.188759    0.744435    0.000000
    6          1           0        0.009123   -2.399977    0.000000
    7          1           0        0.094424    2.466487    0.000000
    8          1           0       -2.120460    1.282070    0.000000
    9          7           0        1.170073   -0.693811    0.000000
   10          8           0        2.364141    1.238892    0.000000
   11          1           0        3.043937    0.568620    0.000000
   12          9           0       -2.342179   -1.306132    0.000000
---------------------------------------------------------------
```
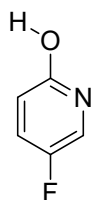

E = -422.6384543 a.u.

```
---------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number      Type         X           Y           Z
---------------------------------------------------------------
    1          6           0        0.049169   -1.349345    0.000000
    2          6           0        1.195654   -0.592183    0.000000
    3          6           0        0.000000    1.331525    0.000000
    4          6           0       -1.211668    0.643577    0.000000
    5          6           0       -1.181904   -0.734224    0.000000
    6          1           0        2.161313   -1.070144    0.000000
    7          1           0       -2.149973    1.170928    0.000000
    8          1           0       -2.083734   -1.320471    0.000000
    9          7           0        1.165351    0.731138    0.000000
   10          8           0        0.054316    2.675998    0.000000
   11          1           0       -0.821497    3.045683    0.000000
   12          9           0        0.132711   -2.683116    0.000000
---------------------------------------------------------------
```
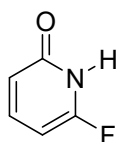
E = -422.6511446 a.u.

```
-----------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type          X            Y            Z
-----------------------------------------------------------------
    1          6           0        1.174014    -1.105842     0.000000
    2          6           0        1.143465     0.234082     0.000000
    3          6           0       -1.280063     0.368926     0.000000
    4          6           0       -1.256442    -1.074863     0.000000
    5          6           0       -0.091490    -1.756683     0.000000
    6          1           0        2.106141    -1.634244     0.000000
    7          1           0        0.041330     1.943501     0.000000
    8          1           0       -2.210014    -1.568048     0.000000
    9          1           0       -0.109505    -2.833275     0.000000
   10          7           0        0.000000     0.940437     0.000000
   11          8           0       -2.252224     1.082456     0.000000
   12          9           0        2.228104     0.983960     0.000000
-----------------------------------------------------------------
```
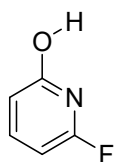
E = -422.6603817 a.u.

```
-----------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type          X            Y            Z
-----------------------------------------------------------------
    1          6           0        1.210812    -1.072021     0.000000
    2          6           0        1.112044     0.299532     0.000000
    3          6           0       -1.128027     0.299239     0.000000
    4          6           0       -1.186965    -1.087677     0.000000
    5          6           0        0.011629    -1.767560     0.000000
    6          1           0        2.168907    -1.554854     0.000000
    7          1           0       -2.136886    -1.587019     0.000000
    8          1           0        0.017956    -2.843931     0.000000
    9          7           0        0.000000     0.981339     0.000000
   10          8           0       -2.266311     0.996512     0.000000
   11          1           0       -2.046058     1.925738     0.000000
   12          9           0        2.223290     1.021058     0.000000
-----------------------------------------------------------------
```
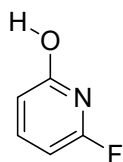
E = -422.6519767 a.u.

```
----------------------------------------------------------------
 Center     Atomic      Atomic         Coordinates (Angstroms)
 Number     Number       Type        X           Y           Z
----------------------------------------------------------------
    1          6           0      -1.235511    1.045152    0.000000
    2          6           0      -1.113706   -0.328042    0.000000
    3          6           0       1.121244   -0.308097    0.000000
    4          6           0       1.156916    1.081783    0.000000
    5          6           0      -0.049153    1.753772    0.000000
    6          1           0      -2.200488    1.514207    0.000000
    7          1           0       2.092599    1.612604    0.000000
    8          1           0      -0.064372    2.829883    0.000000
    9          7           0       0.000000   -0.997622    0.000000
   10          8           0       2.233974   -1.053814    0.000000
   11          1           0       3.006771   -0.499200    0.000000
   12          9           0      -2.220560   -1.056782    0.000000
----------------------------------------------------------------
```
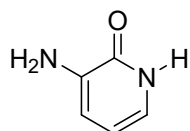

E = -378.765554 a.u.

```
----------------------------------------------------------------
 Center     Atomic      Atomic         Coordinates (Angstroms)
 Number     Number       Type        X           Y           Z
----------------------------------------------------------------
    1          6           0      -0.660829   -0.642025   -0.010713
    2          6           0       0.426385   -1.453610    0.001877
    3          6           0      -0.488074    0.808419   -0.003013
    4          6           0       1.743530   -0.917596    0.008936
    5          1           0       0.293026   -2.522808   -0.002823
    6          7           0      -1.967591   -1.049368   -0.069144
    7          7           0       0.812187    1.230447   -0.006217
    8          8           0      -1.420526    1.590082    0.014205
    9          6           0       1.911406    0.414978    0.001050
   10          1           0       2.597282   -1.568339    0.015454
   11          1           0      -2.191134   -1.959402    0.275138
   12          1           0      -2.633711   -0.329358    0.135670
   13          1           0       0.925832    2.226016    0.000511
   14          1           0       2.866235    0.904679    0.001124
----------------------------------------------------------------
```
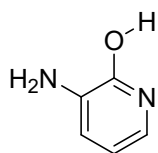
E = -378.7615651 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
---------------------------------------------------------------
    1          6           0       0.555473    0.688101   -0.009387
    2          6           0      -0.621553    1.405663   -0.004594
    3          6           0       0.424266   -0.708567   -0.004213
    4          6           0      -1.840535    0.736511    0.004551
    5          1           0      -0.589209    2.482633   -0.013851
    6          7           0       1.812621    1.262719   -0.071870
    7          7           0      -0.710358   -1.345740    0.003260
    8          8           0       1.568332   -1.423013    0.001265
    9          6           0      -1.840362   -0.637206    0.005682
   10          1           0      -2.766467    1.282822    0.007921
   11          1           0       1.891221    2.182861    0.311573
   12          1           0       2.565320    0.657586    0.190332
   13          1           0      -2.757567   -1.200314    0.010474
   14          1           0       1.330464   -2.347343    0.011463
---------------------------------------------------------------
```
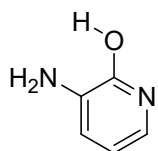

E = -378.7526445 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
---------------------------------------------------------------
    1          6           0       0.000000    0.839891    0.000000
    2          6           0       1.365784    0.673278    0.000000
    3          6           0      -0.795828   -0.315660    0.000000
    4          6           0       1.896124   -0.608757    0.000000
    5          1           0       2.009651    1.537747    0.000000
    6          7           0      -0.686533    2.091851    0.000000
    7          7           0      -0.305927   -1.531981    0.000000
    8          8           0      -2.123120   -0.193919    0.000000
    9          6           0       1.012704   -1.668666    0.000000
   10          1           0       2.957593   -0.777221    0.000000
   11          1           0      -0.487590    2.643412    0.816330
   12          1           0      -0.487590    2.643412   -0.816330
   13          1           0       1.378765   -2.682749    0.000000
   14          1           0      -2.311362    0.747159    0.000000
---------------------------------------------------------------
```
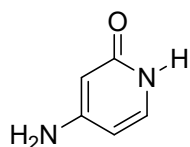
E = -378.7680981 a.u.

```
----------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type         X            Y            Z
----------------------------------------------------------------------
   1           6           0       0.068248    -1.046167    -0.002659
   2           6           0       1.181067    -0.257007    -0.005695
   3           6           0      -1.252934    -0.498167     0.000299
   4           6           0       1.043383     1.168227    -0.003752
   5           7           0      -1.290185     0.899327     0.004331
   6           8           0      -2.295365    -1.118603     0.003567
   7           6           0      -0.195431     1.690522     0.001936
   8           1           0       1.905437     1.808415    -0.016772
   9           1           0      -2.209083     1.297244     0.008466
  10           1           0      -0.373544     2.750747     0.003406
  11           1           0       0.139544    -2.118802    -0.006102
  12           7           0       2.444278    -0.781600    -0.054280
  13           1           0       3.203313    -0.204096     0.240733
  14           1           0       2.552600    -1.753221     0.150609
----------------------------------------------------------------------
```
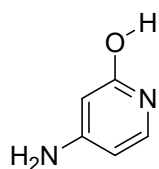

E = -378.767834 a.u.

```
----------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type         X            Y            Z
----------------------------------------------------------------------
   1           6           0       0.038483    -1.001619    -0.005819
   2           6           0       1.204934    -0.253495    -0.007609
   3           6           0      -1.168506    -0.322955     0.000374
   4           6           0       1.089042     1.143046    -0.003601
   5           7           0      -1.294691     0.986441     0.005587
   6           8           0      -2.297433    -1.045473     0.003167
   7           6           0      -0.167553     1.693043     0.003413
   8           1           0       1.962032     1.771501    -0.011383
   9           1           0      -0.285091     2.764590     0.007531
  10           1           0      -3.025519    -0.427639     0.007480
  11           1           0       0.048853    -2.076596    -0.013640
  12           7           0       2.435326    -0.855661    -0.055398
  13           1           0       3.227099    -0.311097     0.216007
  14           1           0       2.489247    -1.820559     0.196794
----------------------------------------------------------------------
```
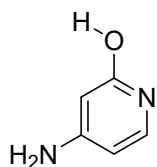
E = -378.7580622 a.u.

```
---------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type            X           Y           Z
---------------------------------------------------------------
  1           6           0       0.000104   -0.976632   -0.005440
  2           6           0       1.193178   -0.267930   -0.007865
  3           6           0      -1.193657   -0.266189    0.001072
  4           6           0       1.117798    1.127004   -0.004297
  5           7           0      -1.274800    1.043637    0.006797
  6           8           0      -2.378833   -0.903393    0.003833
  7           6           0      -0.127207    1.709534    0.003680
  8           1           0       2.007398    1.731773   -0.012090
  9           1           0      -0.211653    2.784630    0.008233
 10           1           0      -2.247309   -1.844902   -0.008181
 11           1           0       0.001630   -2.054321   -0.014849
 12           7           0       2.403417   -0.912556   -0.057199
 13           1           0       3.211119   -0.389334    0.210114
 14           1           0       2.427864   -1.872998    0.216026
---------------------------------------------------------------
```
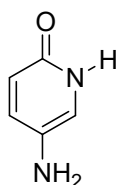

E = -378.7526947 a.u.

```
---------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type            X           Y           Z
---------------------------------------------------------------
  1           6           0      -0.728261   -1.247530   -0.001404
  2           6           0       0.617257   -1.211625   -0.016811
  3           6           0      -1.521251   -0.035217    0.003883
  4           6           0       1.340258    0.020914   -0.002232
  5           7           0      -0.754916    1.110045   -0.001857
  6           8           0      -2.733245    0.020502    0.007769
  7           6           0       0.613792    1.154946    0.014163
  8           1           0      -1.276311    1.965294   -0.002362
  9           1           0       1.052891    2.136053    0.026921
 10           1           0      -1.272607   -2.173737   -0.009128
 11           1           0       1.179395   -2.131153   -0.048071
 12           7           0       2.742804   -0.012444   -0.080602
 13           1           0       3.171941    0.892068   -0.031415
 14           1           0       3.164655   -0.624666    0.593529
---------------------------------------------------------------
```
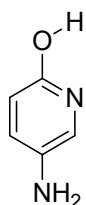
E = -378.7569688 a.u.

```
---------------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type           X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.699060    1.221486    0.000006
   2          6           0       -0.673961    1.203214   -0.010694
   3          6           0        1.366205    0.002029    0.002711
   4          6           0       -1.356042   -0.013054   -0.007785
   5          1           0       -1.225424    2.128964   -0.026482
   6          7           0        0.746562   -1.149355    0.000152
   7          8           0        2.712578   -0.000405    0.009545
   8          6           0       -0.582631   -1.158670   -0.002370
   9          1           0       -1.050716   -2.130995   -0.004295
  10          1           0        2.996086   -0.911510    0.007445
  11          7           0       -2.750594   -0.065200   -0.075165
  12          1           0       -3.145648   -0.944274    0.196960
  13          1           0       -3.218215    0.692498    0.383120
  14          1           0        1.255729    2.140407    0.000784
---------------------------------------------------------------------
```
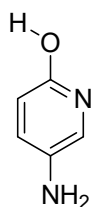

E = -378.7480303 a.u.

```
---------------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type           X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.726164    1.178353   -0.000273
   2          6           0       -0.650569    1.203245   -0.010393
   3          6           0        1.367653   -0.055381    0.002594
   4          6           0       -1.361088    0.009254   -0.007981
   5          1           0       -1.172709    2.145765   -0.025205
   6          7           0        0.712717   -1.187616    0.000254
   7          8           0        2.714926   -0.166651    0.010220
   8          6           0       -0.610042   -1.156270   -0.003124
   9          1           0       -1.106128   -2.115429   -0.005413
  10          1           0        3.115323    0.695258    0.004352
  11          7           0       -2.755573   -0.016942   -0.074510
  12          1           0       -3.167101   -0.886310    0.204251
  13          1           0       -3.210453    0.754011    0.374153
  14          1           0        1.288949    2.096622    0.000960
---------------------------------------------------------------------
```
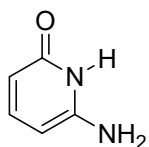
E = -378.7658989 a.u.

```
----------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
----------------------------------------------------------------
   1           6          0        1.363242    1.003882    0.008623
   2           6          0        0.236585    1.755166    0.002088
   3           6          0        1.281407   -0.429800    0.003606
   4           6          0       -1.058431    1.190304    0.003356
   5           7          0       -0.032230   -0.917031   -0.005128
   6           8          0        2.198589   -1.219981   -0.000515
   7           6          0       -1.161737   -0.167043   -0.005868
   8           1          0       -0.095135   -1.915729   -0.074826
   9           1          0        2.345973    1.435480    0.010082
  10           1          0        0.322983    2.829247    0.004040
  11           1          0       -1.939570    1.803017    0.014450
  12           7          0       -2.345925   -0.862005   -0.068335
  13           1          0       -2.374840   -1.741380    0.409931
  14           1          0       -3.167428   -0.312591    0.083857
----------------------------------------------------------------
```
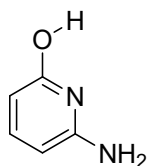
E = -378.7728846 a.u.

```
----------------------------------------------------------------
Center      Atomic      Atomic           Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
----------------------------------------------------------------
   1           6          0        1.253420    1.070370    0.005065
   2           6          0        0.071021    1.783928    0.003982
   3           6          0        1.140177   -0.310386    0.000586
   4           6          0       -1.144862    1.131099   -0.004229
   5           1          0        0.097220    2.860516    0.007455
   6           7          0       -0.003223   -0.961740   -0.001753
   7           8          0        2.256991   -1.050359    0.002960
   8           6          0       -1.133300   -0.262416   -0.008208
   9           1          0        1.992881   -1.967576   -0.007098
  10           1          0        2.219154    1.538032    0.009530
  11           7          0       -2.293209   -0.990704   -0.059254
  12           1          0       -2.202242   -1.958470    0.173558
  13           1          0       -3.132836   -0.550113    0.252922
  14           1          0       -2.073815    1.672016   -0.016173
----------------------------------------------------------------
```
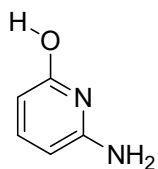
E = -378.7650806 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
---------------------------------------------------------------------
    1          6           0       -1.250177    1.032113    0.004003
    2          6           0       -0.080375    1.770802    0.003877
    3          6           0       -1.120832   -0.350801    0.000178
    4          6           0        1.141427    1.137559   -0.003684
    5          1           0       -0.127379    2.846574    0.007268
    6          7           0        0.031526   -0.978516   -0.002135
    7          8           0       -2.193974   -1.161624    0.002597
    8          6           0        1.145094   -0.259560   -0.007882
    9          1           0       -2.991932   -0.644343    0.004847
   10          1           0       -2.216492    1.504590    0.008355
   11          1           0        2.063140    1.690749   -0.015339
   12          7           0        2.315375   -0.967848   -0.057405
   13          1           0        3.150370   -0.519637    0.255524
   14          1           0        2.234955   -1.941068    0.156390
---------------------------------------------------------------------
```
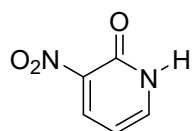

E = -527.8534468 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
---------------------------------------------------------------------
    1          6           0        0.423430    1.047352   -0.085500
    2          6           0       -0.280665   -0.221313    0.006012
    3          6           0        0.361316   -1.411454    0.067939
    4          6           0        1.768815   -1.482067    0.103410
    5          6           0        2.455568   -0.318216    0.055746
    6          7           0        1.810102    0.860348   -0.031635
    7          1           0       -0.232239   -2.307928    0.096331
    8          1           0        2.279839   -2.421983    0.170652
    9          1           0        3.529205   -0.269202    0.082739
   10          8           0       -0.024175    2.150715   -0.224317
   11          1           0        2.330607    1.716334   -0.087810
   12          7           0       -1.734931   -0.231175    0.025485
   13          8           0       -2.294422    0.708894    0.513299
   14          8           0       -2.281950   -1.210515   -0.427045
---------------------------------------------------------------------
```
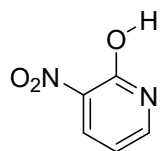
E = -527.8545268 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic        Coordinates (Angstroms)
 Number     Number      Type          X          Y          Z
---------------------------------------------------------------
    1          6          0       -0.492212   0.942459   0.049649
    2          6          0        0.241216  -0.247532  -0.012092
    3          6          0       -0.433962  -1.448682  -0.064952
    4          6          0       -1.813398  -1.446684  -0.084462
    5          6          0       -2.451187  -0.222250  -0.033810
    6          7          0       -1.809446   0.931691   0.039117
    7          1          0        0.135607  -2.359107  -0.091791
    8          1          0       -2.374158  -2.360977  -0.136536
    9          1          0       -3.526848  -0.160750  -0.048175
   10          8          0        0.101335   2.118498   0.154662
   11          7          0        1.697189  -0.278572  -0.018555
   12          8          0        2.284530   0.698787  -0.390311
   13          8          0        2.218812  -1.308916   0.334973
   14          1          0       -0.588953   2.778179   0.211977
---------------------------------------------------------------
```
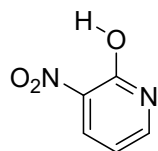

E = -527.8606681 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic        Coordinates (Angstroms)
 Number     Number      Type          X          Y          Z
---------------------------------------------------------------
    1          6          0       -0.239541  -1.052692   0.000000
    2          6          0        0.000000   0.335441   0.000000
    3          6          0        1.301667   0.808985   0.000000
    4          6          0        2.333307  -0.095821   0.000000
    5          6          0        2.001175  -1.444543   0.000000
    6          7          0        0.768156  -1.904676   0.000000
    7          1          0        1.468417   1.870018   0.000000
    8          1          0        3.359388   0.220843   0.000000
    9          1          0        2.777836  -2.192547   0.000000
   10          8          0       -1.437798  -1.591742   0.000000
   11          7          0       -1.077587   1.295908   0.000000
   12          8          0       -2.220983   0.871156   0.000000
   13          8          0       -0.806361   2.463623   0.000000
   14          1          0       -2.098127  -0.889460   0.000000
---------------------------------------------------------------
```
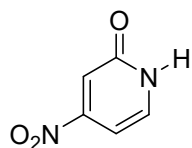
E = -527.8588358 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
---------------------------------------------------------------------
    1          6           0       -0.358789   -1.840511    0.000000
    2          6           0       -0.860982   -0.478514    0.000000
    3          6           0        0.000000    0.551594    0.000000
    4          6           0        1.409780    0.403265    0.000000
    5          6           0        1.874749   -0.859695    0.000000
    6          7           0        1.027912   -1.919188    0.000000
    7          1           0        2.059931    1.252985    0.000000
    8          1           0        2.923575   -1.091867    0.000000
    9          8           0       -1.036923   -2.836836    0.000000
   10          1           0        1.393817   -2.852975    0.000000
   11          1           0       -1.923463   -0.333110    0.000000
   12          7           0       -0.546885    1.925076    0.000000
   13          8           0       -1.739798    2.052853    0.000000
   14          8           0        0.250522    2.824847    0.000000
---------------------------------------------------------------------
```
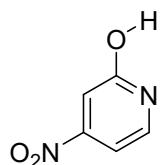

E = -527.860718 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type            X           Y           Z
---------------------------------------------------------------------
    1          6           0       -0.120990   -1.760106    0.000000
    2          6           0       -0.791795   -0.539137    0.000000
    3          6           0        0.000000    0.577078    0.000000
    4          6           0        1.381141    0.501163    0.000000
    5          6           0        1.919018   -0.767116    0.000000
    6          7           0        1.186257   -1.874633    0.000000
    7          1           0        1.989564    1.383531    0.000000
    8          1           0        2.986702   -0.905676    0.000000
    9          8           0       -0.850958   -2.876081    0.000000
   10          1           0       -1.862362   -0.483392    0.000000
   11          7           0       -0.645250    1.901874    0.000000
   12          8           0       -1.846015    1.933192    0.000000
   13          8           0        0.075383    2.863426    0.000000
   14          1           0       -0.252476   -3.620736    0.000000
---------------------------------------------------------------------
```
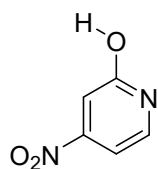
E = -527.8521073 a.u.

```
----------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type          X           Y           Z
----------------------------------------------------------------
   1          6           0      -0.047395   -1.774124    0.000000
   2          6           0      -0.751524   -0.571903    0.000000
   3          6           0       0.000000    0.576099    0.000000
   4          6           0       1.377559    0.545609    0.000000
   5          6           0       1.952752   -0.711323    0.000000
   6          7           0       1.263693   -1.840228    0.000000
   7          1           0       1.959557    1.445784    0.000000
   8          1           0       3.025059   -0.813202    0.000000
   9          8           0      -0.675183   -2.956307    0.000000
  10          1           0      -1.824417   -0.525237    0.000000
  11          7           0      -0.695648    1.873971    0.000000
  12          8           0      -1.897964    1.857000    0.000000
  13          8           0      -0.014995    2.863163    0.000000
  14          1           0      -1.619729   -2.840551    0.000000
----------------------------------------------------------------
```
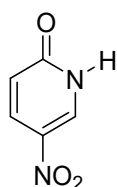

E = -527.864658 a.u.

```
----------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type          X           Y           Z
----------------------------------------------------------------
   1          6           0       0.100846   -2.158095    0.000000
   2          6           0       1.304467   -1.353214    0.000000
   3          6           0       1.256358   -0.008712    0.000000
   4          6           0       0.000000    0.655197    0.000000
   5          6           0      -1.145790   -0.062705    0.000000
   6          7           0      -1.082199   -1.400626    0.000000
   7          1           0      -2.113228    0.402857    0.000000
   8          8           0       0.037400   -3.359066    0.000000
   9          1           0      -1.926895   -1.942465    0.000000
  10          1           0       2.234691   -1.889576    0.000000
  11          1           0       2.151279    0.586102    0.000000
  12          7           0      -0.075199    2.093711    0.000000
  13          8           0      -1.170512    2.603093    0.000000
  14          8           0       0.965692    2.700554    0.000000
----------------------------------------------------------------
```
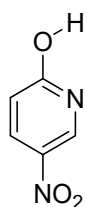
E = -527.86501 a.u.

```
--------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type          X            Y            Z
--------------------------------------------------------------------
   1           6           0        0.044855    -2.008411     0.000000
   2           6           0        1.267264    -1.334925     0.000000
   3           6           0        1.238061     0.033448     0.000000
   4           6           0        0.000000     0.663074     0.000000
   5           6           0       -1.155976    -0.087074     0.000000
   6           7           0       -1.127799    -1.409342     0.000000
   7           1           0       -2.117867     0.392566     0.000000
   8           8           0        0.057040    -3.336754     0.000000
   9           1           0        2.185910    -1.890581     0.000000
  10           1           0        2.137311     0.620742     0.000000
  11           7           0       -0.079077     2.111641     0.000000
  12           8           0       -1.174693     2.612880     0.000000
  13           8           0        0.958427     2.724790     0.000000
  14           1           0       -0.848637    -3.642825     0.000000
--------------------------------------------------------------------
```
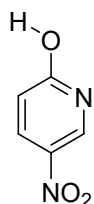

E = -527.8556905 a.u.

```
--------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type          X            Y            Z
--------------------------------------------------------------------
   1           6           0       -0.014084    -2.012170     0.000000
   2           6           0        1.219301    -1.354598     0.000000
   3           6           0        1.222139     0.016398     0.000000
   4           6           0        0.000000     0.666774     0.000000
   5           6           0       -1.169662    -0.068150     0.000000
   6           7           0       -1.171534    -1.386889     0.000000
   7           1           0       -2.122423     0.430318     0.000000
   8           8           0       -0.099761    -3.342996     0.000000
   9           1           0        2.141668    -1.908756     0.000000
  10           1           0        2.134496     0.583130     0.000000
  11           7           0       -0.051319     2.116524     0.000000
  12           8           0       -1.136667     2.638315     0.000000
  13           8           0        0.998321     2.709575     0.000000
  14           1           0        0.764928    -3.740822     0.000000
--------------------------------------------------------------------
```
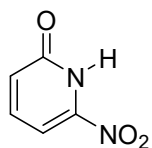
E = -527.8580828 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type        X           Y           Z
---------------------------------------------------------------
    1          6           0       0.018356   -1.852895    0.000000
    2          6           0       1.467701   -1.731184    0.000000
    3          6           0       2.081578   -0.533142    0.000000
    4          6           0       1.334982    0.682102    0.000000
    5          6           0       0.000000    0.563796    0.000000
    6          7           0      -0.637967   -0.626479    0.000000
    7          8           0      -0.601622   -2.884688    0.000000
    8          1           0      -1.643497   -0.635393    0.000000
    9          1           0       2.016233   -2.654865    0.000000
   10          1           0       3.156381   -0.478794    0.000000
   11          1           0       1.795368    1.649335    0.000000
   12          7           0      -0.874638    1.733449    0.000000
   13          8           0      -2.060667    1.519380    0.000000
   14          8           0      -0.356704    2.815167    0.000000
---------------------------------------------------------------
```
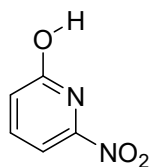

E = -527.8622989 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type        X           Y           Z
---------------------------------------------------------------
    1          6           0      -0.035641   -1.704774    0.000000
    2          6           0       1.358064   -1.772360    0.000000
    3          6           0       2.053859   -0.589527    0.000000
    4          6           0       1.366925    0.621758    0.000000
    5          6           0       0.000000    0.533988    0.000000
    6          7           0      -0.698615   -0.574954    0.000000
    7          8           0      -0.730582   -2.841935    0.000000
    8          1           0       1.845704   -2.729278    0.000000
    9          1           0       3.129653   -0.595744    0.000000
   10          1           0       1.860898    1.572418    0.000000
   11          7           0      -0.798630    1.786882    0.000000
   12          8           0      -1.989793    1.693729    0.000000
   13          8           0      -0.173785    2.818291    0.000000
   14          1           0      -1.661498   -2.626083    0.000000
---------------------------------------------------------------
```
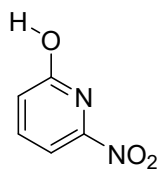
E = -527.8526698 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number       Type          X           Y           Z
---------------------------------------------------------------
    1          6           0       -0.091402   -1.697106    0.000000
    2          6           0        1.301386   -1.787802    0.000000
    3          6           0        2.029475   -0.620732    0.000000
    4          6           0        1.371996    0.601053    0.000000
    5          6           0        0.000000    0.536155    0.000000
    6          7           0       -0.723641   -0.549271    0.000000
    7          8           0       -0.879428   -2.777808    0.000000
    8          1           0        1.790347   -2.746667    0.000000
    9          1           0        3.104726   -0.655595    0.000000
   10          1           0        1.884559    1.541635    0.000000
   11          7           0       -0.769140    1.812617    0.000000
   12          8           0       -1.960557    1.751716    0.000000
   13          8           0       -0.114654    2.826576    0.000000
   14          1           0       -0.361777   -3.576065    0.000000
---------------------------------------------------------------
```
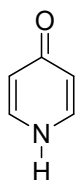

E = -323.4025585 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number       Type          X           Y           Z
---------------------------------------------------------------
    1          6           0        0.000000   -1.182230   -1.036416
    2          6           0        0.000000   -1.221558    0.304982
    3          6           0        0.000000    0.000000    1.100689
    4          6           0        0.000000    1.221558    0.304982
    5          6           0        0.000000    1.182230   -1.036416
    6          7           0        0.000000    0.000000   -1.713728
    7          1           0        0.000000   -2.068715   -1.645018
    8          1           0        0.000000   -2.164125    0.820840
    9          1           0        0.000000    2.164125    0.820840
   10          1           0        0.000000    2.068715   -1.645018
   11          8           0        0.000000    0.000000    2.316101
   12          1           0        0.000000    0.000000   -2.711294
---------------------------------------------------------------
```
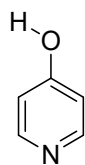
E = -323.4066016 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic              Coordinates (Angstroms)
 Number      Number       Type         X              Y             Z
--------------------------------------------------------------------
     1          6           0        1.144806     -1.150834      0.000000
     2          6           0        1.196601      0.228070      0.000000
     3          6           0        0.000000      0.925139      0.000000
     4          6           0       -1.184625      0.207194      0.000000
     5          6           0       -1.111119     -1.173870      0.000000
     6          7           0        0.021621     -1.856393      0.000000
     7          1           0        2.061935     -1.717773      0.000000
     8          1           0        2.132412      0.756738      0.000000
     9          1           0       -2.140842      0.703731      0.000000
    10          1           0       -2.019642     -1.754825      0.000000
    11          8           0        0.046509      2.269477      0.000000
    12          1           0       -0.831267      2.636879      0.000000
--------------------------------------------------------------------
```
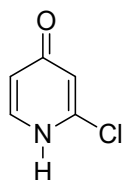

E = -783.0094105 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic              Coordinates (Angstroms)
 Number      Number       Type         X              Y             Z
--------------------------------------------------------------------
     1          6           0        1.658991      0.918031      0.000000
     2          6           0        0.734947      1.887193      0.000000
     3          6           0       -0.689540      1.573319      0.000000
     4          6           0       -0.988670      0.143839      0.000000
     5          6           0        0.000000     -0.758225      0.000000
     6          7           0        1.312140     -0.403698      0.000000
     7          1           0        2.715694      1.114153      0.000000
     8          1           0        1.028135      2.920471      0.000000
     9          1           0       -2.015857     -0.166756      0.000000
    10          8           0       -1.556870      2.421151      0.000000
    11          1           0        2.013138     -1.114847      0.000000
    12         17           0       -0.280323     -2.463605      0.000000
--------------------------------------------------------------------
```
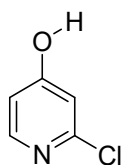
E = -783.0186604 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
---------------------------------------------------------------------
    1          6           0       1.821827   -0.502021    0.000000
    2          6           0       1.075474   -1.656939    0.000000
    3          6           0      -0.307790   -1.535523    0.000000
    4          6           0      -0.869779   -0.271309    0.000000
    5          6           0       0.000000    0.805287    0.000000
    6          7           0       1.301287    0.722244    0.000000
    7          1           0       2.897841   -0.554472    0.000000
    8          1           0       1.535241   -2.627871    0.000000
    9          1           0      -1.934581   -0.121387    0.000000
   10          8           0      -1.040731   -2.658853    0.000000
   11          1           0      -1.971773   -2.460510    0.000000
   12         17           0      -0.684016    2.408375    0.000000
---------------------------------------------------------------------
```
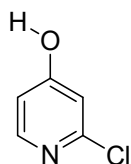

E = -783.0183691 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
---------------------------------------------------------------------
    1          6           0       1.806785   -0.519528    0.000000
    2          6           0       1.040316   -1.665435    0.000000
    3          6           0      -0.340667   -1.523290    0.000000
    4          6           0      -0.884351   -0.251354    0.000000
    5          6           0       0.000000    0.808732    0.000000
    6          7           0       1.304901    0.707435    0.000000
    7          1           0       2.881953   -0.589945    0.000000
    8          1           0       1.505338   -2.636502    0.000000
    9          1           0      -1.947614   -0.106885    0.000000
   10          8           0      -1.186786   -2.564764    0.000000
   11          1           0      -0.711409   -3.389221    0.000000
   12         17           0      -0.652988    2.423168    0.000000
---------------------------------------------------------------------
```
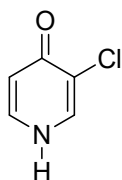
E = -783.0078366 a.u.

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type          X           Y           Z
 ---------------------------------------------------------------------
    1          6           0         1.225001    1.913399    0.000000
    2          6           0        -0.116557    1.884818    0.000000
    3          6           0        -0.865980    0.636542    0.000000
    4          6           0         0.000000   -0.546748    0.000000
    5          6           0         1.339683   -0.447778    0.000000
    6          7           0         1.954675    0.765378    0.000000
    7          1           0         1.789334    2.828170    0.000000
    8          1           0        -0.680304    2.799295    0.000000
    9          1           0         1.978745   -1.310979    0.000000
   10          8           0        -2.074207    0.582812    0.000000
   11          1           0         2.951750    0.807665    0.000000
   12         17           0        -0.742440   -2.105041    0.000000
 ---------------------------------------------------------------------
```
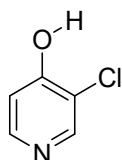

E = -783.0160954 a.u.

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type          X           Y           Z
 ---------------------------------------------------------------------
    1          6           0         1.588066   -1.650242    0.000000
    2          6           0         0.223877   -1.846064    0.000000
    3          6           0        -0.607471   -0.737165    0.000000
    4          6           0         0.000000    0.510850    0.000000
    5          6           0         1.378494    0.600009    0.000000
    6          7           0         2.167802   -0.456858    0.000000
    7          1           0         2.250147   -2.500456    0.000000
    8          1           0        -0.205895   -2.831270    0.000000
    9          8           0        -1.930210   -0.914861    0.000000
   10          1           0        -2.380266   -0.072697    0.000000
   11          1           0         1.847168    1.570250    0.000000
   12         17           0        -0.984817    1.946278    0.000000
 ---------------------------------------------------------------------
```
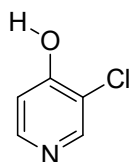
E = -783.0115104 a.u.

```
-----------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number      Type          X           Y           Z
-----------------------------------------------------------------
     1          6          0       1.548106   -1.678482    0.000000
     2          6          0       0.176582   -1.837513    0.000000
     3          6          0      -0.629325   -0.709507    0.000000
     4          6          0       0.000000    0.527772    0.000000
     5          6          0       1.381125    0.573927    0.000000
     6          7          0       2.150474   -0.500836    0.000000
     7          1          0       2.188416   -2.545490    0.000000
     8          1          0      -0.260306   -2.822246    0.000000
     9          8          0      -1.966030   -0.757769    0.000000
    10          1          0      -2.268907   -1.659904    0.000000
    11          1          0       1.873562    1.532150    0.000000
    12         17          0      -0.924516    1.988607    0.000000
-----------------------------------------------------------------
```
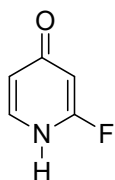

E = -422.6359716 a.u.

```
-----------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number      Type          X           Y           Z
-----------------------------------------------------------------
     1          6          0      -0.110031   -1.686564    0.000000
     2          6          0      -1.269772   -1.019734    0.000000
     3          6          0      -1.310861    0.442840    0.000000
     4          6          0       0.000000    1.080175    0.000000
     5          6          0       1.100343    0.325988    0.000000
     6          7          0       1.089948   -1.025530    0.000000
     7          1          0      -0.045049   -2.758836    0.000000
     8          1          0      -2.203326   -1.550784    0.000000
     9          1          0       0.073995    2.150879    0.000000
    10          8          0      -2.348211    1.070763    0.000000
    11          1          0       1.959660   -1.517717    0.000000
    12          9          0       2.323633    0.825870    0.000000
-----------------------------------------------------------------
```
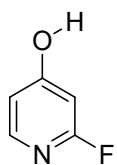
E = -422.6489721 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6           0        -0.100733   -1.702239    0.000000
    2          6           0         1.135518   -1.102834    0.000000
    3          6           0         1.184432    0.287412    0.000000
    4          6           0         0.000000    0.999832    0.000000
    5          6           0        -1.165334    0.258132    0.000000
    6          7           0        -1.253590   -1.034491    0.000000
    7          1           0        -0.179381   -2.776540    0.000000
    8          1           0         2.043182   -1.677122    0.000000
    9          1           0        -0.035012    2.074803    0.000000
   10          8           0         2.389223    0.875269    0.000000
   11          1           0         2.307727    1.823638    0.000000
   12          9           0        -2.310940    0.928077    0.000000
---------------------------------------------------------------------
```
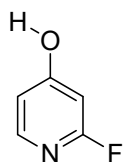

E = -422.6488057 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6           0        -0.119619   -1.692103    0.000000
    2          6           0         1.122646   -1.097243    0.000000
    3          6           0         1.179338    0.292698    0.000000
    4          6           0         0.000000    1.012211    0.000000
    5          6           0        -1.166032    0.278132    0.000000
    6          7           0        -1.263604   -1.018542    0.000000
    7          1           0        -0.202714   -2.766265    0.000000
    8          1           0         2.017644   -1.695410    0.000000
    9          1           0        -0.007262    2.085509    0.000000
   10          8           0         2.332097    0.978319    0.000000
   11          1           0         3.078360    0.387827    0.000000
   12          9           0        -2.310621    0.947712    0.000000
---------------------------------------------------------------------
```
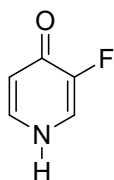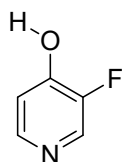
E = -422.6276961 a.u.

```
----------------------------------------------------------------
 Center      Atomic      Atomic           Coordinates (Angstroms)
 Number      Number      Type          X           Y           Z
----------------------------------------------------------------
    1          6          0       -0.864716   -1.701940    0.000000
    2          6          0        0.462586   -1.486580    0.000000
    3          6          0        1.028128   -0.147689    0.000000
    4          6          0        0.000000    0.887611    0.000000
    5          6          0       -1.311597    0.618555    0.000000
    6          7          0       -1.750166   -0.672940    0.000000
    7          1          0       -1.292690   -2.687912    0.000000
    8          1          0        1.146477   -2.315021    0.000000
    9          1          0       -2.051964    1.396619    0.000000
   10          8          0        2.214120    0.097407    0.000000
   11          1          0       -2.730691   -0.856852    0.000000
   12          9          0        0.397852    2.152749    0.000000
----------------------------------------------------------------
```
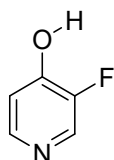
E = -422.6364508 a.u.

```
----------------------------------------------------------------
 Center      Atomic      Atomic           Coordinates (Angstroms)
 Number      Number      Type          X           Y           Z
----------------------------------------------------------------
    1          6          0       -1.139806   -1.576076    0.000000
    2          6          0        0.240641   -1.510940    0.000000
    3          6          0        0.841012   -0.265120    0.000000
    4          6          0        0.000000    0.831705    0.000000
    5          6          0       -1.363313    0.675965    0.000000
    6          7          0       -1.935518   -0.516675    0.000000
    7          1          0       -1.627655   -2.536811    0.000000
    8          1          0        0.848310   -2.397662    0.000000
    9          8          0        2.174198   -0.146680    0.000000
   10          1          0        2.424074    0.773889    0.000000
   11          1          0       -1.998541    1.546656    0.000000
   12          9          0        0.559740    2.052321    0.000000
----------------------------------------------------------------
```

H
O
F

E = -422.6320997 a.u.

```
----------------------------------------------------------------------
Center       Atomic       Atomic              Coordinates (Angstroms)
Number       Number       Type           X            Y            Z
----------------------------------------------------------------------
   1            6            0        -1.128566     1.573659     0.000000
   2            6            0         0.252250     1.489602     0.000000
   3            6            0         0.847868     0.239848     0.000000
   4            6            0         0.000000    -0.855277     0.000000
   5            6            0        -1.361542    -0.673944     0.000000
   6            7            0        -1.929364     0.522527     0.000000
   7            1            0        -1.604524     2.540443     0.000000
   8            1            0         0.854874     2.382663     0.000000
   9            8            0         2.169880     0.026057     0.000000
  10            1            0         2.643813     0.851335     0.000000
  11            1            0        -2.003961    -1.539346     0.000000
  12            9            0         0.510695    -2.082730     0.000000
----------------------------------------------------------------------
```
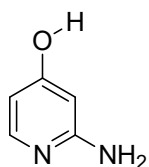
O
N
H
NH₂
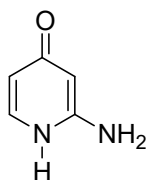
E = -378.7495345 a.u.

```
----------------------------------------------------------------------
Center       Atomic       Atomic              Coordinates (Angstroms)
Number       Number       Type           X            Y            Z
----------------------------------------------------------------------
   1            6            0         0.171288     1.696465     0.002038
   2            6            0         1.320765     1.014945     0.008509
   3            6            0         1.327400    -0.447580    -0.001417
   4            6            0         0.010239    -1.050899     0.007983
   5            6            0        -1.114963    -0.304280    -0.003995
   6            7            0        -1.041460     1.058968     0.004489
   7            1            0         0.124320     2.770424    -0.001445
   8            1            0         2.264063     1.528601     0.018097
   9            1            0        -0.052858    -2.123773     0.036177
  10            8            0         2.357541    -1.095274    -0.000384
  11            1            0        -1.871970     1.582480    -0.179827
  12            7            0        -2.404278    -0.807027    -0.073279
  13            1            0        -2.443585    -1.807188    -0.049182
  14            1            0        -3.048510    -0.403839     0.582073
----------------------------------------------------------------------
```

E =-378.7609986 a.u.

```
---------------------------------------------------------------------
Center      Atomic      Atomic          Coordinates (Angstroms)
Number      Number      Type           X           Y           Z
---------------------------------------------------------------------
    1          6          0       -0.044222    1.708666    0.002394
    2          6          0        1.188275    1.099494    0.006367
    3          6          0        1.207973   -0.290654    0.001751
    4          6          0        0.018918   -0.986728   -0.008301
    5          6          0       -1.172697   -0.256924   -0.008521
    6          7          0       -1.205654    1.066537   -0.000523
    7          1          0       -0.107059    2.785158    0.006330
    8          1          0        2.103562    1.660734    0.012739
    9          1          0        0.003218   -2.064078   -0.028311
   10          8          0        2.406763   -0.901726    0.003945
   11          1          0        2.301172   -1.847251   -0.008468
   12          7          0       -2.385439   -0.897539   -0.059989
   13          1          0       -2.436799   -1.830656    0.291617
   14          1          0       -3.170038   -0.316195    0.155983
---------------------------------------------------------------------
```
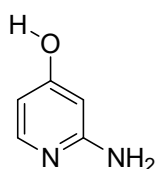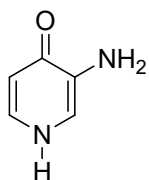

E = -378.761394 a.u.

```
---------------------------------------------------------------------
Center      Atomic      Atomic          Coordinates (Angstroms)
Number      Number      Type           X           Y           Z
---------------------------------------------------------------------
    1          6          0       -0.025095    1.700226    0.002546
    2          6          0        1.198468    1.066900    0.004841
    3          6          0        1.194168   -0.324871    0.000950
    4          6          0       -0.004638   -0.999755   -0.007900
    5          6          0       -1.180335   -0.249615   -0.008413
    6          7          0       -1.192943    1.078570    0.000040
    7          1          0       -0.067268    2.777944    0.007355
    8          1          0        2.115413    1.630424    0.010941
    9          1          0       -0.019138   -2.074587   -0.023960
   10          8          0        2.326854   -1.052472    0.003372
   11          1          0        3.087672   -0.481451    0.003689
   12          7          0       -2.403744   -0.865177   -0.057820
   13          1          0       -2.469360   -1.807573    0.264719
   14          1          0       -3.180751   -0.276045    0.162597
---------------------------------------------------------------------
```
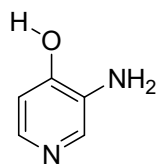
E = -378.74788 a.u.

```
-----------------------------------------------------------------
 Center     Atomic     Atomic        Coordinates (Angstroms)
 Number     Number     Type        X          Y          Z
-----------------------------------------------------------------
    1          6          0      -1.873984   0.519995   0.005066
    2          6          0      -0.808877   1.351047  -0.003426
    3          6          0       0.535423   0.842025  -0.004307
    4          6          0       0.646809  -0.623367  -0.012473
    5          6          0      -0.466115  -1.386417  -0.007073
    6          7          0      -1.714970  -0.817454   0.008591
    7          1          0      -2.888190   0.876281   0.012839
    8          1          0      -0.949297   2.415861   0.002118
    9          1          0      -0.438957  -2.460650  -0.022028
   10          8          0       1.543299   1.532951   0.011563
   11          1          0      -2.516403  -1.411213   0.011324
   12          7          0       1.931992  -1.113428  -0.073246
   13          1          0       2.115086  -1.987891   0.374263
   14          1          0       2.612683  -0.399518   0.114849
-----------------------------------------------------------------
```
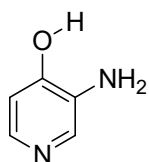

E = -378.750103 a.u.

```
-----------------------------------------------------------------
 Center     Atomic     Atomic        Coordinates (Angstroms)
 Number     Number     Type        X          Y          Z
-----------------------------------------------------------------
    1          6          0       1.131982  -1.623921   0.000000
    2          6          0      -0.245661  -1.548173   0.000000
    3          6          0      -0.826878  -0.291261   0.000000
    4          6          0       0.000000   0.829290   0.000000
    5          6          0       1.367043   0.622783   0.000000
    6          7          0       1.938212  -0.570102   0.000000
    7          1          0       1.613332  -2.588645   0.000000
    8          1          0      -0.859340  -2.430639   0.000000
    9          8          0      -2.153225  -0.151496   0.000000
   10          1          0      -2.330062   0.792997   0.000000
   11          1          0       2.029067   1.476481   0.000000
   12          7          0      -0.643391   2.103346   0.000000
   13          1          0      -0.424928   2.648378   0.815652
   14          1          0      -0.424928   2.648378  -0.815652
-----------------------------------------------------------------
```

H–O

NH$_2$

E = -378.7482322 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic           Coordinates (Angstroms)
 Number      Number       Type          X           Y           Z
--------------------------------------------------------------------
    1           6           0        -1.911609    0.505797    0.005798
    2           6           0        -0.788819    1.317128    0.001773
    3           6           0         0.455361    0.724742   -0.005043
    4           6           0         0.550376   -0.664847   -0.009739
    5           6           0        -0.644084   -1.369846   -0.004050
    6           7           0        -1.844523   -0.812357    0.005493
    7           1           0        -2.895936    0.943798    0.010976
    8           1           0        -0.888254    2.390229    0.006501
    9           8           0         1.622517    1.411211    0.001085
   10           1           0         1.463431    2.348723    0.016505
   11           1           0        -0.614158   -2.449243   -0.009940
   12           7           0         1.787850   -1.284133   -0.073854
   13           1           0         1.825175   -2.211077    0.299946
   14           1           0         2.558960   -0.714524    0.213425
--------------------------------------------------------------------
```
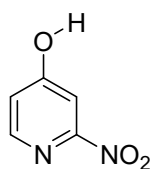
O

N—NO$_2$

H
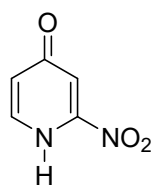
E = -527.8433477 a.u.

```
--------------------------------------------------------------------
 Center      Atomic      Atomic           Coordinates (Angstroms)
 Number      Number       Type          X           Y           Z
--------------------------------------------------------------------
    1           6           0         1.759181   -1.035241    0.000000
    2           6           0         0.898500   -2.066230    0.000000
    3           6           0        -0.542299   -1.856310    0.000000
    4           6           0        -0.939660   -0.444239    0.000000
    5           6           0         0.000000    0.505145    0.000000
    6           7           0         1.329970    0.256133    0.000000
    7           1           0         2.825737   -1.165404    0.000000
    8           1           0         1.262398   -3.076622    0.000000
    9           1           0        -1.980726   -0.185253    0.000000
   10           8           0        -1.355421   -2.752906    0.000000
   11           1           0         1.959672    1.035126    0.000000
   12           8           0         0.592575    2.701316    0.000000
   13           8           0        -1.494977    2.233382    0.000000
   14           7           0        -0.338374    1.932306    0.000000
--------------------------------------------------------------------
```

E = -527.8505467 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0         0.946077    1.800407    0.000000
    2          6           0         2.004579    0.917354    0.000000
    3          6           0         1.729143   -0.442307    0.000000
    4          6           0         0.406977   -0.856206    0.000000
    5          6           0        -0.543937    0.140709    0.000000
    6          7           0        -0.325534    1.422216    0.000000
    7          1           0         1.125450    2.862175    0.000000
    8          1           0         3.022726    1.260940    0.000000
    9          1           0         0.118581   -1.890503    0.000000
   10          8           0         2.760837   -1.295723    0.000000
   11          8           0        -2.808663    0.579720    0.000000
   12          8           0        -2.186502   -1.462889    0.000000
   13          7           0        -1.975995   -0.273848    0.000000
   14          1           0         2.461535   -2.199788    0.000000
---------------------------------------------------------------------
```
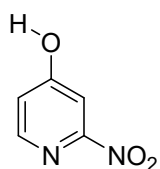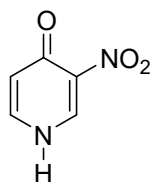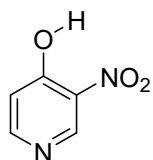

E = -527.8496738 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6           0         0.942378    1.791235   -0.015457
    2          6           0         2.000735    0.901845   -0.005891
    3          6           0         1.721900   -0.455970    0.005650
    4          6           0         0.397148   -0.866285    0.006836
    5          6           0        -0.547176    0.131475   -0.002691
    6          7           0        -0.325142    1.417173   -0.012899
    7          1           0         1.127626    2.852247   -0.025466
    8          1           0         3.014884    1.263836   -0.007697
    9          1           0         0.128649   -1.903925    0.013717
   10          8           0         2.666262   -1.405169    0.015772
   11          8           0        -2.807507    0.587474    0.044580
   12          8           0        -2.202464   -1.458451   -0.040514
   13          7           0        -1.982017   -0.273233    0.000663
   14          1           0         3.538729   -1.024369    0.015718
---------------------------------------------------------------------
```
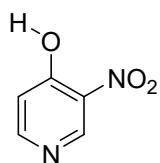
E = -527.8388884 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6           0       0.376219   -1.349126   -0.056013
    2          6           0      -0.275984   -0.169929   -0.005045
    3          6           0       0.428674    1.116447    0.084460
    4          6           0       1.881650    0.947513    0.019797
    5          6           0       2.465352   -0.252585   -0.056779
    6          7           0       1.719043   -1.401607   -0.085971
    7          1           0      -0.160754   -2.278806   -0.078528
    8          1           0       2.475763    1.841960    0.049422
    9          1           0       3.530640   -0.386974   -0.095456
   10          1           0       2.173394   -2.289464   -0.139377
   11          7           0      -1.726234   -0.245665   -0.026330
   12          8           0      -2.326315    0.679002   -0.490325
   13          8           0      -2.233642   -1.259886    0.403881
   14          8           0      -0.093063    2.192168    0.227885
---------------------------------------------------------------------
```
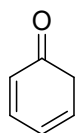

E = -527.857049 a.u.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
    1          6           0       1.324659    0.757825    0.000000
    2          6           0       0.000000    0.327172    0.000000
    3          6           0      -0.288215   -1.043500    0.000000
    4          6           0       0.809875   -1.899593    0.000000
    5          6           0       2.074489   -1.368460    0.000000
    6          7           0       2.346711   -0.061033    0.000000
    7          1           0       1.524755    1.814863    0.000000
    8          1           0       0.642140   -2.960841    0.000000
    9          1           0       2.928657   -2.025278    0.000000
   10          7           0      -1.047005    1.316838    0.000000
   11          8           0      -2.201026    0.916378    0.000000
   12          8           0      -0.749360    2.476295    0.000000
   13          8           0      -1.496034   -1.568222    0.000000
   14          1           0      -2.146986   -0.855657    0.000000
---------------------------------------------------------------------
```
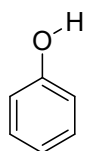
E = -527.8411732 a.u.

```
--------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
--------------------------------------------------------------------
   1           6           0        0.458674    -1.430818    -0.086111
   2           6           0       -0.229876    -0.231486    -0.010837
   3           6           0        0.475519     0.966620     0.065157
   4           6           0        1.861100     0.867131     0.046636
   5           6           0        2.448288    -0.375538    -0.047604
   6           7           0        1.772503    -1.514961    -0.114976
   7           1           0       -0.103857    -2.346947    -0.130577
   8           1           0        2.468566     1.754072     0.110658
   9           1           0        3.522776    -0.456964    -0.064941
  10           7           0       -1.683717    -0.280981    -0.020295
  11           8           0       -2.275465     0.640070    -0.513051
  12           8           0       -2.196910    -1.266718     0.448566
  13           8           0       -0.159464     2.127039     0.184630
  14           1           0        0.463493     2.842858     0.267161
--------------------------------------------------------------------
```


E = -307.339104 a.u.

```
--------------------------------------------------------------------
Center      Atomic      Atomic            Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
--------------------------------------------------------------------
   1           6           0        1.115151    -1.225980     0.000000
   2           6           0        1.276967     0.256145     0.000000
   3           6           0        0.000000     1.074619     0.000000
   4           6           0       -1.268239     0.342206     0.000000
   5           6           0       -1.292428    -0.994604     0.000000
   6           6           0       -0.082365    -1.801727     0.000000
   7           1           0        2.011478    -1.824176     0.000000
   8           1           0        1.861362     0.570524     0.863781
   9           1           0       -2.167307     0.933376     0.000000
  10           1           0       -2.240010    -1.508322     0.000000
  11           1           0       -0.179861    -2.873372     0.000000
  12           8           0        0.044808     2.278436     0.000000
  13           1           0        1.861362     0.570524    -0.863781
--------------------------------------------------------------------
```

E = -307.3696098 a.u.

```
---------------------------------------------------------------------
 Center      Atomic      Atomic            Coordinates (Angstroms)
 Number      Number      Type         X           Y           Z
---------------------------------------------------------------------
    1           6           0      -1.178669   -1.153733    0.000000
    2           6           0      -1.195036    0.230980    0.000000
    3           6           0       0.000000    0.932750    0.000000
    4           6           0       1.206940    0.251908    0.000000
    5           6           0       1.210397   -1.129916    0.000000
    6           6           0       0.021081   -1.842226    0.000000
    7           1           0      -2.110829   -1.692430    0.000000
    8           1           0      -2.132929    0.763296    0.000000
    9           1           0       2.123059    0.815368    0.000000
   10           1           0       2.150916   -1.654028    0.000000
   11           1           0       0.030516   -2.917840    0.000000
   12           8           0       0.047753    2.287170    0.000000
   13           1           0      -0.831036    2.649699    0.000000
---------------------------------------------------------------------
```