

Supplementary information for: Electron Attachment to Isolated and Microhydrated Favipiravir

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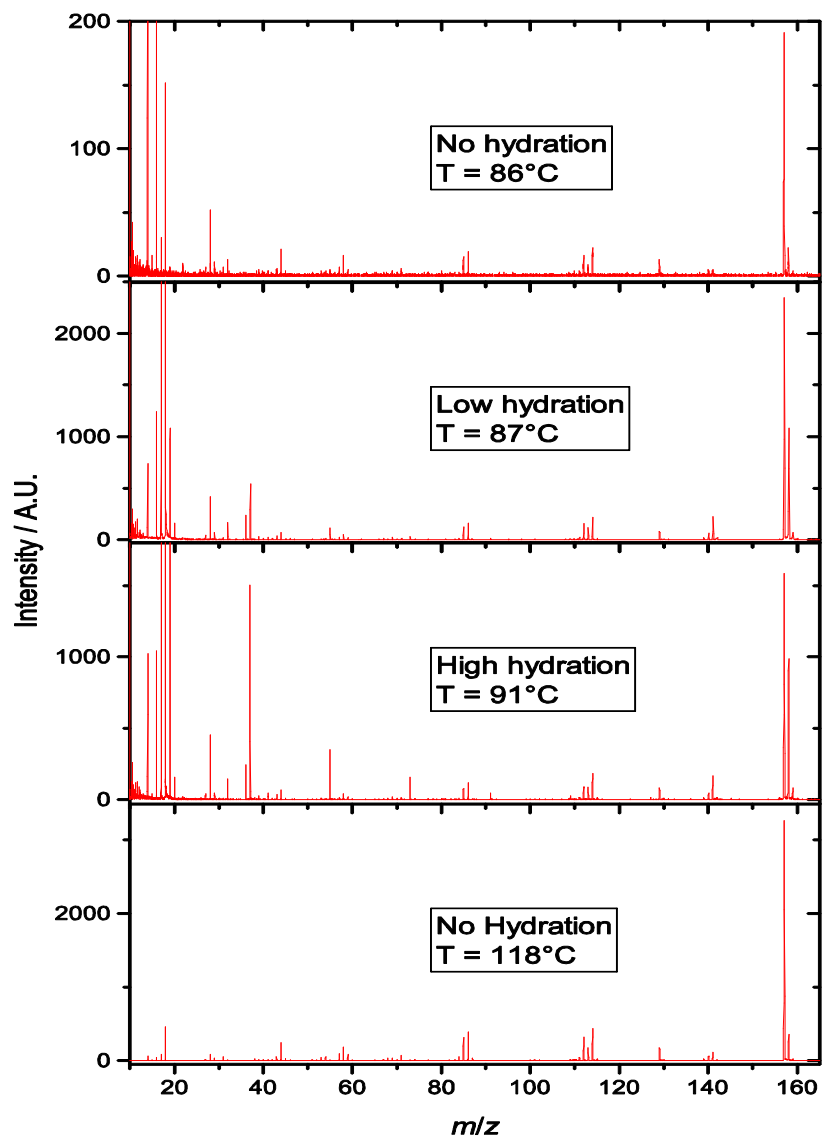
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^bDepartment of Nuclear Chemistry, Faculty of Nuclear Sciences and Physical Engineering, Břehová 7, 11519 Prague, Czech Repu

1. Low m/z part of the electron impact ionization mass spectra presented in Fig. 6.
2. Comparison of the reaction energies calculated using B3LYP and M062x functionals.
3. Cartesian coordinates of the optimized structures favipiravir neutral A,B,C,D, and anion A⁻,B⁻,C⁻,D⁻ conformers discussed in paper.
4. Cartesian coordinates of the optimized structures for fragment anions used to calculate reaction energy thresholds for individual DEA channels.

1. Low m/z part of the electron impact ionization mass spectra presented in Fig. 5.

First panel from top is a positive ion MS from CLUB experiment. Second and third panel are low m/z parts of positive MS presented in Fig. 6 of the paper in the same order. The bottom panel shows a measurement at increased sample temperature to identify possible thermal decomposition products.



2. Comparison of the reaction energies calculated using B3LYP and M062x functionals.

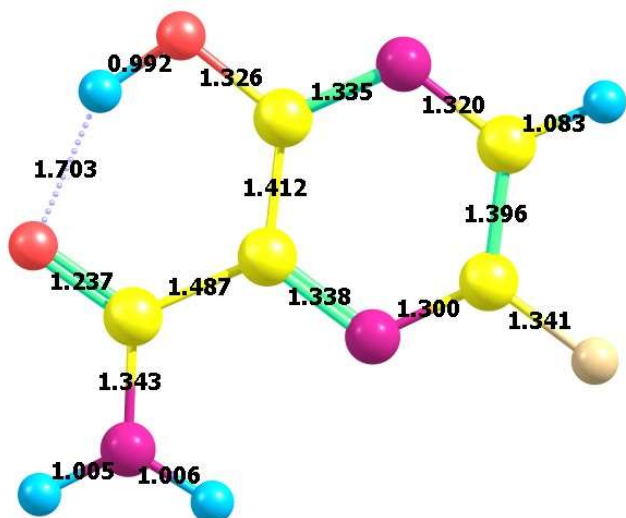
The Truhlar's M062 functionals are becoming still more popular due to excellent performance in describing noncovalent interactions or excited states. Similar to many of our previous studies, the B3LYP in combination with basis set involving diffuse orbitals can well reproduce the experimentally observed reaction thresholds. The order of reaction thresholds for individual fragment ions is preserved also when M062x functional is used, except of the structure D of the OH loss channel. However, the reaction energies using M062x functional seems to be overestimated when open shell anions are formed. Or otherwise, enthalpies of formation of such species seems to be underestimated using M062x. Robustness of the M062x functionals for the anion calculations probably needs more exploration beyond the scope of the present experimental work.

anion m/z	channel		B3LYP	M062x
156	A (M-H)-	H	0.64	1.08
	B (M-H)-	H	1.03	1.38
	C (M-H)-	H	1.03	1.48
	D (M-H)-	H	2.05	2.48
	E (M-H)-	H	2.22	2.64
	F (M-H)-	H	2.5	2.8
140	[M-NH3]-	NH3	0.17	0.95
	A [M-OH]-	OH	2.96	3.61
	B [M-OH]-	OH	3.17	3.82
	C [M-OH]-	OH	4.92	3.84
	D [M-OH]-	OH	5.03	3.5
113	A [M-CONH2]-	CO+NH2	3.24	2.9
	B [M-CONH2]-	CO+NH2	3.46	3.1
	C [M-CONH2]-	CO+NH2	3.63	3.35
112	A [M-CONH3]-	CONH3	0.86	1.66
	B [M-CONH3]-	CONH3	1.96	2.77
	C [M-CONH3]-	CONH3	2.35	3.16
	D [M-CONH3]-	CONH3	2.4	3.21
42	OCN-	C4H4FN2O	1.93	2.67
	OCN-	H2+ C4H2FN2O A	4.1	2.66
	OCN-	H2+ C4H2FN2O B	4.87	2.8
	OCN-	H2+ C4H2FN2O C	4.95	1.99
26	CN-	H2O+ C4H2FN2O A	1.85	2.6
	CN-	C4H4N2O2F	1.97	2.57
	CN-	HF+C4H3N2O2	2.61	3.4
	CN-	H2O+ C4H2FN2O B	2.62	3.27
	CN-	H2O+ C4H2FN2O C	2.7	3.42
19	F-	[M-F] A	1.72	2.5
		[M-F] B	2.15	2.92
		[M-F] C	2.15	3.04
		[M-F] D	2.34	3.21

3. Cartesian coordinates of the optimized structures favipiravir neutral A,B,C,D, and anion A⁻,B⁻,C⁻,D⁻ conformers discussed in paper.

A B3LYP

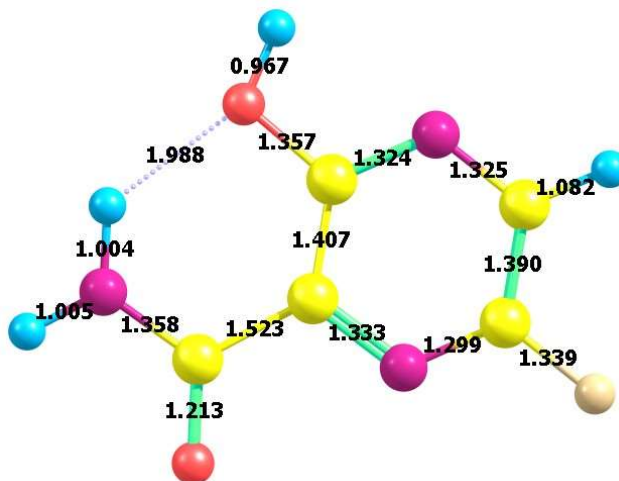
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B B3LYP

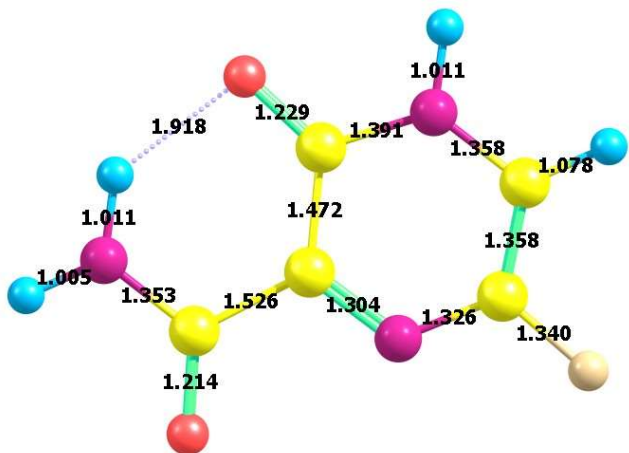
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C B3LYP

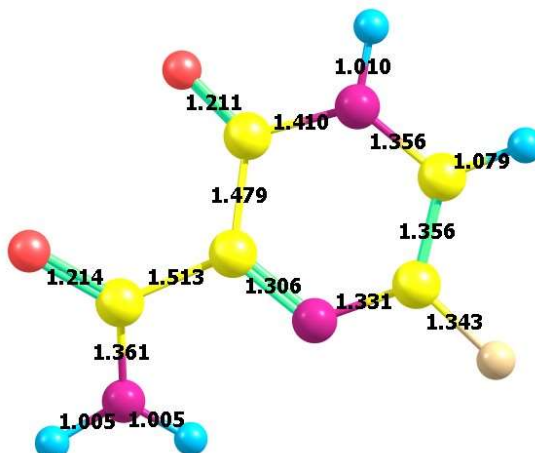
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7	2.458132000	2.756490000	-0.490724000
9	0.246618000	-2.623062000	0.169865000
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D B3LYP

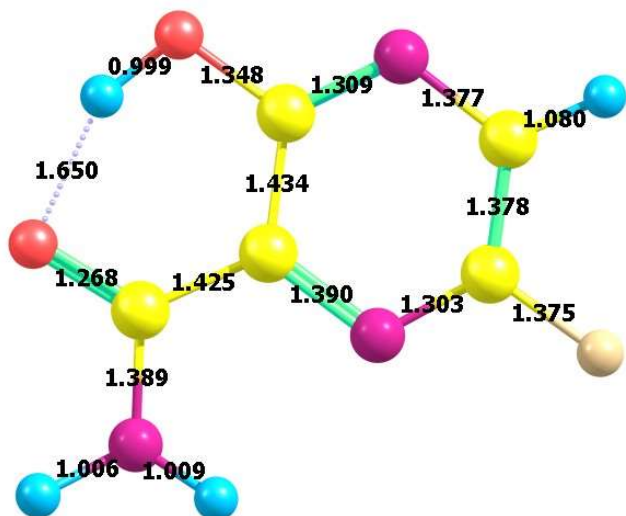
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7	3.613992000	0.650964000	0.001936000
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A- B3LYP

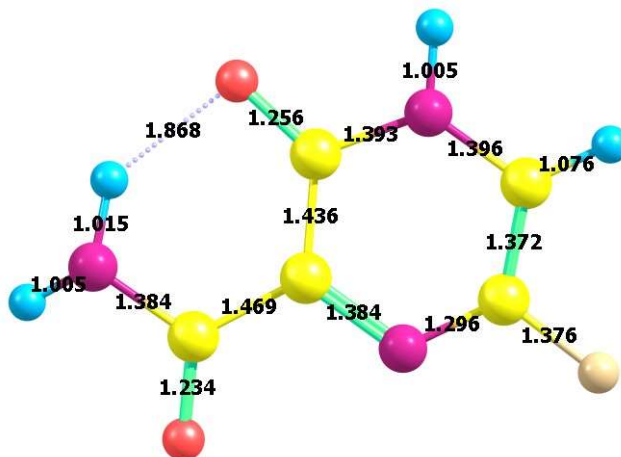
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B- B3LYP

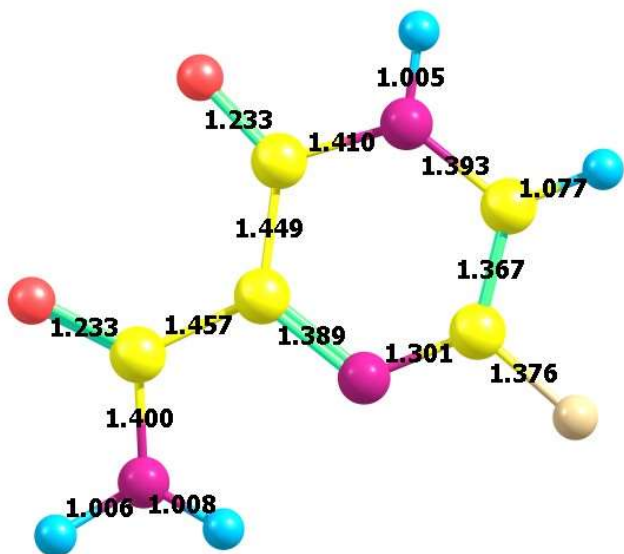
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9	0.251581000	-2.650148000	0.172204000
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C B3LYP

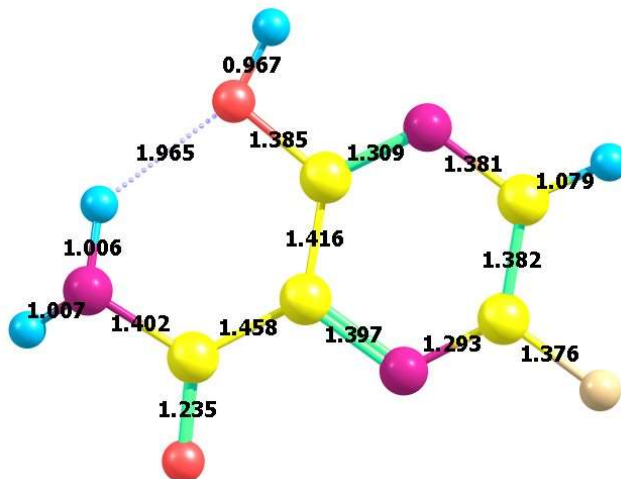
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D B3LYP

Sum of electronic and zero-point Energies=
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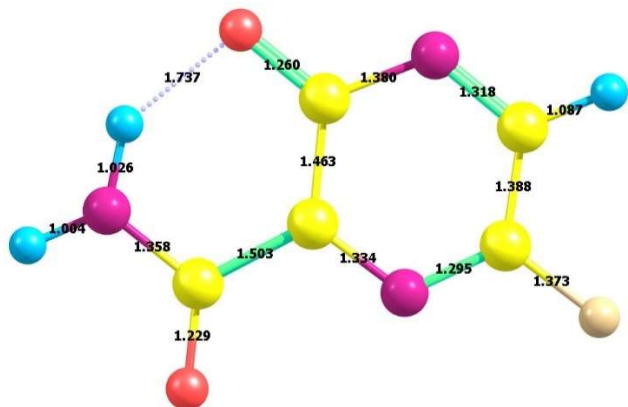
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1	-1.254106000	2.836428000	-0.331965000

4. Cartesian coordinates of the optimized structures for fragment anions used to calculate reaction energy thresholds for individual DEA channels.

m/z 156

A (M-H(15)) ANION B3LYP

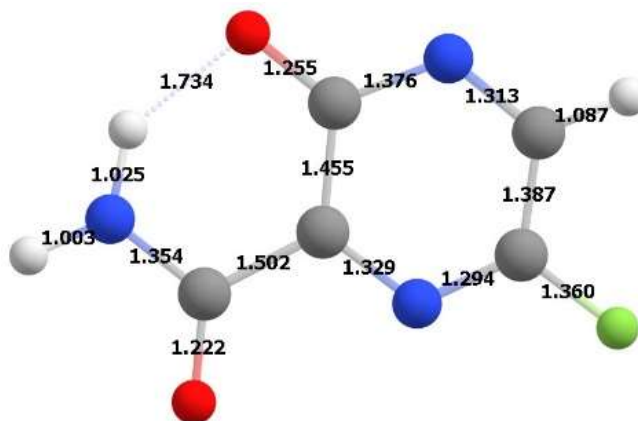
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9	0.404481000	-2.500606000	0.407690000
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1	1.386884000	3.262240000	-0.746438000
1	3.166645000	3.443456000	-0.972675000

A (M-H(15)) ANION M062x

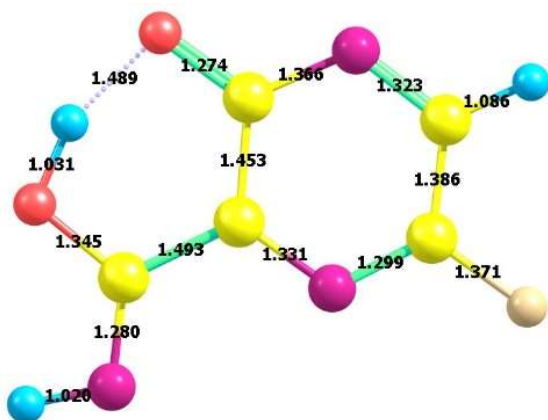
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B (M-H(13)) ANION B3LYP

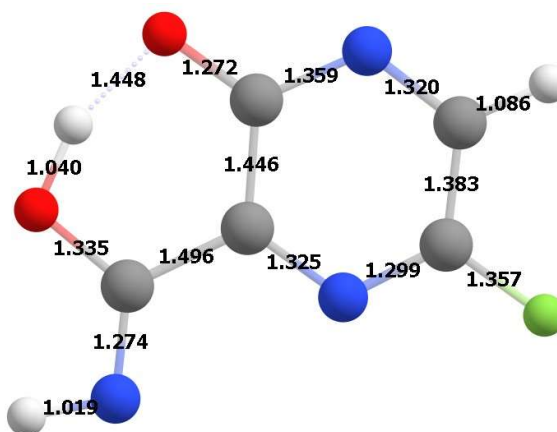
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6	-0.225107000	1.227526000	-0.036310000
8	-0.270863000	2.496466000	-0.137285000
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8	2.198599000	2.570029000	-0.292779000
7	3.453341000	0.633058000	-0.211590000
9	-0.029604000	-2.815077000	0.284966000
1	4.183387000	1.337658000	-0.313820000
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B (M-H(13)) ANION M062x

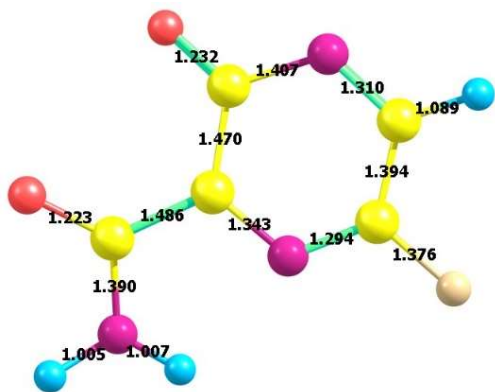
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C (M-H(15)) ANION B3LYP

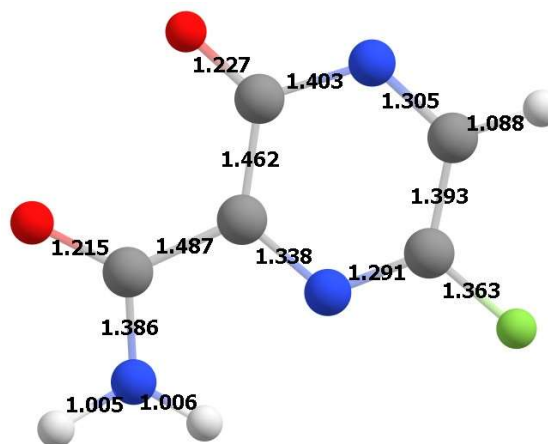
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6	-0.086931000	1.451248000	-0.017940000
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C (M-H(15)) ANION M062x

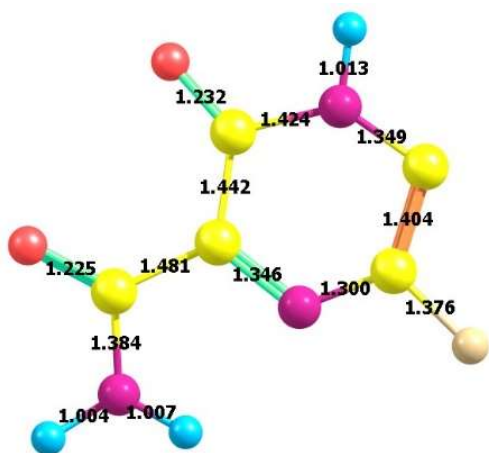
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6	-0.081753000	1.446447000	-0.037186000
8	-0.200412000	2.667574000	-0.033466000
7	-1.221281000	0.629929000	0.021417000
6	2.499413000	1.420453000	-0.242171000
8	2.654556000	2.586675000	-0.546786000
7	3.595156000	0.608734000	0.004007000
9	0.253756000	-2.633116000	0.177936000
1	-1.982447000	-1.282552000	0.137572000
1	3.434120000	-0.384283000	-0.010100000
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D (M-H(12)) ANION B3LYP

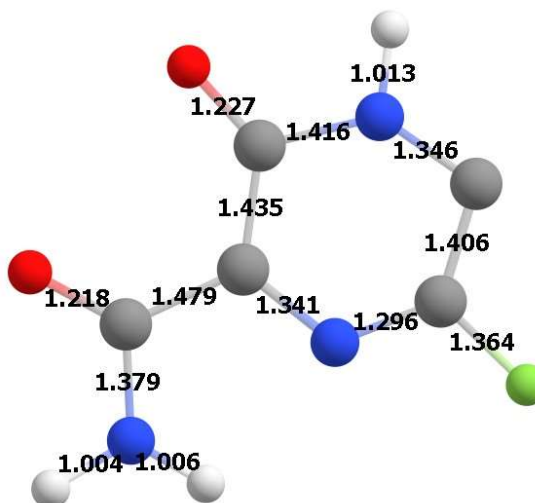
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6	1.211663000	0.767792000	-0.090076000
6	-0.039447000	1.483696000	-0.074854000
8	-0.269964000	2.692432000	-0.128304000
7	-1.142950000	0.590033000	0.028021000
6	2.526445000	1.438130000	-0.213014000
8	2.697275000	2.629147000	-0.440952000
7	3.604988000	0.590824000	-0.027258000
9	0.288929000	-2.610158000	0.173855000
1	-2.015108000	1.104320000	0.033652000
1	3.418998000	-0.398502000	-0.063136000
1	4.487013000	0.937646000	-0.360032000

D (M-H(12)) ANION M062x

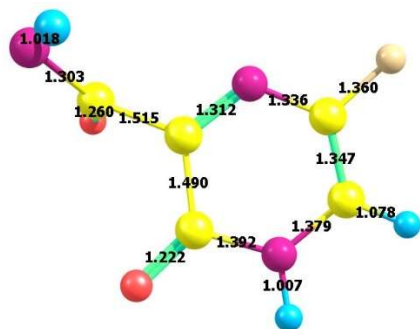
Sum of electronic and zero-point Energies=
-606.851769



6	-1.190325000	-0.750255000	0.118166000
6	0.125237000	-1.246726000	0.096862000
7	1.231933000	-0.578165000	0.004240000
6	1.209598000	0.759753000	-0.088014000
6	-0.032841000	1.477513000	-0.078410000
8	-0.259240000	2.681984000	-0.139232000
7	-1.132143000	0.591261000	0.026826000
6	2.520490000	1.434845000	-0.208065000
8	2.682515000	2.622584000	-0.421050000
7	3.598221000	0.591123000	-0.037190000
9	0.284023000	-2.598954000	0.179417000
1	-2.002108000	1.109636000	0.030216000
1	3.419225000	-0.398112000	-0.079825000
1	4.479567000	0.951051000	-0.355951000

E (M-H(13)) ANION B3LYP

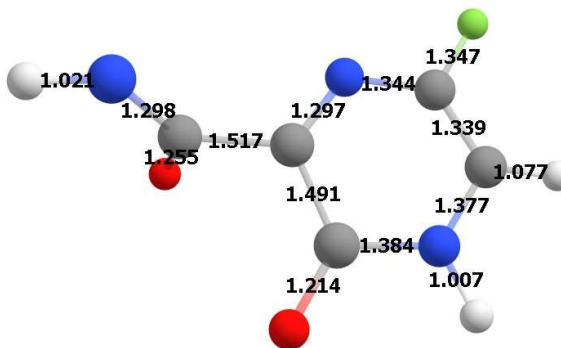
Sum of electronic and zero-point Energies=
-607.062881



6	-1.171153000	-0.718543000	0.026202000
6	-0.016100000	-1.358294000	-0.239060000
7	1.180436000	-0.771385000	-0.332058000
6	1.289973000	0.527789000	-0.183410000
6	0.112917000	1.369009000	0.172125000
8	0.112641000	2.561847000	0.435617000
7	-1.071761000	0.641363000	0.230805000
6	2.601210000	1.223236000	-0.487819000
8	2.516690000	1.759919000	-1.625031000
7	3.602418000	1.207983000	0.345667000
9	-0.030664000	-2.704225000	-0.431475000
1	-2.139665000	-1.186894000	0.091461000
1	-1.888017000	1.181174000	0.470325000
1	3.352142000	0.650958000	1.160064000

E (M-H(13)) ANION M062x

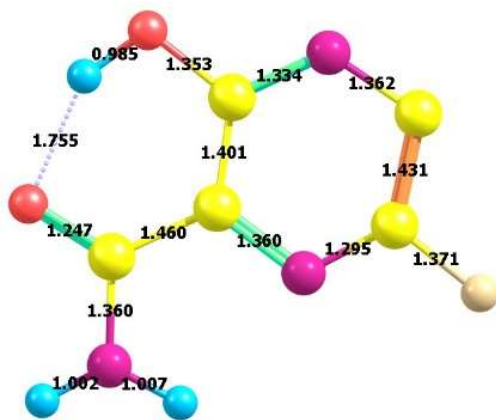
Sum of electronic and zero-point Energies=
-606.845533



6	-1.173028000	-0.816472000	0.210568000
6	-0.017573000	-1.456745000	-0.011093000
7	1.172065000	-0.855798000	-0.184102000
6	1.250495000	0.438308000	-0.151039000
6	0.053956000	1.292567000	0.094738000
8	0.033323000	2.504293000	0.171904000
7	-1.106165000	0.557457000	0.262415000
6	2.553999000	1.147254000	-0.468914000
8	2.593039000	1.528772000	-1.664046000
7	3.375209000	1.235449000	0.532553000
9	-0.003169000	-2.802610000	-0.071125000
1	4.195031000	1.748570000	0.205396000
1	-2.125852000	-1.300112000	0.348979000
1	-1.933492000	1.104214000	0.439412000

F (M-H(12)) ANION B3LYP

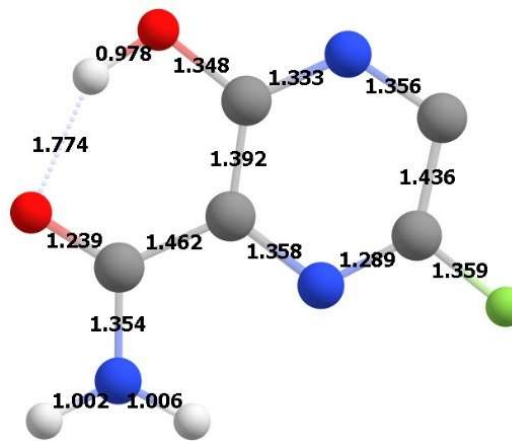
Sum of electronic and zero-point Energies=
-607.052653



6	-1.390170000	-0.806369000	0.144673000
6	-0.078432000	-1.378033000	0.127780000
7	1.073645000	-0.796250000	0.025299000
6	1.032119000	0.559321000	-0.080840000
6	-0.207358000	1.211282000	-0.069358000
8	-0.281146000	2.558318000	-0.167308000
7	-1.361653000	0.551578000	0.037234000
6	2.295995000	1.280695000	-0.197729000
8	2.366218000	2.523071000	-0.277452000
7	3.414755000	0.508568000	-0.225319000
9	0.000178000	-2.742564000	0.235491000
1	3.306645000	-0.482928000	-0.086146000
1	4.312679000	0.953757000	-0.205111000
1	0.648317000	2.876752000	-0.230123000

F (M-H(12)) ANION M062x

Sum of electronic and zero-point Energies=
-606.839264

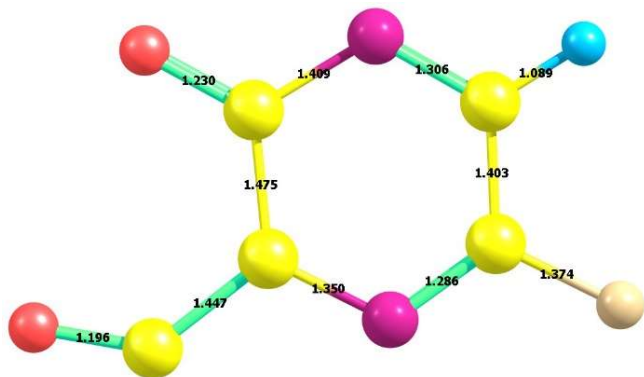


6	-1.386458000	-0.803660000	0.139985000
6	-0.068138000	-1.373275000	0.125302000
7	1.078605000	-0.791868000	0.029680000
6	1.030400000	0.561569000	-0.072583000
6	-0.201671000	1.208768000	-0.068012000
8	-0.282145000	2.550373000	-0.168042000
7	-1.355134000	0.547577000	0.034290000
6	2.297073000	1.283641000	-0.184563000
8	2.372434000	2.515935000	-0.283736000
7	3.406591000	0.508070000	-0.172619000
9	0.008032000	-2.726610000	0.226243000
1	3.290404000	-0.488329000	-0.091949000
1	4.305260000	0.944532000	-0.248626000
1	0.636538000	2.880475000	-0.234279000

m/z = 140

(M-NH₃) ANION B3LYP

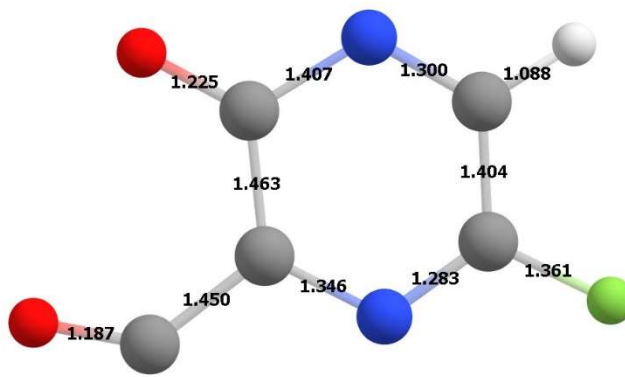
Sum of electronic and zero-point Energies=
-551.085739



6	-0.388579000	-0.403856000	0.054344000
6	0.872614000	-1.017875000	0.043175000
7	1.978496000	-0.366413000	-0.041700000
6	1.909755000	0.979123000	-0.123755000
6	0.623295000	1.700794000	-0.117999000
8	0.516247000	2.923990000	-0.191132000
7	-0.526461000	0.892299000	-0.021828000
6	3.180018000	1.665441000	-0.217613000
8	3.461937000	2.824577000	-0.301931000
9	0.934302000	-2.387717000	0.127104000
1	-1.285143000	-1.017330000	0.128454000

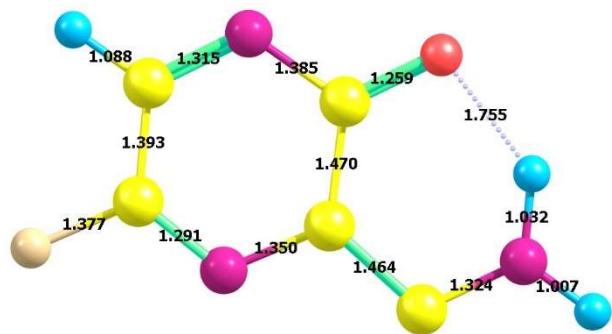
(M-NH₃) ANION M062x

Sum of electronic and zero-point Energies=
-550.887769



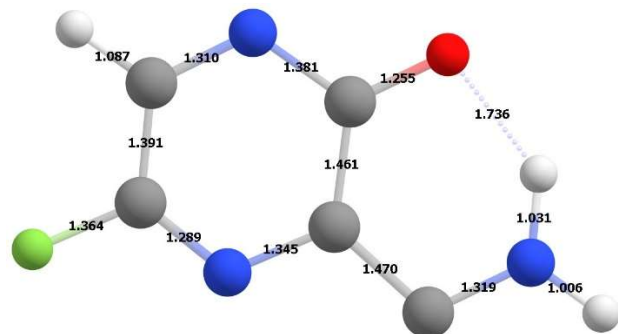
6	-0.383234000	-0.397168000	0.053806000
6	0.876201000	-1.017906000	0.042987000
7	1.979199000	-0.368883000	-0.041713000
6	1.902562000	0.972622000	-0.123237000
6	0.630687000	1.695899000	-0.118308000
8	0.530068000	2.914865000	-0.191125000
7	-0.520547000	0.892869000	-0.022040000
6	3.172140000	1.667778000	-0.217260000
8	3.439154000	2.821813000	-0.300671000
9	0.927644000	-2.375705000	0.126589000
1	-1.277393000	-1.013151000	0.128090000

A (M-OH) anion B3LYP



Sum of electronic and zero-point Energies=
-531.777732

6	-1.080550000	-0.091326000	0.220378000
6	-0.222018000	-1.103378000	-0.201437000
7	1.039174000	-0.932827000	-0.418159000
6	1.563412000	0.296878000	-0.226341000
6	0.698691000	1.398574000	0.218726000
8	1.126970000	2.566404000	0.415476000
7	-0.644009000	1.131309000	0.428298000
6	2.998823000	0.408516000	-0.493521000
7	3.458430000	1.633013000	-0.289014000
9	-0.741139000	-2.363054000	-0.401604000
1	-2.135257000	-0.300310000	0.385413000
1	4.436129000	1.814659000	-0.445398000
1	2.828100000	2.387855000	0.023779000



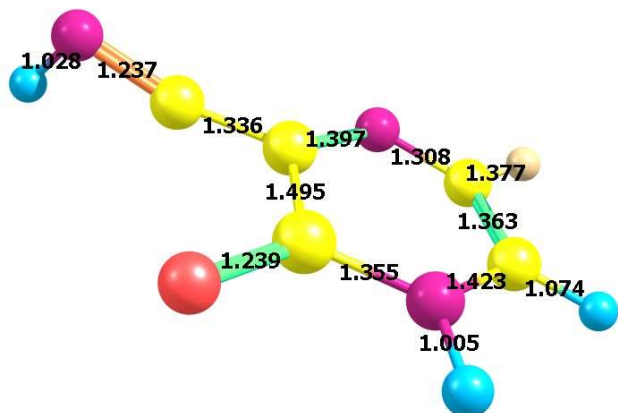
Sum of electronic and zero-point Energies=
-531.582981

6	-1.071869000	-0.087429000	0.219699000
6	-0.218622000	-1.101836000	-0.201932000
7	1.040668000	-0.929858000	-0.417941000
6	1.558021000	0.297005000	-0.225297000
6	0.702382000	1.395693000	0.217289000
8	1.130643000	2.559236000	0.412534000
7	-0.636414000	1.130687000	0.426960000
6	2.999103000	0.406147000	-0.493832000
7	3.447496000	1.629588000	-0.287869000
9	-0.736794000	-2.347986000	-0.399118000
1	-2.125632000	-0.298514000	0.384278000
1	4.424411000	1.813717000	-0.442625000
1	2.813363000	2.379863000	0.024448000

A (M-OH) anion M062x

B (M-OH) anion B3LYP

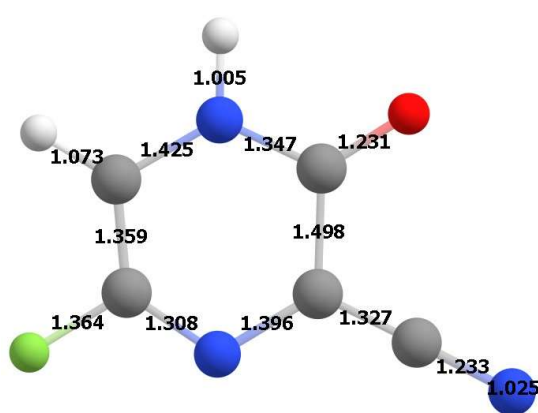
Sum of electronic and zero-point Energies=
-531.770231



6	-0.718314000	-0.392182000	0.205508000
6	0.352645000	-1.120694000	-0.218887000
7	1.587641000	-0.731991000	-0.403740000
6	1.838685000	0.624738000	-0.182653000
6	0.784735000	1.556919000	0.322992000
7	-0.425632000	0.971315000	0.490832000
6	3.020456000	1.180104000	-0.465221000
9	0.123079000	-2.452936000	-0.481680000
1	-1.721351000	-0.748800000	0.347881000
1	-1.147288000	1.581038000	0.834958000
8	0.975984000	2.754486000	0.574566000
7	4.185399000	1.596314000	-0.460071000
1	4.470717000	2.027997000	-1.347885000

B (M-OH) anion B3LYP

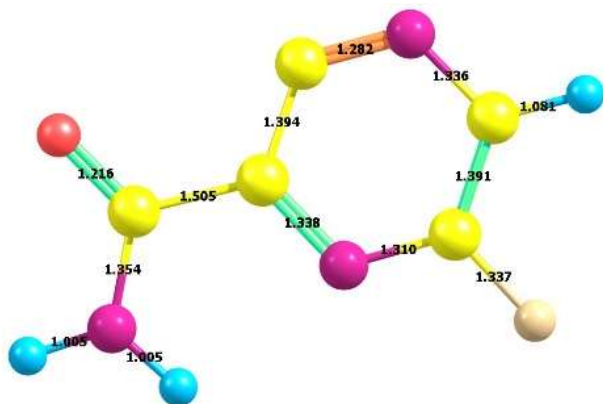
Sum of electronic and zero-point Energies=
-531.575329



6	-0.707843000	-0.389365000	0.212243000
6	0.350137000	-1.119413000	-0.229835000
7	1.584322000	-0.743373000	-0.443963000
6	1.845340000	0.603539000	-0.183521000
6	0.794881000	1.550202000	0.310160000
7	-0.412360000	0.977925000	0.481387000
6	3.034896000	1.155051000	-0.386692000
9	0.107741000	-2.435735000	-0.490050000
1	-1.701335000	-0.754221000	0.388649000
1	-1.133072000	1.599301000	0.805691000
8	1.000251000	2.742558000	0.539040000
7	4.175143000	1.621583000	-0.437079000
1	4.388656000	2.038255000	-1.349429000

C (M-OH) anion B3LYP

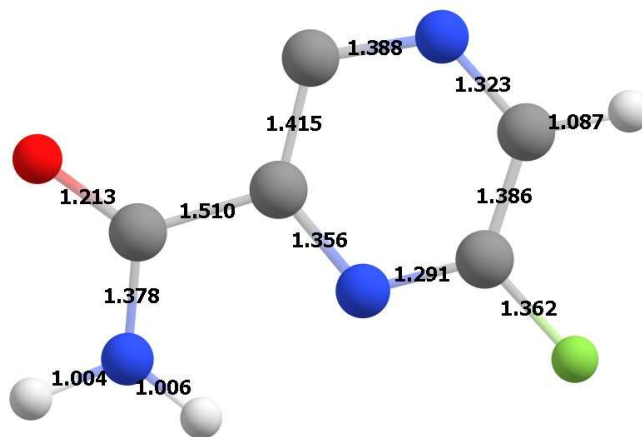
Sum of electronic and zero-point Energies=
-531.705829



6	-1.154018000	-0.635577000	0.120482000
6	0.086221000	-1.265055000	0.108072000
7	1.225260000	-0.626756000	0.007784000
6	1.188848000	0.706911000	-0.087960000
6	-0.057325000	1.330395000	-0.074694000
7	-1.167374000	0.697196000	0.023840000
6	2.471626000	1.484402000	-0.205141000
8	2.460448000	2.697227000	-0.293007000
7	3.589653000	0.721491000	-0.202398000
9	0.142326000	-2.597514000	0.202832000
1	-2.082268000	-1.182460000	0.204190000
1	3.528835000	-0.278787000	-0.125953000
1	4.483738000	1.173418000	-0.276707000

C (M-OH) anion M062x

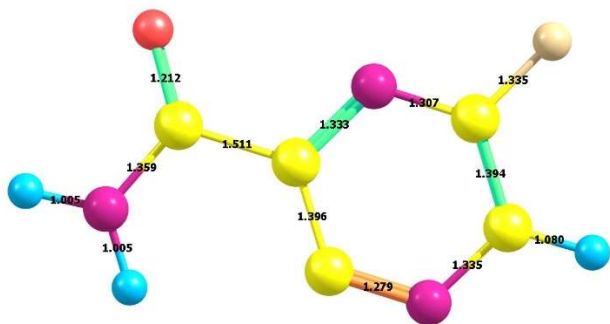
Sum of electronic and zero-point Energies=
-531.574688



6	-1.095800000	-0.639797000	0.128330000
6	0.148612000	-1.245318000	0.060570000
7	1.251607000	-0.581618000	-0.039150000
6	1.115661000	0.766317000	-0.086364000
6	-0.094630000	1.496792000	-0.019572000
7	-1.209305000	0.678043000	0.096604000
6	2.435955000	1.487872000	-0.219705000
8	2.566197000	2.669418000	-0.463317000
7	3.537376000	0.684457000	-0.021902000
9	0.238911000	-2.603273000	0.102876000
1	-1.992524000	-1.248377000	0.212540000
1	3.395023000	-0.310733000	-0.042150000
1	4.418887000	1.071109000	-0.307420000

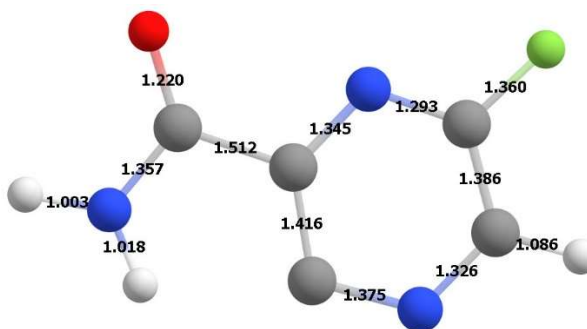
D (M-OH) anion B3LYP

Sum of electronic and zero-point Energies=
-531.701583



6	-1.039449000	-0.540847000	0.363876000
6	0.051720000	-1.287083000	-0.078052000
7	1.208740000	-0.772803000	-0.402041000
6	1.357041000	0.548688000	-0.305161000
6	0.259287000	1.287845000	0.138003000
7	-0.870748000	0.780252000	0.454186000
6	2.692634000	1.150138000	-0.676994000
8	3.624127000	0.471823000	-1.051827000
7	2.739015000	2.502502000	-0.551076000
9	-0.078474000	-2.612116000	-0.181071000
1	-1.986813000	-0.988980000	0.626644000
1	1.948832000	3.032659000	-0.228308000
1	3.597929000	2.974342000	-0.773729000

Sum of electronic and zero-point Energies=
-531.587345



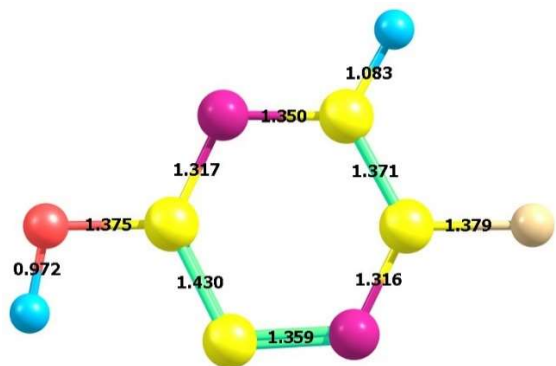
6	-0.980310000	-0.500271000	0.364102000
6	0.077107000	-1.271968000	-0.092097000
7	1.229076000	-0.791262000	-0.427849000
6	1.330741000	0.543573000	-0.300775000
6	0.323641000	1.430052000	0.150816000
7	-0.860816000	0.814663000	0.480870000
6	2.677223000	1.120763000	-0.676294000
8	3.652989000	0.460686000	-0.991830000
7	2.681072000	2.476831000	-0.627542000
9	-0.092999000	-2.616957000	-0.199259000
1	-1.922563000	-0.970844000	0.629955000
1	1.833208000	2.893439000	-0.247174000
1	3.555473000	2.957715000	-0.728473000

D (M-OH) anion M062x

m/z = 113

A (M - CONH₂) ANION B3LYP

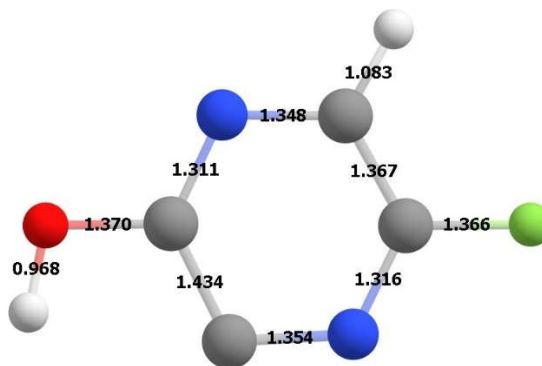
Sum of electronic and zero-point Energies=
-438.286173



6	-1.139801000	-0.625140000	0.097733000
6	0.090398000	-1.229348000	0.117256000
7	1.247254000	-0.607091000	0.038366000
6	1.259493000	0.747335000	-0.072246000
6	-0.046527000	1.330040000	-0.088466000
8	-0.087035000	2.699507000	-0.198946000
7	-1.210490000	0.718470000	-0.010513000
9	0.140794000	-2.603223000	0.226948000
1	-2.063471000	-1.187351000	0.165263000
1	0.859614000	2.917543000	-0.239355000

A (M - CONH₂) ANION M062x

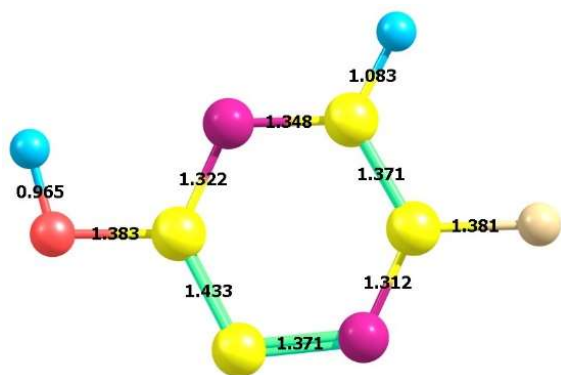
Sum of electronic and zero-point Energies=
-438.131018



6	-1.137572000	-0.622327000	0.097209000
6	0.088144000	-1.226585000	0.117085000
7	1.245801000	-0.606503000	0.038353000
6	1.264294000	0.743124000	-0.072005000
6	-0.046160000	1.324450000	-0.087942000
8	-0.087866000	2.689163000	-0.198015000
7	-1.206513000	0.719084000	-0.010659000
9	0.136051000	-2.586973000	0.225783000
1	-2.058715000	-1.187023000	0.165228000
1	0.852767000	2.914330000	-0.238997000

B (M-CONH₂) ANION B3LYP

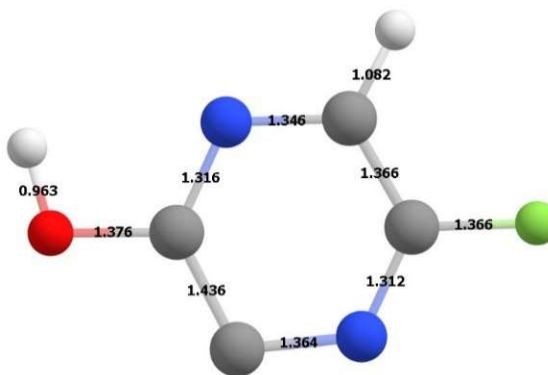
Sum of electronic and zero-point Energies=
-438.278037



6	-1.146133000	-0.703767000	0.116352000
6	0.101104000	-1.271576000	0.097919000
7	1.235357000	-0.616178000	0.028708000
6	1.243846000	0.752971000	-0.032444000
6	-0.083654000	1.293255000	-0.010005000
8	-0.208496000	2.669120000	-0.066616000
7	-1.231160000	0.640315000	0.059352000
9	0.186088000	-2.648292000	0.155389000
1	-2.059158000	-1.283775000	0.173449000
1	-1.159713000	2.831368000	-0.040425000

B (M-CONH₂) ANION M062x

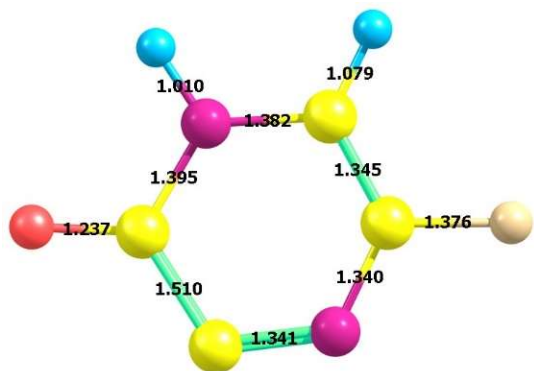
Sum of electronic and zero-point Energies=
-438.123211



6	-1.144974000	-0.701583000	0.115603000
6	0.098291000	-1.268260000	0.097466000
7	1.232958000	-0.612805000	0.028635000
6	1.244201000	0.749941000	-0.032380000
6	-0.087347000	1.288124000	-0.009591000
8	-0.207815000	2.658032000	-0.066079000
7	-1.230649000	0.640453000	0.059082000
9	0.183338000	-2.630819000	0.155321000
1	-2.054467000	-1.285367000	0.173596000
1	-1.155455000	2.825724000	-0.039974000

C (M-CONH₂) ANION B3LYP

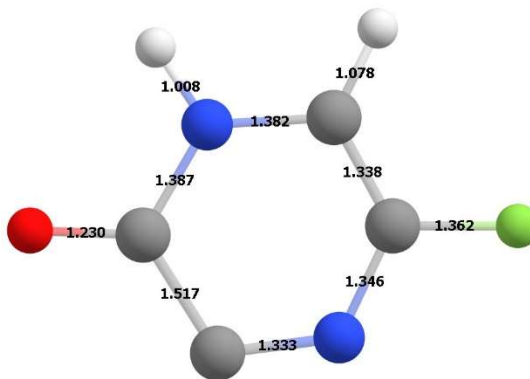
Sum of electronic and zero-point Energies=
-438.272027



6	-1.123153000	-0.751352000	0.109040000
6	0.116885000	-1.271049000	0.087904000
7	1.259637000	-0.576774000	-0.002521000
6	1.290298000	0.761359000	-0.085062000
6	-0.056683000	1.442730000	-0.069344000
8	-0.233692000	2.664995000	-0.135475000
7	-1.184224000	0.626647000	0.028109000
9	0.250587000	-2.638104000	0.166035000
1	-2.039728000	-1.316175000	0.182265000
1	-2.077207000	1.098162000	0.037519000

C (M-CONH₂) ANION B3LYP

Sum of electronic and zero-point Energies=
-438.113499

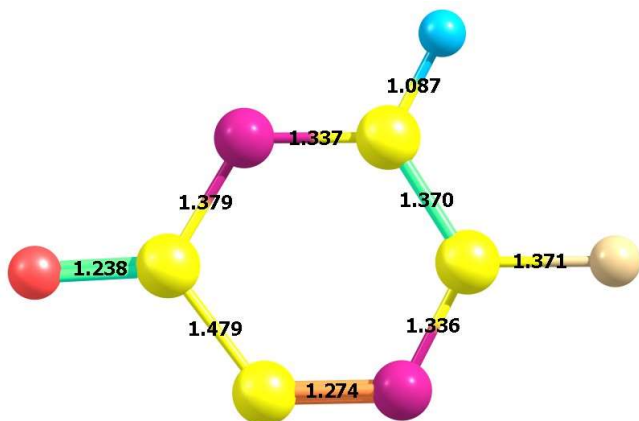


6	-1.122592000	-0.751011000	0.109160000
6	0.111444000	-1.268650000	0.088251000
7	1.259492000	-0.572776000	-0.002679000
6	1.294861000	0.756843000	-0.084880000
6	-0.061890000	1.435798000	-0.068467000
8	-0.234539000	2.651749000	-0.134945000
7	-1.183785000	0.626812000	0.028133000
9	0.249459000	-2.621691000	0.164547000
1	-2.036485000	-1.318617000	0.182473000
1	-2.073244000	1.101983000	0.036876000

m/z= 113

A (M-CONH₃) anion B3LYP

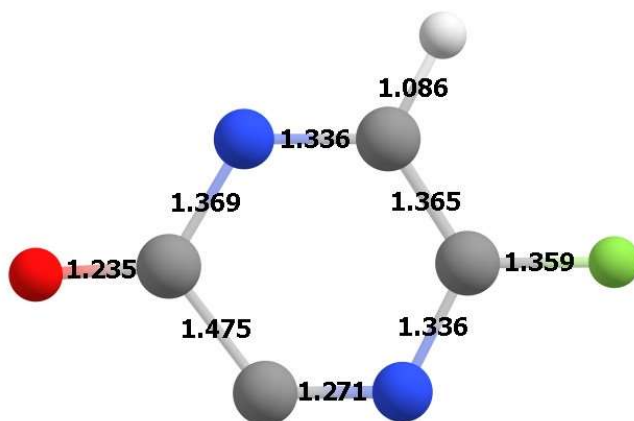
Sum of electronic and zero-point Energies=
-437.690066



6	-1.079699000	-0.691554000	0.103548000
6	0.144851000	-1.305734000	0.089068000
7	1.262774000	-0.580162000	-0.002356000
6	1.154174000	0.687527000	-0.074698000
6	-0.108816000	1.457329000	-0.067747000
8	-0.173134000	2.691850000	-0.140070000
7	-1.212628000	0.636710000	0.028741000
9	0.278596000	-2.667651000	0.166240000
1	-1.986178000	-1.286034000	0.178224000

A (M-CONH₃) anion M062

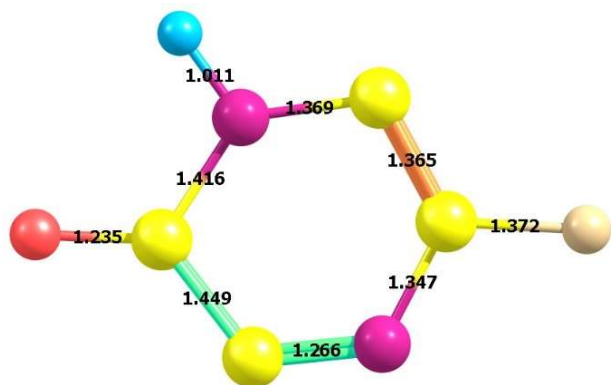
Sum of electronic and zero-point Energies=
-437.531560



6	-1.075893000	-0.687893000	0.102978000
6	0.143845000	-1.300767000	0.088696000
7	1.265903000	-0.581103000	-0.002401000
6	1.143981000	0.681752000	-0.073898000
6	-0.115131000	1.449444000	-0.067086000
8	-0.165919000	2.681229000	-0.139608000
7	-1.214018000	0.639048000	0.028623000
9	0.274918000	-2.651324000	0.165509000
1	-1.977747000	-1.288107000	0.178138000

B (M-CONH₃) anion B3LYP

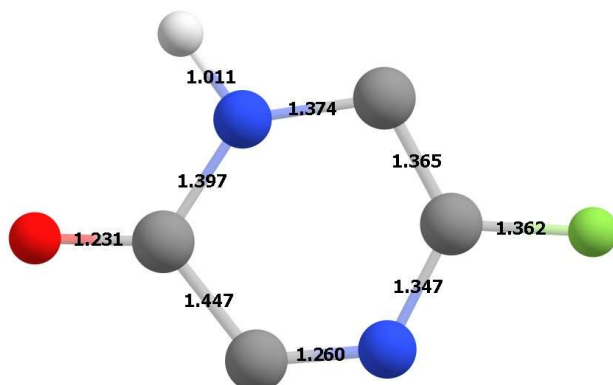
Sum of electronic and zero-point Energies=
-437.649686



6	-1.174427000	-0.771885000	0.112537000
6	0.089351000	-1.288125000	0.090330000
7	1.206863000	-0.541987000	-0.002346000
6	1.198873000	0.721730000	-0.078718000
6	-0.034490000	1.482596000	-0.072176000
8	-0.216561000	2.702084000	-0.139035000
7	-1.132174000	0.594224000	0.028040000
9	0.314371000	-2.639162000	0.162954000
1	-2.009336000	1.097144000	0.034624000

B (M-CONH₃) anion B3LYP

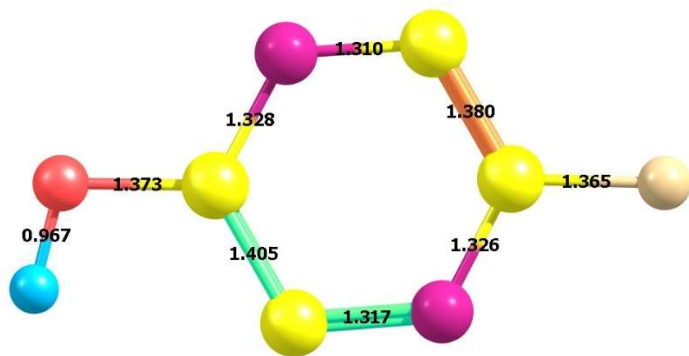
Sum of electronic and zero-point Energies=
-437.490612



6	-1.176898000	-0.774012000	0.113035000
6	0.090370000	-1.281707000	0.090025000
7	1.214481000	-0.544528000	-0.002360000
6	1.184638000	0.712966000	-0.077380000
6	-0.044710000	1.476427000	-0.071729000
8	-0.212446000	2.694005000	-0.138751000
7	-1.125325000	0.596807000	0.027598000
9	0.315446000	-2.622681000	0.161549000
1	-2.003086000	1.099342000	0.034224000

C (M-CONH₃) anion B3LYP

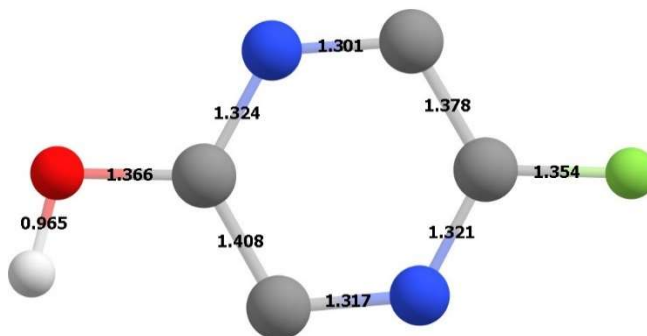
Sum of electronic and zero-point Energies=
-437.635417



6	-1.167669000	-0.629914000	0.098365000
6	0.060100000	-1.260527000	0.120204000
7	1.206988000	-0.599655000	0.038667000
6	1.247866000	0.712388000	-0.069199000
6	-0.002906000	1.353078000	-0.091209000
8	-0.087242000	2.718834000	-0.200381000
7	-1.142526000	0.675869000	-0.008599000
9	0.160620000	-2.617596000	0.228133000
1	0.838470000	2.995602000	-0.245221000

C (M-CONH₃) anion M062x

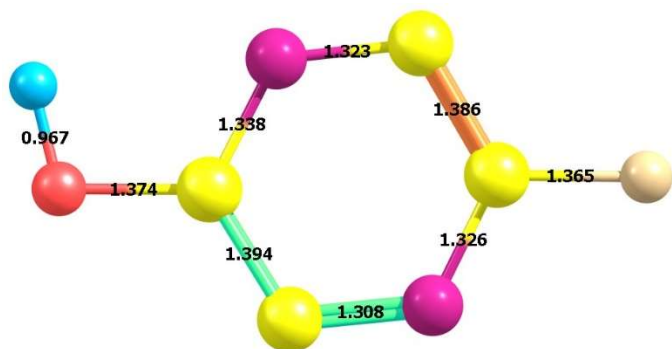
Sum of electronic and zero-point Energies=
-437.476264



6	-1.161768000	-0.623366000	0.097751000
6	0.060299000	-1.259823000	0.120520000
7	1.200828000	-0.597455000	0.038794000
6	1.252768000	0.714488000	-0.069502000
6	-0.002498000	1.350845000	-0.091039000
8	-0.089582000	2.709592000	-0.199651000
7	-1.136348000	0.672765000	-0.008512000
9	0.156565000	-2.605817000	0.226861000
1	0.833437000	2.986853000	-0.244462000

D (M-CONH₃) anion B3LYP

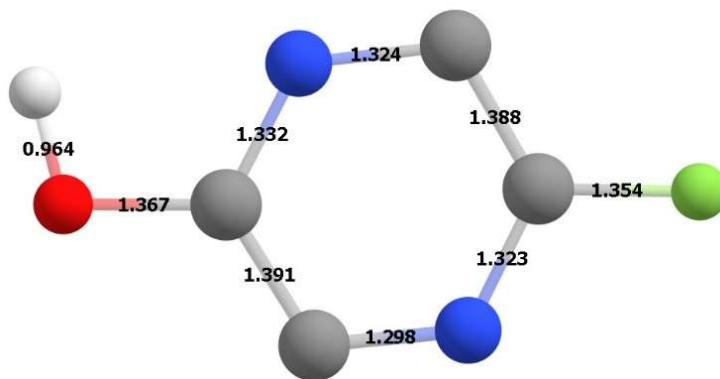
Sum of electronic and zero-point Energies=
-437.633642



6	-1.184147000	-0.715641000	0.118014000
6	0.077788000	-1.289297000	0.099338000
7	1.200781000	-0.587830000	0.028659000
6	1.197411000	0.718839000	-0.029327000
6	-0.054975000	1.329922000	-0.012524000
8	-0.199634000	2.694839000	-0.068049000
7	-1.178199000	0.606210000	0.059039000
9	0.234116000	-2.644327000	0.153766000
1	-1.155911000	2.834494000	-0.040685000

D (M-CONH₃) anion B3LYP

Sum of electronic and zero-point Energies=
-437.474418



6	-1.188076000	-0.716735000	0.118186000
6	0.076918000	-1.286672000	0.099338000
7	1.195710000	-0.584033000	0.028678000
6	1.191043000	0.713129000	-0.028868000
6	-0.056016000	1.328946000	-0.012439000
8	-0.197811000	2.687934000	-0.067814000
7	-1.171890000	0.605473000	0.058830000
9	0.238569000	-2.629794000	0.152919000
1	-1.151218000	2.828962000	-0.040600000

m/z = 42

OCN anion B3LYP



Sum of electronic and zero-point Energies=
-168.190620

6	0.00000000	0.07134200	0.00000000
8	-0.00411700	-1.15459300	0.00000000
7	0.00470500	1.25838400	0.00000000

OCN anion M062x

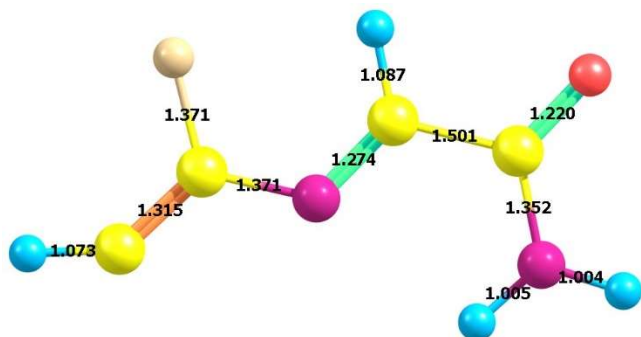


Sum of electronic and zero-point Energies=
-168.128403

6	-0.00038600	0.07291100	0.00000000
8	-0.00392800	-1.15535000	0.00000000
7	0.00490200	1.25757200	0.00000000

(M-OCN) neutral B3LYP

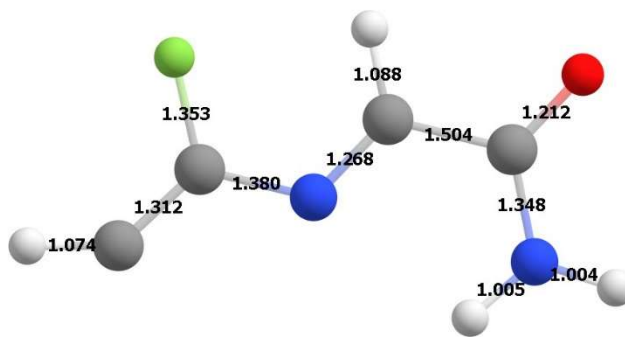
Sum of electronic and zero-point Energies=
-439.385104



6	-1.17562200	-1.23234200	-0.90526200
6	-0.58128200	-0.44206200	-0.03884400
7	0.61892500	0.17847900	-0.26866400
6	1.15523700	0.93602500	0.60434100
6	2.47028900	1.60802200	0.33443800
8	2.96621900	2.33038100	1.18315900
7	3.01702900	1.34634900	-0.87393100
9	-1.17827900	-0.21000700	1.17329800
1	-2.06740900	-1.82233500	-0.99754200
1	2.54352600	0.73904900	-1.52021600
1	3.89645200	1.76651900	-1.11622600
1	0.72581000	1.15365900	1.57941700

(M-OCN) neutral M062x

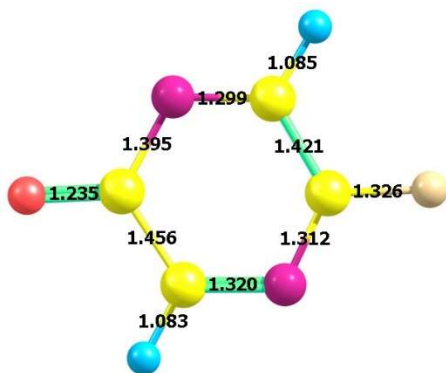
Sum of electronic and zero-point Energies=
-439.214551



6	-1.16507200	-1.22966300	-0.91066600
6	-0.57616700	-0.44092900	-0.04332800
7	0.63308300	0.17903900	-0.28505700
6	1.14952600	0.92933200	0.59694300
6	2.46758200	1.60617900	0.33653200
8	2.95467000	2.32163600	1.18547400
7	3.01126500	1.34625000	-0.86898300
9	-1.14963700	-0.19791900	1.15759400
1	-2.06844600	-1.80755600	-0.96236200
1	2.53354600	0.73911800	-1.51226800
1	3.89119700	1.76650900	-1.10911500
1	0.70934900	1.13974100	1.56920500

A (M-OCN - H₂) neutral B3LYP

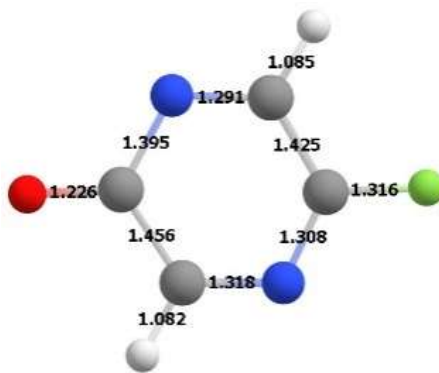
Sum of electronic and zero-point Energies=
-438.243019



6	-0.148280000	-0.123292000	0.026965000
6	1.118496000	-0.767031000	0.017546000
7	2.269364000	-0.143346000	-0.067213000
6	2.195125000	1.172257000	-0.147146000
6	0.934497000	1.900405000	-0.142962000
8	0.916978000	3.133060000	-0.220155000
7	-0.249541000	1.169392000	-0.050400000
9	1.149018000	-2.090253000	0.099663000
1	-1.049020000	-0.724106000	0.100338000
1	3.114713000	1.739309000	-0.219257000

A (M-OCN - H₂) neutral M062x

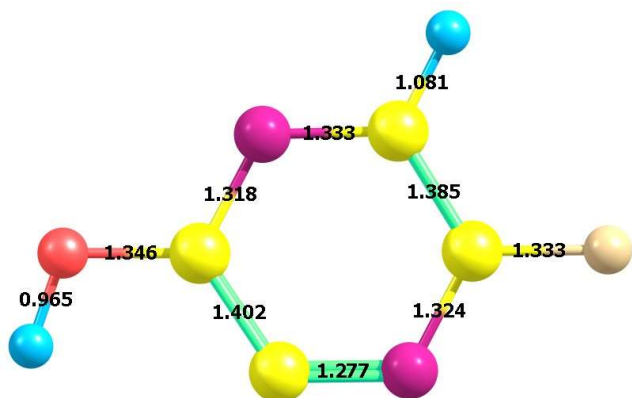
Sum of electronic and zero-point Energies=
-438.080695



6	-0.147787000	-0.117796000	0.026560000
6	1.122424000	-0.763215000	0.017169000
7	2.271334000	-0.144551000	-0.067270000
6	2.193222000	1.168396000	-0.146843000
6	0.933268000	1.897553000	-0.142818000
8	0.921741000	3.120661000	-0.219286000
7	-0.252006000	1.167119000	-0.050193000
9	1.143422000	-2.076246000	0.099237000
1	-1.043198000	-0.726246000	0.100094000
1	3.108932000	1.740721000	-0.219271000

B (M-OCN - H₂) neutral B3LYP

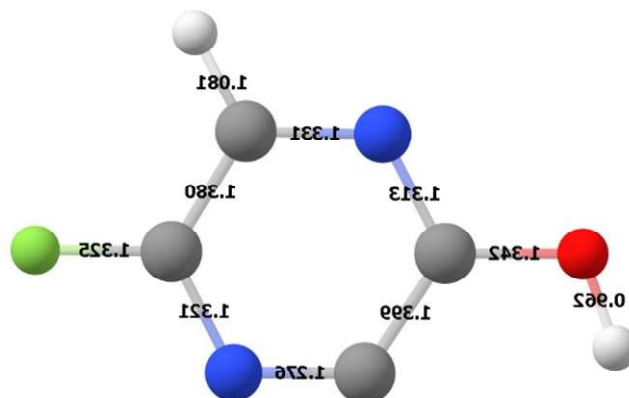
Sum of electronic and zero-point Energies=
-438.214809



6	0.010367000	-0.323574000	0.033303000
6	1.226830000	-0.984977000	0.026896000
7	2.360522000	-0.306460000	-0.060551000
6	2.300708000	0.966924000	-0.138289000
6	1.094610000	1.681366000	-0.135550000
8	1.015265000	3.022270000	-0.216955000
7	-0.033683000	1.005870000	-0.048564000
9	1.291875000	-2.313665000	0.107923000
1	-0.922361000	-0.866036000	0.104248000
1	1.907216000	3.384678000	-0.275082000

B (M-OCN - H₂) neutral M062x

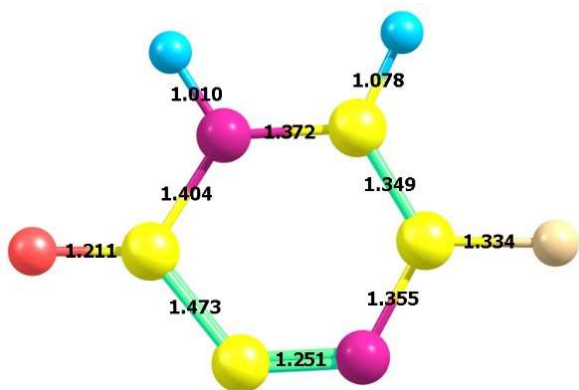
Sum of electronic and zero-point Energies=
-438.056152



6	0.013386000	-0.320645000	0.032974000
6	1.227469000	-0.977151000	0.026352000
7	2.363470000	-0.308498000	-0.060608000
6	2.293497000	0.963035000	-0.137950000
6	1.090603000	1.677333000	-0.135574000
8	1.017602000	3.014410000	-0.216701000
7	-0.035016000	1.007327000	-0.048853000
9	1.288968000	-2.298414000	0.107270000
1	-0.915900000	-0.868176000	0.104416000
1	1.907270000	3.377173000	-0.273946000

C (M-OCN - H₂) neutral B3LYP

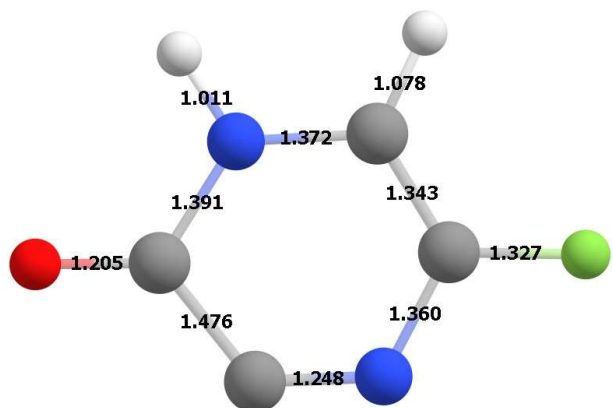
Sum of electronic and zero-point Energies=
-438.211802



6	0.282558000	-0.196286000	0.014580000
6	1.485377000	-0.807763000	0.005569000
7	2.626475000	-0.082462000	-0.085143000
6	2.596817000	1.166260000	-0.162577000
6	1.385017000	2.004394000	-0.167566000
8	1.294798000	3.209414000	-0.239829000
7	0.257623000	1.172444000	-0.070630000
9	1.608568000	-2.134052000	0.084230000
1	-0.656306000	-0.721427000	0.084756000
1	-0.629576000	1.655873000	-0.066013000

C (M-OCN - H₂) neutral M062x

Sum of electronic and zero-point Energies=
-438.050683



6	0.285909000	-0.194317000	0.014240000
6	1.482961000	-0.802022000	0.005204000
7	2.634147000	-0.084309000	-0.085333000
6	2.590739000	1.161024000	-0.161963000
6	1.375140000	1.997342000	-0.166719000
8	1.298170000	3.198148000	-0.239203000
7	0.257845000	1.175054000	-0.070827000
9	1.605635000	-2.120516000	0.083518000
1	-0.650278000	-0.723643000	0.084818000
1	-0.628916000	1.659634000	-0.066358000

m/z = 26

CN ANION B3LYP

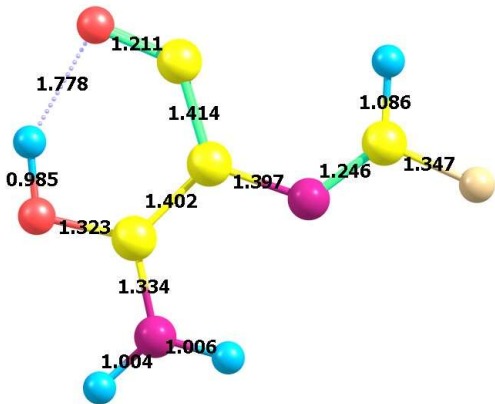
Sum of electronic and zero-point Energies=
-92.890709



6	0.533905000	0.218193000	-0.141014000
7	1.516365000	0.835086000	0.020490000

[M-CN] NEUTRAL B3LYP

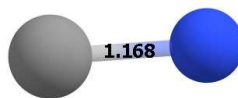
Sum of electronic and zero-point Energies=
-514.683598



6	-0.300464000	-1.471779000	0.170689000
7	0.703225000	-0.743316000	0.053463000
6	0.651113000	0.649275000	-0.045092000
6	-0.522932000	1.436529000	-0.026238000
8	-0.651685000	2.638123000	-0.105453000
6	1.885971000	1.300921000	-0.172930000
8	1.988570000	2.615942000	-0.275198000
7	3.044727000	0.640866000	-0.201025000
9	-0.139265000	-2.806170000	0.258370000
1	3.022338000	-0.361651000	-0.123868000
1	3.911418000	1.139658000	-0.289079000
1	1.082816000	3.002021000	-0.244005000
1	-1.349082000	-1.194106000	0.216967000

CN ANION M062x

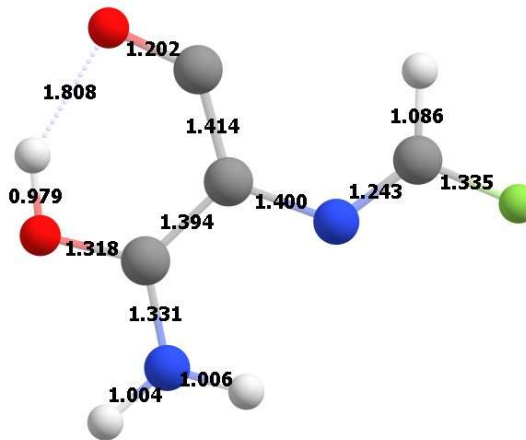
Sum of electronic and zero-point Energies=
-92.855928



6	0.535370000	0.219113000	-0.140773000
7	1.514900000	0.834166000	0.020249000

[M-CN] NEUTRAL M062x

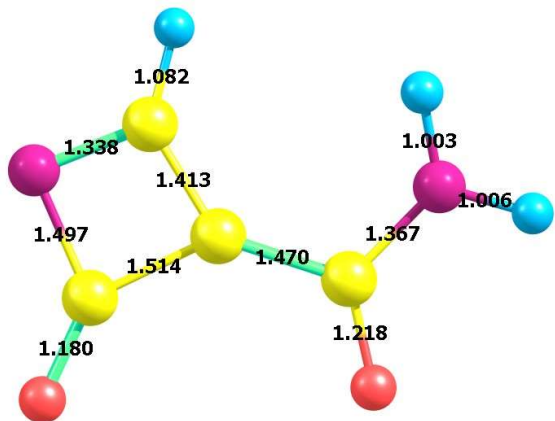
Sum of electronic and zero-point Energies=
-514.490503



6	-0.294283000	-1.460501000	0.169455000
7	0.721912000	-0.754919000	0.052369000
6	0.661539000	0.640068000	-0.045306000
6	-0.520964000	1.414348000	-0.025069000
8	-0.671123000	2.604703000	-0.101470000
6	1.884576000	1.297398000	-0.172054000
8	1.984870000	2.607911000	-0.273905000
7	3.043050000	0.643570000	-0.199564000
9	-0.164734000	-2.786724000	0.257742000
1	3.023600000	-0.359570000	-0.124218000
1	3.904996000	1.150295000	-0.290109000
1	1.087445000	2.998795000	-0.245335000
1	-1.334135000	-1.149061000	0.214065000

[M - CN - HF] NEUTRAL B3LYP

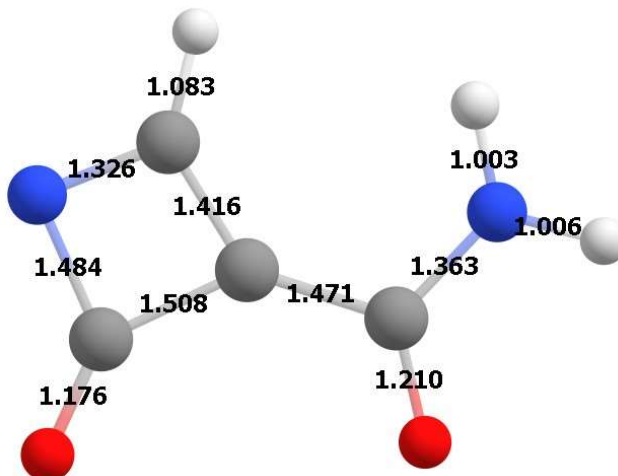
Sum of electronic and zero-point Energies=
-414.179403



6	-0.235907000	-0.338346000	0.052712000
6	0.658293000	0.747802000	-0.074315000
6	-0.604682000	1.578200000	-0.162643000
8	-0.946784000	2.700388000	-0.290862000
7	-1.399404000	0.317700000	-0.016624000
6	2.103897000	1.012882000	-0.090478000
8	2.535011000	2.152290000	-0.107696000
7	2.911285000	-0.090295000	-0.060970000
1	-0.126961000	-1.407568000	0.177785000
1	2.557869000	-1.024630000	-0.155999000
1	3.905049000	0.054912000	-0.120958000

[M - CN - HF] NEUTRAL M062x

Sum of electronic and zero-point Energies=-
414.016461

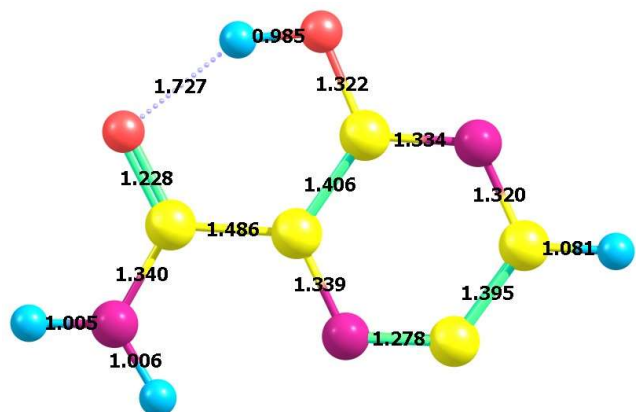


6	-0.233323000	-0.334394000	0.042971000
6	0.663106000	0.754540000	-0.077104000
6	-0.603570000	1.569455000	-0.154036000
8	-0.947109000	2.687754000	-0.271386000
7	-1.387446000	0.316528000	-0.016556000
6	2.109453000	1.019375000	-0.097483000
8	2.538918000	2.150442000	-0.135661000
7	2.903895000	-0.087341000	-0.047789000
1	-0.120849000	-1.404960000	0.157479000
1	2.536226000	-1.016694000	-0.133252000
1	3.898363000	0.048630000	-0.117232000

m/z=19

A (M-F) NEUTRAL B3LYP

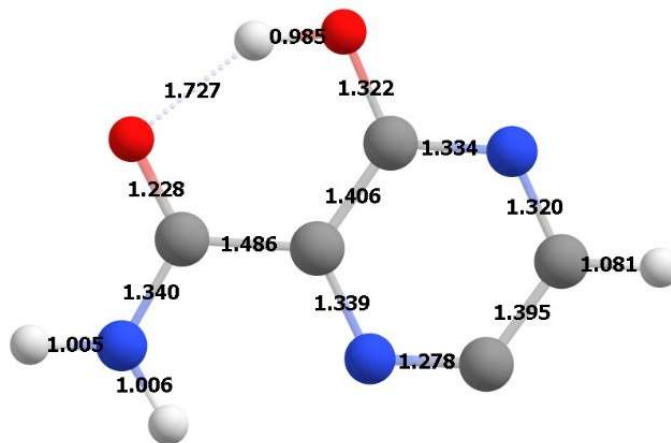
Sum of electronic and zero-point Energies=
-507.687708



6	-1.130656000	-0.629962000	0.098241000
6	0.112632000	-1.263607000	0.088644000
7	1.222747000	-0.636250000	0.005281000
6	1.190714000	0.700030000	-0.077260000
6	-0.047302000	1.366721000	-0.070717000
8	-0.141198000	2.683342000	-0.150333000
7	-1.190874000	0.686273000	0.017353000
6	2.465834000	1.456406000	-0.175582000
8	2.464633000	2.682400000	-0.253119000
7	3.582181000	0.714849000	-0.173394000
1	-2.060926000	-1.175923000	0.169110000
1	3.519001000	-0.286752000	-0.107938000
1	4.472577000	1.175992000	-0.238124000
1	0.775896000	3.039179000	-0.208652000

A (M-F) NEUTRAL M062x

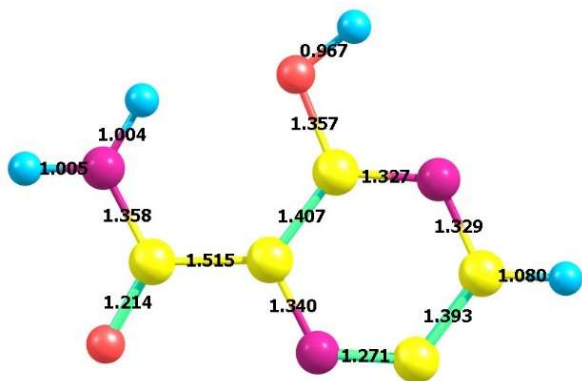
Sum of electronic and zero-point Energies=
-507.495662



6	-1.130656000	-0.629962000	0.098241000
6	0.112632000	-1.263607000	0.088644000
7	1.222747000	-0.636250000	0.005281000
6	1.190714000	0.700030000	-0.077260000
6	-0.047302000	1.366721000	-0.070717000
8	-0.141198000	2.683342000	-0.150333000
7	-1.190874000	0.686273000	0.017353000
6	2.465834000	1.456406000	-0.175582000
8	2.464633000	2.682400000	-0.253119000
7	3.582181000	0.714849000	-0.173394000
1	-2.060926000	-1.175923000	0.169110000
1	3.519001000	-0.286752000	-0.107938000
1	4.472577000	1.175992000	-0.238124000
1	0.775896000	3.039179000	-0.208652000

B (M-F) NEUTRAL B3LYP

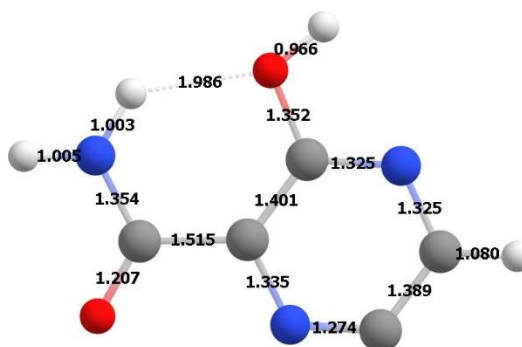
Sum of electronic and zero-point Energies=
-507.671892



6	-1.063425000	-0.604484000	0.213384000
6	0.168301000	-1.240363000	0.075190000
7	1.253690000	-0.611911000	-0.133307000
6	1.280905000	0.724094000	-0.234883000
6	0.039999000	1.373296000	-0.096292000
8	-0.052804000	2.724223000	-0.180965000
7	-1.095431000	0.721343000	0.121440000
6	2.637632000	1.351207000	-0.484103000
8	3.627724000	0.655495000	-0.581126000
7	2.670676000	2.705027000	-0.588891000
1	-1.992802000	-1.125596000	0.390662000
1	1.847845000	3.274734000	-0.507515000
1	3.566512000	3.129843000	-0.754186000
1	-0.984654000	2.953513000	-0.058158000

B (M-F) NEUTRAL M062x

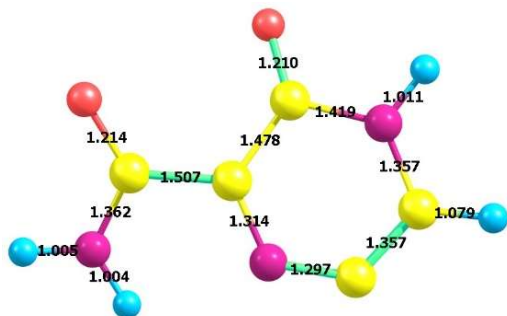
Sum of electronic and zero-point Energies=
-507.480239



6	-1.057237000	-0.595820000	0.212011000
6	0.170582000	-1.230870000	0.074330000
7	1.264072000	-0.612237000	-0.134830000
6	1.276834000	0.719448000	-0.234091000
6	0.044653000	1.372622000	-0.096922000
8	-0.044454000	2.718627000	-0.182045000
7	-1.090577000	0.725803000	0.120464000
6	2.631624000	1.350768000	-0.483308000
8	3.615395000	0.657812000	-0.579768000
7	2.660100000	2.700550000	-0.586935000
1	-1.986105000	-1.117844000	0.388966000
1	1.836362000	3.267736000	-0.504726000
1	3.556874000	3.123533000	-0.752166000
1	-0.973951000	2.950292000	-0.059732000

D (M-F) NEUTRAL B3LYP

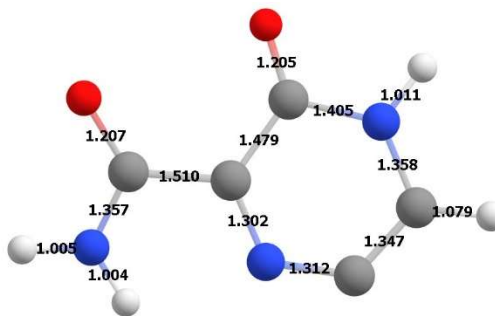
Sum of electronic and zero-point Energies=
-507.664798



6	-1.188459000	-0.846246000	0.126739000
6	0.063231000	-1.369836000	0.124615000
7	1.135177000	-0.645140000	0.035328000
6	1.123966000	0.665664000	-0.053794000
6	-0.159342000	1.396975000	-0.008922000
8	-0.352822000	2.591836000	-0.003785000
7	-1.262542000	0.506939000	0.054758000
6	2.436278000	1.387055000	-0.219172000
8	2.504232000	2.546181000	-0.574387000
7	3.524831000	0.617229000	0.059205000
1	-2.108845000	-1.407028000	0.180906000
1	-2.159090000	0.974756000	0.070849000
1	3.427901000	-0.370064000	0.216485000
1	4.430613000	1.004059000	-0.139546000

D (M-F) NEUTRAL M062x

Sum of electronic and zero-point Energies=
-507.469514

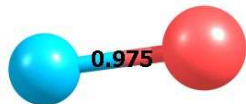


6	-1.182304000	-0.840055000	0.125478000
6	0.057665000	-1.367268000	0.120275000
7	1.152429000	-0.650073000	0.029060000
6	1.121407000	0.648746000	-0.055621000
6	-0.158403000	1.388962000	-0.007770000
8	-0.334351000	2.581076000	-0.000304000
7	-1.255933000	0.514331000	0.055598000
6	2.429923000	1.383190000	-0.221947000
8	2.483377000	2.534516000	-0.580591000
7	3.517015000	0.621943000	0.061284000
1	-2.104215000	-1.397778000	0.180676000
1	-2.151417000	0.984194000	0.074420000
1	3.418849000	-0.364728000	0.220497000
1	4.421087000	1.015325000	-0.131775000

SMALL NEUTRAL FRAGMENTS:

OH NEUTRAL B3LYP

Sum of electronic and zero-point Energies=
-75.760188



8	0.886911000	0.063699000	0.006281000
1	1.163358000	0.989580000	-0.126806000

OH NEUTRAL M062x

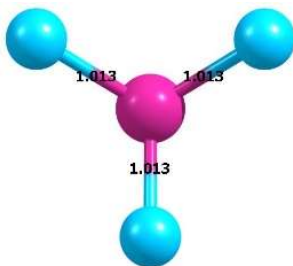
Sum of electronic and zero-point Energies=
-75.725231



8	0.887387000	0.065291000	0.006052000
1	1.162882000	0.987988000	-0.126577000

NH₃ NEUTRAL B3LYP

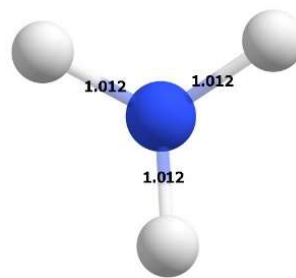
Sum of electronic and zero-point Energies=
-56.554675



7	0.261019000	0.059110000	0.080922000
1	-0.104048000	-0.752585000	0.564379000
1	-0.369962000	0.829340000	0.266563000
1	0.212991000	-0.135866000	-0.911863000

NH₃ NEUTRAL M062x

Sum of electronic and zero-point Energies=
-56.518493



7	0.262250000	0.059363000	0.081140000
1	-0.104372000	-0.751278000	0.563342000
1	-0.369789000	0.827731000	0.266094000
1	0.211910000	-0.135816000	-0.910575000

H₂ NEUTRAL B3LYP

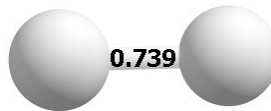
Sum of electronic and zero-point Energies=
-1.169954



1	0.919888000	0.174144000	-0.009594000
1	1.130381000	0.879135000	-0.110931000

H₂ NEUTRAL M062x

Sum of electronic and zero-point Energies=
-1.158705

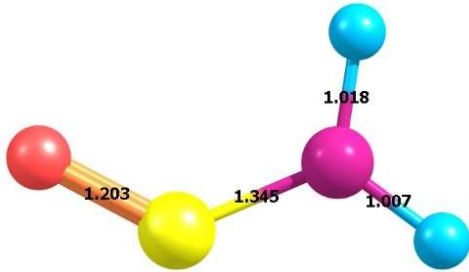


1	0.920433000	0.175971000	-0.009857000
1	1.129836000	0.877308000	-0.110668000

1 -0.307588000 0.848426000 0.368481000

CONH₂ NEUTRAL B3LYP

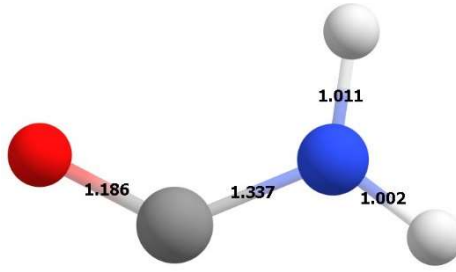
Sum of electronic and zero-point Energies=
-169.199205



6	-4.150300000	2.847700000	0.345270000
8	-3.286580000	3.373860000	-0.305540000
7	-5.030690000	1.898150000	-0.019000000
1	-5.038110000	1.511860000	-0.960470000
1	-5.704070000	1.550200000	0.644590000

CONH₂ NEUTRAL M062x

Sum of electronic and zero-point Energies=
-169.204081



6	-4.152392000	2.841772000	0.335189000
8	-3.297971000	3.365866000	-0.299559000
7	-5.030299000	1.898230000	-0.019421000
1	-5.031610000	1.519198000	-0.957080000
1	-5.697477000	1.556705000	0.645721000

CO NEUTRAL B3LYP

Sum of electronic and zero-point Energies=
-113.353802



6	-0.069886000	-0.483665000	0.577116000
8	-0.253379000	0.607934000	0.371610000

CO NEUTRAL M062x

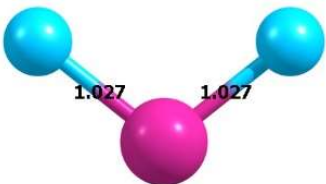
Sum of electronic and zero-point Energies=
-113.315065



6	-0.070247000	-0.481517000	0.576712000
8	-0.253018000	0.605786000	0.372014000

NH₂ NEUTRAL B3LYP

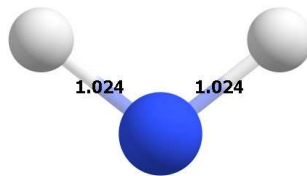
Sum of electronic and zero-point Energies=
-55.887617



7	0.036084000	-0.009040000	-0.080239000
1	-0.045020000	-0.713595000	0.662551000

NH₂ NEUTRAL M062x

Sum of electronic and zero-point Energies=
-55.852724

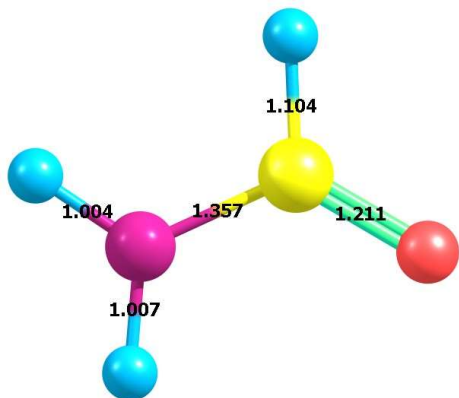


7	0.035450000	-0.008805000	-0.078466000
1	-0.044900000	-0.712545000	0.661448000

1 -0.307073000 0.847141000 0.367811000

CONH₃ NEUTRAL B3LYP

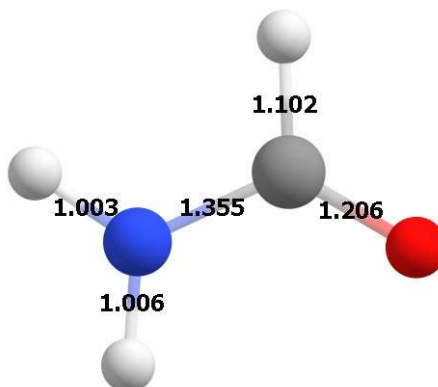
Sum of electronic and zero-point Energies=
-169.924989



8	1.578050000	0.079204000	0.369598000
6	1.902412000	-0.212571000	-0.759804000
7	3.182526000	-0.325013000	-1.195270000
1	1.166311000	-0.418231000	-1.556270000
1	3.940635000	-0.159398000	-0.554134000
1	3.389646000	-0.570640000	-2.146310000

CONH₃ NEUTRAL M062x

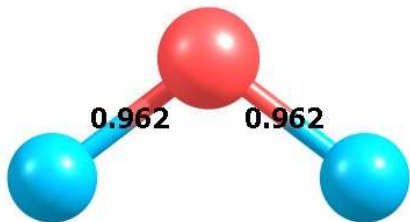
Sum of electronic and zero-point Energies=
-169.848616



8	1.585537000	0.077788000	0.364348000
6	1.902965000	-0.213211000	-0.761644000
7	3.181345000	-0.325089000	-1.196182000
1	1.164533000	-0.417254000	-1.553112000
1	3.934395000	-0.158230000	-0.549928000
1	3.390805000	-0.570653000	-2.145671000

H₂O NEUTRAL B3LYP

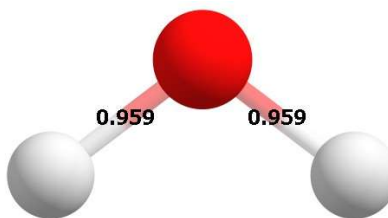
Sum of electronic and zero-point Energies=
-76.444953



8	0.748012000	0.288466000	-0.196845000
1	1.648320000	0.385159000	-0.520944000
1	0.679073000	0.906294000	0.537003000

H₂O NEUTRAL M062x

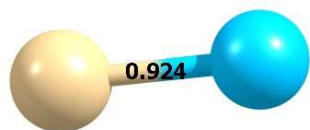
Sum of electronic and zero-point Energies=
-76.408546



8	0.749701000	0.289974000	-0.195949000
1	1.647181000	0.384588000	-0.521043000
1	0.678524000	0.905357000	0.536205000

HF NEUTRAL B3LYP

Sum of electronic and zero-point Energies=
-100.480794



9	1.418164000	0.767622000	-0.090986000
1	0.632105000	0.285657000	-0.029538000

HF NEUTRAL M062x

Sum of electronic and zero-point Energies=
-100.443533



1	0.894766000	0.090006000	0.002500000
9	1.155503000	0.963273000	-0.123025000