Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information of

IR-VUV spectroscopy of pyridine dimer, trimer and pyridine-ammonia complexes in a supersonic jet

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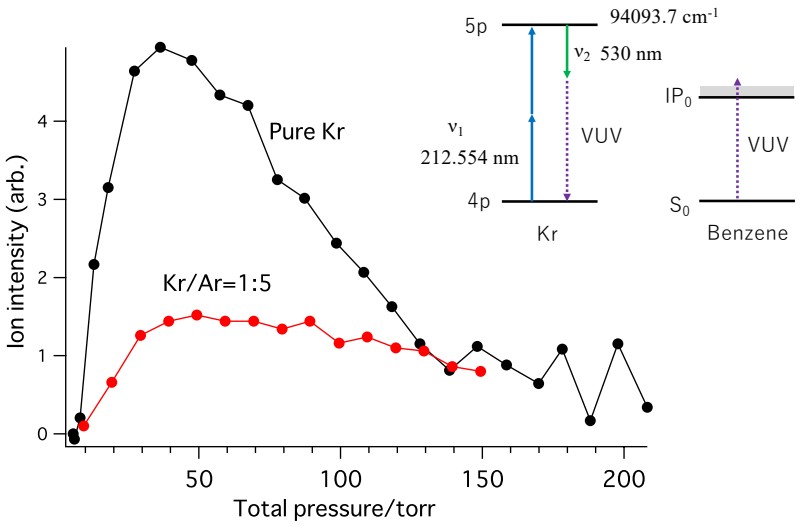

Fig. S1 Plots of the VUV ionization signal intensity of benzene monomer vs. total pressure of pure Kr gas and Kr/Ar (1:5) mixture gas. Pure Kr gives 4 times stronger ion signal. Laser power of ν_1 is 1 mJ/pulse and that of ν_2 is 4 mJ/pulse.

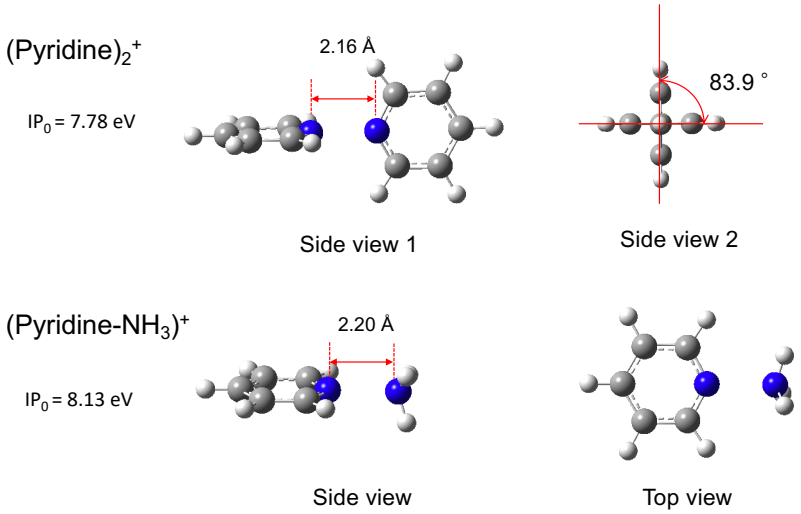

Fig. S2 Ground state structures of $(pyridine)_2^+$ and $[pyridine\text{-}NH_3]^+$ cations calculated at the ωB97X-D/aug-cc-pVDZ level. IP_0s are obtained at the same level of calculation.

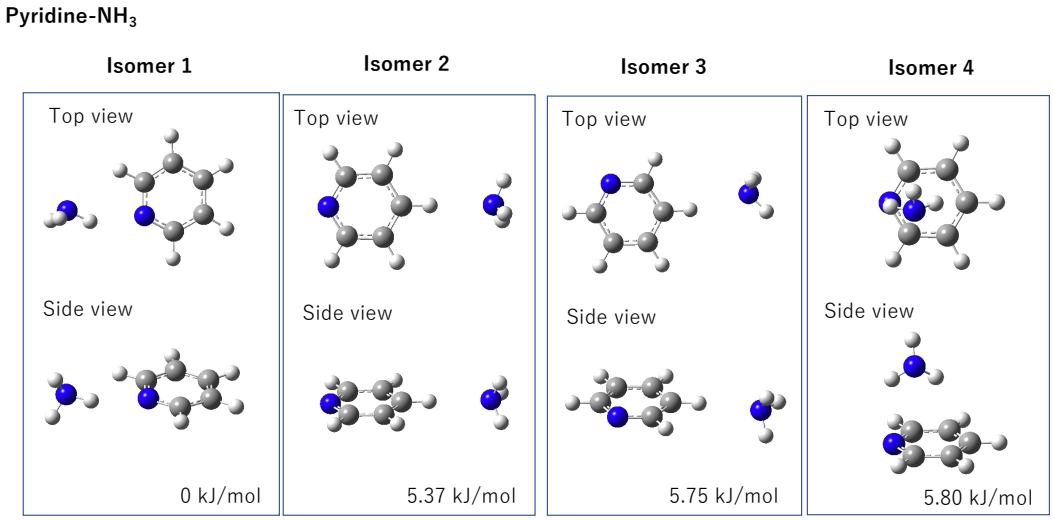

Fig. S3 Stable isomers of pyridine-NH_3 complexes and their relative (ZPE corrected) energies calculated at the ωB97X-D/aug-cc-pVDZ level.

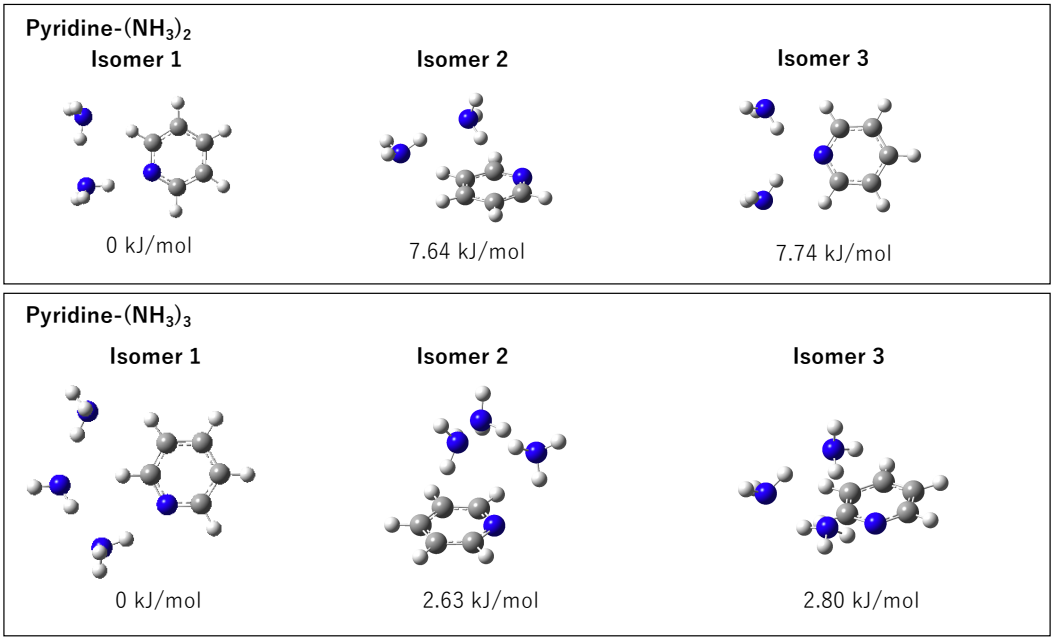

Fig. S4 Three lowest energy isomers of pyridine-$(NH_3)_2$ and pyridine-$(NH_3)_3$ complexes and their relative (ZPE corrected) energies calculated at the ωB97X-D/aug-cc-pVDZ level.

Table S1 Cartesian coordinates of the stable structures of $(pyridine)_2$, $(pyridine)_3$ and $(pyridine)_m$-$(ammonia)_n$ calculated at the ωB97XD/aug-cc-pVDZ.

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$(pyridine)_m$-$(ammonia)_n$, (m, n) = (2, 0)

****

22

1 Relative E0+Ezero= 0.0 kJ/mol

C 2.398645 -1.018827 0.807388

C 1.421227 -1.652814 1.567761

C 0.308380 -2.175883 0.914404

C 0.227661 -2.044185 -0.471054

C 2.220755 -0.942288 -0.572808

H 3.291061 -0.600645 1.269798

H 1.530464 -1.746432 2.647873

H -0.484909 -2.681670 1.463630

H -0.632457 -2.444773 -1.012194

H 2.973734 -0.456844 -1.196927

N 1.160692 -1.442067 -1.214080

C 3.150931 -4.527399 0.961096

C 5.147338 -3.430352 0.872079

C 5.073735 -3.294675 -0.513393

C 3.962764 -3.813147 -1.173566

C 2.980026 -4.446712 -0.419717

H 2.393631 -5.012458 1.580250

H 6.005965 -3.033695 1.418478

H 5.871007 -2.789442 -1.057346

H 3.859294 -3.716763 -2.254008

H 2.088781 -4.861244 -0.887632

N 4.209164 -4.032083 1.608889

22

2 Relative E0+Ezero= 0.8349088850146933 kJ/mol

C -0.086508 3.493070 -0.626409

C -0.158027 3.353338 0.756382

C 0.769523 4.033084 1.539616

C 1.727652 4.820507 0.902600

C 0.912318 4.304135 -1.162834

H -0.786865 2.979476 -1.283762
H -0.915283 2.719003 1.216155
H 0.764115 3.944833 2.624768
H 2.470197 5.364525 1.490419
H 0.995658 4.431419 -2.244386
N 1.810823 4.960596 -0.423392
C 2.934439 1.501942 1.294512
C 1.230442 -0.012656 1.297878
C 1.188968 -0.052031 -0.095003
C 2.082299 0.743065 -0.808051
C 2.976002 1.539016 -0.098552
H 3.619892 2.118325 1.879346
H 0.542440 -0.624201 1.885877
H 0.469936 -0.693004 -0.603901
H 2.079178 0.745924 -1.898089
H 3.684737 2.189392 -0.608382
N 2.083291 0.745460 1.992766
22
3 Relative E0+Ezero= 1.3127498191181999 kJ/mol
C 0.379034 -5.356971 -3.051821
C 0.439837 -5.338218 -4.440692
C -0.001781 -4.199231 -5.109865
C -0.481603 -3.129694 -4.356784
C -0.122435 -4.233462 -2.394498
H 0.726215 -6.215643 -2.479724
H 0.829891 -6.193270 -4.992675
H 0.024925 -4.135497 -6.197045
H -0.834092 -2.222004 -4.851717
H -0.179491 -4.218009 -1.304283
N -0.546900 -3.133704 -3.021633
C 4.110321 -5.369023 -3.333706
C 3.233281 -3.796001 -1.935725
C 2.994466 -2.911599 -2.987622
C 3.345584 -3.304085 -4.274352
C 3.918093 -4.561142 -4.452616
H 4.555733 -6.360639 -3.440493

H 2.965010 -3.516628 -0.914914
H 2.529297 -1.946277 -2.795516
H 3.170946 -2.645116 -5.124757
H 4.210843 -4.914907 -5.440478
N 3.778658 -5.004932 -2.090974
22
4 Relative E0+Ezero= 4.358329399120212 kJ/mol
C 1.700242 -2.896990 1.999321
C 1.034756 -2.984433 0.778931
C 0.035198 -2.057431 0.499499
C -0.258717 -1.080490 1.451300
C 1.332868 -1.884135 2.883298
H 2.490072 -3.598120 2.266167
H 1.292223 -3.762424 0.059371
H -0.514487 -2.083286 -0.440456
H -1.037866 -0.337327 1.263681
H 1.835354 -1.788420 3.848356
N 0.375162 -0.988377 2.626678
C -1.730834 1.701639 3.119648
C -3.322394 2.505200 1.687575
C -3.689816 3.518078 2.571505
C -3.024369 3.605576 3.791912
C -2.024799 2.678606 4.071406
H -0.951674 0.958499 3.307314
H -3.824849 2.409440 0.722504
H -4.479653 4.219182 2.304612
H -3.281874 4.383587 4.511437
H -1.475143 2.704505 5.011377
N -2.364676 1.609472 1.944254
22
5 Relative E0+Ezero= 4.681265854674329 kJ/mol
C -1.902669 -0.419928 2.877011
C -1.876348 -1.197084 1.721962
C -2.339991 -0.638756 0.533972
C -2.808622 0.674776 0.554657
C -2.393199 0.882269 2.787711

H -1.544618 -0.816843 3.826197
H -1.499113 -2.219460 1.749407
H -2.342346 -1.205914 -0.396367
H -3.177861 1.141307 -0.361500
H -2.427583 1.518361 3.674948
N -2.839829 1.432632 1.654299
C -0.527060 -4.027208 3.731376
C 1.045591 -2.435428 3.280797
C 1.379190 -3.029184 2.064169
C 0.707098 -4.188065 1.685027
C -0.269023 -4.699544 2.536622
H -1.287411 -4.400972 4.419828
H 1.549784 -1.522899 3.604264
H 2.145745 -2.586113 1.430080
H 0.936982 -4.681030 0.740370
H -0.824381 -5.601958 2.285049
N 0.112155 -2.915740 4.107567

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (3, 0)

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33

1 Relative E0+Ezero= 0.0 kJ/mol

C 4.282874 -2.286641 -0.909231

C 5.370863 -1.429069 -1.069644

C 4.125847 0.398784 -0.507520

C 2.975790 -0.367866 -0.319593

H 4.398799 -3.356101 -1.081516

H 6.343983 -1.825078 -1.368412

H 4.083287 1.478767 -0.357740

H 2.051971 0.128476 -0.024963

C 1.713505 1.226716 -4.993845

C 2.171287 0.048890 -4.403345

C 3.437021 0.044471 -3.824418

C 4.190236 1.214746 -3.862590

C 3.640861 2.336540 -4.480378

N 2.425187 2.356721 -5.038296

H 3.825574 -0.849250 -3.337144

H 0.722574 1.264464 -5.450800

H 1.542046 -0.840019 -4.392580

H 5.175540 1.260505 -3.401554

H 4.202603 3.271731 -4.522755

C 0.912762 3.595517 0.442960

C 0.569774 4.816035 -0.135012

C 0.709592 4.960599 -1.513579

C 1.185743 3.881729 -2.252911

C 1.500963 2.704139 -1.576006

N 1.370580 2.550942 -0.254076

H 0.451729 5.900089 -2.002990

H 0.814801 3.448599 1.520625

H 0.202589 5.632435 0.485711

H 1.319035 3.937670 -3.332308

H 1.879627 1.838812 -2.124297

N 5.306542 -0.107550 -0.877432

C 3.058452 -1.741459 -0.526260
H 2.184524 -2.379480 -0.392509
33
2 Relative E0+Ezero= 0.14702797965527478 kJ/mol
C -2.267030 1.508584 2.989070
C -1.974796 0.520342 2.049699
C 0.149892 0.264977 2.845872
C -0.040647 1.235786 3.829191
H -3.249969 1.977604 3.003188
H -2.729612 0.209949 1.324264
H 1.113909 -0.238577 2.753747
H 0.774043 1.486268 4.507013
C 3.363558 1.910323 2.942447
C 3.709192 1.303106 1.736974
C 4.012314 -0.055022 1.743337
C 3.961975 -0.742908 2.953569
C 3.608890 -0.038769 4.104447
N 3.310631 1.264198 4.111524
H 4.278896 -0.568219 0.819463
H 3.109439 2.971818 2.966570
H 3.730504 1.883446 0.816476
H 4.189129 -1.806564 3.010651
H 3.557808 -0.548746 5.068557
C 1.903330 1.637144 -1.353693
C 0.888725 1.550473 -0.401720
C 0.643821 2.657291 0.406355
C 1.423260 3.796855 0.227136
C 2.417388 3.777201 -0.751230
N 2.664829 2.721945 -1.533641
H -0.135392 2.626585 1.167783
H 2.122202 0.787156 -2.003552
H 0.314647 0.633359 -0.279441
H 1.270149 4.689447 0.832730
H 3.048102 4.653833 -0.913899
N -0.792582 -0.098316 1.969872
C -1.277497 1.870131 3.901066

H -1.467826 2.634739 4.654517
33
3 Relative E0+Ezero= 0.2704264626282083 kJ/mol
N 1.272252 -3.375307 -0.503359
C 1.687786 -3.223294 0.758080
C 0.161093 -2.722973 -0.862129
C 1.032001 -2.426805 1.696614
C -0.565347 -1.900518 -0.002763
C -0.118794 -1.746801 1.306899
H 2.594041 -3.767410 1.032731
H -0.162609 -2.864163 -1.895508
H 1.422794 -2.342858 2.710223
H -1.456073 -1.383316 -0.357496
H -0.656569 -1.096401 1.996262
N 1.473017 2.307431 -1.461661
C 1.869465 2.937056 -0.351361
C 1.649164 0.982965 -1.509982
C 2.441086 2.286503 0.742075
C 2.213108 0.238703 -0.476023
C 2.613711 0.906117 0.677140
H 1.716836 4.018017 -0.331080
H 1.313872 0.485629 -2.422195
H 2.738955 2.854394 1.622365
H 2.323725 -0.839738 -0.574217
H 3.049414 0.357566 1.512090
N -2.182214 0.839077 1.360540
C -3.381156 0.407728 0.956438
C -1.409805 1.443830 0.452052
C -3.855845 0.557125 -0.346057
C -1.792069 1.652425 -0.872792
C -3.043159 1.197590 -1.279094
H -3.995518 -0.084426 1.713251
H -0.427252 1.772828 0.795547
H -4.842105 0.181793 -0.615979
H -1.111109 2.154182 -1.558782
H -3.380062 1.338883 -2.306294

33
4 Relative E0+Ezero= 1.7302042612524406 kJ/mol
C -1.439101 -1.174247 0.126689
C -2.083120 -2.152158 -0.629301
C -3.424652 -2.750063 1.114000
C -2.848569 -1.798404 1.953672
H -0.643734 -0.576066 -0.314240
H -1.798008 -2.316857 -1.670471
H -4.226203 -3.395525 1.480251
H -3.194180 -1.694728 2.981674
C 1.590554 -3.460039 0.016902
C 0.498601 -4.321485 -0.058190
C -0.271500 -4.520762 1.084438
C 0.088897 -3.851840 2.249234
C 1.201790 -3.013137 2.218372
N 1.948716 -2.812052 1.129658
H -1.145064 -5.170741 1.059807
H 2.210122 -3.281015 -0.864624
H 0.251467 -4.815210 -0.996781
H -0.485994 -3.963804 3.166947
H 1.508064 -2.474737 3.117816
C 1.489633 0.551441 1.225211
C 2.091688 0.319483 -0.011367
C 1.668440 1.070589 -1.103421
C 0.657820 2.011744 -0.913137
C 0.120652 2.161513 0.364114
N 0.523423 1.452202 1.423829
H 2.111339 0.921049 -2.088204
H 1.798370 -0.030594 2.094250
H 2.857774 -0.448463 -0.097109
H 0.287306 2.620148 -1.737055
H -0.676894 2.885024 0.544284
N -3.058153 -2.935173 -0.158223
C -1.830403 -0.992613 1.449350
H -1.348146 -0.234421 2.066121
33

5 Relative E0+Ezero= 2.200168696461833 kJ/mol
C 2.127328 -1.005021 -0.285943
C 2.843249 -1.625859 0.736607
C 0.985464 -1.817563 2.048745
C 0.179378 -1.202271 1.091911
H 2.631436 -0.690172 -1.197888
H 3.914391 -1.804812 0.626232
H 0.557860 -2.149618 2.996978
H -0.881329 -1.050054 1.286455
C 2.459443 1.329665 2.971860
C 2.976375 0.536668 3.995214
C 3.372858 1.158658 5.175767
C 3.235318 2.540858 5.281060
C 2.708881 3.240786 4.196998
N 2.324888 2.657401 3.057517
H 3.782588 0.576389 6.001544
H 2.140156 0.874118 2.032271
H 3.062934 -0.539649 3.853680
H 3.531081 3.072614 6.184606
H 2.589800 4.325167 4.247034
C 4.111376 1.804398 -1.362678
C 3.531352 2.352694 -0.220072
C 2.180647 2.688076 -0.251954
C 1.473399 2.462362 -1.429871
C 2.146233 1.904746 -2.516902
N 3.441189 1.573673 -2.496707
H 1.705794 3.102135 0.637869
H 5.169062 1.532361 -1.367390
H 4.121386 2.506742 0.682030
H 0.415466 2.709847 -1.510985
H 1.617280 1.713311 -3.453264
N 2.294801 -2.030433 1.887164
C 0.764703 -0.788510 -0.101771
H 0.173485 -0.297052 -0.873563
33
6 Relative E0+Ezero= 2.6438781353575136 kJ/mol

C 2.808999 2.369191 -0.997668
C 3.010800 1.984720 -2.323528
C 2.908857 -0.230053 -1.788146
C 2.695702 0.047098 -0.439418
H 2.780436 3.425758 -0.733823
H 3.141091 2.738526 -3.102836
H 2.956707 -1.264220 -2.135808
H 2.566508 -0.765585 0.273236
C 0.041723 -0.187990 1.792320
C -0.262770 -1.424654 1.225711
C 0.527712 -2.518766 1.564851
C 1.585102 -2.328018 2.451806
C 1.803709 -1.047770 2.960158
N 1.052364 0.011592 2.643876
H 0.323768 -3.503084 1.143581
H -0.556004 0.689152 1.540024
H -1.096497 -1.520981 0.532764
H 2.233169 -3.151789 2.747871
H 2.624342 -0.865241 3.656827
C -2.680987 0.168620 -1.015798
C -1.636392 1.081612 -1.158429
C -0.525055 0.709751 -1.909715
C -0.512612 -0.553736 -2.493110
C -1.609250 -1.390415 -2.291813
N -2.678308 -1.050815 -1.563603
H 0.317826 1.387842 -2.036792
H -3.563962 0.428036 -0.427856
H -1.698148 2.062070 -0.687561
H 0.332802 -0.883020 -3.094937
H -1.629535 -2.387823 -2.736026
N 3.057953 0.710699 -2.726119
C 2.642485 1.377418 -0.033661
H 2.462034 1.626597 1.012024
33
7 Relative E0+Ezero= 2.7095156264402798 kJ/mol
C -2.543524 -0.297060 6.934828

C -3.208121 0.013521 5.749214
C -1.509514 -0.821861 4.472583
C -0.757971 -1.166231 5.596032
H -3.001791 -0.068826 7.896381
H -4.191236 0.488057 5.776948
H -1.127197 -1.030591 3.472513
H 0.217567 -1.633416 5.470562
C -4.372432 -5.423340 3.128970
C -4.022276 -5.844653 4.411373
C -3.686871 -4.878317 5.357793
C -3.714297 -3.539893 4.979836
C -4.079292 -3.224044 3.670657
N -4.403730 -4.140774 2.752894
H -3.405888 -5.165431 6.371359
H -4.639104 -6.155529 2.363874
H -4.015112 -6.905888 4.656438
H -3.450593 -2.748289 5.679331
H -4.094811 -2.181710 3.348624
C 0.215007 -3.828174 3.501530
C -0.945035 -4.126162 2.791065
C -1.199817 -3.432089 1.611732
C -0.274518 -2.479760 1.191996
C 0.856136 -2.255878 1.978596
N 1.105824 -2.907427 3.118712
H -2.111675 -3.623000 1.046311
H 0.435341 -4.350686 4.434839
H -1.639390 -4.876732 3.164622
H -0.425044 -1.909672 0.276230
H 1.595538 -1.510055 1.679478
N -2.711391 -0.240288 4.534490
C -1.288626 -0.898223 6.854549
H -0.735192 -1.151850 7.759040
33
8 Relative E0+Ezero= 2.874922103515153 kJ/mol
C 1.995249 -4.952499 1.818152
C 1.522269 -3.651272 1.982218

C -0.580983 -4.378353 2.492762
C -0.211520 -5.714562 2.351000
H 3.036782 -5.117413 1.546045
H 2.193454 -2.802344 1.841365
H -1.605878 -4.115931 2.763130
H -0.944233 -6.505301 2.507713
C 4.830958 -2.283956 1.251973
C 4.174341 -1.078792 1.008874
C 3.384567 -0.969371 -0.133034
C 3.289676 -2.070478 -0.979229
C 3.985020 -3.231389 -0.643251
N 4.743938 -3.351054 0.450198
H 2.838539 -0.049280 -0.339033
H 5.452106 -2.402220 2.141981
H 4.265007 -0.251347 1.711159
H 2.682121 -2.038264 -1.882517
H 3.922945 -4.114244 -1.282888
C 1.121461 -0.024098 2.303177
C 1.556183 -0.477220 3.548279
C 2.489532 0.285070 4.243812
C 2.944697 1.469177 3.666693
C 2.441430 1.835428 2.418854
N 1.547978 1.110496 1.738096
H 2.857219 -0.036369 5.218583
H 0.401874 -0.617964 1.737289
H 1.162965 -1.412916 3.941384
H 3.674277 2.101894 4.170744
H 2.774527 2.759368 1.941038
N 0.261938 -3.355854 2.316447
C 1.106878 -6.006881 2.008357
H 1.435546 -7.039972 1.892204
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9 Relative E0+Ezero= 2.924806596511207 kJ/mol
N 0.475994 -2.696857 -1.209687
C 0.699649 -3.504730 -0.168464
C -0.533946 -1.826775 -1.106016

C -0.056020 -3.481871 1.003133
C -1.353548 -1.728594 0.017789
C -1.107359 -2.572553 1.095907
H 1.528634 -4.207725 -0.274006
H -0.693619 -1.160735 -1.955714
H 0.179900 -4.162486 1.820078
H -2.156967 -0.994760 0.043961
H -1.719866 -2.519693 1.996146
N -1.764930 1.490477 -1.460679
C -0.896270 1.658697 -0.458929
C -3.059617 1.400191 -1.139825
C -1.267720 1.738455 0.883398
C -3.538292 1.475791 0.167842
C -2.619354 1.649166 1.201381
H 0.155752 1.725146 -0.740755
H -3.753092 1.260303 -1.971677
H -0.502517 1.845303 1.650308
H -4.606553 1.396284 0.365029
H -2.952486 1.707807 2.237812
N 1.978676 1.003974 1.462579
C 1.965331 -0.060784 0.654069
C 2.521644 2.128555 0.985236
C 2.487005 -0.056170 -0.639691
C 3.065705 2.241777 -0.293103
C 3.049610 1.121813 -1.121992
H 1.504968 -0.965237 1.056052
H 2.520169 2.986936 1.660528
H 2.428510 -0.955870 -1.250155
H 3.490342 3.187633 -0.626816
H 3.462992 1.169815 -2.129407
33
10 Relative E0+Ezero= 3.1873565605437864 kJ/mol
C -0.674429 -2.443838 0.358321
C -1.196930 -1.749130 1.447751
C -1.135665 0.236771 0.326200
C -0.611657 -0.362670 -0.818456

H -0.492544 -3.515072 0.424564
H -1.437551 -2.276973 2.372674
H -1.324027 1.312183 0.345669
H -0.391410 0.239753 -1.698656
C 4.097871 0.772935 2.557910
C 3.533327 1.780234 3.337726
C 2.147893 1.810963 3.480944
C 1.388173 0.839618 2.835347
C 2.052468 -0.122393 2.075312
N 3.381242 -0.167532 1.934831
H 1.668848 2.580482 4.086828
H 5.180704 0.719510 2.427213
H 4.170205 2.520197 3.821023
H 0.301992 0.813824 2.909778
H 1.486173 -0.897820 1.554294
C 1.554870 -5.237968 -0.562547
C 1.810002 -5.337448 0.804942
C 2.525138 -4.314046 1.423302
C 2.959639 -3.240910 0.650484
C 2.650583 -3.242365 -0.708967
N 1.959306 -4.211718 -1.317516
H 2.739074 -4.351942 2.491603
H 0.993622 -6.021577 -1.076222
H 1.452162 -6.199106 1.367478
H 3.507943 -2.403500 1.083585
H 2.969327 -2.410445 -1.340135
N -1.428892 -0.432025 1.445206
C -0.378178 -1.734908 -0.803089
H 0.038452 -2.247450 -1.669595
33
11 Relative E0+Ezero= 3.218862556120241 kJ/mol
C -0.424890 -0.177873 -0.715476
C -1.486653 -0.802592 -1.365086
C -1.403414 0.661752 -3.111470
C -0.332067 1.355717 -2.547661
H -0.077031 -0.549054 0.246670

H -1.970774 -1.670912 -0.912973
H -1.818169 0.975265 -4.071767
H 0.096297 2.213483 -3.064776
C 1.282820 0.300552 2.494250
C 0.399863 -0.632468 3.037046
C -0.954071 -0.308119 3.098477
C -1.363643 0.931411 2.617481
C -0.398125 1.791657 2.096352
N 0.902853 1.494374 2.027119
H -1.677028 -1.009967 3.514473
H 2.349588 0.076949 2.430239
H 0.771359 -1.588963 3.402411
H -2.409302 1.232389 2.638720
H -0.690895 2.768786 1.709082
C -3.410058 3.100308 0.635758
C -3.363277 2.019855 -0.243377
C -4.174916 0.919142 0.014444
C -4.989507 0.945452 1.143731
C -4.954040 2.072932 1.964560
N -4.182991 3.138427 1.726008
H -4.168330 0.061946 -0.658044
H -2.792902 3.983184 0.455785
H -2.702428 2.040460 -1.107970
H -5.644148 0.109973 1.389093
H -5.578517 2.123789 2.858949
N -1.983507 -0.397280 -2.538059
C 0.164610 0.929691 -1.317969
H 0.985463 1.451171 -0.825979
33
12 Relative E0+Ezero= 3.4814125198543358 kJ/mol
C -2.315266 0.620252 0.362099
C -2.447348 1.988293 0.134460
C -0.593818 2.039020 -1.198764
C -0.370334 0.673524 -1.028427
H -3.035919 0.095518 0.987944
H -3.270177 2.544214 0.589525

H 0.069279 2.632835 -1.831285
H 0.472171 0.193786 -1.523825
C -3.406001 0.151163 -2.932405
C -2.946396 1.304136 -3.565545
C -1.864405 1.199485 -4.434076
C -1.288289 -0.053164 -4.625109
C -1.823556 -1.143796 -3.940483
N -2.864836 -1.057987 -3.108152
H -1.474854 2.078397 -4.946536
H -4.250415 0.203649 -2.242746
H -3.418481 2.264648 -3.368882
H -0.437009 -0.188737 -5.291270
H -1.393047 -2.139496 -4.068843
C 0.203661 4.351412 -5.123365
C -0.761385 4.630551 -6.090382
C -2.061942 4.900705 -5.669766
C -2.335428 4.881255 -4.305227
C -1.299981 4.586081 -3.417633
N -0.048899 4.322110 -3.811471
H -2.846855 5.121920 -6.393208
H 1.232885 4.137222 -5.418909
H -0.494801 4.634647 -7.146211
H -3.335857 5.088008 -3.927125
H -1.488854 4.537370 -2.343270
N -1.612007 2.695743 -0.632134
C -1.253274 -0.052739 -0.236528
H -1.126465 -1.125906 -0.098481
33
13 Relative E0+Ezero= 3.7649664806394005 kJ/mol
C 2.156716 -1.654123 -3.651464
C 2.434865 -2.897930 -3.086853
C 4.220508 -2.074903 -1.927244
C 4.027943 -0.789933 -2.434945
H 1.316369 -1.537699 -4.334450
H 1.813625 -3.762843 -3.328540
H 5.039966 -2.260584 -1.231983

H 4.689631 0.014381 -2.119661
C 0.211866 -0.353563 2.067527
C 0.514487 -1.232219 1.027824
C 1.295493 -0.769702 -0.027484
C 1.734980 0.550004 0.004699
C 1.373799 1.346455 1.089124
N 0.627401 0.915498 2.110640
H 1.562122 -1.425381 -0.855709
H -0.398162 -0.687339 2.910008
H 0.145129 -2.256822 1.050342
H 2.359117 0.952510 -0.790374
H 1.707611 2.384477 1.143224
C 4.353495 -1.146287 1.478131
C 3.738353 -0.786668 2.675455
C 3.914226 0.508767 3.149486
C 4.707618 1.382984 2.410724
C 5.285525 0.920417 1.230299
N 5.118147 -0.319173 0.759773
H 3.429453 0.835685 4.068541
H 4.215817 -2.151084 1.073321
H 3.116608 -1.504065 3.207961
H 4.874851 2.408332 2.737762
H 5.917107 1.580586 0.631658
N 3.445631 -3.118028 -2.238909
C 2.974546 -0.575709 -3.317750
H 2.786360 0.413835 -3.734745
33
14 Relative E0+Ezero= 3.8988669624363035 kJ/mol
C -3.107561 -2.981350 -1.288120
C -4.103073 -2.058447 -0.968466
C -2.932767 -0.337952 -1.899868
C -1.880575 -1.176116 -2.261879
H -3.227410 -4.031318 -1.023831
H -5.008227 -2.383100 -0.450161
H -2.888702 0.728530 -2.128920
H -1.006008 -0.773489 -2.768509

C 1.536950 -4.235418 -1.622474
C 1.780103 -2.883650 -1.386546
C 1.629866 -1.988210 -2.441443
C 1.248898 -2.484494 -3.684737
C 1.023154 -3.855579 -3.813410
N 1.158272 -4.725570 -2.808430
H 1.794274 -0.923888 -2.279417
H 1.648336 -4.964872 -0.817483
H 2.070893 -2.528160 -0.399600
H 1.117223 -1.826275 -4.542777
H 0.713610 -4.274593 -4.772956
C -0.373125 -1.176518 0.815220
C -1.620993 -0.821813 1.322114
C -2.015103 0.509573 1.242843
C -1.138032 1.427554 0.671285
C 0.092800 0.970241 0.204334
N 0.480576 -0.306957 0.267649
H -2.994089 0.822388 1.603745
H -0.048650 -2.218675 0.843445
H -2.275533 -1.581056 1.746158
H -1.400463 2.480787 0.581950
H 0.804724 1.667332 -0.243089
N -4.030284 -0.757313 -1.262797
C -1.969302 -2.529302 -1.949800
H -1.166509 -3.216567 -2.215196
33
15 Relative E0+Ezero= 4.161416926170398 kJ/mol
C -3.188872 3.059185 -1.909837
C -2.602878 3.105380 -3.172973
C -2.246191 0.853638 -3.189302
C -2.817592 0.698021 -1.926563
H -3.537802 3.972275 -1.432136
H -2.498520 4.058234 -3.695346
H -1.857741 -0.013672 -3.727960
H -2.880698 -0.289171 -1.470360
C -2.885075 2.578165 2.357128

C -2.944335 3.839261 1.764489
C -4.184859 4.306869 1.338733
C -5.302970 3.496614 1.518487
C -5.130342 2.249498 2.119577
N -3.947653 1.786603 2.535309
H -4.274914 5.286715 0.869148
H -1.929694 2.180397 2.706515
H -2.038748 4.425216 1.612067
H -6.294076 3.818040 1.200965
H -5.986445 1.589751 2.274577
C 0.018816 5.211973 -1.354871
C 0.608018 4.654837 -2.488354
C 0.796793 3.276070 -2.529978
C 0.388913 2.517800 -1.437632
C -0.200849 3.172284 -0.359186
N -0.384666 4.494530 -0.302556
H 1.238890 2.800769 -3.404748
H -0.136051 6.291071 -1.289563
H 0.905599 5.292012 -3.319980
H 0.500063 1.435074 -1.426608
H -0.554966 2.600031 0.500241
N -2.135310 2.029596 -3.813371
C -3.301464 1.827321 -1.272221
H -3.753065 1.749785 -0.283484
33
16 Relative E0+Ezero= 4.337325401770757 kJ/mol
C 0.795443 2.810846 -2.693741
C 1.915919 2.060485 -2.346515
C 2.405768 3.429452 -0.589645
C 1.300907 4.239917 -0.844129
H 0.175211 2.511154 -3.536614
H 2.174588 1.167091 -2.917948
H 3.073616 3.655938 0.244232
H 1.091659 5.096738 -0.205271
C -2.065524 0.913970 -1.639645
C -1.290192 -0.205107 -1.942388

C -0.190021 -0.489598 -1.138213
C 0.084119 0.359646 -0.070279
C -0.755131 1.450271 0.147150
N -1.814728 1.734847 -0.615996
H 0.442094 -1.353876 -1.340025
H -2.935950 1.162345 -2.251170
H -1.549994 -0.838886 -2.789504
H 0.940783 0.187266 0.577771
H -0.562171 2.134808 0.975325
C 2.591064 -2.751981 -0.125496
C 3.177629 -1.487788 -0.091622
C 3.516112 -0.873968 -1.295073
C 3.260173 -1.563211 -2.478084
C 2.669924 -2.824755 -2.404111
N 2.331661 -3.418286 -1.255540
H 3.940766 0.129703 -1.305257
H 2.310725 -3.255312 0.802041
H 3.358855 -0.991926 0.861332
H 3.511129 -1.133932 -3.447589
H 2.454603 -3.387338 -3.315150
N 2.718194 2.354754 -1.319264
C 0.477256 3.922549 -1.920765
H -0.405699 4.521002 -2.141548
33
17 Relative E0+Ezero= 4.4607238847436905 kJ/mol
C 3.426795 1.200602 0.499316
C 2.063884 1.080500 0.771706
C 2.350444 1.685611 2.951964
C 3.725406 1.839479 2.786572
H 3.798633 0.986245 -0.500759
H 1.373238 0.778566 -0.017255
H 1.889938 1.867809 3.925766
H 4.347239 2.145386 3.627229
C 2.110311 1.376169 -2.820115
C 0.810515 1.879965 -2.780564
C -0.235862 0.994550 -2.543469

C 0.063092 -0.353569 -2.353432
C 1.397048 -0.753401 -2.413059
N 2.412086 0.086706 -2.642581
H -1.266790 1.346215 -2.498344
H 2.946759 2.054935 -2.989687
H 0.647484 2.947103 -2.920368
H -0.720003 -1.084389 -2.156749
H 1.664079 -1.801472 -2.264152
C 1.691219 4.238805 -0.332953
C 2.059997 4.558969 0.971978
C 3.350006 5.025612 1.199054
C 4.211094 5.155918 0.112356
C 3.738927 4.816931 -1.154101
N 2.502367 4.366845 -1.386181
H 3.681939 5.274405 2.206839
H 0.691567 3.850304 -0.536962
H 1.354419 4.415954 1.788017
H 5.231981 5.514371 0.238132
H 4.387149 4.913956 -2.027679
N 1.522171 1.315351 1.970586
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H 5.345456 1.701823 1.359701
33
18 Relative E0+Ezero= 4.4843533817245165 kJ/mol
C -2.829727 2.067095 1.569801
C -2.052815 2.012758 2.725743
C -1.987660 4.285233 2.901781
C -2.762200 4.451592 1.754698
H -3.143983 1.153857 1.066121
H -1.753486 1.048089 3.141721
H -1.631742 5.156482 3.455951
H -3.011699 5.451448 1.402285
C -3.048808 1.443669 -1.980946
C -3.019454 2.698763 -2.586638
C -4.204731 3.426302 -2.649554
C -5.358600 2.871765 -2.101207

C -5.274032 1.613100 -1.505330
N -4.144960 0.901544 -1.441198
H -4.225064 4.413991 -3.109971
H -2.139505 0.842126 -1.919231
H -2.085056 3.107727 -2.966429
H -6.309062 3.403156 -2.124264
H -6.156796 1.156021 -1.053978
C -0.156160 3.364867 -0.487892
C 0.553533 3.450391 0.707414
C 0.930096 4.708764 1.165065
C 0.583844 5.822814 0.405083
C -0.123214 5.625991 -0.779926
N -0.491665 4.423484 -1.230566
H 1.474500 4.818433 2.102599
H -0.479238 2.391516 -0.861274
H 0.781097 2.550957 1.276325
H 0.852958 6.830201 0.720193
H -0.405495 6.479421 -1.400178
N -1.630109 3.093969 3.389388
C -3.190417 3.316965 1.073078
H -3.787577 3.402280 0.166422
33
19 Relative E0+Ezero= 4.74427784582724 kJ/mol
C 2.761415 -0.383397 -3.044753
C 3.279890 0.301147 -4.142280
C 4.369457 1.797417 -2.811526
C 3.906353 1.185215 -1.647998
H 2.114583 -1.247104 -3.189907
H 3.045885 -0.029112 -5.156563
H 5.012259 2.677900 -2.748537
H 4.175756 1.587357 -0.672688
C 1.158272 3.269396 -0.379075
C 1.879865 4.279535 -1.012621
C 1.936445 4.280480 -2.403950
C 1.269406 3.275154 -3.096668
C 0.573673 2.311511 -2.368805

N 0.513739 2.298678 -1.032141
H 2.495390 5.048283 -2.938895
H 1.094800 3.240739 0.711051
H 2.382859 5.046171 -0.424345
H 1.294057 3.225269 -4.183647
H 0.043611 1.507341 -2.882802
C -0.652409 -1.960536 -3.592202
C -0.087551 -3.148085 -3.128746
C 0.339475 -3.205342 -1.803748
C 0.181963 -2.075603 -1.006133
C -0.390228 -0.933134 -1.567003
N -0.803187 -0.868309 -2.837649
H 0.786719 -4.114673 -1.402034
H -0.999909 -1.883460 -4.624527
H 0.014607 -4.003841 -3.794559
H 0.499592 -2.071488 0.035904
H -0.500181 -0.020799 -0.976917
N 4.070138 1.374655 -4.042697
C 3.080415 0.072714 -1.769127
H 2.677114 -0.423377 -0.887475
33
20 Relative E0+Ezero= 4.802038837717407 kJ/mol
C -2.348580 -0.407455 -0.097570
C -3.734153 -0.523253 0.003992
C -3.600365 -2.686911 0.710701
C -2.207907 -2.680660 0.643747
H -1.890925 0.520909 -0.440105
H -4.375118 0.324923 -0.245975
H -4.130708 -3.587256 1.028378
H -1.642972 -3.574675 0.903996
C -0.425724 0.334554 -2.947677
C -0.309121 0.163574 -4.326134
C -0.373569 1.290496 -5.140318
C -0.551700 2.535377 -4.540322
C -0.660401 2.595686 -3.152047
N -0.601771 1.521599 -2.358504

H -0.289995 1.202504 -6.223921
H -0.386709 -0.540100 -2.297201
H -0.182432 -0.839409 -4.730497
H -0.609414 3.447519 -5.133199
H -0.804394 3.556459 -2.653122
C -1.183682 -4.147055 -2.728674
C -2.226289 -4.998848 -2.368106
C -3.520498 -4.486926 -2.335213
C -3.714539 -3.147891 -2.660304
C -2.603666 -2.382475 -3.007463
N -1.356503 -2.861363 -3.047336
H -4.362574 -5.117998 -2.051343
H -0.157111 -4.517807 -2.764401
H -2.022238 -6.039634 -2.119590
H -4.703721 -2.695191 -2.628979
H -2.721392 -1.327406 -3.261236
N -4.362785 -1.635473 0.399007
C -1.570397 -1.515752 0.228590
H -0.483970 -1.470665 0.154015
33
21 Relative E0+Ezero= 4.80728983698015 kJ/mol
C -0.173649 3.453845 5.195141
C -0.623576 4.474731 4.357753
C 1.477469 4.842731 3.539212
C 2.024634 3.833199 4.329918
H -0.876383 2.927950 5.839870
H -1.682838 4.732757 4.326177
H 2.114580 5.420750 2.866551
H 3.089737 3.611627 4.277640
C -3.756395 2.632634 1.957995
C -3.632747 2.111893 0.670667
C -2.877148 2.818394 -0.258937
C -2.276775 4.009935 0.139610
C -2.456554 4.440157 1.452653
N -3.185033 3.772986 2.354172
H -2.748402 2.441458 -1.273517

H -4.339140 2.097714 2.710042
H -4.108255 1.166218 0.416448
H -1.669614 4.596766 -0.548366
H -1.976878 5.356397 1.801564
C -1.225995 -0.658027 1.068156
C -0.394861 0.062716 0.211631
C 0.133752 1.270039 0.660880
C -0.191466 1.703020 1.941973
C -1.034288 0.906826 2.715193
N -1.547666 -0.255375 2.300454
H 0.782206 1.867299 0.019776
H -1.654271 -1.610091 0.746753
H -0.170603 -0.319742 -0.783517
H 0.184848 2.644706 2.335591
H -1.313568 1.227717 3.719681
N 0.179915 5.164063 3.540196
C 1.178052 3.122952 5.177893
H 1.565175 2.323155 5.809031
33
22 Relative E0+Ezero= 4.846672331749203 kJ/mol
C -1.092848 -4.300946 3.006316
C -2.462568 -4.040664 2.942475
C -2.414105 -2.833161 4.877763
C -1.042972 -3.029177 5.030768
H -0.614026 -4.899100 2.231795
H -3.058641 -4.431836 2.115168
H -2.973846 -2.248979 5.611347
H -0.505407 -2.592322 5.870493
C -0.216523 1.514342 1.384592
C -0.808423 0.251794 1.361917
C -1.127014 -0.355881 2.573258
C -0.838599 0.328160 3.750265
C -0.248675 1.587093 3.662780
N 0.063907 2.181837 2.507340
H -1.589587 -1.341957 2.601042
H 0.043037 2.017401 0.450304

H -1.016430 -0.238417 0.411553
H -1.058410 -0.109396 4.721733
H -0.009774 2.145341 4.569979
C 2.494552 -0.650019 5.419125
C 2.989267 0.563175 4.943998
C 3.030527 0.771470 3.567971
C 2.576258 -0.242108 2.730948
C 2.090899 -1.412605 3.308539
N 2.049139 -1.628941 4.626216
H 3.392492 1.712529 3.155788
H 2.455278 -0.845547 6.492896
H 3.328987 1.326666 5.642401
H 2.569979 -0.121862 1.649222
H 1.706128 -2.214737 2.675275
N -3.123010 -3.320696 3.853541
C -0.366681 -3.780113 4.073599
H 0.707242 -3.935592 4.167827

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (1, 1)

****

15

1 Relative E0+Ezero= 0.0 kJ/mol

C -2.913129 -0.886338 1.018455

C -2.099278 -0.667134 -0.091467

C -1.826775 1.543067 0.430208

C -2.628325 1.426880 1.565065

C -3.183050 0.185811 1.865208

H -3.322993 -1.877397 1.209254

H -1.867894 -1.486187 -0.775508

H -1.370928 2.496938 0.156024

H -2.810360 2.295268 2.196896

H -3.815039 0.056161 2.744091

N -1.561746 0.519312 -0.389083

N 0.151409 2.569193 -2.061750

H -0.160850 2.785003 -3.004623

H 1.154304 2.412866 -2.115041

H -0.278498 1.680500 -1.798035

15

2 Relative E0+Ezero= 4.977947313616251 kJ/mol

C -1.010798 -0.234299 0.689446

C -1.938876 -0.926515 1.466615

C -3.628483 0.477327 0.858584

C -2.780951 1.236440 0.052425

C -1.438347 0.874957 -0.037218

H 0.027933 -0.562370 0.657328

H -1.629373 -1.799588 2.045977

H -4.685490 0.739593 0.946176

H -3.170621 2.095191 -0.493755

H -0.742109 1.444054 -0.658142

N -3.228303 -0.588006 1.559063

N 0.803021 2.670890 -2.103478

H 0.572325 3.655012 -2.211737

H 1.768266 2.632511 -1.786797

H 0.786677 2.264470 -3.035204

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (1, 2)

****

19

1 Relative E0+Ezero= 0.0 kJ/mol

C 3.168650 -3.528383 1.666484

C 2.719786 -3.335325 0.362169

C 1.691327 -1.360607 0.905111

C 2.095277 -1.465887 2.236621

C 2.847776 -2.569776 2.625180

H 3.755305 -4.410479 1.919861

H 2.953197 -4.066969 -0.414413

H 1.098657 -0.504863 0.567669

H 1.818636 -0.689220 2.948390

H 3.180094 -2.683713 3.657605

N 1.996635 -2.278759 -0.021050

N 0.656753 -1.141192 -2.613661

H -0.035760 -1.776834 -2.999454

H 1.333100 -0.967026 -3.351680

H 1.146751 -1.644855 -1.867383

N -0.162031 1.124156 -0.586858

H 0.013382 0.486310 -1.370813

H 0.198462 2.035304 -0.856784

H -1.169929 1.225862 -0.504347

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (1, 3)

****

23

1 Relative E0+Ezero= 0.0 kJ/mol

C 1.873063 -4.763301 -0.711963

C 2.983945 -3.923872 -0.674717

C 1.675408 -2.064468 -0.431360

C 0.501018 -2.814780 -0.457319

C 0.604974 -4.195084 -0.601056

H 2.005755 -5.838797 -0.824215

H 3.990970 -4.337726 -0.758313

H 1.623784 -0.980800 -0.314540

H -0.451347 -2.293803 -0.362918

H -0.287750 -4.820954 -0.625993

N 2.898733 -2.596615 -0.537475

N 4.332960 0.144439 -0.411288

H 4.098580 -0.852343 -0.461784

H 5.250302 0.216396 0.019663

H 4.438560 0.467996 -1.368995

N 1.787830 1.198201 1.104967

H 1.823648 0.743192 2.013766

H 1.810025 2.197767 1.287147

H 2.665219 0.960261 0.626622

N -0.961462 0.205987 -0.168400

H -1.049287 0.609246 -1.097657

H -0.101196 0.589552 0.238808

H -1.737412 0.574388 0.375130

23

2 Relative E0+Ezero= 2.628125137569286 kJ/mol

C 1.602933 3.143796 1.350403

C 0.817616 2.526829 2.322738

C 2.649407 1.837967 3.498477

C 3.524002 2.422142 2.583250

C 2.986727 3.092586 1.485798

H 1.132019 3.631479 0.498935

H -0.269616 2.532523 2.238835
H 3.038113 1.303965 4.367950
H 4.600852 2.349157 2.730605
H 3.637279 3.557453 0.744753
N 1.319017 1.885301 3.381812
N -0.789573 -0.337619 2.454219
H -0.417982 0.144132 3.271191
H 0.028397 -0.662981 1.931959
H -1.289179 -1.156763 2.786781
N -1.094140 1.281809 -0.203255
H -1.589710 2.168688 -0.167996
H -1.229557 0.818985 0.703369
H -1.578846 0.715572 -0.894668
N 1.633710 -0.258637 0.439595
H 0.972951 0.402870 0.025132
H 2.084286 -0.758026 -0.321561
H 2.355358 0.293944 0.896079
23
3 Relative E0+Ezero= 2.8040336133188872 kJ/mol
C 1.419570 1.471599 1.837748
C 0.556799 2.274064 1.093901
C -0.853058 0.524456 0.668235
C -0.057726 -0.359680 1.396224
C 1.103059 0.123582 1.992460
H 2.317764 1.897563 2.282960
H 0.774604 3.334549 0.952060
H -1.755953 0.170567 0.166759
H -0.344595 -1.406662 1.483288
H 1.752592 -0.537407 2.566827
N -0.559435 1.820126 0.516074
N -2.077276 1.909692 -2.244655
H -1.773939 2.271883 -1.339563
H -2.551864 1.026000 -2.056341
H -2.765762 2.554713 -2.619717
N -2.288258 -1.314161 -1.849205
H -2.698448 -1.572207 -2.742983

H -2.290684 -2.159452 -1.284482
H -1.307786 -1.073802 -2.034048
N 0.445377 0.109764 -2.400768
H -0.207425 0.883835 -2.559907
H 1.053164 0.051412 -3.212544
H 1.030234 0.376729 -1.613195
23
4 Relative E0+Ezero= 3.6021855033451406 kJ/mol
C -2.761516 -1.459245 0.733795
C -2.229980 -0.413044 -0.019237
C -2.780415 1.128256 1.576858
C -3.335899 0.154611 2.405237
C -3.326155 -1.169217 1.972751
H -2.728213 -2.477240 0.347833
H -1.784350 -0.609486 -0.996461
H -2.774491 2.175874 1.884479
H -3.765137 0.432626 3.367045
H -3.751026 -1.959570 2.592126
N -2.236031 0.861579 0.386481
N -1.385814 1.752126 -2.545256
H -1.137842 2.672700 -2.894116
H -1.525286 1.834215 -1.536889
H -2.299155 1.507658 -2.933030
N -3.790414 -0.238566 -3.110360
H -4.228720 -0.311275 -2.195803
H -2.952449 -0.824460 -3.087138
H -4.434025 -0.653431 -3.778035
N -0.726461 -1.191310 -3.144832
H -0.669683 -0.172289 -3.022073
H -0.552225 -1.381377 -4.127983
H 0.051675 -1.601239 -2.634958
23
5 Relative E0+Ezero= 4.912309822682727 kJ/mol
C -0.471622 4.533027 -0.330739
C -1.808302 4.319414 0.005196
C -1.549400 2.053786 -0.034950

C -0.200302 2.155586 -0.372300
C 0.350561 3.425806 -0.524153
H -0.089563 5.547890 -0.437108
H -2.479125 5.166959 0.162584
H -2.013416 1.072822 0.089494
H 0.406231 1.260604 -0.506084
H 1.403266 3.535812 -0.785479
N -2.350383 3.107121 0.153361
N 2.603817 1.808932 1.568728
H 2.839042 2.031427 0.598507
H 3.389253 2.089639 2.148298
H 1.818392 2.401211 1.825095
N 1.760071 -0.823758 0.147582
H 2.004495 -0.142996 0.874706
H 2.395646 -1.610288 0.246845
H 0.832398 -1.178608 0.363931
N 2.979218 1.513506 -1.596081
H 2.551557 0.636886 -1.281754
H 3.925955 1.291308 -1.891051
H 2.479430 1.803550 -2.432784

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (2, 1)

****

26

1 Relative E0+Ezero= 0.0 kJ/mol

C 1.125100 0.658837 0.474374

C 2.166056 0.085284 -0.250576

C 3.269025 0.879540 -0.553964

C 3.274898 2.207598 -0.128596

C 1.229159 1.995052 0.854284

H 0.235546 0.082833 0.724927

H 2.085906 -0.947216 -0.592957

H 4.112975 0.483373 -1.118192

H 4.125977 2.854020 -0.355735

H 0.423885 2.471728 1.417378

N 2.278380 2.770195 0.561355

C 0.295050 1.127013 -2.801040

C -1.713954 1.349642 -1.739322

C -1.493924 2.702894 -1.492503

C -0.302893 3.274163 -1.933964

C 0.609252 2.470076 -2.608985

H 0.999494 0.463984 -3.306543

H -2.635923 0.870139 -1.404292

H -2.239674 3.290376 -0.958821

H -0.083693 4.324157 -1.743625

H 1.560958 2.865523 -2.958889

N -0.841592 0.565122 -2.379056

N 0.233605 -2.346446 -1.613289

H -0.293279 -1.524463 -1.918714

H 0.296803 -2.969982 -2.413739

H -0.341508 -2.826554 -0.925918

26

2 Relative E0+Ezero= 0.2809284611536933 kJ/mol

C -0.030732 -1.167456 1.532025

C -0.026560 -2.434757 0.955247

C 0.153485 -2.539286 -0.420314

C 0.315522 -1.369652 -1.158551
C 0.141173 -0.060376 0.704007
H -0.169473 -1.033538 2.604023
H -0.174724 -3.325645 1.564841
H 0.146081 -3.506190 -0.919344
H 0.440269 -1.415108 -2.241594
H 0.139434 0.947569 1.124270
N 0.311297 -0.147357 -0.618179
C -2.997562 -3.326431 -2.094875
C -3.305464 -2.268262 -0.099831
C -3.121578 -1.012454 -0.674813
C -2.857162 -0.932380 -2.039374
C -2.799125 -2.120279 -2.765113
H -2.955829 -4.272838 -2.639030
H -3.508157 -2.359310 0.969597
H -3.166693 -0.115511 -0.058676
H -2.664343 0.031835 -2.512981
H -2.596502 -2.115986 -3.835734
N -3.243825 -3.414854 -0.784061
N -1.068686 1.902446 -2.646047
H -0.490575 1.373604 -1.987659
H -0.477141 2.133150 -3.439942
H -1.298794 2.784799 -2.196708
26
3 Relative E0+Ezero= 0.4778409341035066 kJ/mol
C -3.195430 -3.244167 -1.016143
C -1.926254 -3.556180 -1.496228
C -1.376728 -2.758379 -2.495105
C -2.123818 -1.682694 -2.968726
C -3.858177 -2.144231 -1.556833
H -3.666922 -3.836950 -0.233478
H -1.371346 -4.403252 -1.093084
H -0.379557 -2.947470 -2.888069
H -1.717287 -1.027912 -3.741210
H -4.853657 -1.870663 -1.201132
N -3.342693 -1.372082 -2.517208

C 0.446627 -1.240340 0.072919
C 0.734205 0.180351 -1.687723
C -0.497512 0.793727 -1.469500
C -1.280773 0.344097 -0.409834
C -0.797484 -0.690949 0.383404
H 0.850350 -2.060965 0.670310
H 1.373891 0.508189 -2.510232
H -0.865515 1.583817 -2.122072
H -2.258249 0.789197 -0.227755
H -1.374195 -1.081731 1.220865
N 1.208739 -0.823910 -0.941581
N -3.419087 1.806147 -2.863100
H -4.177751 2.255439 -2.356754
H -3.536400 2.070086 -3.837791
H -3.582093 0.797395 -2.808332
26
4 Relative E0+Ezero= 0.9162993737364444 kJ/mol
C -3.010234 1.278206 1.359074
C -1.833321 0.652027 0.960239
C -1.102712 1.206621 -0.087176
C -1.591263 2.366883 -0.686991
C -3.410425 2.432256 0.686544
H -3.618981 0.879482 2.169881
H -1.494129 -0.263151 1.445384
H -0.197254 0.724629 -0.457694
H -1.044277 2.827742 -1.512432
H -4.333029 2.943226 0.971493
N -2.723325 2.977488 -0.321133
C -2.932036 -0.605882 -2.093464
C -3.339546 -2.316639 -0.636974
C -4.577181 -1.787223 -0.277857
C -4.988657 -0.598086 -0.874264
C -4.148879 0.006984 -1.803620
H -2.243590 -0.149883 -2.806910
H -2.985478 -3.246518 -0.187317
H -5.198662 -2.298024 0.456384

H -5.945349 -0.146100 -0.613004
H -4.414056 0.948963 -2.280092
N -2.524520 -1.746247 -1.528727
N 0.644830 -1.362259 -1.534127
H 1.020681 -1.440881 -2.475523
H 1.161854 -2.027668 -0.965522
H -0.323050 -1.691931 -1.571974
26
5 Relative E0+Ezero= 1.1000843482309166 kJ/mol
C 3.713107 -1.738875 0.988837
C 2.605307 -2.553385 1.207620
C 2.785751 -3.932424 1.238082
C 4.069732 -4.438872 1.038155
C 4.952779 -2.348877 0.805006
H 3.596585 -0.657146 0.925994
H 1.616620 -2.113170 1.335924
H 1.949114 -4.610557 1.402886
H 4.244049 -5.517310 1.051232
H 5.842936 -1.741359 0.627071
N 5.142517 -3.672990 0.822082
C 0.680715 -2.725733 -1.941181
C 2.843155 -2.024216 -2.156001
C 3.311671 -3.327803 -2.302743
C 2.391028 -4.369586 -2.261105
C 1.044723 -4.063305 -2.078892
H -0.365665 -2.450476 -1.794389
H 3.540783 -1.185089 -2.166406
H 4.377098 -3.517148 -2.419923
H 2.718722 -5.404179 -2.360915
H 0.286168 -4.843776 -2.038661
N 1.555217 -1.716050 -1.978394
N 1.868644 0.887791 -0.154287
H 1.042261 1.137107 0.382786
H 2.109468 1.710288 -0.701029
H 1.584969 0.163025 -0.818123
26

6 Relative E0+Ezero= 1.8746067415748289 kJ/mol
C 1.215569 -2.482691 -4.417628
C 0.161747 -3.309646 -4.044319
C -0.936937 -2.739798 -3.406634
C -0.928323 -1.368239 -3.166300
C 1.128772 -1.123206 -4.125698
H 2.104792 -2.882631 -4.901897
H 0.203073 -4.382436 -4.228237
H -1.781691 -3.347356 -3.085627
H -1.772277 -0.890783 -2.664151
H 1.947646 -0.450304 -4.386987
N 0.081437 -0.563657 -3.513699
C 2.955977 -4.401365 -1.752306
C 1.513493 -2.879377 -0.854884
C 2.388418 -1.818751 -1.086761
C 3.614305 -2.100854 -1.683806
C 3.906867 -3.418524 -2.025207
H 3.154181 -5.445113 -2.006981
H 0.543047 -2.695348 -0.389669
H 2.106627 -0.796297 -0.829705
H 4.328570 -1.301409 -1.883710
H 4.854007 -3.687981 -2.492034
N 1.777393 -4.150297 -1.175817
N 1.152761 1.409399 -1.247102
H 1.579181 2.273228 -1.571248
H 0.706691 0.973154 -2.057578
H 0.408152 1.680746 -0.610426
26
7 Relative E0+Ezero= 1.927116734202254 kJ/mol
C -4.508445 0.768897 -4.361469
C -3.292826 0.104754 -4.505664
C -2.323318 0.264245 -3.520137
C -2.622529 1.085127 -2.432286
C -4.703828 1.561807 -3.232058
H -5.297988 0.673616 -5.106375
H -3.106263 -0.534561 -5.368721

H -1.368815 -0.262459 -3.565404
H -1.884467 1.231424 -1.640557
H -5.646968 2.094303 -3.088944
N -3.784978 1.725680 -2.275232
C -3.889694 -3.472870 -3.422057
C -3.458571 -2.164415 -1.601232
C -4.753491 -1.650595 -1.591857
C -5.644847 -2.089109 -2.565250
C -5.205522 -3.022553 -3.500666
H -3.512068 -4.202599 -4.141297
H -2.730233 -1.830977 -0.860006
H -5.040597 -0.905240 -0.852463
H -6.664082 -1.704315 -2.599671
H -5.866462 -3.395518 -4.282042
N -3.023373 -3.059632 -2.492393
N 0.008856 -2.225653 -3.048170
H -0.877406 -2.697347 -2.851556
H 0.478429 -2.765897 -3.769899
H 0.581053 -2.309792 -2.212155
26
8 Relative E0+Ezero= 2.0032562238105047 kJ/mol
C -1.678251 0.355848 -0.344218
C -0.974480 0.667171 0.815921
C -0.314179 1.890850 0.890825
C -0.390863 2.754925 -0.200978
C -1.689604 1.294646 -1.375520
H -2.192073 -0.598518 -0.471030
H -0.937512 -0.036653 1.648206
H 0.249007 2.178551 1.778308
H 0.112444 3.724181 -0.171667
H -2.228131 1.080102 -2.300661
N -1.065374 2.475140 -1.319643
C 0.691186 -1.425130 -1.891345
C 0.071271 -0.464573 -3.867576
C 0.894656 0.637337 -3.653198
C 1.649952 0.684578 -2.484571

C 1.550785 -0.371829 -1.585829
H 0.572569 -2.258661 -1.196366
H -0.537791 -0.529464 -4.771354
H 0.927342 1.446983 -4.380057
H 2.292875 1.538337 -2.273208
H 2.112016 -0.376987 -0.652899
N -0.039535 -1.482662 -3.007751
N -2.773768 -2.577065 -1.802177
H -1.951078 -2.394331 -2.381578
H -2.793135 -3.577051 -1.620605
H -3.588921 -2.376313 -2.375544
26
9 Relative E0+Ezero= 2.368200673466563 kJ/mol
C -1.634291 2.022174 0.340457
C -2.008582 2.199879 -0.988697
C -2.142634 3.496305 -1.479323
C -1.899276 4.562394 -0.614131
C -1.415522 3.159810 1.117122
H -1.486128 1.029828 0.769552
H -2.189636 1.338793 -1.632795
H -2.434699 3.684838 -2.512204
H -2.000815 5.591126 -0.967628
H -1.114642 3.056671 2.161449
N -1.543389 4.410958 0.664649
C 1.644652 1.817927 -0.263428
C 2.073900 2.634669 1.825265
C 2.043034 3.952148 1.375943
C 1.798661 4.187377 0.025668
C 1.601289 3.096883 -0.814471
H 1.471906 0.941192 -0.890249
H 2.259636 2.414955 2.878635
H 2.191754 4.773905 2.074571
H 1.746223 5.204599 -0.360534
H 1.393101 3.229247 -1.874781
N 1.876957 1.578121 1.029975
N -0.185386 -0.674241 1.932133

H 0.076825 -1.637465 1.741039
H 0.635293 -0.096088 1.735460
H -0.352643 -0.617783 2.933343
26
10 Relative E0+Ezero= 3.6336914990708378 kJ/mol
C 1.755236 -3.151342 -0.138131
C 1.029417 -2.676758 -1.227618
C -0.359193 -2.753503 -1.186353
C -0.960317 -3.300995 -0.054863
C 1.057041 -3.683674 0.944274
H 2.843624 -3.111204 -0.122212
H 1.537633 -2.250775 -2.092767
H -0.972101 -2.385841 -2.007632
H -2.047494 -3.358907 0.020062
H 1.594449 -4.062879 1.815690
N -0.275309 -3.764011 0.994381
C -0.814591 -0.493503 1.731904
C -2.162569 0.235996 0.036666
C -1.098405 0.850395 -0.621795
C 0.168308 0.772679 -0.048839
C 0.312912 0.087449 1.153443
H -0.741619 -1.047025 2.669898
H -3.169167 0.281168 -0.384790
H -1.265822 1.378661 -1.559744
H 1.027060 1.240329 -0.531155
H 1.282535 -0.003746 1.640464
N -2.035899 -0.426461 1.189449
N -2.306833 -2.874320 3.340257
H -3.006756 -3.488724 3.744714
H -2.791720 -2.215648 2.732102
H -1.708412 -3.441250 2.738344
26
11 Relative E0+Ezero= 4.804664337348778 kJ/mol
C -3.604118 1.604061 -0.897297
C -3.555738 0.759126 0.206435
C -3.317758 1.316321 1.460115

C -3.135899 2.694184 1.551054
C -3.410722 2.970257 -0.697520
H -3.778028 1.216257 -1.899632
H -3.692210 -0.315806 0.090109
H -3.264910 0.697349 2.354800
H -2.939921 3.162368 2.517630
H -3.430817 3.659712 -1.543693
N -3.183449 3.516642 0.498958
C -0.109211 0.472323 0.164816
C -0.247210 2.017462 -1.512529
C -0.457830 1.029339 -2.474451
C -0.495736 -0.300462 -2.067175
C -0.319205 -0.587156 -0.715770
H 0.035117 0.281720 1.230269
H -0.221868 3.074565 -1.785160
H -0.591814 1.305335 -3.519617
H -0.657533 -1.101170 -2.789548
H -0.340088 -1.611923 -0.346646
N -0.070566 1.751992 -0.213982
N -0.365051 4.931156 -0.032182
H 0.088406 5.704236 0.445773
H -1.347289 4.937596 0.240847
H 0.016589 4.066676 0.351757
26
12 Relative E0+Ezero= 4.865050829168802 kJ/mol
C -3.137452 3.024376 -2.710484
C -4.098060 2.189246 -2.148898
C -4.471896 2.399558 -0.823046
C -3.863788 3.435773 -0.118328
C -2.593744 4.035304 -1.920220
H -2.793216 2.893449 -3.735000
H -4.546841 1.384113 -2.731155
H -5.219259 1.772185 -0.338974
H -4.129463 3.624878 0.923806
H -1.830501 4.699639 -2.327609
N -2.940546 4.244896 -0.647134

C 0.304661 2.268274 -2.419040
C 0.679711 4.135096 -3.673058
C 0.944665 4.907171 -2.542369
C 0.872136 4.304615 -1.288240
C 0.550435 2.951342 -1.229344
H 0.040257 1.208838 -2.400717
H 0.724522 4.583036 -4.668307
H 1.189790 5.963593 -2.645592
H 1.013667 4.886759 -0.378339
H 0.470218 2.434032 -0.274404
N 0.357967 2.838028 -3.627188
N -0.849436 6.084751 0.955856
H -1.059043 7.063557 0.776929
H -1.575981 5.537674 0.484953
H -0.976026 5.945536 1.954941

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (2, 2)

****

30

1 Relative E0+Ezero= 0.0 kJ/mol

C 2.497431 -4.699774 -0.236701

C 1.105346 -4.720110 -0.283747

C 0.410232 -3.738298 0.416635

C 1.132612 -2.777425 1.118588

C 3.127453 -3.695771 0.495553

H 3.091506 -5.443363 -0.766969

H 0.559827 -5.453226 -0.879345

H -0.677829 -3.704410 0.398429

H 0.615051 -1.983942 1.660875

H 4.217712 -3.649773 0.544307

N 2.468720 -2.743573 1.162876

C 1.051237 -2.330213 -2.662587

C -0.943777 -1.412076 -2.039789

C -0.313950 -0.407984 -1.307490

C 1.078127 -0.387483 -1.260304

C 1.773430 -1.369255 -1.960556

H 1.568949 -3.123658 -3.204786

H -2.034026 -1.458195 -2.088661

H -0.908167 0.335553 -0.777307

H 1.623482 0.345717 -0.664663

H 2.861492 -1.403037 -1.942217

N -0.284862 -2.364220 -2.707014

N -1.265556 -5.393141 -2.574513

H -2.232240 -5.434282 -2.262164

H -1.056440 -4.409039 -2.764664

H -1.235787 -5.878372 -3.467310

N 3.449011 0.285380 1.030632

H 3.420703 0.770799 1.923372

H 3.239689 -0.698595 1.221218

H 4.415285 0.325976 0.716945

30

2 Relative E0+Ezero= 1.4886582948678007 kJ/mol
C -2.621501 0.942145 2.830256
C -3.052905 1.995918 3.629717
C -2.425195 3.232712 3.497543
C -1.400020 3.356811 2.563153
C -1.579870 1.165226 1.928843
H -3.077196 -0.044658 2.899569
H -3.864479 1.858965 4.344987
H -2.724707 4.088260 4.101498
H -0.885625 4.311148 2.432464
H -1.190907 0.352455 1.309508
N -0.981244 2.352892 1.788764
C 1.839737 2.485371 3.959222
C 1.978574 0.494057 2.855900
C 0.993546 -0.081682 3.654006
C 0.415388 0.692414 4.655708
C 0.846622 2.006321 4.812079
H 2.195752 3.513552 4.052316
H 2.441759 -0.081128 2.053240
H 0.676373 -1.107000 3.472166
H -0.367992 0.284336 5.293629
H 0.416387 2.656115 5.572754
N 2.405598 1.752596 2.997165
N 1.512229 1.897301 -0.060982
H 1.570217 2.458595 -0.905366
H 0.696798 2.218889 0.469024
H 2.320202 2.128885 0.513142
N 0.350551 -1.013460 0.073233
H -0.078115 -1.243229 -0.819675
H 0.839974 -0.119492 -0.058472
H 1.063307 -1.721438 0.230635
30
3 Relative E0+Ezero= 1.4886582948678007 kJ/mol
C 1.195962 -2.374395 -2.191252
C -0.072163 -1.798598 -2.178967
C -0.437058 -1.019087 -1.086327

C 0.480869 -0.845233 -0.051966
C 2.037623 -2.147361 -1.103893
H 1.531003 -2.991260 -3.024320
H -0.760914 -1.952091 -3.010151
H -1.411772 -0.537827 -1.029136
H 0.227596 -0.217113 0.803761
H 3.035816 -2.589638 -1.078952
N 1.697858 -1.400564 -0.049681
C 2.243212 1.636596 -1.737090
C 0.587178 2.579390 -0.474802
C -0.310699 2.554586 -1.541069
C 0.117328 2.036618 -2.759250
C 1.421980 1.559868 -2.859446
H 3.269474 1.267089 -1.777331
H 0.271254 2.943352 0.503290
H -1.325698 2.925720 -1.406703
H -0.557807 1.993386 -3.614266
H 1.800007 1.130244 -3.785856
N 1.846024 2.141714 -0.565766
N -0.496297 1.333639 2.638249
H -0.936672 0.586751 3.169769
H 0.515939 1.156110 2.662778
H -0.660426 2.186040 3.167736
N 2.522796 0.725318 2.153401
H 3.342740 0.815704 2.745264
H 2.570439 -0.187734 1.698899
H 2.610424 1.401969 1.392855
30
4 Relative E0+Ezero= 1.661941270836788 kJ/mol
C 0.268621 2.655790 -2.558714
C -0.270871 1.468448 -3.042070
C -0.253770 0.346010 -2.218556
C 0.295351 0.467184 -0.944134
C 0.800919 2.669550 -1.270357
H 0.286394 3.558430 -3.167964
H -0.689603 1.414716 -4.047147

H -0.652454 -0.609481 -2.555400
H 0.324940 -0.393851 -0.273855
H 1.254216 3.577644 -0.870131
N 0.812509 1.602931 -0.466954
C 3.480920 0.052705 -1.926789
C 2.736382 0.059659 -4.091662
C 2.485057 -1.309502 -4.073287
C 2.758196 -2.015942 -2.903622
C 3.264192 -1.321232 -1.810063
H 3.861499 0.631902 -1.081068
H 2.532300 0.645031 -4.990804
H 2.089013 -1.807418 -4.957530
H 2.579254 -3.090187 -2.849404
H 3.491374 -1.826719 -0.872594
N 3.225192 0.735409 -3.048565
N 3.780334 2.325176 0.527521
H 2.806098 2.069302 0.686460
H 4.103641 2.821596 1.352390
H 3.779019 2.989668 -0.250182
N 3.780397 3.744557 -2.355586
H 3.559895 2.809278 -2.713308
H 3.231393 4.409963 -2.892769
H 4.754127 3.923063 -2.586013
30
5 Relative E0+Ezero= 2.399706669341503 kJ/mol
C 2.670757 1.268575 -1.435436
C 3.779827 2.074136 -1.191989
C 3.628543 3.454388 -1.271151
C 2.368883 3.968742 -1.573826
C 1.459574 1.881393 -1.742562
H 2.753326 0.185917 -1.360189
H 4.728923 1.614141 -0.921971
H 4.462934 4.128343 -1.083065
H 2.212321 5.048290 -1.622029
H 0.569268 1.279051 -1.936011
N 1.296575 3.207809 -1.808997

C 4.061780 3.231625 2.471673
C 2.114871 2.255314 1.784501
C 1.461032 3.481471 1.684667
C 2.176716 4.631348 2.007558
C 3.503923 4.507110 2.410358
H 5.100988 3.098553 2.780222
H 1.591575 1.332287 1.528906
H 0.428049 3.541222 1.338599
H 1.704541 5.611503 1.937905
H 4.101773 5.378854 2.674091
N 3.388562 2.118714 2.168030
N 4.525248 -0.536017 0.811096
H 4.214409 0.260947 1.374867
H 3.997606 -1.343898 1.132042
H 5.492963 -0.714962 1.067089
N -1.321632 4.084296 -0.250745
H -2.074751 3.419082 -0.404827
H -1.699928 4.999543 -0.479693
H -0.596342 3.878816 -0.943027
30
6 Relative E0+Ezero= 2.5047266545963525 kJ/mol
C -2.408120 0.387200 1.113148
C -1.949562 1.139771 2.192013
C -1.023649 2.148302 1.952097
C -0.582052 2.350945 0.646104
C -1.917305 0.678245 -0.156357
H -3.125658 -0.419808 1.252083
H -2.298586 0.931444 3.202717
H -0.622501 2.753555 2.762957
H 0.177201 3.104369 0.429404
H -2.256864 0.108617 -1.023714
N -1.017713 1.638020 -0.396224
C 0.554795 -1.331834 1.803626
C 0.974415 -0.573085 3.911667
C 1.788270 0.455185 3.437880
C 1.975155 0.582462 2.063694

C 1.346580 -0.339302 1.230258
H 0.042611 -2.061294 1.172421
H 0.807376 -0.693698 4.984692
H 2.255986 1.147800 4.137190
H 2.560421 1.399265 1.635320
H 1.445738 -0.270671 0.147913
N 0.359047 -1.457046 3.120409
N 3.088235 3.125185 0.024072
H 2.521251 2.958974 -0.815275
H 3.080267 4.128065 0.191940
H 4.047020 2.891853 -0.221317
N 1.169797 2.497842 -2.413880
H 0.858222 3.263228 -3.005408
H 1.495881 1.767145 -3.040555
H 0.340917 2.134371 -1.932969
30
7 Relative E0+Ezero= 2.982567588699859 kJ/mol
C -0.095326 1.735377 0.723818
C -1.133794 2.123833 1.566124
C -1.230859 3.463292 1.929069
C -0.279781 4.352358 1.431659
C 0.804644 2.706255 0.285594
H 0.027035 0.697935 0.413682
H -1.845237 1.397725 1.957448
H -2.016415 3.790645 2.608601
H -0.323790 5.410019 1.700732
H 1.632453 2.431905 -0.372495
N 0.725974 3.995959 0.625475
C 1.383584 2.166906 3.962470
C -0.445039 2.677721 5.234844
C -0.074816 4.017503 5.325457
C 1.090415 4.427842 4.685841
C 1.834443 3.483649 3.982857
H 1.939166 1.402903 3.416428
H -1.367026 2.327886 5.701165
H -0.698316 4.719885 5.876380

H 1.408589 5.469728 4.722454
H 2.738965 3.761385 3.445185
N 0.268411 1.760435 4.576605
N -1.947079 -0.318105 3.980879
H -1.073480 0.192368 4.148285
H -2.107183 -0.904929 4.794983
H -1.778674 -0.953109 3.205097
N -3.745759 2.321027 3.923690
H -4.317755 2.362055 4.762962
H -4.396547 2.306208 3.142292
H -3.272383 1.411616 3.929764
30
8 Relative E0+Ezero= 3.0193245838375415 kJ/mol
C -1.983271 -0.391652 -1.208472
C -2.272052 0.966255 -1.298197
C -3.369680 1.356305 -2.061831
C -4.131349 0.372340 -2.689683
C -2.807338 -1.295583 -1.877353
H -1.145067 -0.739899 -0.606832
H -1.650570 1.683289 -0.761634
H -3.640439 2.406534 -2.167386
H -4.998802 0.648424 -3.293763
H -2.608981 -2.368485 -1.821683
N -3.868214 -0.935851 -2.606239
C -3.992672 -1.183723 1.395291
C -2.747322 0.554448 2.200371
C -3.699070 1.490084 1.803284
C -4.848513 1.036809 1.162951
C -4.998722 -0.330155 0.949477
H -4.076661 -2.260440 1.238327
H -1.820541 0.880046 2.674449
H -3.528017 2.550801 1.979007
H -5.608596 1.739151 0.821290
H -5.867828 -0.732910 0.432610
N -2.885601 -0.761225 2.012812
N 0.043193 -1.662545 1.573902

H 0.550230 -1.905237 2.420303
H -0.946384 -1.580953 1.828443
H 0.128517 -2.463434 0.953584
N 0.397824 1.394202 0.728249
H 0.377788 0.400165 0.979778
H 1.017111 1.475095 -0.074622
H 0.864293 1.879928 1.489860
30
9 Relative E0+Ezero= 3.465659522364593 kJ/mol
C -3.300801 2.189041 2.192860
C -3.181348 0.901779 1.677162
C -2.139499 0.096198 2.126626
C -1.260998 0.614621 3.075011
C -2.373427 2.610834 3.142211
H -4.087791 2.863267 1.859480
H -3.883096 0.537321 0.926841
H -1.993665 -0.911544 1.740993
H -0.415894 0.021342 3.425761
H -2.429423 3.618094 3.557382
N -1.373042 1.843790 3.585895
C -0.007547 3.282427 0.903994
C -1.519464 4.595814 -0.186899
C -1.836603 3.577597 -1.085134
C -1.185937 2.352540 -0.956550
C -0.250556 2.198563 0.061746
H 0.714005 3.180535 1.715254
H -2.012137 5.567913 -0.263516
H -2.574977 3.749023 -1.867968
H -1.409379 1.530347 -1.637288
H 0.282022 1.264697 0.236544
N -0.622584 4.465093 0.794889
N 2.109318 0.625725 1.946493
H 2.801188 0.967056 1.283395
H 2.016785 1.351547 2.665677
H 2.532318 -0.180539 2.398991
N 1.504321 2.851646 4.144244

H 1.878263 2.706622 5.077516
H 1.566722 3.850089 3.961831
H 0.507307 2.616496 4.175200
30
10 Relative E0+Ezero= 4.311070405755529 kJ/mol
C -5.354700 -0.056380 1.425130
C -4.952641 -1.039579 2.324767
C -3.689227 -0.939370 2.898860
C -2.878480 0.134323 2.540198
C -4.471733 0.981454 1.138814
H -6.328344 -0.096473 0.939626
H -5.604135 -1.880583 2.559072
H -3.319210 -1.693629 3.590795
H -1.868756 0.216883 2.943218
H -4.753291 1.764084 0.431498
N -3.254061 1.085768 1.679558
C -4.663908 -2.903687 -1.134555
C -2.776666 -2.362327 0.028840
C -2.573670 -1.209980 -0.730132
C -3.481490 -0.913351 -1.741757
C -4.553122 -1.778398 -1.950094
H -5.491951 -3.602683 -1.274821
H -2.080493 -2.599963 0.834348
H -1.731219 -0.558107 -0.505821
H -3.362841 -0.019530 -2.355039
H -5.291571 -1.590857 -2.728922
N -3.799135 -3.203170 -0.161179
N -0.530887 1.655844 0.305466
H -1.466024 1.709349 0.721550
H 0.029447 2.385315 0.737161
H -0.623346 1.911892 -0.673939
N 0.156921 -1.243735 1.461868
H 0.055382 -0.315240 1.039734
H 0.874621 -1.165838 2.177454
H 0.541286 -1.851720 0.742748
30

11 Relative E0+Ezero= 4.623504862485677 kJ/mol
C -1.539408 -0.726935 -2.717277
C -2.081674 -1.660228 -3.594520
C -1.724610 -2.999677 -3.445908
C -0.834809 -3.339060 -2.428704
C -0.661507 -1.168045 -1.726454
H -1.790402 0.330634 -2.782141
H -2.773897 -1.353472 -4.379168
H -2.123497 -3.769743 -4.104937
H -0.531715 -4.378777 -2.288232
H -0.251661 -0.456543 -1.007977
N -0.308047 -2.450150 -1.580417
C -2.536534 -2.888003 0.894502
C -3.178663 -1.600291 2.666135
C -4.071964 -0.872286 1.881383
C -4.178301 -1.187852 0.528213
C -3.393754 -2.219259 0.022740
H -1.896674 -3.690125 0.523988
H -3.062055 -1.369831 3.726841
H -4.662232 -0.071127 2.324600
H -4.855425 -0.632710 -0.120969
H -3.425138 -2.496977 -1.029913
N -2.419765 -2.592852 2.192101
N 0.689297 -1.996850 1.452815
H 0.004351 -2.449446 2.055525
H 0.549031 -2.367164 0.510915
H 1.610003 -2.293354 1.761498
N -0.783258 0.749155 1.001904
H -0.196290 -0.039446 1.295386
H -0.573163 1.528294 1.619516
H -1.744177 0.476586 1.196387
30
12 Relative E0+Ezero= 4.728524848039012 kJ/mol
C -2.534991 -0.236035 -0.226216
C -1.794746 0.129532 -1.346474
C -1.180182 1.380534 -1.358646

C -1.340095 2.207453 -0.248417
C -2.628776 0.659317 0.839939
H -3.029669 -1.204362 -0.164001
H -1.694721 -0.547409 -2.195251
H -0.587549 1.713311 -2.209772
H -0.875475 3.195425 -0.226123
H -3.166473 0.376375 1.748384
N -2.045427 1.863807 0.833077
C -0.357189 -1.038865 2.733605
C 0.818848 -0.570318 4.632747
C 1.674077 0.297537 3.954448
C 1.482710 0.484276 2.586518
C 0.445301 -0.199545 1.961400
H -1.193947 -1.570599 2.279178
H 0.943067 -0.739200 5.704359
H 2.470583 0.812611 4.490062
H 2.129090 1.154826 2.020130
H 0.246148 -0.080830 0.897443
N -0.181459 -1.232104 4.043605
N -3.373903 -0.587959 3.949073
H -2.737143 -1.266123 4.363201
H -2.954895 0.329500 4.132994
H -4.240961 -0.634982 4.476523
N -1.707465 2.100310 3.951393
H -0.762766 1.751121 4.095197
H -1.802506 2.285964 2.950349
H -1.768000 2.992100 4.433592

****

$(pyridine)_m$-$(ammonia)_n$, (m, n) = (2, 3)

****

34

1 Relative E0+Ezero= 0.0 kJ/mol

C 3.645975 0.160214 1.921095

C 3.220724 1.430038 2.307313

C 1.925288 1.824693 1.990061

C 1.109288 0.926150 1.304823

C 2.751201 -0.660784 1.238393

H 4.652261 -0.193637 2.143287

H 3.893638 2.101946 2.840973

H 1.532248 2.811907 2.232365

H 0.092618 1.213174 1.031693

H 3.052510 -1.661831 0.922316

N 1.501877 -0.297133 0.933166

C 2.160244 1.396758 -2.030903

C 0.581718 2.939021 -1.442314

C 1.532547 3.768483 -0.852212

C 2.864066 3.366449 -0.870555

C 3.187031 2.151845 -1.469150

H 2.376270 0.434305 -2.498275

H -0.474115 3.213112 -1.424092

H 1.223946 4.687362 -0.358776

H 3.636506 3.980724 -0.408082

H 4.211877 1.784587 -1.490818

N 0.879572 1.777328 -2.031412

N -0.565411 4.151683 1.903112

H -0.904786 5.049882 1.567652

H -1.097668 3.431293 1.400811

H -0.855681 4.093142 2.876251

N -2.365522 1.914581 0.527474

H -2.017859 1.090177 0.017341

H -2.870531 1.557035 1.334797

H -3.068263 2.349689 -0.064968

N -1.024919 -0.439826 -0.953336

H -0.267312 -0.793618 -0.365863
H -1.456468 -1.236134 -1.411903
H -0.567755 0.125557 -1.670374
34
2 Relative E0+Ezero= 0.6327454126528951 kJ/mol
C 0.073045 0.266953 5.690908
C -0.067453 -0.809736 4.817076
C -0.560753 -0.568739 3.538957
C -0.891662 0.740020 3.187167
C -0.291430 1.536099 5.243496
H 0.458290 0.132332 6.700866
H 0.210277 -1.817704 5.125566
H -0.675176 -1.374065 2.815206
H -1.261328 0.964444 2.184701
H -0.194615 2.400451 5.903835
N -0.766234 1.779986 4.018336
C 1.535859 -2.500783 0.998116
C 0.845920 -0.373007 0.522918
C -0.347944 -0.824637 -0.039318
C -0.585664 -2.195200 -0.070656
C 0.375791 -3.054358 0.460137
H 2.307573 -3.145210 1.424276
H 1.045562 0.698504 0.590455
H -1.067334 -0.090211 -0.401361
H -1.509898 -2.590229 -0.493098
H 0.233878 -4.134471 0.460411
N 1.776631 -1.186311 1.034662
N 0.912747 3.164493 1.715872
H 1.346242 4.058444 1.503611
H 0.277222 3.316525 2.498402
H 1.647145 2.548570 2.082001
N -1.492506 2.305519 -0.091099
H -1.432209 2.667230 -1.039046
H -2.268086 2.795490 0.348101
H -0.640534 2.608351 0.397443
N 2.760267 0.984435 3.035301

H 3.722920 1.072303 3.346919
H 2.202134 0.777369 3.860484
H 2.706555 0.160449 2.431729
34
3 Relative E0+Ezero= 1.3862638086473524 kJ/mol
C 0.017536 -2.746651 2.964007
C -1.098575 -2.649761 3.788758
C -0.907575 -2.543702 5.165463
C 0.395167 -2.543738 5.657303
C 1.278601 -2.733778 3.556916
H -0.047158 -2.821837 1.878933
H -2.104199 -2.654258 3.367316
H -1.750749 -2.465022 5.850889
H 0.580562 -2.465861 6.730780
H 2.171837 -2.791801 2.932824
N 1.475863 -2.638090 4.876663
C 2.462559 0.216442 2.083917
C 0.295206 0.660120 2.643989
C 0.615229 0.803964 3.992528
C 1.941722 0.638463 4.380003
C 2.887246 0.337891 3.404762
H 3.174430 -0.045258 1.300088
H -0.737535 0.774525 2.309033
H -0.164277 1.027463 4.719252
H 2.229495 0.725838 5.427455
H 3.932680 0.170632 3.655943
N 1.193402 0.374749 1.697257
N 4.404942 -2.677475 1.693009
H 4.558670 -3.674860 1.567043
H 5.158343 -2.214730 1.191188
H 4.549211 -2.486053 2.691302
N 4.558048 -2.353252 4.838293
H 4.922695 -1.586203 5.396690
H 3.552586 -2.418072 5.034333
H 4.981444 -3.198796 5.211449
N 1.548540 -2.373070 0.054953

H 2.454384 -2.436199 0.526017
H 1.710716 -2.548826 -0.932213
H 1.245203 -1.403692 0.143210
34
4 Relative E0+Ezero= 2.058391716069301 kJ/mol
C 3.022934 -0.716632 -0.143508
C 2.358413 0.218629 0.647696
C 1.050345 0.559774 0.319627
C 0.464536 -0.053297 -0.786498
C 2.347949 -1.266647 -1.231025
H 4.048194 -1.015959 0.071182
H 2.856789 0.676437 1.502762
H 0.478682 1.298340 0.880015
H -0.556447 0.201234 -1.075098
H 2.842614 -1.997601 -1.873992
N 1.091094 -0.948883 -1.556443
C 1.937754 3.374306 -3.604817
C 0.124476 2.893856 -2.300824
C 0.588756 3.694953 -1.259169
C 1.794461 4.367021 -1.430187
C 2.485375 4.204831 -2.629729
H 2.458287 3.218963 -4.552026
H -0.813657 2.346996 -2.192747
H 0.011529 3.752081 -0.337503
H 2.194996 5.003126 -0.640283
H 3.434704 4.707766 -2.810621
N 0.777742 2.727266 -3.455266
N -1.925668 2.281689 0.640363
H -2.177392 1.659465 1.404738
H -2.515636 3.103356 0.745560
H -2.228847 1.816027 -0.223295
N -0.704836 -0.006839 -3.985030
H -0.091116 -0.614545 -3.439302
H -0.848913 -0.452484 -4.885850
H -0.176060 0.852392 -4.150903
N -2.903783 0.824623 -2.014083

H -3.426004 0.009333 -1.703476
H -3.582527 1.433971 -2.463364
H -2.261697 0.500194 -2.752888
34
5 Relative E0+Ezero= 2.922181096879836 kJ/mol
C 3.408533 3.672542 2.024520
C 2.125696 3.926806 1.543633
C 1.458942 2.915950 0.858295
C 2.107039 1.694301 0.680106
C 3.964296 2.414132 1.798401
H 3.973244 4.431709 2.564310
H 1.656154 4.898736 1.696611
H 0.460740 3.069935 0.451447
H 1.621447 0.889737 0.124947
H 4.967134 2.182416 2.163077
N 3.335326 1.436729 1.139850
C 0.757936 2.266535 -2.358542
C -1.431900 2.412563 -1.705837
C -1.449473 3.792966 -1.887929
C -0.285156 4.418623 -2.333258
C 0.843489 3.642038 -2.572141
H 1.634323 1.632929 -2.509946
H -2.325167 1.889797 -1.358088
H -2.357120 4.360065 -1.684775
H -0.259839 5.498336 -2.483531
H 1.796607 4.066955 -2.882635
N -0.353813 1.654508 -1.934034
N 4.026076 3.301819 -1.937358
H 3.912248 2.283229 -1.972703
H 5.013690 3.489418 -2.087844
H 3.828157 3.574581 -0.976502
N 0.790162 -1.178455 -1.473464
H 0.526701 -1.604167 -0.588993
H 0.198006 -0.352751 -1.606614
H 0.541794 -1.844540 -2.199082
N 3.673343 0.119946 -1.753306

H 3.996088 0.196939 -0.789050
H 2.801072 -0.417272 -1.715707
H 4.353770 -0.445964 -2.251876
34
6 Relative E0+Ezero= 3.2004840587006425 kJ/mol
C -2.234983 1.290790 0.280802
C -3.414557 1.663523 -0.354841
C -4.195994 0.672781 -0.945405
C -3.755996 -0.646650 -0.875000
C -1.885649 -0.058663 0.305649
H -1.595443 2.025585 0.766206
H -3.723757 2.708333 -0.387834
H -5.127533 0.913161 -1.456270
H -4.340015 -1.447953 -1.332615
H -0.981919 -0.391152 0.821184
N -2.626294 -1.016383 -0.264730
C -3.199612 -0.597517 3.171984
C -2.695183 1.512455 3.892346
C -3.951474 1.996619 3.533149
C -4.864939 1.112049 2.964625
C -4.482183 -0.212863 2.782629
H -2.861812 -1.625397 3.020849
H -1.955686 2.179301 4.340830
H -4.202806 3.043748 3.697670
H -5.856212 1.452403 2.664709
H -5.155823 -0.941116 2.333922
N -2.315197 0.244049 3.718299
N 0.067260 -1.614708 2.691199
H 0.845583 -1.966177 3.241351
H -0.386112 -0.887786 3.246828
H -0.613028 -2.375620 2.619350
N -2.142099 -3.617172 1.586978
H -2.524557 -2.937964 0.926660
H -1.351386 -4.032569 1.093176
H -2.836894 -4.346376 1.717315
N 0.223936 -2.897523 -0.252882

H 0.437382 -2.318589 0.562014
H 1.004144 -2.817315 -0.898152
H -0.583099 -2.466437 -0.701247
34
7 Relative E0+Ezero= 3.77546847946337 kJ/mol
C -3.544152 -1.954729 0.529266
C -4.682107 -1.761683 1.306011
C -5.928877 -2.037491 0.746192
C -5.979849 -2.495894 -0.568692
C -3.705112 -2.415837 -0.776646
H -2.541101 -1.725335 0.887321
H -4.602481 -1.392533 2.328694
H -6.848525 -1.898231 1.313028
H -6.940114 -2.717360 -1.038649
H -2.832880 -2.543857 -1.420161
N -4.894190 -2.685002 -1.325552
C -4.942822 1.250469 -2.828095
C -3.004976 1.654699 -3.963480
C -2.228088 1.141529 -2.926055
C -2.867793 0.656415 -1.789352
C -4.257909 0.717079 -1.738035
H -6.033612 1.302975 -2.820723
H -2.531287 2.036575 -4.870451
H -1.142977 1.112601 -3.015755
H -2.294461 0.219672 -0.971304
H -4.806293 0.339224 -0.876009
N -4.340716 1.709359 -3.931024
N -3.882025 -1.933740 -4.195651
H -4.154153 -0.960544 -4.314315
H -4.189460 -2.424847 -5.029898
H -4.427135 -2.298508 -3.411233
N -0.335861 -1.193253 -0.276149
H -0.504421 -1.494801 -1.244045
H 0.252826 -0.365112 -0.321556
H 0.231934 -1.914937 0.160145
N -0.927975 -2.092085 -3.242344

H -0.346033 -1.513338 -3.842817
H -0.635646 -3.050353 -3.417740
H -1.888353 -2.011486 -3.604494
34
8 Relative E0+Ezero= 4.095779435087632 kJ/mol
C 0.512718 -0.140055 2.058071
C 0.209783 -1.427105 1.623630
C -0.581364 -1.573191 0.487299
C -1.035656 -0.428999 -0.160229
C 0.022702 0.942186 1.329838
H 1.135359 0.031112 2.935157
H 0.599142 -2.314475 2.121704
H -0.819709 -2.563084 0.103564
H -1.655117 -0.508542 -1.055567
H 0.270138 1.963474 1.623840
N -0.743046 0.812284 0.243097
C 1.465005 -2.004035 -2.617932
C 2.593364 -1.350932 -0.743572
C 2.408036 -0.000514 -1.027772
C 1.703391 0.337906 -2.178610
C 1.225138 -0.684291 -2.995190
H 1.097040 -2.829629 -3.231134
H 3.125907 -1.654359 0.159958
H 2.770013 0.781224 -0.360661
H 1.516993 1.385433 -2.414252
H 0.666216 -0.470390 -3.905562
N 2.134887 -2.344465 -1.512993
N 2.512923 3.251464 -0.223974
H 2.442651 3.921939 0.536894
H 3.256164 3.591383 -0.829045
H 1.642737 3.319209 -0.761697
N 1.372131 -4.479323 0.731690
H 2.212275 -4.895765 1.124685
H 0.804452 -5.255187 0.400351
H 1.666089 -3.954003 -0.096503
N -0.311426 3.195425 -1.690092

H -0.573239 2.955282 -2.642552
H -0.619201 2.422472 -1.089087
H -0.871202 4.005957 -1.440392
34
9 Relative E0+Ezero= 4.468600383637804 kJ/mol
C 3.990702 3.036038 -3.640676
C 3.362892 1.812417 -3.862792
C 2.125503 1.589594 -3.266146
C 1.577489 2.588200 -2.466472
C 3.358818 3.973168 -2.826375
H 4.959811 3.263848 -4.083104
H 3.823864 1.023635 -4.457872
H 1.606109 0.642485 -3.398712
H 0.622274 2.432479 -1.961714
H 3.828413 4.939503 -2.629599
N 2.175465 3.763437 -2.241946
C 4.341912 0.541080 -0.820828
C 2.423633 -0.666911 -0.542427
C 1.836395 0.334069 0.227310
C 2.569002 1.491719 0.474427
C 3.852579 1.595236 -0.052973
H 5.335193 0.599866 -1.270014
H 1.878249 -1.588323 -0.758351
H 0.819560 0.245795 0.607046
H 2.122970 2.304447 1.045987
H 4.459462 2.486112 0.100834
N 3.650888 -0.575933 -1.067342
N 0.978552 4.754311 0.459608
H 1.393349 4.565196 -0.459469
H 0.361164 5.553216 0.342533
H 1.733207 5.069986 1.063584
N -0.739902 2.212219 1.326654
H -0.228852 3.062701 1.066320
H -1.655648 2.269990 0.888837
H -0.902628 2.263354 2.328972
N 3.955864 -1.478575 -4.104336

H 3.928364 -1.351006 -3.088667
H 3.172258 -2.079540 -4.346647
H 4.795379 -2.013311 -4.310763
34
10 Relative E0+Ezero= 4.4948553802500015 kJ/mol
C 1.851005 -3.301418 -2.365446
C 1.322220 -4.013310 -1.293647
C 0.030957 -3.711445 -0.865074
C -0.670634 -2.706451 -1.528367
C 1.064650 -2.318358 -2.963646
H 2.858327 -3.490301 -2.732569
H 1.905787 -4.788084 -0.796221
H -0.425342 -4.238290 -0.028263
H -1.680458 -2.438343 -1.212393
H 1.453024 -1.733813 -3.799249
N -0.173067 -2.018771 -2.560219
C 2.556133 0.531015 -2.174859
C 3.542103 0.409512 -4.233893
C 4.609890 -0.335161 -3.736859
C 4.628482 -0.644172 -2.377321
C 3.579758 -0.203342 -1.577012
H 1.709429 0.868411 -1.575031
H 3.497670 0.671396 -5.293198
H 5.407760 -0.658462 -4.404666
H 5.448114 -1.223630 -1.950968
H 3.507765 -0.430085 -0.513649
N 2.527738 0.839876 -3.476337
N -0.615945 1.060950 -3.252183
H -1.299959 1.378763 -3.931812
H 0.310212 1.237721 -3.644461
H -0.702629 0.045215 -3.179208
N -0.317301 1.659169 -0.229012
H -0.528945 1.555325 -1.230504
H -1.207532 1.670929 0.261121
H 0.082274 2.586373 -0.107893
N 1.479904 -0.724623 0.881985

H 0.883668 0.046849 0.561113
H 1.163757 -1.557237 0.389804
H 1.265530 -0.874213 1.864061
34
11 Relative E0+Ezero= 4.57624586882251 kJ/mol
C -2.912193 -2.033322 -4.239880
C -4.120129 -2.492407 -4.754426
C -5.171977 -1.589237 -4.887001
C -4.968364 -0.269847 -4.488664
C -2.809831 -0.693797 -3.869416
H -2.064906 -2.703822 -4.106751
H -4.242491 -3.537297 -5.038510
H -6.137890 -1.898944 -5.283940
H -5.774341 0.461931 -4.574692
H -1.880315 -0.308401 -3.444039
N -3.815691 0.180153 -3.985088
C -2.833616 -3.328341 -0.707834
C -4.969002 -2.975310 -1.423067
C -4.875985 -1.602876 -1.199911
C -3.678905 -1.087368 -0.712989
C -2.635523 -1.972264 -0.452606
H -2.033329 -4.047250 -0.517216
H -5.892598 -3.406168 -1.815395
H -5.719573 -0.952855 -1.425699
H -3.552199 -0.015080 -0.568057
H -1.684991 -1.613153 -0.061011
N -3.972916 -3.834930 -1.190077
N -2.442849 2.039989 -1.783924
H -1.563483 1.582644 -2.034293
H -3.120584 1.721065 -2.479409
H -2.313669 3.035707 -1.940118
N 0.054676 -0.006711 -1.750713
H -0.231596 0.139988 -0.777646
H 0.038108 -1.009571 -1.916912
H 1.025929 0.282372 -1.825545
N -1.353225 0.905976 0.920561

H -1.996613 0.414849 1.535750
H -0.902691 1.620512 1.484962
H -1.916242 1.390669 0.213411
34
12 Relative E0+Ezero= 4.820417335137006 kJ/mol
C -0.709323 2.816519 3.441635
C -2.083499 3.026063 3.422354
C -2.674179 3.458734 2.236849
C -1.859820 3.659570 1.124968
C 0.017063 3.041149 2.272674
H -0.200941 2.464104 4.337278
H -2.687368 2.848679 4.312292
H -3.746704 3.636939 2.170606
H -2.291258 3.997483 0.180423
H 1.092656 2.852131 2.250122
N -0.539198 3.455647 1.130008
C -0.874323 -0.850608 3.574242
C -0.191763 -0.019783 1.558499
C -1.501164 0.060752 1.087606
C -2.535233 -0.336328 1.928285
C -2.215994 -0.802995 3.201448
H -0.590356 -1.213518 4.564435
H 0.635891 0.312902 0.930789
H -1.693067 0.448003 0.088558
H -3.573612 -0.278246 1.601476
H -2.989549 -1.126543 3.896917
N 0.126939 -0.466989 2.777648
N 2.982507 0.812406 2.199813
H 3.225019 0.124528 1.481676
H 3.796491 0.925076 2.796514
H 2.255429 0.367255 2.762242
N 1.838031 2.073468 -0.493176
H 2.334925 1.965209 0.395341
H 2.448642 2.597691 -1.113127
H 1.031033 2.668700 -0.300524
N 2.708683 -0.941807 -0.442772

H 1.961311 -1.617147 -0.306238
H 2.275080 -0.059773 -0.731759
H 3.267513 -1.277440 -1.221659
34
13 Relative E0+Ezero= 4.941190318478568 kJ/mol
C 1.789898 -4.786574 2.575510
C 2.099365 -4.575789 3.915117
C 1.080864 -4.183129 4.781442
C -0.203515 -4.015946 4.264756
C 0.471818 -4.600619 2.163447
H 2.557813 -5.058764 1.854367
H 3.118994 -4.708128 4.277122
H 1.273439 -4.003577 5.838553
H -1.023084 -3.701529 4.914215
H 0.196156 -4.751579 1.118534
N -0.514572 -4.219231 2.981098
C 1.827347 -3.339768 -0.649903
C 0.728454 -4.252425 -2.435580
C 1.847085 -4.992156 -2.813245
C 3.004604 -4.886048 -2.044416
C 2.996588 -4.042405 -0.937298
H 1.787421 -2.675087 0.215559
H -0.195800 -4.317015 -3.013542
H 1.805101 -5.636765 -3.690412
H 3.897633 -5.454754 -2.305313
H 3.858029 -3.915942 -0.281488
N 0.706674 -3.439387 -1.374962
N -1.008063 -1.878687 0.758556
H -1.798242 -1.297307 0.496821
H -0.688693 -2.357062 -0.087201
H -1.358044 -2.593573 1.395146
N 1.558310 -1.275123 2.412311
H 1.682118 -0.303231 2.682874
H 0.700693 -1.321042 1.847389
H 1.355479 -1.785968 3.269155
N 4.343738 -2.656009 1.792678

H 3.438664 -2.196929 1.952617
H 4.721986 -2.881215 2.709269
H 4.960225 -1.946985 1.403466

Table S2 Sub-matrices (cm^{-1}) of the quantum states (>4000 cm^{-1}) in pyridine calculated by 10-D anharmonic Hamiltonian discussed in main text.

2v23	2669.5	12.1	0.0	0.0	0.0	-2.3	0.0	-0.2	0.0	-4.9	0.0	11.8	0.0	0.0	12.3	0.0	0.1	0.0	0.0	0.0
v22+v23	12.1	2758.3	0.0	11.9	0.0	4.8	0.0	0.0	0.0	-7.3	-1.5	-18.5	0.0	0.0	-3.9	0.0	-0.1	0.0	0.0	-0.1
v5+v23	0.0	0.0	2813.6	0.0	-8.6	0.0	0.5	0.0	10.4	0.0	0.0	0.0	0.0	2.9	0.0	1.7	0.0	0.0	0.0	0.0
2v22	0.0	11.9	0.0	2855.2	0.0	-0.4	0.0	0.3	0.0	-10.1	6.5	-11.5	0.0	0.0	23.2	0.0	0.1	0.1	0.0	0.1
v5+v22	0.0	0.0	-8.6	0.0	2913.2	0.0	0.8	0.0	-39.1	-0.1	0.0	0.0	-0.2	25.3	0.0	4.7	0.0	0.0	-0.2	0.0
v21+v23	-2.3	4.8	0.0	-0.4	0.0	2954.6	0.0	0.7	0.0	0.4	8.8	27.2	0.0	0.0	14.8	0.0	-0.4	-2.4	0.0	0.2
v4+v23	0.0	0.0	0.5	0.0	0.8	0.0	2967.7	0.0	9.5	0.0	0.0	0.0	-8.7	0.2	0.0	-0.8	0.0	0.0	-1.8	0.0
2v5	-0.2	0.0	0.0	0.3	0.0	0.7	0.0	2968.4	0.0	-18.5	0.5	-15.5	0.0	0.0	17.2	0.0	-0.4	0.2	0.0	0.1
v20	0.0	0.0	10.4	0.0	-39.1	0.0	9.5	0.0	3033.5	0.0	0.0	0.0	-20.5	-0.2	0.0	13.2	0.0	0.0	-12.9	0.0
v3	-4.9	-7.3	0.0	-10.1	-0.1	0.4	0.0	-18.5	0.0	3037.1	18.5	0.6	0.0	0.0	0.0	0.0	30.6	-4.5	0.0	-3.7
v21+v22	0.0	-1.5	0.0	6.5	0.0	8.8	0.0	0.5	0.0	18.5	3051.3	-17.8	0.0	0.0	2.2	0.0	-0.1	6.5	0.0	-0.6
v2	11.8	-18.5	0.0	-11.5	0.0	27.2	0.0	-15.5	0.0	0.6	-17.8	3057.5	0.0	0.0	-1.7	0.0	-4.0	13.2	0.0	-14.6
v4+v22	0.0	0.0	0.0	0.0	-0.2	0.0	-8.7	0.0	-20.5	0.0	0.0	0.0	3061.6	-33.6	0.0	0.4	0.0	0.0	-4.6	0.0
v19	0.0	0.0	2.9	0.0	25.3	0.0	0.2	0.0	-0.2	0.0	0.0	0.0	-33.6	3072.0	0.0	14.3	0.0	0.0	15.9	0.0
v1	12.3	-3.9	0.0	23.2	0.0	14.8	0.0	17.2	0.0	0.0	2.2	-1.7	0.0	0.0	3091.2	0.0	11.5	18.1	0.0	13.4
v5+v21	0.0	0.0	1.7	0.0	4.7	0.0	-0.8	0.0	13.2	0.0	0.0	0.0	0.4	14.3	0.0	3104.2	0.0	0.0	-0.4	0.0
v4+v5	0.1	-0.1	0.0	0.1	0.0	-0.4	0.0	-0.4	0.0	30.6	-0.1	-4.0	0.0	0.0	11.5	0.0	3118.4	0.1	0.0	-0.4
2v21	0.0	0.0	0.0	0.1	0.0	-2.4	0.0	0.2	0.0	-4.5	6.5	13.2	0.0	0.0	18.1	0.0	0.1	3243.0	0.0	-0.2
v4+v21	0.0	0.0	0.0	0.0	-0.2	0.0	-1.8	0.0	-12.9	0.0	0.0	0.0	-4.6	15.9	0.0	-0.4	0.0	0.0	3257.5	0.0
2v4	0.0	-0.1	0.0	0.1	0.0	0.2	0.0	0.1	0.0	-3.7	-0.6	-14.6	0.0	0.0	13.4	0.0	-0.4	-0.2	0.0	3268.4

Table S3 Sub-matrices (cm^{-1}) of the quantum states involved in the Fermi resonance of NH_3 moiety in pyridine−$(NH_3)_n$ complexes calculated by *ab initio* anharmonic algorithms. In pyridine−$(NH_3)_2$ and pyridine−$(NH_3)_3$, the ammonia molecules are labeled from their hydrogen bond connection from pyridine. The common features are same for all three complexes: (1) The strongest (> 40 cm^{-1}) coupling occurs between $\nu_4 + \nu_4$' and ν_3', (2) coupling between $2\nu_4$' and ν_1 and coupling $2\nu_4$ and ν_3 are second largest with the strength slightly less than 40 cm^{-1} and (3) coupling between $2\nu_4$ and ν_1 and coupling $2\nu_4$' and ν_3 are relatively weaker with the strength slightly more than 15 cm^{-1}.

P1N2(1)	$2\nu_4$	$\nu_4+\nu_4'$	$2\nu_4'$	ν_1	ν_3	ν_3'
$2\nu_4$	3225.1	0.0	0.4	18.1	37.3	0.0
$\nu_4+\nu_4'$	0.0	3257.1	0.0	0.0	0.0	-44.6
$2\nu_4'$	0.4	0.0	3287.0	37.6	-17.1	0.0
ν_1	18.1	0.0	37.6	3235.3	6.3	0.0
ν_3	37.3	0.0	-17.1	6.3	3371.7	0.0
$\nu3'$	0.0	-44.6	0.0	0.0	0.0	3420.3
P1N2(2)	$2\nu_4$	$\nu_4+\nu_4'$	$2\nu_4'$	ν_1	ν_3	ν_3'
$2\nu_4$	3229.2	0.0	0.4	18.1	37.3	0.0
$\nu_4+\nu_4'$	0.0	3265.0	0.0	0.0	0.0	-44.6
$2\nu_4'$	0.4	0.0	3298.7	37.6	-17.1	0.0
ν_1	18.1	0.0	37.6	3231.5	6.3	0.0
ν_3	37.3	0.0	-17.1	6.3	3370.4	0.0
ν_3'	0.0	-44.6	0.0	0.0	0.0	3419.0

P1N3(1)	$2\nu_4$	$\nu_4+\nu_4'$	$2\nu_4'$	ν_1	ν_3	ν_3'
$2\nu_4$	3227.4	-0.2	-0.4	-17.6	-37.1	-1.0
$\nu_4+\nu_4'$	-0.2	3258.7	0.2	-0.9	1.5	-44.2
$2\nu_4'$	-0.4	0.2	3288.1	37.4	-16.6	-0.9
ν_1	-17.6	-0.9	37.4	3232.3	6.3	0.1
ν_3	-37.1	1.5	-16.6	6.3	3368.1	-0.1
ν_3'	-1.0	-44.2	-0.9	0.1	-0.1	3417.3
P1N3(2)	$2\nu_4$	$\nu_4+\nu_4'$	$2\nu_4'$	ν_1	ν_3	ν_3'
$2\nu_4$	3236.3	-0.2	-0.4	-17.6	-37.1	-1.0
$\nu_4+\nu_4'$	-0.2	3271.8	0.2	-0.9	1.5	-44.2
$2\nu_4'$	-0.4	0.2	3305.6	37.4	-16.6	-0.9
ν_1	-17.6	-0.9	37.4	3211.9	6.3	0.1
ν_3	-37.1	1.5	-16.6	6.3	3356.9	-0.1
ν_3'	-1.0	-44.2	-0.9	0.1	-0.1	3409.3
P1N3(3)	$2\nu_4$	$\nu_4+\nu_4'$	$2\nu_4'$	ν_1	ν_3	ν_3'
$2\nu_4$	3234.6	-0.2	-0.4	-17.6	-37.1	-1.0
$\nu_4+\nu_4'$	-0.2	3268.7	0.2	-0.9	1.5	-44.2
$2\nu_4'$	-0.4	0.2	3301.2	37.4	-16.6	-0.9
ν_1	-17.6	-0.9	37.4	3231.8	6.3	0.1
ν_3	-37.1	1.5	-16.6	6.3	3366.4	-0.1
ν_3'	-1.0	-44.2	-0.9	0.1	-0.1	3413.7

Table S4 Assignments on the spectral features related to Fermi resonance of NH_3 moiety in pyridine−$(NH_3)_n$ complexes calculated by *ab initio* anharmonic algorithms. Similar to Table S3, the ammonia molecules, in pyridine−$(NH_3)_2$ and pyridine−$(NH_3)_3$, are labeled from their hydrogen bond connection from pyridine.

P1N2(1)		P1N2(2)		
Freq(cm^{-1})	Intensity	Freq(cm^{-1})		
3186.50	51.54	3188.73	40.95	$2\nu_4$
3212.18	140.27	3214.14	83.42	$2\nu_4'$
3228.92	0.17	3236.14	0.12	$\nu_4+\nu_4'$
3296.22	76.28	3302.47	33.45	ν_1
3381.33	69.97	3380.71	42.49	ν_3
3427.07	0.33	3425.85	0.06	ν_3'

P1N3(1)		P1N3(2)		P1N3(3)		
Freq(cm^{-1})	Intensity	Freq(cm^{-1})	Intensity	Freq(cm^{-1})	Intensity	
3187.5	60.5	3183.7	124.7	3191.6	51.5	$2\nu_4$
3212.1	121.9	3213.4	53.9	3217.9	73.1	$2\nu_4'$
3230.5	0.4	3243.2	0.1	3239.7	0.1	$\nu_4+\nu_4'$
3295.9	67.2	3304.0	27.5	3304.5	30.9	ν_1
3377.9	60.0	3368.0	43.4	3377.3	45.3	ν_3
3424.2	0.5	3417.3	0.2	3421.5	0.2	ν_3'