

SUPPLEMENTARY MATERIAL

Isotope exchange in reactions between D₂O and size-selected ionic water clusters containing pyridine, H⁺(pyridine)_m(H₂O)_n

Mauritz Johan Ryding^a, Alexey S. Zatula^b, Patrik Urban Andersson^{a,*}, and Einar Uggerud^{b,*}

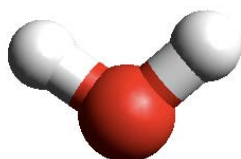
^a Department of Chemistry, Atmospheric Science, University of Gothenburg, SE-412 96 Göteborg, Sweden.

^b Mass Spectrometry Laboratory and Centre of Theoretical and Computational Chemistry, Department of Chemistry, University of Oslo, POB 1033 Blindern, N-0315 Oslo, Norway.

*Corresponding authors (e-mail: einar.uggerud@kjemi.uio.no).

Cartesian coordinates (Å) and energies (Hartree) for the most stable structures, as calculated by B3LYP/6-311+G**.

H₂O

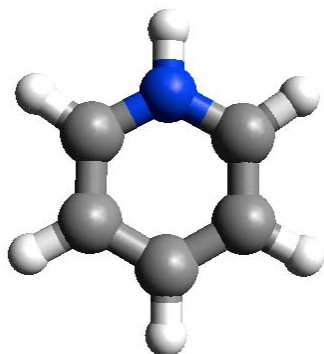


H	0.76357	-0.46819	0.00000
O	0.00000	0.11705	0.00000
H	-0.76357	-0.46819	0.00000

Zero-point correction=	0.021283 (Hartree/Particle)
Thermal correction to Energy=	0.024119
Thermal correction to Enthalpy=	0.025063
Thermal correction to Gibbs Free Energy=	0.002986
Sum of electronic and zero-point Energies=	-76.437181
Sum of electronic and thermal Energies=	-76.434345
Sum of electronic and thermal Enthalpies=	-76.433401
Sum of electronic and thermal Free Energies=	-76.455478

Electronic Energy= -76.4584639

1P-1W

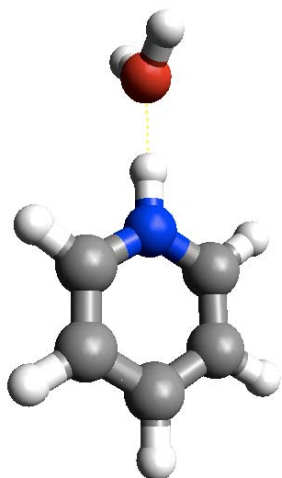


N	0.00000	1.30753	0.00000
C	-1.18836	0.66523	0.00000
C	-1.20965	-0.71552	0.00000
C	0.00001	-1.41266	0.00000
C	1.20965	-0.71553	0.00000
C	1.18835	0.66523	0.00000
H	-2.07663	1.28254	0.00000
H	-2.15977	-1.23289	0.00000
H	-0.00002	-2.49628	0.00000
H	2.15979	-1.23287	0.00000
H	2.07662	1.28253	0.00000
H	0.00002	2.32372	0.00000

Zero-point correction=	0.102571 (Hartree/Particle)
Thermal correction to Energy=	0.106954
Thermal correction to Enthalpy=	0.107898
Thermal correction to Gibbs Free Energy=	0.075070
Sum of electronic and zero-point Energies=	-248.616486
Sum of electronic and thermal Energies=	-248.612103
Sum of electronic and thermal Enthalpies=	-248.611159
Sum of electronic and thermal Free Energies=	-248.643987

ELECTRONIC ENERGY =-248.7190567

1P-1W

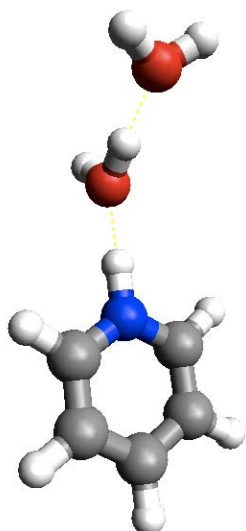


H	3.86261	0.00002	0.77198
N	0.52109	0.00000	0.00000
C	-0.12609	1.18191	0.00000
C	-1.50821	1.20813	0.00000
C	-2.20656	-0.00000	-0.00000
C	-1.50820	-1.20813	-0.00000
C	-0.12608	-1.18191	0.00000
H	0.49121	2.07028	0.00000
H	-2.02495	2.15849	0.00000
H	-3.29009	-0.00001	-0.00000
H	-2.02495	-2.15849	-0.00000
H	0.49122	-2.07028	0.00000
O	3.28437	-0.00001	0.00000
H	3.86261	0.00002	-0.77197
H	1.56053	-0.00000	0.00000

Zero-point correction=	0.126459 (Hartree/Particle)
Thermal correction to Energy=	0.134332
Thermal correction to Enthalpy=	0.135276
Thermal correction to Gibbs Free Energy=	0.093656
Sum of electronic and zero-point Energies=	-325.078704
Sum of electronic and thermal Energies=	-325.070832
Sum of electronic and thermal Enthalpies=	-325.069887
Sum of electronic and thermal Free Energies=	-325.111507

ELECTRONIC ENERGY = -325.2051636

1P-2W

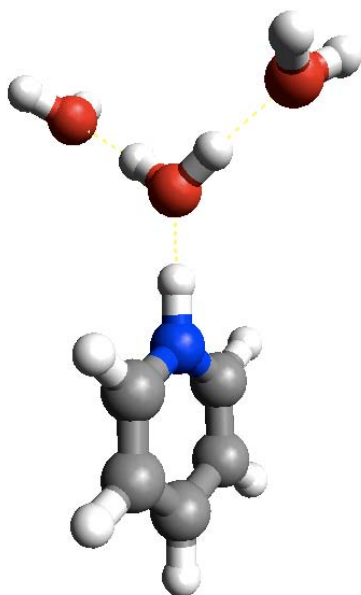


H	-4.86577	0.77327	-1.06778
N	0.31981	0.00078	0.29550
C	0.94880	1.17984	0.13493
C	2.28832	1.20725	-0.20813
C	2.96457	-0.00059	-0.38186
C	2.28683	-1.20773	-0.20907
C	0.94735	-1.17893	0.13402
H	0.35113	2.06841	0.28864
H	2.78930	2.15746	-0.33570
H	4.01428	-0.00114	-0.65037
H	2.78664	-2.15847	-0.33736
H	0.34853	-2.06684	0.28706
O	-4.35390	0.00112	-0.80317
H	-4.86618	-0.76967	-1.07096
H	-0.70042	0.00110	0.55846
H	-2.63791	-0.00226	1.85152
O	-2.27572	-0.00173	0.95961
H	-3.03653	-0.00142	0.33711

Zero-point correction=	0.150772 (Hartree/Particle)
Thermal correction to Energy=	0.161793
Thermal correction to Enthalpy=	0.162737
Thermal correction to Gibbs Free Energy=	0.112119
Sum of electronic and zero-point Energies=	-401.534133
Sum of electronic and thermal Energies=	-401.523113
Sum of electronic and thermal Enthalpies=	-401.522169
Sum of electronic and thermal Free Energies=	-401.572786

ELECTRONIC ENERGY = -401.6849056

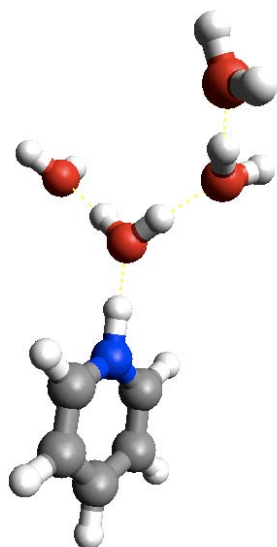
1P-3W



H	3.78476	2.72480	0.77023
N	-0.75072	-0.00000	-0.00000
C	-1.40108	-0.00002	1.17677
C	-2.78445	-0.00001	1.20681
C	-3.48383	0.00000	0.00000
C	-2.78445	0.00002	-1.20681
C	-1.40109	0.00001	-1.17677
H	-0.78371	-0.00003	2.06529
H	-3.30062	-0.00002	2.15748
H	-4.56731	0.00001	0.00001
H	-3.30062	0.00003	-2.15747
H	-0.78372	0.00002	-2.06529
O	3.36783	2.32392	0.00002
H	3.78472	2.72483	-0.77020
H	0.32095	-0.00001	-0.00000
H	2.43292	-0.79465	-0.00001
O	1.86366	0.00000	-0.00002
H	2.43292	0.79466	-0.00000
H	3.78474	-2.72482	0.77021
O	3.36783	-2.32392	-0.00001
H	3.78478	-2.72478	-0.77022

Zero-point correction= 0.174587 (Hartree/Particle)
 Thermal correction to Energy= 0.189141
 Thermal correction to Enthalpy= 0.190085
 Thermal correction to Gibbs Free Energy= 0.129628
 Sum of electronic and zero-point Energies= -477.986710
 Sum of electronic and thermal Energies= -477.972156
 Sum of electronic and thermal Enthalpies= -477.971212
 Sum of electronic and thermal Free Energies= -478.031669
 ELECTRONIC ENERGY = -478.1612968

1P-4W



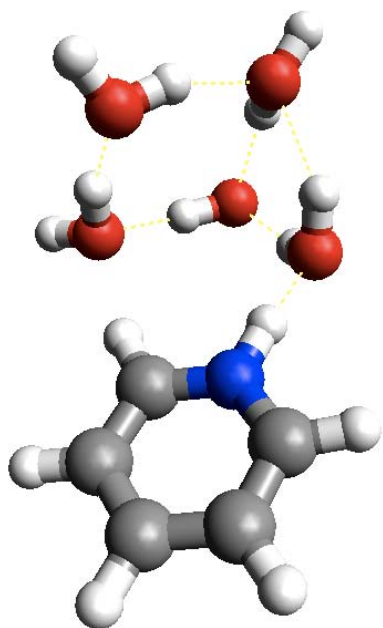
H	-2.25438	3.72068	-1.39043
N	1.37199	0.06534	0.02310
C	1.80413	-0.50908	-1.11233
C	3.10682	-0.96607	-1.21076
C	3.95574	-0.81913	-0.11401
C	3.48242	-0.22000	1.05307
C	2.17011	0.21794	1.09344
H	1.08211	-0.58483	-1.91469
H	3.44645	-1.42702	-2.12858
H	4.97960	-1.16941	-0.16842
H	4.11791	-0.09309	1.91925
H	1.72496	0.69187	1.95833
O	-1.84238	3.46778	-0.55748
H	-2.02037	4.18647	0.05849
H	0.34961	0.41514	0.07740
H	-1.83239	0.34110	0.46718
O	-1.07573	0.89169	0.15829
H	-1.39826	1.78053	-0.08325
H	-3.69975	-1.19826	0.51396
O	-3.04488	-0.71336	1.05249
H	-3.40344	-0.66941	1.94377
H	-5.73817	-1.77887	-0.82703
H	-4.98412	-3.08227	-0.49727
O	-4.92313	-2.12261	-0.44665

Zero-point correction=	0.198775 (Hartree/Particle)
Thermal correction to Energy=	0.216606
Thermal correction to Enthalpy=	0.217550
Thermal correction to Gibbs Free Energy=	0.147249
Sum of electronic and zero-point Energies=	-554.437663
Sum of electronic and thermal Energies=	-554.419832
Sum of electronic and thermal Enthalpies=	-554.418888

Sum of electronic and thermal Free Energies= -554.489189

ELECTRONIC ENERGY = -554.636438

1P-5W



H	3.60911	-0.87030	-0.01123
N	-1.45178	-0.61044	-0.05148
C	-1.53825	0.71922	-0.24203
C	-2.77372	1.34070	-0.17226
C	-3.90585	0.57238	0.09581
C	-3.78215	-0.80433	0.28725
C	-2.52667	-1.37791	0.20603
H	-0.60700	1.23779	-0.44838
H	-2.84335	2.40917	-0.32614
H	-4.88040	1.04236	0.15435
H	-4.64341	-1.42502	0.49478
H	-2.34123	-2.43575	0.33756
O	3.44891	-1.07913	0.92834
H	4.21956	-1.55854	1.25153
H	-0.49879	-1.07115	-0.11149
H	1.46865	-1.47217	-1.01439
O	0.92174	-1.81073	-0.28016
H	1.55094	-1.85568	0.45773
H	2.43650	0.58024	-1.55929
O	2.81913	-0.31584	-1.69507
H	3.23755	-0.32839	-2.56240
O	1.54188	1.94458	-0.78197
H	1.82309	1.89234	0.16190
H	1.72795	2.84242	-1.07730
H	2.54919	1.79146	2.51470
O	2.23610	1.29966	1.74935
H	2.77176	0.48565	1.68582

Zero-point correction=

0.228548 (Hartree/Particle)

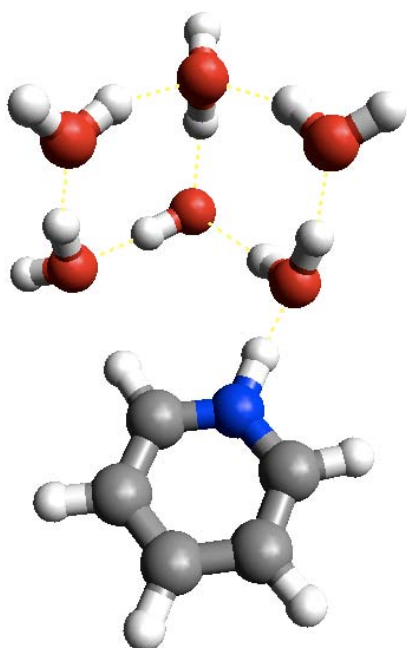
Thermal correction to Energy=

0.246403

Thermal correction to Enthalpy=	0.247347
Thermal correction to Gibbs Free Energy=	0.181861
Sum of electronic and zero-point Energies=	-630.888473
Sum of electronic and thermal Energies=	-630.870618
Sum of electronic and thermal Enthalpies=	-630.869674
Sum of electronic and thermal Free Energies=	-630.935160

ELECTRONIC ENERGY = -631.1170211

1P-6W



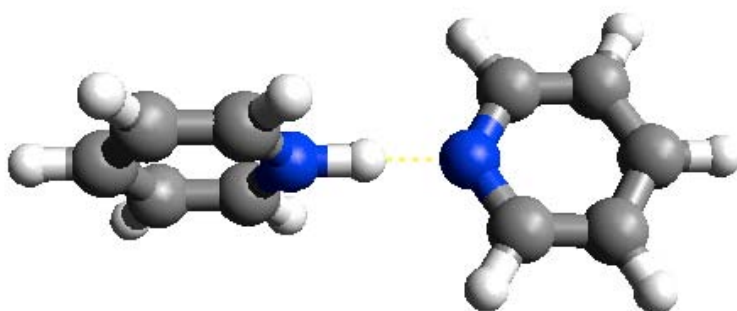
H	3.56306	0.17378	0.54971
N	-1.83107	0.52936	0.22046
C	-1.90724	-0.79905	0.02322
C	-3.12345	-1.37660	-0.30231
C	-4.25023	-0.56409	-0.41983
C	-4.13944	0.81028	-0.20739
C	-2.90165	1.33615	0.11627
H	-0.98419	-1.35835	0.14071
H	-3.18258	-2.44514	-0.46027
H	-5.20983	-0.99816	-0.67441
H	-4.99653	1.46505	-0.28988
H	-2.72833	2.38848	0.29930
O	3.93996	0.35447	-0.33692
H	4.89744	0.38667	-0.23247
H	-0.87996	0.96378	0.46855
H	1.07473	1.09393	1.39200
O	0.45849	1.63535	0.86622
H	1.01067	2.04792	0.16306
H	1.88843	-1.08777	1.58905
O	2.33492	-0.25706	1.87797
H	2.59944	-0.37594	2.79690
O	1.04839	-2.31361	0.61036
H	1.54241	-2.26268	-0.24208
H	1.09133	-3.23333	0.89393
H	2.75394	-2.11603	-2.42728
O	2.50753	-1.74011	-1.57747
H	3.14049	-1.02961	-1.36597
H	2.94767	1.86657	-0.98515
O	2.17528	2.45207	-1.07891

H 2.50472 3.32632 -1.30873

Zero-point correction=	0.253227 (Hartree/Particle)
Thermal correction to Energy=	0.273925
Thermal correction to Enthalpy=	0.274869
Thermal correction to Gibbs Free Energy=	0.202153
Sum of electronic and zero-point Energies=	-707.342570
Sum of electronic and thermal Energies=	-707.321873
Sum of electronic and thermal Enthalpies=	-707.320929
Sum of electronic and thermal Free Energies=	-707.393645

ELECTRONIC ENERGY = -707.5957978

2P-0W

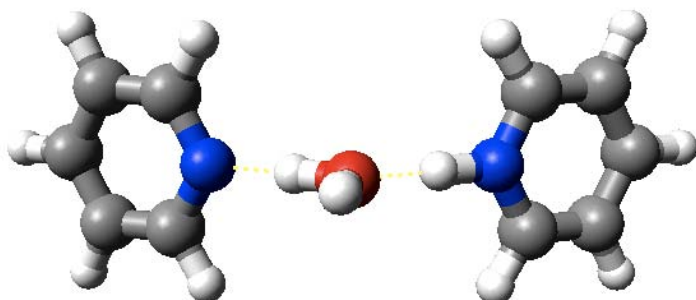


N	-1.36012	-0.00000	-0.00000
C	-2.01393	-1.03511	-0.55615
C	-3.39765	-1.06275	-0.57117
C	-4.09763	0.00000	0.00000
C	-3.39764	1.06276	0.57117
C	-2.01393	1.03511	0.55615
H	-1.40028	-1.82073	-0.97837
H	-3.91344	-1.90044	-1.02136
H	-5.18112	0.00001	0.00001
H	-3.91342	1.90045	1.02137
H	-1.40027	1.82072	0.97836
H	-0.25644	-0.00001	-0.00000
C	2.02105	0.55836	-1.01060
C	3.40923	0.58052	-1.05020
H	1.43427	0.99989	-1.80945
H	3.91952	1.04245	-1.88567
N	1.33458	-0.00001	-0.00001
C	4.11629	0.00001	0.00000
C	2.02105	-0.55834	1.01061
H	5.19983	0.00001	0.00000
C	3.40923	-0.58053	1.05020
H	1.43427	-0.99986	1.80946
H	3.91952	-1.04247	1.88566

Zero-point correction=	0.190985 (Hartree/Particle)
Thermal correction to Energy=	0.201301
Thermal correction to Enthalpy=	0.202245
Thermal correction to Gibbs Free Energy=	0.152181
Sum of electronic and zero-point Energies=	-496.918906
Sum of electronic and thermal Energies=	-496.908591
Sum of electronic and thermal Enthalpies=	-496.907647
Sum of electronic and thermal Free Energies=	-496.957710

ELECTRONIC ENERGY = -497.1098914

2P-1W

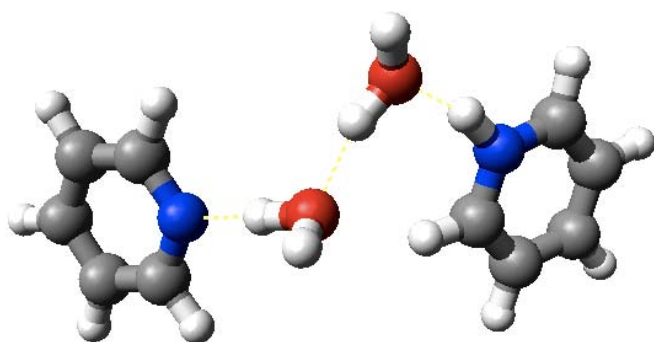


H	0.88527	-0.00004	1.08225
N	-2.40275	-0.00000	0.39065
C	-2.99004	1.17727	0.11152
C	-4.23903	1.20695	-0.48293
C	-4.87046	0.00000	-0.78340
C	-4.23897	-1.20695	-0.48306
C	-2.98998	-1.17728	0.11140
H	-2.43307	2.06589	0.37756
H	-4.70546	2.15759	-0.70415
H	-5.84906	0.00000	-1.24849
H	-4.70535	-2.15759	-0.70439
H	-2.43297	-2.06589	0.37733
O	-0.03389	-0.00007	1.52565
H	0.10156	0.00002	2.47855
H	-1.43921	-0.00001	0.85330
C	3.00005	-1.15150	0.09488
C	4.26961	-1.19901	-0.46927
H	2.46420	-2.06331	0.33732
H	4.73680	-2.15400	-0.67403
N	2.37092	-0.00002	0.37302
C	4.91653	0.00005	-0.75694
C	2.99996	1.15150	0.09482
H	5.90750	0.00008	-1.19541
C	4.26951	1.19907	-0.46934
H	2.46404	2.06327	0.33721
H	4.73663	2.15408	-0.67414

Zero-point correction=	0.216158 (Hartree/Particle)
Thermal correction to Energy=	0.229325
Thermal correction to Enthalpy=	0.230269
Thermal correction to Gibbs Free Energy=	0.171179
Sum of electronic and zero-point Energies=	-573.369907
Sum of electronic and thermal Energies=	-573.356739
Sum of electronic and thermal Enthalpies=	-573.355795
Sum of electronic and thermal Free Energies=	-573.414886

ELECTRONIC ENERGY = -573.5860641

2P-2W



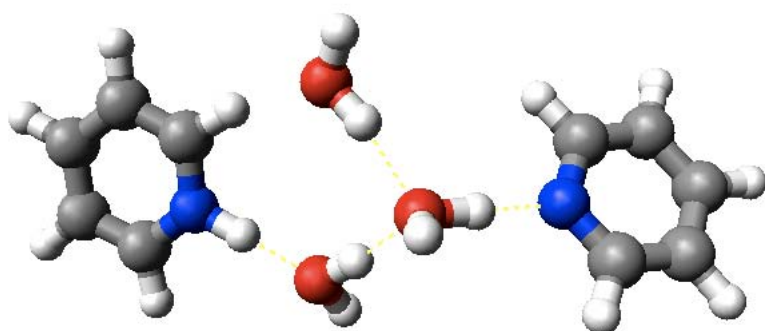
H	-1.25998	0.50051	1.07481
N	3.01425	0.60813	-0.12909
C	4.20500	0.66833	-0.75157
C	4.99447	-0.46355	-0.83973
C	4.53149	-1.65310	-0.27583
C	3.29151	-1.68396	0.36129
C	2.53872	-0.52393	0.42327
H	4.48889	1.62793	-1.16258
H	5.95183	-0.41179	-1.34059
H	5.13519	-2.55098	-0.33388
H	2.90985	-2.59344	0.80546
H	1.56397	-0.44515	0.89400
O	-0.38557	0.77542	1.49754
H	-0.57033	0.88943	2.43616
H	2.40566	1.46634	-0.05543
C	-3.40260	0.91271	-0.43638
C	-4.62467	0.61051	-1.02704
H	-2.93389	1.87857	-0.59427
H	-5.12037	1.34183	-1.65300
N	-2.73988	0.05146	0.34908
C	-5.18701	-0.64132	-0.79208
C	-3.28779	-1.15213	0.57057
H	-6.13901	-0.91010	-1.23458
C	-4.50530	-1.54113	0.02303
H	-2.72823	-1.82506	1.21238
H	-4.90621	-2.52447	0.23448
H	1.12135	3.45099	0.36591
O	1.18018	2.50629	0.19740
H	0.48093	2.04004	0.71842

Zero-point correction= 0.241807 (Hartree/Particle)
Thermal correction to Energy= 0.257775
Thermal correction to Enthalpy= 0.258720

Thermal correction to Gibbs Free Energy=	0.192638
Sum of electronic and zero-point Energies=	-649.818749
Sum of electronic and thermal Energies=	-649.802780
Sum of electronic and thermal Enthalpies=	-649.801836
Sum of electronic and thermal Free Energies=	-649.867917

ELECTRONIC ENERGY = -650.0605557

2P-3W

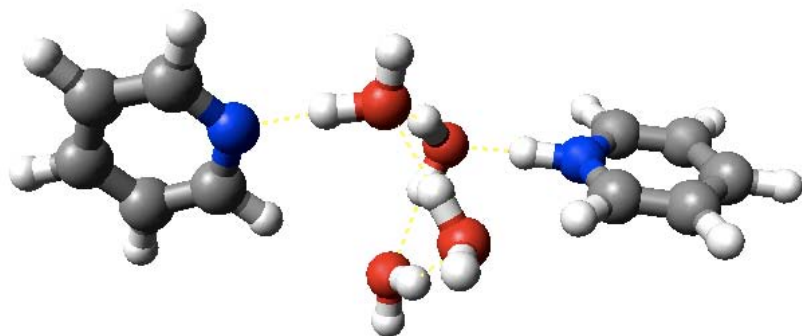


H	1.93785	-0.21710	1.02292
N	-3.33598	-0.54812	-0.15938
C	-4.37391	-1.35412	-0.45375
C	-5.63916	-0.82181	-0.60860
C	-5.81256	0.55498	-0.45317
C	-4.71923	1.36118	-0.14475
C	-3.46844	0.78215	0.00119
H	-4.15265	-2.40830	-0.55362
H	-6.47022	-1.47260	-0.84480
H	-6.79650	0.99342	-0.57045
H	-4.82731	2.42970	-0.01536
H	-2.56157	1.32669	0.25509
O	1.01515	-0.27218	1.44256
H	1.14759	-0.48049	2.37425
H	-2.38253	-0.97680	-0.05350
C	4.38926	-1.03102	0.44736
C	5.64947	-0.93880	-0.13263
H	4.12366	-1.88399	1.06354
H	6.37933	-1.72216	0.02842
N	3.44366	-0.09369	0.28721
C	5.94313	0.17517	-0.91463
C	3.73327	0.97660	-0.46716
H	6.91559	0.28030	-1.38111
C	4.96585	1.15207	-1.08603
H	2.94613	1.71553	-0.57608
H	5.15117	2.03463	-1.68526
H	-0.49890	-2.34809	-0.44494
O	-0.90588	-1.70258	0.14088
H	-0.17363	-1.24120	0.61525
H	-0.45640	2.72867	1.33569
O	-0.73380	1.89418	0.94614
H	-0.04512	1.24068	1.17172

Zero-point correction=	0.266597 (Hartree/Particle)
Thermal correction to Energy=	0.285687
Thermal correction to Enthalpy=	0.286631
Thermal correction to Gibbs Free Energy=	0.212543
Sum of electronic and zero-point Energies=	-726.270460
Sum of electronic and thermal Energies=	-726.251370
Sum of electronic and thermal Enthalpies=	-726.250426
Sum of electronic and thermal Free Energies=	-726.324515

ELECTRONIC ENERGY = -726.5370575

2P-4W

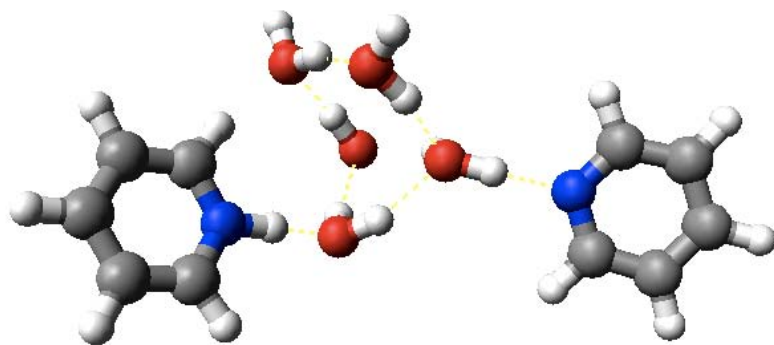


H	1.79851	-1.12535	0.42696
N	-3.29173	-0.14586	-0.56855
C	-3.56629	0.09209	0.72698
C	-4.87921	0.06724	1.16760
C	-5.89525	-0.20508	0.25236
C	-5.57882	-0.44729	-1.08478
C	-4.25123	-0.41070	-1.47239
H	-2.71051	0.29405	1.36409
H	-5.09794	0.25862	2.20963
H	-6.92847	-0.22852	0.57795
H	-6.34653	-0.66073	-1.81640
H	-3.91944	-0.58594	-2.48747
O	0.81947	-1.35917	0.58370
H	0.78446	-2.30639	0.75479
H	-2.26037	-0.11684	-0.88351
C	4.42946	-1.40576	0.25468
C	5.72260	-0.97739	-0.02253
H	4.24286	-2.42071	0.59062
H	6.55655	-1.65772	0.09563
N	3.35677	-0.61165	0.12746
C	5.91187	0.33364	-0.45166
C	3.54378	0.65138	-0.28604
H	6.90600	0.70121	-0.67766
C	4.80189	1.16324	-0.58551
H	2.65224	1.26458	-0.37472
H	4.90409	2.18905	-0.91683
H	-0.40713	0.84022	-1.13375
O	-0.77836	-0.04825	-1.31235
H	-0.19786	-0.65532	-0.80841
H	-0.00216	1.90358	0.80406
O	0.25888	2.19687	-0.09007
H	0.18847	3.15598	-0.11678
O	-0.52104	0.56491	2.04685
H	-0.00745	-0.19272	1.68733
H	-0.27505	0.64245	2.97483

Zero-point correction=	0.292955 (Hartree/Particle)
Thermal correction to Energy=	0.313719
Thermal correction to Enthalpy=	0.314663
Thermal correction to Gibbs Free Energy=	0.239499
Sum of electronic and zero-point Energies=	-802.721267
Sum of electronic and thermal Energies=	-802.700503
Sum of electronic and thermal Enthalpies=	-802.699559
Sum of electronic and thermal Free Energies=	-802.774723

ELECTRONIC ENERGY = -803.0142222

2P-5W



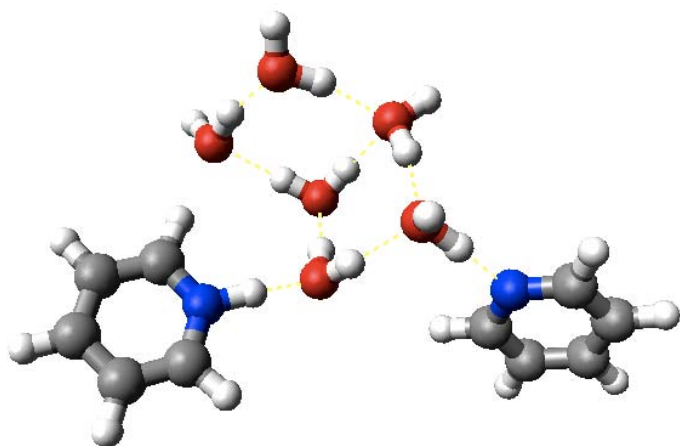
H	-1.18030	1.25382	0.84709
N	3.31971	-0.85013	0.25518
C	3.98150	0.22875	-0.20039
C	5.25235	0.07941	-0.73133
C	5.82109	-1.19201	-0.78346
C	5.10897	-2.29116	-0.30185
C	3.84440	-2.08794	0.21963
H	3.46546	1.18077	-0.12021
H	5.78352	0.94810	-1.09660
H	6.81397	-1.32740	-1.19568
H	5.52563	-3.28906	-0.32789
H	3.22582	-2.88193	0.61685
O	-1.23961	0.62131	0.11464
H	-2.19965	0.33799	0.03319
H	2.33920	-0.71970	0.66719
H	0.87308	0.20097	1.93372
O	0.93492	-0.57747	1.34748
H	0.14729	-0.46067	0.77633
H	0.99359	2.51313	1.54014
O	0.38690	2.03118	2.14214
H	0.29901	2.55720	2.94339
O	2.03118	2.90107	0.08110
H	1.47678	2.60743	-0.68152
H	2.27235	3.81809	-0.08644
H	0.11893	1.91352	-2.59558
O	0.47043	1.67102	-1.73401
H	-0.26652	1.27661	-1.21452
H	-4.40091	1.47353	-1.21354
C	-4.75446	0.54884	-0.76874
H	-6.78055	0.78425	-1.44448
C	-6.08420	0.16195	-0.89647
N	-3.84451	-0.17618	-0.10324
C	-4.24269	-1.32454	0.46198
C	-6.48982	-1.03234	-0.30679

C	-5.55069	-1.79120	0.38648
H	-3.48232	-1.88703	0.99417
H	-7.51824	-1.36494	-0.38560
H	-5.82185	-2.72588	0.86118

Zero-point correction=	0.318612 (Hartree/Particle)
Thermal correction to Energy=	0.342117
Thermal correction to Enthalpy=	0.343061
Thermal correction to Gibbs Free Energy=	0.259174
Sum of electronic and zero-point Energies=	-879.172834
Sum of electronic and thermal Energies=	-879.149330
Sum of electronic and thermal Enthalpies=	-879.148385
Sum of electronic and thermal Free Energies=	-879.232272

ELECTRONIC ENERGY = -879.4914461

2P-6W



H	-2.40340	0.34508	-1.16369
N	2.83673	-1.33203	-0.08528
C	3.02451	-2.62223	-0.41498
C	4.30428	-3.13126	-0.53769
C	5.38839	-2.28231	-0.31067
C	5.16403	-0.95103	0.03368
C	3.86117	-0.49053	0.14328
H	2.13040	-3.21201	-0.56870
H	4.44681	-4.17024	-0.80295
H	6.40051	-2.65878	-0.40013
H	5.98535	-0.27166	0.21846
H	3.60810	0.53051	0.41702
O	-1.52753	0.75198	-1.47452
H	-1.51141	0.68239	-2.43523
H	1.82676	-0.96449	0.00400
C	-3.62695	-1.11201	0.60148
C	-4.69564	-1.72285	1.24840
H	-2.61154	-1.23031	0.96601
H	-4.52196	-2.32613	2.13059
N	-3.77962	-0.35140	-0.49280
C	-5.97813	-1.53871	0.73864
C	-5.01722	-0.17738	-0.97822
H	-6.83360	-2.00009	1.21794
C	-6.14291	-0.75067	-0.39749
H	-5.10568	0.44443	-1.86325
H	-7.12175	-0.58044	-0.82788
H	0.37240	0.25227	0.90202
O	0.37919	-0.48178	0.23104
H	-0.19745	-0.16323	-0.49012
H	1.38179	1.99510	1.80098
O	0.46654	1.66103	1.84033
H	-0.06315	2.32057	1.36315
O	1.79599	3.77054	-0.92246

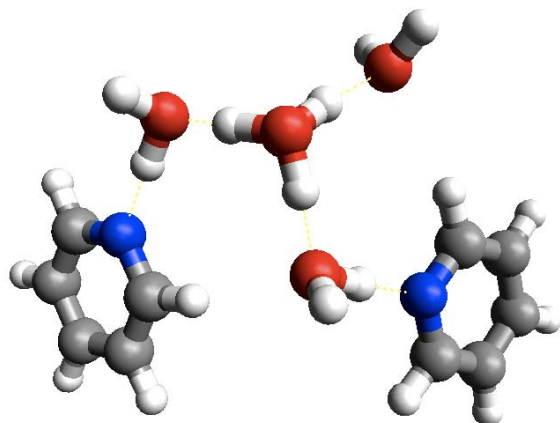
H	1.95173	4.55691	-1.45327
H	0.83033	3.68861	-0.79561
H	3.62182	3.09064	1.67084
H	2.75931	3.07030	0.37187
O	3.08620	2.51471	1.11533
H	-1.59652	3.76470	-0.22551
H	-1.18168	2.35844	-0.77322
O	-0.85740	3.15043	-0.28665

Zero-point correction=	0.343783 (Hartree/Particle)
Thermal correction to Energy=	0.369884
Thermal correction to Enthalpy=	0.370828
Thermal correction to Gibbs Free Energy=	0.281270
Sum of electronic and zero-point Energies=	-955.623814
Sum of electronic and thermal Energies=	-955.597714
Sum of electronic and thermal Enthalpies=	-955.596770
Sum of electronic and thermal Free Energies=	-955.686327

ELECTRONIC ENERGY = -955.9675975

Cartesian coordinates (Å) and energies (Hartree) for hydroxonium-containing structures for clusters with 2 pyridines, by B3LYP/6-31G*.

2P-4W



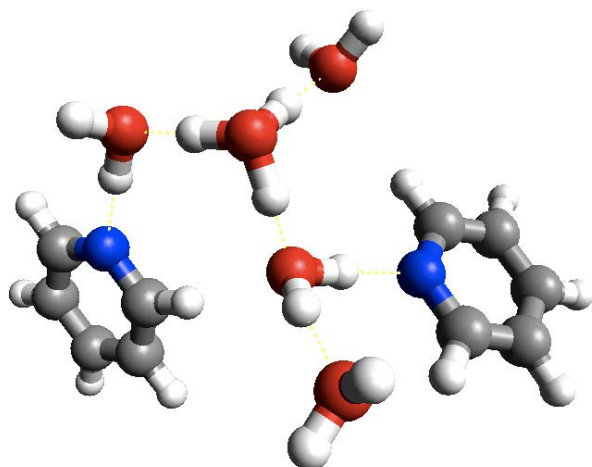
H	0.21372	1.80414	1.25674
O	0.52892	0.41091	1.68789
H	1.34032	0.01443	1.21087
H	0.73460	0.38045	2.63592
C	3.45837	0.16435	-0.36111
C	4.59572	-0.31739	-1.00422
H	3.13724	1.19594	-0.48761
H	5.18079	0.33926	-1.63985
N	2.69676	-0.60130	0.43779
C	4.95998	-1.65020	-0.81122
C	3.05106	-1.88377	0.61785
H	5.84183	-2.05788	-1.29649
C	4.17152	-2.45020	0.01569
H	2.40949	-2.47229	1.26900
H	4.41672	-3.49203	0.19371
H	2.25647	4.33392	-0.59583
O	1.76899	3.53053	-0.84031
H	1.48873	3.66858	-1.75955
H	0.57538	3.08189	0.25250
H	-1.06962	2.70772	0.51311
O	-0.07518	2.75529	0.93886
H	-4.74411	-3.42817	-0.30460
H	-5.89094	-1.53482	-1.49106
C	-4.97597	-1.37417	-0.93053
C	-4.33508	-2.42267	-0.27050
C	-4.41662	-0.10136	-0.85720
C	-3.15982	-2.15791	0.43295
H	-2.62984	-2.94537	0.95885
H	-4.88170	0.74440	-1.35735
N	-3.28768	0.15847	-0.17829
C	-2.67028	-0.85423	0.45335

H	-1.75353	-0.60397	0.98298
H	-2.97417	3.16390	0.45687
H	-2.70358	1.69380	-0.11818
O	-2.33332	2.65219	-0.06230

Zero-point correction=	0.290150 (Hartree/Particle)
Thermal correction to Energy=	0.311103
Thermal correction to Enthalpy=	0.312047
Thermal correction to Gibbs Free Energy=	0.233603
Sum of electronic and zero-point Energies=	-802.410957
Sum of electronic and thermal Energies=	-802.390003
Sum of electronic and thermal Enthalpies=	-802.389059
Sum of electronic and thermal Free Energies=	-802.467503

ELECTRONIC ENERGY = -802.7011062

2P-5W



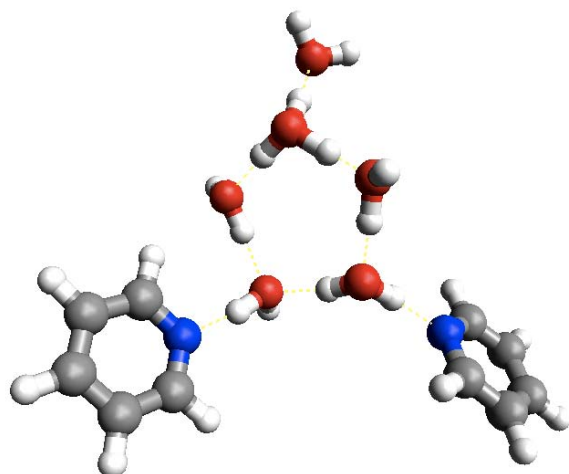
H	0.13967	1.56331	1.14714
O	0.45876	0.23918	1.28827
H	1.26680	0.01474	0.71556
H	0.72706	-0.01149	2.20501
C	3.08885	0.16923	-1.28315
C	4.24475	-0.22700	-1.95195
H	2.43979	0.94122	-1.69007
H	4.50646	0.22638	-2.90258
N	2.71466	-0.35744	-0.10641
C	5.04739	-1.21117	-1.37436
C	3.49355	-1.30017	0.44797
H	5.95455	-1.54491	-1.86960
C	4.66640	-1.75693	-0.14847
H	3.15975	-1.68907	1.40723
H	5.26340	-2.52124	0.33830
H	1.69795	4.09129	-1.21820
O	1.06238	3.36143	-1.29389
H	0.45402	3.62578	-2.00294
H	0.28847	2.93860	0.15884
H	-1.20398	2.60880	0.77728
O	-0.17443	2.59817	0.97583
H	-4.71439	-3.46520	-1.03033
H	-6.18223	-1.47397	-1.46558
C	-5.19408	-1.35924	-1.03225
C	-4.37534	-2.46198	-0.78895
C	-4.71671	-0.09211	-0.70690
C	-3.11357	-2.25327	-0.23196
H	-2.44412	-3.08312	-0.02939
H	-5.32090	0.79451	-0.88305
N	-3.50479	0.11405	-0.16773
C	-2.71798	-0.95042	0.06345
H	-1.74074	-0.74210	0.49454
H	-3.19731	2.96705	1.09551
H	-2.97708	1.68606	0.18118

O	-2.62913	2.61791	0.39143
H	1.03007	-1.35118	4.17644
O	1.51789	-0.70226	3.64613
H	1.96041	-0.12890	4.29091

Zero-point correction=	0.314416 (Hartree/Particle)
Thermal correction to Energy=	0.338886
Thermal correction to Enthalpy=	0.339830
Thermal correction to Gibbs Free Energy=	0.252624
Sum of electronic and zero-point Energies=	-878.816165
Sum of electronic and thermal Energies=	-878.791694
Sum of electronic and thermal Enthalpies=	-878.790750
Sum of electronic and thermal Free Energies=	-878.877956

ELECTRONIC ENERGY = -879.1305802

2P-6W(a)



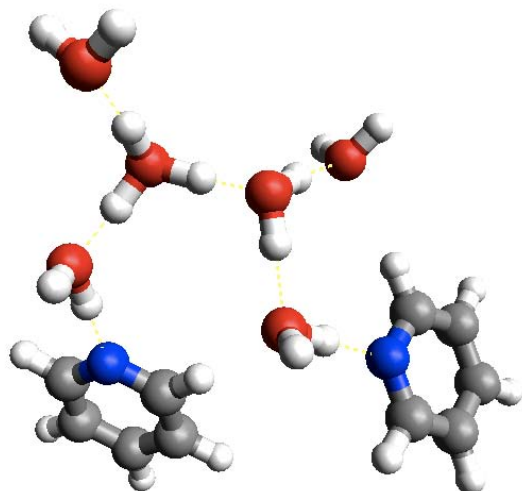
H	-0.25764	3.13433	1.13824
O	-0.88618	-0.12686	-1.28738
H	-1.61058	-0.76645	-0.95373
H	-0.61847	-0.46185	-2.15784
C	-3.01301	-2.92137	-0.16081
C	-4.16756	-3.55104	0.29696
H	-2.09960	-3.48524	-0.33264
H	-4.16577	-4.61946	0.48618
N	-2.95488	-1.60450	-0.41334
C	-5.31157	-2.77964	0.50267
C	-4.05850	-0.86493	-0.21210
H	-6.22952	-3.23800	0.85876
C	-5.25603	-1.40997	0.24420
H	-3.96401	0.19775	-0.42351
H	-6.12191	-0.77291	0.39214
H	-1.15669	6.77481	0.00219
O	-0.60646	6.04096	-0.31458
H	0.30738	6.36067	-0.25185
H	-1.63816	3.10818	0.02421
H	-0.95224	4.55592	0.37519
O	-1.19096	3.66057	0.75315
H	7.05829	-2.42987	-0.23235
H	6.56689	-0.39251	-1.61651
C	5.82541	-0.80217	-0.93815
C	6.09442	-1.93345	-0.16748
C	4.57540	-0.19813	-0.82077
C	5.10391	-2.41431	0.68878
H	5.27001	-3.28993	1.30805
H	4.32826	0.68690	-1.40253
N	3.61700	-0.65509	-0.00111
C	3.88407	-1.74307	0.73783
H	3.08335	-2.07972	1.39220
H	1.99437	-0.01055	0.34540
H	0.44712	0.01768	-0.05038

O	1.07959	0.22070	0.67496
H	-2.48249	2.57316	-1.93620
O	-2.28079	2.16434	-1.08103
H	-1.72580	1.35927	-1.27095
H	0.95865	1.60875	1.16974
H	0.78801	2.45832	2.52889
O	0.82563	2.56984	1.56509

Zero-point correction=	0.340090 (Hartree/Particle)
Thermal correction to Energy=	0.366146
Thermal correction to Enthalpy=	0.367090
Thermal correction to Gibbs Free Energy=	0.273668
Sum of electronic and zero-point Energies=	-955.226092
Sum of electronic and thermal Energies=	-955.200036
Sum of electronic and thermal Enthalpies=	-955.199092
Sum of electronic and thermal Free Energies=	-955.292515

ELECTRONIC ENERGY = -955.5661822

2P-6W(b)



H	-0.29208	-2.02469	-0.72966
O	0.39501	-0.66830	-1.43923
H	1.33848	-0.53733	-1.11694
H	0.47774	-0.81596	-2.39435
C	3.49842	-1.02811	0.44840
C	4.80734	-0.88161	0.90378
H	2.81801	-1.73635	0.91642
H	5.16326	-1.47848	1.73749
N	3.00191	-0.31803	-0.57786
C	5.63950	0.03972	0.26820
C	3.80848	0.56724	-1.18373
H	6.66542	0.17786	0.59690
C	5.12992	0.78027	-0.79826
H	3.37421	1.12444	-2.01081
H	5.74050	1.50744	-1.32366
H	1.38764	-4.26871	1.80394
O	1.03572	-3.36462	1.80030
H	0.75850	-3.19629	2.71460
H	-0.14482	-3.03292	0.48441
H	-2.01063	-2.48930	0.13564
O	-0.72690	-2.80530	-0.27733
H	-0.53215	5.46592	0.75340
H	-2.97326	5.21456	1.28791
C	-2.40840	4.40015	0.84617
C	-1.05251	4.53493	0.54755
C	-3.03330	3.18807	0.56366
C	-0.37747	3.45411	-0.01980
H	0.67763	3.51739	-0.26637
H	-4.08814	3.03654	0.77912
N	-2.38733	2.14629	0.01729
C	-1.08154	2.27766	-0.26950
H	-0.59578	1.40857	-0.70945

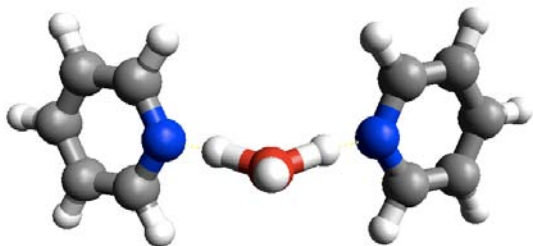
H	-4.03731	-0.06903	-1.40436
H	-3.27173	0.74252	-0.27651
O	-3.85337	-0.07226	-0.45288
H	-3.64183	-2.98284	0.09574
O	-3.02757	-2.27756	0.45098
H	-3.34840	-1.35372	0.07179
H	-5.55186	-4.20957	-0.08377
O	-4.74311	-4.04598	-0.59385
H	-4.43641	-4.92028	-0.88025

Zero-point correction=	0.339282 (Hartree/Particle)
Thermal correction to Energy=	0.366760
Thermal correction to Enthalpy=	0.367704
Thermal correction to Gibbs Free Energy=	0.271629
Sum of electronic and zero-point Energies=	-955.220364
Sum of electronic and thermal Energies=	-955.192887
Sum of electronic and thermal Enthalpies=	-955.191942
Sum of electronic and thermal Free Energies=	-955.288017

ELECTRONIC ENERGY = -955.5596461

Proton transfer transition structures for clusters with two pyridines by B3LYP/6-31G*.
Cartesian coordinates (Å) and energies (Hartree) for corresponding transition states.

2P-1W_TS

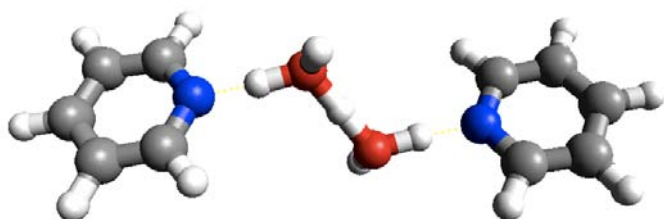


H	1.06686	-0.28806	0.87231
N	-2.23358	-0.08654	0.36665
C	-2.92365	-1.16308	-0.04726
C	-4.19579	-1.04607	-0.59388
C	-4.76048	0.22553	-0.70913
C	-4.03636	1.33787	-0.27497
C	-2.76957	1.14102	0.26052
H	-2.42737	-2.12093	0.07342
H	-4.72952	-1.93224	-0.91927
H	-5.75326	0.34858	-1.13109
H	-4.44440	2.34002	-0.34780
H	-2.15932	1.96519	0.61687
O	0.00000	-0.60011	1.32734
H	0.00000	-0.55612	2.29596
H	-1.06686	-0.28807	0.87231
C	2.92367	-1.16308	-0.04723
C	4.19581	-1.04607	-0.59385
H	2.42740	-2.12093	0.07347
H	4.72955	-1.93225	-0.91921
N	2.23358	-0.08653	0.36665
C	4.76048	0.22554	-0.70913
C	2.76956	1.14102	0.26049
H	5.75326	0.34859	-1.13109
C	4.03635	1.33788	-0.27500
H	2.15929	1.96520	0.61682
H	4.44437	2.34003	-0.34786

Zero-point correction=	0.210974 (Hartree/Particle)
Thermal correction to Energy=	0.223429
Thermal correction to Enthalpy=	0.224373
Thermal correction to Gibbs Free Energy=	0.167368
Sum of electronic and zero-point Energies=	-573.197518
Sum of electronic and thermal Energies=	-573.185063
Sum of electronic and thermal Enthalpies=	-573.184118
Sum of electronic and thermal Free Energies=	-573.241124

ELECTRONIC ENERGY = -573.408492

2P-2W_TS

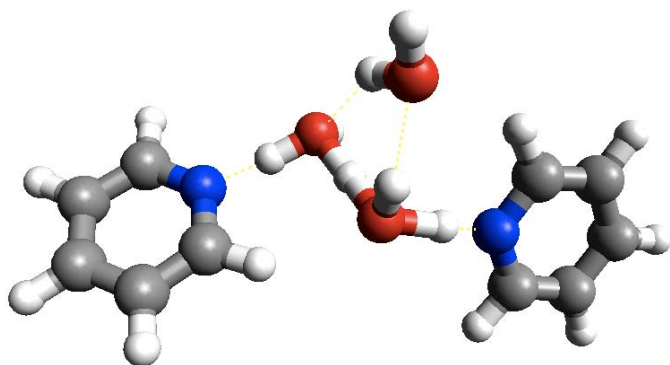


H	1.83554	0.39216	0.48832
N	-3.25378	-0.15009	-0.24336
C	-4.04365	-1.21141	-0.00734
C	-5.40872	-1.08256	0.22648
C	-5.97156	0.19434	0.21359
C	-5.15036	1.29589	-0.03205
C	-3.79493	1.07969	-0.25626
H	-3.55474	-2.18154	-0.00947
H	-6.01298	-1.96386	0.41287
H	-7.03416	0.32925	0.39165
H	-5.54967	2.30425	-0.05112
H	-3.11434	1.90362	-0.45257
O	0.78552	0.64709	0.65466
H	0.59906	0.55001	1.60309
H	-1.83554	-0.39228	-0.48826
C	3.79500	-1.07970	0.25624
C	5.15043	-1.29581	0.03199
H	3.11446	-1.90367	0.45256
H	5.54980	-2.30415	0.05103
N	3.25378	0.15005	0.24338
C	5.97157	-0.19422	-0.21366
C	4.04358	1.21142	0.00735
H	7.03416	-0.32907	-0.39175
C	5.40865	1.08265	-0.22651
H	3.55462	2.18152	0.00951
H	6.01286	1.96399	-0.41291
H	-0.59905	-0.55024	-1.60299
O	-0.78553	-0.64727	-0.65455
H	-0.00000	-0.00009	0.00005

Zero-point correction= 0.235552 (Hartree/Particle)
Thermal correction to Energy= 0.250342
Thermal correction to Enthalpy= 0.251286
Thermal correction to Gibbs Free Energy= 0.186305
Sum of electronic and zero-point Energies= -649.599093
Sum of electronic and thermal Energies= -649.584304
Sum of electronic and thermal Enthalpies= -649.583359
Sum of electronic and thermal Free Energies= -649.648340

ELECTRONIC ENERGY = -649.834645

2P-3W_TS



H	-2.07030	0.77538	-0.76422
N	2.75384	-0.39263	0.15235
C	3.27821	-1.60980	-0.06181
C	4.62548	-1.77394	-0.35950
C	5.43877	-0.64066	-0.43030
C	4.88196	0.61904	-0.20134
C	3.52603	0.70681	0.09117
H	2.59170	-2.44738	0.01290
H	5.02634	-2.76730	-0.52884
H	6.49563	-0.73941	-0.65904
H	5.48629	1.51851	-0.24520
H	3.01991	1.64846	0.28914
O	-0.79555	1.29922	-0.92079
H	-0.46280	1.22199	-1.82864
H	1.58793	-0.22799	0.45586
C	-2.91657	-0.73745	0.46105
C	-4.03370	-1.44004	0.89302
H	-1.90742	-0.91318	0.82572
H	-3.92444	-2.22243	1.63567
N	-3.03849	0.23765	-0.45968
C	-5.28235	-1.11765	0.35685
C	-4.23116	0.56600	-0.98605
H	-6.17018	-1.65319	0.67901
C	-5.38419	-0.10021	-0.59561
H	-4.23113	1.36747	-1.71700
H	-6.33960	0.17437	-1.02842
H	0.43845	0.72425	1.35456
O	0.36325	-0.03399	0.73371
H	-0.15975	0.57315	-0.17387
H	0.53345	3.43226	1.56082
O	0.74843	2.63144	1.05968
H	0.13466	2.61394	0.29718

Zero-point correction=

0.260952 (Hartree/Particle)

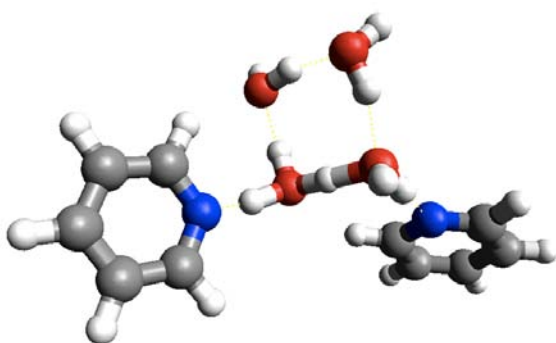
Thermal correction to Energy=

0.277240

Thermal correction to Enthalpy=	0.278184
Thermal correction to Gibbs Free Energy=	0.213476
Sum of electronic and zero-point Energies=	-726.000760
Sum of electronic and thermal Energies=	-725.984473
Sum of electronic and thermal Enthalpies=	-725.983529
Sum of electronic and thermal Free Energies=	-726.048236

ELECTRONIC ENERGY = -726.261712

2P-4W_TS



H	-2.16476	0.41953	-0.87095
N	2.68758	-0.67223	0.09440
C	3.06258	-1.89679	-0.30959
C	4.39284	-2.21788	-0.55539
C	5.36329	-1.23098	-0.37258
C	4.97020	0.03901	0.05063
C	3.61877	0.28139	0.27569
H	2.26800	-2.62722	-0.43324
H	4.65910	-3.21788	-0.88055
H	6.41090	-1.45045	-0.55575
H	5.69526	0.83065	0.20615
H	3.24987	1.24650	0.61458
O	-0.94846	1.01121	-1.17647
H	-0.62726	0.74582	-2.05300
H	1.42395	-0.29938	0.37724
C	-2.92026	-0.87091	0.62895
C	-3.99367	-1.54647	1.19389
H	-1.90837	-0.90926	1.02191
H	-3.84234	-2.15909	2.07563
N	-3.09157	-0.10535	-0.46485
C	-5.25457	-1.41777	0.60691
C	-4.29731	0.03325	-1.04280
H	-6.10970	-1.93625	1.02967
C	-5.41014	-0.61650	-0.52711
H	-4.34079	0.67255	-1.91819
H	-6.37607	-0.49540	-1.00451
H	0.63418	0.96538	1.17056
O	0.39469	0.13139	0.66149
H	-0.17152	0.51775	-0.24912
H	0.86250	3.02206	0.76913
O	1.27940	2.46905	1.48806
H	1.12057	2.93167	2.32411
O	0.01895	3.50609	-0.62574
H	-0.46279	2.69215	-0.92096
H	-0.63987	4.21390	-0.58006

Zero-point correction=

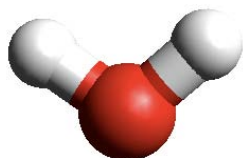
0.287094 (Hartree/Particle)

Thermal correction to Energy=	0.306411
Thermal correction to Enthalpy=	0.307355
Thermal correction to Gibbs Free Energy=	0.233893
Sum of electronic and zero-point Energies=	-802.414484
Sum of electronic and thermal Energies=	-802.395167
Sum of electronic and thermal Enthalpies=	-802.394223
Sum of electronic and thermal Free Energies=	-802.467685

ELECTRONIC ENERGY = -802.701578

Structures for proposed mechanism of H/D exchange in clusters containing two pyridines.
Cartesian coordinates (Å) and energies (Hartree), by B3LYP/6-31G*.

H2O

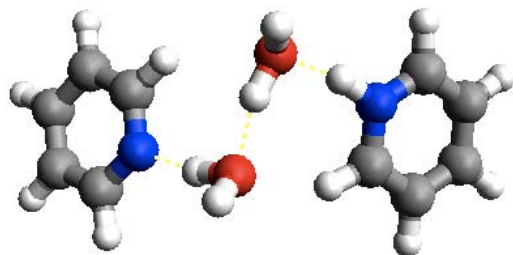


H	0.76155	-0.47898	0.00000
O	0.00000	0.11975	0.00000
H	-0.76155	-0.47899	0.00000

Zero-point correction=	0.015401 (Hartree/Particle)
Thermal correction to Energy=	0.018247
Thermal correction to Enthalpy=	0.019191
Thermal correction to Gibbs Free Energy=	-0.003986
Sum of electronic and zero-point Energies=	-76.393553
Sum of electronic and thermal Energies=	-76.390707
Sum of electronic and thermal Enthalpies=	-76.389763
Sum of electronic and thermal Free Energies=	-76.412940

ELECTRONIC ENERGY = -76.408954

A



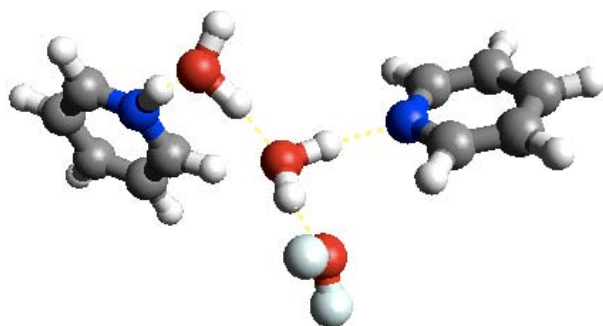
H	-1.13596	-0.44340	1.36625
N	2.66865	0.59510	0.07223
C	3.70843	1.05963	-0.64823
C	4.68694	0.18539	-1.09282
C	4.56987	-1.17283	-0.78106
C	3.47838	-1.62396	-0.03505
C	2.52486	-0.70882	0.38759
H	3.72105	2.12500	-0.84748
H	5.52223	0.56240	-1.67175
H	5.32579	-1.87461	-1.11989
H	3.36349	-2.67186	0.21765
H	1.63709	-0.95633	0.96616
O	-0.27927	-0.31168	1.89268
H	-0.52028	-0.46009	2.82048
H	1.91546	1.26393	0.41289
C	-2.73571	0.80531	-0.23685
C	-3.85022	1.06072	-1.03181
H	-1.94784	1.54584	-0.11640
H	-3.94772	2.01292	-1.54306
N	-2.56014	-0.35285	0.42103
C	-4.82681	0.07145	-1.14973
C	-3.50265	-1.30101	0.30219
H	-5.70998	0.23664	-1.75983
C	-4.64970	-1.13370	-0.46998
H	-3.32750	-2.22494	0.84780
H	-5.38374	-1.93032	-0.53305
H	0.67360	2.75433	1.60274
O	0.58783	2.01802	0.97774
H	0.16595	1.26101	1.47591

Zero-point correction=	0.243720 (Hartree/Particle)
Thermal correction to Energy=	0.259127
Thermal correction to Enthalpy=	0.260071
Thermal correction to Gibbs Free Energy=	0.196957
Sum of electronic and zero-point Energies=	-649.604337
Sum of electronic and thermal Energies=	-649.588930
Sum of electronic and thermal Enthalpies=	-649.587986

Sum of electronic and thermal Free Energies= -649.651099

ELECTRONIC ENERGY = -649.8480563

B



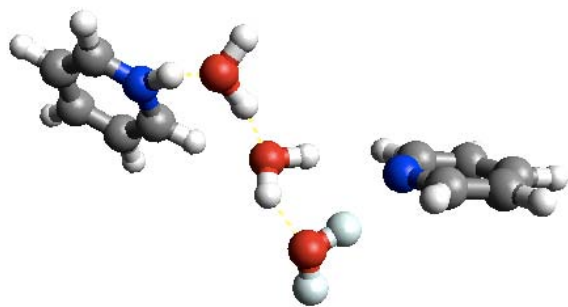
H	-0.99748	0.34833	-0.16215
N	3.14644	-0.01074	0.63566
C	2.76803	-0.18897	-0.64655
C	3.68851	-0.66032	-1.57252
C	4.99169	-0.93925	-1.15450
C	5.35191	-0.73955	0.18186
C	4.39620	-0.26729	1.06721
H	1.73225	0.06827	-0.86550
H	3.38548	-0.80388	-2.60347
H	5.72501	-1.30852	-1.86492
H	6.35669	-0.94480	0.53308
H	4.59203	-0.08181	2.11716
O	-0.16052	0.89798	-0.17865
H	-0.46670	1.78270	-0.47767
H	0.51682	1.03086	1.32520
C	-2.94772	-1.67895	0.04000
C	-4.26076	-2.14097	0.09746
H	-2.11254	-2.37455	0.08066
H	-4.46096	-3.20403	0.18454
N	-2.63243	-0.37929	-0.06762
C	-5.29788	-1.20994	0.03965
C	-3.63656	0.51102	-0.12527
H	-6.33392	-1.53321	0.08173
C	-4.97955	0.14315	-0.07467
H	-3.34183	1.55394	-0.21951
H	-5.75421	0.90164	-0.12451
H	2.40408	0.35819	1.31776
O	1.17632	1.00131	2.08464
H	0.75888	0.48184	2.78869
D	-1.31883	4.08336	-0.23112
O	-1.41860	3.31508	-0.81415
D	-1.50359	3.68333	-1.70698

Zero-point correction= 0.261577 (Hartree/Particle)
Thermal correction to Energy= 0.280822

Thermal correction to Enthalpy=	0.281766
Thermal correction to Gibbs Free Energy=	0.208055
Sum of electronic and zero-point Energies=	-726.014282
Sum of electronic and thermal Energies=	-725.995037
Sum of electronic and thermal Enthalpies=	-725.994093
Sum of electronic and thermal Free Energies=	-726.067804

ELECTRONIC ENERGY = -726.2758585

TS1



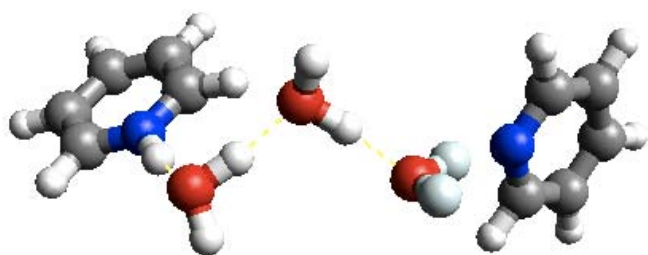
H	-0.80336	0.16397	0.18236
N	3.49855	-0.34854	-0.54186
C	3.17860	0.60891	0.35215
C	4.18110	1.38887	0.91050
C	5.50696	1.16240	0.53293
C	5.80528	0.15873	-0.39367
C	4.76746	-0.59280	-0.92173
H	2.12032	0.69649	0.58673
H	3.92424	2.15791	1.63006
H	6.30506	1.76220	0.95953
H	6.82521	-0.04099	-0.70170
H	4.91085	-1.39153	-1.64038
O	0.04795	-0.21907	0.46274
H	-0.25346	-0.77682	1.22687
H	0.70522	-1.28567	-0.70979
C	-3.36713	1.22580	-0.31660
C	-4.62490	1.76775	-0.56892
H	-2.48723	1.86695	-0.32669
H	-4.72818	2.82440	-0.79363
N	-3.16077	-0.06610	-0.00584
C	-5.73138	0.91833	-0.54519
C	-4.23646	-0.87508	0.00001
H	-6.72847	1.30180	-0.74068
C	-5.53099	-0.43332	-0.26682
H	-4.04966	-1.92081	0.23613
H	-6.35929	-1.13403	-0.24421
H	2.69638	-0.93173	-0.94353
O	1.37090	-1.73870	-1.29803
H	1.01289	-1.70541	-2.19809
D	-1.81430	-1.27405	2.98893
O	-1.55839	-1.56922	2.10154
D	-2.21576	-1.17182	1.49591

Zero-point correction= 0.261284 (Hartree/Particle)
Thermal correction to Energy= 0.278970
Thermal correction to Enthalpy= 0.279914

Thermal correction to Gibbs Free Energy=	0.210083
Sum of electronic and zero-point Energies=	-726.005626
Sum of electronic and thermal Energies=	-725.987939
Sum of electronic and thermal Enthalpies=	-725.986995
Sum of electronic and thermal Free Energies=	-726.056827

ELECTRONIC ENERGY = -726.266910

C



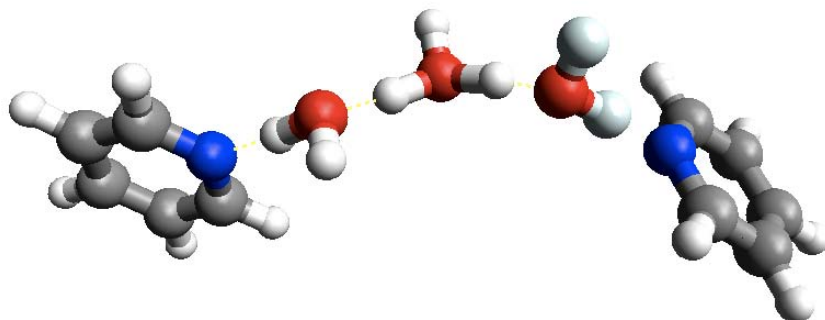
H	-0.70088	1.98689	-2.03129
N	-3.83823	0.26595	0.22217
C	-3.05317	-0.59165	-0.46082
C	-3.48202	-1.89453	-0.67101
C	-4.72437	-2.28978	-0.16920
C	-5.51565	-1.37431	0.53142
C	-5.04181	-0.08493	0.71438
H	-2.11125	-0.18008	-0.81745
H	-2.85164	-2.58429	-1.22056
H	-5.07692	-3.30486	-0.32435
H	-6.48500	-1.65294	0.92861
H	-5.59156	0.68685	1.24088
O	-0.82675	1.63801	-1.13558
H	0.06994	1.71514	-0.68567
H	-1.98323	2.49436	-0.23291
C	4.33482	-0.14355	-1.09138
C	5.47896	-0.93300	-0.99943
H	3.95273	0.17251	-2.05922
H	6.00170	-1.24108	-1.89916
N	3.64568	0.27149	-0.01763
C	5.92986	-1.30909	0.26600
C	4.08599	-0.09412	1.19635
H	6.81933	-1.92260	0.37583
C	5.21912	-0.88153	1.38749
H	3.50271	0.26398	2.04143
H	5.53460	-1.14856	2.39090
H	-3.47177	1.26304	0.35845
O	-2.77971	2.69553	0.33494
H	-2.43216	3.03981	1.17218
D	1.83520	2.81655	0.12361
O	1.44765	1.92990	0.17143
D	2.21614	1.30457	0.01782

Zero-point correction= 0.261612 (Hartree/Particle)
Thermal correction to Energy= 0.280464

Thermal correction to Enthalpy=	0.281408
Thermal correction to Gibbs Free Energy=	0.206224
Sum of electronic and zero-point Energies=	-726.014759
Sum of electronic and thermal Energies=	-725.995908
Sum of electronic and thermal Enthalpies=	-725.994963
Sum of electronic and thermal Free Energies=	-726.070148

ELECTRONIC ENERGY = -726.2763717

TS2



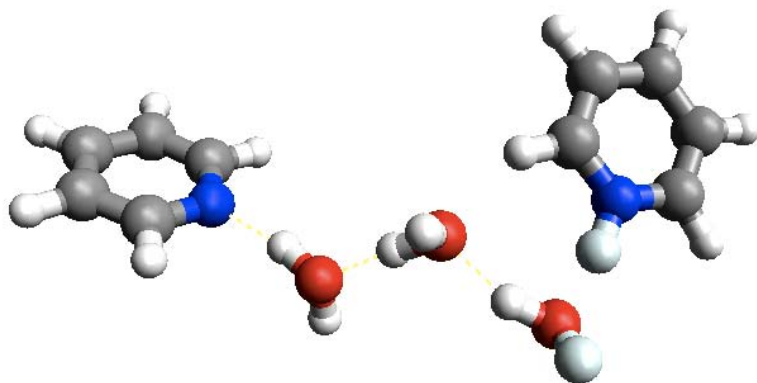
H	-0.16140	-1.51798	1.80056
N	-4.11011	-0.07188	-0.20466
C	-4.18477	1.26826	-0.17485
C	-5.38687	1.95162	-0.01348
C	-6.56222	1.21219	0.12251
C	-6.49010	-0.18061	0.09222
C	-5.24409	-0.77926	-0.07342
H	-3.24579	1.80496	-0.28472
H	-5.39766	3.03643	0.00391
H	-7.51750	1.71287	0.24943
H	-7.37916	-0.79414	0.19378
H	-5.13885	-1.86076	-0.10362
O	0.03154	-1.08020	0.95466
H	1.01216	-1.47313	0.50430
H	-0.80520	-1.25205	0.29794
C	4.69724	0.21823	1.13828
C	5.81859	1.04157	1.11422
H	4.21059	-0.04243	2.07434
H	6.22322	1.43554	2.04045
N	4.15651	-0.29681	0.02200
C	6.40106	1.34143	-0.11789
C	4.71834	-0.00651	-1.16326
H	7.27758	1.98012	-0.17200
C	5.84064	0.80792	-1.27890
H	4.24528	-0.44620	-2.03716
H	6.26268	1.01582	-2.25639
H	-2.72701	-0.93219	-0.39896
O	-1.91114	-1.54724	-0.51382
H	-1.70708	-1.56292	-1.46189
D	2.35867	-2.75259	0.12619
O	2.07922	-1.84852	-0.08824
D	2.92080	-1.21185	0.00903

Zero-point correction= 0.255418 (Hartree/Particle)
Thermal correction to Energy= 0.273157

Thermal correction to Enthalpy=	0.274101
Thermal correction to Gibbs Free Energy=	0.200375
Sum of electronic and zero-point Energies=	-726.007436
Sum of electronic and thermal Energies=	-725.989696
Sum of electronic and thermal Enthalpies=	-725.988752
Sum of electronic and thermal Free Energies=	-726.062478

ELECTRONIC ENERGY = -726.2628535

D



H	-0.56442	1.89272	1.74280
N	3.72686	0.04575	-0.24657
C	3.99183	-1.18757	-0.70259
C	5.23823	-1.79471	-0.56605
C	6.25760	-1.08903	0.07363
C	5.99018	0.19415	0.55045
C	4.71275	0.71868	0.36699
H	3.17187	-1.70367	-1.19650
H	5.40237	-2.79484	-0.95406
H	7.24211	-1.53080	0.19703
H	6.75315	0.77979	1.05301
H	4.45803	1.71533	0.71959
O	-0.79568	1.51436	0.88015
H	-1.93988	2.42479	0.01536
H	0.07819	1.50248	0.38015
C	-3.24140	-0.53392	0.52335
C	-3.70487	-1.82199	0.75082
H	-2.27198	-0.15440	0.84073
H	-3.08245	-2.52815	1.28851
N	-4.01657	0.34417	-0.14525
C	-4.96939	-2.18225	0.27897
C	-5.23778	0.02477	-0.61545
H	-5.34884	-3.18534	0.44799
C	-5.74603	-1.24857	-0.41405
H	-5.77146	0.80632	-1.14402
H	-6.72935	-1.50176	-0.79356
H	2.24899	1.00746	-0.32750
O	1.54002	1.71470	-0.31627
H	1.54923	2.10505	-1.20231
D	-3.09522	3.49393	-0.10931
O	-2.76912	2.66330	-0.48775
D	-3.62091	1.32547	-0.30065

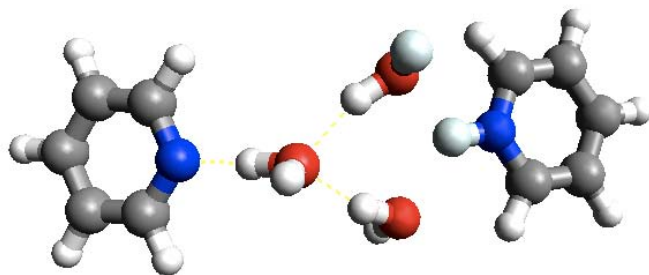
Zero-point correction=

0.261520 (Hartree/Particle)

Thermal correction to Energy=	0.280330
Thermal correction to Enthalpy=	0.281275
Thermal correction to Gibbs Free Energy=	0.206629
Sum of electronic and zero-point Energies=	-726.014248
Sum of electronic and thermal Energies=	-725.995438
Sum of electronic and thermal Enthalpies=	-725.994493
Sum of electronic and thermal Free Energies=	-726.069139

ELECTRONIC ENERGY = -726.275768

TS3



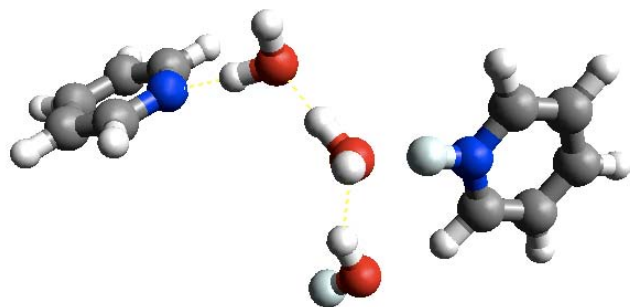
H	0.64124	-1.91950	-0.61467
N	-3.49011	-0.09152	0.26215
C	-4.25935	-1.14028	-0.07044
C	-5.50505	-1.00227	-0.67742
C	-5.97461	0.28241	-0.95167
C	-5.18059	1.37684	-0.60853
C	-3.94820	1.14200	-0.00407
H	-3.85733	-2.12346	0.16212
H	-6.08987	-1.88186	-0.92583
H	-6.94200	0.42792	-1.42324
H	-5.50684	2.39340	-0.80235
H	-3.29882	1.96611	0.28097
O	1.00421	-1.65681	0.24453
H	0.19823	0.83781	1.26728
H	0.21583	-1.37020	0.76219
C	3.92973	-1.13571	-0.11877
C	5.25234	-1.07990	-0.53184
H	3.38147	-2.04257	0.10486
H	5.81787	-1.99735	-0.64781
N	3.23293	0.00617	0.02962
C	5.82792	0.16707	-0.79200
C	3.75564	1.22323	-0.20878
H	6.86125	0.23108	-1.11893
C	5.07164	1.33185	-0.63117
H	3.08154	2.05576	-0.04935
H	5.49392	2.31046	-0.82855
H	-1.98155	-0.28791	1.02735
O	-1.09338	-0.39145	1.50725
H	-1.31796	-0.60726	2.42570
D	1.24824	1.62741	2.07771
O	1.06356	1.30296	1.18347
D	2.24321	-0.05145	0.34633

Zero-point correction= 0.261320 (Hartree/Particle)
Thermal correction to Energy= 0.279639
Thermal correction to Enthalpy= 0.280584
Thermal correction to Gibbs Free Energy= 0.209410

Sum of electronic and zero-point Energies=	-726.014798
Sum of electronic and thermal Energies=	-725.996479
Sum of electronic and thermal Enthalpies=	-725.995534
Sum of electronic and thermal Free Energies=	-726.066708

ELECTRONIC ENERGY = -726.276118

E



H	-0.92266	0.80562	2.48947
N	3.46123	-0.39922	0.25578
C	4.30389	0.51860	0.75438
C	5.54866	0.78946	0.19113
C	5.93798	0.07445	-0.94174
C	5.06786	-0.88174	-1.46556
C	3.84300	-1.08386	-0.83395
H	3.96468	1.05251	1.63892
H	6.19439	1.54109	0.63344
H	6.90214	0.25824	-1.40664
H	5.33030	-1.46225	-2.34401
H	3.13490	-1.82034	-1.20619
O	-0.90066	0.53151	1.55954
H	-0.93456	2.11581	0.47576
H	-0.12788	-0.12027	1.46522
C	-3.91109	-1.23776	0.56090
C	-5.09992	-1.49983	-0.09774
H	-3.45985	-1.91447	1.27712
H	-5.62994	-2.42534	0.09571
N	-3.24984	-0.08673	0.32224
C	-5.59098	-0.55333	-1.00394
C	-3.69230	0.84677	-0.54632
H	-6.52260	-0.73868	-1.52984
C	-4.88128	0.62741	-1.22928
H	-3.05464	1.72730	-0.64160
H	-5.24066	1.37618	-1.92597
H	1.90881	-0.84041	0.90186
O	1.02185	-1.19153	1.22458
H	1.23624	-1.78575	1.95914
D	-0.74162	3.15643	-0.66085
O	-1.41168	2.75651	-0.08776
D	-2.34776	0.10299	0.83422

Zero-point correction= 0.260918 (Hartree/Particle)

Thermal correction to Energy= 0.280150

Thermal correction to Enthalpy= 0.281095

Thermal correction to Gibbs Free Energy= 0.205259

Sum of electronic and zero-point Energies=	-726.011247
Sum of electronic and thermal Energies=	-725.992015
Sum of electronic and thermal Enthalpies=	-725.991071
Sum of electronic and thermal Free Energies=	-726.066906

ELECTRONIC ENERGY = -726.2721653