

# Proton affinities of candidates for positively charged ambient ions in the boreal forest

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## Supplementary material

Table 1. The values for the zero-point-corrected electronic energy (CBS-QB3 (0K)), the calculated standard enthalpy @ 298.15 K (CBS-QB3 Enthalpy) and the Gibbs Free Energy @ 298.15 K (CBS-QB3 Free Energy) for both neutral and protonated cases of the listed molecule species. All values are in Hartrees.

	Neutral			Protonated		
	CBS-QB3 (0K)	CBS-QB3 Enthalpy	CBS-QB3 Free Energy	CBS-QB3 (0K)	CBS-QB3 Enthalpy	CBS-QB3 Free Energy
Ammonia	-56.460175	-56.456364	-56.479245	-56.783193	-56.779396	-56.802848
Methylamine	-95.668471	-95.664102	-95.691391	-96.008720	-96.004308	-96.031912
Dimethylamine	-134.884710	-134.879339	-134.910191	-135.236092	-135.230616	-135.261855
Trimethylamine	-174.106381	-174.099935	-174.133744	-174.464720	-174.458120	-174.492378

Pyrroline	-210.962672	-210.957149	-210.990120	-211.315555	-211.309887	-211.343231
3-Pyrroline	-210.962672	-210.957149	-210.990120	-211.315551	-211.309878	-211.343248
<b>Alkyl amine(4) (C<sub>4</sub>H<sub>11</sub>N):</b>						
Ethanamine, N-ethyl-	-213.341913	-213.333993	-213.372116	-213.701638	-213.693567	-213.732091
1-Butanamine	-213.347735	-213.339750	-213.378021	-213.696082	-213.687954	-213.726615
Ethanamine, N,N-dimethyl-	-213.333501	-213.325691	-213.363246	-213.695939	-213.687968	-213.726027
2-Propanamine, N-methyl-	-213.340218	-213.332286	-213.370177	-213.700562	-213.692578	-213.730560
<b>Pyridine (C<sub>5</sub>H<sub>5</sub>N):</b>						
Pyridine	-247.830972	-247.825719	-247.858384	-248.181853	-248.176502	-248.209363
Bicyclo[1.1.0]butane-1-carbonitrile	-247.670872	-247.663770	-247.700222	-248.001343	-287.413275	-287.451195
Cis-1-cyano-1,3-butadiene	-247.791293	-247.784133	-247.820883	-248.099952	-248.091968	-248.130419
Cyclopropene-3-carbonitrile, 1-methyl-	-247.745696	-247.738425	-247.775552	-248.059234	-248.051374	-248.089500
2,4-Pentadienenitrile	-247.791287	-247.784128	-247.820875	-248.099955	-248.091972	-248.130420
4-Cyano-1-butyne	-247.764901	-247.757435	-247.795045	-248.061498	-248.053599	-248.092042
Trans-1-cyano-1,3-butadiene	-247.791299	-247.784140	-247.820888	-248.099950	-248.091968	-248.130412
<b>Alkyl pyrroline(1) (C<sub>5</sub>H<sub>9</sub>N):</b>						
Pentanenitrile	-250.203002	-250.194744	-250.234323	-250.507043	-250.498332	-250.538734
2-Propyn-1-amine, N,N-dimethyl-	-250.121328	-250.113024	-250.152009	-250.477642	-250.469197	-250.508656
Propane, 2-isocyano-2-methyl-	-250.179953	-250.171536	-250.210329	-250.508103	-250.499454	-250.538594
2,5-Dihydro-1-methylpyrrole	-250.166421	-250.159538	-250.195526	-250.527419	-250.520533	-250.556698
<b>Alkyl amine(5) (C<sub>5</sub>H<sub>13</sub>N):</b>						
1-Pentanamine	-252.573486	-252.564200	-252.605957	-252.922510	-252.913036	-252.955311
N-ethyl-N-methylethanamine	-252.560322	-252.551100	-252.592524	-252.926428	-252.917101	-252.958852
N,N-dimethyl-2-propanamine	-252.560785	-252.551722	-252.592340	-252.927091	-252.917845	-252.958780

Tropylium	-269.723224	-269.716779	-269.751995	-270.122314	-270.115857	-270.151396
<b>Alkyl pyridine(1) (C<sub>6</sub>H<sub>7</sub>N):</b>						
2-Methylpyridine	-287.064925	-287.057874	-287.095251	-287.422171	-287.415027	-287.452503
4-Methylpyridine	-287.063082	-287.055972	-287.094025	-287.420469	-287.413275	-287.451195
Aniline	-287.068121	-287.061296	-287.097325	-287.401524	-287.394303	-287.432206
3-Methylpyridine	-287.062347	-287.055286	-287.092706	-287.418324	-287.411196	-287.448500
1-Cyclopentene-1-carbonitrile	-287.039738	-287.032444	-287.070059	-287.349863	-287.341894	-287.380724
2-Cyclopentene-1-carbonitrile	-287.035217	-287.027994	-287.065534	-287.342557	-287.334841	-287.373305
3-Methylenecyclobutanenitrile	-287.004177	-286.996519	-287.035031	-287.309182	-287.301019	-287.340525
Bicyclo[2.1.0]pentane-1-carbonitrile	-286.994631	-286.987580	-287.024407	-287.307794	-287.299935	-287.338256
N-2-propynyl-2-propyn-1-amine	-286.914537	-286.905475	-286.947165	-287.261704	-287.252745	-287.294389
5-Hexynenitrile	-286.991557	-286.982769	-287.023994	-287.291594	-287.282370	-287.324396
7-Azenorbornadiene	-286.976191	-286.970397	-287.004289	-287.338185	-287.332346	-287.366359
2,4-Hexadienenitrile	-287.022791	-287.014098	-287.054686	-287.336211	-287.326955	-287.368520
<b>Alkyl amine(6) (C<sub>6</sub>H<sub>15</sub>N):</b>						
Triethylamine	-291.785425	-291.774940	-291.819541	-292.156950	-292.146399	-292.190982
1-Hexanamine	-291.799254	-291.788619	-291.833946	-292.148617	-292.137791	-292.183653
N,N,2-trimethyl-2-propanamine	-291.788881	-291.778450	-291.821897	-292.158335	-292.147770	-292.191802
<b>Alkyl pyridine(2) (C<sub>7</sub>H<sub>9</sub>N):</b>						
2,6-Dimethylpyridine	-326.298986	-326.290029	-326.332880	-326.662159	-326.653072	-326.696394
2,4-Dimethylpyridine	-326.297034	-326.288114	-326.330643	-326.660455	-326.651336	-326.695207
o-Toluidine	-326.299752	-326.291391	-326.330822	-326.635475	-326.626650	-326.667735
N-methylaniline	-326.284144	-326.275874	-326.315521	-326.629582	-326.621273	-326.661527

p-Aminotoluene	-326.298322	-326.289575	-326.331044	-326.635544	-326.626401	-326.669787
3-Methylbenzenamine	-326.298909	-326.290230	-326.331200	-326.635554	-326.626486	-326.669168
3,5-Dimethylpyridine	-326.293676	-326.284770	-326.327028	-326.654457	-326.645449	-326.687749
2,5-Dimethylpyridine	-326.296091	-326.287180	-326.329460	-326.658085	-326.649107	-326.691223
2,3-Dimethylpyridine	-326.295839	-326.287354	-326.327441	-326.657942	-326.649273	-326.689857
2-Ethylpyridine	-326.289536	-326.281319	-326.321978	-326.649119	-326.640807	-326.681372
3,4-Dimethylpyridine	-326.294421	-326.285953	-326.325979	-326.656435	-326.647826	-326.688169
3-Ethylpyridine	-326.286308	-326.278129	-326.318434	-326.645042	-326.636716	-326.677477
Benzylamine	-326.286135	-326.277939	-326.318053	-326.635858	-326.627530	-326.667741
4-Ethylpyridine	-326.287511	-326.279328	-326.319652	-326.647392	-326.639069	-326.679520
Cyclohexenecarbonitrile	-326.272596	-326.264375	-326.304122	-326.585833	-326.576899	-326.617930
Bicyclo[3.1.0]hexane-1-carbonitrile	-326.257390	-326.249525	-326.288278	-326.571987	-326.563405	-326.603432
N-Methyl-di(2-propynyl)-amine	-326.129750	-326.119380	-326.164525	-326.491006	-326.480663	-326.525297
2-Cyclohexene-1-carbonitrile	-326.267314	-326.259134	-326.298856	-326.575270	-326.566575	-326.607257
4,4-Dimethyl-2-pentynonitrile	-326.229031	-326.218825	-326.262720	-326.533998	-326.523013	-326.568329
4-Cyanocyclohexene	-326.269251	-326.261047	-326.300741	-326.575818	-326.567103	-326.607725
1-Cyclopentylacetonitrile	-326.265029	-326.256337	-326.297650	-326.569629	-326.560425	-326.602967
1-Allylpyrrole	-326.134109	-326.125511	-326.166349	-326.494456	-326.485741	-326.527039

**Alkyl pyridine(3) (C<sub>8</sub>H<sub>11</sub>N):**

2,6-Xylidine	-365.531200	-365.521276	-365.564091	-365.869086	-365.858512	-365.903907
2-(i-C <sub>3</sub> H <sub>7</sub> )-pyridine	-365.519602	-365.510060	-365.553114	-365.879817	-365.870136	-365.913808
2-Propylpyridine	-365.516995	-365.507402	-365.551356	-365.877054	-365.867330	-365.911493
4-Isopropylpyridine	-365.516870	-365.507281	-365.550645	-365.876755	-365.866991	-365.910940
3-Ethylaniline	-365.524780	-365.514947	-365.558598	-365.861432	-365.851202	-365.897060
Quinoline	-401.194180	-401.186502	-401.225354	-401.553519	-401.545686	-401.584806

**Alkyl amine (8) (C<sub>8</sub>H<sub>19</sub>N):**

Diisopropylethylamine	-370.238460	-370.225132	-370.275818	-370.613177	-370.600173	-370.649890
1-Octanamine	-370.250855	-370.237496	-370.289956	-370.600569	-370.587020	-370.640006
(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	-370.254280	-370.241344	-370.289935	-370.626039	-370.612957	-370.661815

**Alkyl pyridine(4) (C<sub>9</sub>H<sub>13</sub>N):**

2,6-Diethylpyridine	-404.749405	-404.738214	-404.785985	-405.116715	-405.105315	-405.154048
N-ethyl-N-methyl-benzenamine	-404.728830	-404.717818	-404.764682	-405.088469	-405.077442	-405.124206
N,N,3-trimethyl-benzenamine	-404.731507	-404.719954	-404.767760	-405.090493	-405.078994	-405.127057

**Alkyl quinoline(1) (C<sub>10</sub>H<sub>9</sub>N):**

1-Naphthalenamine	-440.429086	-440.419818	-440.461870	-440.773812	-440.764214	-440.807355
8-Methyl-quinoline	-440.426428	-440.417035	-440.459669	-440.788332	-440.778845	-440.821516

**Alkyl pyridine(5) (C<sub>10</sub>H<sub>15</sub>N):**

N,N-diethylaniline	-443.956091	-443.943912	-443.993418	-444.317813	-444.305569	-444.355093
N,N,2,6-tetramethylbenzenamine	-443.955057	-443.942101	-443.992178	-444.316643	-444.303826	-444.353367
N,N,3,5-tetramethylbenzenamine	-443.962397	-443.948924	-444.001809	-444.323838	-444.310388	-444.363729
2-Methyl-4,6-diethylpyridine	-443.981407	-443.968336	-444.020635	-444.352865	-444.339558	-444.393198

**Alkyl quinoline(2) (C<sub>11</sub>H<sub>11</sub>N):**

2,7-Dimethylquinoline	-479.660130	-479.648805	-479.696176	-480.029231	-480.017651	-480.066447
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