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Supporting Information

Protonation Sites in Pyrimidine and Pyrimidinamines in the Gas Phase

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Tables of HF/6-31G(d,p) optimized geometries and uncorrected harmonic frequencies in cm^{-1} .

Pyrimidine (1)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.002782	.000000	1.297253
2	7	1.177892	.000000	.709794
3	7	-1.180715	.000000	.704850
4	6	1.173469	.000000	-.611003
5	6	-1.170958	.000000	-.616155
6	6	.002721	.000000	-1.345820
7	1	-.005061	.000000	2.372645
8	1	2.134453	.000000	-1.096460
9	1	-2.130104	.000000	-1.105194
10	1	.005773	.000000	-2.419151

Pyrimidine (1)

Frequencies -- 415, 461, 683, 751, 788, 911, 1095, 1103, 1130, 1155, 1161, 1162, 1212, 1258, 1355, 1512, 1569, 1637, 1798, 1799, 3348, 3353, 3370, 3392.

(1H)-Pyrimidinium Cation (1a⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.160416	.611782	.000000
2	7	.000000	1.276134	.000000
3	7	-1.221007	-.683155	.000000
4	6	1.176702	.628201	.000000
5	6	-.079464	-1.357536	.000000
6	6	1.169119	-.736363	.000000
7	1	-2.062410	1.194684	.000000
8	1	-.013786	2.277841	.000000
9	1	2.066228	1.228528	.000000
10	1	-.160114	-2.429467	.000000
11	1	2.081478	-1.298946	.000000

(1H)-Pyrimidinium Cation (**1a**⁺)

Frequencies -- 383, 446, 670, 726, 729, 860, 950, 1093, 1105, 1140, 1145, 1170, 1171, 1199, 1263, 1363, 1423, 1514, 1611, 1715, 1800, 1830, 3392, 3409, 3410, 3423, 3803.

(1H)-Pyrimidinium Radical (**1a**[•])

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.992189	-.874636	.013001
2	7	-1.237510	.491422	-.085784
3	7	.169666	-1.407849	.015055
4	6	-.134940	1.358472	.014221
5	6	1.268726	-.585007	-.016667
6	6	1.123033	.816983	.011845
7	1	-1.866460	-1.499151	.056752
8	1	-2.114317	.814321	.253142
9	1	-.345677	2.408878	.034214
10	1	2.228895	-1.062212	-.020443
11	1	1.984693	1.458282	.037044

(1H)-Pyrimidinium Radical (**1a**[•])

Frequencies -- 229, 420, 444, 629, 644, 668, 705, 718, 924, 954, 1004, 1040, 1066, 1131, 1210, 1278, 1442, 1467, 1533, 1612, 1651, 1723, 3357, 3364, 3387, 3401, 3872.

(2H)-Pyrimidinium (**1b**⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.000000	1.319305	.000000
2	7	1.225073	.630035	.000000
3	7	-1.224987	.629979	.000000
4	6	1.232711	-.650018	.000000
5	6	-1.232728	-.650153	.000000
6	6	-.000052	-1.359979	.000000
7	1	-.000103	2.004355	.854934
8	1	-.000103	2.004355	-.854934
9	1	2.171489	-1.173213	.000000
10	1	-2.171621	-1.173125	.000000
11	1	.000139	-2.437396	.000000

(2H)-Pyrimidinium (**1b**⁺)

Frequencies -- 272, 379, 459, 615, 686, 865, 973, 1029, 1072, 1076, 1097, 1109, 1181, 1229, 1311, 1373, 1409, 1534, 1537, 1562, 1705, 1739, 3127, 3148, 3372, 3390, 3393.

(5H)-Pyrimidinium (1c⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.000687	-1.330260	.000000
2	7	-.000518	-.745791	1.208481
3	7	-.000518	-.745791	-1.208481
4	6	-.000518	.540797	1.226694
5	6	-.000518	.540797	-1.226694
6	6	.000781	1.367144	.000000
7	1	.004241	-2.405819	.000000
8	1	-.001399	1.027780	2.188500
9	1	-.001399	1.027780	-2.188500
10	1	-.860210	2.041281	.000000
11	1	.863413	2.039174	.000000

(5H)-Pyrimidinium (1c⁺)

Frequencies -- 153, 332, 384, 637, 702, 748, 928, 952, 1042, 1095, 1142, 1217, 1233, 1323, 1326, 1449, 1501, 1513, 1527, 1531, 1713, 1825, 3150, 3179, 3363, 3364, 3402.

2-Pyrimidyl radical(1d[•])

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.000059	-1.328186	.000000
2	7	.000058	-.776949	1.190716
3	7	.000058	-.776949	-1.190716
4	6	.000058	.557770	1.189882
5	6	.000058	.557770	-1.189882
6	6	-.000198	1.284234	.000000
7	1	-.000170	1.045048	2.148240
8	1	-.000170	1.045048	-2.148240
9	1	-.000335	2.357668	.000000

2-Pyrimidyl Radical (1d[•])

Frequencies -- 412, 438, 652, 737, 783, 848, 1019, 1045, 1053, 1106, 1173, 1190, 1237, 1381, 1478, 1562, 1650, 1655, 3360, 3367, 3390,

2-Pyrimidinamine (2)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.857083	-.000038	-.006258
2	7	-.254667	-1.184619	.001454
3	7	-.254673	1.184623	.001448
4	6	1.061475	-1.167235	.002469
5	6	1.061412	1.167260	.002472
6	6	1.803314	-.000002	-.000735
7	7	-2.209347	-.000002	-.044195
8	1	1.546877	-2.129154	.008258
9	1	1.546854	2.129163	.008263
10	1	2.875473	.000060	.000505
11	1	-2.676570	-.854684	.142155
12	1	-2.676534	.854697	.142173

2-Pyrimidinamine (2) Frequencies -- 214, 326, 441, 459, 545, 583, 647, 703, 877, 911, 964, 1093, 1121, 1121, 1140, 1182, 1223, 1272, 1448, 1496, 1616, 1620, 1781, 1783, 1819, 3339, 3342, 3400, 3857, 3997.

(1H)-Pyrimidine-2-ammonium (2a⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.892014	-.039898	-.000040
2	7	-.206483	1.118023	.000016
3	7	-.258542	-1.209029	-.000008
4	1	-.697641	1.987851	.000134
5	6	1.155662	1.133188	-.000024
6	6	1.042444	-1.207980	.000010
7	6	1.830249	-.031172	-.000012
8	7	-2.209180	-.031927	.000013
9	1	1.615505	2.102251	.000036
10	1	1.515754	-2.174121	.000130
11	1	2.900509	-.066802	-.000011
12	1	-2.755832	.798558	-.000032
13	1	-2.676911	-.912038	-.000001

(1H)-Pyrimidine-2-ammonium (2a⁺)

Frequencies -- 194, 420, 438, 450, 541, 596, 624, 692, 765, 873, 897, 954, 1076, 1104, 1123, 1150, 1152, 1231, 1314, 1414, 1493, 1560, 1602, 1723, 1796, 1831, 1862, 3380, 3413, 3430, 3813, 3832, 3951

(1H)-Pyrimidine-2-ammonium radical (2a[•])

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.873042	-.092994	.004387

2	7	.250988	1.143755	.064172
3	7	.278643	-1.212956	.017963
4	1	.738625	1.879570	-.397307
5	6	-1.158912	1.172771	-.000662
6	6	-1.110813	-1.217387	.001726
7	6	-1.838287	-.026029	-.010670
8	7	2.248437	-.011773	-.089544
9	1	-1.617106	2.140784	.007218
10	1	-1.582101	-2.180234	-.007211
11	1	-2.912565	-.034490	-.025477
12	1	2.663323	.653882	.527223
13	1	2.673169	-.910862	-.021268

(1H)-Pyrimidine-2-ammonium radical (**2a**)

Frequencies -- 190, 306, 390, 437, 493, 532, 605, 628, 646, 682, 723, 843, 901, 942, 1044, 1054, 1117, 1194, 1285, 1339, 1451, 1474, 1522, 1625, 1657, 1774, 1866, 3364, 3388, 3404, 3787, 3842, 3903

NH₃-Pyrimidine-2-ammonium (**2b**⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.742060	.000714	-.000505
2	7	-.208491	1.178653	-.000728
3	7	-.209708	-1.179296	-.000655
4	6	1.123167	1.179475	-.000008
5	6	1.119520	-1.181183	-.000055
6	6	1.842813	-.000501	.000864
7	7	-2.219729	.002505	.000235
8	1	1.603582	2.139916	-.000190
9	1	1.599745	-2.141846	-.000070
10	1	2.915143	-.001836	.001509
11	1	-2.556003	.955238	-.051038
12	1	-2.579019	-.524527	-.785238
13	1	-2.578592	-.431007	.841284

NH₃-Pyrimidine-2-ammonium (**2b**⁺)

Frequencies -- 43, 240, 396, 466, 521, 622, 691, 828, 901, 927, 1109, 1120, 1142, 1146, 1176, 1199, 1207, 1255, 1355, 1449, 1578, 1615, 1649, 1767, 1767, 1769, 1851, 3392, 3398, 3416, 3601, 3702, 3716.

(5H)-Pyrimidine-2-ammonium (**2c**⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.000441	.912319	.000000
2	7	-.000790	.296698	1.226226

3	7	-.000790	.296698	-1.226226
4	6	-.000790	-.972170	1.231301
5	6	-.000790	-.972170	-1.231301
6	6	-.000639	-1.811392	.000000
7	7	.002854	2.198074	.000000
8	1	-.001420	-1.463606	2.190757
9	1	-.001420	-1.463606	-2.190757
10	1	-.867137	-2.472193	.000000
11	1	.864386	-2.473915	.000000
12	1	.003670	2.696759	.865741
13	1	.003670	2.696759	-.865741

(5H)-Pyrimidine-2-ammonium (2c⁺)

Frequencies -- 99, 344, 396, 456, 610, 666, 694, 802, 814, 908, 965, 976, 989, 1041, 1074, 1153, 1187, 1335, 1442, 1507, 1527, 1529, 1597, 1677, 1794, 1877, 1899, 3183, 3217, 3356, 3357, 3776, 3914

4-Pyrimidinamine (3)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.058061	-1.137940	.002189
2	7	-.260934	-1.165965	-.001150
3	7	1.838695	-.082287	.005478
4	6	-.882723	.003279	-.007423
5	7	-2.237578	-.020181	-.044063
6	6	1.203944	1.087505	.002734
7	6	-.159999	1.205317	-.003975
8	1	1.546585	-2.097089	.005394
9	1	1.825126	1.967122	.005734
10	1	-.648150	2.161611	-.012976
11	1	-2.671829	-.897384	.125274
12	1	-2.748709	.795808	.193566

4-Pyrimidinamine (3)

Frequencies -- 225, 337, 428, 433, 506, 604, 615, 747, 870, 911, 952, 1091, 1107, 1141, 1155, 1188, 1262, 1334, 1474, 1484, 1557, 1657, 1781, 1789, 1816, 3346, 3358, 3380, 3845, 3979

(1H)-pyrimidin-4-ammonium (3a⁺)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	.987550	-1.184516	.000184
2	7	-.296484	-1.182033	.000135
3	7	1.733627	-.071564	-.000164
4	6	-.937399	.004074	-.000547
5	7	-2.246821	-.031683	.000080

6	6	1.133573	1.147861	.000001
7	6	-.207311	1.231970	.000166
8	1	1.512297	-2.122253	.000346
9	1	1.779063	2.004583	.000094
10	1	-.703990	2.181944	.000801
11	1	-2.707799	-.915783	.000015
12	1	-2.799637	.795188	-.000119
13	1	2.729342	-.143059	-.000317

(1H)-pyrimidin-4-ammonium (**3a⁺**)

Frequencies -- 186, 443, 447, 540, 590, 598, 676, 709, 755, 850, 929, 942, 1083, 1123, 1124, 1128, 1150, 1270, 1331, 1460, 1525, 1538, 1674, 1709, 1774, 1831, 1855, 3400, 3404, 3420, 3810, 3845, 3948

(3H)-pyrimidin-4-ammonium (**3b⁺**)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.150176	-1.108439	-.000017
2	7	.212860	-1.101505	-.000002
3	7	-1.856435	-.049841	-.000017
4	6	.915504	.046896	-.000107
5	7	2.234074	.007874	.000045
6	6	-1.190815	1.131487	.000067
7	6	.163801	1.238678	-.000047
8	1	-1.611108	-2.078765	-.000110
9	1	-1.806810	2.011260	.000123
10	1	.658497	2.189771	-.000303
11	1	2.749950	-.843430	-.000986
12	1	2.757565	.854582	.000896
13	1	.688524	-1.980848	.000820

(3H)-pyrimidin-4-ammonium (**3b⁺**)

Frequencies -- 219, 384, 437, 460, 532, 578, 584, 735, 776, 835, 924, 932, 1071, 1091, 1125, 1162, 1171, 1235, 1362, 1422, 1515, 1549, 1601, 1724, 1808, 1831, 1861, 3396, 3403, 3412, 3814, 3824, 3943

NH₃-pyrimidin-4-ammonium (**3c⁺**)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.097970	-1.166888	-.000011
2	7	-.226955	-1.148115	-.000003
3	7	1.869679	-.100850	.000003
4	6	-.767691	.033475	-.000014
5	7	-2.246935	-.019553	.000007
6	6	1.287143	1.079298	.000047
7	6	-.098939	1.226622	-.000023
8	1	1.572144	-2.129409	-.000016

9	1	1.929029	1.941509	-.000046
10	1	-.574873	2.188865	-.000063
11	1	-2.515480	-.997141	-.000870
12	1	-2.646042	.419583	.819417
13	1	-2.646204	.421179	-.818457

NH₃-pyrimidin-4-ammonium (**3c⁺**)

Frequencies -- 88, 236, 391, 429, 552, 583, 737, 816, 879, 925, 1095, 1102, 1108, 1154, 1157, 1189, 1228, 1288, 1335, 1471, 1550, 1637, 1651, 1761, 1767, 1782, 1849, 3382, 3397, 3413, 3591, 3693, 3705

(5H)-pyrimidin-4-ammonium (**3d⁺**)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-.987063	-1.216295	.000109
2	7	.302742	-1.213156	.000803
3	7	-1.849066	-.138555	-.001119
4	6	.918638	-.020326	.000631
5	7	2.209965	-.017913	-.001147
6	6	-1.326160	1.013281	-.000852
7	6	.149873	1.264249	.001472
8	1	-1.469964	-2.176604	.001793
9	1	-1.978219	1.871675	-.002198
10	1	.413528	1.858285	.874915
11	1	.416377	1.862289	-.868256
12	1	2.692051	-.895233	-.001756
13	1	2.749013	.821493	-.002415

(5H)-pyrimidin-4-ammonium (**3d⁺**)

Frequencies -- 67, 280, 436, 457, 558, 562, 698, 737, 812, 872, 907, 1007, 1066, 1106, 1110, 1193, 1219, 1334, 1472, 1482, 1507, 1519, 1574, 1683, 1710, 1854, 1881, 3189, 3232, 3357, 3402, 3768, 3906.