How H-bonding modifies molecular structure and pi-electron delocalization in the ring of pyridine/pyridinium derivatives involved in H-bond complexation.

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General Information

Pyridine and its derivatives play a very important role in heterocyclic chemistry.¹ Hydrogen bonding is one of the most important terms used in chemistry, biochemistry and related fields.² Both pyridine and hydrogen bond are the subject of numerous research and papers.³ The number of papers treating both topics are permanently increasing, see Figure S1. Nowadays, every hour a paper appears dealing with hydrogen bond and every four hours – a paper with the word “pyridine” included in its title or abstract or as a keyword (Figure S1). Every day a paper is published in which the terms “pyridine” (Py) and “hydrogen bond” (HB) are in the title or abstract, or as a keyword (Figure S2).

Figure S1. The number of papers in which Py (pyridine), HB (H-bonded or H-bonding or hydrogen bond*) appears in the title or abstract, or as a keyword, published every day within the last decade.³

¹ Pozharski, A.F.; Soldatenkov, A.T.; Katritzky, A.R. *Heterocycles in Life and Society*. Wiley, New York, **1997**. Katritzky, A.R.; Rees, C.W.; Scriven, E.F.V., Eds, *Comprehensive Heterocyclic Chemistry II*. Pergamon Press, Oxford, **1996**. Katritzky, A.R.; Rees, C.W., Eds, *Comprehensive Heterocyclic Chemistry*. Pergamon Press, Oxford, **1984**.

² Jeffrey, G.A. *An Introduction to Hydrogen Bonding*. Oxford University Press: Oxford, **1997**. Desiraju, G.R.; Steiner, T. *The weak Hydrogen Bonding in Structural Chemistry and Biology*. Oxford University Press, **1999**.

³ Institute for Scientific Information, Philadelphia (1996 – 2005). Retrieved in June 2005.

Figure S2. The number of papers in which both Py (pyridine) and HB (H-bonded or H-bonding or hydrogen bond*) appear in the title or abstract, or as a keyword, published every day within the last decade.³

Geometries of 397 H-bonded complexes of variously substituted pyridine and pyridinium cation derivatives (287 hits) with various oxygen and nitrogen acids/bases were retrieved from CSD⁴ with the following restrictions: (1) the searches were performed for substituted pyridine (pyridinium cation) interacting with a nitrogen or oxygen acid (base) with an intermolecular contact between the nitrogen of pyridine (pyridinium cation) and the nearest O or N atom in acid (base) equal to or less than the sum of their van der Waals radii;⁵ (2) the searches were restricted to structure measurements with the reported mean estimated standard deviation (e.s.d.) of the CC bond $\leq 0.005 \text{ \AA}$ (corresponding to AS flag = 1). The data were retrieved for polysubstituted pyridine/pyridinium cation (by any of the following substituents: halogen, -Me, -Et, -CHCH₂, -CN, -COOH, -COOMe, -COOEt, -COOPr, -COMe, -COPh, -CONH₂, -CF₃, -NH₂, -NMe₂, -NO₂, -OH, -OMe, -Ph, -SH, -H) interacting with N or O atom in acid/base partner. Sometimes the molecules of the solvent were present in the crystal lattice.

⁴ The Cambridge Structure Database, the 5.26 version, November 2004, updated February 2005.

⁵ Bondi, A. *J. Phys. Chem.* **1964**, 68, 441-451.

A large majority of pyridine structures under study (nearly 80% hits) have been published within the last decade. The number of measurements is still increasing, as shown in Figure S3.

Figure S3. The number of hits pyridine under study published every year within the last decade. The Cambridge Database was updated in February 2005 therefore the data for previous year are incomplete.

B3LYP/6-311+G** level of theory was employed to optimize the molecules' geometries of 4-X-pyridine and 4-X-pyridinium cation ($X = \text{NO}_2, \text{H}, \text{OH}, \text{NH}_2, \text{O}^-$). All ab initio calculations were performed using the *Gaussian03* series of programs. The optimized molecules correspond to minima (no imaginary frequencies). The optimized geometries are reported on pages S5 and S6.

XYZ coordinates of 4-X-pyridine and 4-X-pyridinium cation

4-NO ₂ -pyridine <i>E</i> =-452.909787 hartree				4-NO ₂ -pyridinium <i>E</i> =-453.253666 hartree			
N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.335783	C	0.000000	0.000000	1.350309
C	1.160201	0.000000	2.109255	C	1.204452	0.000000	2.028531
C	2.367129	0.000000	1.426841	C	2.368917	0.000000	1.271621
C	2.406644	0.000000	0.040692	C	2.356172	0.000000	-0.117242
C	1.181191	0.000000	-0.624049	C	1.125514	0.000000	-0.746347
H	0.972899	0.000000	1.816921	H	-0.963675	0.000000	1.842150
H	1.130434	0.000000	3.189688	H	1.242708	0.000000	3.109972
N	3.641228	0.000000	2.194284	N	3.695551	0.000000	1.983649
H	3.349075	0.000000	-0.488580	H	3.278888	0.000000	-0.682582
H	1.152091	0.000000	-1.709017	H	1.002771	0.000000	-1.821282
O	4.682574	0.000000	1.554535	H	-0.896362	0.000000	-0.481284
O	3.562131	0.000000	3.413924	O	4.681446	0.000000	1.274524
				O	3.649414	0.000000	3.197219

pyridine <i>E</i> =-248.351212 hartree				pyridinium <i>E</i> =-248.719068 hartree			
N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.336490	C	0.000000	0.000000	1.350823
C	1.161313	0.000000	2.108187	C	1.204546	0.000000	2.026086
C	2.391142	0.000000	1.456215	C	2.393178	0.000000	1.293609
C	2.406022	0.000000	0.064052	C	2.354903	0.000000	-0.102073
C	1.187759	0.000000	-0.613544	C	1.130151	0.000000	-0.739940
H	-0.976031	0.000000	1.813877	H	-0.965429	0.000000	1.838729
H	1.097371	0.000000	3.189991	H	1.207812	0.000000	3.107945
H	3.317383	0.000000	2.020045	H	3.346493	0.000000	1.808899
H	3.338100	0.000000	-0.488791	H	3.261810	0.000000	-0.691941
H	1.163649	0.000000	-1.699753	H	1.009500	0.000000	-1.814904
				H	-0.893931	0.000000	-0.483210

4-OH-pyridine <i>E</i> =-323.601551 hartree				4-OH-pyridinium <i>E</i> =-323.975952 hartree			
N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.338801	C	0.000000	0.000000	1.352747
C	1.147258	0.000000	2.123104	C	1.185588	0.000000	2.043454
C	2.383995	0.000000	1.478503	C	2.397248	0.000000	1.323556
C	2.409047	0.000000	0.083342	C	2.360925	0.000000	-0.085748
C	1.194281	0.000000	-0.597408	C	1.148821	0.000000	-0.721837
H	-0.975990	0.000000	1.815740	H	-0.965257	0.000000	1.840978
H	1.095124	0.000000	3.204546	H	1.171173	0.000000	3.126434
O	3.506616	0.000000	2.245923	O	3.592637	0.000000	1.890286
H	3.346658	0.000000	-0.463650	H	3.283248	0.000000	-0.650907
H	1.187846	0.000000	-1.683861	H	1.047028	0.000000	-1.798631
H	4.290368	0.000000	1.685295	H	-0.887691	0.000000	-0.490449
				H	3.558242	0.000000	2.857300

4-NH2-pyridine E=-303.732400 hartree

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.338215
C	1.144558	0.000000	2.124535
C	2.400351	-0.000068	1.498487
C	2.411320	-0.001721	0.095346
C	1.202211	-0.001272	-0.587642
H	-0.976595	0.001358	1.815111
H	1.063618	-0.003650	3.206378
N	3.572542	-0.047601	2.230210
H	3.347758	-0.006755	-0.452371
H	1.201884	-0.001072	-1.674469
H	4.422123	0.229503	1.763937
H	3.526286	0.227745	3.198769

4-NH2-pyridinium E=-304.121447 hartree

N	1.785908	0.000144	-0.023371
C	1.121554	1.184460	0.001057
C	-0.242893	1.215983	0.025242
C	-0.980448	0.000009	0.010512
C	-0.242531	-1.215960	0.025571
C	1.121826	-1.184432	0.001024
H	1.727458	2.080338	-0.003668
H	-0.749899	2.172186	0.040097
N	-2.318304	-0.000173	-0.025318
H	-0.749506	-2.172167	0.040407
H	1.728093	-2.080072	-0.004344
H	2.798476	0.000116	-0.048379
H	-2.846261	-0.859783	-0.039053
H	-2.846626	0.859223	-0.037378

4-O(-)-pyridine E=-323.053159 hartree

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.349837
C	1.122101	0.000000	2.156557
C	2.453022	0.000000	1.591614
C	2.426929	0.000000	0.145803
C	1.232977	0.000000	-0.550112
H	-0.988173	0.000000	1.814649
H	1.022753	0.000000	3.238985
O	3.511839	0.000000	2.278778
H	3.374780	0.000000	-0.386301
H	1.254453	0.000000	-1.641841

4-O(-)pyridinium E=-323.599785 hartree

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.372899
C	1.158318	0.000000	2.074091
C	2.462049	0.000000	1.405824
C	2.375104	0.000000	-0.056739
C	1.182614	0.000000	-0.697989
H	-0.976169	0.000000	1.841936
H	1.139611	0.000000	3.156345
O	3.531735	0.000000	2.016454
H	3.297756	0.000000	-0.622799
H	1.090086	0.000000	-1.776956
H	-0.874236	0.000000	-0.499361

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