Hydrogen Bonding Interactions Can Decrease Clar Sextet Character in Acridone Pigments

Zhili Wen,[a] Lucas José Karas,[a] Judy I. Wu [a,*]

[a]Department of Chemistry, University of Houston, Houston, TX 77004, USA

Correspondence: jiwu@central.uh.edu

Table of Contents

1. Computed IMS plots, GIMIC plots, and NICS(1)$_{zz}$ values of the monomers and hydrogen-bonded dimers of 2-hydroxylpyridine and 2-pyridone.

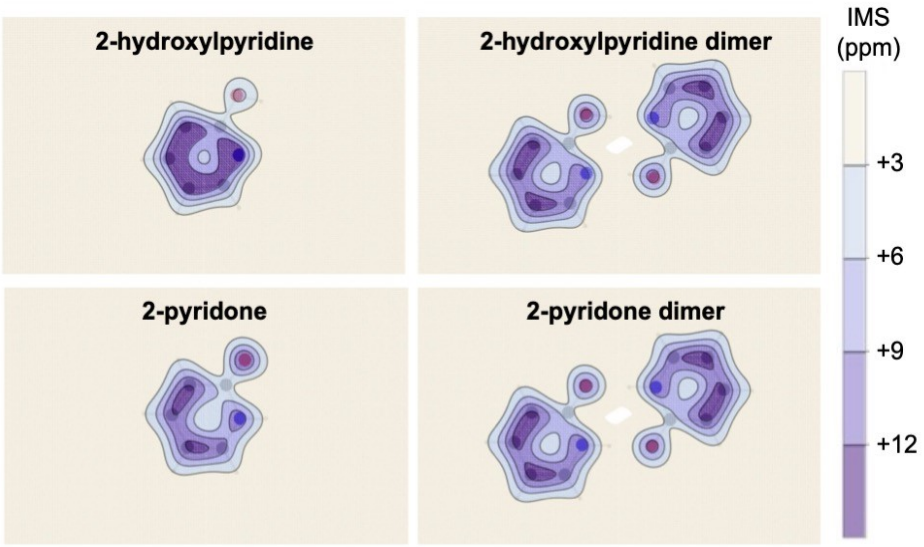

Figure S1. Computed IMS plots of 2-hydroxylpyridine and 2-pyridone and their dimers.

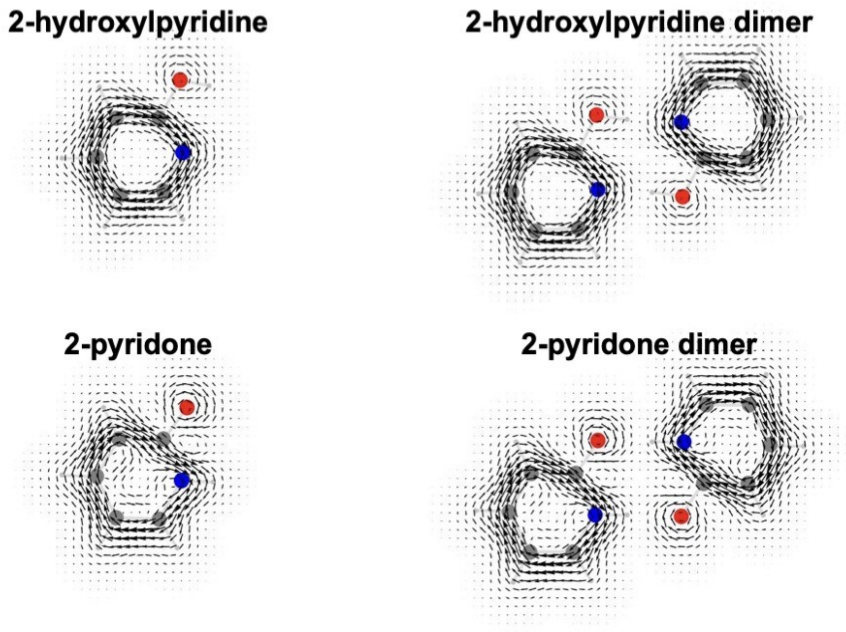

Figure S2. Computed GIMIC plots of 2-hydroxylpyridine and 2-pyridone and their dimers.

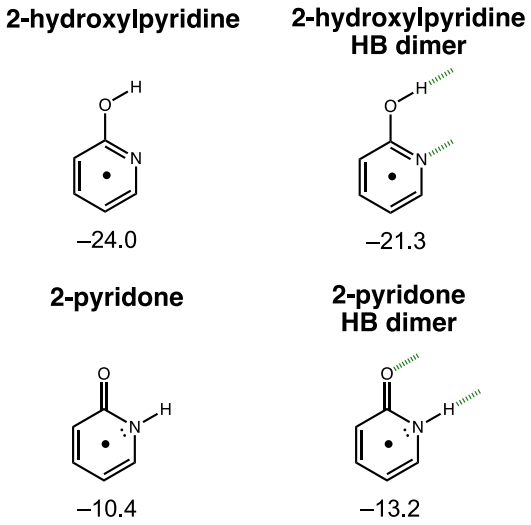

Figure S3. Computed NICS(1)$_{zz}$ values (in ppm) of 2-hydroxylpyridine and 2-pyridone and their dimers.

2. Computed HOMO, LUMO levels (in eV) of 1, 2, and 3

Table S1. Computed HOMO, LUMO levels (in eV) of the monomer, hydrogen-bonded trimer, doubly protonated form, and tautomeric form of **1**, **2**, and **3**.

1	Monomer	Hydrogen-bonded trimer	Doubly protonated	Tautomer
HOMO	–7.31	–7.22	–14.33	–6.93
LUMO	–4.08	–4.27	–11.83	–4.49
2				
HOMO	–7.50	–7.40	–15.33	–7.30
LUMO	–3.98	–4.10	–12.49	–4.27
3				
HOMO	–7.82	–7.34	–15.10	–7.61
LUMO	–3.82	–3.36	–11.33	–3.56

3. Computed IMS plots, GIMIC plots, and NICS(1)$_{zz}$ values of 3, 3-pro, 3-taut, and chrysene

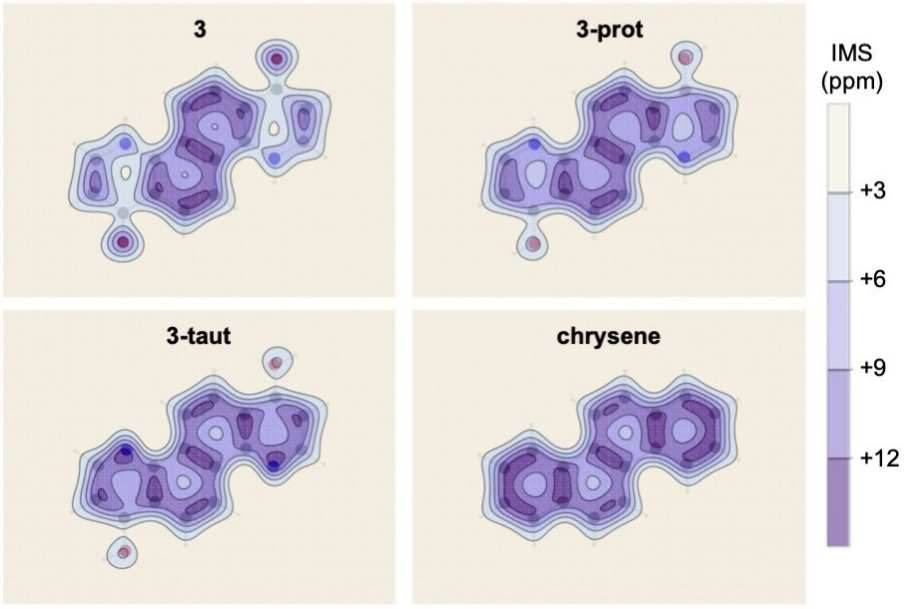

Figure S4. Computed IMS plots of **3**, **3-pro**, **3-taut**, and **chrysene**.

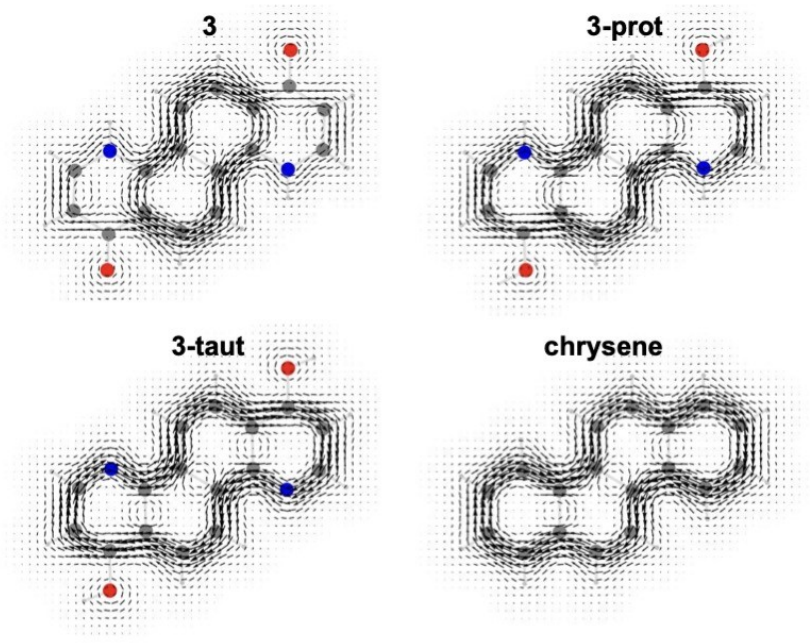

Figure S5. Computed GIMIC plots of **3**, **3-pro**, **3-taut**, and **chrysene**.

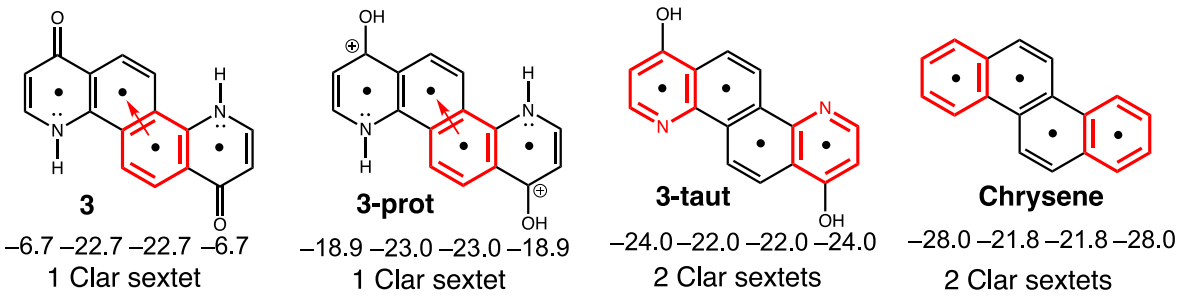

Figure S6. Computed NICS(1)$_{zz}$ values (in ppm) of **3**, **3-pro**, **3-taut**, and **chrysene**.

4. Computed NICS(1)$_{zz}$ values of 1-hb, 2-hb, and 3-hb

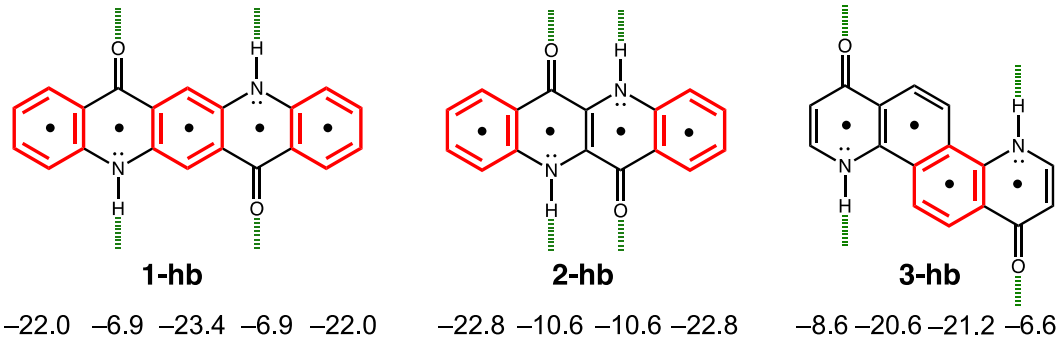

Figure S7. Computed NICS(1)$_{zz}$ values (in ppm) of 1-hb, 2-hb, and 3-hb.

5. Full reference of Gaussian16 program

Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

6. Optimized Cartesian coordinates at B3LYP-D3/6-311+G(d,p) in the gas-phase

1

	X	Y	Z
H	-4.83057	2.49335	0.00000
H	4.83057	-2.49335	0.00000
C	-4.86111	1.40855	0.00000
C	4.86111	-1.40855	0.00000
C	-4.94186	-1.38332	0.00000
C	4.94186	1.38332	0.00000
C	-3.65667	0.67844	0.00000
C	3.65667	-0.67844	0.00000
C	-6.07148	0.74158	0.00000
C	6.07148	-0.74158	0.00000
C	-6.12077	-0.66333	0.00000
C	6.12077	0.66333	0.00000
C	-3.69481	-0.73359	0.00000
C	3.69481	0.73359	0.00000
N	-2.44652	1.33451	0.00000
N	2.44652	-1.33451	0.00000
H	-6.99230	1.31402	0.00000
H	6.99230	-1.31402	0.00000
H	-7.07651	-1.17305	0.00000
H	7.07651	1.17305	0.00000
C	-2.45111	-1.52402	0.00000
C	2.45111	1.52402	0.00000
H	-4.93739	-2.46668	0.00000
H	4.93739	2.46668	0.00000
C	-1.22757	0.68126	0.00000
C	1.22757	-0.68126	0.00000
H	-2.44484	2.34315	0.00000
H	2.44484	-2.34315	0.00000
O	-2.44332	-2.75149	0.00000
O	2.44332	2.75149	0.00000
C	-0.03123	1.39594	0.00000
C	0.03123	-1.39594	0.00000
C	-1.19419	-0.73535	0.00000
C	1.19419	0.73535	0.00000
H	-0.01750	2.48058	0.00000
H	0.01750	-2.48058	0.00000

Total Electronic Energy = –1029.66945 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

1-tau

	X	Y	Z
H	-4.73754	2.48948	0.00000
H	4.73754	-2.48948	0.00000
C	-4.79888	1.40798	0.00000
C	4.79888	-1.40798	0.00000
C	-4.90299	-1.41235	0.00000
C	4.90299	1.41235	0.00000
C	-3.56024	0.68437	0.00000
C	3.56024	-0.68437	0.00000
C	-5.99513	0.75272	0.00000
C	5.99513	-0.75272	0.00000
C	-6.05153	-0.67587	0.00000
C	6.05153	0.67587	0.00000
C	-3.62799	-0.76332	0.00000
C	3.62799	0.76332	0.00000
N	-2.42179	1.37438	0.00000
N	2.42179	-1.37438	0.00000
H	-6.92086	1.31754	0.00000
H	6.92086	-1.31754	0.00000
H	-7.01588	-1.17041	0.00000
H	7.01588	1.17041	0.00000
C	-2.42701	-1.46981	0.00000
C	2.42701	1.46981	0.00000
H	-4.93353	-2.49433	0.00000

H	4.93353	2.49433	0.00000
C	-1.25981	0.68341	0.00000
C	1.25981	-0.68341	0.00000
O	-2.48901	-2.82064	0.00000
O	2.48901	2.82064	0.00000
C	-0.05540	1.40126	0.00000
C	0.05540	-1.40126	0.00000
C	-1.18911	-0.76754	0.00000
C	1.18911	0.76754	0.00000
H	-0.16117	2.48197	0.00000
H	0.16117	-2.48197	0.00000
H	-1.60591	-3.20544	0.00000
H	1.60591	3.20544	0.00000

Total Electronic Energy = –1029.61910 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

1-pro

	X	Y	Z
H	-4.82495	2.49409	0.00000
H	4.82495	-2.49409	0.00000
C	-4.84718	1.41022	0.00000
C	4.84718	-1.41022	0.00000
C	-4.93727	-1.41539	0.00000
C	4.93727	1.41539	0.00000
C	-3.64640	0.68054	0.00000
C	3.64640	-0.68054	0.00000
C	-6.04620	0.73224	0.00000
C	6.04620	-0.73224	0.00000
C	-6.09516	-0.68612	0.00000
C	6.09516	0.68612	0.00000
C	-3.67522	-0.75060	0.00000
C	3.67522	0.75060	0.00000
N	-2.44028	1.32227	0.00000
N	2.44028	-1.32227	0.00000
H	-6.97256	1.29470	0.00000
H	6.97256	-1.29470	0.00000
H	-7.05519	-1.18642	0.00000
H	7.05519	1.18642	0.00000
C	-2.45916	-1.45558	0.00000
C	2.45916	1.45558	0.00000
H	-4.95910	-2.49665	0.00000
H	4.95910	2.49665	0.00000
C	-1.23186	0.68021	0.00000
C	1.23186	-0.68021	0.00000
H	-2.44953	2.33551	0.00000
H	2.44953	-2.33551	0.00000
O	-2.54652	-2.77351	0.00000
O	2.54652	2.77351	0.00000
C	-0.03825	1.40051	0.00000
C	0.03825	-1.40051	0.00000
C	-1.20094	-0.75246	0.00000
C	1.20094	0.75246	0.00000
H	-0.10117	2.48305	0.00000
H	0.10117	-2.48305	0.00000
H	1.70303	3.24195	0.00000
H	-1.70303	-3.24195	0.00000

Total Electronic Energy = –1030.30425 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 1 (5.38i cm^{-1})

1-hb

	X	Y	Z
H	-4.52887	2.92745	0.00000
H	4.52894	-2.92730	0.00000
H	4.39802	-9.88376	0.00000
H	-4.39792	9.88394	0.00000
H	-4.71104	-4.03247	0.00000
H	4.71112	4.03260	0.00000
C	-4.69062	1.85794	0.00000

C	4.69069	-1.85779	0.00000
C	4.53628	-8.80758	0.00000
C	-4.53617	8.80776	0.00000
C	-4.86469	-5.10339	0.00000
C	4.86477	5.10352	0.00000
C	-5.04405	-0.91409	0.00000
C	5.04410	0.91424	0.00000
C	4.88759	-6.03849	0.00000
C	-4.88749	6.03867	0.00000
C	-5.20369	-7.87887	0.00000
C	5.20380	7.87899	0.00000
C	-3.55900	1.01302	0.00000
C	3.55906	-1.01288	0.00000
C	3.40670	-7.96265	0.00000
C	-3.40659	7.96283	0.00000
C	-3.73092	-5.94164	0.00000
C	3.73101	5.94178	0.00000
C	-5.95581	1.31333	0.00000
C	5.95587	-1.31318	0.00000
C	5.80373	-8.26388	0.00000
C	-5.80363	8.26407	0.00000
C	-6.12894	-5.65666	0.00000
C	6.12903	5.65678	0.00000
C	-6.14322	-0.08420	0.00000
C	6.14328	0.08436	0.00000
C	5.98865	-6.86809	0.00000
C	-5.98854	6.86827	0.00000
C	-6.30928	-7.05307	0.00000
C	6.30938	7.05319	0.00000
C	-3.73324	-0.39257	0.00000
C	3.73329	0.39271	0.00000
C	3.57779	-6.55789	0.00000
C	-3.57768	6.55807	0.00000
C	-3.90097	-7.34503	0.00000
C	3.90107	7.34517	0.00000
N	-2.30514	1.56170	0.00000
N	2.30520	-1.56156	0.00000
N	2.14518	-8.49617	0.00000
N	-2.14507	8.49635	0.00000
N	-2.47369	-5.38383	0.00000
N	2.47378	5.38399	0.00000
H	-6.81813	1.97098	0.00000
H	6.81820	-1.97083	0.00000
H	6.66497	-8.92226	0.00000
H	-6.66487	8.92245	0.00000
H	-6.99420	-5.00267	0.00000
H	6.99429	5.00278	0.00000
H	-7.14423	-0.49814	0.00000
H	7.14429	0.49830	0.00000
H	6.98919	-6.45350	0.00000
H	-6.98908	6.45369	0.00000
H	-7.30832	-7.47210	0.00000
H	7.30842	7.47221	0.00000
C	-2.57707	-1.28412	0.00000
C	2.57713	1.28426	0.00000
C	2.41790	-5.66165	0.00000
C	-2.41780	5.66183	0.00000
C	-2.73862	-8.24037	0.00000
C	2.73873	8.24052	0.00000
H	-5.15829	-1.98929	0.00000
H	5.15834	1.98944	0.00000
H	5.00213	-4.96338	0.00000
H	-5.00203	4.96356	0.00000
H	-5.30018	-8.95787	0.00000
H	5.30030	8.95799	0.00000
C	-1.16388	0.79483	0.00000
C	1.16394	-0.79469	0.00000
C	0.99578	-7.72753	0.00000
C	-0.99567	7.72770	0.00000
C	-1.32863	-6.14283	0.00000

C	1.32873	6.14299	0.00000
H	-2.22575	2.57986	0.00000
H	2.22580	-2.57972	0.00000
H	2.04357	-9.50011	0.00000
H	-2.04346	9.50029	0.00000
H	-2.40154	-4.36560	0.00000
H	2.40161	4.36576	0.00000
O	-2.68919	-2.52099	0.00000
O	2.68924	2.52113	0.00000
O	2.54346	-4.42722	0.00000
O	-2.54336	4.42740	0.00000
O	-2.82954	-9.46664	0.00000
O	2.82966	9.46679	0.00000
C	0.09677	1.39083	0.00000
C	-0.09671	-1.39069	0.00000
C	-0.26008	-8.32921	0.00000
C	0.26019	8.32938	0.00000
C	-0.06730	-5.54498	0.00000
C	0.06740	5.54515	0.00000
C	-1.25887	-0.62467	0.00000
C	1.25893	0.62481	0.00000
C	1.09685	-6.31206	0.00000
C	-1.09675	6.31224	0.00000
C	-1.41839	-7.56169	0.00000
C	1.41849	7.56185	0.00000
H	0.19479	2.46713	0.00000
H	-0.19473	-2.46699	0.00000
H	-0.37191	-9.40835	0.00000
H	0.37203	9.40852	0.00000
H	0.02919	-4.46871	0.00000
H	-0.02911	4.46888	0.00000

Total Electronic Energy = –3089.08253 a.u.
Point Group = C_s
Number of Imaginary Frequency = 6 (16.19*i* cm^{-1}, 11.35*i* cm^{-1}, 7.86*i* cm^{-1}, 2.94*i* cm^{-1}, 1.74*i* cm^{-1}, 0.88*i* cm^{-1})

2

	X	Y	Z
C	-4.78956	-0.97758	0.00000
C	4.78956	0.97758	0.00000
C	-3.55599	-1.59486	0.00000
C	3.55599	1.59486	0.00000
C	-2.38174	-0.81423	0.00000
C	2.38174	0.81423	0.00000
C	-2.47728	0.60048	0.00000
C	2.47728	-0.60048	0.00000
C	-3.75269	1.19868	0.00000
C	3.75269	-1.19868	0.00000
C	-4.89583	0.42752	0.00000
C	4.89583	-0.42752	0.00000
C	-1.27460	1.43586	0.00000
C	1.27460	-1.43586	0.00000
C	-0.01420	0.68795	0.00000
C	0.01420	-0.68795	0.00000
H	-1.03538	-2.41662	0.00000
H	1.03538	2.41662	0.00000
H	-5.68751	-1.58502	0.00000
H	5.68751	1.58502	0.00000
H	-3.47688	-2.67663	0.00000
H	3.47688	2.67663	0.00000
H	-3.79685	2.28108	0.00000
H	3.79685	-2.28108	0.00000
H	-5.87278	0.89541	0.00000
H	5.87278	-0.89541	0.00000
O	-1.27137	2.67063	0.00000
O	1.27137	-2.67063	0.00000
N	-1.14619	-1.40878	0.00000
N	1.14619	1.40878	0.00000

Total Electronic Energy = –875.99250 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-tau

	X	Y	Z
C	-4.72871	-0.98473	0.00000
C	4.72871	0.98473	0.00000
C	-3.50621	-1.59660	0.00000
C	3.50621	1.59660	0.00000
C	-2.30145	-0.82813	0.00000
C	2.30145	0.82813	0.00000
C	-2.42276	0.61540	0.00000
C	2.42276	-0.61540	0.00000
C	-3.71696	1.21626	0.00000
C	3.71696	-1.21626	0.00000
C	-4.83966	0.43693	0.00000
C	4.83966	-0.43693	0.00000
C	-1.24532	1.37087	0.00000
C	1.24532	-1.37087	0.00000
C	0.01013	0.71144	0.00000
C	-0.01013	-0.71144	0.00000
H	-5.63141	-1.58551	0.00000
H	5.63141	1.58551	0.00000
H	-3.41054	-2.67575	0.00000
H	3.41054	2.67575	0.00000
H	-3.78359	2.29712	0.00000
H	3.78359	-2.29712	0.00000
H	-5.82165	0.89518	0.00000
H	5.82165	-0.89518	0.00000
O	-1.26791	2.70784	0.00000
O	1.26791	-2.70784	0.00000
N	-1.12253	-1.46709	0.00000
N	1.12253	1.46709	0.00000
H	0.33095	-2.98799	0.00000
H	-0.33095	2.98799	0.00000

Total Electronic Energy = –875.96635 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-pro

	X	Y	Z
C	-4.76829	-0.99691	0.00000
C	4.76829	0.99691	0.00000
C	-3.53830	-1.61056	0.00000
C	3.53830	1.61056	0.00000
C	-2.37306	-0.82041	0.00000
C	2.37306	0.82041	0.00000
C	-2.47016	0.61530	0.00000
C	2.47016	-0.61530	0.00000
C	-3.76654	1.20618	0.00000
C	3.76654	-1.20618	0.00000
C	-4.88606	0.41916	0.00000
C	4.88606	-0.41916	0.00000
C	-1.28147	1.36670	0.00000
C	1.28147	-1.36670	0.00000
C	-0.02117	0.70013	0.00000
C	0.02117	-0.70013	0.00000
H	-1.07691	-2.41997	0.00000
H	1.07691	2.41997	0.00000
H	-5.66654	-1.60310	0.00000
H	5.66654	1.60310	0.00000
H	-3.45805	-2.69171	0.00000
H	3.45805	2.69171	0.00000
H	-3.88332	2.28410	0.00000
H	3.88332	-2.28410	0.00000
H	-5.86971	0.87181	0.00000
H	5.86971	-0.87181	0.00000
O	-1.19250	2.68671	0.00000
O	1.19250	-2.68671	0.00000
N	-1.14093	-1.40544	0.00000
N	1.14093	1.40544	0.00000
H	2.03995	-3.15518	0.00000

H	-2.03995	3.15518	0.00000

Total Electronic Energy = –876.60423 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-hb

	X	Y	Z
C	-4.75910	-1.08393	0.00000
C	-3.51573	-1.67236	0.00000
C	-2.35664	-0.86410	0.00000
C	-2.48329	0.54829	0.00000
C	-3.77658	1.11457	0.00000
C	-4.89904	0.32012	0.00000
C	-1.30487	1.40211	0.00000
C	-0.02700	0.69336	0.00000
C	0.02713	-0.69430	0.00000
C	1.30513	-1.40283	0.00000
H	-1.03137	-2.45849	0.00000
H	-5.64392	-1.71088	0.00000
H	-3.38660	-2.74546	0.00000
H	-3.85629	2.19297	0.00000
H	-5.88632	0.76617	0.00000
H	1.03102	2.45753	0.00000
C	2.35674	0.86352	0.00000
C	2.48350	-0.54885	0.00000
C	3.77684	-1.11495	0.00000
C	4.89921	-0.32034	0.00000
C	4.75912	1.08369	0.00000
C	3.51566	1.67199	0.00000
H	3.85671	-2.19334	0.00000
H	5.88653	-0.76628	0.00000
H	5.64387	1.71075	0.00000
H	3.38638	2.74510	0.00000
O	-1.35155	2.64423	0.00000
O	1.35221	-2.64498	0.00000
N	1.11629	1.43805	0.00000
N	-1.11628	-1.43890	0.00000
C	-5.05110	-8.04405	0.00000
C	-3.79883	-8.61667	0.00000
C	-2.65194	-7.79477	0.00000
C	-2.78875	-6.38287	0.00000
C	-4.08800	-5.83449	0.00000
C	-5.20283	-6.64253	0.00000
C	-1.61472	-5.51044	0.00000
C	-0.32710	-6.20080	0.00000
C	-0.26813	-7.58151	0.00000
C	0.99987	-8.31684	0.00000
H	-1.24252	-9.34182	0.00000
H	-5.92851	-8.68054	0.00000
H	-3.67842	-9.69438	0.00000
H	-4.18168	-4.75702	0.00000
H	-6.19467	-6.20718	0.00000
H	0.75066	-4.44335	0.00000
C	2.06130	-6.05418	0.00000
C	2.18394	-7.46686	0.00000
C	3.46775	-8.04809	0.00000
C	4.59741	-7.26092	0.00000
C	4.46614	-5.85710	0.00000
C	3.22615	-5.25700	0.00000
H	3.52363	-9.12984	0.00000
H	5.58180	-7.71331	0.00000
H	5.35510	-5.23584	0.00000
H	3.10797	-4.18245	0.00000
O	-1.68543	-4.27046	0.00000
O	1.00261	-9.55168	0.00000
N	0.82210	-5.46337	0.00000
N	-1.40160	-8.33935	0.00000
C	-4.46496	5.86040	0.00000
C	-3.22538	5.25944	0.00000
C	-2.06000	6.05584	0.00000

C	-2.18172	7.46860	0.00000
C	-3.46513	8.05071	0.00000
C	-4.59531	7.26430	0.00000
C	-0.99712	8.31787	0.00000
C	0.27041	7.58177	0.00000
C	0.32852	6.20103	0.00000
C	1.61577	5.50995	0.00000
H	-0.75016	4.44425	0.00000
H	-5.35435	5.23975	0.00000
H	-3.10790	4.18484	0.00000
H	-3.52031	9.13250	0.00000
H	-5.57940	7.71736	0.00000
H	1.24594	9.34151	0.00000
C	2.65435	7.79359	0.00000
C	2.79032	6.38162	0.00000
C	4.08920	5.83239	0.00000
C	5.20455	6.63973	0.00000
C	5.05368	8.04133	0.00000
C	3.80176	8.61475	0.00000
H	4.18214	4.75485	0.00000
H	6.19612	6.20377	0.00000
H	5.93148	8.67728	0.00000
H	3.68205	9.69254	0.00000
O	-0.99912	9.55270	0.00000
O	1.68586	4.27016	0.00000
N	1.40434	8.33895	0.00000
N	-0.82114	5.46426	0.00000

Total Electronic Energy = –2627.99915 a.u.
Point Group = C_s
Number of Imaginary Frequency = 6 (26.75*i* cm^{-1}, 24.19*i* cm^{-1}, 24.02*i* cm^{-1}, 17.83*i* cm^{-1}, 5.77*i* cm^{-1}, 2.68*i* cm^{-1})

3

	X	Y	Z
C	-0.62106	-4.61355	0.00000
C	0.62106	4.61355	0.00000
C	0.68084	-3.96575	0.00000
C	-0.68084	3.96575	0.00000
C	0.63176	-2.48027	0.00000
C	-0.63176	2.48027	0.00000
C	-0.58140	-1.78801	0.00000
C	0.58140	1.78801	0.00000
C	-1.76231	-3.88458	0.00000
C	1.76231	3.88458	0.00000
C	1.84147	-1.74880	0.00000
C	-1.84147	1.74880	0.00000
C	-0.61917	-0.35086	0.00000
C	0.61917	0.35086	0.00000
C	1.83966	-0.38200	0.00000
C	-1.83966	0.38200	0.00000
H	2.76323	-2.31729	0.00000
H	-2.76323	2.31729	0.00000
H	-0.65762	-5.69437	0.00000
H	0.65762	5.69437	0.00000
H	-2.63665	-2.03210	0.00000
H	2.63665	2.03210	0.00000
H	-2.74533	-4.33922	0.00000
H	2.74533	4.33922	0.00000
H	2.79586	0.12797	0.00000
H	-2.79586	-0.12797	0.00000
O	-1.74559	4.58157	0.00000
O	1.74559	-4.58157	0.00000
N	-1.75512	-2.51644	0.00000
N	1.75512	2.51644	0.00000

Total Electronic Energy = –875.96823 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

3-tau

	X	Y	Z
C	-0.59813	-4.54321	0.00000

C	0.59813	4.54321	0.00000
C	0.61842	-3.89057	0.00000
C	-0.61842	3.89057	0.00000
C	0.64838	-2.47256	0.00000
C	-0.64838	2.47256	0.00000
C	-0.60184	-1.79683	0.00000
C	0.60184	1.79683	0.00000
C	-1.77122	-3.76765	0.00000
C	1.77122	3.76765	0.00000
C	1.86593	-1.73071	0.00000
C	-1.86593	1.73071	0.00000
C	-0.61188	-0.35011	0.00000
C	0.61188	0.35011	0.00000
C	1.84541	-0.36731	0.00000
C	-1.84541	0.36731	0.00000
H	2.80411	-2.27032	0.00000
H	-2.80411	2.27032	0.00000
H	-0.65728	-5.62667	0.00000
H	0.65728	5.62667	0.00000
H	-2.73660	-4.26760	0.00000
H	2.73660	4.26760	0.00000
H	2.76316	0.20481	0.00000
H	-2.76316	-0.20481	0.00000
O	-1.81509	4.53596	0.00000
O	1.81509	-4.53596	0.00000
N	-1.79232	-2.44962	0.00000
N	1.79232	2.44962	0.00000
H	-1.67679	5.48926	0.00000
H	1.67679	-5.48926	0.00000

Total Electronic Energy = –875.96371 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

3-pro

	X	Y	Z
C	-0.61217	-4.59439	0.00000
C	0.61217	4.59439	0.00000
C	0.60864	-3.91599	0.00000
C	-0.60864	3.91599	0.00000
C	0.62913	-2.48203	0.00000
C	-0.62913	2.48203	0.00000
C	-0.59132	-1.78178	0.00000
C	0.59132	1.78178	0.00000
C	-1.77815	-3.86019	0.00000
C	1.77815	3.86019	0.00000
C	1.85185	-1.75664	0.00000
C	-1.85185	1.75664	0.00000
C	-0.62183	-0.34298	0.00000
C	0.62183	0.34298	0.00000
C	1.84236	-0.39393	0.00000
C	-1.84236	0.39393	0.00000
H	2.78469	-2.30383	0.00000
H	-2.78469	2.30383	0.00000
H	-0.66152	-5.67601	0.00000
H	0.66152	5.67601	0.00000
H	-2.64440	-2.03483	0.00000
H	2.64440	2.03483	0.00000
H	-2.75522	-4.32639	0.00000
H	2.75522	4.32639	0.00000
H	2.80176	0.10836	0.00000
H	-2.80176	-0.10836	0.00000
O	-1.78584	4.51213	0.00000
O	1.78584	-4.51213	0.00000
N	-1.75443	-2.51645	0.00000
N	1.75443	2.51645	0.00000
H	-1.73443	5.47967	0.00000
H	1.73443	-5.47967	0.00000

Total Electronic Energy = –876.63443 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

3-hb

	X	Y	Z
C	-1.80467	-5.26413	0.00000
C	-2.61430	-4.06098	0.00000
C	-1.83664	-2.79859	0.00000
C	-0.43876	-2.79319	0.00000
C	-0.44907	-5.19430	0.00000
C	-2.52567	-1.56642	0.00000
C	0.29700	-1.55823	0.00000
C	-0.43757	-0.34052	0.00000
C	-1.85641	-0.37606	0.00000
C	2.37614	-0.31799	0.00000
C	1.71914	-1.51373	0.00000
H	-3.60652	-1.61600	0.00000
H	-2.30348	-6.22371	0.00000
H	1.23022	-4.02493	0.00000
H	0.17946	-6.07613	0.00000
H	-2.41279	0.54941	0.00000
H	3.45108	-0.28302	0.00000
H	2.31229	-2.42089	0.00000
C	0.28432	0.90490	0.00000
C	0.27291	3.29011	0.00000
C	1.63290	3.37228	0.00000
C	2.44234	2.18179	0.00000
C	1.68490	0.91656	0.00000
H	-1.40737	2.15406	0.00000
H	-0.36603	4.16409	0.00000
H	2.12409	4.33576	0.00000
O	3.68917	2.20448	0.00000
O	-3.84983	-4.06468	0.00000
N	0.22280	-4.00552	0.00000
N	-0.38973	2.10622	0.00000
C	-4.72744	4.54108	0.00000
C	-4.38136	3.14048	0.00000
C	-5.52777	2.21238	0.00000
C	-6.84632	2.68036	0.00000
C	-6.02758	4.93705	0.00000
C	-5.30482	0.81631	0.00000
C	-7.96236	1.77265	0.00000
C	-7.68820	0.37573	0.00000
C	-6.33828	-0.07293	0.00000
C	-10.34785	1.32581	0.00000
C	-9.31297	2.21996	0.00000
H	-4.28572	0.47427	0.00000
H	-3.93252	5.27406	0.00000
H	-7.99901	4.39737	0.00000
H	-6.31776	5.98017	0.00000
H	-6.09741	-1.12926	0.00000
H	-11.38076	1.65169	0.00000
H	-9.55319	3.27691	0.00000
C	-8.79755	-0.53760	0.00000
C	-9.61557	-2.79715	0.00000
C	-10.91292	-2.40755	0.00000
C	-11.27262	-0.99960	0.00000
C	-10.11339	-0.06766	0.00000
H	-7.64095	-2.25958	0.00000
H	-9.31755	-3.83817	0.00000
H	-11.70741	-3.14115	0.00000
O	-12.43236	-0.59089	0.00000
O	-3.20384	2.73640	0.00000
N	-7.05581	4.04485	0.00000
N	-8.58190	-1.90023	0.00000
C	7.80493	-4.77978	0.00000
C	6.62386	-3.93627	0.00000
C	6.90635	-2.48173	0.00000
C	8.21244	-1.98390	0.00000
C	9.04903	-4.23820	0.00000
C	5.82797	-1.56975	0.00000
C	8.47336	-0.56995	0.00000

C	7.35680	0.31108	0.00000
C	6.04001	-0.22100	0.00000
C	9.98800	1.32619	0.00000
C	9.78964	-0.02716	0.00000
H	4.83234	-1.99315	0.00000
H	7.67382	-5.85334	0.00000
H	10.20411	-2.54686	0.00000
H	9.94706	-4.84377	0.00000
H	5.19452	0.45122	0.00000
H	10.98317	1.75401	0.00000
H	10.66114	-0.67221	0.00000
C	7.59453	1.73030	0.00000
C	6.74417	3.96307	0.00000
C	7.98264	4.52010	0.00000
C	9.17295	3.69163	0.00000
C	8.90118	2.23144	0.00000
H	5.57059	2.30463	0.00000
H	5.83537	4.55193	0.00000
H	8.10402	5.59491	0.00000
O	10.32156	4.14096	0.00000
O	5.47015	-4.37890	0.00000
N	9.25792	-2.88906	0.00000
N	6.53978	2.61598	0.00000

Total Electronic Energy = –2627.95999 a.u.
Point Group = C_s
Number of Imaginary Frequency = 2 (65.86*i* cm^{-1}, 54.20*i* cm^{-1})

2-hydroxylpyridine

	X	Y	Z
C	2.22881	0.81645	0.00000
C	3.56183	1.24648	0.00000
C	4.54644	0.27153	0.00000
C	4.18080	-1.07825	0.00000
C	2.82657	-1.38582	0.00000
N	1.85910	-0.45791	0.00000
H	5.59210	0.55869	0.00000
H	3.78888	2.30418	0.00000
H	4.92322	-1.86598	0.00000
H	2.49056	-2.41843	0.00000
O	1.24958	1.75148	0.00000
H	0.40796	1.27429	0.00000

Total Electronic Energy = –323.61917 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-hydroxylpyridine dimer

	X	Y	Z
C	-1.89627	-0.70837	0.00000
C	-3.23467	-1.14641	0.00000
C	-4.23934	-0.19877	0.00000
C	-3.90956	1.16379	0.00000
C	-2.56819	1.50125	0.00000
N	-1.57688	0.59238	0.00000
H	-5.27786	-0.51089	0.00000
H	-3.43702	-2.20922	0.00000
H	-4.67080	1.93283	0.00000
H	-2.25006	2.53914	0.00000
O	-0.92757	-1.61673	0.00000
H	-0.01695	-1.18304	0.00000
C	1.89627	0.70837	0.00000
C	3.23467	1.14641	0.00000
C	4.23934	0.19877	0.00000
C	3.90956	-1.16379	0.00000
C	2.56819	-1.50125	0.00000
N	1.57688	-0.59238	0.00000
H	5.27786	0.51089	0.00000
H	3.43702	2.20922	0.00000
H	4.67080	-1.93283	0.00000
H	2.25006	-2.53914	0.00000
O	0.92757	1.61673	0.00000

H	0.01695	1.18304	0.00000

Total Electronic Energy = –647.27038 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-pyridone

	X	Y	Z
C	2.15576	0.91606	0.00000
C	3.56976	1.24235	0.00000
C	4.52772	0.27211	0.00000
C	4.18553	-1.11243	0.00000
C	2.86573	-1.44550	0.00000
N	1.90849	-0.47373	0.00000
H	5.57526	0.55497	0.00000
H	3.81504	2.29609	0.00000
H	4.94352	-1.88243	0.00000
H	2.50949	-2.46785	0.00000
O	1.22012	1.70502	0.00000
H	0.92811	-0.72424	0.00000

Total Electronic Energy = –323.621130 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0

2-pyridone dimer

	X	Y	Z
C	1.86545	0.80882	0.00000
C	3.22434	1.28298	0.00000
C	4.27643	0.40787	0.00000
C	4.06309	-0.99490	0.00000
C	2.77196	-1.44244	0.00000
N	1.73003	-0.57392	0.00000
H	5.29150	0.79123	0.00000
H	3.36466	2.35566	0.00000
H	4.88651	-1.69482	0.00000
H	2.50423	-2.49162	0.00000
O	0.85474	1.53926	0.00000
H	0.75709	-0.94581	0.00000
C	-1.86545	-0.80882	0.00000
C	-3.22434	-1.28298	0.00000
C	-4.27643	-0.40787	0.00000
C	-4.06309	0.99490	0.00000
C	-2.77196	1.44244	0.00000
N	-1.73003	0.57392	0.00000
H	-5.29150	-0.79123	0.00000
H	-3.36466	-2.35566	0.00000
H	-4.88651	1.69482	0.00000
H	-2.50423	2.49162	0.00000
O	-0.85474	-1.53926	0.00000
H	-0.75709	0.94581	0.00000

Total Electronic Energy = –647.27871 a.u.
Point Group = C_{2h}
Number of Imaginary Frequency = 0