Quantum-Chemical Investigation on Indole: Vibrational Force Field and Theoretical Determination of its Aqueous pK_a Value

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Table S1. Equilibrium Geometries of Indole computed with B3LYP functional

	cc-pVTZ			aug-cc-pVTZ			cc-pVQZ		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.670004	0.000000	-0.240873	0.669847	0.000000	-0.240694	0.669736	0.000000	-0.240797
C	-0.748519	0.000000	-0.241002	-0.748297	0.000000	-0.240732	-0.748321	0.000000	-0.240722
C	-1.164245	0.000000	-1.612700	-1.164401	0.000000	-1.612636	-1.164151	0.000000	-1.612502
C	-0.032652	0.000000	-2.375368	-0.033011	0.000000	-2.375780	-0.032617	0.000000	-2.374893
C	-1.422904	0.000000	0.987085	-1.423205	0.000000	0.987282	-1.422863	0.000000	0.987069
C	-0.687764	0.000000	2.158145	-0.687807	0.000000	2.158457	-0.687568	0.000000	2.157859
C	0.717314	0.000000	2.133957	0.717601	0.000000	2.134125	0.717410	0.000000	2.133484
C	1.413681	0.000000	0.937872	1.413979	0.000000	0.937696	1.413589	0.000000	0.937411
N	1.076272	0.000000	-1.556006	1.076437	0.000000	-1.556451	1.075985	0.000000	-1.555790
H	-2.504792	0.000000	1.017636	-2.504893	0.000000	1.018084	-2.504111	0.000000	1.017788
H	-1.198556	0.000000	3.111721	-1.198408	0.000000	3.111909	-1.197891	0.000000	3.110982
H	1.264204	0.000000	3.067228	1.264489	0.000000	3.067156	1.264067	0.000000	3.066156
H	2.495961	0.000000	0.922262	2.496058	0.000000	0.922187	2.495240	0.000000	0.921771
H	0.079254	0.000000	-3.446075	0.078916	0.000000	-3.446397	0.079280	0.000000	-3.444972
H	-2.174522	0.000000	-1.984320	-2.174454	0.000000	-1.984827	-2.173790	0.000000	-1.984189
H	2.028437	0.000000	-1.871379	2.028485	0.000000	-1.872012	2.027577	0.000000	-1.871004

Table S2. Equilibrium Geometries of Protonated indole computed with B3LYP functional

	cc-pVTZ			aug-cc-pVTZ			cc-pVQZ		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.000000	0.688195	0.000000	0.000000	0.687952	0.000000	0.000000	0.687830	0.000000
C	0.384463	-0.654073	0.000000	0.384630	-0.654197	0.000000	0.384470	-0.654090	0.000000
C	2.259702	0.729096	0.000000	2.259569	0.729237	0.000000	2.258783	0.729667	0.000000
C	-0.592160	-1.633269	0.000000	-0.592116	-1.633393	0.000000	-0.591850	-1.633197	0.000000
C	-1.926202	-1.227007	0.000000	-1.926190	-1.227030	0.000000	-1.925706	-1.226963	0.000000
C	-2.281825	0.123468	0.000000	-2.281850	0.123478	0.000000	-2.281300	0.123254	0.000000
C	-1.313538	1.120872	0.000000	-1.313408	1.120887	0.000000	-1.313128	1.120542	0.000000
N	1.191986	1.462168	0.000000	1.191754	1.462193	0.000000	1.191333	1.461868	0.000000
H	-0.337767	-2.683771	0.000000	-0.338022	-2.683881	0.000000	-0.337606	-2.683163	0.000000
H	-2.705566	-1.975776	0.000000	-2.705515	-1.975713	0.000000	-2.704674	-1.975361	0.000000
H	-3.326430	0.399167	0.000000	-3.326386	0.399141	0.000000	-3.325386	0.398771	0.000000
H	-1.580137	2.168334	0.000000	-1.579906	2.168322	0.000000	-1.579465	2.167518	0.000000
H	3.249771	1.160308	0.000000	3.249415	1.160988	0.000000	3.248173	1.161155	0.000000
H	1.203750	2.476641	0.000000	1.203262	2.476518	0.000000	1.202399	2.475752	0.000000
C	1.887822	-0.707232	0.000000	1.887912	-0.707114	0.000000	1.887793	-0.706909	0.000000
H	2.321453	-1.210189	0.872459	2.321800	-1.209820	0.872420	2.321428	-1.209273	0.872041
H	2.321453	-1.210189	-0.872459	2.321800	-1.209820	-0.872420	2.321428	-1.209273	-0.872041

Table S3. Equilibrium Geometries of Indole computed with M06 functional

	cc-pVTZ			aug-cc-pVTZ			cc-pVQZ		
	X	Y	Z	X	Y	Z	X	Y	Z
H	0.074686	-2.692926	0.000000	0.075194	-2.693321	0.000000	0.074708	-2.691768	0.000000
C	0.423568	-1.667700	0.000000	0.423657	-1.667887	0.000000	0.423315	-1.667834	0.000000
C	1.358408	0.997737	0.000000	1.358015	0.997944	0.000000	1.358150	0.997950	0.000000
C	-0.489689	-0.612304	0.000000	-0.489418	-0.612347	0.000000	-0.489434	-0.612145	0.000000
C	1.771136	-1.386435	0.000000	1.771202	-1.386261	0.000000	1.770687	-1.386412	0.000000
C	2.234471	-0.065604	0.000000	2.234416	-0.065272	0.000000	2.233941	-0.065473	0.000000
C	0.000000	0.709854	0.000000	0.000000	0.709481	0.000000	0.000000	0.709751	0.000000
H	2.488375	-2.196976	0.000000	2.488612	-2.196701	0.000000	2.487329	-2.195716	0.000000
H	3.300215	0.122833	0.000000	3.300149	0.123287	0.000000	3.298413	0.122515	0.000000
H	1.717009	2.019644	0.000000	1.716533	2.019993	0.000000	1.716802	2.018453	0.000000
C	-1.914762	-0.527162	0.000000	-1.914474	-0.527262	0.000000	-1.914579	-0.527163	0.000000
H	-2.613052	-1.346887	0.000000	-2.613674	-1.346597	0.000000	-2.612202	-1.346035	0.000000
C	-2.235095	0.792961	0.000000	-2.235217	0.792683	0.000000	-2.234367	0.792998	0.000000
H	-3.201330	1.269019	0.000000	-3.201545	1.268887	0.000000	-3.199384	1.269096	0.000000
N	-1.086474	1.546958	0.000000	-1.086553	1.547086	0.000000	-1.086210	1.546600	0.000000
H	-1.048804	2.548509	0.000000	-1.048486	2.548374	0.000000	-1.048481	2.547219	0.000000

Table S4. Equilibrium Geometries of Protonated indole computed with M06 functional

	cc-pVTZ			aug-cc-pVTZ			cc-pVQZ		
	X	Y	Z	X	Y	Z	X	Y	Z
C	0.000000	0.684767	0.000000	0.000000	0.684261	0.000000	0.000000	0.684522	0.000000
C	0.382866	-0.651015	0.000000	0.383287	-0.651397	0.000000	0.382627	-0.651100	0.000000
C	2.249222	0.721341	0.000000	2.248831	0.721970	0.000000	2.248532	0.721946	0.000000
C	-0.590367	-1.626527	0.000000	-0.590136	-1.626754	0.000000	-0.590182	-1.626669	0.000000
C	-1.917565	-1.220471	0.000000	-1.917264	-1.220517	0.000000	-1.917310	-1.220412	0.000000
C	-2.271283	0.124362	0.000000	-2.271198	0.124336	0.000000	-2.270830	0.124401	0.000000
C	-1.307224	1.117354	0.000000	-1.307006	1.117214	0.000000	-1.306827	1.117493	0.000000
N	1.189275	1.457526	0.000000	1.188469	1.457598	0.000000	1.188987	1.457384	0.000000
H	-0.336049	-2.677480	0.000000	-0.336301	-2.677924	0.000000	-0.336293	-2.676645	0.000000
H	-2.698151	-1.968661	0.000000	-2.697960	-1.968692	0.000000	-2.697274	-1.967673	0.000000
H	-3.316481	0.399648	0.000000	-3.316538	0.399351	0.000000	-3.315006	0.399323	0.000000
H	-1.571391	2.165865	0.000000	-1.570964	2.165993	0.000000	-1.571189	2.164896	0.000000
H	3.243156	1.145498	0.000000	3.242441	1.147046	0.000000	3.241651	1.145856	0.000000
H	1.202662	2.470876	0.000000	1.200871	2.470552	0.000000	1.201450	2.470093	0.000000
C	1.875492	-0.703566	0.000000	1.875656	-0.703287	0.000000	1.875761	-0.704079	0.000000
H	2.312244	-1.207948	0.869726	2.313072	-1.207235	0.869745	2.311564	-1.207072	0.869470
H	2.312244	-1.207948	-0.869726	2.313072	-1.207235	-0.869745	2.311564	-1.207072	-0.869470

Table S5. Equilibrium Geometries of Indole computed with MP2 level of theory

	cc-pVTZ			aug-cc-pVTZ		
	X	Y	Z	X	Y	Z
C	0.000000	0.714630	0.000000	0.000000	0.714264	0.000000
C	-0.497108	-0.617083	0.000000	-0.496670	-0.617615	0.000000
C	-1.921681	-0.529769	0.000000	-1.921575	-0.531653	0.000000
C	-2.241462	0.807150	0.000000	-2.243629	0.805451	0.000000
C	0.420083	-1.681405	0.000000	0.421391	-1.681740	0.000000
C	1.775270	-1.396842	0.000000	1.777002	-1.395680	0.000000
C	2.244946	-0.068064	0.000000	2.245862	-0.065986	0.000000
C	1.366679	1.004315	0.000000	1.366281	1.006348	0.000000
N	-1.086517	1.552976	0.000000	-1.088279	1.552318	0.000000
H	0.072077	-2.706058	0.000000	0.074172	-2.707532	0.000000
H	2.491413	-2.207185	0.000000	2.494502	-2.205969	0.000000
H	3.310117	0.118507	0.000000	3.311722	0.121390	0.000000
H	1.729337	2.023991	0.000000	1.727938	2.027227	0.000000
H	-3.204443	1.289070	0.000000	-3.207269	1.287769	0.000000
H	-2.626833	-1.343149	0.000000	-2.626650	-1.346204	0.000000
H	-1.046415	2.556395	0.000000	-1.048430	2.556763	0.000000

Table S6. Equilibrium Geometries of Protonated Indole computed with MP2 level of theory

	cc-pVTZ			aug-cc-pVTZ		
	X	Y	Z	X	Y	Z
C	0.000000	0.686808	0.000000	0.000000	0.686515	0.000000
C	0.388983	-0.654592	0.000000	0.389187	-0.655003	0.000000
C	2.258850	0.726740	0.000000	2.259931	0.726439	0.000000
C	-0.590007	-1.638897	0.000000	-0.590337	-1.639222	0.000000
C	-1.923887	-1.228634	0.000000	-1.924426	-1.228400	0.000000
C	-2.281945	0.126608	0.000000	-2.282384	0.127285	0.000000
C	-1.314782	1.127419	0.000000	-1.314678	1.128154	0.000000
N	1.188521	1.460772	0.000000	1.188753	1.460395	0.000000
H	-0.334296	-2.688962	0.000000	-0.335074	-2.690274	0.000000
H	-2.704904	-1.975566	0.000000	-2.706462	-1.975478	0.000000
H	-3.327046	0.399754	0.000000	-3.328277	0.400675	0.000000
H	-1.579014	2.175460	0.000000	-1.578223	2.177294	0.000000
H	3.245928	1.164896	0.000000	3.247205	1.165982	0.000000
H	1.204941	2.477004	0.000000	1.204426	2.477281	0.000000
C	1.887016	-0.706872	0.000000	1.886968	-0.706952	0.000000
H	2.314686	-1.204736	0.876282	2.314784	-1.205567	0.876922
H	2.314686	-1.204736	-0.876282	2.314784	-1.205567	-0.876922

Table S7. Gas phase anharmonic wavenumbers (cm^{-1}) of indole computed at B3LYP level of theory combined with 6-311++G(df, pd) and cc-pVTZ basis set compared to experimental data (taken from Ref. 23).

Mode	Symmetry	Exp.	6-311++G(df, pd)	cc-pVTZ
1	A'	3524	3507	3510
2	A'	3140	3132	3132
3	A'	3119	3111	3111
4	A'	3090	3058	3059
5	A'	3072	3042	3033
6	A'	3058	3043	3042
7	A'	3051	3013	3012
8	A'	1625	1615	1619
9	A'	1580	1577	1580
10	A'	1519	1516	1520
11	A'	1486	1492	1497
12	A'	1458	1451	1452
13	A'	1411	1402	1408
14	A'	1347	1357	1360
15	A'	1333	1329	1331
16	A'	1276	1273	1274
17	A'	1245	1247	1247
18	A'	1205	1202	1206
19	A'	1150	1163	1165
20	A'	1121	1127	1129
21	A'	1093	1086	1090
22	A'	1067	1068	1072
23	A'	1014	1019	1025
24	A'	899	900	900
25	A'	877	881	882
26	A'	758	762	765
27	A'	607	612	614
28	A'	543	548	551
29	A'	397	401	406
30	A"	961	987	996
31	A"	925	947	945
32	A"	850	863	869
33	A"	840	850	854
34	A"	764	760	793
35	A"	738	741	748
36	A"	715	717	725
37	A"	601	602	613
38	A"	570	576	591
39	A"	419	425	437
40	A"	387	444	474
41	A"	241	246	254
42	A"	207	211	225