A Comprehensive Study of N-Butyl-1H-Benzimidazole

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Supplementary Materials

Table S1. Condensed Fukui functions for NBB

Atoms	f_r^+	f_r^-	f_r^0	Δf(r)
C1	-18,8264	2,3029	-8,2618	-21,1293
C2	13,0512	-7,4194	2,8159	20,4706
C3	-6,3062	-3,0305	-4,6684	-3,2757
C4	11,3780	-5,7455	2,8163	17,1235
C5	12,1912	-5,1466	3,5223	17,3378
C6	2,1966	-4,0100	-0,9067	6,2066
C7	-15,9949	-7,7970	-11,8960	-8,1979
H8	-5,3944	-6,3091	-5,8518	0,9147
H9	-4,3771	-7,4156	-5,8964	3,0385
H10	-10,0579	-7,0430	-8,5505	-3,0149
H11	-30,9569	-5,8619	-18,4094	-25,0950
H12	-31,7882	-6,9532	-19,3707	-24,8350

C13	44,7673	1,0525	22,9099	43,7148
H14	-26,8419	-3,3110	-15,0765	-23,5309
H15	4,8414	-3,0603	0,8905	7,9017
C16	8,3801	2,5912	5,4857	5,7889
H17	31,6032	-0,4020	15,6006	32,0052
H18	-14,5065	-2,2840	-8,3953	-12,2225
C19	6,0125	1,0261	3,5193	4,9864
H20	-40,8605	-0,8910	-20,8758	-39,9695
H21	-46,2341	-0,9343	-23,5842	-45,2998
C22	148,0819	-3,1314	72,4753	151,2133
H23	-37,8624	-0,2530	-19,0577	-37,6094
H24	-57,6031	-1,9546	-29,7789	-55,6485
H25	-23,4681	-0,7722	-12,1202	-22,6959
N26	-3,0917	-3,8957	-3,4937	0,8040
N27	-6,1914	-9,4666	-7,8290	3,2752

Table S2. Second order perturbation theory analysis of Fock matrix in NBO basis for N-Butyl-1H-benzimidazole.

Donor (i)	Type	ED/e	Acceptor(j)	Type	ED/e	$E^{(2)a}$(KJ mol^{-1})	E(j)-E(i)[b] (a.u)	F(i.j)[c] (a.u)
C1-C2	σ	1.96	C1-C6	σ*	0.03	4.63	1.24	0.068
C1-C2	σ	1.96	C1-N26	σ*	0.03	0.86	1.12	0.028
C1-C2	σ	1.96	C6-H11	σ*	0.01	2.42	1.12	0.046
C1-C2	π	1.59	C3-C4	π*	0.31	18.89	0.28	0.067
C1-C2	π	1.59	C7-N27	π*	0.35	14.45	0.25	0.055
C1-C6	σ	1.97	C1 –C2	σ*	0.03	4.57	1.25	0.068
C1-C6	σ	1.97	C1-N26	σ*	0.03	2.82	1.15	0.051
C1-C6	σ	1.97	C6-H11	σ*	0.01	1.04	1.15	0.031
C1-N26	σ	1.98	C1-C2	σ*	0.03	1.03	1.34	0.033
C1-N26	σ	1.98	C2-C3	σ*	0.02	2.53	1.37	0.053

C2-C3	σ	1.97	C1-C2	σ*	0.03	3.55	1.24	0.059
C2-C3	σ	1.97	C3-H8	σ*	0.01	0.95	1.15	0.030
C2-N27	σ	1.98	C1-C2	σ*	0.03	1.17	1.31	0.035
C2-N27	σ	1.98	C7-H12	σ*	0.02	5.04	1.18	0.069
C2-N27	σ	1.98	C7-N27	σ*	0.01	0.71	1.34	0.028
C3-C4	σ	1.97	C2-C3	σ*	0.02	3.01	1.27	0.055
C3-C4	σ	1.97	C2-N27	σ*	0.02	5.47	1.17	0.071
C3-C4	π	1.72	C1-C2	π *	0.5	17.97	0.28	0.066
C3-C4	π	1.72	C5-C6	σ*	0.01	19.46	0.28	0.067
C3-H8	σ	1.98	C1-C2	σ*	0.03	4.09	1.06	0.059
C4-C5	π	1.71	C3-C4	π*	0.31	2.62	1.28	0.052
C5-C6	π	1.72	C1-C2	π*	0.47	19.58	0.28	0.070
C5-C6	π	1.72	C3-C4	π*	0.31	17.74	0.29	0.065
C7-N26	σ	1.98	C1-C6	σ*	0.02	4.68	1.37	0.072
C7-N27	σ	1.98	C2-C3	σ*	0.02	5.70	1.42	0.081
C7-N27	π	1.88	C1-C2	π*	0.47	18.41	0.34	0.078
N26	LP(1)	1.57	C1-C2	π*	0.47	35.08	0.29	0.091
N26	LP(1)	1.57	C7-N27	π*	0.35	50.10	0.26	0.105
N27	LP(1)	1.57	C1-C2	π*	0.47	5.88	0.92	0.066
N27	LP(2)	1.83	C7-N26	π*	0.35	7.60	0.81	0.071
C7-N27	π*	1.88	C1-C2	π*	0.47	73.61	0.50	0.061

Table S3. Calculated natural bond orbitals (NBO) and the polarization coefficient for each hybrid in selected bonds of the C1 using the B3LYP/6-311++G(d,p) in the gas phase for NBB.

Occupancy (a.u.)	Bond (A-B)[a]	Energy (a.u.)	ED_A (%)	ED_B (%)	NBO	S(%)(A)	S(%)(B)	P(%) (A)	P(%) (B)
1.96507	σ (C1-C2)	-0.67599	51.00	49.00	0.7142 ($sp^{2.03}$) + 0.7000 ($sp^{2.09}$)	32.94	32.33	67.01	67.62

1.58979	π (C1-C2)	-0.25537	49.97	50.03	0.7069 ($sp^{1.00}$) + 0.7073 ($sp^{1.00}$)	0.00	0.00	99.97	99.97
1.97476	σ (C1-C6)	-0.71441	51.65	48.35	0.7187 ($sp^{1.51}$) +0.6953 ($sp^{1.94}$)	39.85	33.98	60.12	65.97
1.98139	σ(C1-N26)	-0.80177	37.55	62.45	0.6128 ($sp^{2.70}$) +0.7903 ($sp^{2.0}$)	27.03	33.28	72.87	66.67
1.97699	σ(C2-C3)	-0.70264	51.29	48.71	0.7161($sp^{1.62}$) +0.6980 ($sp^{1.90}$)	38.21	34.44	61.76	65.51
1.97730	σ(C2-N27)	-0.77181	41.98	58.02	0.6479 ($sp^{2.42}$) +0.7617 ($sp^{2.10}$)	29.19	32.20	70.71	67.71
1.97685	σ(C3-C4)	-0.70116	50.49	49.51	0.7105 ($sp^{1.75}$) +0.7037 ($sp^{1.78}$)	36.35	35.96	63.61	64.00
1.72398	π(C3-C4)	-0.25652	49.07	50.93	0.7005 ($sp^{1.00}$) +0.7137 ($sp^{1.00}$)	0.00	0.00	99.95	99.96
1.97965	σ(C3-H8)	-0.51968	61.00	39.00	0.7810 ($sp^{2.42}$) +0.6245 ($sp^{0.00}$)	29.21	99.96	70.75	0.04
1.97934	σ(C4-C5)	-0.69084	49.95	50.05	0.7068 ($sp^{1.81}$) +0.7075 ($sp^{1.80}$)	35.54	35.73	64.42	64.23
1.97989	σ(C4-H9)	-0.51316	60.65	39.35	0.7788 ($sp^{2.51}$) +0.6273 ($sp^{0.00}$)	28.52	99.95	71.44	0.05
1.97559	σ(C5-C6)	-0.70186	49.23	50.77	0.7017 ($sp^{1.79}$) +0.7125 ($sp^{1.75}$)	35.79	36.41	64.16	63.55
1.72737	π(C5-C6)	-0.25897	49.34	50.66	0.7017 ($sp^{1.00}$) +0.7125 ($sp^{1.00}$)	0.00	0.00	99.95	99.95
1.97953	σ(C5-H10)	-0.51465	60.67	39.33	0.7789 ($sp^{2.51}$) +0.6272 ($sp^{0.00}$)	28.48	99.95	71.47	0.05

1.97870	σ(C6-H11)	-0.52629	61.22	38.78	0.7824 ($sp^{2.37}$) +0.6272 ($sp^{0.00}$)	29.62	99.95	70.34	0.05
1.98436	σ(C7-H12)	-0.56257	60.57	39.43	0.7782 ($sp^{1.93}$) +0.6280 ($sp^{0.00}$)	34.14	99.94	95.82	0.06
1.98559	σ(C7-N26)	-0.80774	36.04	63.96	0.6004 ($sp^{2.27}$) +0.7997 ($sp^{2.11}$)	30.57	32.14	69.31	67.81
1.98933	σ(C22-H24)	-0.49246	60.09	39.91	0.6004 ($sp^{3.25}$) +0.7997 ($sp^{0.04}$)	23.52	99.96	76.42	0.07
1.98359	σ(C7-N27)	-0.32006	41.30	58.70	0.6426 ($sp^{1.82}$) +0.7662 ($sp^{1.84}$)	35.38	35.38	64.53	64.77
1.97887	σ(C13-C16)	-0.61557	50.81	49.19	0.7128 ($sp^{2.27}$) +0.7014 ($sp^{2.69}$)	30.57	27.08	69.39	72.88
1.57449	LP (1) (N26)	-0.26555	-	-	($sp^{99.99}$)	99.94	-	66.99	-
1.92917	LP (1) (N27)	-0.37999	-	-	($sp^{69.99}$)	99.99	-	0.052	

Table S4. Theoretical wavenumber (cm^{-1}) of N-Butyl-1H-benzimidazole calculated by means of VEDA 4 program

No	Theoretical Wavenumber (cm^{-1})		TED (<10%)	Experimental Wavenumber (cm^{-1})	No	Theoretical Wavenumber (cm^{-1})		TED (<10%)	Experimental Wavenumber (cm^{-1})
	Scaled	I_{IR}	Assignments			Scaled	I_{IR}	Assignments	
1	3110,892	1.60	νCH (99)		37	1136,174	6.91	νCC (11) + δHCC (34)+ δHCC (17)	
2	3089,168	11.15	νCH (63) + νCH (24)	3100	38	1114,614	10.62	δHCC (16)	1080
3	3080,708	18.92	νCH (40) + νCH (34)	3001	39	1092,948	3.23	νCC (14)+ τHCCC (10)	
4	3070,247	11.86	νCH (10) + νCH (44)		40	1084,247	5.04	νNC (11)	
5	3059,912	0.21	νCH (47)		41	1054,498	11.05	δCCC (10) + δNCN (25)	1006
6	2987,045	40.60	νCH (74)		42	1023,222	0.66	νCC (37)	
7	2983,835	75.32	νCH (11) + νCH (23)	2900	43	993,271	8.48	δHCC (13)+ δHCC (11) + δCCC (19)	

8	2979,127	0.41	νCH (31) + νCH (23)		44	976,7484	2.51	νCC (34)	
9	2953,903	4.87	νCH (18) + νCH (37)		45	943,4034	0.06	τHCCC (33) + τHCCC (16)	
10	2936,887	57.30	νCH (28) + νCH (59)		46	914,0031	3.06	τHCCC (13)	
11	2926,823	8.74	νCH (45)		47	908,6566	2.36	τHCCC (27) + τHCCC (35)	
12	2923,439	31.22	νCH (18) + νCH (27)+ νCH (18)+νCH (22)		48	882,1953	0.29	νCC (24) + νCC (15) + τHCCC (16)	
13	2919,968	6.63	νCH (39) + νCH (19)		49	866,4462	4.09	δCCC (22) + δNCN (12)	
14	2904,78	19.81	νCH (43) + νCH (51)		50	832,9659	7.67	τHCCC (13) + τHCNC (51)	863
15	1597,821	20.17	νCC (18)+ νCC (18)	1615	51	820,4071	1.20	τHCCC (17)+ τHCCC (12)+ τHCCC (21)+ τCNCN (12)+	
16	1563,035	1.77	νCC (10)		52	759,083	7.54	νCC (11) + δCNC (13) + δCNC (15)	
17	1477,889	90.25	νNC (40)	1490	53	747,8005	4.06	τHCCC (18)	
18	1463,426	5.42	δHCH (15)		54	730,0403	9.33	νNC (10) + νNC (21) + δNCN (12)	
19	1462,159	2.21	δHCH (13)		55	723,6981	78.49	τHCCC (11) + τHCCC (22)	740
20	1451,689	5.91	δHCH (19) + δHCH (28)		56	713,7788	3.15	δHCC (15) + τHCCC (21) + τHCCC (23)	
21	1451,118	8.75	δHCH (39)		57	617,3405	2.30	τCNCN (30)	
22	1442,176	3.04	δHCH (29) + δHCH (12)		58	593,8279	3.08	νCC (12) + δCNC (14)	
23	1440,667	2.15	δHCH (10) + δHCH (43) δHCH (28)		59	567,5116	0.66	τHCCC (10) + τCCCN (29)+ τCCNC (12)	
24	1430,313	46.54	δCNC (12) + δHCC (15) δHCC (17)		60	533,809	0.30	δCCC (14)	
25	1362,531	8.82	νNC (13) + δHCC (21)		61	468,9753	5.34	δCNC (26)	
26	1354,409	14.76	τHCNC (12)		62	416,5845	7.03	δCCC (16) + τCNCC (28)	
27	1344,277	25.83	νNC (12)+ νNC (24)	1300	63	415,0472	1.36	δCCC (23)	
28	1335,46	6.02	τHCNC (13)+ τHCCC (12)		64	257,0141	0.88	δCNC (21)	
29	1316,057	18.57	νCC (15)	1310	65	237,3977	0.45	τHCCC (17) + τHCCC (21)	
30	1287,014	0.34	δHCC (31)		66	218,9029	0.43	δCNC (21)	
31	1272,309	3.95	δHCC (14) + δHCC (11) + δHCC (13)		67	218,6418	1.68	τCCCN (36) + τCNCN (16)	
32	1264,603	36.54	νNC (18)	1275	68	166,7633	1.96	δCCC (22) + τCCNC (14)	
33	1251,407	5.24	τHCCC (18)		69	113,6667	0.01	τCCCC (65)	
34	1231,8	28.36	δHCC (16)	1225	70	62,98702	0.02	τCCCN (71)	
35	1184,968	30.99	δHCN (10)+ δHCC (10)	1200	71	37,4345	0.38	τCCNC (60) + τCCCC (10)	
36	1180,54	6.48	νNC (17) + δHCN (29)						

ν ;stretching. δ; bending. τ; torsion vibrations.

Table S5. Mulliken atomic charges of N-Butyl-1H-benzimidazole

Atoms	Charges	Atoms	Charges

C1	0.14132	H15	0.17715
C2	-0.22164	C16	0.06192
C3	-0.32792	H17	0.1531
C4	-0.31576	H18	0.13609
C5	-0.2385	C19	-0.24316
C6	-0.20609	H20	0.12718
C7	0.305	H21	0.1295
H8	0.18349	C22	-0.61749
H9	0.15194	H23	0.13986
H10	0.17072	H24	0.14482
H11	0.13464	H25	0.13988
H12	0.18223	N26	0.20546
C13	-0.55373	N27	-0.12611
H14	0.16612		