

Supporting Information Tables

for

Normal Vibrational Mode Analysis and Assignment of Benzimidazole by ab initio and Density Functional Calculations, and Polarized Infrared and Raman Spectroscopy

By

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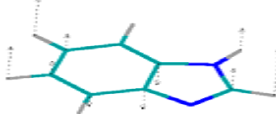
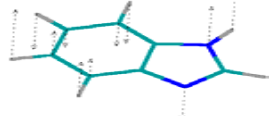
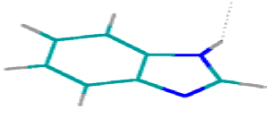
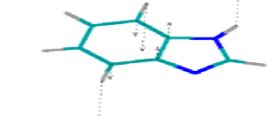
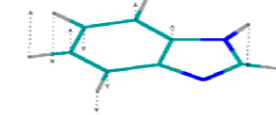
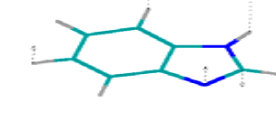
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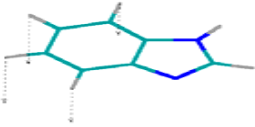
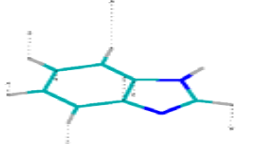
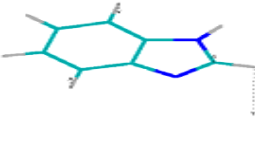
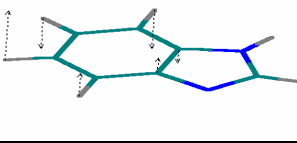
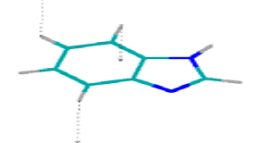
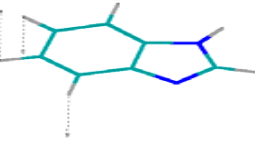
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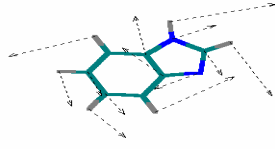
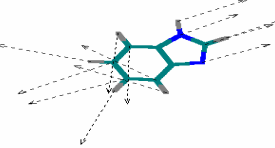
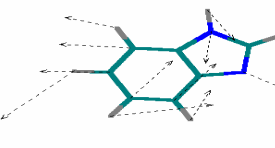
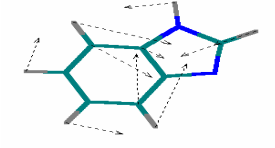
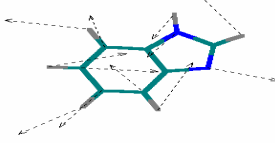
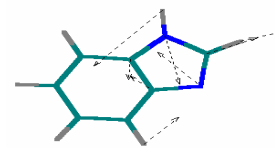
Table 1S: Observed and estimated frequencies (cm^{-1}), relative intensities, and assignments for the out-of-plane fundamental modes for Benzimidazole.

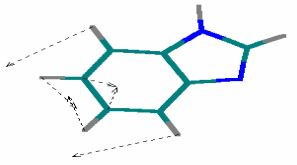
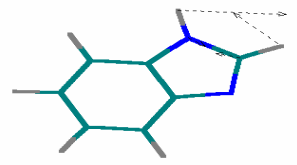
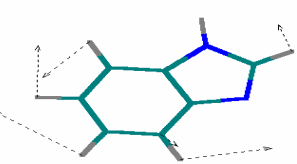
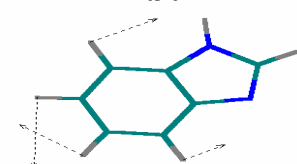
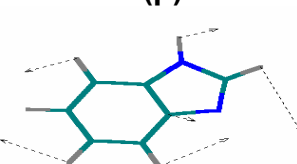
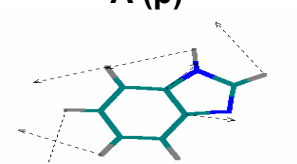
Solid IR	Solid Ram	Gas-like	Assignments/Symmetry	Single Crys. Pol-Ram ^e	ab initio levels	Calculated Modes ^f	IR-Vector Representation ^g
244(m) ^a 242 ^b 242(m)^c	 246(w) ^b 247(w)^c	 ^d	Lattice or fundamentals ^a ^b ^d	aa = 244 (vw) bb = 242 (w) cc = 254 (w) ab = ac = 254 (w) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	260 [218] (9.70) 244 [205] (12.09) 236 [227] (8.08) 225 [217] (7.32) 227 (7.55) 218 (6.66)	A''(dp) 
272(m) ^a 274 ^b 270(m)^c	 269(vw) ^b 272(vw)^c	 ^d	 ^a ^b ^d	aa = bb = 273 (vw) cc = 274 (w) ab = ac = bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	297 [249] (6.00) 279 [234] (1.81) 268 [258] (4.84) 257 [247] (2.12) 258 (4.16) 248 (1.65)	A''(dp) 
628(m) ^a 628(s) ^b 626(m)^c	 628(m) ^b 625(m)^c	 449 (vs)^c 459/449 (109) ^d	NH out-of-plane ^a A'', f ^b NH bending ^d	aa = 623 (s) bb = 624 (m) cc = 623 (vs) ab = 633 (s) ac = 632 (vw) bc = 635 (m)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	658 [552] (84.30) 435 [365] (154.62) 600 [578] (126.72) 429 [413] (82.53) 557 (117.96) 406 (99.94)	A''(dp) 
425(s) ^a 424(s) ^b 424(s)^c	 425(sh) ^b 424(w)^c	 425 (s)^c 420 (11) ^d	Ring torsion ^a A'', f ^b Bond torsion ^d	aa = 426 (w) bb = 427 (w) cc = 426 (w) ab = ac = 425 (w) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	506 [424] (20.50) 475 [398] (1.38) 456 [439] (15.95) 439 [423] (32.28) 438 (14.51) 421 (2.11)	A''(dp) 
579(w) ^a 578(w) ^b 578(w)^c	 581(vw) ^b 580(w)^c	 586 (w)^c 578 (5) ^d	 ^a A'', f ^b Bond torsion ^d	aa = 580 (w) bb = 581 (w) cc = 580 (w) ab = ac = bc = 585 (vw)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	687 [578] (67.35) 638 [535] (3.42) 616 [593] (4.70) 589 [567] (4.37) 592 (1.63) 570 (4.36)	A''(dp) 
637(m) ^a ^b 635(m)^c	 637(w) ^b 636(m)^c	 647 (w)^c 637 (3) ^d	Im-ring torsion ^a A', f ^b Bond torsion ^d	aa = 632 (w) bb = 632 (w) cc = 631 (w) ab = 643 (m) ac = 641 (vw) bc = 641 (m)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	724 [607] (18.09) 705 [591] (0.12) 658 [634] (0.03) 652 [628] (1.62) 632 (1.13) 630 (2.11)	A''(dp) 

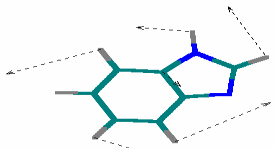
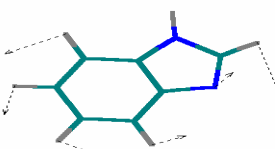
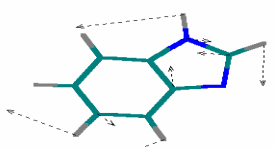
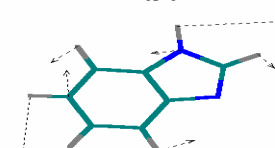
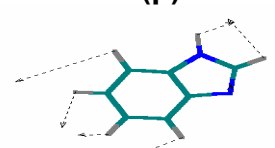
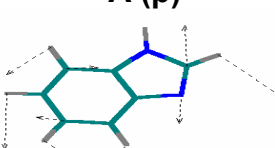
744(vs) ^a			Bz-out-of-plane bend ^a	aa = bb = 748 (w) cc = ab = ac = bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	888 [744] (148.45) 840 [704] (56.20) 785 [756] (105.26) 758 [730] (52.84) 751 (88.12) 731 (45.57)	A''(dp) 
740(vs) ^b	748(w) ^b		A'', f ^b				
746(vs)^c	746(w)^c	743 (vs)^c	C4H, C3H bend ^d				
		742 (93) ^d					
751(vs) ^a			Bz-CH out-of-plane bend ^a	aa = 750 (sh) bb = 755 (s) cc = ab = ac = 760 (w) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	936 [785] (1.04) 854 [716] (27.82) 836 [805] (0.42) 779 [750] (5.74) 798 (1.65) 750 (3.80)	A''(dp) 
760(m) ^b	752(vw) ^b		A'', f ^b				
752(vs)^c	755(w)^c	766 (m)^c	Ring torsion ^d				
		766 (10) ^d					
848(m) ^a			Im-CH out plane bend ^a	aa = 855 (m) bb = 855 (m) cc = 851 (w) ab = ac = bc = 853 (vw)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1065 [893] (0.17) 1022 [857] (3.38) 879 [846] (7.00) 849 [818] (4.69) 823 (8.39) 797 (8.79)	A''(dp) 
848(s) ^b	851(w) ^b		A'' ^b				
847(w)^c	848(w)^c	 ^c					
		 ^d	 ^d				
.... ^a			 ^a	aa = 896 (w) bb = 896 (w) cc = 890 (w) ab = 888 (w) ac = 895 (w) bc = 892 (w)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1035 [868] (3.13) 964 [793] (0.04) 929 [895] (0.15) 866 [834] (3.91) 883 (0.23) 830 (1.85)	A''(dp) 
880(m) ^b	884(w) ^b		A'' ^b				
887(m)^c	890(w)^c	860 (m)^c	C5H, C3H, C2H, C7H bend ^d				
		858 (9) ^d					
890(s) ^a			Im-in-plane bend ^a	aa = 905 (vw) bb = 906 (vw) cc = 904 (vw) ab = 905 (vw) ac = 905 (vw) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1137 [953] (9.93) 1064 [877] (3.59) 990 [953] (6.78) 932 [898] (2.17) 940 (5.71) 890 (1.79)	A''(dp) 
890(vw) ^b	892(w) ^b		A'' ^b				
902(w)^c	905(vw)^c	903 (m)^c	C2H, C5H, C7H bend ^d				
		902/899 (12) ^d					
935(m) ^a			Bz-in-plane bend ^a	aa = 934 (vw) bb = 937 (w) cc = 932 (vw) ab = 941 (vw) ac = 937 (vw) bc = 937 (vw)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1183 [992] (0.03) 1104 [925] (0.02) 1032 [994] (0.06) 975 [939] (0.06) 981 (0.12) 933 (0.06)	A''(dp) 
929(m) ^b	936(vw) ^b		A'' ^b				
933(w)^c	934(w)^c	931(w)^c	C2H, C3H, C5H bend ^d				
		949/944 (21) ^d					

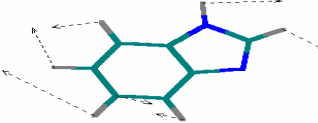
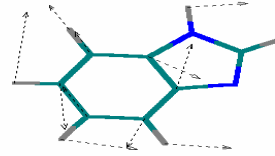
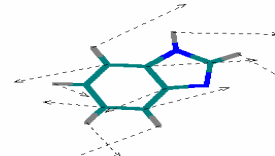
Abbreviations: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; f, fundamental; A'', Symmetry; dp, depolarized.
a IR of KBr-Discs Ref. (19), b polarized IR of partially oriented BZI-solid and Raman of powder BZI Ref. (17), c this work, d FT-IR of gas-like BZI trapping in Ar-Matrix Ref. (25), e polarized Raman from a single crystal of BZI based on its unit cell axes notation Ref (17), f Computed vibrational modes [its scaled value] (its intensity in km/mol), g estimated mode symmetry, (polarization), and graphical representation.

Table 2S: Observed and estimated frequencies (cm^{-1}), relative intensities, and assignments for the in-plane fundamental modes for Benzimidazole.

Solid IR	Solid Ram	Gas-like	Assignments/Symmetry	Single Crys. Pol-Ram ^e	ab initio levels	Calculated Modes ^f	IR-Vector Representation ^g
.... ^a 419(m) ^b 419(s)^c	422(w) ^b 418(w)^c	417(m)^c 411 (11) ^d	 ^a A', f ^b Angle bend ^d	aa = 419 (w) bb = cc = 419 (w) ab = ac = bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	449 [405] (9.70) 448 [404] (8.74) 419 [403] (8.55) 418 [403] (7.53) 405 (7.98) 405 (7.05)	A'(p) 
544(w) ^a 544(w) ^b 542(w)^c	547(w) ^b 544(m)^b	538(vw)^c 542 (1) ^d	Ring torsiona ^a A', f ^b Angle bend ^d	aa = 548 (m) bb = 550 (s) cc = 550 (w) ab = 550 (w) ac = 551 (w) bc = 551 (m)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	603 [544] (0.71) 590 [532] (0.33) 564 [543] (0.30) 553 [533] (0.14) 546 (0.26) 537 (0.15)	A'(p) 
619(m) ^a 619(m) ^b 618(m)^c	620(m) ^b 617(m)^c	621(vw)^c 620 (<1) ^d	In-plane ring bend ^a A', f ^b Angle bend ^d	aa = bb = 617 (sh) cc = ab = ac = bc = 623 (vw)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	698 [629] (0.33) 676 [610] (0.26) 645 [621] (0.12) 629 [606] (0.09) 623 (0.08) 610 (0.05)	A'(p) 
770(s) ^a 772(w) ^b 768(s)^c	780(vs) ^b 778(vs)^c	780(m)^c 776 (9) ^d	In-plane ring bend ^a A', f ^b Angle bend & bond stretch ^d	aa = 784 (vs) bb = 785 (vs) cc = 781 (vs) ab = 780 (s) ac = 785 (s) bc = 786 (s)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	843 [760] (6.84) 844 [761] (8.08) 790 [761] (3.91) 793 [764] (4.57) 762 (3.10) 767 (3.89)	A'(p) 
.... ^a ^b 876(m)^c	 ^b 881(w)^c	877(m)^c 877 (14) ^d	 ^a ^b Angle bend ^d	aa = 885 (w) bb = 885 (w) cc = ab = ac = 884 (vw) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	963 [868] (2.21) 954 [860] (2.10) 896 [863] (3.40) 890 [857] (3.22) 864 (3.60) 863 (3.39)	A'(p) 
960(s) ^a 955(vs) ^b 958(s)^c	962(vw) ^b 958(w)^c	947(s)^c 926 (3) ^d	Im-ring in-plane bend ^a A', f ^b Angle bend & bond stretch ^d	aa = 966 (m) bb = 962 (w) cc = 962 (s) ab = ac = 967 (w) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1033 [931] (0.44) 1023 [922] (1.43) 953 [918] (0.70) 945 [910] (1.90) 916 (0.64) 912 (1.85)	A'(p) 

1007(s) ^a 1006(m) ^b 1005(m)^c	1008(s) ^b 1004(vs)^c	1011(m)^c 1009 (9) ^d	Bz in-plane bend ^a A', f ^b Mainly C3C4 stretch (st) ^d	aa = 1010 (s) bb = 1012 (s) cc = 1009 (s) ab = 1009 (s) ac = 1010 (s) bc = 1011 (s)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1103 [995] (3.22) 1107 [998] (3.64) 1037 [999] (3.24) 1037 [999] (3.55) 1003 (2.76) 1005 (3.14)	A'(p) 
1138(s) ^a 1138(m) ^b 1134(s)^c	1139(m) ^b 1135(s)^c	1082(s)^c 1080 (23) ^d	NH in-plane bend ^a A', f ^b N1H bend & N1C7 stretch ^d	aa = 1140 (s) bb = 1142 (s) cc = 1134 (s) ab = ac = 1139 (m) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1159 [1045] (35.64) 1197 [1079] (29.37) 1081 [1041] (19.38) 1107 [1066] (16.45) 1030 (17.99) 1061 (14.89)	A'(p) 
1115(m) ^a 1115(w) ^b 1112(w)^c	1112(w) ^b 1110(m)^c	1115(w)^c 1112 (3) ^d	Bz in-plane CH bend ^a A', f ^b C2H, C3H bend & C2C3 st ^d	aa = 1118 (m) bb = 1117 (s) cc = ab = 1114 (s) ac = bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1226 [1105] (0.18) 1222 [1102] (0.99) 1140 [1098] (0.84) 1138 [1096] (1.16) 1099 (1.56) 1103 (1.24)	A'(p) 
1162(m) ^a 1155(m) ^b 1158(w)^c	1160(vw) ^b 1163(vw)^c	1163(vw)^c 1161/1148 (2) ^d	Bz in-plane CH bend ^a A', f ^b C5H, C3H, C4H bend ^d	aa = 1163 (w) bb = 1162 (w) cc = 1168 (w) ab = 1160 (w) ac = 1161 (w) bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1272 [1147] (13.82) 1238 [1116] (7.55) 1196 [1152] (12.22) 1182 [1138] (1.53) 1152 (16.37) 1151 (2.57)	A'(p) 
1207(s) ^a 1200(m) ^b 1202(m)^c	1206(w) ^b 1204(w)^c	1199(w)^c 1178 (<1) ^d	Bz in-plane CH bend ^a A', f ^b C2H bend & C1N2 stretch ^d	aa = 1211 (m) bb = 1209 (m) cc = 1207 (w) ab = 1208 (w) ac = bc =	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1294 [1167] (6.33) 1306 [1178] (0.54) 1214 [1169] (1.13) 1212 [1167] (1.27) 1176 (1.83) 1170 (1.23)	A'(p) 
1251(vs) ^a 1250(m) ^b 1246(vs)^c	1251(w) ^b 1250(m)^c	1254(vs)^c 1256/1253(22) ^d	Ring stretch ^a A', fb Mainly C5H bend ^d	aa = 1253 (m) bb = 1253 (m) cc = 1256 (s) ab = 1250 (w) ac = 1252 (w) bc = 1253 (m)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1339 [1207] (38.30) 1369 [1234] (39.29) 1263 [1216] (23.08) 1287 [1239] (16.63) 1219 (17.80) 1241 (22.07)	A'(p) 

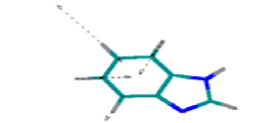
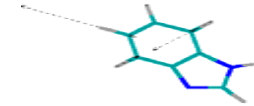
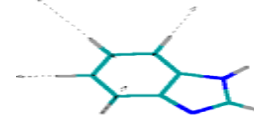
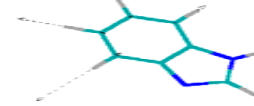
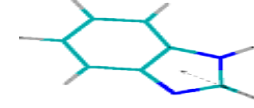
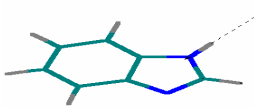
1280(vs) ^a 1263(vs) ^b 1274(vs)^c	1277(vs) ^b 1277(vs)^c	1264(vs)^c 1274/1265(34) ^d	Bz in-plane bend ^a A', f ^b C2H bend, N1C6, C1N2 st ^d	aa = 1279 (vs) bb = 1278 (vs) cc = 1282 (vs) ab = 1279 (vs) ac = 1279 (s) bc = 1277 (vs)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1380 [1244] (26.23) 1381 [1245] (22.48) 1287 [1239] (37.98) 1298 [1250] (29.83) 1236 (34.78) 1253 (26.83)	A'(p) 
1308(s) ^a 1295(vs) ^b 1300(s)^c	1306(w) ^b 1304(m)^c	1306(m)^c 1304 (12) ^d	 A', f C3H, C7H bend C7N2 st	aa = 1306 (w) bb = 1308 (s) cc = 1308 (w) ab = 1312 (s) ac = 1310 (m) bc = 1306 (s)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1434 [1293] (6.00) 1414 [1275] (5.35) 1337 [1288] (5.88) 1347 [1297] (7.62) 1292 (5.50) 1299 (5.11)	A'(p) 
1353(s) ^a 1340(w) ^b 1345(w)^c	1349(w) ^b 1345(m)^c	1346(m)^c 1357/1342(30) ^d	 ^a A', f ^b C1C6 stretch ^d	aa = 1351 (m) bb = 1350 (m) cc = 1353 (s) ab = 1355 (w) ac = 1350 (w) bc = 1350 (w)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1457 [1314] (10.67) 1482 [1336] (10.82) 1376 [1325] (17.02) 1394 [1342] (35.14) 1334 (12.47) 1349 (36.89)	A'(p) 
1412(vs) ^a 1410(w) ^b 1410(vs)^c	1414(m) ^b 1412(s)^c	1394(vs)^c 1396/1384(39) ^d	Ring stretch ^a A', f ^b N1H, C4H bend & N1C7 st ^d	aa = bb = 1417 (s) cc = 1413 (w) ab = ac = 1414 (vs) bc = 1414 (sh)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1535 [1384] (54.15) 1566 [1412] (88.60) 1416 [1364] (13.43) 1435 [1382] (26.76) 1367 (3.50) 1390 (9.66)	A'(p) 
1456(s) ^a 1460(s) ^b 1459(w)^c	1463(w) ^b 1463(w)^c	1458(s)^c 1454/1448(35) ^d	Ring stretch ^a A', f ^b C2H, C5H bend & C1C6 st ^d	aa = 1467 (sh) bb = 1465 (w) cc = 1465 (w) ab = 1465 (w) ac = bc = 1464 (w)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1615 [1456] (49.86) 1624 [1464] (34.02) 1466 [1412] (40.46) 1497 [1442] (22.59) 1403 (33.61) 1445 (22.44)	A'(p) 
1478(s) ^a 1485(vs) ^b 1478(s)^c	1481(m) ^b 1480(m)^c	1494(sh)^c 1504/1500(35) ^d	Ring stretch ^a A', fb C7H bend & N2C7 std	aa = 1480 (m) bb = 1484 (m) cc = 1484 (m) ab = ac = bc = 1486 (s)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1642 [1481] (6.37) 1663 [1500] (2.18) 1506 [1450] (0.48) 1538 [1481] (2.93) 1454 (1.03) 1478 (12.70)	A'(p) 

1495(w) ^a 1505(w) ^b 1494(m)^c	1500(w) ^b 1498(m)^c	1503(vs)^c 1494/1489 (3) ^d	751 + 744 ^a A', f ^b C4H, C3H bend & C2C3 st ^d	aa = bb = 1504 (m) cc = 1505 (s) ab = 1503 (vw) ac = 1502 (w) bc = 1503 (s)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1669 [1505] (24.89) 1720 [1551] (71.15) 1540 [1483] (5.10) 1553 [1496] (32.14) 1490 (3.78) 1491 (8.50)	A'(p) 
1588(w) ^a 1589(w) ^b 1588(m)^c	1592(m) ^b 1590(s)^c	1593(w)^c 1594/1580(3) ^d	NH in-plane bend ^a A', f ^b C1C6, C4C3, C1C2 st ^d	aa = 1591 (w) bb = 1595 (s) cc = 1589 (w) ab = 1595 (w) ac = 1595 (s) bc = 1593 (m)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1748 [1576] (4.83) 1786 [1610] (2.88) 1613 [1553] (4.39) 1640 [1579] (3.18) 1551 (4.14) 1576 (2.93)	A'(p) 
1620(w) ^a 1620(w) ^b 1620(w)^c	1620(w) ^b 1623(w)^c	1621(vw)^c 1627 (10) ^d	Im-CH out plane bend ^a A', f ^b C2C1, C5C6, C3C4 st ^d	aa = 1626 (w) bb = cc = ab = ac = bc = 1624 (w)	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	1790 [1614] (7.30) 1827 [1647] (13.03) 1652 [1591] (5.20) 1680 [1618] (6.70) 1586 (5.08) 1613 (6.29)	A'(p) 

Abbreviations: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; f, fundamental; A', Symmetry; p, polarized.

^a IR of KBr-Discs Ref. (19), ^b polarized IR of partially oriented BZI-solid and Raman of powder BZI Ref. (17), ^c this work, ^d FT-IR of gas-like BZI trapped in Ar-Matrix Ref. (25), ^e polarized Raman from a single crystal of BZI based on its unit cell axes notation Ref (17), ^f Computed vibrational modes [its scaled value] (its intensity in km/mol), ^g estimated mode symmetry, polarization and graphical representation.

Table 3S: Observed and estimated frequencies (cm^{-1}), relative intensities, and assignments of the XH-stretching fundamentals for Benzimidazole.

Solid IR	Solid Ram	Gas-like	Assignments/Symmetry	ab initio levels	Calculated Modes ^f	IR-Vector Representation ^g
3065 ^a 3062(w)^c	 ^c	3066(w)^c 3033 (1) ^d	 ^a C3H, C4H, C5H stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3357 [2997] (1.04) 3358 [2998] (0.39) 3196 [3077] (0.21) 3185 [3067] (0.35) 3110 [3094] (0.14) 3098 [3083] (0.16)	A'(p) 
3040 ^a 2926(m)^c	2930(w)^c	3088(m)^c 3052 (9) ^d	 ^a C3H, C5H stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3371 [3010] (10.94) 3370 [3009] (17.58) 3207 [3088] (10.14) 3196 [3077] (15.00) 3121 [3105] (12.28) 3108 [3092] (18.01)	A'(p) 
3097 ^a 3094(w)^c	3091(w)^c	3095(sh)^c 3064 (1) ^d	 ^a C2H, C4H, C5H stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3383 [3021] (17.50) 3383 [3021] (32.55) 3219 [3100] (16.54) 3208 [3089] (28.75) 3133 [3117] (21.30) 3120 [3104] (33.70)	A'(p) 
.... ^a 3115(m)^c	3112(m)^c	3114(w)^c 3076 (13) ^d	 ^a C2H, C3H stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3398 [3034] (7.49) 3396 [3032] (16.03) 3232 [3113] (7.55) 3219 [3099] (13.72) 3147 [3131] (11.13) 3131 [3115] (17.57)	A'(p) 
.... ^a 3038(w)^c	3021(sh)^c	3145(w)^c 3093 (3) ^d	CH stretch ^a C7H stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3456 [3086] (4.23) 3437 [3069] (9.25) 3281 [3160] (2.19) 3256 [3136] (4.40) 3195 [3179] (3.68) 3172 [3156] (5.62)	A'(p) 
3005(b) ^a 3423(b)^c	3055(vs)^c	3509(vs)^c 3508/3502 (172) ^d	NH stretch ^a NH stretch ^d	HF/3-21G* HF/6-31G* B3LYP/3-21G* B3LYP/6-31G* BLYP/3-21G* BLYP/6-31G*	3857 [3444] (107.93) 3920 [3500] (96.18) 3594 [3461] (60.08) 3656 [3521] (52.39) 3466 [3449] (36.54) 3532 [3514] (30.74)	A'(p) 

Abbreviations: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; b, broad; f, fundamental; A', Symmetry; p, polarized, ^a IR of KBr-Discs Ref. (19), ^b polarized IR of partially oriented BZI-solid and Raman of powder BZI Ref. (17), ^c this work, ^d FT-IR of gas-like BZI in Ar-Matrix Ref. (25), ^f Computed vibrational modes [its scaled value] (its intensity in km/mol), ^g estimated mode symmetry, (polarization), and graphical representation.