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Supplement: A combined experimental and theoretical study on vibrational and electronic properties of (5-methoxy-1*H*-indol-1-yl) (5-methoxy-1*H*-indol-2-yl)methanone

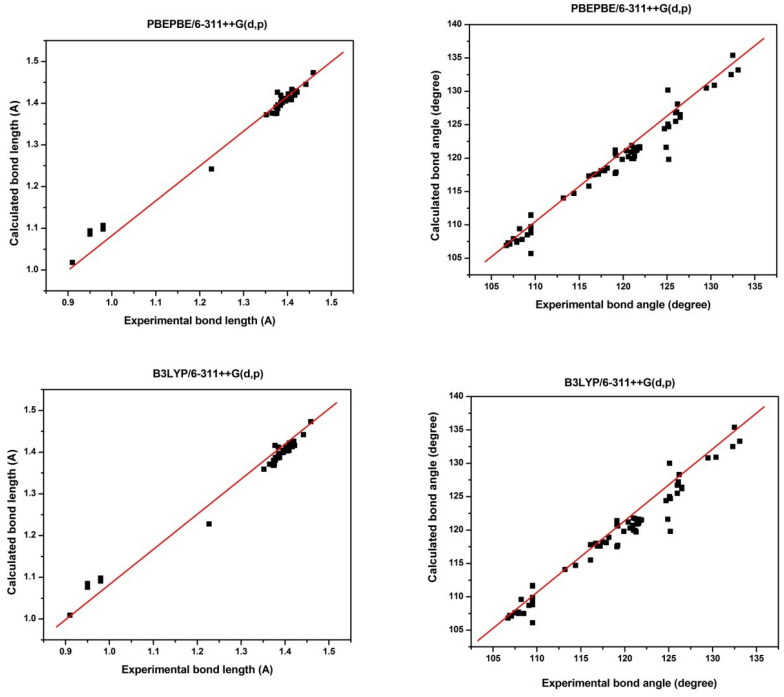

Figure S1: Linear regression graphs for the experimental and calculated bond lengths and bond angles.

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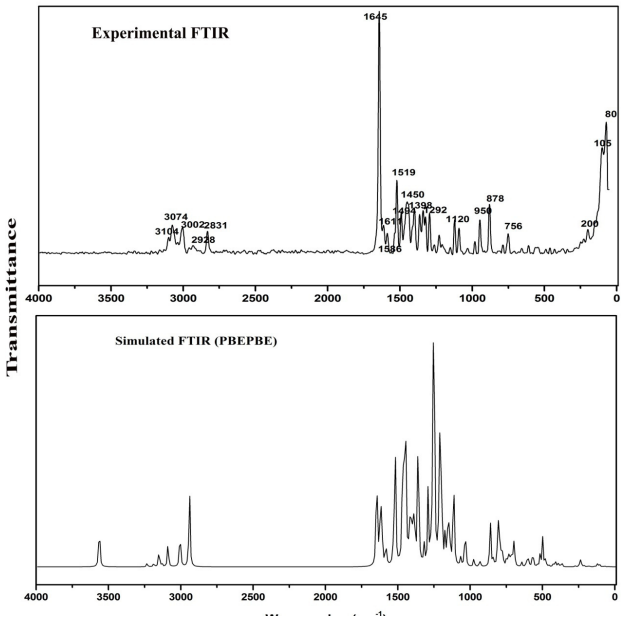

Figure S2: Experimental and simulated (PBEPBE) FT-IR spectra of the MIMIM molecule.

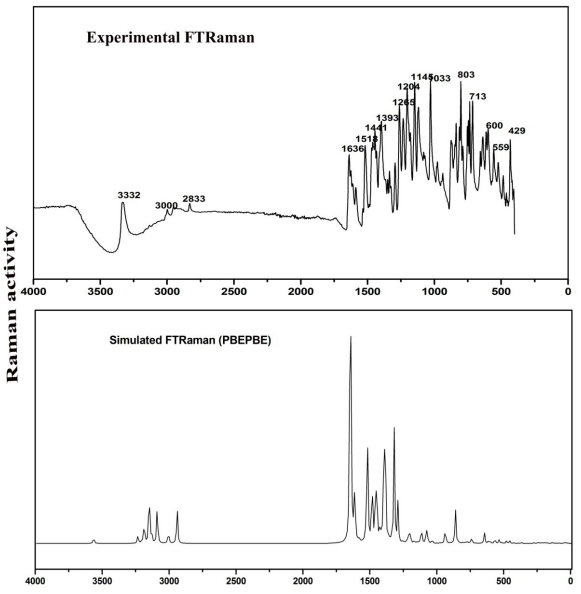

Figure S3: Experimental and simulated (PBEPBE) FR-Raman spectra of the MIMIM molecule.

Table S1: Selected optimized some geometrical parameters of bond lengths (Å) and bond angles (°) of the title molecule.

Bond lengths (Å)	XRD values	Method PBEPBE	B3LYP	Bond angles (°)	XRD values	Method PBEPBE	B3LYP
C1-C2	1.415	1.427	1.421	C2-C1-C6	121.6	121.2	121.0
C1-C6	1.378	1.396	1.387	C2-C1-O21	113.2	114.0	114.1
C1-O21	1.376	1.376	1.369	C6-C1-O21	125.2	124.7	124.7
C2-C3	1.374	1.390	1.380	C1-C2-C3	121.9	121.5	121.5
C2-H25	0.950	1.093	1.084	C1-C2-H25	119.1	117.7	117.5
C3-C4	1.405	1.409	1.403	C3-C2-H25	119.1	121.0	120.9
C3-H26	0.950	1.094	1.085	C2-C3-C4	116.9	117.6	117.6
C4-C5	1.410	1.433	1.422	C2-C3-H26	119.1	120.7	120.8
C4-N7	1.365	1.376	1.371	C4-C3-H26	119.1	121.2	121.4
C5-C6	1.417	1.419	1.413	C3-C4-C5	121.9	121.7	121.5
C5-C9	1.420	1.429	1.426	C3-C4-N7	129.5	130.5	130.8
C6-H27	0.950	1.092	1.083	C5-C4-N7	108.5	107.8	107.5
N7-C8	1.378	1.387	1.381	C4-C5-C6	119.9	119.8	119.8
N7-H28	0.910	1.018	1.009	C4-C5-C9	106.7	106.9	106.8
C8-C9	1.388	1.401	1.387	C6-C5-C9	133.1	133.2	133.3
C8-C10	1.459	1.473	1.473	C1-C6-C5	117.5	118.1	118.2
C9-H29	0.950	1.088	1.079	C1-C6-H27	121.2	121.3	121.7
C10-N11	1.387	1.407	1.397	C5-C6-H27	121.2	119.9	119.9
C10-O20	1.227	1.242	1.228	C4-N7-C8	108.2	109.4	109.6
N11-C12	1.409	1.408	1.404	C4-N7-H28	126.2	128.1	128.3
N11-C15	1.407	1.413	1.411	C8-N7-H28	124.9	121.6	121.6
C12-C13	1.352	1.372	1.359	C9-C8-N7	109.1	108.5	108.7
C12-H30	0.950	1.086	1.076	C10-C8-N7	116.1	115.8	115.5
C13-C14	1.442	1.445	1.442	C9-C8-C10	132.5	135.4	135.4
C13-H31	0.950	1.089	1.081	C5-C9-C8	106.9	107.3	107.2
C14-C15	1.402	1.422	1.412	C5-C9-H29	126.5	126.5	126.4

Continued **Table S1:** Selected optimized some geometrical parameters of bond lengths (Å) and bond angles (°) of the title molecule.

Bond lengths (Å)	XRD values	Method PBEPBE	B3LYP	Bond angles (°)	XRD values	Method PBEPBE	B3LYP
C14-C16	1.396	1.411	1.404	C8-C9-H29	126.5	126.1	126.2
C15-C19	1.396	1.405	1.399	C8-C10-N11	118.2	118.5	118.9
C16-C17	1.385	1.402	1.393	C8-C10-O20	121.3	120.3	119.7
C16-H32	0.950	1.092	1.083	N11-C10-O20	120.4	121.1	121.2
C17-C18	1.385	1.419	1.412	C10-N11-C12	126.1	126.9	127.2
C17-O23	1.373	1.375	1.368	C10-N11-C15	125.1	125.1	125.0
C18-C19	1.384	1.395	1.386	C12-N11-C15	107.5	107.9	107.6
C18-H33	0.950	1.093	1.084	N11-C12-C13	109.5	109.7	109.9
C19-H34	0.950	1.090	1.081	N11-C12-H30	125.2	119.8	119.8
O21-C22	1.377	1.426	1.416	C13-C12-H30	125.1	130.2	130.0
C22-H35	0.980	1.098	1.091	C12-C13-C14	107.9	107.6	107.7
C22-H36	0.980	1.106	1.098	C12-C13-H31	126.0	125.5	125.5
C22-H37	0.980	1.106	1.098	C14-C13-H31	126.0	126.8	126.7
O23-C24	1.422	1.426	1.416	C13-C14-C15	107.1	107.1	107.1
C24-H38	0.980	1.106	1.098	C13-C14-C16	132.3	132.5	132.5
C24-H39	0.980	1.099	1.091	C15-C14-C16	120.6	120.2	120.3
C24-H40	0.980	1.107	1.098	C14-C15-N11	107.9	107.4	107.5
				C19-C15-N11	130.4	130.9	130.9
				C14-C15-C19	121.7	121.6	121.4
				C14-C16-C17	117.9	118.1	118.1
				C14-C16-H32	121.0	119.9	120.0
				C17-C16-H32	121.0	121.9	121.8
				C16-C17-C18	120.9	120.9	120.7
				C16-C17-O23	124.7	124.4	124.4
				C18-C17-O23	114.4	114.7	114.7
				C17-C18-C19	121.6	121.5	121.6
				C17-C18-H33	119.2	117.9	117.7
				C19-C18-H33	119.2	120.4	120.6
				C15-C19-C18	117.2	117.6	117.6
				C15-C19-H34	121.4	121.1	120.9
				C18-C19-H34	121.4	121.2	121.3
				C1-O21-C22	116.1	117.3	117.8
				O21-C22-H35	109.5	108.8	106.1
				O21-C22-H36	109.5	111.4	111.6
				O21-C22-H37	109.5	111.4	111.6
				H35-C22-H36	109.5	109.4	109.2
				H36-C22-H37	109.5	109.4	109.2
				H35-C22-H37	109.5	109.3	108.8
				C17-O23-C24	116.7	117.5	118.0
				O23-C24-H38	109.5	111.4	111.7
				O23-C24-H39	109.5	105.7	106.1
				O23-C24-H40	109.5	111.5	111.7
				H38-C24-H39	109.5	109.4	109.1
				H38-C24-H40	109.5	109.3	108.9
				H39-C24-H40	109.5	109.4	109.1

Table S2: Second order perturbation theory analysis of Fock matrix in NBO basis for the title compound.

Donor (i)	Type of bond	Occupancy	Acceptor (j)	Type of bond	Occupancy	E2 (kJ mol–1)[a]	E(j) –E(i) (a.u.)[b]	F(i, j) (a.u.)[c]
C1-C2	σ	1.97383	C1-C6	σ*	0.02355	3.96	1.25	0.063
			C2-C3	σ*	0.01173	2.71	1.27	0.053
`			C2-H25	σ*	0.01188	1.03	1.13	0.031
			C3-H26	σ*	0.01427	2.56	1.13	0.048
			C6-H27	σ*	0.01395	2.33	1.12	0.046
			O21-C22	σ*	0.00956	2.93	0.97	0.048
C1-C6	σ	1.72417	C1-C2	σ*	0.02355	4.00	1.25	0.063
			C2-H25	σ*	0.01188	1.76	1.15	0.040
			C5-C6	σ*	0.02249	3.48	1.26	0.059
			C5-C9	σ*	0.02012	4.38	1.22	0.065
			C6-H27	σ*	0.01395	1.41	1.14	0.036
C1-C6	π		C2-C3	π*	0.30779	17.5	0.29	0.064
			C4-C5	π*	0.46479	18.0	0.29	0.068
C1-O21	σ	1.98990	C1-C2	σ*	0.02355	0.52	1.40	0.024
			C1-C6	σ*	0.02709	0.84	`1.42	0.031
			C2-C3	σ*	0.01173	1.61	1.44	0.043
			C5-C6	σ*	0.02249	1.27	1.42	0.038
C2-C3	σ	1.73347	C1-C2	σ*	0.02355	2.58	1.24	0.051
			C1-O21	σ*	0.03248	2.86	1.03	0.049
			C2-H25	σ*	0.01188	1.13	1.14	0.032
			C3-C4	σ*	0.02327	3.54	1.27	0.060
			C3-H26	σ*	0.01427	1.18	1.13	0.033
			C4-N7	σ*	0.02673	6.06	1.11	0.073
C2-C3	π		C1-C6	π*	0.34600	19.03	0.28	0.067
			C4-C5	π*	0.46479	18.84	0.29	0.070
C3-C4	σ	1.97466	C2-C3	σ*	0.01173	2.90	1.29	0.055
			C2-H25	σ*	0.01188	2.31	1.15	0.046
			C3-H26	σ*	0.01427	1.28	1.14	0.034
			C4-C5	σ*	0.03128	5.06	1.27	0.072
			C4-N7	σ*	0.02673	2.19	1.12	0.044
			C5-C9	σ*	0.02012	1.68	1.22	0.040
			N7-C8	σ*	0.01861	1.60	1.09	0.037
C4-C5	σ	1.96382	C3-C4	σ*	0.02327	4.95	1.25	0.070
			C3-H26	σ*	0.01427	2.53	1.11	0.048
			C4-N7	σ*	0.02673	0.97	1.09	0.029
			C5-C6	σ*	0.02249	4.12	1.24	0.064
			C5-C9	σ*	0.02012	2.63	1.19	0.050
			C6-H27	σ*	0.01395	2.35	1.11	0.046
			N7-H28	σ*	0.02657	1.71	1.08	0.038
			C9-H29	σ*	0.01281	3.07	1.13	0.053
C4-N7	σ	1.98247	C2-C3	σ*	0.01173	0.98	1.35	0.033
			C3-C4	σ*	0.02327	2.11	1.34	0.047
			C4-C5	σ*	0.03128	1.54	1.33	0.041
			C5-C6	σ*	0.02249	3.14	1.33	0.058
			N7-C8	σ*	0.01861	0.99	1.16	0.030
			N7-H28	σ*	0.02657	0.75	1.17	0.027
			C8-C10	σ*	0.05625	3.01	1.17	0.053

Continued **Table S2:** Second order perturbation theory analysis of Fock matrix in NBO basis for the title compound.

Donor (i)	Type of bond	Occupancy	Acceptor (j)	Type of bond	Occupancy	E2 (kJ mol–1)[a]	E(j) –E(i) (a.u.)[b]	F(i, j) (a.u.)[c]
C5-C6	σ	1.96946	C1-C6	σ*	0.02709	3.22	1.25	0.057
			C1-O21	σ*	0.03248	4.93	1.02	0.063
			C4-C5	σ*	0.03128	4.48	1.25	0.067
			C4-N7	σ*	0.02673	1.89	1.10	0.041
			C5-C9	σ*	0.02012	3.92	1.20	0.062
			C6-H27	σ*	0.01395	1.35	1.13	0.035
			C8-C9	σ*	0.01813	0.76	1.26	0.028
C5-C9	σ	1.96660	C1-C6	σ*	0.02709	1.52	1.22	0.039
			C3-C4	σ*	0.02327	4.41	1.23	0.066
			C4-C5	σ*	0.03128	2.96	1.22	0.054
			C4-N7	σ*	0.02673	0.87	1.08	0.027
			C5-C6	σ*	0.02249	4.00	1.22	0.063
			N7-C8	σ*	0.01861	1.09	1.05	0.030
			C8-C9	σ*	0.01813	2.74	1.23	0.052
			C8-C10	σ*	0.05625	7.03	1.06	0.078
			C9-H29	σ*	0.01281	1.18	1.11	0.032
C10-O20	σ	1.97964	C8-C9	σ*	0.01813	2.33	1.63	0.055
			C8-C10	σ*	0.05625	1.50	1.46	0.042
			N11-C12	σ*	0.02524	1.42	1.41	0.040
			C8-C9	σ*	0.01813	5.90	0.41	0.048
C12-C13	σ	1.97869	C10-N11	σ*	0.08628	2.48	1.05	0.046
			N11-C12	σ*	0.02524	0.68	1.08	0.024
			C12-H30	σ*	0.01378	1.99	1.19	0.044
			C13-C14	σ*	0.02319	2.51	1.23	0.050
			C13-H31	σ*	0.01304	1.67	1.17	0.039
			C14-C16	σ*	0.02239	5.09	1.31	0.073
			C15-C19	σ*	0.02297	0.54	1.31	0.024
C13-C14	σ		N11-C12	σ*	0.02524	0.93	0.99	0.027
			N11-C15	σ*	0.03437	0.99	0.98	0.028
			C12-C13	σ*	0.00952	2.42	1.26	0.050
			C12-H30	σ*	0.01378	4.33	1.10	0.062
			C13-H31	σ*	0.01304	1.04	1.08	0.030
			C14-C15	σ*	0.02907	2.64	1.22	0.051
			C14-C16	σ*	0.02239	3.71	1.22	0.060
			C15-C19	σ*	0.02297	4.27	1.22	0.065
			C16-C17	σ*	0.02809	1.87	1.21	0.042
C15-C19	σ	1.97554	N11-C12	σ*	0.02524	1.24	1.04	0.032
			N11-C15	σ*	0.03437	1.44	1.03	0.034
			C13-C14	σ*	0.02319	2.08	1.20	0.044
			C14-C15	σ*	0.02907	5.15	1.27	0.072
			C18-C19	σ*	0.01429	2.83	1.28	0.054
			C18-H33	σ*	0.01236	2.07	1.15	0.044
			C19-H34	σ*	0.01351	1.57	1.17	0.038
C16-C17	σ	1.97831	C13-C14	σ*	0.02319	4.35	1.20	0.064
			C14-C16	σ*	0.02239	3.69	1.28	0.061
			C16-H32	σ*	0.01414	1.42	1.14	0.036
			C17-C18	σ*	0.02358	4.16	1.26	0.065
			C18-H33	σ*	0.01236	1.93	1.15	0.042

Continued **Table S2:** Second order perturbation theory analysis of Fock matrix in NBO basis for the title compound.

Donor (i)	Type of bond	Occupancy	Acceptor (j)	Type of bond	Occupancy	E2 (kJ mol–1)[a]	E(j) –E(i) (a.u.)[b]	F(i, j) (a.u.)[c]
O23-C24	σ	1.99043	C16-C17	σ*	0.02809	0.51	0.83	0.020
			C17-C18	σ*	0.02358	2.03	1.37	0.047
N7	LP1	1.70693	C4-C5	σ*	0.03128	0.90	0.88	0.027
			N7-H28	σ*	0.02657	1.72	0.72	0.034
			C8-C9	σ*	0.01813	0.69	0.89	0.024
N11	LP1	1.67682	C10-O20	σ*	0.01013	0.53	0.89	0.021
O20	LP1	1.97779	C8-C10	σ*	0.05625	1.47	1.10	0.036
			C10-N11	σ*	0.08628	0.79	1.02	0.026
O21	LP1	1.96183	C1-C2	σ*	0.02355	0.54	1.08	0.022
			C1-C6	σ*	0.02709	6.82	1.10	0.077
			C22-H35	σ*	0.00922	2.80	0.93	0.046
			C22-H36	σ*	0.01932	1.52	0.92	0.033
O23	LP1	1.96205	C16-C17	σ*	0.02809	6.83	1.09	0.077
			C17-C18	σ*	0.02358	0.50	1.10	0.021
			C24-H38	σ*	0.01937	1.56	0.91	0.034

[a] E(2) means energy of hyper-conjugative interactions; [b] Energy difference between donor and acceptor (i) and (j) NBO orbitals; [c] F(i, j) is the Fock matrix element between (i) and (j) NBO orbitals.

Table S3: Detailed assignments of vibrational bands of the title molecule along with potential total energy distribution (PED).

NO	Experimental		Theoretical B3LYP/ 6-311++G(d,p)		Theoretical PBEPBE/ 6-311++G(d,p)		I^m	S	Vibrational assignment
	FT-IR	FT-Raman	Unscaled	scaled	Unscaled	scaled			
			3549	3400	3563	3414	92.17	81.13	γNH(100)
			3529	3381	3233	3097	6.30	90.16	γCH(98)
			3384	3242	3204	3069	0.45	31.02	γCH(100)
			3303	3164	3190	3056	3.67	122.06	γCH(97)
			3257	3120	3181	3047	1.53	75.66	γCH(97)
			3256	3119	3153	3020	7.73	87.34	γCH(100)
			3254	3117	3153	3020	11.14	87.46	γCH(100)
			3216	3081	3148	3016	5.56	282.54	γCH(96)
	3074		3215	3080	3144	3012	3.74	156.70	γCH(98)
			3197	3063	3130	2998	5.34	88.75	γCH(96)
			3159	3026	3089	2959	21.94	217.77	γCH_3(94)
			3157	3024	3088	2958	23.35	213.92	γCH_3(96)
	3000	3000	3124	2993	3006	2879	38.61	58.73	γCH_3(91)
			3122	2991	3005	2879	38.22	78.42	γCH_3(95)
			3044	2916	2940	2817	66.92	241.06	γCH_3(98)
		2883	3043	2915	2940	2816	78.41	157.25	γCH_3(92)
			1728	1655	1646	1618	215.78	2853.10	γCC(73)
	1636		1667	1639	1626	1598	65.85	55.95	γCO(69)
			1650	1622	1612	1585	126.90	443.45	γCC(75)
			1649	1621	1583	1556	34.87	15.30	γCC(72)
	1606		1637	1609	1577	1550	9.61	10.69	γCC(69)
	1586		1616	1589	1531	1505	24.29	39.05	γCC(59)
			1558	1532	1519	1493	262.07	962.23	γCC(68)+ γCO(21)
	1522	1518	1513	1487	1484	1458	4.54	515.38	γCO(75)+ γCC(19)
	1486		1512	1486	1466	1441	215.80	11.58	γCO(72)

Continued **Table S3**: Detailed assignments of vibrational bands of the title molecule along with potential total energy distribution (PED).

NO	Experimental		Theoretical B3LYP/ 6-311++G(d,p)		Theoretical PBEPBE/ 6-311++G(d,p)		I^m	S	Vibrational assignment
	FT-IR	FT-Raman	Unscaled	scaled	Unscaled	scaled			
			1502	1476	1462	1437	6.93	5.63	γCC(69)
			1499	1474	1458	1433	62.32	349.09	γCC(68)
			1498	1473	1452	1428	55.19	120.87	γCC(61)
			1497	1472	1447	1422	237.86	185.41	γCO(72)+ γCC(19)
		1469	1489	1464	1442	1417	10.29	19.82	γCO(79)
		1461	1481	1456	1441	1417	9.50	16.79	γCC(68)+ γCO(19)
		1441	1467	1442	1428	1403	8.22	66.94	γCC(56)
		1435	1463	1438	1419	1395	71.01	37.86	γCC(57)+βCHC(13)
		1381	1397	1373	1408	1384	51.75	14.00	γCC(60)+βCHC(15)
	1365		1385	1361	1394	1370	125.04	1009.20	γCN(63)+βCHC(11)
			1361	1338	1383	1359	41.33	405.83	γCN(66)
	1335		1358	1335	1359	1336	310.60	40.09	γCN(61)
	1296	1296	1316	1294	1338	1315	1.16	34.69	γCC(64)+ γCN(19)
			1305	1283	1318	1296	31.12	738.33	βCHC(49)+γCC(12)
	1265	1265	1287	1265	1291	1269	119.66	263.37	βCHC(69)
		1238	1261	1240	1267	1246	63.82	1.10	γCN(66)+βCHC(16)
			1252	1231	1251	1230	649.94	15.40	γCN(72)+γCN(26)
	1207	1204	1224	1203	1222	1201	22.97	26.50	βCCN(45)
			1203	1183	1211	1191	152.60	16.77	βCHC(53)+ βCCN(14)
			1199	1179	1204	1184	197.04	93.22	βCHC(68)
		1175	1194	1174	1194	1173	50.82	17.05	βCHC(59)
	1155		1175	1155	1174	1154	44.27	7.17	βCHC(56)
		1146	1164	1144	1165	1145	6.15	6.42	βCHC(59)
			1159	1139	1152	1133	87.70	2.91	βCHC(55)
			1158	1138	1143	1124	63.31	10.25	βCHC(55)
			1156	1136	1130	1111	0.53	1.56	βCHN(58)
	1120	1120	1135	1116	1129	1109	0.43	1.71	βCHN(54)
			1124	1105	1115	1096	167.87	110.60	βCCC(69)+ βCHN(15)
		1079	1094	1075	1110	1078	29.54	6.21	βCOC(53)+βCCC(21)
		1065	1078	1060	1078	1060	1.22	115.61	βCCC(59)+βCOC(14)
		1031	1054	1036	1065	1047	14.31	16.85	βCHO(48)
	1020		1035	1017	1035	1017	56.23	20.34	βCCN(55)
		978	1031	1013	1033	1016	26.71	4.00	βCNC(58)
	948		971	954	974	957	14.69	4.02	βCCC(64)+βCNC(15)
		938	957	941	937	922	2.77	72.97	βCCC(62)
			954	938	933	917	8.46	20.30	βCHC(67)+βCCC(18)
			946	930	923	907	0.84	2.74	βCNC(63)
			942	926	904	888	0.01	1.77	βCCC(48)
		874	881	866	861	846	84.25	235.95	βCCC(55)
			870	855	839	825	12.80	9.27	βCCC(62)
		838	841	827	810	797	22.50	1.40	βCCC(67)
			837	823	806	792	47.89	3.44	βCCC(59)
			832	818	801	787	37.08	1.12	βCCO(70)+βCCC(15)
		803	823	809	793	780	26.79	0.48	βCCO(74)
	788	788	811	797	783	770	2.75	9.02	βCNC(64)+βCCO(17)

Continued **Table S3**: Detailed assignments of vibrational bands of the title molecule along with potential total energy distribution (PED).

NO	Experimental		Theoretical B3LYP/ 6-311++G(d,p)		Theoretical PBEPBE/ 6-311++G(d,p)		I^m	S	Vibrational assignment
	FT-IR	FT-Raman	Unscaled	scaled	Unscaled	scaled			
			785	772	782	768	31.29	0.05	βCNC(60)
			778	765	772	759	7.10	10.45	βCNC(55)
			773	760	751	738	8.88	3.41	βCCN(74)+βCNC(24)
	754	755	763	750	742	729	5.89	20.61	βCNC(48)
		738	748	735	734	722	3.03	8.94	βCCN(63)
			744	731	729	717	28.34	0.84	βCOH(47)
	704	713	719	707	711	699	31.47	2.06	βCNC(43)+βCOH(14)
			700	688	695	683	46.07	0.24	φCCCH(72)
	653	659	661	650	644	633	7.56	62.54	φCHOC(82)
		640	648	637	614	603	3.53	12.20	φCCCH(45) +φCHOC(18)
			643	632	606	596	2.14	1.97	φCCCH(61)
		612	626	615	603	592	12.69	6.19	φCCCH(48)
			614	604	596	586	8.37	3.65	φCCCH(39)
	601	600	610	600	570	561	7.33	4.80	φCCNH(59)
			571	561	565	556	20.73	21.18	φCCCH(74)
	559	559	570	560	534	525	2.53	20.58	φCCCO(49)+φCCCH(18)
			537	528	516	508	19.07	3.54	φCCNC(42)+φCCCO(11)
		517	520	511	499	490	47.73	0.84	φCOCH(44)
	489	486	489	481	479	471	13.48	15.82	φCCNC(50)+φCOCH(13)
	458	458	460	452	454	447	2.03	13.56	φCNCC(48)+φCCNC(15)
	433	433	443	435	424	416	5.86	0.46	φCCNC(47)
			433	426	422	415	1.58	3.47	φCCNC(41)
		419	430	423	408	401	8.02	0.31	φCHOH(45)
			402	395	389	382	6.16	1.01	φCHOH(55)
			397	390	377	370	1.01	0.60	φCNCC(42)+φCHOH(17)
	375		377	371	367	361	5.72	0.32	φCHOH(53)+φCNCC(14)
			368	362	364	357	1.09	3.46	φCCCH(37)
	280		284	279	275	271	1.44	4.06	φCCCH(68)
			261	257	250	246	0.12	2.23	φCCCH(61)
	235		234	230	245	240	2.70	1.13	φCHOH(55)+φCCCH(12)
			221	217	236	232	12.23	3.53	φCCNC(43)+φCCOH(16)
	203		200	197	234	230	2.43	0.66	φCCCC(35)
			175	172	213	210	2.08	4.88	φCCCC(43)
			172	169	190	187	0.42	5.03	φCNCC(45)
			149	146	179	176	2.22	3.25	φCCNC(53)
			129	127	164	161	0.15	1.44	φCH_3 wagging(62)
	107		114	112	137	135	1.08	5.02	φCH_3 wagging (59)
	80		83	82	118	116	6.65	1.41	φCCON(54)
			57	56	104	102	3.30	0.99	φCCCN(49)
			45	44	86	84	0.35	1.80	φCNCC(43)
			39	38	70	69	1.46	0.25	φCNCC(46)
			30	29	45	44	0.48	4.03	φCOCC(41)
			28	28	38	37	0.25	3.78	φCH_3 triggering(49)
			19	19	20	19	0.14	2.52	φCH_3 triggering (45)

β: in-plane bending; γ: out-of-plane bending; I: IR intensity, S: Raman scattering activity