

Spectroscopic Investigations, Quantum Chemical, Molecular Docking and Drug Likeness Studies of 3-Fluorobenzamide

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Table S1 — Molecular orbital contributions of 3-fluorobenzamide

Gas phase		TD-DFT/ B3LYP/6-31++G(d,p)			Gas phase		TD-DFT/ B3LYP/6-311++G(d,p)		
Energy (eV)	Oscillator strength	Computed wavelength (nm)	Major contributions	Assignment	Energy (eV)	Oscillator strength	Computed wavelength (nm)	Major contributions	Assignment
4.462	0.006	277.9	H-1→L (49.08%)	$\pi \rightarrow \pi^*$	4.492	0.007	276.0	H-1→L (46.66%)	$\pi \rightarrow \pi^*$
4.892	0.040	253.5	H-1→L (39.58%)	$\pi \rightarrow \pi^*$	4.911	0.038	252.5	H-1→L (41.38%)	$\pi \rightarrow \pi^*$
5.508	0.114	225.1	H-2→L (68.12%)	$\pi \rightarrow \pi^*$	5.517	0.104	224.7	H-2→L (66.66%)	$\pi \rightarrow \pi^*$
Methanol									
4.683	0.015	264.8	H-2→L (41.38%)	$\pi \rightarrow \pi^*$	4.703	0.016	263.6	H→L (38.05%)	$\pi \rightarrow \pi^*$
4.881	0.041	254.0	H→L (45.46%)	$\pi \rightarrow \pi^*$	4.906	0.039	252.7	H→L (42.69%)	$\pi \rightarrow \pi^*$
5.423	0.199	228.6	H-1→L (46.87%)	$\pi \rightarrow \pi^*$	5.440	0.186	227.9	H-1→L (40.86%)	$\pi \rightarrow \pi^*$
Ethanol									
4.679	0.015	265.0	H-2→L (40.72%)	$\pi \rightarrow \pi^*$	4.699	0.016	263.9	H→L (38.01%)	$\pi \rightarrow \pi^*$
4.880	0.042	254.1	H→L (45.72%)	$\pi \rightarrow \pi^*$	4.904	0.040	252.8	H→L (42.91%)	$\pi \rightarrow \pi^*$
5.421	0.202	228.7	H-1→L (45.33%)	$\pi \rightarrow \pi^*$	5.438	0.189	228.0	H-1→L (41.48%)	$\pi \rightarrow \pi^*$

Table S2 — Second-order perturbation theory analysis of Fock matrix for 3-fluorobenzamide by NBO analysis

Donor(i)	ED (i) (e)	Acceptor (j)	ED (j) (e)	E(2) (Kcal/mol)	E (j) -E (i) (arb. units)	F(i,j) (arb. units)
σ (C1-C2)	1.97	σ^* (C1-C6)	0.02	3.91	1.28	0.06
σ (C1-C2)	1.97	σ^* (C3-F8)	0.03	3.99	0.97	0.06
π (C1-C2)	1.67	π^* (C3-C4)	0.36	22.25	0.28	0.07
π (C1-C2)	1.67	π^* (C5-C6)	0.31	18.21	0.29	0.07
π (C1-C2)	1.67	π^* (C12-O13)	0.27	15.14	0.31	0.06
σ (C1-C6)	1.97	σ^* (C1-C2)	0.02	3.92	1.26	0.06
σ (C2-C3)	1.98	σ^* (C1-C2)	0.02	3.09	1.29	0.06
σ (C2-C3)	1.98	σ^* (C1-C12)	0.07	3.15	1.14	0.05
σ (C2-C3)	1.98	σ^* (C3-C4)	0.03	4.18	1.29	0.07
σ (C2-H7)	1.98	σ^* (C3-C4)	0.03	3.91	1.10	0.06
σ (C3-C4)	1.98	σ^* (C2-C3)	0.03	4.24	1.28	0.07
π (C3-C4)	1.65	π^* (C1-C2)	0.38	19.50	0.29	0.07
π (C3-C4)	1.65	π^* (C5-C6)	0.31	18.97	0.30	0.07
σ (C4-C5)	1.97	σ^* (C3-F8)	0.03	4.39	0.97	0.06
σ (C4-H9)	1.98	σ^* (C2-C3)	0.03	3.97	1.09	0.06
σ (C4-H9)	1.98	σ^* (C5-C6)	0.01	3.44	1.11	0.06
σ (C5-C6)	1.98	σ^* (C1-C6)	0.02	3.02	1.27	0.06
π (C5-C6)	1.65	π^* (C1-C2)	0.38	21.97	0.27	0.07
π (C5-C6)	1.65	π^* (C3-C4)	0.36	20.86	0.27	0.07
σ (C5-H10)	1.98	σ^* (C1-C6)	0.02	3.72	1.09	0.06
σ (C5-H10)	1.98	σ^* (C3-C4)	0.03	3.13	1.08	0.05
σ (C6-H11)	1.98	σ^* (C1-C2)	0.02	4.74	1.07	0.06
σ (C6-H11)	1.98	σ^* (C4-C5)	0.01	3.78	1.08	0.06
π (C12-O13)	1.98	π^* (C1-C2)	0.38	3.75	0.41	0.04
σ (N14-H15)	1.99	σ^* (C1-C12)	0.07	3.67	1.08	0.06
σ (N14-H16)	1.99	σ^* (C12-O13)	0.02	3.49	1.27	0.06
LP(2)F8	1.97	σ^* (C2-C3)	0.03	5.87	0.98	0.07
LP(2)F8	1.97	σ^* (C3-C4)	0.03	5.89	0.98	0.07
LP(3)F8	1.93	π^* (C3-C4)	0.36	17.84	0.43	0.09
LP(2)O13	1.87	σ^* (C1-C12)	0.07	18.72	0.66	0.10
LP(2)O13	1.87	σ^* (C12-N14)	0.07	24.90	0.69	0.12
LP(1)N14	1.77	π^* (C12-O13)	0.27	43.56	0.33	0.11
π^* (C1-C2)	0.38	π^* (C12-O13)	0.27	86.70	0.02	0.07
π^* (C3-C4)	0.36	π^* (C5-C6)	0.31	181.81	0.01	0.08
π^* (C12-O13)	0.27	σ^* (C12-O13)	0.02	4.24	0.55	0.11

Table S3 — Mulliken atomic charges for 3-fluorobenzamide
Atomic Charges (Mulliken)

Atoms	B3LYP/6-31++G(d,p)			B3LYP/6-311++G(d,p)		
	Gas phase	Methanol	Ethanol	Gas phase	Methanol	Ethanol
C1	0.732	0.671	0.672	1.279	1.223	1.224
C2	-0.451	-0.402	-0.403	-0.483	-0.462	-0.463
C3	-0.107	-0.083	-0.083	-0.513	-0.480	-0.480
C4	0.164	0.161	0.161	0.168	0.155	0.155
C5	0.050	-0.008	-0.007	-0.125	-0.177	-0.176
C6	-0.642	-0.629	-0.629	-0.694	-0.690	-0.690
H7	0.125	0.146	0.146	0.179	0.213	0.212
F8	-0.328	-0.341	-0.341	-0.167	-0.183	-0.183
H9	0.147	0.165	0.164	0.200	0.227	0.226
H10	0.134	0.153	0.153	0.183	0.211	0.211
H11	0.148	0.143	0.143	0.192	0.191	0.191
C12	0.385	0.425	0.425	-0.089	-0.042	-0.043
O13	-0.507	-0.591	-0.590	-0.319	-0.405	-0.404
N14	-0.501	-0.505	-0.505	-0.354	-0.382	-0.381
H15	0.352	0.367	0.367	0.320	0.340	0.340
H16	0.297	0.329	0.328	0.223	0.261	0.261

Table S4 — Fukui functions of 3-fluorobenzamide

Atoms	B3LYP/6-31++G(d,p)							B3LYP/6-311++G(d,p)						
	Mulliken Charges			Fukui functions				Mulliken Charges			Fukui functions			
	q(N+1)	q(N)	q(N-1)	f_k^+	f_k^-	f_k^0	$\Delta f(r)$	q(N+1)	q(N)	q(N-1)	f_k^+	f_k^-	f_k^0	$\Delta f(r)$
C1	2.082	0.732	0.873	1.350	-0.141	0.605	1.491	1.640	1.279	1.337	0.361	-0.058	0.152	0.419
C2	-1.879	-0.451	-0.447	-1.428	-0.004	-0.716	-1.425	-0.571	-0.483	-0.486	-0.088	0.003	-0.043	-0.091
C3	0.919	-0.107	-0.046	1.026	-0.061	0.482	1.087	-0.074	-0.513	-0.415	0.439	-0.097	0.171	0.536
C4	-0.349	0.164	0.258	-0.513	-0.093	-0.303	-0.420	-0.176	0.168	0.221	-0.344	-0.053	-0.199	-0.291
C5	0.671	0.050	0.068	0.621	-0.018	0.302	0.639	0.204	-0.125	-0.088	0.329	-0.037	0.146	0.366
C6	-1.058	-0.642	-0.595	-0.416	-0.047	-0.232	-0.369	-1.403	-0.694	-0.664	-0.709	-0.030	-0.370	-0.679
H7	-0.431	0.125	0.171	-0.556	-0.046	-0.301	-0.510	0.052	0.179	0.239	-0.127	-0.059	-0.093	-0.068
F8	-0.338	-0.328	-0.234	-0.010	-0.094	-0.052	0.084	-0.205	-0.167	-0.070	-0.037	-0.098	-0.067	0.061
H9	0.040	0.147	0.211	-0.106	-0.064	-0.085	-0.042	0.109	0.200	0.277	-0.091	-0.077	-0.084	-0.014
H10	0.052	0.134	0.195	-0.082	-0.061	-0.072	-0.021	0.113	0.183	0.258	-0.075	-0.071	-0.073	-0.004
H11	0.067	0.148	0.195	-0.081	-0.047	-0.064	-0.035	0.116	0.192	0.253	-0.076	-0.061	-0.069	-0.015
C12	1.082	0.385	0.374	0.697	0.011	0.354	0.685	0.079	-0.089	-0.058	0.168	-0.031	0.069	0.199
O13	-0.539	-0.507	-0.302	-0.032	-0.205	-0.119	0.173	-0.425	-0.319	-0.117	-0.107	-0.202	-0.154	0.095
N14	-0.477	-0.501	-0.437	0.023	-0.064	-0.020	0.087	-0.284	-0.354	-0.306	0.069	-0.048	0.011	0.118
H15	-0.499	0.352	0.389	-0.851	-0.037	-0.444	-0.814	0.054	0.320	0.360	-0.265	-0.041	-0.153	-0.224
H16	-0.342	0.297	0.327	-0.640	-0.029	-0.334	-0.611	-0.229	0.223	0.259	-0.452	-0.036	-0.244	-0.416

Table S5 — ^{13}C and ^1H NMR chemical shifts for 3-fluorobenzamide

Atoms	B3LYP/6-31++G(d,p)			B3LYP/6-311++G(d,p)		
	Gas phase	Methanol	Ethanol	Gas phase	Methanol	Ethanol
C2	99.41	100.87	118.36	127.04	127.01	127.02
C4	104.95	106.18	123.68	127.06	128.45	128.43
C6	113.11	112.39	129.93	130.99	131.03	131.03
C5	116.66	117.26	134.77	135.05	136.19	136.17
C1	123.72	123.34	140.87	144.33	144.23	144.23
C3	151.35	151.42	168.94	172.39	172.16	172.16
C12	151.26	153.91	171.39	193.09	196.68	196.63
H16	5.47	6.15	6.14	1.55	1.90	1.89
H15	4.97	5.42	5.42	1.55	1.90	1.89
H9	7.57	7.81	7.80	7.48	7.74	7.73
H10	7.83	8.04	8.03	7.72	7.97	7.97
H11	8.42	8.34	8.33	8.29	8.33	8.33
H7	7.56	7.87	7.86	8.95	8.98	8.98

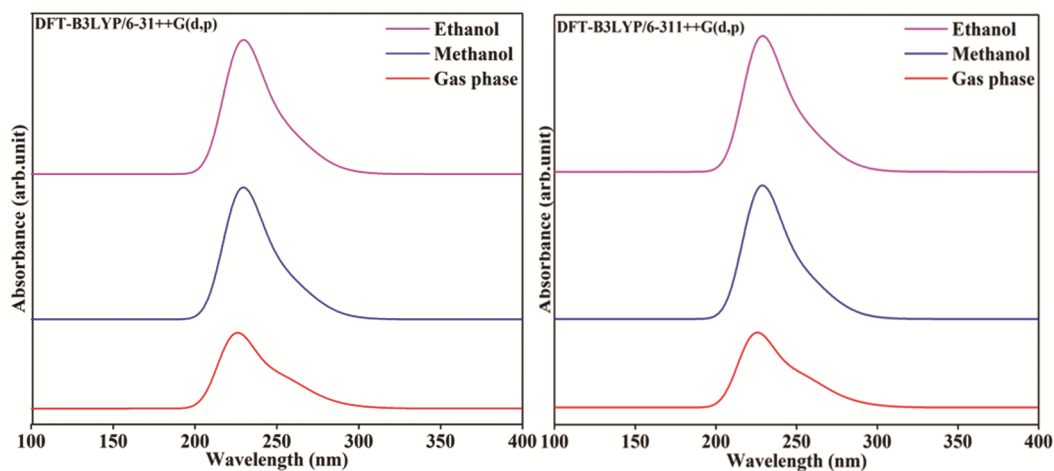


Fig. S1 — UV plot of 3-fluorobenzamide

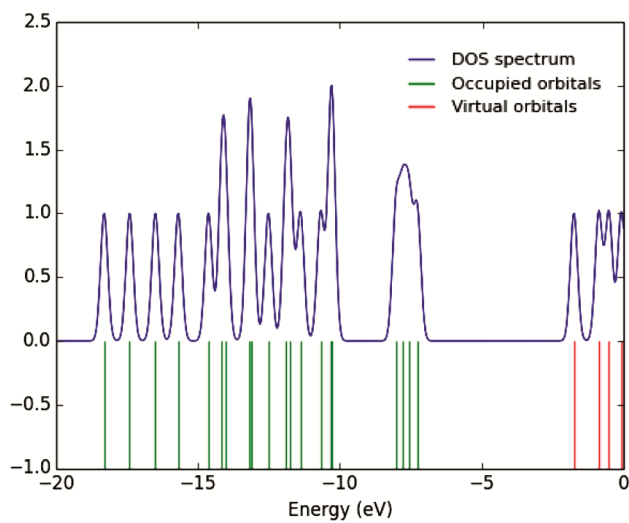


Fig. S2 — DOS Spectrum of 3-fluorobenzamide

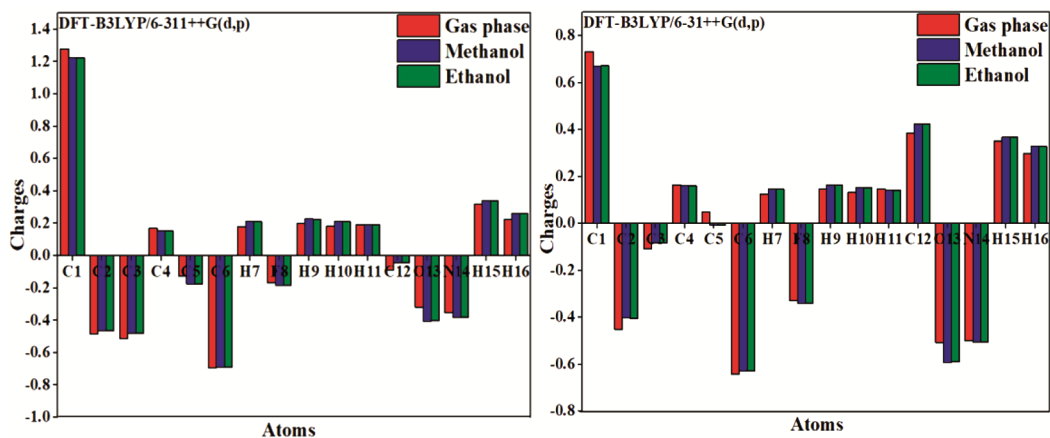


Fig. S3 — Mulliken charges plot for 3-fluorobenzamide

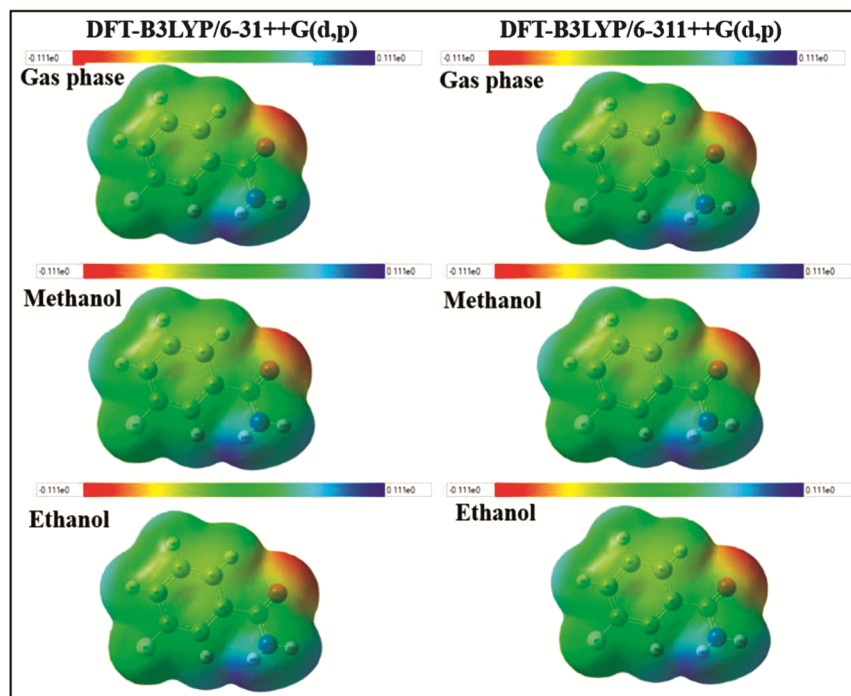
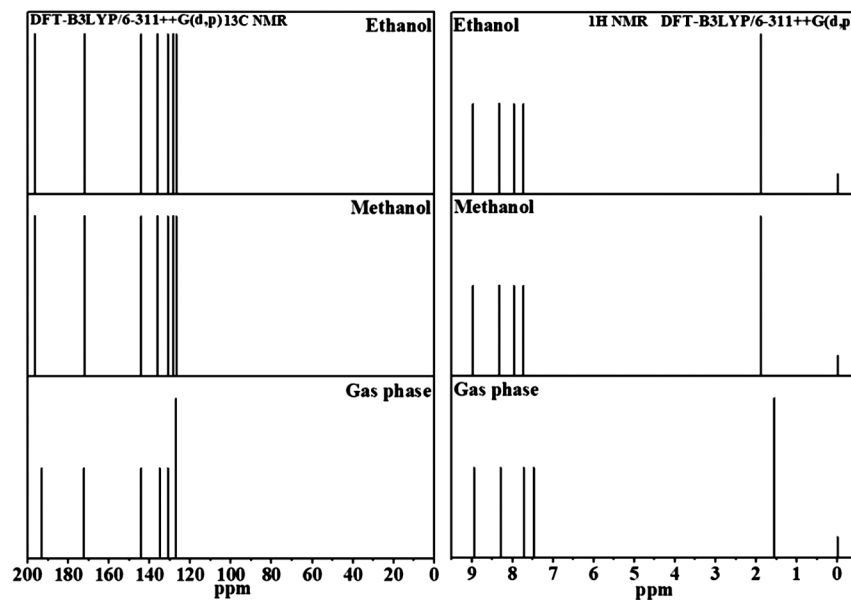


Fig. S4 — MEP plot of 3-fluorobenzamide

Fig. S5 — ^{13}C and ^1H NMR plot of 3-fluorobenzamide by B3LYP/6-311++G(d,p) method