Solid State Structure and Environmental Polarization Effect of a Novel Asymmetric Azine

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Supplementary Information:

Table S1: Vibrational assignments, experimental and calculated wave numbers in cm^{-1} of $C_{17}H_{17}N_3O_3$ at CAM-B3LYP/6-311+G(d)

Mode nº	Unscaled Freq.	Scaled Freq[a].	$I^{infrared}$	FT-IR[b]	IR assingments
1	8.35	8.00	0.01		Γ C3C4C7N2 + Γ C9C10C11N3
2	18.73	17.94	0.02		Γ C12C13O3C16
3	32.12	30.77	0.15		β C7N2N3
4	35.00	33.53	1.03		Γ C7N2N3C9 + Γ C11C12C13C14
5	48.68	46.64	0.00		Γ NO2 + R1
6	57.04	54.64	0.01		Γ O2N1C1C6
7	83.52	80.01	0.09		β N1C1C2C6
8	90.04	86.26	0.66		β C9N2N3
9	107.57	103.05	13.77		Γ C7N2N3C9 + Γ C12C13O3C16
10	117.58	112.64	1.11		Γ C12C13O3C16 + Γ C13O3C16C17
11	159.59	152.89	0.69		β C14C13O3
12	184.61	176.86	2.34		Γ HC8C7C4
13	187.46	179.59	0.10		r CH3 8
14	201.31	192.85	1.55		Γ C11C10C9N3
15	233.13	223.34	0.44		Γ C2C3C4C7 + β C4C7C8N2
16	247.75	237.34	0.75		Γ HC17C16O3
17	255.23	244.51	0.11		Γ CH3 + Γ CH2
18	299.56	286.98	2.23		β C8C7N2
19	308.49	295.53	1.92		ρ C1C2N1
20	331.24	317.33	5.03		Γ H9C9N2N3
21	377.50	361.65	1.84		ρ O3C16C17
22	416.19	398.71	2.07		Γ R2
23	420.65	402.98	0.48		ρ C8C7N2
24	425.49	407.62	0.04		Γ R1
25	434.03	415.80	1.22		Γ R2
26	474.20	454.28	3.44		ν C1N1
27	485.11	464.74	1.22		β C4C7C8
28	486.11	465.69	4.72		β C1C2C6N1 + β C12C13C14O3
29	548.24	525.21	2.01	533(w)	r NO2
30	551.47	528.31	0.87		ν C4C7
31	552.82	529.60	12.16		Γ H15C15C14O1+ Γ H12C12C11C8
32	573.70	549.60	15.85		Γ H8bC8C7C4
33	640.64	613.73	50.69		ρ C8C11N2+ ρ

Mode nº	Unscaled Freq.	Scaled Freq[a].	$I^{infrared}$	FT-IR[b]	IR assingments
					C13C14C15+ ρ C8N2N3
34	652.75	625.33	0.27		β R1
35	655.47	627.94	1.37		β R2
36	713.98	683.99	23.90	690(w)	ω NO_2
37	716.88	686.77	1.05		ρ NO_2?
38	750.25	718.74	1.02		Γ R2
39	753.75	722.09	4.20	752(w)	ω NO_2 + β N1C2C3C4 + β O1C13C14C15
40	792.93	759.63	6.25		ν C7C22
41	825.28	790.62	5.44		ρ N3N2C8 + ρ C14O1C17
42	831.50	796.58	5.55		Γ H18bC18C17O1
43	851.06	815.32	11.04		Γ R2 + rCH2
44	866.11	829.73	41.60		TR1+TR2 + rCH2
45	866.87	830.46	7.11		Γ H1C1C3C4+ Γ H15C15C14C13
46	890.04	852.66	36.63	854(w)	ρ NO_2 + ν N1C3
47	892.46	854.98	39.74		Γ C5H5C4C3 + Γ H4C4C5C6
48	903.39	865.45	39.80		ν C8C11 + ν C11C16
49	956.18	916.02	19.15		ν C17C18 + ν C17O1
50	979.37	938.24	1.05		Γ CHR2 + Γ H8C8N2N3
51	994.77	952.99	4.08		ν C7C22
52	995.23	953.43	0.07		Γ CH R2
53	1006.11	963.85	0.73		Γ H3C3C2C1
54	1029.58	986.34	8.27		Γ H6C6C5C4
55	1032.61	989.24	1.63		Γ H5C5C6C1
56	1038.92	995.29	0.36		rCHR2
57	1044.24	1000.38	12.48		rCHR1
58	1076.44	1031.23	79.36		ν N2N3
59	1077.39	1032.14	0.26		rCH3; C8
60	1094.63	1048.66	83.32	1050(w)	ν sym $C_{16}O_3$
61	1141.02	1093.10	0.96		ν N2N3
62	1147.59	1099.39	71.52		ν C1N1
63	1149.19	1100.92	1.45		rH6C6C5+ r H3C3C2
64	1151.70	1103.33	32.64		ρ H15C15C14H14
65	1159.28	1110.59	32.69		β CH3 17 + β C13O3C16
66	1197.39	1147.10	3.75		β H16C16C17
67	1202.55	1152.04	179.24		β CH R2
68	1219.85	1168.62	0.39		ν C5C6 + ν C2C3
69	1266.01	1212.84	23.03		ν C9C10
70	1310.39	1255.35	419.25	1251(vs)	ν C13O3
71	1328.72	1272.91	44.47		ν C4C7
72	1330.82	1274.93	0.95		Γ C16 + C13
73	1338.68	1282.46	0.93		ν CR1 + B CH3
74	1340.82	1284.51	203.94		ν CR2 + ν C13O13

Mode nº	Unscaled Freq.	Scaled Freq[a].	$I^{infrared}$	FT-IR[b]	IR assingments
75	1354.30	1297.42	129.86		ν CR2
76	1357.44	1300.43	21.12		ν CR1
77	1406.48	1347.41	0.50		ρ H9C9N3
78	1421.60	1361.89	42.68		β CH3; C8
79	1422.57	1362.82	4.76		β CH3 17 + β C16
80	1433.00	1372.81	543.32	1388(w)	ν sym NO2
81	1454.74	1393.64	50.41		β C16C17
82	1462.28	1400.86	8.67		ν CR1 + β CH3 8
83	1477.62	1415.56	13.45		ν C14C15 + ν C11C12
84	1500.95	1437.91	8.01		β CH3 8
85	1507.92	1444.59	9.38		β CH3 17
86	1521.54	1457.64	5.71		ρ CH3 17
87	1522.53	1458.58	11.48		ρ CH3 8
88	1542.32	1477.54	56.77	1477(w)	ρ C16 + ρ CH3 17
89	1554.97	1489.66	18.71		ν Rr1 + rCHR1
90	1576.40	1510.19	145.34		ν C14C13 + ν C13O13
91	1631.11	1562.60	183.19	1575(w)	V asym NO_2
92	1642.95	1573.95	48.57		ν R2
93	1665.95	1595.98	279.04		ν C5C6 + ν C2C3 + ν C10C15 + ν C13C13 + ν N1O1 + ν C7N2 + ν C9N3
94	1685.56	1614.77	44.67		ν CR1 + ν N1O2
95	1689.06	1618.12	345.81		ν C1C2 + ν C5C4 + ν C14C15 + ν C11C12 + ν N1O2
96	1702.95	1631.43	30.01		ν CR1 + ν CR2 + ν C7N2 + ν C9N3
97	1732.10	1659.35	259.71	1618(w)	ν C7N2 + ν C9N3
98	3040.87	2913.15	26.91	2929(vw)	ν sym CH2
99	3069.26	2940.35	21.88		ν sym CH3; C8
100	3070.59	2941.63	23.49		ν sym CH3; C17
101	3081.06	2951.66	25.35	2986(vw)	ν asym CH2
102	3106.25	2975.79	19.47		ν C9h9
103	3120.44	2989.38	10.02		ν asym C8H8aH8b
104	3140.19	3008.30	23.11		ν asym CH3; C17
105	3148.62	3016.38	27.50		ν asym C17H17aH17b
106	3191.69	3057.64	8.70		ν C15H15
107	3204.73	3070.13	3.04		ν C8H8c
108	3219.24	3084.03	4.92		ν C11H11
109	3221.92	3086.60	6.35		ν C14H14
110	3229.82	3094.17	3.56		ν C3H3
111	3236.86	3100.91	11.99		ν C12H12
112	3241.54	3105.40	1.75		ν C5H5
113	3252.37	3115.77	0.96		ν C2H2
114	3254.00	3117.33	0.16		ν C5H5 + ν C6H6

R1 and R2; first and second ring, ν; stretching, β; in plane bending, ; out of plane bending, ρ; scissoring, Γ; torsion, ω; wagging, r; rocking, t; twisting; IR intensities, [$I^{Infrared}$ (K mmol−1)] a Scale factor 0.958 [56] b Intensity: vs; very strong, s; strong, m; medium, w; weak, vw; very weak

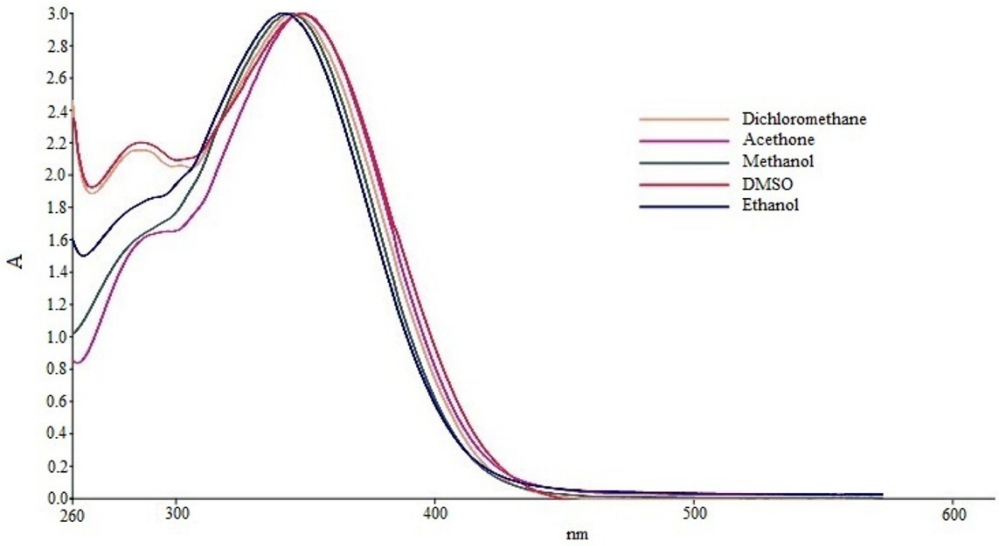


Figure S1: UV–vis spectrum of NPT-HI

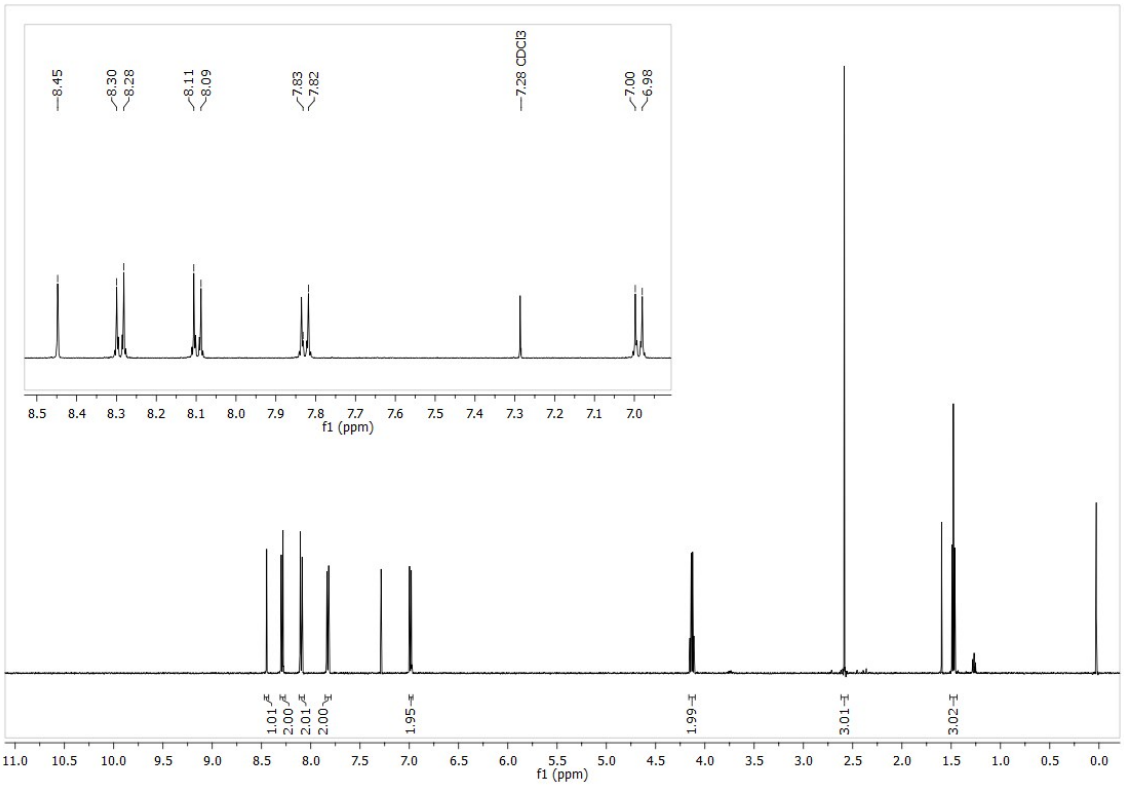
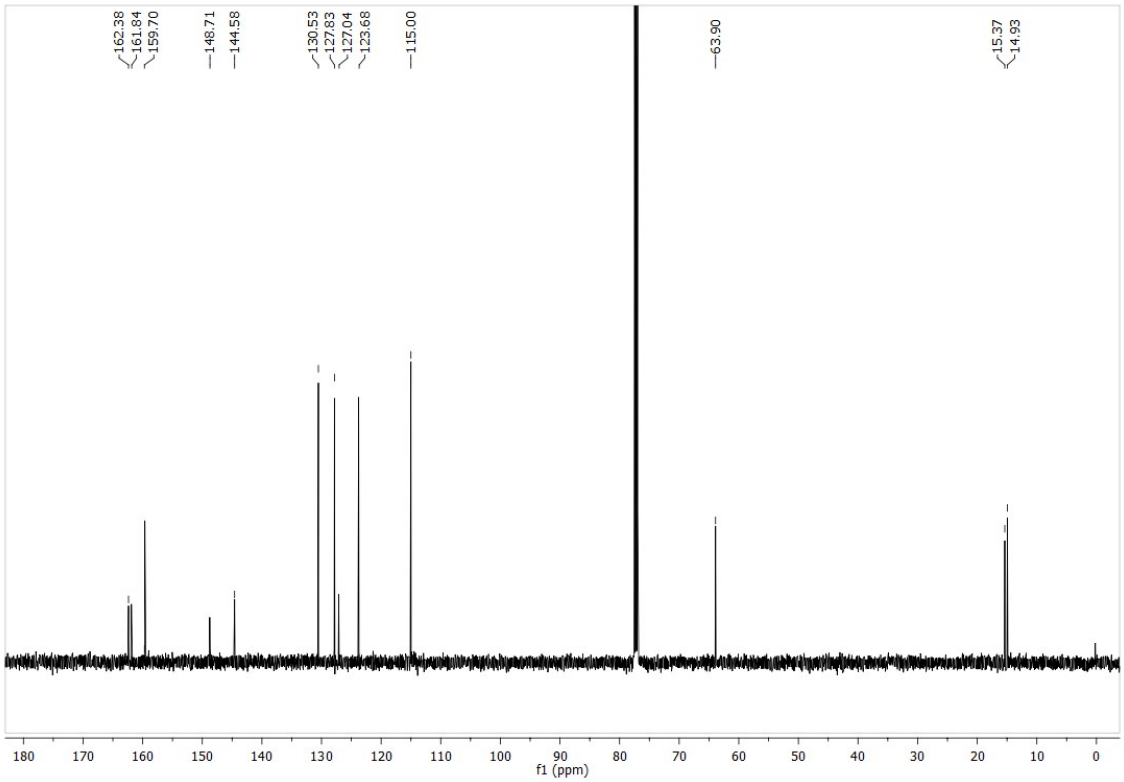


Figure S2: ^{1}H NMR spectrum of NPT-HI (CDCl3, 500 MHz)



(b)

Figure S3: ^{13}C NMR spectrum of NPT-HI (CDCl3, 125 MHz)

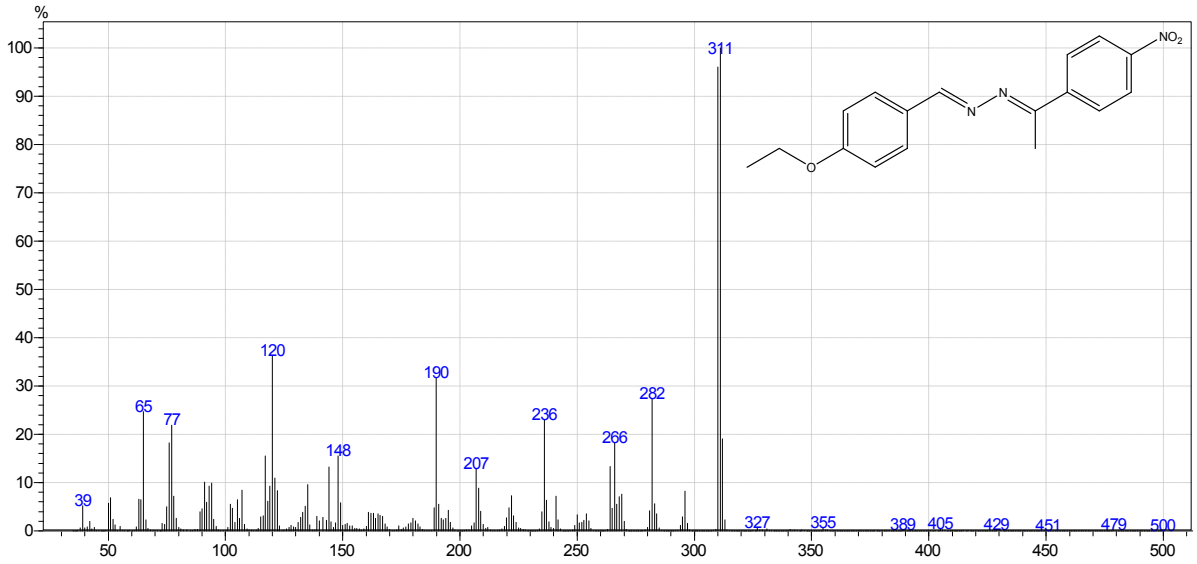


Figure S4: Mass Spectrum of NPT-HI

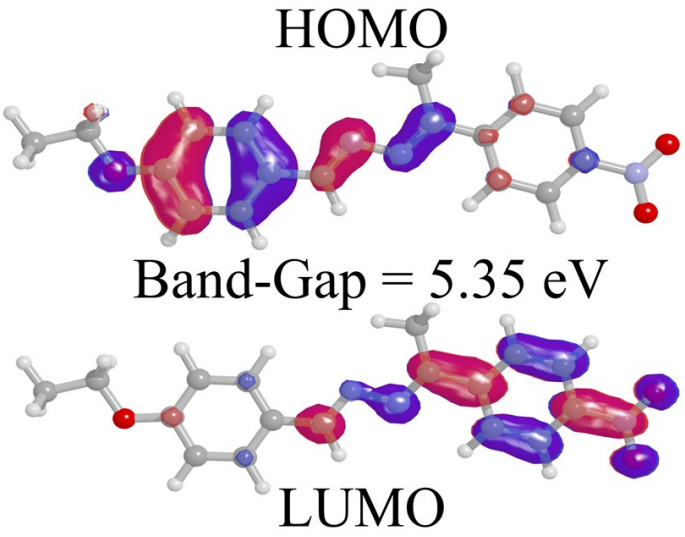


Figure S5: Molecular orbital plots, showing HOMO-LUMO as obtained in the CAM-B3LYP/6-311+G(d) level of theory for ACETONE solvent, for the NPT-HI molecule.

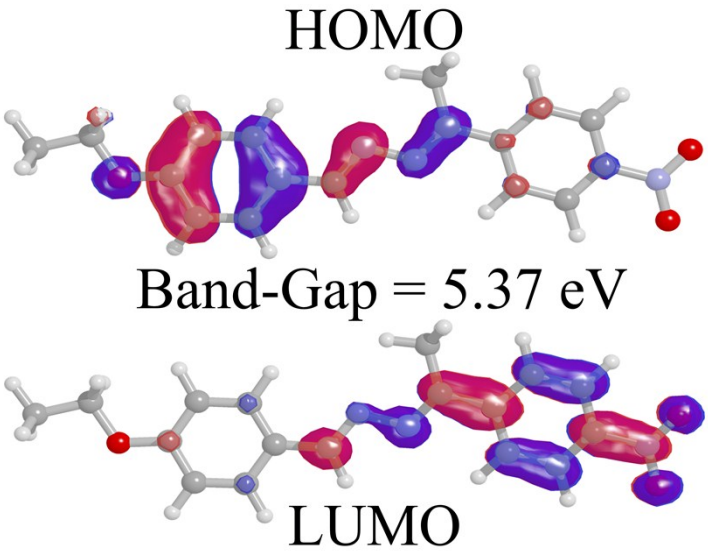


Figure S6: Molecular orbital plots, showing HOMO-LUMO as obtained in the CAM-B3LYP/6-311+G(d) level of theory for Dichloromethane solvent, for the NPT-HI molecule.

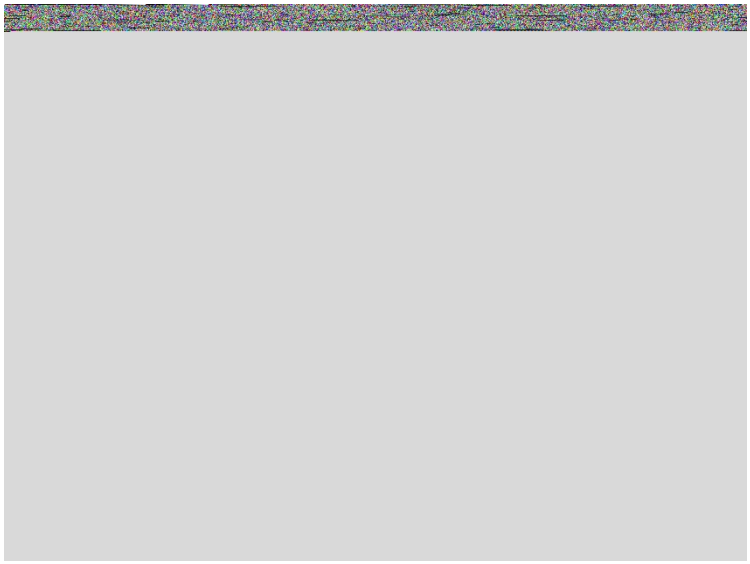


Figure S7: Molecular orbital plots, showing HOMO-LUMO as obtained in the CAM-B3LYP/6-311+G(d) level of theory for ETHANOL solvent, for the NPT-HI molecule.

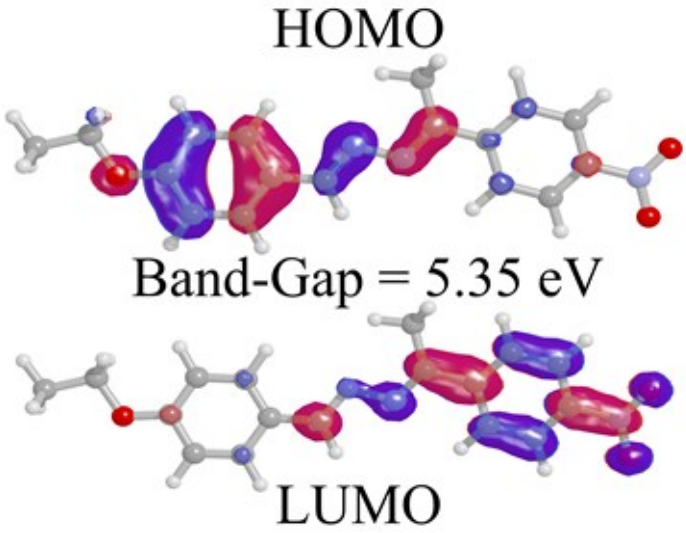


Figure S8: Molecular orbital plots, showing HOMO-LUMO as obtained in the CAM-B3LYP/6-311+G(d) level of theory for METHANOL solvent, for the NPT-HI molecule.

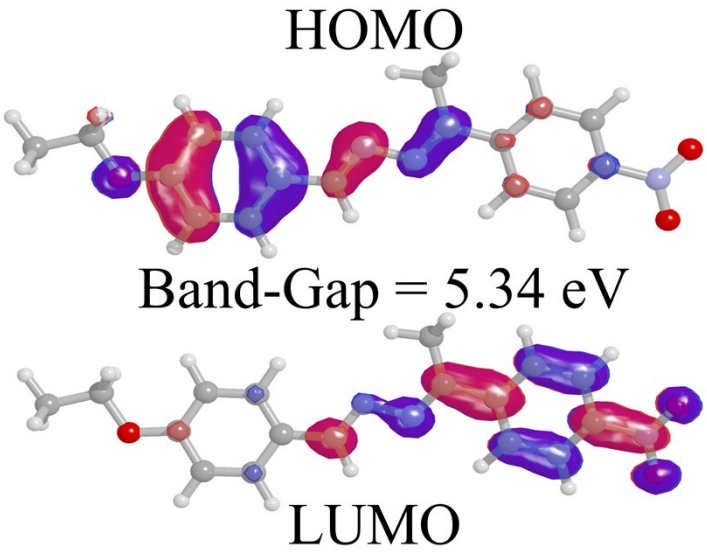


Figure S9: Molecular orbital plots, showing HOMO-LUMO as obtained in the CAM-B3LYP/6-311+G(d) level of theory for WATER solvent, for the NPT-HI molecule.