Supporting Information

3-Pyridylvinyl benzoxazole derived multifunctional organic materials - from solid state photoreactivity to photophysical and electrochemical properties

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1. Crystallography

Table S1: Crystallographic data

	3-PVBO	**[3-MPVBO]I**	**[3-MPVBO](OTf)**	**PBOCB**
CCDC number	2306976	2306977	2306978	2306979
Empirical formula	$C_{14}H_{10}N_2O$	$C_{15}H_{13}N_2O_3I$	$C_{16}H_{13}F_3N_2O_4S$	$C_{28}H_{20}N_4O_2$
Formula weight ($g.mol^{-1}$)	222.24	396.17	386.34	444.48
Temperature (K)	295 K	286 K	295 K	296 K
Radiation, λ (Å)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
Crystal Colour, habit	Block, Colourless	Block, Colourless	Block, colourless	Block, colourless
Crystal size (mm^3)	0.400 × 0.220 × 0.210	0.260 × 0.150 × 0.130	0.360 × 0.210 × 0.100	0.250 ×0.180 × 0.140
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
Unit cell dimensions				
a (Å)	6.5833(13)	7.203(3)	6.6963(6)	6.4328(15)
b (Å)	13.825(3)	16.679(7)	7.3887(6)	9.342(3)
c (Å)	24.715(9)	13.419(6)	17.6221(16)	9.841(3)
α (º)	90	90	80.201(3)	105.347(8)
β (º)	91.627(9)	92.582(14)	81.214(3)	105.020(7)
γ (º)	90	90	76.968(3)	91.233(6)
Volume ($Å^3$)	2248.5(11)	1610.5(12)	831.08(13)	548.2(3)
Z	8	4	2	1
Calculated density ($Mg.m^{-3}$)	1.313	1.634	1.544	1.346
μ (mm^{-1})	0.085	1.999	0.252	0.087
F(000)	928	776	396	232
θ range (°)	2.21 to 27.05	2.24 to 25.26	2.36 to 26.37	2.23 to 27.10
Reflections collected	39886	20041	24592	16103
Independent reflections	4600	2850	3392	2215
Parameters/ restraints	427/228	355/538	292/114	324/692
GooF on F^2	1.121	1.089	1.074	1.100
R_1 [I>2σ(I)] [a]	0.0518(3764)	0.0957(2071)	0.0517(3014)	0.0405(1873)
wR_2 (all data) [b]	0.1215(4600)	0.2344(2850)	0.1371(3392)	0.0975(2215)
Maximum/minimum residual electron density ($e.Å^{-3}$)	0.211/-0.140	2.080/-1.577	0.301/ -0.204	0.120/-0.122

2. Additional crystallographic diagrams

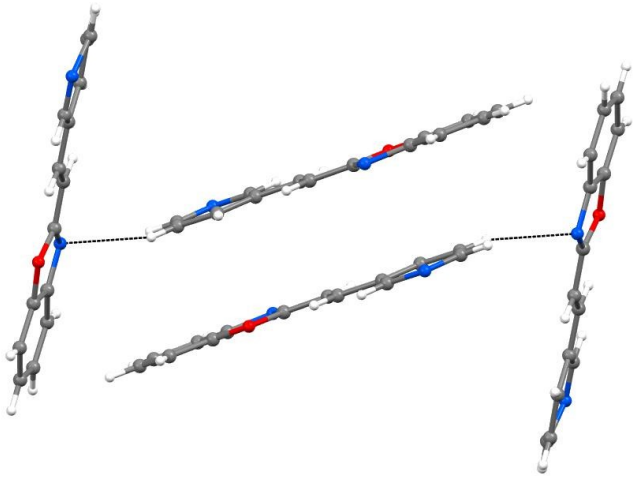


Fig. S1: Arrangement of two types of molecules of **3-PVBO** in its crystal structure. A pair of **3-PVBO** molecules stack in parallel via C−H···N interaction.

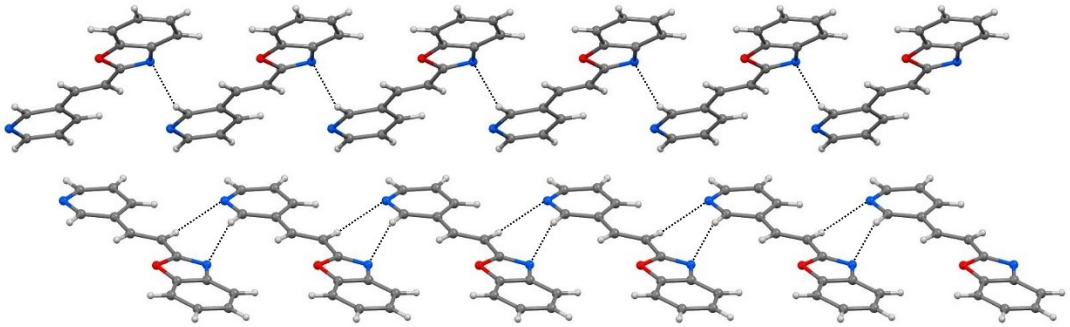


Fig. S2: Arrangement of two types of molecules of **3-PVBO** in its crystal structure via various C−H···N interactions.

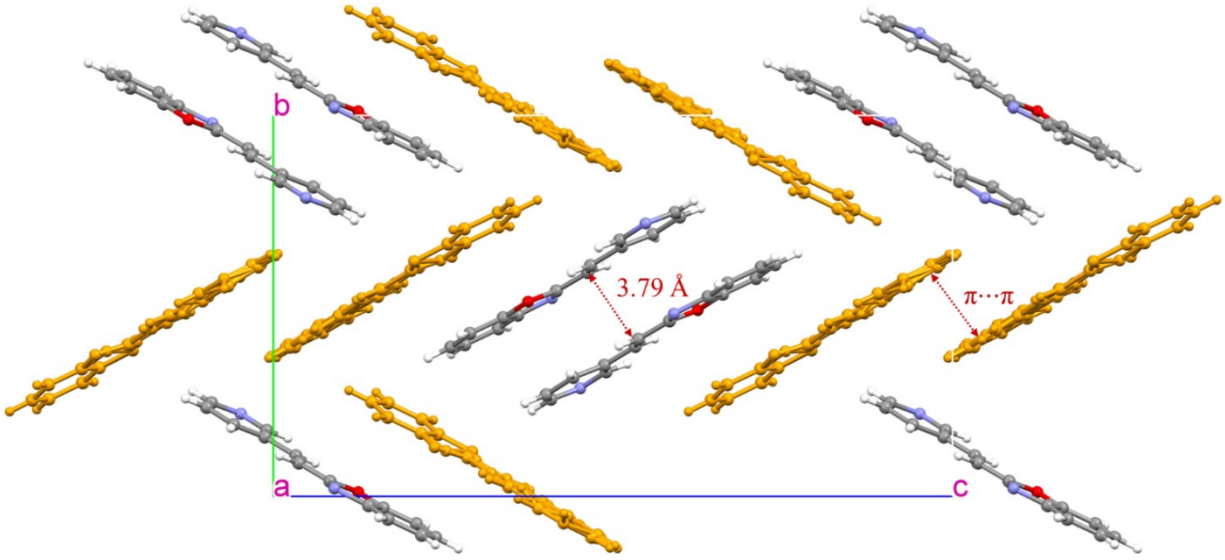


Fig. S3: Crystal packing of two types of **3-PVBO** molecules are shown. The disordered molecules are shown in orange to distinguish them from the other. Only one type (more ordered) of molecules is found to stack in a parallel arrangement, suitable for photodimerization reaction in the solid state.

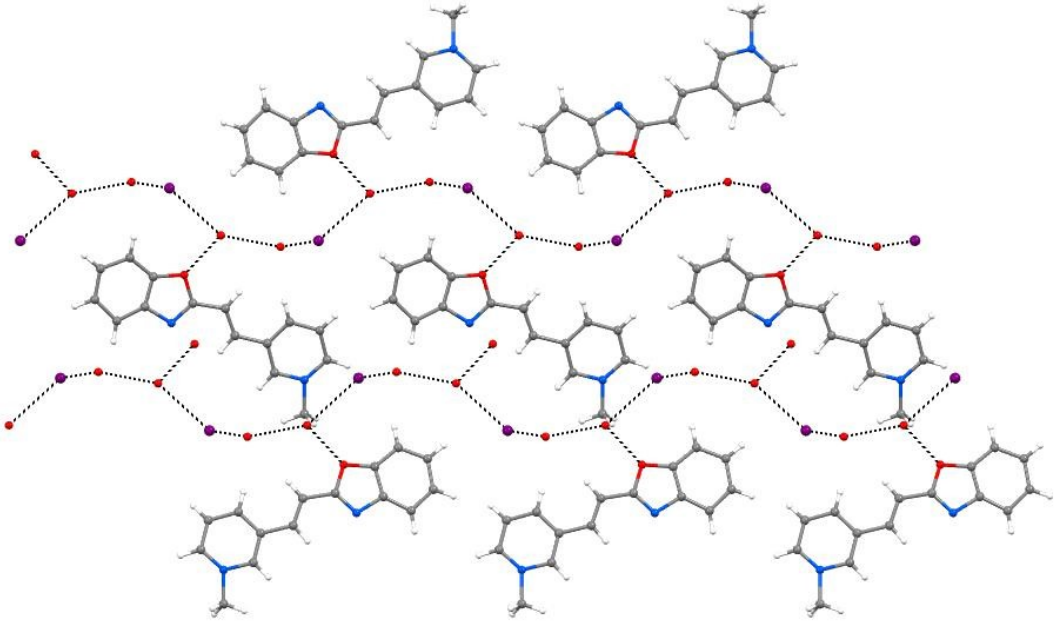


Fig. S4: Crystal packing of **[3-MPVBO]I**, viewed approximately along the *c*-direction, showing hydrogen bonding interaction between **3-MPVBO** cations, lattice water and iodide anions. One-dimensional zig-zag hydrogen bonded network, formed between lattice water and iodide anions, can be observed.

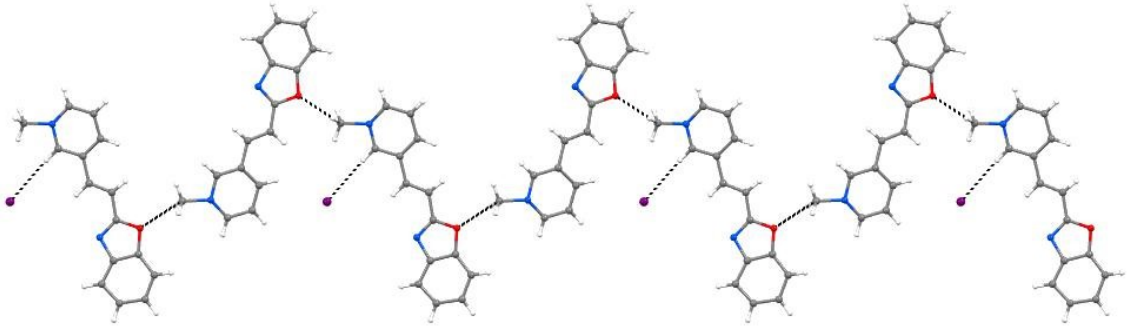


Fig. S5: Crystal packing of **[3-MPVBO]I** showing C−H···O and C−H···I weak interactions, viewed approximately along the *a*-direction.

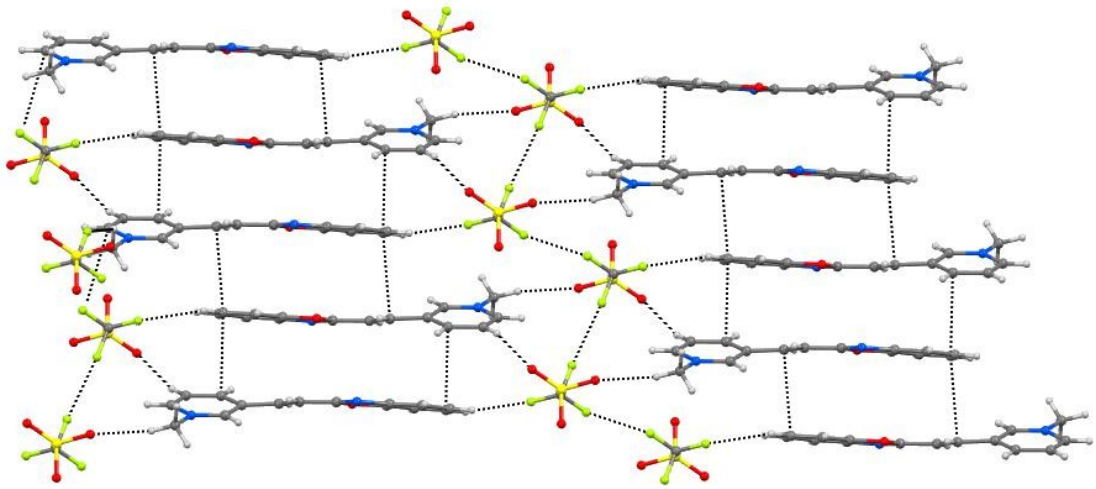


Fig. S6: Crystal packing of **[3-MPVBO](OTf)** showing various weak interactions between **3-MPVBO** cations and triflate anions, viewed approximately along the *a*-direction.

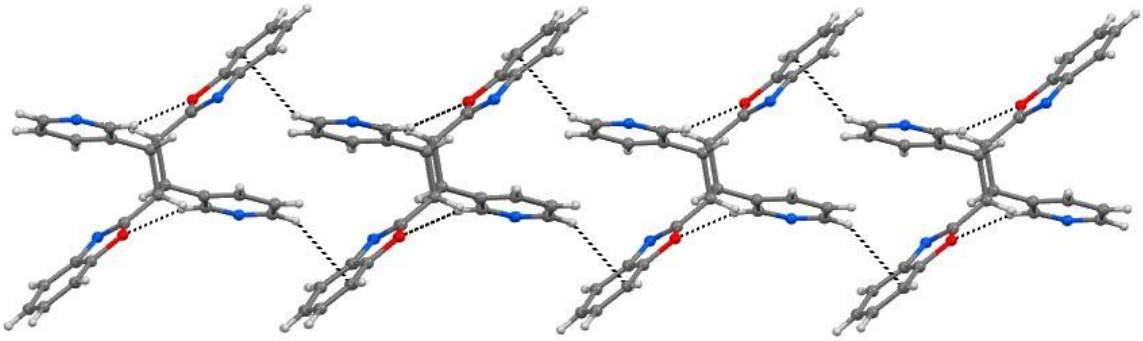


Fig. S7: Crystal packing of **PBOCB** showing C−H···N, C−H···O and C−H··· π weak interactions, viewed approximately along the *a*-direction.

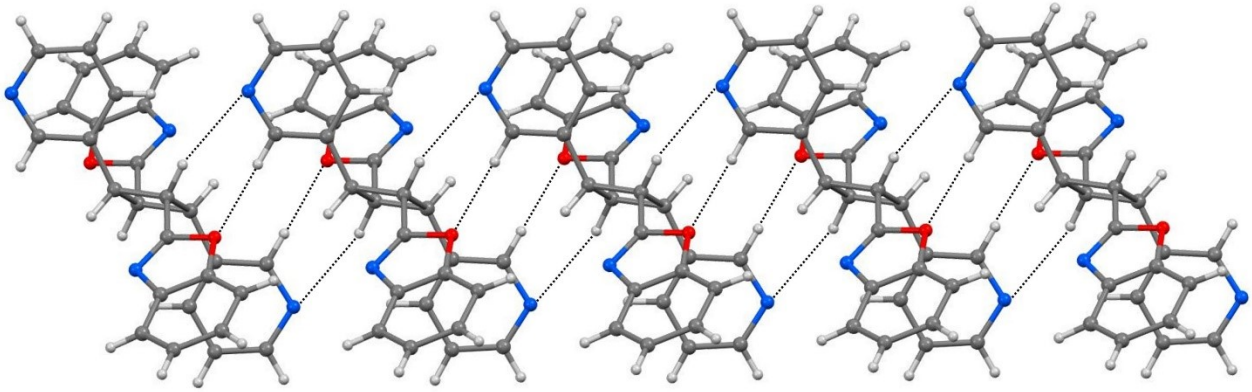


Fig. S8: Crystal packing of **PBOCB** showing intermolecular C−H···N and C−H···O weak interactions, viewed approximately along the *c*-direction.

3. Analysis of Hirshfeld surfaces

Plotting of Hirshfeld Surface can be done using a variety of characteristics, including curvedness, electrostatic potential, shaped index, and d_{norm} (normalised distance). Here, the HS is mapped using the d_{norm} to visually show the interactions using two distinct colours to indicate the direction of acting interactions. Red spots indicate the positions of strong interactions between a pair of neighbouring molecules.

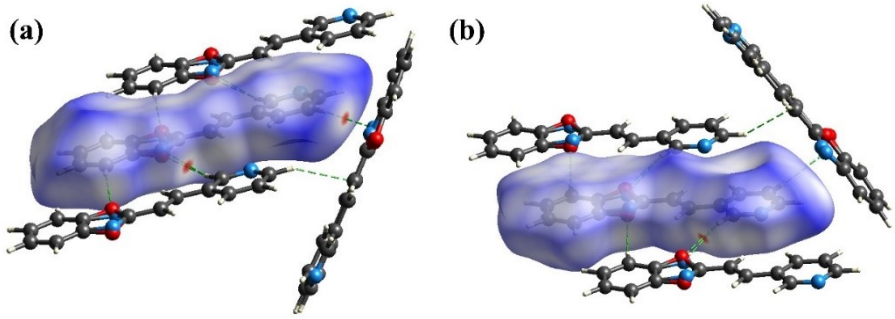


Fig. S9: Hirshfeld surface for **3-PVBO**. The C−H···N are shown in different viewing directions (a) and (b).

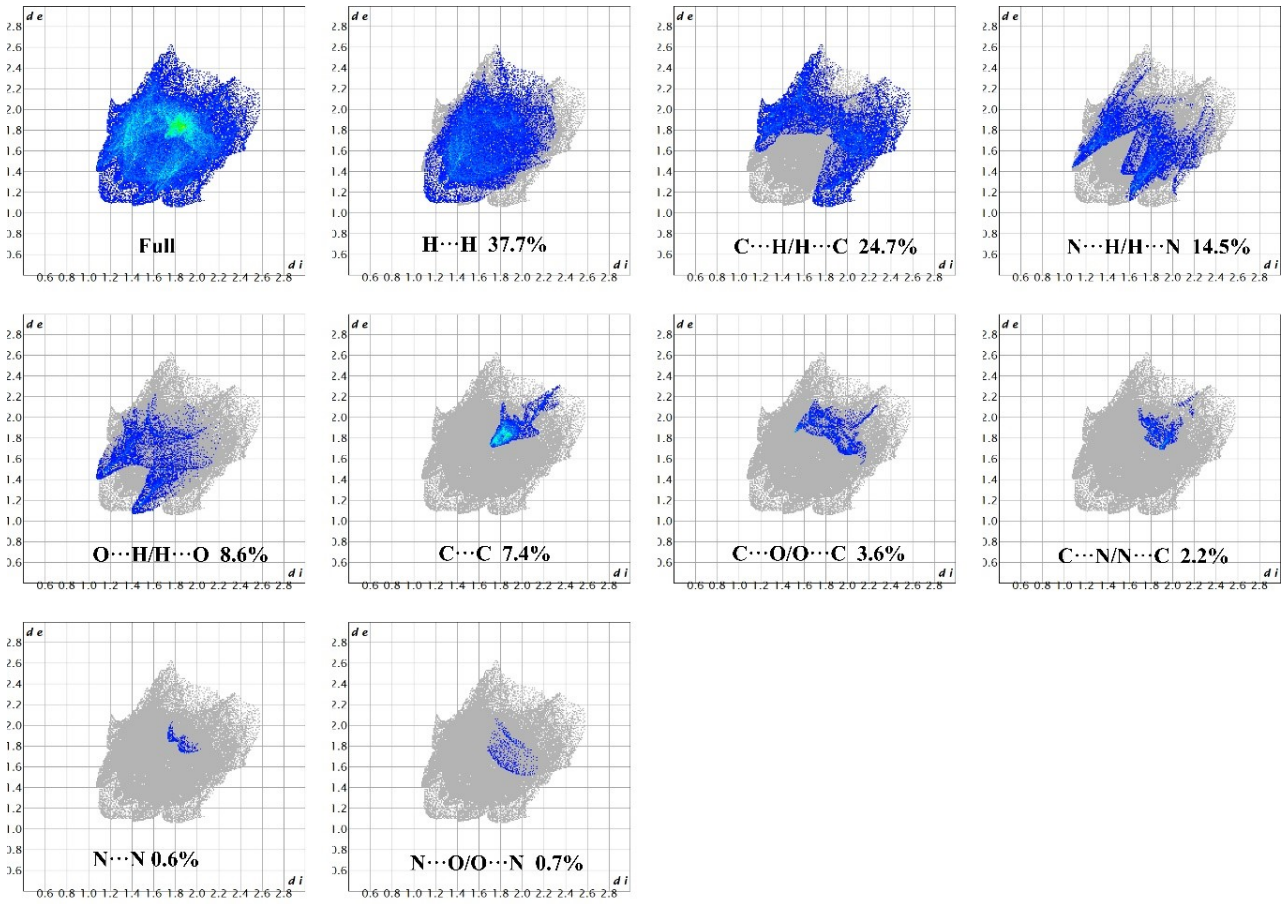


Fig. S10: Full fingerprint plot is resolved for various types of interactions and the percentage of their contributions to the total Hirshfeld surface area is presented for **3-PVBO**.

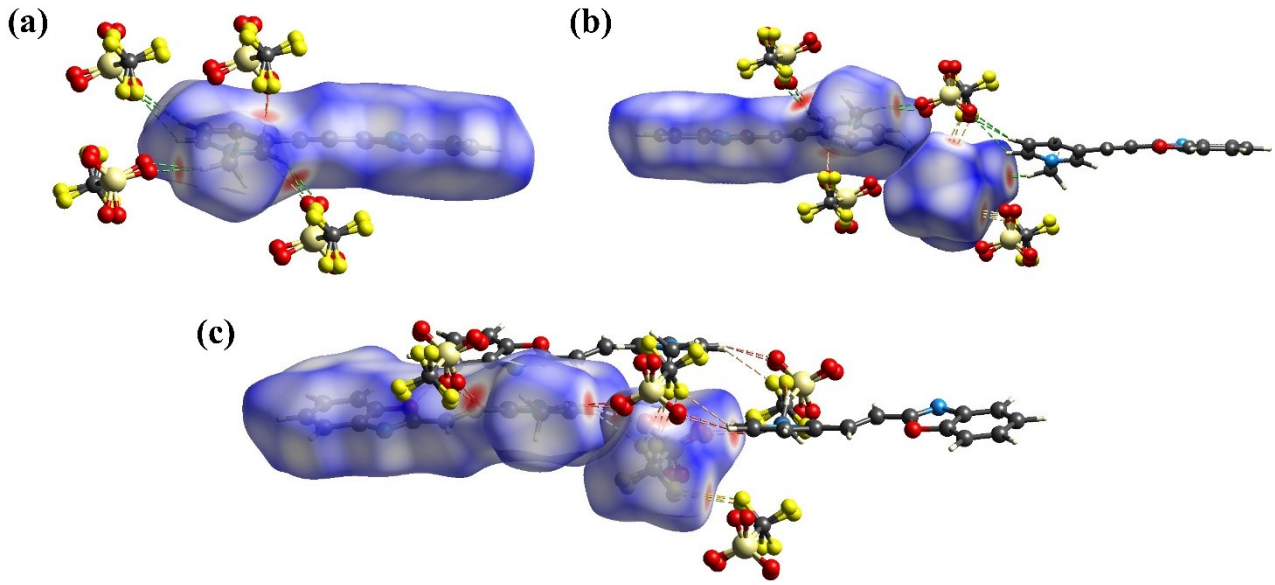


Fig. S11: Hirshfeld surface for **[3-MPVBO](OTf)**. Various interactions like C−H···O, C−H···F between the cation and triflate anion are shown in different angles in (a), (b) and (c).

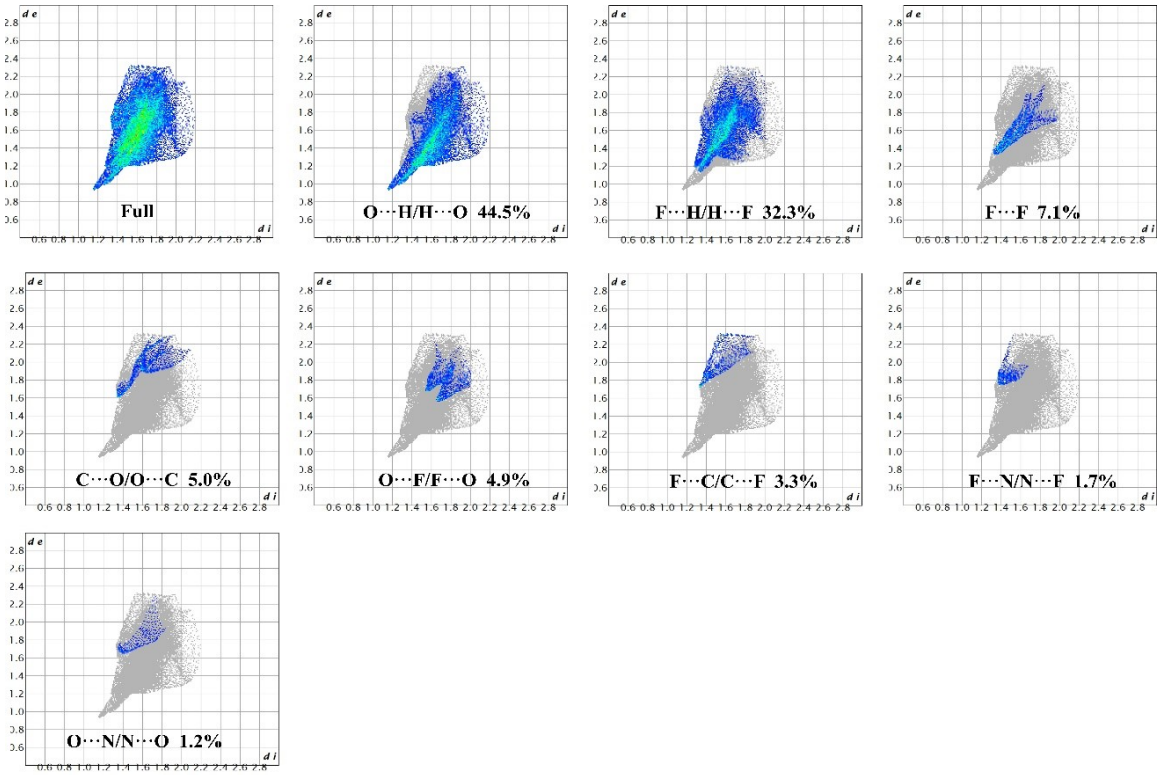


Fig. S12: Full fingerprint plot is resolved for various types of interactions and the percentage of their contributions to the total Hirshfeld surface area is presented for **[3-MPVBO](OTf)**.

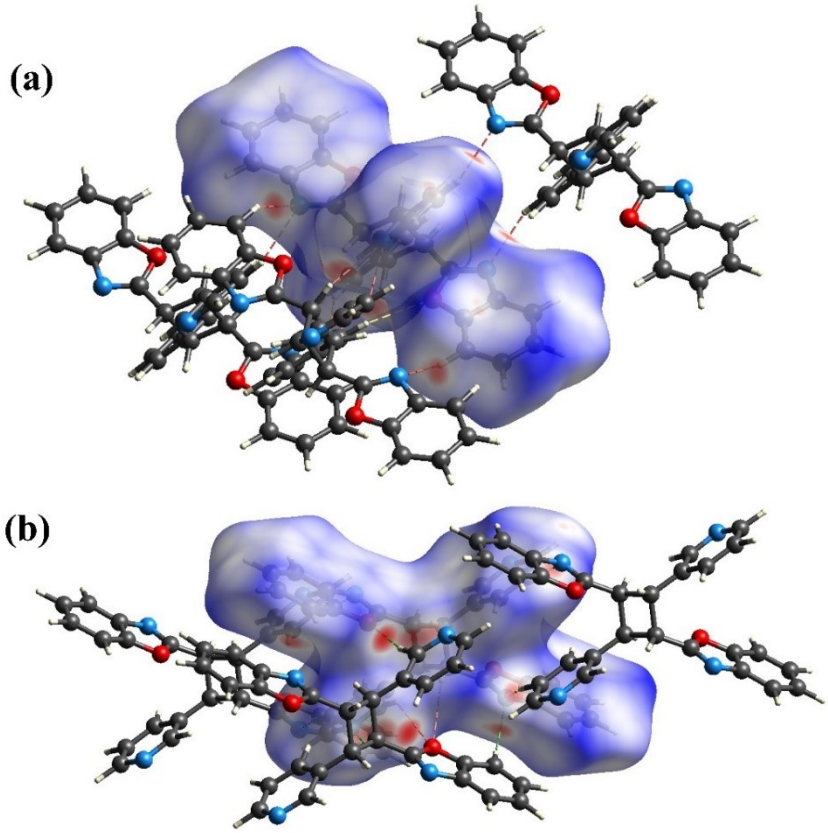


Fig. S13: Hirshfeld surface for **PBOCB**. Various interactions like C−H···N, C−H···π are shown in different angles in (a) and (b).

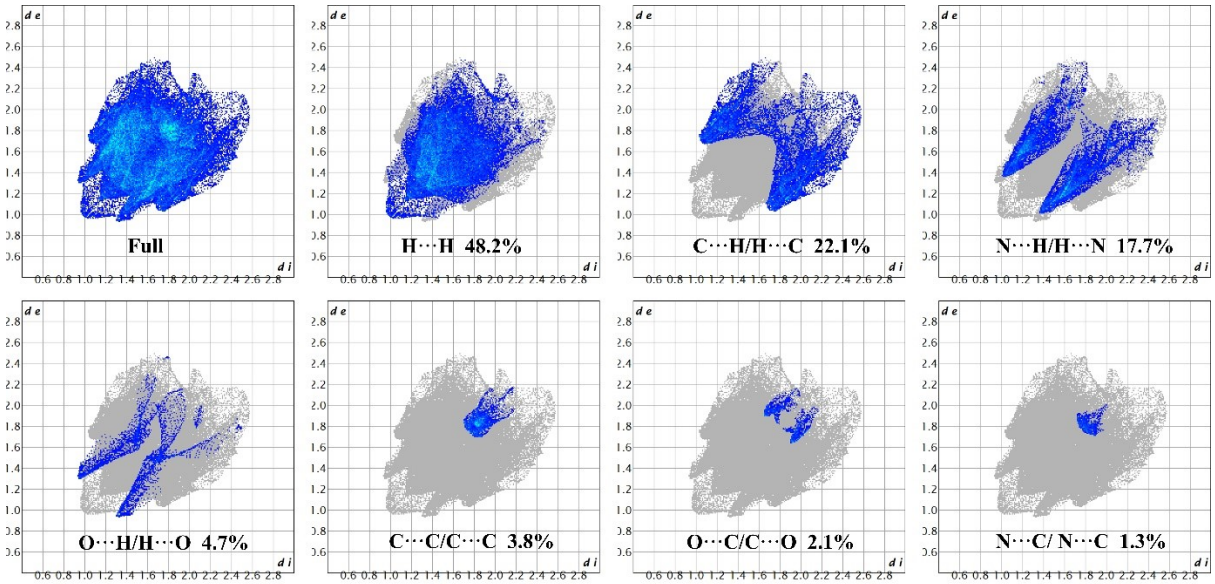


Fig. S14: Full fingerprint plot is resolved for various types of interactions and the percentage of their contributions to the total Hirshfeld surface area is presented for **PBOCB**.

4. NMR spectroscopy

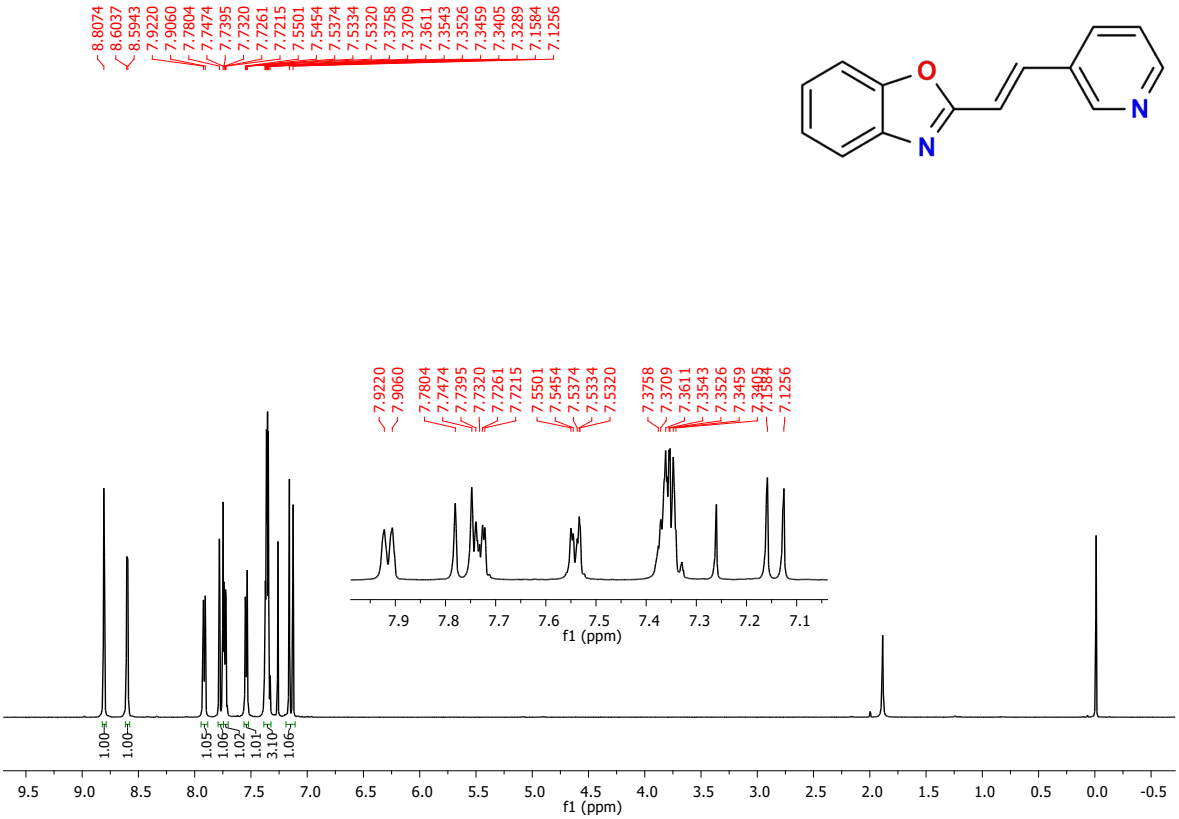


Fig. S15: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **3-PVBO.**

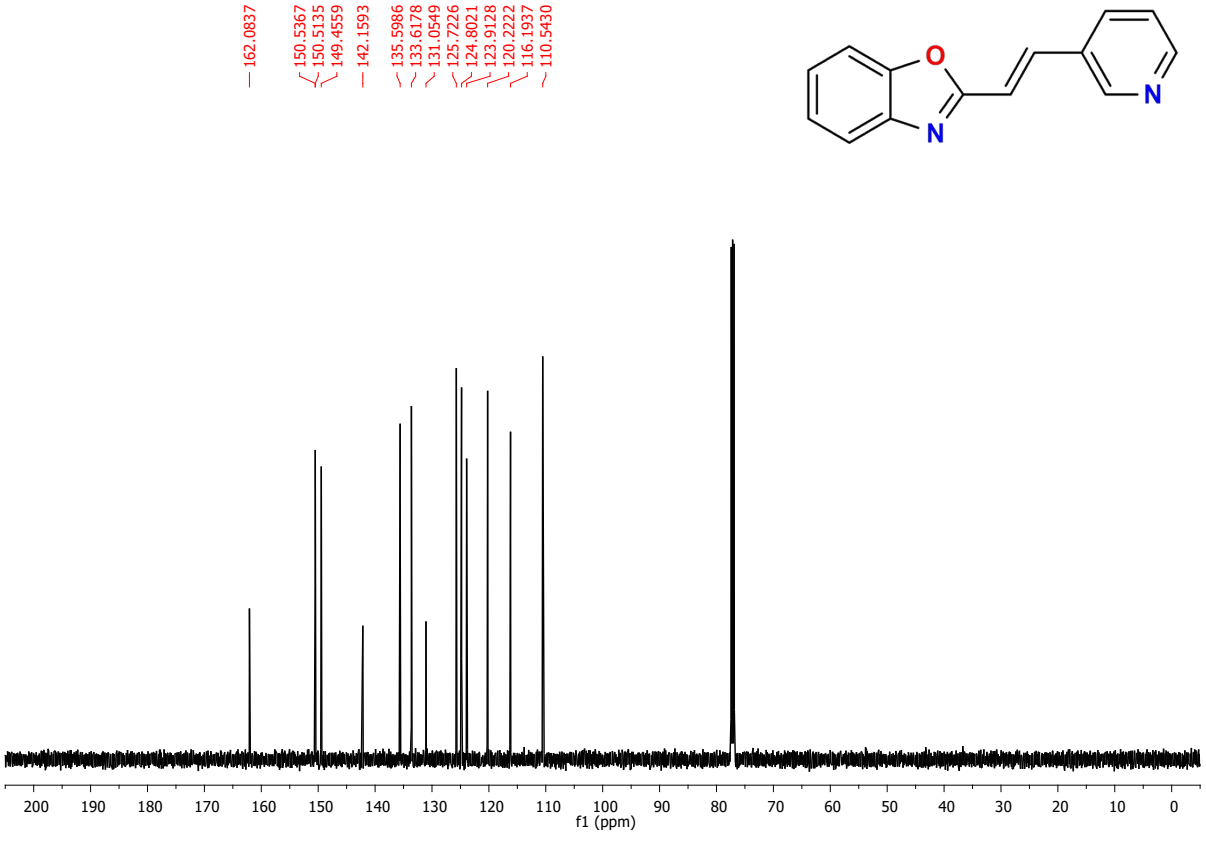


Fig. S16: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **3-PVBO.**

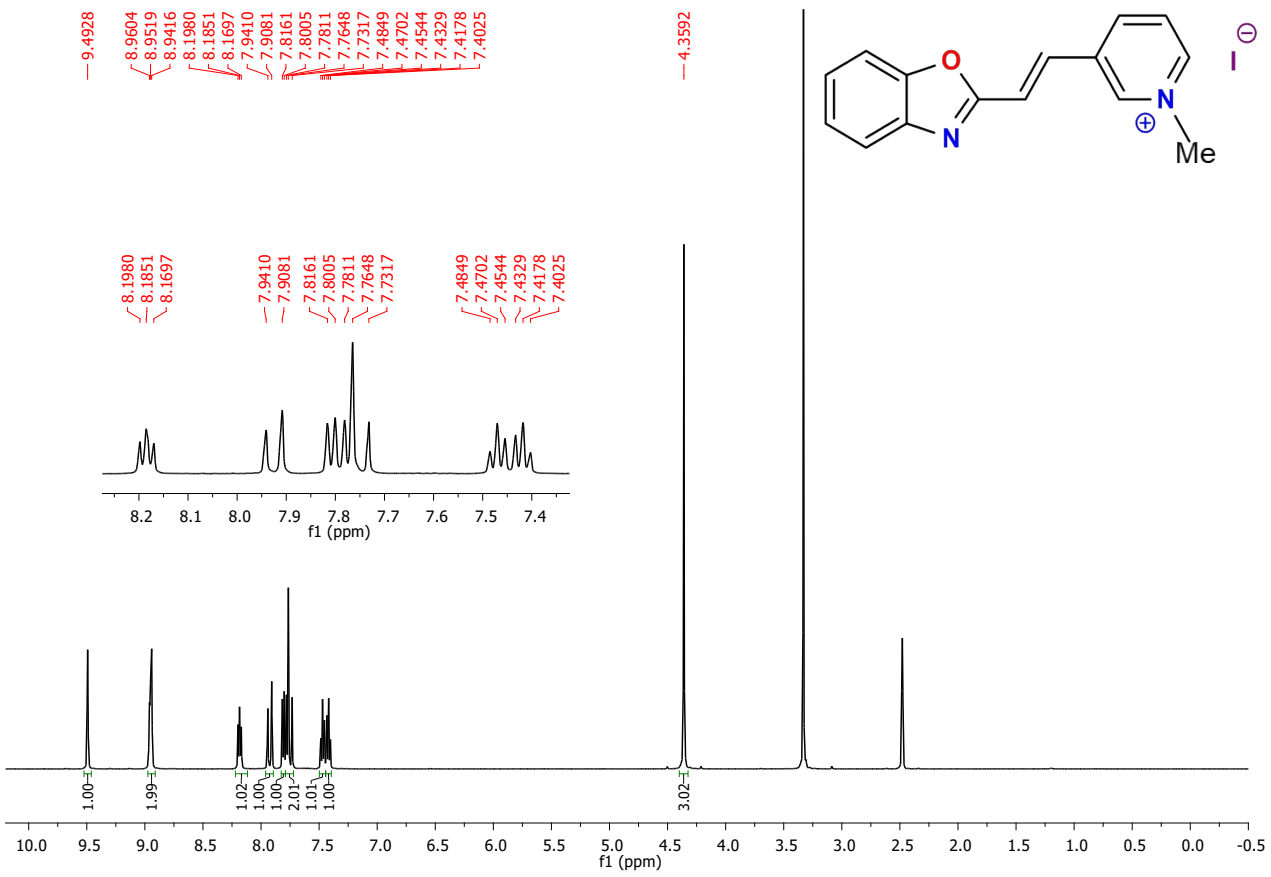


Fig. S17: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **[3-MPVBO]I.**

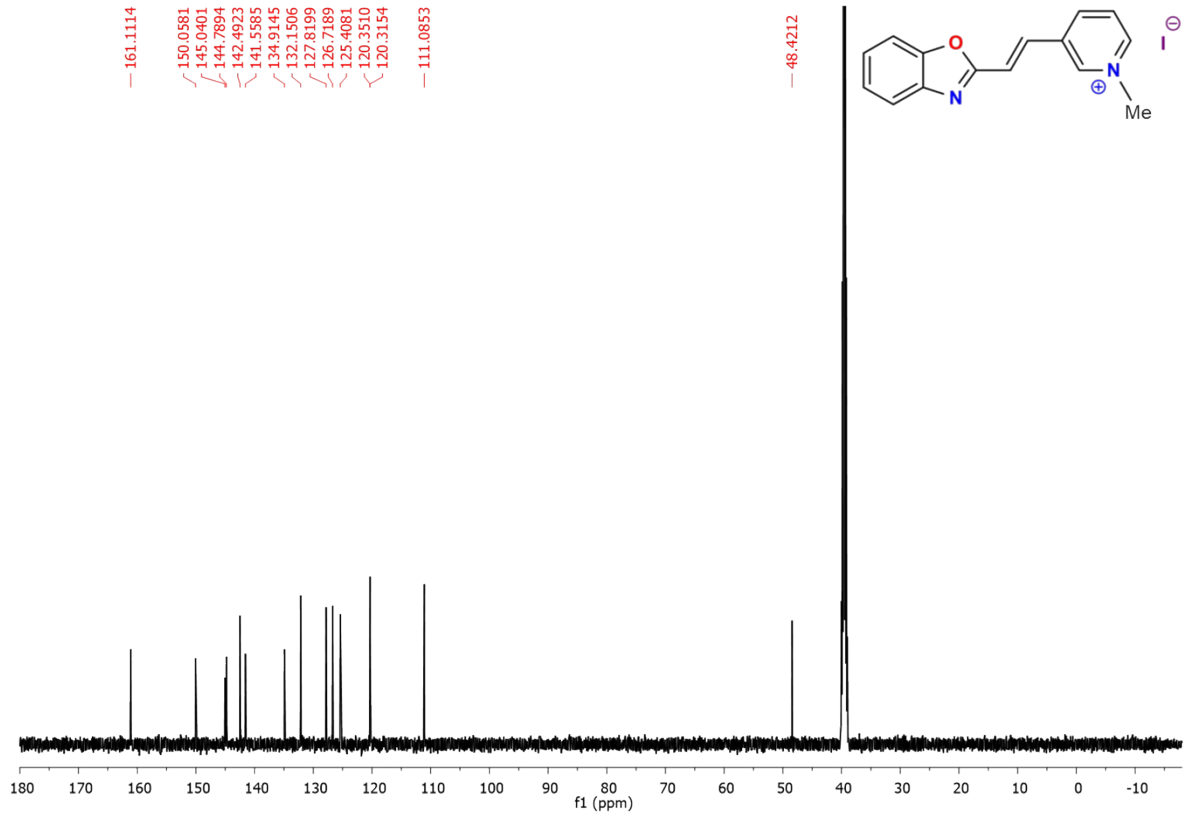


Fig. S18: ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of **[3-MPVBO]I.**

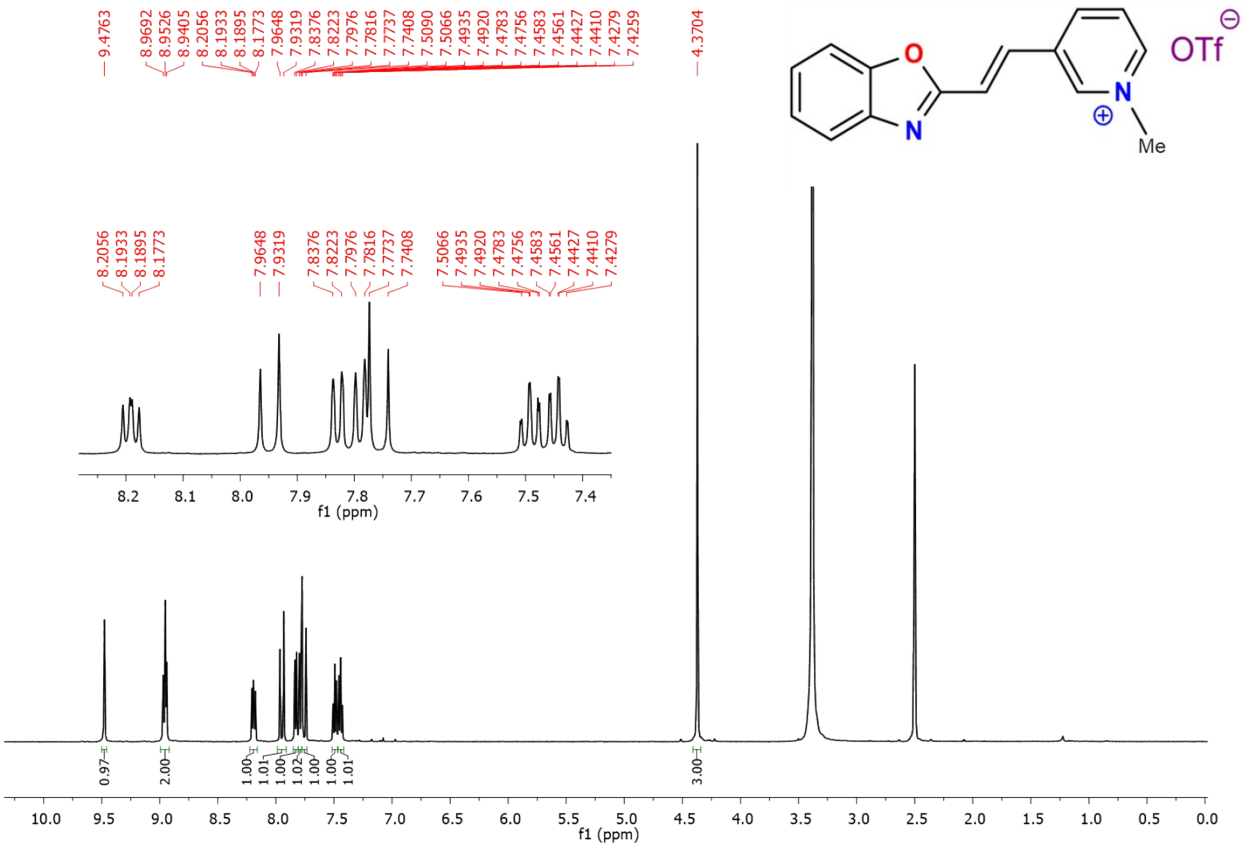


Fig. S19: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **[3-MPVBO](OTf)**.

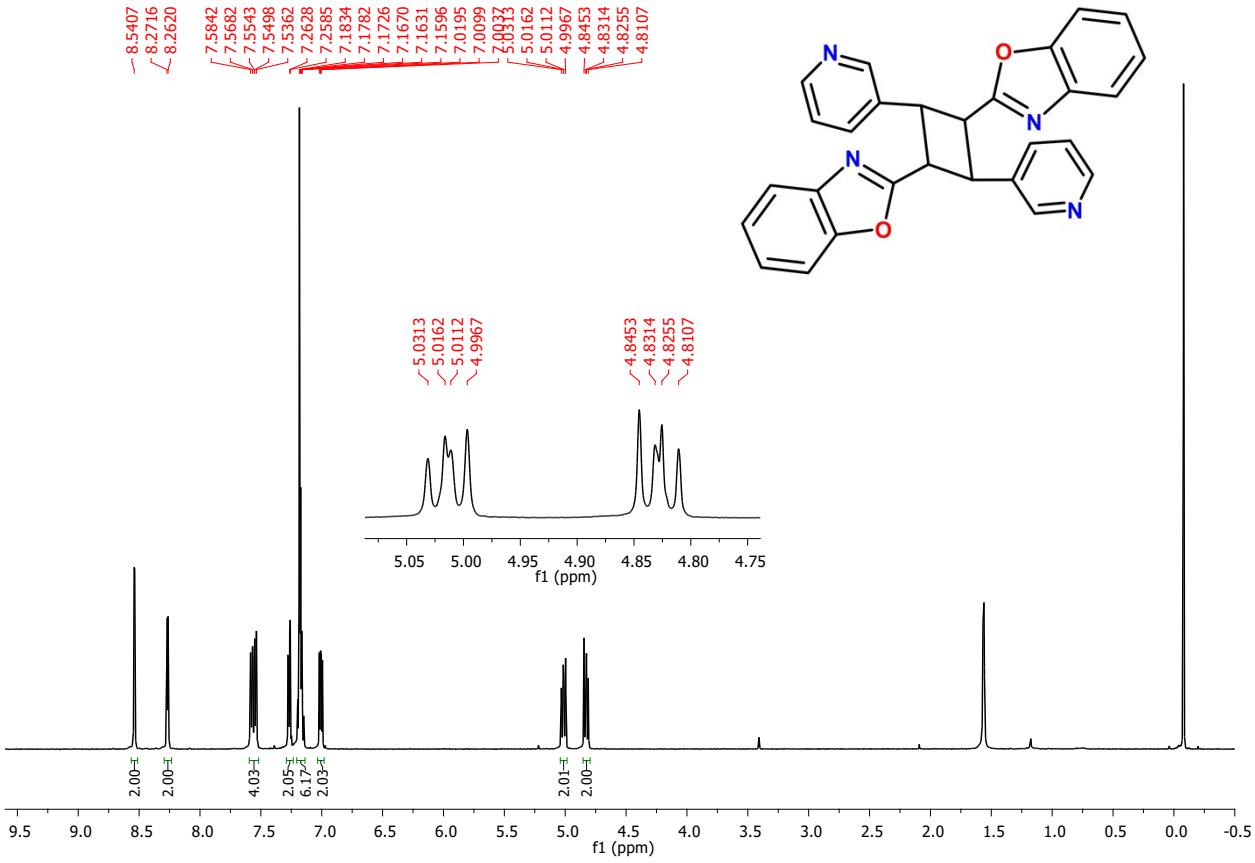


Fig. S20: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **PBOCB**.

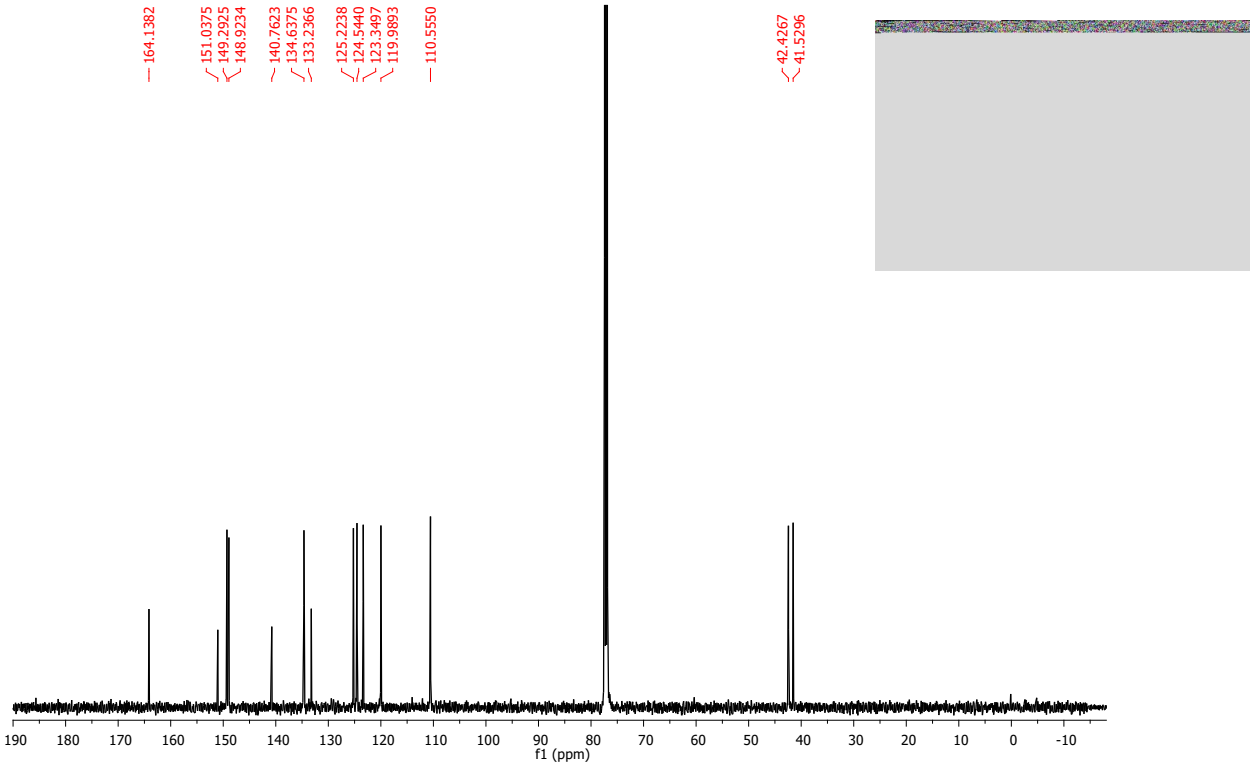


Fig. S21: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **PBOCB**.

5. Mass spectrometry

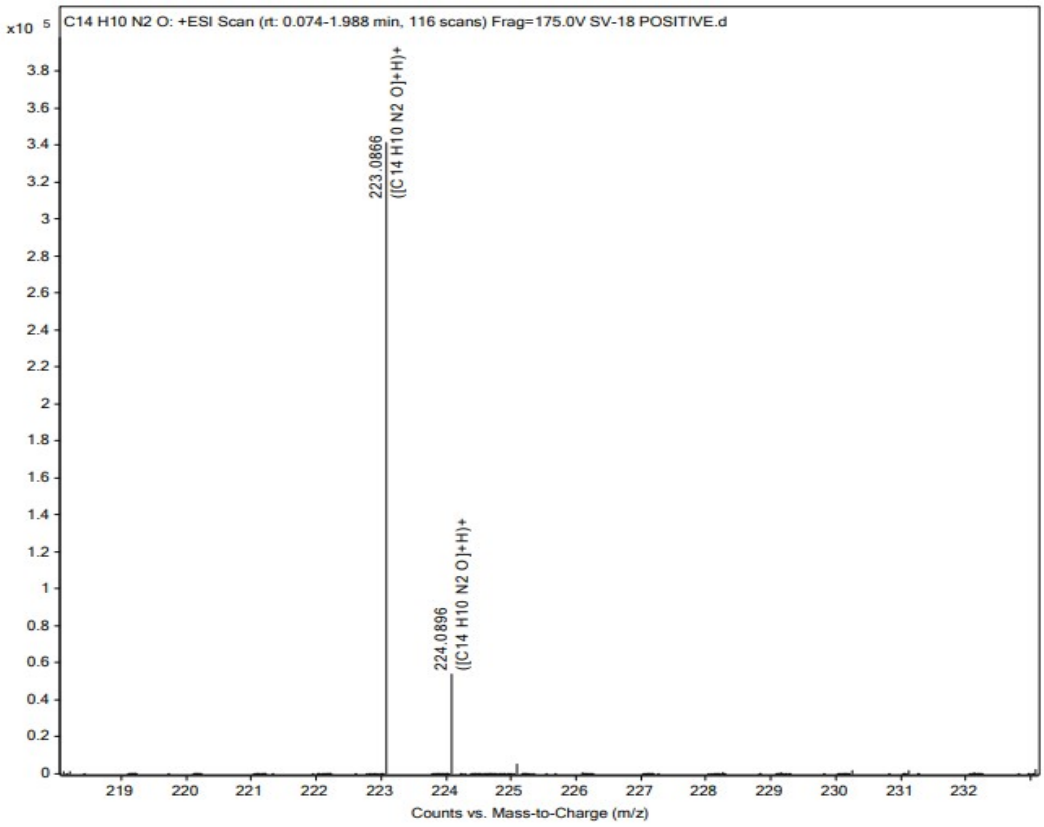


Fig. S22: HR-MS spectrum of **3-PVBO**.

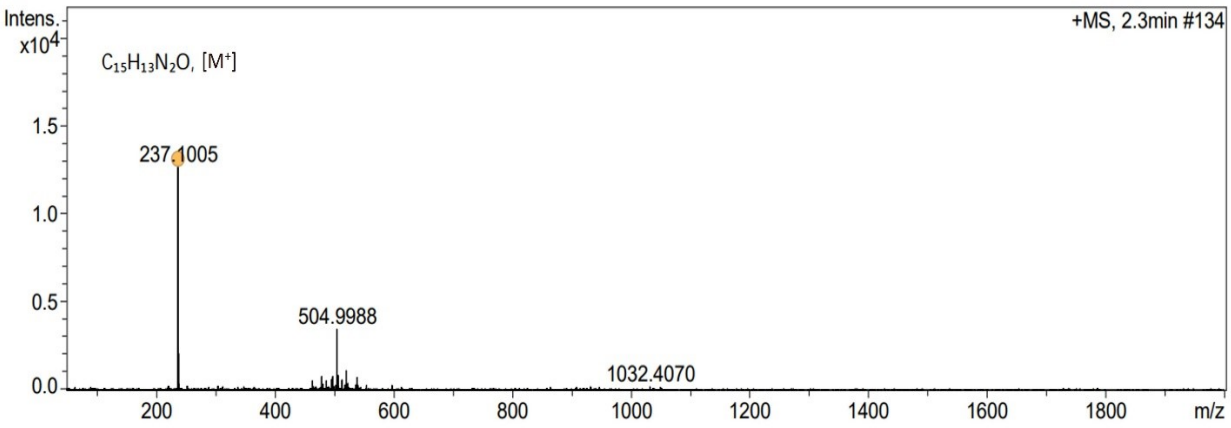


Fig. S23: HR-MS spectrum of **[3-MPVBO]I**.

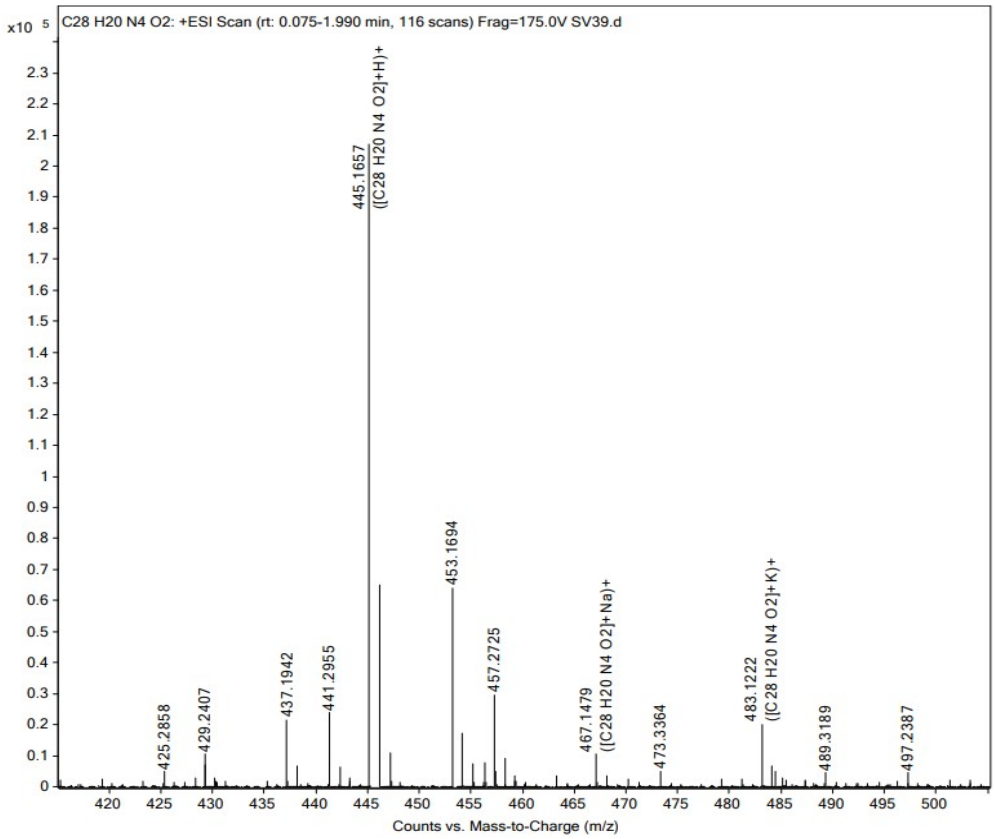


Fig. S24: HR-MS spectrum of **PBOCB**.

6. FT-IR spectroscopy

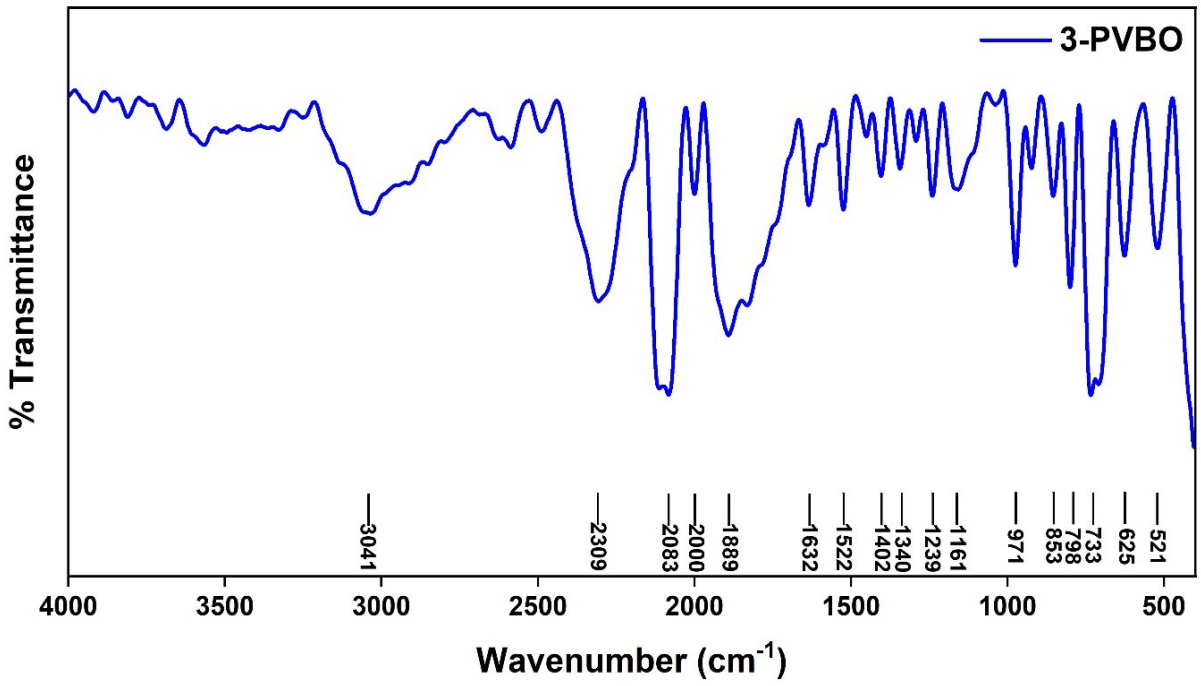


Fig. S25: FT-IR (ATR, cm^{-1}) spectrum of **3-PVBO**.

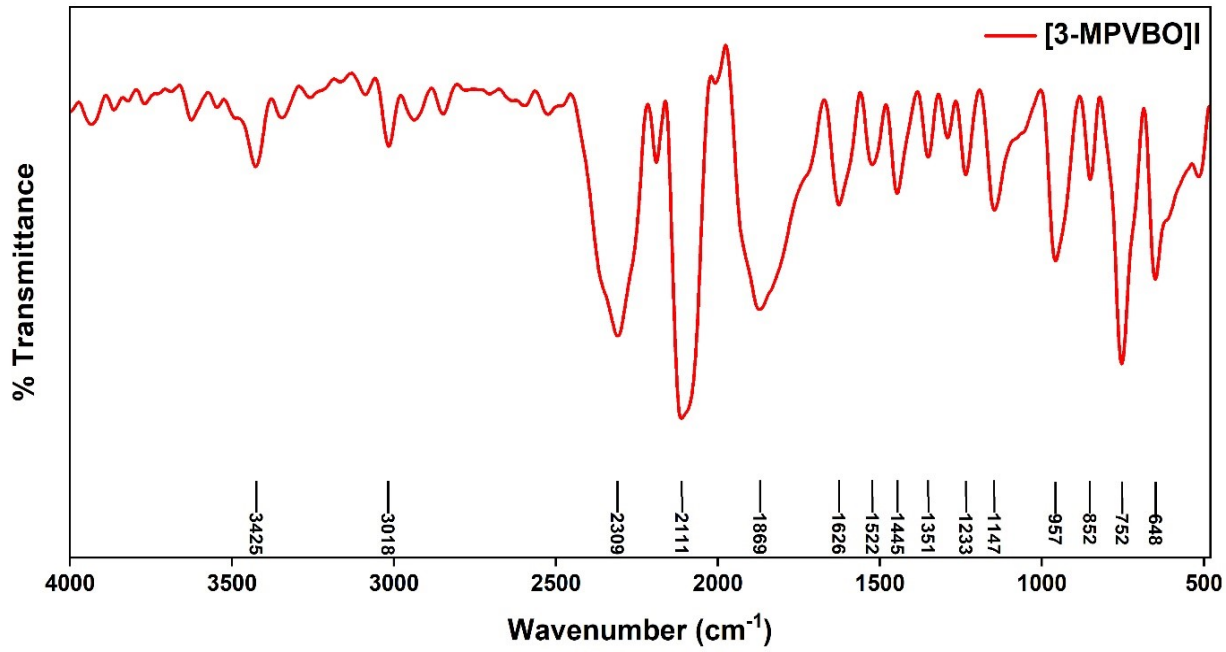


Fig. S26: FT-IR (ATR, cm^{-1}) spectrum of **[3-MPVBO]I**.

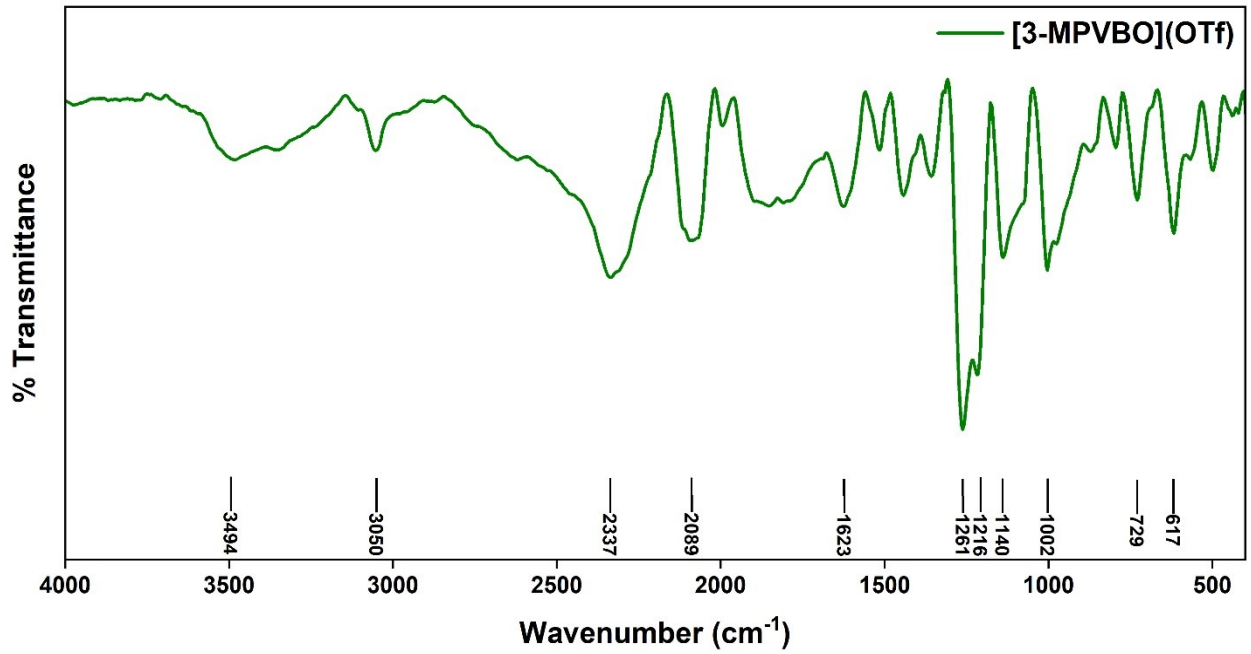


Fig. S27: FT-IR (ATR, cm^{-1}) spectrum of **[3-MPVBO](OTf)**.

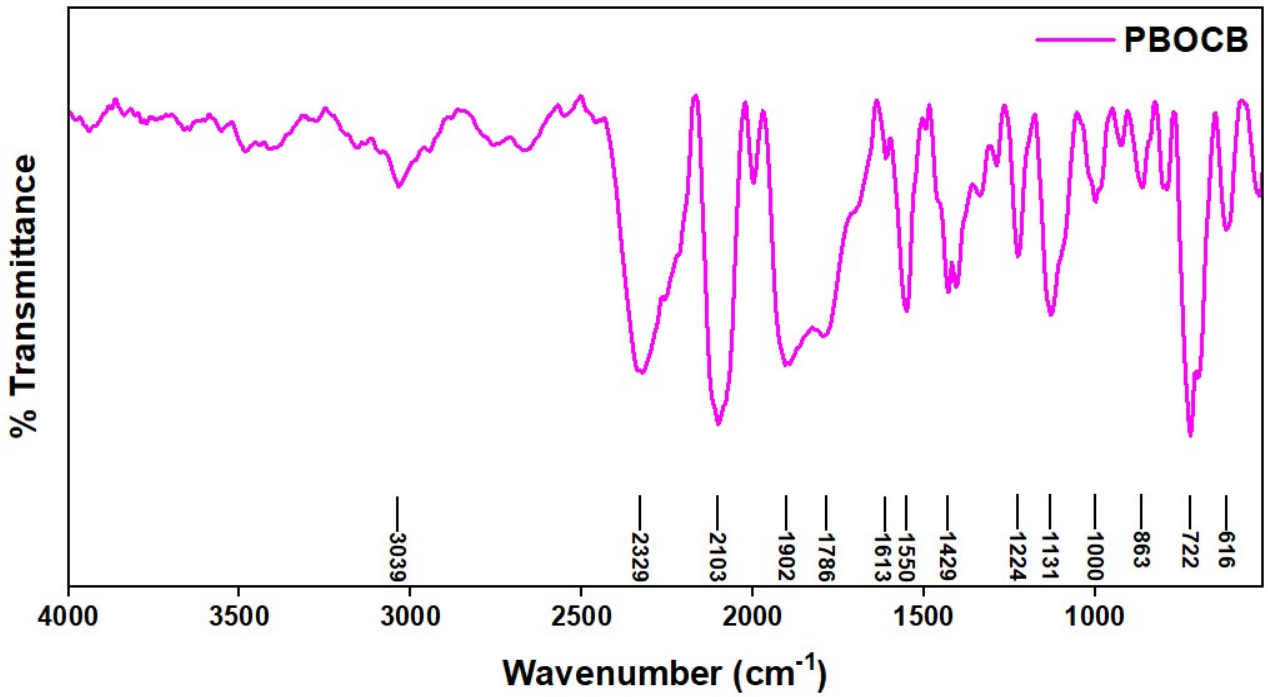


Fig. S28: FT-IR (ATR, cm^{-1}) spectrum of **PBOCB**.

7. Thermogravimetric analysis

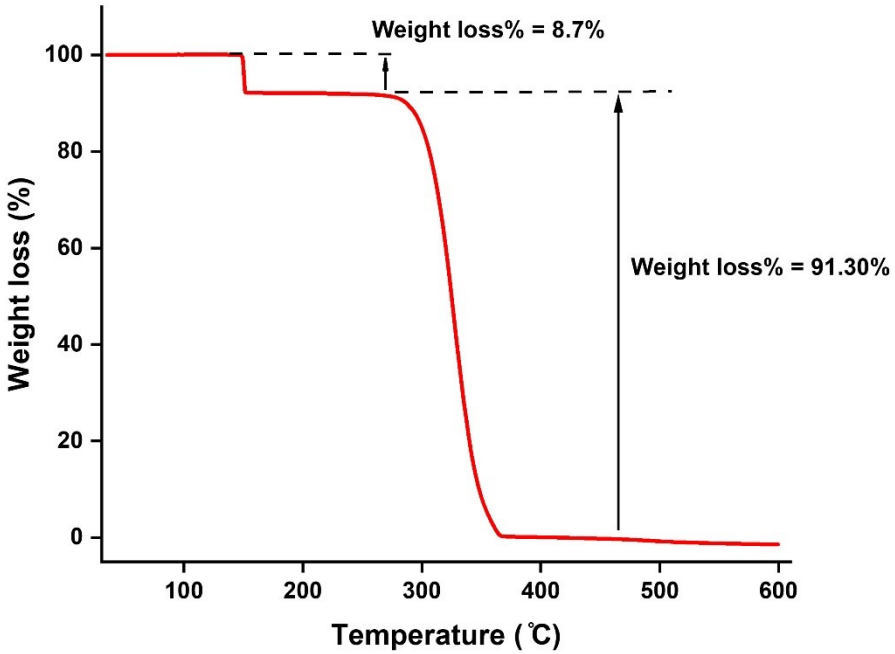


Fig. S29: Thermogravimetric analysis curve of **[3-MPVBO]I**.

8. UV-Vis absorption and emission spectra

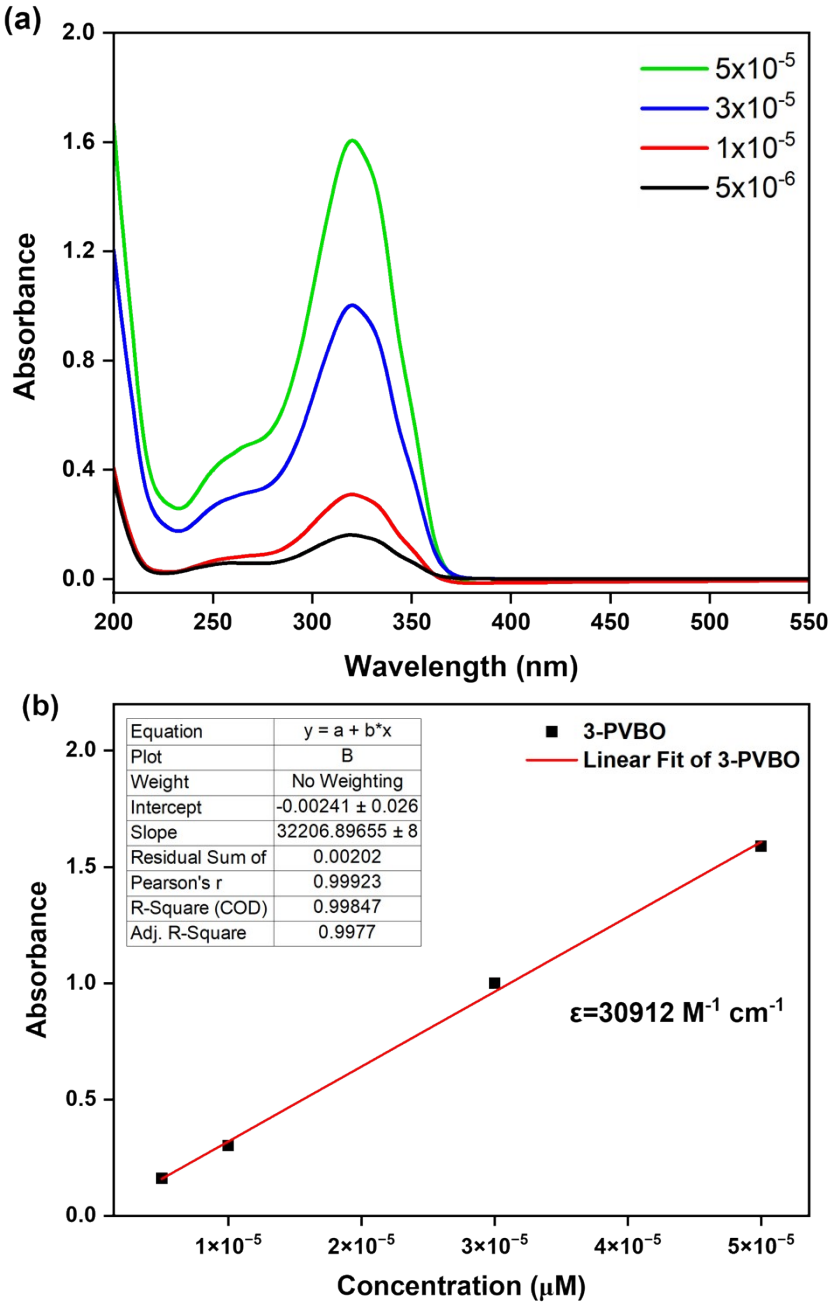


Fig. S30: (a) Absorbance of **3-PVBO** at various concentrations in MeCN; (b) calibration curve for **3-PVBO**.

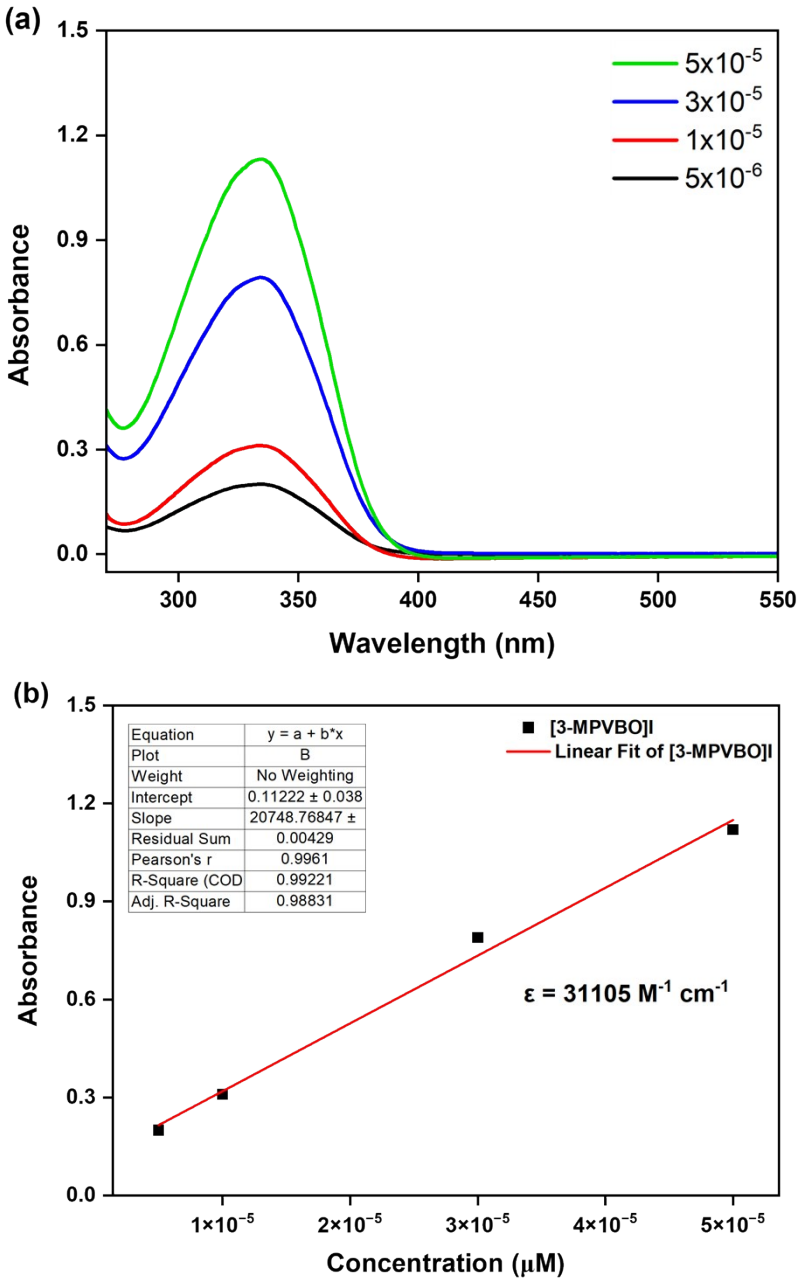


Fig. S31: (a) Absorbance of **[3-MPVBO]I** at various concentrations in MeCN; (b) calibration curve for **[3-MPVBO]I**.

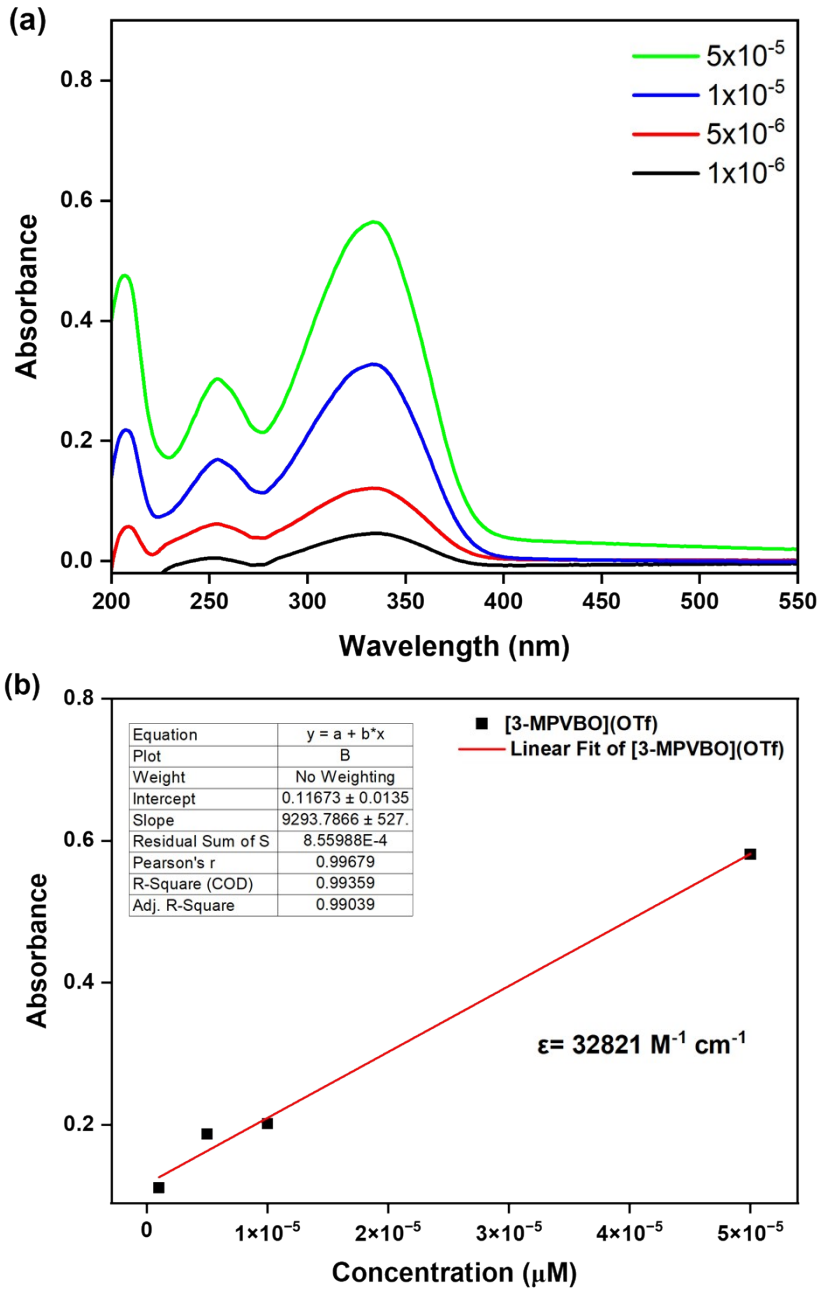


Fig. S32: (a) Absorbance of **[3-MPVBO](OTf)** at various concentrations in MeCN; (b) calibration curve for **[3-MPVBO](OTf)**.

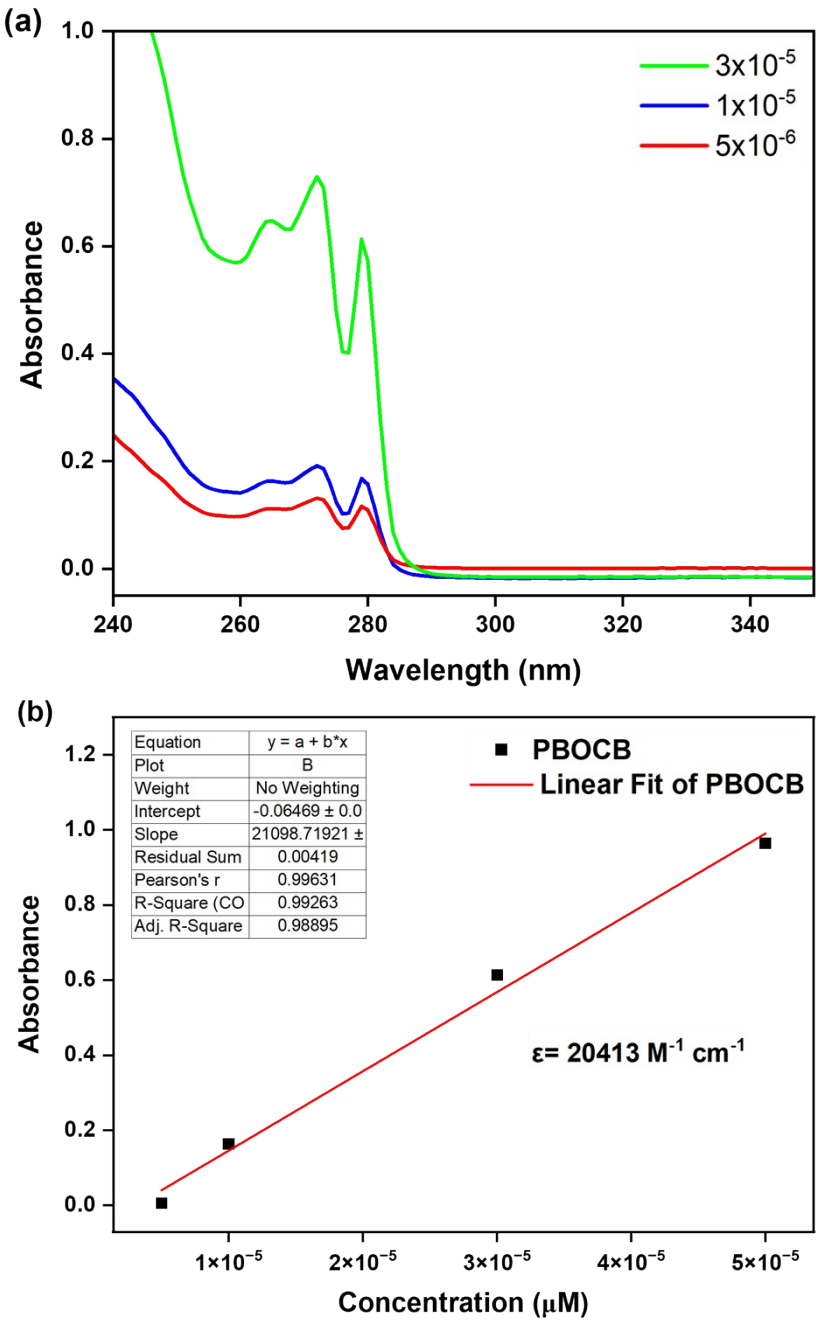


Fig. S33: (a) Absorbance of **PBOCB** at various concentrations in MeCN; (b) calibration curve for **PBOCB**.

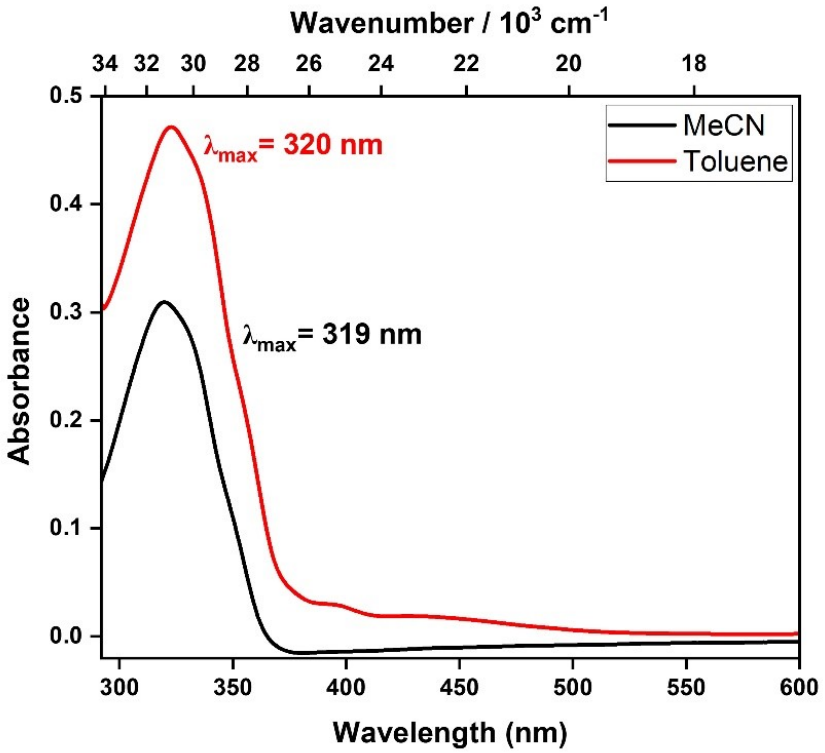


Fig. S34: Absorbance of **3-PVBO** in MeCN and toluene ($c = 1 \times 10^{-5}$ M).

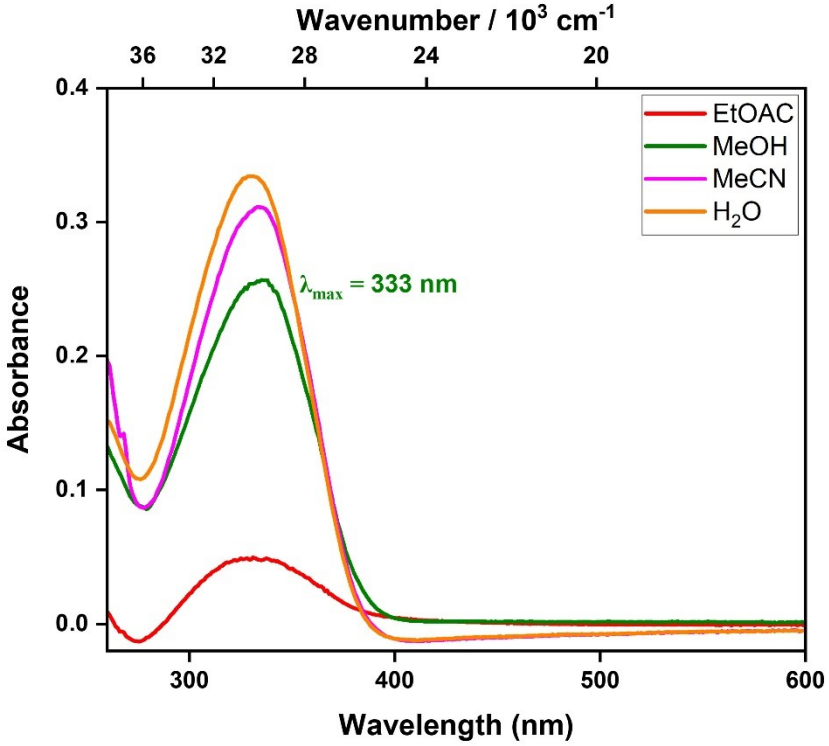


Fig. S35: Absorbance of **[3-MPVBO]I** in different solvents ($c = 1 \times 10^{-5}$ M).

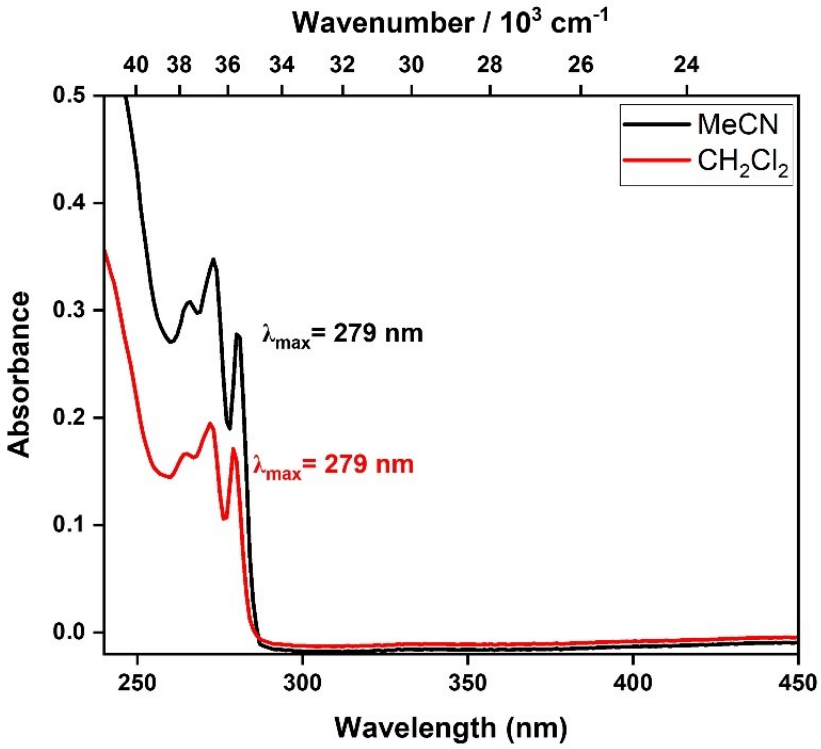


Fig. S36: Absorbance of **PBOCB** in MeCN and CH_2Cl_2 (c = 1 × 10^{-5} M).

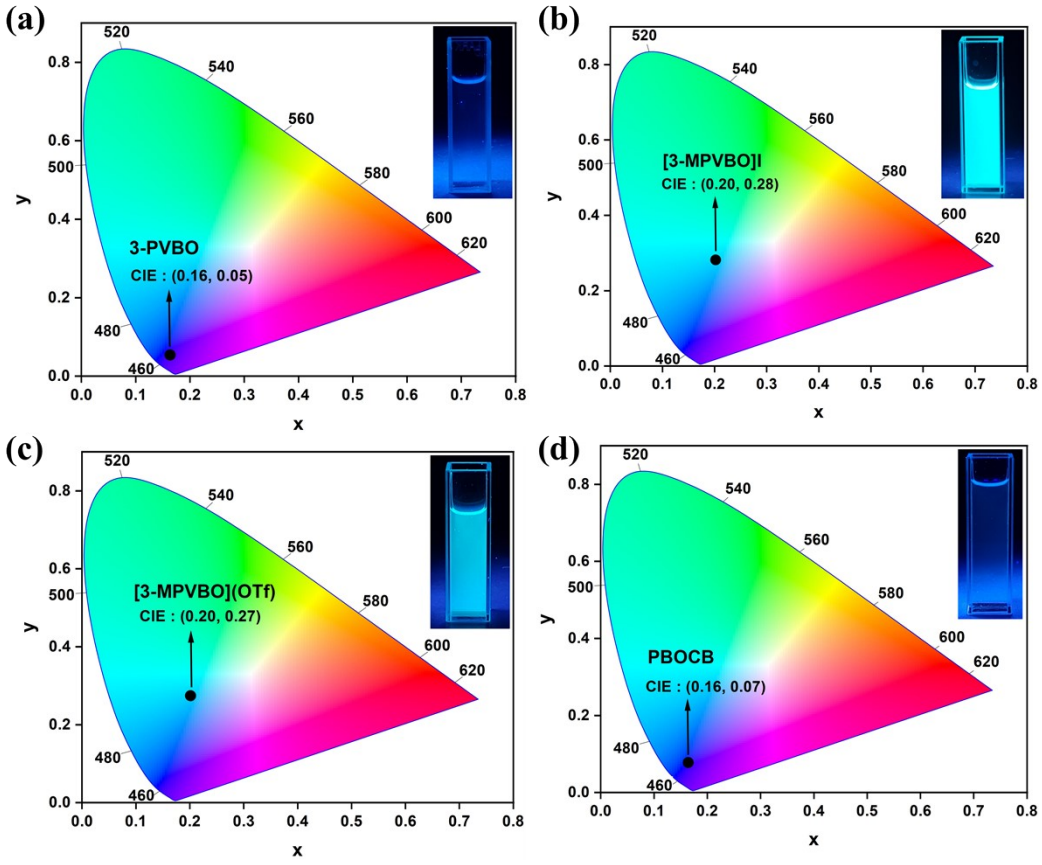


Fig. S37: CIE colour coordinates of (a) **3-PVBO**, (b) **[3-MPVBO]I**, (c) **[3-MPVBO](OTf)** and (d) **PBOCB** in MeCN (c = 1 × 10^{-5} M).

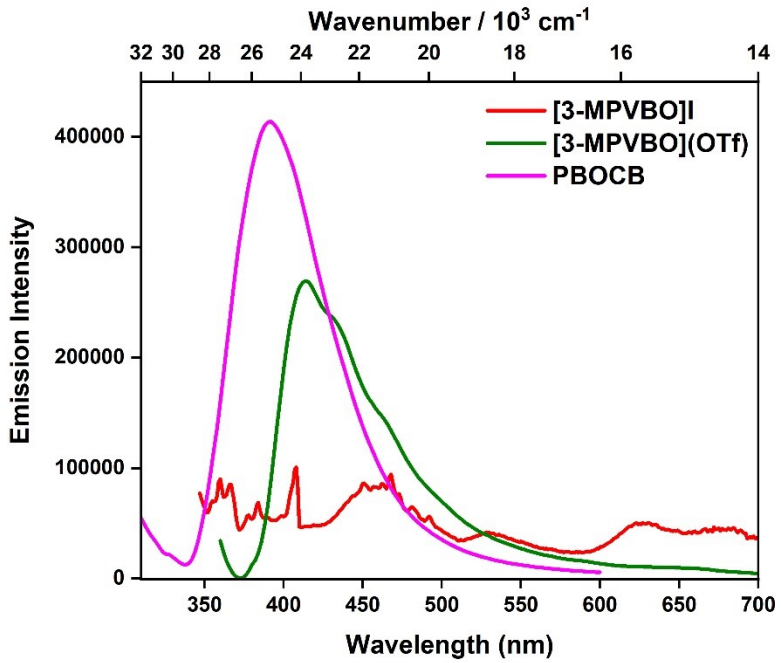


Fig. S38: Emission spectra of **[3-MPVBO]I**, **[3-MPVBO](OTf)**, **PBOCB** in the solid state.

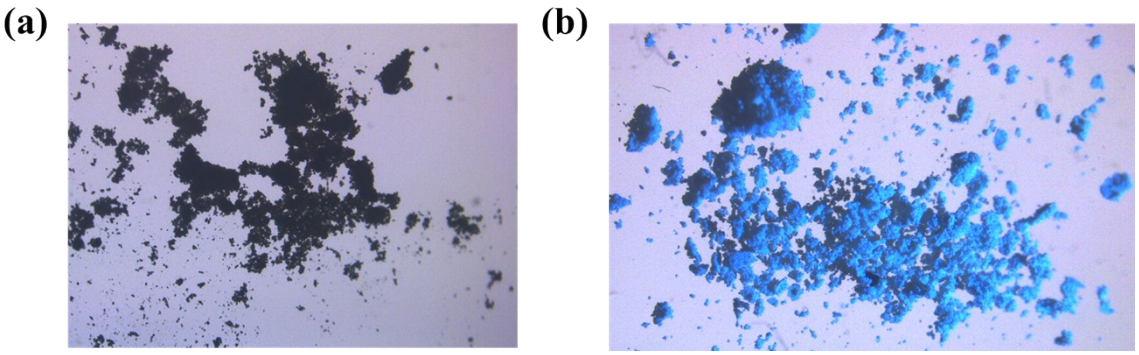


Fig. S39: Photographs of the crystalline solids of (a) **[3-MPVBO]I**, and (b) **[3-MPVBO](OTf)** exposed under UV light (λ ~ 360 nm).

9. Electrochemistry

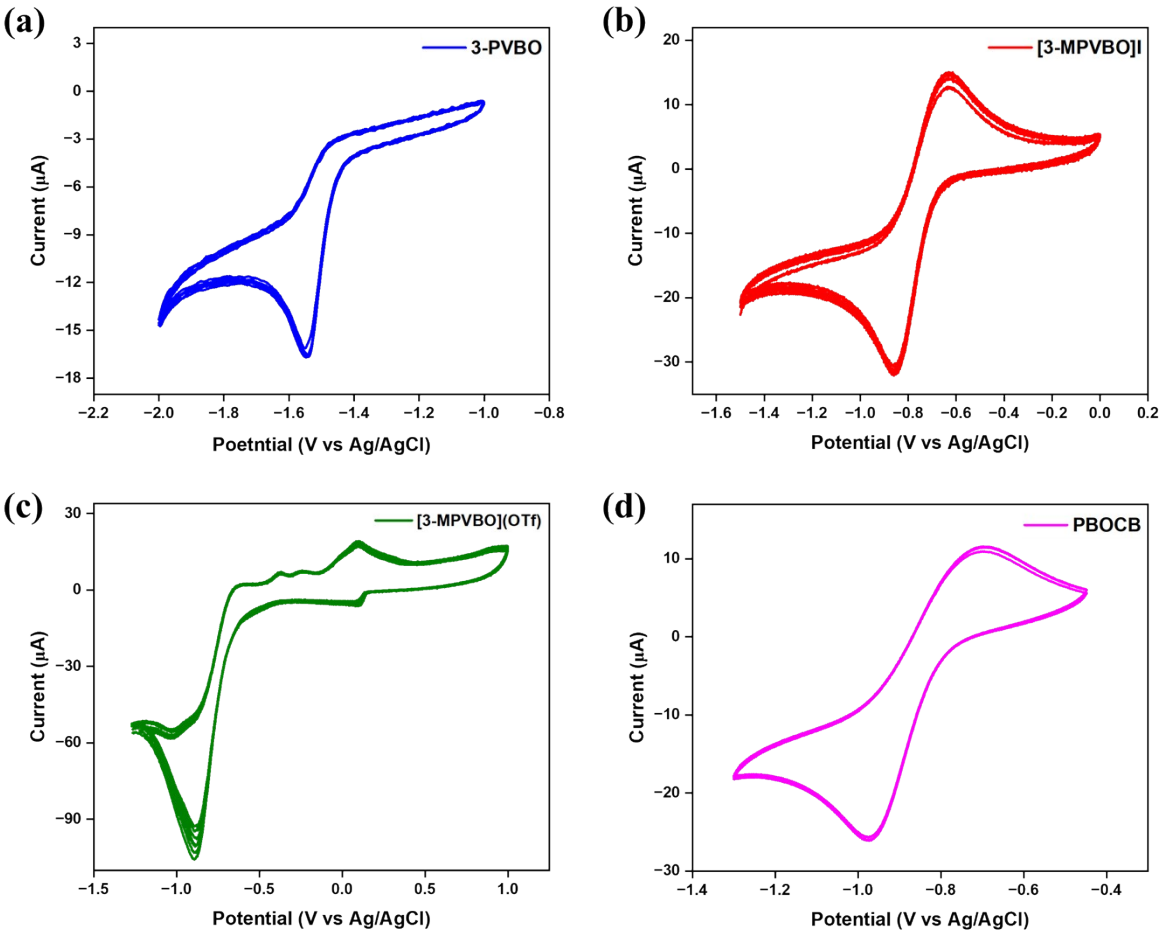
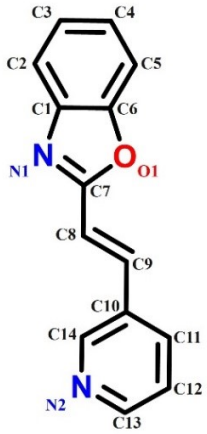


Fig. S40: Cyclic Voltammetry of (a) **3-PVBO**, (b) **[3-MPVBO]I**, (c) **[3-MPVBO](OTf)**, and (d) **PBOCB** at a scan rate of 50 mV/s.

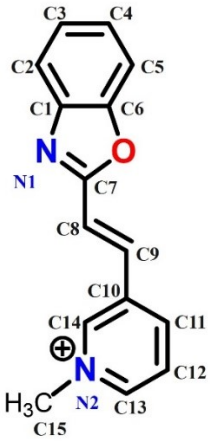
10. DFT Calculations

Table S2: Comparison of selected experimentally (crystallography) determined and theoretically optimized (B3LYP/6-31G*(d) function) structural parameters for **3-PVBO**.



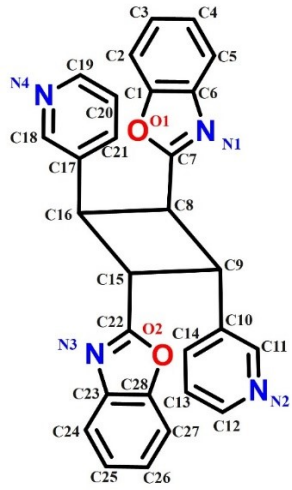
Atoms	Experimental (crystallography) bond length (Å)		Calculated (DFT) bond length (Å)
More ordered		**More disordered**	
C1-C2	1.396	1.380	1.399
C1-N1	1.396	1.396	1.389
N1-C7	1.278	1.295	1.303
O1-C7	1.377	1.380	1.384
C8-C9	1.312	1.317	1.351
C14-N2	1.329	1.290	1.335
N2-C13	1.325	1.295	1.339
C6-O1	1.376	1.402	1.371
	Experimental bond angle (°)		**Calculated bond angle (°)**
C6-O1-C7	103.64	105.59	104.27
O1-C7-C8	118.36	118.08	115.84
C1-N1-C7	105.10	103.38	104.76
N1-C7-C8	126.69	127.62	129.44
C8-C9-C10	126.07	126.40	126.83
C9-C10-C14	118.53	118.78	118.75
C9-C10-C11	124.78	124.75	124.69
C14-N2-C13	115.57	116.52	117.36

Table S3: Comparison of selected experimentally (crystallography) determined and theoretically optimized (B3LYP/6-31G*(d) function) structural parameters for **[3-MPVBO](OTf)**.



Atoms	Experimental bond length (Å)	Calculated bond length (Å)
C1-C2	1.389	1.403
C1-N1	1.398	1.383
N1-C7	1.290	1.307
O1-C7	1.370	1.376
C6-O1	1.377	1.373
C8-C9	1.310	1.355
C14-N2	1.330	1.351
N2-C13	1.343	1.354
N2-C15	1.480	1.485
	Experimental bond angle (°)	**Calculated bond angle (°)**
C6-01-C7	103.87	104.01
O1-C7-C8	118.29	119.40
C1-N1-C7	104.58	104.64
N1-C7-C8	126.57	125.48
C8-C9-C10	124.50	126.04
C9-C10-C14	121.11	123.46
C9-C10-C11	121.50	120.31
C14-N2-C13	121.24	121.55
C14-N2-C15	118.81	118.40
C13-N2-C13	119.91	120.04

Table S4: Comparison of selected experimentally (crystallography) determined and theoretically optimized (B3LYP/6-31G*(d) function) structural parameters for **PBOCB**.

	Atoms	**Experimental bond length (Å)**	**Calculated bond length (Å)**
	C1-C2	1.369	1.387
	C1-O1	1.398	1.375
	O1-C7	1.427	1.379
	C6-N1	1.396	1.397
	N1-C7	1.271	1.297
	C8-C9	1.584	1.586
	C8-C16	1.544	1.556
	C9-C15	1.544	1.585
	C15-16	1.584	1.555
	C11-N2	1.344	1.338
	N2-C12	1.331	1.339
	C22-O2	1.427	1.379
	C22-N3	1.271	1.296
	N3-C23	1.396	1.397
	C18-N4	1.344	1.339
	N4-C19	1.331	1.338
		Experimental bond angle (°)	**Calculated bond angle (°)**
	C1-O1-C7	102.68	104.30
	C6-N1-C7	103.32	104.72
	N1-C7-C8	133.86	126.88
	C8-C9-C15	89.40	86.73
	C9-C15-C16	90.60	89.56
	C16-C8-C9	90.60	89.48
	C8-C9-C10	117.42	119.81
	C9-C10-C11	119.20	124.44
	C11-N2-C12	115.05	117.77

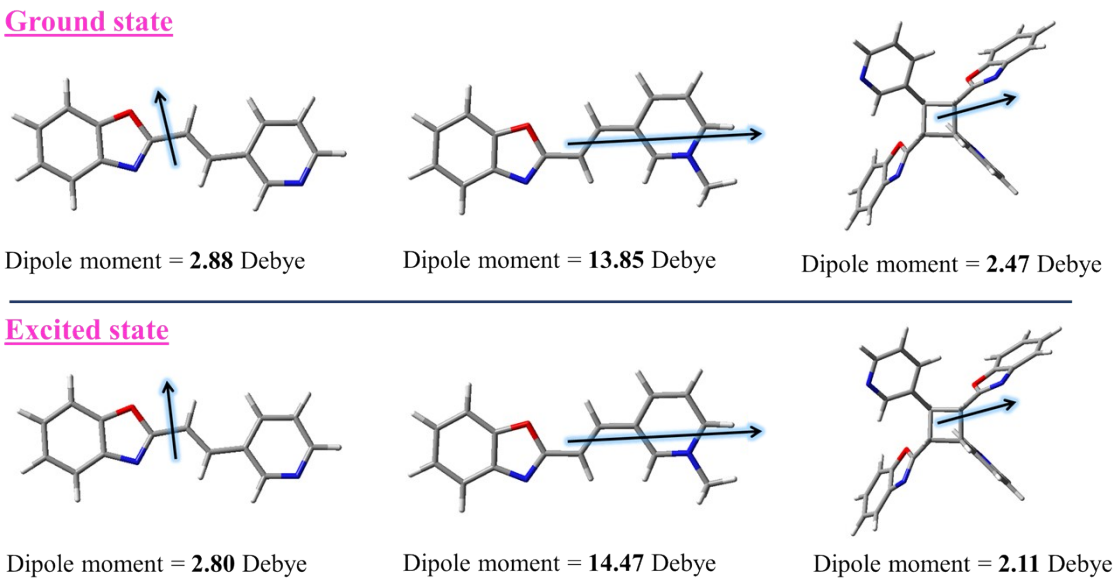


Fig. S41: Computed values and directions of dipole moment for **3-PVBO**, **3-MPVBO** and **PBOCB** in B3LYP/6-31G*(d) function.

Catalogue of Cartesian Co-ordinates ground state Optimized Geometries from B3LYP/6-31G*(d):

3-PVBO

1	6	-0.049240828	-0.019311123	0.008627157
2	6	0.041265833	-0.001713143	0.001518197
3	6	-0.031603805	-0.049139491	0.004460017
4	6	0.027107707	0.024034059	0.000001525
5	6	-0.020245028	0.024318955	-0.000556230
6	6	0.023116440	-0.031009175	0.001587131
7	6	0.036161812	0.117958466	-0.037230330
8	1	0.007849754	0.002041895	0.000078502
9	1	0.001545941	-0.009810911	-0.000920485
10	1	-0.002216151	-0.009275632	-0.000333979
11	1	-0.008323010	0.000727778	0.000356913
12	6	0.128838467	-0.023693382	0.049748062
13	1	-0.031314047	-0.000249260	-0.023448877
14	6	-0.137245250	-0.006653237	0.002393544
15	1	0.015797866	0.001100745	0.013934022
16	6	0.031240406	0.034567413	-0.008364258
17	6	-0.002157895	-0.037339856	-0.035925665
18	6	0.000298090	-0.001547019	-0.009178830
19	1	-0.001352425	-0.008246478	-0.009398057
20	6	-0.000201662	-0.000313020	-0.013111409
21	1	-0.001720319	-0.007001424	0.005082625
22	6	-0.000932819	0.017541355	0.044309797
23	1	-0.000996088	-0.000062894	0.007554355
24	1	-0.000108741	0.004141980	0.012391328
25	7	0.005188699	0.016798012	-0.008648602
26	7	-0.051826338	-0.041617560	0.000964132
27	8	0.021073391	0.003752945	-0.005890585

3-MPVBO

1	6	0.070397863	0.002906979	0.016200566
2	6	0.063218048	-0.036173913	-0.000845503

3	6	-0.069498654	0.040914336	0.002620825
4	6	0.059630664	0.026849870	0.029400958
5	6	0.011848450	-0.039656591	-0.008052393
6	6	-0.061151706	-0.008540369	-0.014422140
7	7	0.000293522	0.040499359	0.002181112
8	6	0.000404121	-0.019298911	0.002543057
9	8	-0.001882419	-0.034934404	-0.045590123
10	6	-0.047861791	0.039911640	0.028910844
11	6	0.037276652	-0.024350778	-0.014549569
12	6	-0.011809288	0.055349568	0.029378471
13	6	0.060267397	-0.000293599	-0.001521050
14	7	-0.062068165	-0.002153843	0.000368244
15	6	-0.019987525	0.077946741	0.042380769
16	6	0.021778910	-0.059795756	-0.032644550
17	6	-0.038094427	-0.049863632	-0.025908722
18	1	-0.004947697	0.010105855	0.002849407
19	1	-0.008068723	-0.006372849	-0.004704046
20	1	-0.003855438	-0.008623691	-0.005405790
21	1	-0.002704268	0.010469924	0.004745906
22	1	-0.012842308	-0.011093574	-0.005580487
23	1	0.001226668	0.010350227	0.005687889
24	1	0.009181098	-0.013444906	-0.007412493
25	1	0.009306457	-0.003158600	-0.001881325
26	1	0.012289547	0.002802958	0.001221795
27	1	-0.007778526	0.007749042	0.004354216
28	6	-0.007280293	0.003486912	0.002017770
29	1	-0.005520119	-0.012687194	0.008487475
30	1	-0.005746785	0.000194145	-0.015255788
31	1	0.013978735	0.000905053	0.000424675

PBOCB

1	6	0.046454835	0.018899065	-0.080729278
2	6	-0.058312984	0.032595345	0.080541522
3	6	0.012412155	-0.050681974	-0.034485527
4	6	0.034106255	-0.009505433	-0.061074119
5	6	-0.032492472	-0.017383843	0.056509334
6	6	-0.019050775	-0.049172796	0.033830157
7	6	0.006132432	0.029185139	-0.027494732
8	1	-0.005703853	-0.004269996	0.008965228
9	1	-0.001236983	0.010382498	0.003772807
10	1	0.001069310	0.011610105	-0.001154510
11	1	0.005479612	-0.004396073	-0.009323521
12	6	0.042933657	0.073079573	-0.057244042
13	6	-0.067917128	-0.048888831	0.100809680
14	1	-0.018414358	-0.002950712	0.015744085
15	6	-0.000706085	0.011931503	-0.023186615
16	6	-0.011355086	-0.008898883	0.012942388
17	6	0.036843044	-0.004368312	0.008794276
18	6	-0.006814653	-0.000694841	0.001054120
19	1	0.008854475	0.004231974	-0.005790900
20	1	-0.013293849	-0.002478596	0.002491031
21	6	-0.004983269	0.019693993	-0.030844742
22	1	0.012188819	-0.001732171	0.003049961
23	1	-0.002814612	-0.007297790	0.011315017
24	7	0.000333513	0.019461104	0.031755440
25	7	-0.014580935	-0.007027880	0.010996772
26	8	0.047781154	0.018234724	-0.020576901
27	1	0.016168645	-0.002121439	0.002737656
28	6	-0.000491465	0.032099073	-0.051338416
29	1	0.019295095	-0.007126462	-0.003768998
30	6	-0.041442718	-0.012957160	0.007672454
31	6	-0.004076439	-0.018834579	0.014627348

32	6	-0.016661572	0.006998148	-0.001060248
33	6	0.035068886	0.015769648	-0.032008474
34	6	-0.005031666	0.001390569	0.005151685
35	1	0.010998445	-0.006510504	-0.000135616
36	1	0.007156633	0.021382289	-0.008425055
37	6	0.013765122	-0.022584154	0.026780712
38	1	0.007494987	0.000911653	-0.010275386
39	1	-0.008729375	0.008240972	-0.006888214
40	7	-0.017077989	0.011518497	-0.001124530
41	6	-0.009784571	0.009946973	0.014786240
42	7	-0.010173316	0.004621012	-0.028509676
43	8	-0.032245179	-0.081423806	0.018761260
44	6	-0.015788622	-0.070897157	0.059458844
45	6	0.045429747	0.039670593	-0.016079667
46	6	-0.040503448	0.069274305	-0.066160885
47	6	0.046936635	-0.009566143	0.039283884
48	6	0.013858037	0.051857401	-0.041117480
49	6	0.011638384	-0.048009859	0.050751431
50	1	-0.010787663	-0.020825007	0.000925726
51	1	0.003890913	0.009112478	-0.005983839
52	1	-0.009726464	-0.000234957	-0.005402267
53	1	-0.010672589	-0.004257690	-0.001568313
54	1	0.004579331	-0.007001587	0.008242897

Catalogue of Cartesian Co-ordinates ground state Optimized Geometries from Cam-B3LYP/6-31G*(d):

3-PVBO

1	6	0.080444771	0.023270231	-0.025446147
2	6	-0.068834563	0.008561567	0.066240807
3	6	0.027141240	-0.039177739	-0.045676071
4	6	0.066847156	0.010280147	-0.037614471
5	6	-0.065416101	-0.028767011	0.020950397
6	6	-0.033630486	-0.037642373	-0.008459680
7	6	-0.001320010	-0.024230737	-0.000280194
8	1	-0.019984230	-0.008165903	0.007634954
9	1	0.002883635	0.001546213	-0.003223526
10	1	0.005709660	0.011283681	0.005205608
11	1	0.000905156	-0.002919888	-0.002139968
12	6	0.034345128	0.030529993	0.045985512
13	1	-0.016857994	-0.002007757	0.006419761
14	6	-0.030230567	-0.022627402	-0.036821812
15	1	0.014469276	0.006992470	-0.000308789
16	6	0.013485267	0.024586575	0.021898258
17	6	0.069743001	-0.064876801	-0.054858039
18	6	-0.016274740	-0.007686510	-0.002204541
19	1	-0.002223511	-0.015716025	0.011346000
20	6	-0.047606505	0.009147365	0.019752965
21	1	-0.015373277	-0.000266205	-0.001206792
22	6	0.028852991	-0.008435343	0.104056663
23	1	0.010795022	0.003896156	-0.013556215
24	1	-0.002838759	-0.019727656	0.010607192
25	7	-0.028697876	0.090792436	-0.066760143
26	7	-0.024112819	0.030798253	0.013024887
27	8	0.017779133	0.030562262	-0.034566617

3-MPVBO

1	6	0.004881412	0.001936761	0.000081635
2	6	0.004529160	-0.001698295	-0.000034517
3	6	0.001120324	-0.005553159	0.000011200
4	6	-0.003699284	-0.006743098	-0.000012720
5	6	0.000170296	0.005934727	-0.000023560
6	6	-0.002908536	0.004888238	-0.000029213
7	7	0.008751988	-0.010524870	0.000012938
8	6	-0.016055723	0.001872788	0.000033994
9	8	0.000063097	0.008864816	0.000012478
10	6	0.011465009	-0.007964175	-0.000042921
11	6	-0.010309403	0.007886953	-0.000010695
12	6	0.010457856	0.001290612	0.000003823
13	6	0.001338779	-0.006495158	0.000002562
14	7	0.000036054	-0.003438599	0.000007891
15	6	-0.007756171	0.000701791	0.000005062
16	6	-0.000429080	0.004971605	-0.000004107
17	6	-0.000271078	0.006428748	-0.000001345
18	1	0.000567605	0.000441600	-0.000015445
19	1	0.000653216	-0.000256285	-0.000009690
20	1	0.000082350	-0.000628273	0.000005774
21	1	-0.000020002	0.000671277	-0.000003241
22	1	-0.000130881	-0.000517366	0.000010298
23	1	-0.000153718	0.000589262	0.000006752
24	1	0.000056946	-0.000247240	-0.000000277
25	1	-0.000291953	0.000013050	-0.000000042
26	1	-0.000353185	0.000478623	0.000000148
27	1	0.000164430	0.000478840	0.000000173
28	6	-0.001681819	-0.002058855	0.000010763
29	1	0.000207934	-0.000631501	0.000593282
30	1	0.000191269	-0.000625632	-0.000614138
31	1	-0.000676894	-0.000067186	0.000003135

PBOCB

1	6	-0.000684798	-0.001126448	-0.004839231
2	6	0.001075436	0.000703213	0.003625371
3	6	0.003890618	-0.000060950	0.003568695
4	6	-0.003370077	0.001819248	0.003405846
5	6	-0.004445228	0.001418045	0.000950392
6	6	-0.002480720	-0.000626601	-0.004542070
7	6	0.007321964	-0.003146305	-0.002525952
8	1	0.000316478	0.000107211	0.000677542
9	1	-0.000326412	0.000274948	0.000664791
10	1	-0.000774157	0.000208348	0.000015546
11	1	-0.000443758	-0.000045427	-0.000601563
12	6	-0.004953312	-0.000997084	-0.000045346
13	6	0.000056144	-0.001868187	0.002327156
14	1	-0.000027777	0.000211939	0.000655188
15	6	-0.000058237	0.004070420	-0.000144035
16	6	-0.004822274	0.001739185	0.000128342
17	6	0.004349457	0.002300957	-0.000449694
18	6	-0.004215399	-0.002687141	0.000513689
19	1	-0.000479216	0.000112762	0.000026996
20	1	0.000590347	0.000215883	-0.000047978
21	6	-0.000589895	-0.005098629	0.000639332
22	1	-0.000829457	-0.000432003	0.000077470
23	1	-0.000008295	-0.000969504	0.000113551
24	7	-0.007705790	0.000233982	-0.006360839
25	7	0.006150371	-0.003250250	0.000025484

26	8	0.004437760	0.000619388	0.006789486
27	1	-0.000114918	-0.000337070	-0.000818462
28	6	0.000070231	0.003975851	-0.003348621
29	1	-0.000017242	-0.000103483	-0.001022098
30	6	0.004751770	-0.001077061	0.000003392
31	6	0.000029981	-0.004242023	-0.001341511
32	6	-0.000097538	-0.000184583	-0.005064742
33	6	0.000103193	-0.003337076	0.003403865
34	6	-0.000098681	0.003644970	-0.003451174
35	1	-0.000014499	-0.000115265	-0.000753851
36	1	0.000003387	-0.000130925	0.000381266
37	6	-0.000028944	0.005097572	0.001073360
38	1	-0.000018942	0.000654356	-0.000677816
39	1	-0.000002909	0.000936049	0.000266245
40	7	0.000126601	0.001434180	0.006674731
41	6	-0.007236028	-0.003233304	-0.002468243
42	7	0.007523033	0.000840454	-0.006501216
43	8	-0.004277528	0.000044808	0.006901744
44	6	0.000601851	-0.000808689	-0.004910696
45	6	0.002388159	-0.000267472	-0.004627156
46	6	-0.001014002	0.000441468	0.003696899
47	6	-0.003788915	-0.000406474	0.003648880
48	6	0.004416877	0.001508648	0.000923183
49	6	0.003389076	0.001726359	0.003431177
50	1	0.000106289	-0.000328124	-0.000832707
51	1	-0.000305658	0.000054731	0.000694173
52	1	0.000334653	0.000244785	0.000674899
53	1	0.000768267	0.000233964	0.000010438
54	1	0.000428660	0.000006355	-0.000614126