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## Supporting Information

## for

## AIE-active Boron Complexes Based on Benzothiazole-hydrazone Chelates

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**Figure S1**. Absorption spectra of **6a** (a), **6b** (b), **7a** (c) and **7b** (d) in various solvents such as hexane, toluene, dichloromethane (DCM), tetrahydrofuran (THF), acetonitrile (ACN), dimethylformamide (DMF), ethanol, ethylene glycol (glycol) and glycerol, respectively.



**Figure S2**.Changes in the  $F_{max}$  of **6a** (a), **6b** (b), **7a** (c) and **7b** (d) in THF/water mixtures (10  $\mu$ M) with varied volumetric fractions of water ( $f_w$ ).



Figure S3. Crystal packing structures of 6a (a), 6b (b), 7a (c) and 7b (d). The blue dotted lines show intermolecular interactions within 6-7.



Figure S4. Calculated absorption spectra of 6a, 6b, 7a and 7b.

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Compound	State	λ [nm]	f	HOMO	LUMO	$E_{\rm g}({\rm eV})$	
				(eV)	(eV)		
6a	$S_1$	411	0.6862	-6.16	-2.75	3.41	
6b	$\mathbf{S}_1$	465	0.1922				
	$S_2$	355	0.4950	-6.61	-2.72	3.89	
7a	$\mathbf{S}_1$	405	0.8369	-6.19	-2.76	3.43	
	$S_5$	300	0.2615				
7b	$S_2$	354	0.4844	-6.61	-2.71	3.90	
	$S_8$	278	0.1551				

Table S1. HOMO, LUMO and energy gaps of compounds 6-7.













S9









Meas. m/z # Formula Score m/z err [mDa] err [ppm] mSigma rdb e Conf N-Rule

## $\begin{array}{c} -8 & 20 \\ 8 & 18 \\ 7 & 97 \\ 7 & 97 \\ 7 & 92 \\ 7 & 92 \\ 7 & 92 \\ 7 & 92 \\ 7 & 92 \\ 7 & 92 \\ 7 & 7 \\ 7 & 92 \\ 7 & 7 \\ 7 & 52 \\ 7 & 7 \\ 7$



--0.28 --0.07 ---0.14



Z-matrix and total energy of 6a, 6b, 7a and 7b. Compound 6a

Symbolic Z-matrix: Charge = 0 Multiplicity = 1 S -2.76431 1.74164 -0.02261

В		0.37753	-0.87241	0.28659
F		0.4038	-1.40842	1.56582
F		0.54922	-1.84685	-0.67635
Ν		-1.0008	-0.15039	0.06421
Ν		1.27842	1.52775	0.1389
Ν		1.48349	0.24262	0.13775
Ν		-0.25377	4.58167	0.23351
С		-3.31784	0.07344	-0.1326
С		-4.62668	-0.39295	-0.26154
Н		-5.46435	0.29474	-0.3046
С		-4.82097	-1.76963	-0.33575
Н		-5.8289	-2.15962	-0.43644
С		-3.73281	-2.65753	-0.28723
Н		-3.9119	-3.72596	-0.35405
С		-2.42771	-2.19583	-0.16092
Н		-1.5858	-2.87622	-0.14026
С		-2.22604	-0.81263	-0.0764
С		-1.12081	1.17604	0.09572
С		0.03526	2.0075	0.16489
С		-0.10331	3.42739	0.20126
С		2.85471	-0.1439	-0.01533
С		3.72635	0.64578	-0.77663
Н		3.35381	1.54547	-1.25305
С		5.05741	0.26111	-0.9203
Н		5.72856	0.87448	-1.5146
С		5.52372	-0.91109	-0.31881
Н		6.5607	-1.2109	-0.4387
С		4.64832	-1.69593	0.43486
Н		5.00339	-2.60424	0.913
С		3.31554	-1.31889	0.59352
Н		2.64635	-1.91332	1.20307
Compound	6b			
Symbolic Z-	-matrix:			
Charge =	0 Multiplicity	= 1		
S		3.29211	1.81016	-0.1082
F		0.13693	-1.9507	0.52821
F		0 61103	-1 72006	-1 70149

5	J.2J211	1.01010	-0.1062
F	0.13693	-1.9507	0.52821
F	0.61103	-1.72006	-1.70149
Ν	1.67835	-0.21234	-0.15342
Ν	-0.77552	-0.02944	-0.63478
Ν	-0.65114	1.25056	-0.83927
Ν	0.72028	4.35619	-1.25173
В	0.40023	-1.06478	-0.49622
С	3.9105	0.23347	0.37306
С	5.20198	-0.09528	0.7872

Н	5.98014	0.65822	0.84596
С	5.45744	-1.42171	1.12444
Н	6.45336	-1.70499	1.45021
С	4.44538	-2.39417	1.0539
Н	4.66998	-3.41977	1.32925
С	3.15757	-2.06946	0.64364
Н	2.37089	-2.81206	0.60418
С	2.89596	-0.73878	0.29394
С	1.72851	1.0972	-0.39329
С	0.55613	1.81349	-0.78068
С	-2.12982	-0.51774	-0.63423
С	-2.45754	-1.52604	-1.51857
Н	-1.69947	-1.90763	-2.19215
С	-3.7714	-2.04243	-1.5599
Н	-4.01063	-2.82716	-2.27115
С	-4.7382	-1.54363	-0.71819
Н	-5.75302	-1.93136	-0.75158
С	-4.43007	-0.52007	0.21743
С	-3.09684	0.01078	0.28087
С	-2.80734	0.99816	1.26265
Н	-1.80429	1.39931	1.34117
С	-3.78679	1.45214	2.11828
Н	-3.54271	2.20437	2.86306
С	-5.10706	0.94815	2.03838
Н	-5.86963	1.3213	2.71604
С	-5.4169	-0.01824	1.10967
Н	-6.42449	-0.42146	1.04688
С	0.62506	3.21494	-1.04121
Compound 7a			
Symbolic Z-matrix:			

0 Multiplicity = $1$		
1.32294	1.9883	0.15535
3.22787	-2.41777	-0.98919
2.77543	-2.3881	1.256
-3.24835	-2.26551	1.08856
-3.43823	-2.04626	-1.18079
2.30716	-0.39774	-0.02793
-1.25934	-2.46178	-0.24126
-1.21153	-3.46819	-0.38399
-2.38031	-0.23269	0.04161
-1.21075	0.32032	0.07917
1.00734	-2.51907	-0.28097
2.37907	-1.98543	0.00151
-2.64616	-1.80025	-0.07529
	0 Multiplicity = 1 1.32294 3.22787 2.77543 -3.24835 -3.43823 2.30716 -1.25934 -1.21153 -2.38031 -1.21075 1.00734 2.37907 -2.64616	0 Multiplicity = 1 1.32294 1.9883 3.22787 -2.41777 2.77543 -2.3881 -3.24835 -2.26551 -3.43823 -2.04626 2.30716 -0.39774 -1.25934 -2.46178 -1.21153 -3.46819 -2.38031 -0.23269 -1.21075 0.32032 1.00734 -2.51907 2.37907 -1.98543 -2.64616 -1.80025

С	4.76686	0.05885	-0.09139
Н	5.03201	-0.98574	-0.19566
С	5.73618	1.05535	-0.04866
Н	6.78383	0.77758	-0.10821
С	5.38534	2.41091	0.06321
Н	6.16347	3.16719	0.09253
С	4.0501	2.80238	0.13253
Н	3.77711	3.84926	0.21361
С	3.0758	1.80481	0.09347
С	3.42415	0.44572	-0.01062
С	1.15347	0.25991	0.04373
С	-0.10344	-0.41745	0.01446
С	-0.10147	-1.85018	-0.1632
С	-3.48112	0.68439	0.01853
С	-4.70973	0.30221	0.57398
Н	-4.81475	-0.67018	1.03745
С	-5.78098	1.19411	0.54682
Н	-6.72985	0.89659	0.98357
С	-5.63763	2.46009	-0.02434
Н	-6.47666	3.1495	-0.04284
С	-4.40947	2.83366	-0.57755
Н	-4.29122	3.81208	-1.03424
С	-3.33253	1.95097	-0.56344
Н	-2.38377	2.22766	-1.00867
Compound 7b			
Symbolic Z-matrix:			
Charge = 0 Multiplicity	= 1		
S	-1.53674	-1.76188	-0.825
F	-4.12923	2.34493	0.09046
F	-3.30879	1.52834	2.06774
F	2.17438	3.16878	-1.26343
F	2.70752	2.8003	0.9304
Ν	-2.82576	0.30655	0.04324
Ν	0.37926	2.89425	0.31641
Н	0.18793	3.84598	0.62187
Ν	1.80062	0.94255	-0.34255
Ν	0.73948	0.20253	-0.38565
0	-1.85166	2.55593	0.54258
В	-3.0825	1.7202	0.72423
В	1.82206	2.51123	-0.08962
С	-3.28689	-1.87796	-0.6432
С	-4.11163	-2.97085	-0.91081
Н	-3.70073	-3.90653	-1.27503
С	-5.48009	-2.82078	-0.6979

Н	-6.14423	-3.6557	-0.89843
С	-6.01038	-1.60562	-0.2338
Н	-7.08128	-1.51306	-0.08254
С	-5.19117	-0.51334	0.03114
Н	-5.5983	0.42984	0.37344
С	-3.81402	-0.66184	-0.17129
С	-1.60218	-0.11962	-0.25501
С	-0.45874	0.72845	-0.13221
С	-0.66637	2.10392	0.25663
С	3.0419	0.24648	-0.55815
С	3.87097	0.69513	-1.56696
Н	3.56664	1.54517	-2.16485
С	5.09421	0.04021	-1.83017
Н	5.72497	0.40023	-2.63728
С	5.47258	-1.04922	-1.08071
Н	6.4093	-1.56125	-1.28486
С	4.6558	-1.51993	-0.01806
С	3.41199	-0.86216	0.27101
С	2.64597	-1.32086	1.3782
Н	1.71756	-0.82453	1.63355
С	3.07251	-2.38655	2.13982
Н	2.47431	-2.71601	2.98469
С	4.28291	-3.05423	1.83588
Н	4.6019	-3.89741	2.44193
С	5.05602	-2.62511	0.78211
Н	5.99508	-3.12031	0.54817