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Rational design of organoboron heteroarene derivatives as luminescent and charge transport materials for organic light-emitting diodes

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Table S1 The calculated total energies of the compounds under investigation in different space groups.

Space groups	**1a**	**1b**	**1c**	**1d**	**2a**	**2b**	**2c**	2d
C2	95.66051472	116.9983839	128.8217775	138.2400842	101.8331040	133.9608482	149.3996535	103.2337225
		3	2	5	7	6	7	9
C2/c	103.7561810	120.5923107	132.5515364	138.9258335	95.46939511	135.3544498	147.6496528	109.4781795
	3	0	9	2		9	1	6
Cc	96.15214464	118.0373413	132.0090549	131.8166024	94.08141538	134.2814809	148.1600322	104.5028136
		4	0	0		1	1	0
$P2_1$	98.08297935	116.9255814	124.4582684	135.8100776	96.16346672	129.3756082	148.4334685	100.8740793
		8	6	3		7	2	1
$P2_1/c$	99.11753329	124.5224884	129.2447034	140.0392959	102.6304258	134.4401830	151.1377558	103.4832714
		4	0	0	0	6	9	3
$P2_12_12_1$	97.30101171	119.3371527	130.0478584	130.6612599	95.29268896	133.0813255	149.1507421	103.4205879
		9	6	2		0	5	8
$P\bar{1}$	92.70361903	119.2886535	129.1663201	138.9254990	95.78282161	134.6923374	147.3417531	109.6988072
		5	8	5		3	4	6
Pbca	100.5684337	122.9088167	133.5082367	139.1814249	105.8022419	132.6362013	147.1060899	95.46072459
	9	4	4	4	0	1	1	
Pbcn	102.8838496	124.3606208	128.5318619	147.7618202	97.50136797	138.4997464	148.1978459	109.3856478
	1	7	9	3		3	3	2
$Pna2_1$	96.05303336	121.8149678	130.5619881	136.8646066	95.96388915	136.5622693	144.0890066	97.96619460
		8	0	4		1	0	

Table S2 The calculated crystal cell parameters of the compounds under investigation with the lowest total energies.

Species	space groups	a	b	c	□α	□β	□γ
1a	$P\bar{1}$	9.954	11.483	10.665	99.5	104.6	117.8
1b	$P2_1$	10.213	13.321	9.304	90.0	103.8	90.0
1c	$P2_1$	8.922	9.610	14.601	90.0	112.2	90.0
1d	$P2_12_12_1$	12.074	13.900	15.048	90.0	90.0	90.0
2a	*Cc*	22.027	9.721	9.428	90.0	96.6	90.0
2b	*Pbca*	29.388	15.488	11.710	90.0	90.0	90.0
2c	$Pna2_1$	24.278	9.273	10.011	90.0	90.0	90.0
2d	*Pbca*	17.153	16.703	17.298	90.0	90.0	90.0

Table S3 Center−center distance and the corresponding hole and electron coupling between the dimer in all of the nearest neighbor pathways for **1d** and **2d** in different space groups.

Species	Space groups	Pathway	Distance (Å)	Electron coupling (eV)	Hole coupling (eV)
1d	*Cc*	1	8.367	1.50×10^{-3}	1.47×10^{-4}
		2	8.367	1.50×10^{-3}	1.47×10^{-4}
		3	10.99	-1.45×10^{-14}	5.27×10^{-17}
		4	10.99	-1.45×10^{-14}	5.27×10^{-17}
		5	8.523	1.28×10^{-4}	8.63×10^{-6}
		6	8.523	1.28×10^{-4}	8.63×10^{-6}
		7	15.544	2.34×10^{-24}	3.47×10^{-25}
		8	9.611	9.54×10^{-4}	1.18×10^{-5}
		9	13.590	1.40×10^{-10}	7.40×10^{-11}
	Drift mobility			5.02×10^{-4}	5.36×10^{-6}

2d	*Pna2₁*	1	10.338	4.04×10^{-4}	1.48×10^{-4}
		2	10.338	4.04×10^{-4}	1.48×10^{-4}
		3	7.135	-5.12×10^{-4}	2.2×10^{-4}
		4	11.287	-5.8×10^{-3}	-1.71×10^{-4}
		5	7.135	-5.12×10^{-4}	2.2×10^{-4}
		6	11.287	-8.73×10^{-4}	3.42×10^{-4}
		7	14.008	2.85×10^{-4}	-4.65×10^{-5}
		8	14.008	2.85×10^{-4}	-4.65×10^{-5}
	Drift mobility			1.56×10^{-2}	2.66×10^{-5}

Table S4 Center−center distance and the corresponding hole and electron coupling between the dimer in all of the nearest neighbor pathways for the crystal structures of **1a**–**1c** and **2a**–**2c** with the lowest total energies.

Species	Space groups	Pathway	Distance (Å)	Electron coupling (eV)	Hole coupling (eV)
1a	*P*$\bar{1}$	1	9.954	2.93×10^{-5}	1.90×10^{-5}
		2	9.954	1.53×10^{-4}	-6.58×10^{-5}
		3	11.142	-4.89×10^{-6}	5.52×10^{-6}
		4	11.142	-4.88×10^{-6}	5.56×10^{-6}
		5	5.691	-6.10×10^{-3}	-1.11×10^{-2}
		6	13.229	1.68×10^{-6}	-5.38×10^{-7}
		7	8.651	1.07×10^{-2}	-1.97×10^{-2}
		8	16.128	2.43×10^{-4}	1.97×10^{-5}
1b	*P2₁*	1	10.213	5.60×10^{-3}	1.40×10^{-3}
		2	10.213	5.60×10^{-3}	1.40×10^{-3}
		3	9.304	-8.91×10^{-6}	5.20×10^{-6}
		4	9.304	-8.91×10^{-6}	5.20×10^{-6}
		5	10.120	1.61×10^{-4}	1.67×10^{-4}
		6	6.872	4.10×10^{-3}	-1.50×10^{-3}
		7	10.120	1.61×10^{-4}	1.67×10^{-4}
1c	*P2₁*	1	8.922	-1.90×10^{-3}	-2.29×10^{-2}
		2	8.922	-1.90×10^{-3}	-2.29×10^{-2}
		3	9.610	1.08×10^{-4}	-1.81×10^{-5}
		4	9.610	1.08×10^{-4}	-1.81×10^{-5}
		5	9.104	$-8.2683e\text{-}007\times10^{-5}$	$3.0995e\text{-}007\times10^{-5}$
		6	9.104	-8.27×10^{-7}	3.10×10^{-7}
		7	8.534	-1.10×10^{-5}	7.94×10^{-6}
		8	8.534	-1.10×10^{-5}	7.93×10^{-6}
2a	*Cc*	1	9.721	-1.10×10^{-3}	7.86×10^{-4}
		2	9.721	-1.10×10^{-3}	7.86×10^{-4}
		3	12.468	7.13×10^{-5}	-5.11×10^{-5}
		4	12.468	7.13×10^{-5}	-5.11×10^{-5}
		5	12.039	1.90×10^{-4}	-2.25×10^{-4}
		6	6.599	-5.20×10^{-3}	-1.86×10^{-2}
		7	6.599	-5.20×10^{-3}	-1.86×10^{-2}
2b	*Pbca*	1	11.710	1.08×10^{-18}	2.38×10^{-18}
		2	11.710	1.08×10^{-18}	2.38×10^{-18}
		3	13.861	1.21×10^{-5}	-1.07×10^{-5}
		4	5.414	-3.40×10^{-3}	-1.38×10^{-2}
		5	7.632	3.38×10^{-5}	-4.53×10^{-5}
		6	8.358	1.93×10^{-4}	-1.30×10^{-3}

		7	14.482	-2.26×10^{-5}	8.26×10^{-5}
		8	8.358	1.93×10^{-4}	-1.30×10^{-3}
		9	7.632	3.38×10^{-5}	-4.53×10^{-5}
		10	14.482	-2.26×10^{-5}	8.26×10^{-5}
2c	$Pna2_1$	1	10.011	3.47×10^{-6}	-6.19×10^{-5}
		2	10.011	3.47×10^{-6}	-6.19×10^{-5}
		3	9.273	-2.00×10^{-3}	9.70×10^{-3}
		4	9.273	-2.00×10^{-3}	9.70×10^{-3}
		5	8.639	-1.02×10^{-2}	-1.40×10^{-2}
		6	8.840	8.12×10^{-8}	5.40×10^{-7}
		7	9.549	-5.76×10^{-4}	2.77×10^{-4}
		8	9.549	1.70×10^{-3}	2.90×10^{-3}