Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C
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Supporting Information

Tuning the Solid State Emission of Meso -$Me_3SiC_6H_4$ BODIPYs by Tuning Their Solid State Structure

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Table S1: Crystallographic data for **4** and **6-9**

	4	**6**	**7**	**8**	**9**
Empirical formula	C_{20} H_{23} B F_2 N_2 Si	C_{20} H_{23} B F_2 N_2 Si	C_{22} H_{27} B F_2 N_2 Si	C_{22} H_{27} B F_2 N_2 Si	C_{22} H_{27} B F_2 N_2 Si
Formula weight	368.3	368.3	396.36	396.36	396.36
Temperature(k)	293(2)	293(2)	296(2)	296(2)	273(2)
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
space group	P2(1)/c	P2(1)/c	P-1	Pna2(1)	P-1
a/ Å	9.301(4)	6.880(3)	9.0644(18)	30.7303(15)	8.957(4)
b/ Å	12.332(5)	10.870(5)	13.838(3)	6.5809(3)	14.264(7)
c/ Å	17.567(7)	26.448(12)	17.166(3)	20.9330(10)	17.227(8)
α/deg	90	90	84.182(9)	90	81.589(9)
β/deg	103.820(9)	93.084(9)	89.033(10)	90	88.643(8)
γ/deg	90	90	78.190(9)	90	87.439(9)
V/$Å^3$	1956.7(14)	1975.1(16)	2096.8(7)	4233.3(3)	2174.7(18)
Crystal size	0.15 x 0.09 x 0.05 mm	0.1 x 0.08 x 0.06 mm	0.12 x 0.08 x 0.05 mm	0.12 x 0.09 x 0.06 mm	0.1 x 0.08 x 0.06 mm
z	4	4	4	8	4
Dc, g cm^{-3}	1.25	1.239	1.256	1.244	1.211
Final R [I>2s(I)]	R1 = 0.1272, wR2 = 0.3024	R1 = 0.1176, wR2 = 0.2670	R1 = 0.1080, wR2 = 0.2556	R1 = 0.0686, wR2 = 0.1624	R1 = 0.0870, wR2 = 0.2063
R (all data)	R1 = 0.3129, wR2 = 0.3528	R1 = 0.1964, wR2 = 0.3110	R1 = 0.1584, wR2 = 0.2772	R1 = 0.0965, wR2 = 0.1849	R1 = 0.1493, wR2 = 0.2428
Reflections collected	20558	22422	43472	82961	24860
Theta range for data collection	2.04 to 28.06 deg.	1.54 to 27.99 deg	1.19 to 30.66 deg	1.33 to 30.64 deg	1.74 to 28.09 deg.
Absorption coefficient	0.144 mm^{-1}	0.142 mm^{-1}	0.139 mm^{-1}	0.138 mm^{-1}	0.134mm^{-1}
Goodness-of-fit on F^2	1.053	1.036	1.104	1.019	1.066

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Table S2. Computed Structure of **4.**
4 Energy = -1399.83666977 a.u. (-38090.96 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	-5.491163	-0.000860	-0.000981
2	7	2.850749	-1.248387	0.028023
3	7	2.841264	1.253820	-0.027147
4	5	3.776927	0.006230	0.000102
5	9	4.581624	0.033199	1.147995
6	9	4.580982	-0.014715	-1.148385
7	6	-3.590235	-0.023229	-0.007189
8	6	-2.849470	-0.701408	-0.992224
9	1	-3.364072	-1.241393	-1.782503
10	6	-1.453151	-0.704225	-0.991953
11	1	-0.911850	-1.227012	-1.774728
12	6	-0.738305	-0.011095	-0.002131
13	6	-1.462483	0.676467	0.986961
14	1	-0.927669	1.201824	1.772455
15	6	-2.857056	0.660674	0.982183
16	1	-3.378482	1.192801	1.774911
17	6	0.747221	-0.005225	-0.000191
18	6	1.454274	-1.218473	0.044982
19	6	0.991075	-2.556369	0.147217
20	1	-0.044781	-2.857339	0.203587
21	6	2.112343	-3.374308	0.176548
22	1	2.138259	-4.452909	0.248594
23	6	3.252093	-2.537629	0.104358
24	6	1.445056	1.213377	-0.044544
25	6	0.971778	2.547706	-0.146792
26	1	-0.066332	2.840823	-0.203474
27	6	2.086867	3.374119	-0.175635
28	1	2.104647	4.452894	-0.247526
29	6	3.232891	2.546054	-0.103435
30	6	-6.090573	1.750588	-0.399737
31	1	-5.748719	2.069930	-1.390597
32	1	-5.717247	2.478476	0.329623
33	1	-7.185890	1.801672	-0.389616
34	6	-6.110954	-0.504082	1.715056
35	1	-5.743476	0.173406	2.494096
36	1	-5.783726	-1.516837	1.975421
37	1	-7.206580	-0.485098	1.752861
38	6	-6.146507	-1.208601	-1.300576
39	1	-7.242708	-1.213990	-1.289382
40	1	-5.810271	-2.234311	-1.111534
41	1	-5.832723	-0.931822	-2.313474
42	6	4.666914	2.963043	-0.113547
43	1	5.183849	2.606591	0.783247
44	1	5.191004	2.536057	-0.974847
45	1	4.740769	4.051923	-0.157304
46	6	4.689154	-2.944020	0.114108
47	1	5.202692	-2.585520	-0.783846
48	1	5.210855	-2.511606	0.974128
49	1	4.770969	-4.032253	0.159741

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Table S3. Computed Structure of **5.**
5 Energy = -1399.83685068 a.u. (-38090.96 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.778851	-1.049379	0.236037
2	7	2.277358	1.368473	-0.173179
3	5	3.406890	0.378275	0.246898
4	9	3.864802	0.690092	1.535091
5	9	4.466864	0.444342	-0.668073
6	6	-3.523525	-1.332717	-1.363098
7	6	-2.479599	-1.901857	-2.098702
8	1	-2.698507	-2.592400	-2.908402
9	6	-1.155128	-1.584832	-1.800347
10	1	-0.344249	-2.017561	-2.377971
11	6	-0.865285	-0.679900	-0.765100
12	6	-1.927974	-0.113387	-0.041962
13	6	-3.271318	-0.428212	-0.315830
14	6	0.542186	-0.331860	-0.436435
15	6	1.446219	-1.340799	-0.065055
16	6	1.254185	-2.735844	0.112942
17	1	0.320810	-3.261718	-0.025572
18	6	2.474832	-3.267917	0.505602
19	1	2.700803	-4.301391	0.729471
20	6	3.401838	-2.200158	0.577261
21	6	0.967552	1.005552	-0.495826
22	6	0.274409	2.179823	-0.889744
23	1	-0.754112	2.218303	-1.217637
24	6	1.170374	3.235329	-0.786872
25	1	0.987023	4.277978	-1.007168
26	6	2.405583	2.704014	-0.343523
27	1	-4.545963	-1.602319	-1.613849
28	1	-1.684458	0.570922	0.767158
29	14	-4.667599	0.353051	0.712595
30	6	-6.334938	-0.343610	0.154562
31	1	-7.143458	0.099665	0.747570
32	1	-6.541196	-0.119852	-0.898246
33	1	-6.389516	-1.430210	0.286469
34	6	-4.386600	-0.045636	2.540930
35	1	-4.399047	-1.127050	2.717114
36	1	-3.423025	0.336736	2.896046
37	1	-5.169940	0.404743	3.162064
38	6	-4.642527	2.229561	0.462279
39	1	-4.817123	2.492127	-0.587250
40	1	-5.420269	2.715653	1.063187
41	1	-3.679328	2.661178	0.757465
42	6	4.842289	-2.261474	0.967059
43	1	5.479737	-1.865298	0.170142
44	1	5.031148	-1.653844	1.858117
45	1	5.131538	-3.294159	1.174117
46	6	3.682223	3.437962	-0.094342
47	1	4.040953	3.263739	0.924972
48	1	4.469271	3.092858	-0.773096
49	1	3.533592	4.510026	-0.241488

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Table S4. Computed Structure of **6.**
6 Energy = -1399.83025106 a.u. (-38090.78 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.973539	-1.236119	0.049804
2	7	1.809747	1.221662	-0.403250
3	5	2.775183	0.102430	0.099935
4	9	3.175721	0.371848	1.416808
5	9	3.894997	0.023747	-0.737924
6	6	-4.172232	-0.766509	-2.034929
7	6	-3.092948	-1.027021	-2.878686
8	1	-3.254567	-1.364739	-3.898200
9	6	-1.795012	-0.850482	-2.400041
10	1	-0.946321	-1.048557	-3.048732
11	6	-1.561440	-0.408922	-1.087229
12	6	-2.640997	-0.143830	-0.207517
13	6	-3.938551	-0.339059	-0.726400
14	1	-4.798638	-0.156285	-0.089205
15	6	-0.128105	-0.236909	-0.688879
16	6	0.628421	-1.353241	-0.311137
17	6	0.261573	-2.719064	-0.200081
18	1	-0.719325	-3.119384	-0.413690
19	6	1.388770	-3.408653	0.224286
20	1	1.480061	-4.469414	0.413381
21	6	2.435036	-2.464515	0.374529
22	6	0.469996	1.028764	-0.752362
23	6	-0.056024	2.275435	-1.178112
24	1	-1.067942	2.439006	-1.520234
25	6	0.969759	3.205062	-1.075960
26	1	0.930827	4.258199	-1.318177
27	6	2.114787	2.525230	-0.591471
28	1	-5.190925	-0.899378	-2.388373
29	14	-2.520184	0.460865	1.610986
30	6	-4.102966	-0.081944	2.504444
31	1	-4.018168	0.170845	3.568133
32	1	-5.000596	0.418681	2.125287
33	1	-4.264628	-1.163479	2.434320
34	6	-2.435750	2.351586	1.658382
35	1	-1.502978	2.728409	1.227762
36	1	-3.268739	2.801375	1.105811
37	1	-2.493884	2.705372	2.694964
38	6	-1.053998	-0.267838	2.553932
39	1	-1.028495	-1.360878	2.491702
40	1	-0.087934	0.109635	2.208227
41	1	-1.151754	0.002337	3.612828
42	6	3.840413	-2.717405	0.811888
43	1	3.967190	-3.768768	1.079249
44	1	4.547963	-2.466831	0.014425
45	1	4.099002	-2.095885	1.674976
46	6	3.468703	3.092336	-0.316498
47	1	4.225644	2.615637	-0.947680
48	1	3.471770	4.167572	-0.508044
49	1	3.763015	2.914980	0.723022

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Table S5. Computed Structure of **7.**
7 Energy = -1478.47355267 a.u. (-40230.74 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	5.449396	0.000021	-0.001106
2	7	-2.887206	-1.247639	-0.001338
3	7	-2.887041	1.247767	-0.001443
4	5	-3.812396	0.000123	-0.002599
5	9	-4.620722	0.000089	-1.151871
6	9	-4.623710	0.000266	1.144579
7	6	3.549015	-0.000122	0.018567
8	6	2.808081	-0.000168	1.214467
9	1	3.322254	-0.000196	2.172090
10	6	1.410403	-0.000182	1.214365
11	1	0.866759	-0.000237	2.155450
12	6	0.700836	-0.000140	0.007367
13	6	1.419909	-0.000112	-1.195977
14	1	0.882937	-0.000079	-2.140855
15	6	2.815730	-0.000110	-1.184408
16	1	3.336385	-0.000119	-2.140009
17	6	-0.794731	-0.000074	0.002438
18	6	-1.485026	-1.224497	0.000932
19	6	-1.024772	-2.584717	0.001856
20	6	-2.169586	-3.375832	0.000211
21	1	-2.200828	-4.457543	0.000352
22	6	-3.299989	-2.531718	-0.001573
23	6	-1.484865	1.224435	0.000997
24	6	-1.024424	2.584593	0.001895
25	6	-2.169130	3.375862	0.000039
26	1	-2.200227	4.457576	0.000025
27	6	-3.299649	2.531899	-0.001843
28	6	6.059131	1.546111	-0.907251
29	1	5.724144	2.459150	-0.402406
30	1	5.687436	1.582309	-1.937568
31	1	7.154573	1.568345	-0.949998
32	6	6.059070	-1.545404	-0.908450
33	1	5.689017	-1.579793	-1.939421
34	1	5.722265	-2.458771	-0.405407
35	1	7.154553	-1.568800	-0.949465
36	6	6.104446	-0.000657	1.772997
37	1	7.200661	-0.000274	1.768112
38	1	5.779518	-0.887298	2.329163
39	1	5.778928	0.885179	2.330104
40	6	-4.739260	2.930152	-0.003656
41	1	-5.253767	2.530027	-0.883215
42	1	-5.255345	2.531890	0.875861
43	1	-4.826384	4.018996	-0.004814
44	6	-4.739654	-2.929773	-0.003425
45	1	-5.256128	-2.530181	0.875241
46	1	-5.253661	-2.530836	-0.883836
47	1	-4.826928	-4.018606	-0.003142
48	6	0.376893	3.122320	0.003952
49	1	0.942205	2.797795	0.882921
50	1	0.944806	2.798114	-0.873455
51	1	0.348889	4.215599	0.003983
52	6	0.376472	-3.122636	0.003525
53	1	0.943991	-2.798803	-0.874283
54	1	0.942268	-2.797898	0.882094
55	1	0.348316	-4.215912	0.003903

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Table S6. Computed Structure of **8.**
8 Energy = -1478.47361262 a.u. (-40230.75 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-2.586971	-1.247311	-0.122881
2	7	-2.586944	1.247348	-0.122811
3	5	-3.470633	0.000036	-0.398801
4	9	-3.900191	0.000070	-1.736920
5	9	-4.586584	0.000037	0.454748
6	6	3.527463	-0.000121	1.724600
7	6	2.510379	-0.000131	2.684218
8	1	2.760666	-0.000180	3.741615
9	6	1.172254	-0.000089	2.289340
10	1	0.379720	-0.000093	3.032498
11	6	0.845523	-0.000046	0.926157
12	6	1.876294	-0.000023	-0.022635
13	6	3.234160	-0.000061	0.348821
14	6	-0.585068	-0.000020	0.488782
15	6	-1.245812	-1.224279	0.286254
16	6	-0.806207	-2.584604	0.421603
17	6	-1.901676	-3.375625	0.088436
18	1	-1.931818	-4.457354	0.080276
19	6	-2.982546	-2.531381	-0.241797
20	6	-1.245759	1.224261	0.286236
21	6	-0.806097	2.584565	0.421587
22	6	-1.901541	3.375633	0.088448
23	1	-1.931624	4.457364	0.080241
24	6	-2.982463	2.531432	-0.241728
25	1	4.561154	-0.000177	2.059964
26	1	1.599677	0.000015	-1.075213
27	14	4.594170	0.000025	-0.980879
28	6	6.293123	-0.000708	-0.150200
29	1	7.083332	-0.000382	-0.910045
30	1	6.441946	0.885236	0.477454
31	1	6.441646	-0.887446	0.476407
32	6	4.407552	-1.544081	-2.059863
33	1	4.523770	-2.459598	-1.469023
34	1	3.424541	-1.583076	-2.542774
35	1	5.165179	-1.558548	-2.852363
36	6	4.408419	1.544945	-2.058843
37	1	4.525002	2.460006	-1.467365
38	1	5.166169	1.559578	-2.851223
39	1	3.425492	1.584738	-2.541857
40	6	-4.360877	-2.928092	-0.658846
41	1	-5.105881	-2.545255	0.046212
42	1	-4.607287	-2.510475	-1.640151
43	1	-4.440190	-4.016594	-0.703967
44	6	-4.360789	2.928210	-0.658725
45	1	-4.607164	2.510810	-1.640136
46	1	-5.105807	2.545204	0.046219
47	1	-4.440112	4.016721	-0.703627
48	6	0.534034	3.123203	0.829544
49	1	0.824409	2.794956	1.832274
50	1	1.330402	2.804053	0.150357
51	1	0.504675	4.216459	0.826776
52	6	0.533957	-3.123303	0.829371
53	1	1.330123	-2.804454	0.149793
54	1	0.824743	-2.794806	1.831893
55	1	0.504455	-4.216556	0.826911

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Table S7. Computed Structure of **9.**
9 Energy = -1478.46797979 a.u. (-40230.59 eV)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.994667	-1.238982	-0.142242
2	7	1.946029	1.253352	-0.198245
3	5	2.843557	0.031031	0.138455
4	9	3.220740	0.068884	1.492956
5	9	3.989180	0.035854	-0.672163
6	6	-4.190458	-0.161531	-1.860482
7	6	-3.168719	-0.193563	-2.808734
8	1	-3.397643	-0.249293	-3.869132
9	6	-1.841501	-0.155454	-2.381511
10	1	-1.036275	-0.183680	-3.111023
11	6	-1.521130	-0.081443	-1.017792
12	6	-2.541202	-0.046561	-0.032669
13	6	-3.870815	-0.091815	-0.502158
14	1	-4.688503	-0.073878	0.211611
15	6	-0.063668	-0.044106	-0.667330
16	6	0.636739	-1.250634	-0.493702
17	6	0.227232	-2.621591	-0.610322
18	6	1.355469	-3.384197	-0.323325
19	1	1.413955	-4.464786	-0.318533
20	6	2.426402	-2.512751	-0.035033
21	6	0.591253	1.195565	-0.557872
22	6	0.139852	2.541261	-0.777244
23	6	1.238738	3.358794	-0.529410
24	1	1.262375	4.438422	-0.599806
25	6	2.334425	2.544858	-0.172990
26	1	-5.230900	-0.192540	-2.171656
27	14	-2.286772	0.095116	1.868001
28	6	-3.937885	-0.319964	2.704729
29	1	-3.795290	-0.308946	3.791924
30	1	-4.726540	0.405347	2.475801
31	1	-4.304642	-1.316369	2.433097
32	6	-1.819553	1.864066	2.352239
33	1	-0.857316	2.168045	1.929473
34	1	-2.577216	2.586259	2.027606
35	1	-1.741415	1.934784	3.444015
36	6	-0.991328	-1.100542	2.549715
37	1	-1.177322	-2.134114	2.238917
38	1	0.028645	-0.840032	2.255570
39	1	-1.036228	-1.071801	3.645654
40	6	3.828504	-2.875152	0.331140
41	1	3.919053	-3.958359	0.439311
42	1	4.531281	-2.534982	-0.436596
43	1	4.124868	-2.395769	1.269222
44	6	3.720345	2.976707	0.178881
45	1	4.439826	2.615069	-0.563091
46	1	3.773372	4.066895	0.222464
47	1	4.025599	2.564321	1.145556
48	6	-1.110440	-3.195758	-0.974853
49	1	-1.909734	-2.835385	-0.321170
50	1	-1.402373	-2.937853	-1.997900
51	1	-1.073332	-4.286227	-0.899977
52	6	-1.204295	3.042450	-1.217707
53	1	-1.466067	2.681235	-2.217354
54	1	-2.007693	2.726054	-0.547474
55	1	-1.195404	4.135737	-1.245955