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Acceptor-regulated luminescence in carbazole-based charge transfer complexes

Si-Si Wang,[a] Kechang Li,[c] Xiaohui Ma,*[a,b] Pengchong Xue*[d]

a. Department of Translational Medicine, The First Hospital of Jilin University, Changchun, P. R. China. Email: ma_xh@jlu.edu.cn.

b. Department of Oncology, The First Hospital of Jilin University, Changchun, P. R. China.

c. College of Chemistry, Jilin University, Changchun, P. R. China.

d. Tianjin Key Laboratory of Structure and Performance for Functional Molecules, College of Chemistry, Tianjin Normal University, Tianjin, P. R. China. Email: xuepengchong@126.com; hxxyxpc@tjnu.edu.cn

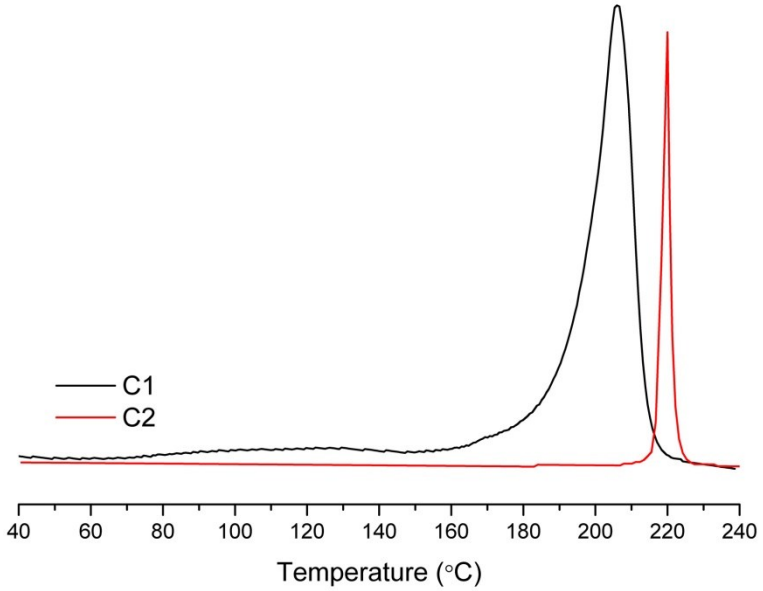

Figure S1. DSC curves of C1 and C2.

Table S1. Crystal data of C1 and C2.

Identification code	C1	C2
Empirical formula	$C_{44}H_{24}F_8N_6$	$C_{48}H_{28}N_{10}$
Formula weight	788.69	744.25
Color	yellow	red
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
Unit cell dimensions ($Å^3$)	1757.9(3)	1954.2(10)
a (Å)	7.1682(7)	15.694(5)
b (Å)	8.2406(9)	7.226(2)
c (Å)	29.792(3)	17.313(5)
α (°)	90	90
β (°)	92.704(8)	95.538
α (°)	90	90
Z	2	4
Density (g/cm^3)	1.490	1.266
Absorption coefficient	0.120	0.078

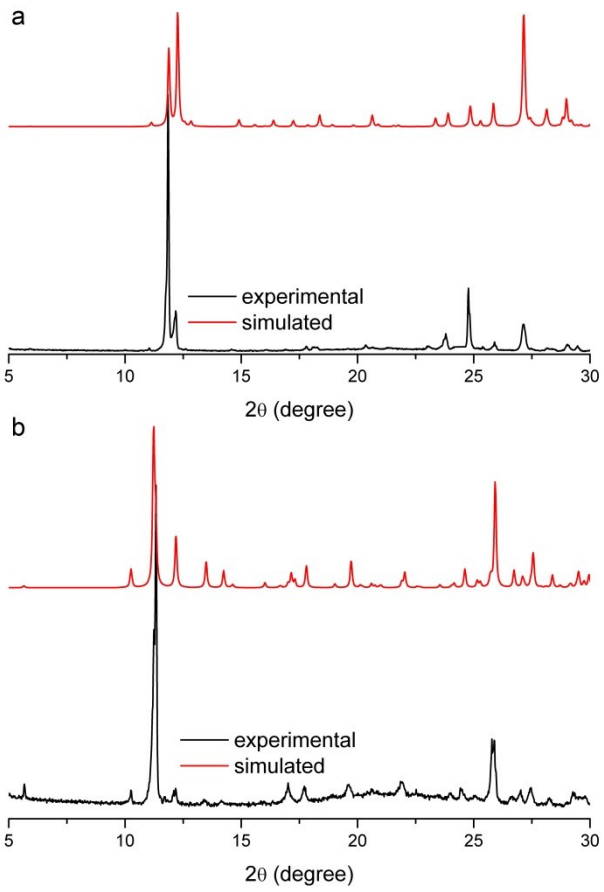

Figure S2. Powder XRD patterns of C1 and C2.

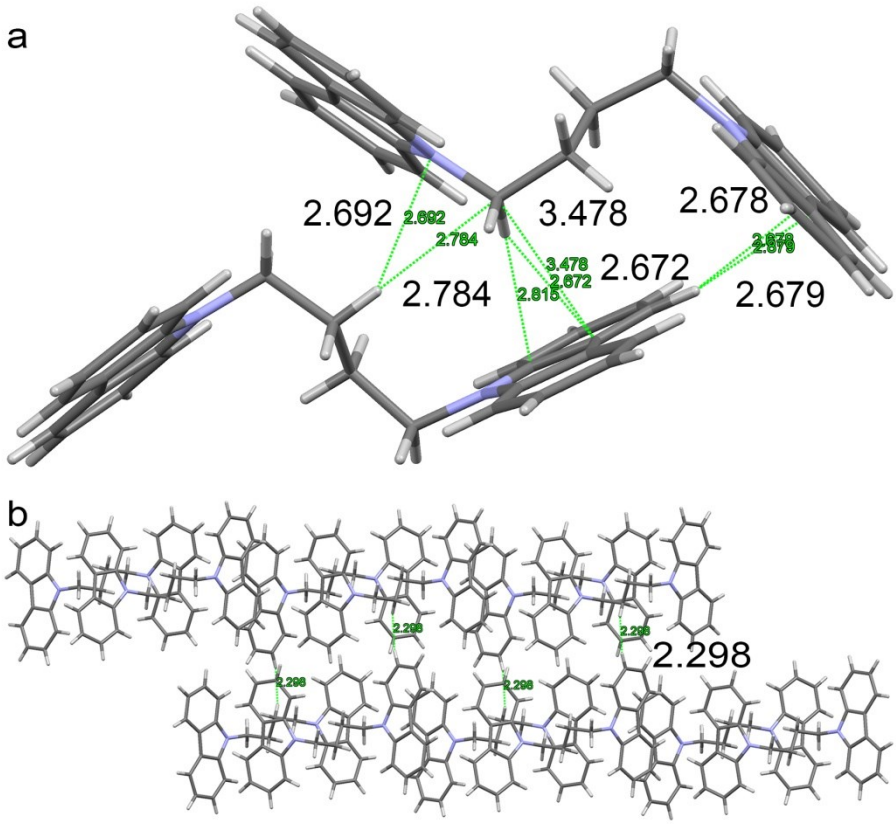

Figure S3. (a) Intermolecular weak interactions between two CC4C molecules in 1D stacking and (b) C-H···H-C interactions between 2D sheets.

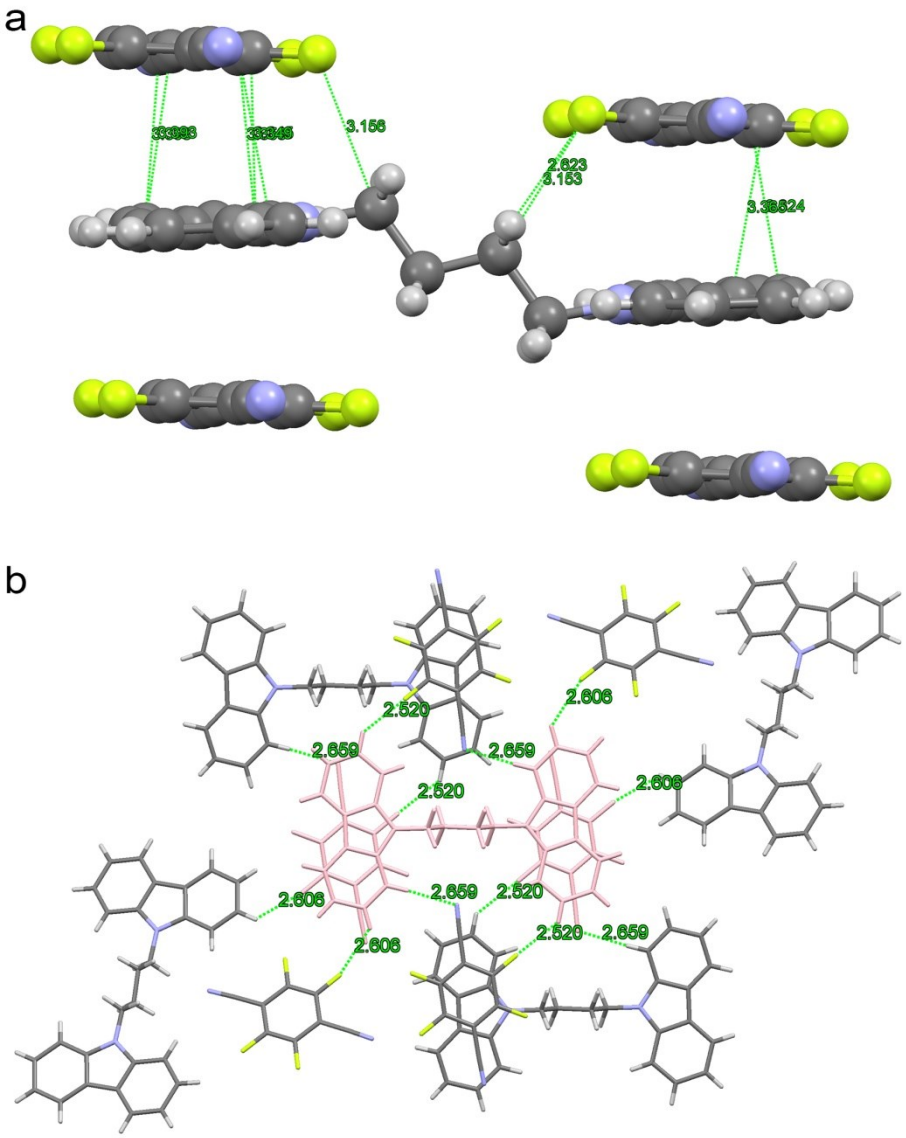

Figure S4. Intermolecular interactions in (a) intra-column and (b) inter-column in C1 crystal.

Table S2. The distance data of short interactions in Figure S2a.

Number	Object 1	Object 2	Length (Å)
1	C12	C6	3.393(2)
2	C12	C8	3.398(3)
3	C9	C2	3.349(2)
4	C9	C1	3.356(2)
5	C10	C1	3.345(2)
6	C5	C15	3.365(3)
7	C4	C20	3.324(2)
8	F1	C22	3.153(2)
9	F1	H22A	2.623
10	C21	F2	3.156(2)

Table S3. The distance data of short interactions in Figure S2b.

Number	Object 1	Object 2	Length (Å)
1	N_2	H_{17}	2.659
2	H_{11}	F_1	2.52
3	F_1	H_{11}	2.52
4	H_{17}	N2	2.659
5	H_{18}	F_3	2.606
6	F_3	H_{18}	2.606
7	H_{17}	N_2	2.659
8	F_1	H_{11}	2.52
9	H_{18}	F_3	2.606
10	N_2	H_{17}	2.659
11	H_{11}	F_1	2.52
12	F_3	H_{18}	2.606

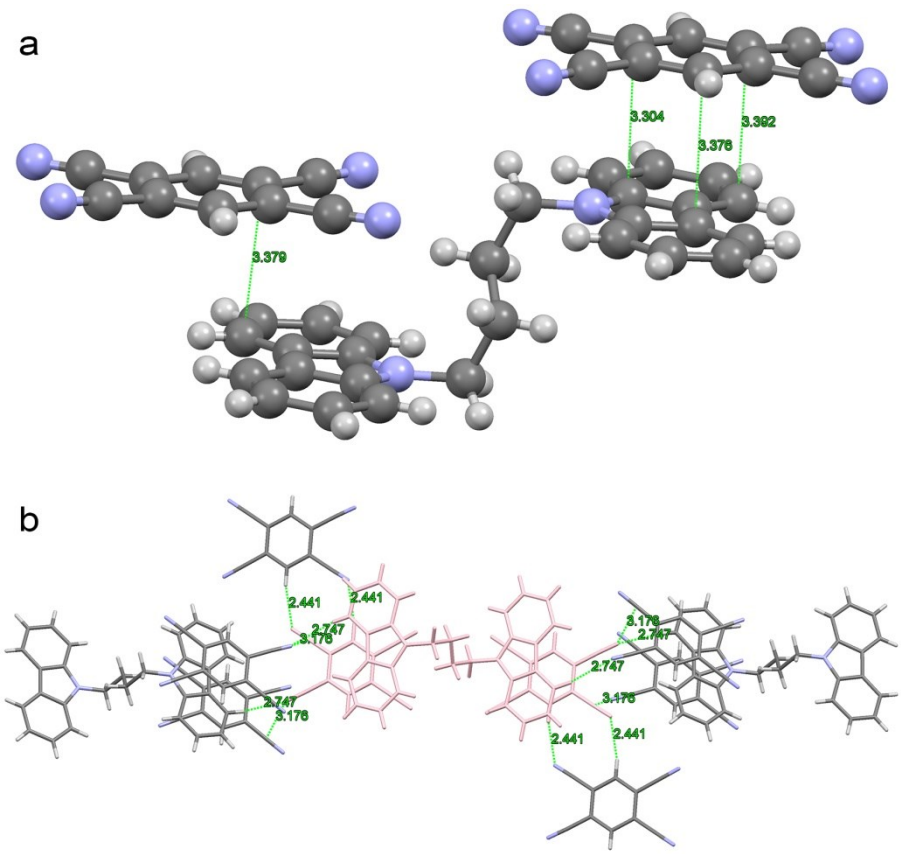

Figure S5. Intermolecular interactions in (a) intra-column and (b) inter-column in C2 crystal.

Table S4. The distance data of short interactions in Figure S3a.

Number	Object1	Object2	Length (Å)
1	C_{17}	C_{12}	3.304(2)
2	C_{21}	C_{6}	3.376(3)
3	C_{19}	C_{8}	3.392(3)
4	C_{16}	C_{5}	3.379(3)

Table S5. The distance data of short interactions in Figure S3b.

Number	Object1	Object2	Length (Å)
1	H_{18}	N=	2.441
2	N_4	H_{18}	2.441
3	C_{23}	N_5	3.176(3)
4	N_5	C_{23}	3.176(3)
5	N_5	H_8	2.747
6	H_8	N_5	2.747
7	H_{18}	N_4	2.441
8	N_4	H_{18}	2.441
9	H_8	N_5	2.747
10	C_{23}	N_5	3.176(3)
11	N_5	H_8	2.747
12	N_5	C_{23}	3.176(3)

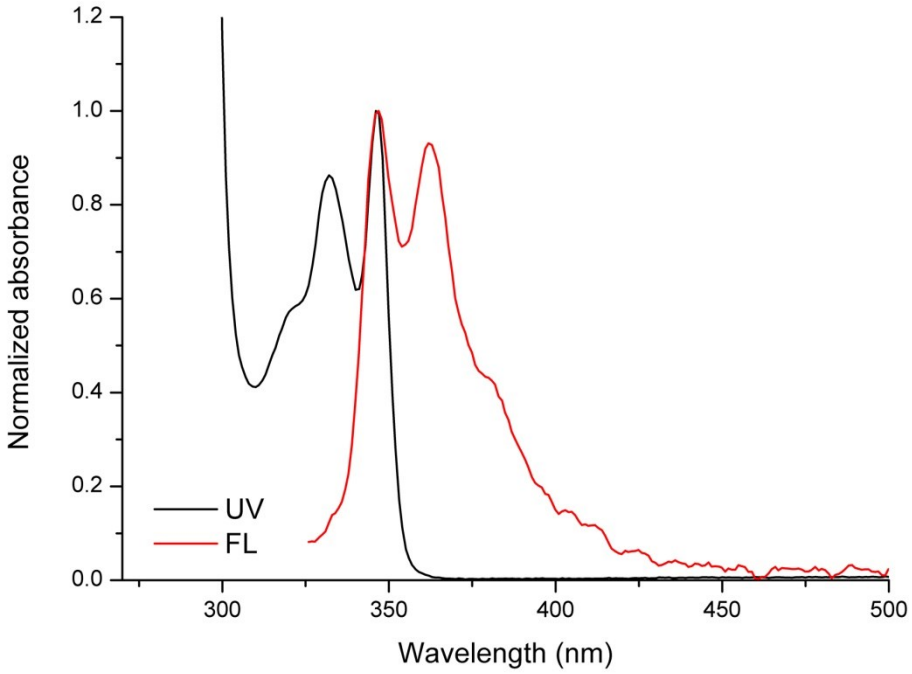

Figure S6. Normalized absorption and emission spectra of CC4C in toluene (10^{-5} M).

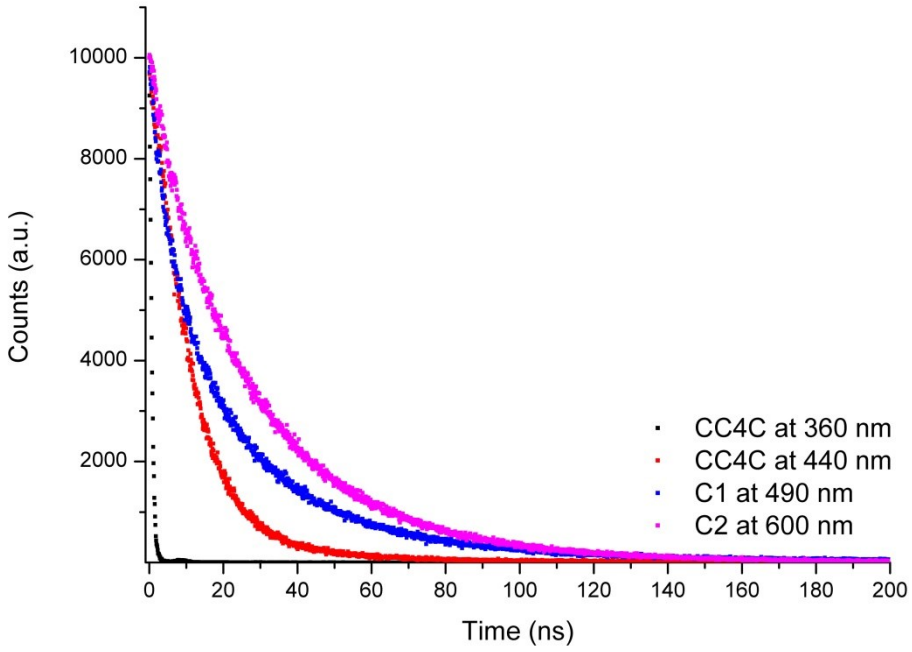

Figure S7. Decay curves of CC4C, C1 and C2 crystals. λ_{ex} is 340 nm for CC4C and C1 crystals, and is 460 nm for C2 crystals.

Table S6. Electron transition data of C1 and C2 by quantum chemical calculations.

	Transition	Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
C1 (2:1)	$S_0 \rightarrow S_1$	H-1→L (40.8 %) H→L (58.0 %)	3.1723	390.83	0.0009
	$S_0 \rightarrow S_2$	H-1→L+1 (51.8 %) H→L+1 (46.8 %)	3.1827	389.55	0.0008
C2 (2:1)	$S_0 \rightarrow S_1$	H-1→L+1 (47.0 %) H→L (52.3 %)	2.7142	456.80	0.0145
	$S_0 \rightarrow S_2$	H-1→L (47.1 %) H→L+1 (52.2 %)	2.7154	456.59	0.0007

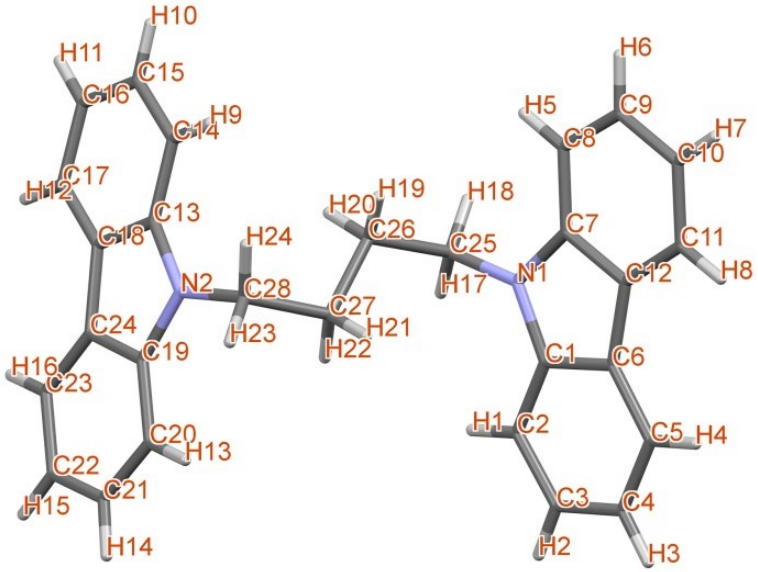

Table S7. Atom coordinates in CC4C crystal.

Number	Label	X	Y	Z
1	N1	0.18109(19)	0.65960(19)	0.26657(7)
2	N2	0.46579(18)	0.54281(19)	0.08511(7)
3	C1	0.2768(2)	0.6410(2)	0.30842(9)
4	C2	0.4173(2)	0.6922(2)	0.31337(10)
5	H1	0.4614	0.7485	0.2857
6	C3	0.4897(3)	0.6583(3)	0.35975(10)
7	H2	0.5853	0.6924	0.3641
8	C4	0.4263(3)	0.5748(3)	0.40069(10)
9	H3	0.4795	0.5524	0.432
10	C5	0.2869(3)	0.5247(2)	0.39593(9)
11	H4	0.2441	0.468	0.4237
12	C6	0.2102(2)	0.5587(2)	0.34974(9)
13	C7	0.0522(2)	0.5928(2)	0.28070(9)
14	C8	-0.0761(2)	0.5883(3)	0.25220(9)
15	H5	-0.0859	0.6355	0.2183
16	C9	-0.1884(3)	0.5118(3)	0.27564(10)
17	H6	-0.2772	0.5066	0.2573
18	C10	-0.1754(3)	0.4420(3)	0.3254(1)
19	H7	-0.2542	0.3885	0.3399
20	C11	-0.0487(3)	0.4503(2)	0.35363(9)
21	H8	-0.0401	0.404	0.3877
22	C12	0.0664(2)	0.5273(2)	0.33158(9)
23	C13	0.3949(2)	0.6251(2)	0.04517(8)
24	C14	0.2522(2)	0.6227(2)	0.03012(9)
25	H9	0.1864	0.5577	0.0478
26	C15	0.2092(2)	0.7171(3)	-0.01110(9)

27	H10	0.1119	0.7177	-0.0218
28	C16	0.3058(2)	0.8127(2)	-0.03777(9)
29	H11	0.273	0.8774	-0.066
30	C17	0.4478(2)	0.8139(2)	-0.02339(9)
31	H12	0.5131	0.8783	-0.0416
32	C18	0.4941(2)	0.7189(2)	0.01838(8)
33	C19	0.6090(2)	0.5809(2)	0.08409(8)
34	C20	0.7200(2)	0.5261(3)	0.11611(9)
35	H13	0.7041	0.4527	0.1436
36	C21	0.8546(2)	0.5830(3)	0.10619(9)
37	H14	0.9327	0.5458	0.1269
38	C22	0.8788(2)	0.6934(3)	0.06664(10)
39	H15	0.9723	0.7318	0.0615
40	C23	0.7681(2)	0.7472(2)	0.03492(9)
41	H16	0.7849	0.822	0.0079
42	C24	0.6313(2)	0.6903(2)	0.04313(8)
43	C25	0.2071(2)	0.7417(2)	0.21732(9)
44	H17	0.2891	0.813	0.2227
45	H18	0.1232	0.8072	0.2084
46	C26	0.2373(2)	0.6340(2)	0.17054(9)
47	H19	0.1553	0.5626	0.1653
48	H20	0.2443	0.6994	0.1384
49	C27	0.3715(2)	0.5355(2)	0.17596(9)
50	H21	0.3607	0.4607	0.2055
51	H22	0.4528	0.6051	0.1847
52	C28	0.4035(2)	0.4442(2)	0.12563(9)
53	H23	0.4698	0.3574	0.1344
54	H24	0.3143	0.3974	0.1115

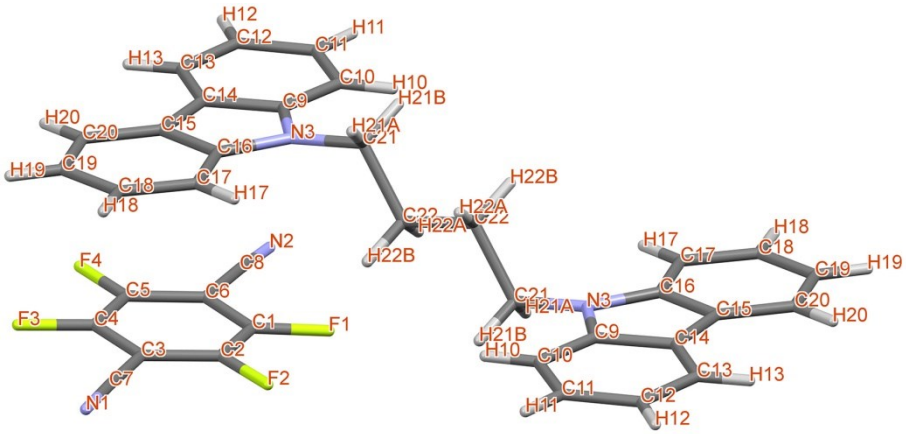

Table S8. Atom coordinates in C1 crystal.

Number	Label	X	Y	Z
1	N3	0.3343(2)	0.1899(2)	0.41561(5)
2	C9	0.2784(2)	0.3514(2)	0.41476(6)
3	C10	0.2252(2)	0.4497(2)	0.45000(7)
4	H10	0.2287	0.4121	0.4795
5	C11	0.1669(2)	0.6060(3)	0.43932(7)
6	H11	0.1289	0.6741	0.4621
7	C12	0.1638(2)	0.6636(3)	0.39525(7)
8	H12	0.1226	0.7687	0.3892
9	C13	0.2207(2)	0.5674(2)	0.36046(7)
10	H13	0.2207	0.6076	0.3313
11	C14	0.2784(2)	0.4085(2)	0.36986(6)
12	C15	0.3381(2)	0.2754(2)	0.34265(6)
13	C16	0.3713(2)	0.1430(2)	0.37212(6)
14	C17	0.4322(2)	-0.0060(2)	0.35667(7)
15	H17	0.4552	-0.0924	0.3762
16	C18	0.4576(2)	-0.0213(3)	0.31114(7)
17	H18	0.4969	-0.1203	0.3
18	C19	0.4257(2)	0.1079(3)	0.28159(7)
19	H19	0.4454	0.0941	0.2512
20	C20	0.3651(2)	0.2562(3)	0.29690(6)
21	H20	0.3428	0.3418	0.277
22	C21	0.3265(2)	0.0806(2)	0.45394(7)
23	H21A	0.2874	-0.0256	0.4431
24	H21B	0.2318	0.1198	0.4735
25	C22	0.5086(2)	0.0622(2)	0.48144(6)
26	H22A	0.544	0.1661	0.4945
27	H22B	0.6062	0.0289	0.4619
28	N3	0.6657(2)	-0.1899(2)	0.58439(5)
29	C9	0.7216(2)	-0.3514(2)	0.58524(6)
30	C10	0.7748(2)	-0.4497(2)	0.55000(7)

31	H10	0.7713	-0.4121	0.5205
32	C11	0.8331(2)	-0.6060(3)	0.56068(7)
33	H11	0.8711	-0.6741	0.5379
34	C12	0.8362(2)	-0.6636(3)	0.60475(7)
35	H12	0.8774	-0.7687	0.6108
36	C13	0.7793(2)	-0.5674(2)	0.63954(7)
37	H13	0.7793	-0.6076	0.6687
38	C14	0.7216(2)	-0.4085(2)	0.63014(6)
39	C15	0.6619(2)	-0.2754(2)	0.65735(6)
40	C16	0.6287(2)	-0.1430(2)	0.62788(6)
41	C17	0.5678(2)	0.0060(2)	0.64333(7)
42	H17	0.5448	0.0924	0.6238
43	C18	0.5424(2)	0.0213(3)	0.68886(7)
44	H18	0.5031	0.1203	0.7
45	C19	0.5743(2)	-0.1079(3)	0.71841(7)
46	H19	0.5546	-0.0941	0.7488
47	C20	0.6349(2)	-0.2562(3)	0.70310(6)
48	H20	0.6572	-0.3418	0.723
49	C21	0.6735(2)	-0.0806(2)	0.54606(7)
50	H21A	0.7126	0.0256	0.5569
51	H21B	0.7682	-0.1198	0.5265
52	C22	0.4914(2)	-0.0622(2)	0.51856(6)
53	H22A	0.456	-0.1661	0.5055
54	H22B	0.3938	-0.0289	0.5381
55	F1	0.81058(15)	0.31716(14)	0.45392(4)
56	F2	0.91610(14)	0.04480(14)	0.41189(4)
57	F3	0.82926(16)	0.30763(16)	0.27225(4)
58	F4	0.71176(16)	0.57614(15)	0.31417(4)
59	N1	0.9802(2)	-0.0922(2)	0.30281(7)
60	N2	0.6598(2)	0.7069(2)	0.42817(7)
61	C1	0.8117(2)	0.3137(2)	0.40907(6)
62	C2	0.8670(2)	0.1760(2)	0.38751(7)
63	C3	0.8738(2)	0.1705(2)	0.34118(7)
64	C4	0.8213(2)	0.3089(3)	0.31683(6)
65	C5	0.7634(3)	0.4460(3)	0.33833(7)
66	C6	0.7583(2)	0.4516(2)	0.38483(7)
67	C7	0.9324(3)	0.0254(3)	0.31920(7)
68	C8	0.7020(3)	0.5951(3)	0.40823(7)

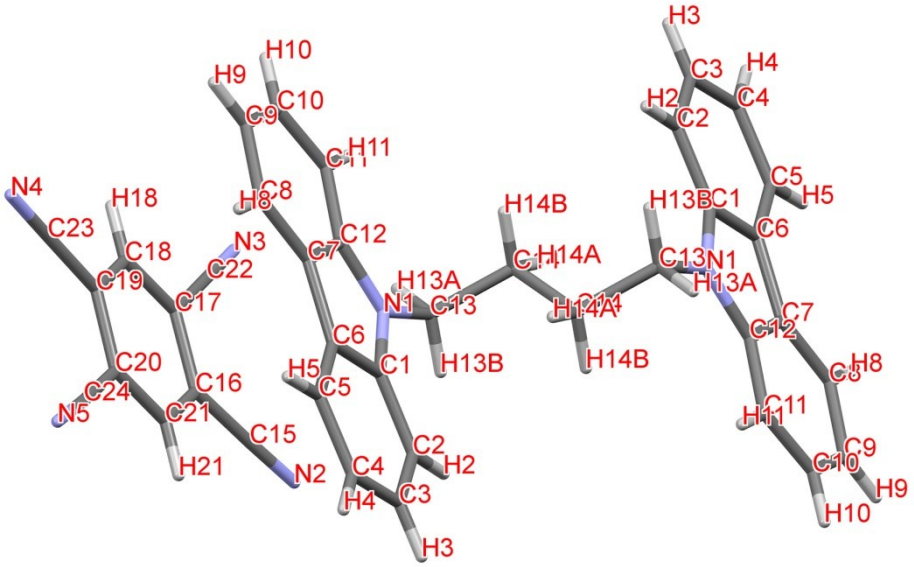

Table S9. Atom coordinates in C2 crystal.

Number	Label	X	Y	Z
1	N1	0.35705(9)	0.16804(19)	0.43434(8)
2	C1	0.33980(11)	0.1006(2)	0.35918(10)
3	C2	0.39279(13)	0.0884(3)	0.29957(11)
4	H2	0.449513	0.127219	0.306575
5	C3	0.35839(14)	0.0170(3)	0.22993(11)
6	H3	0.392984	0.005483	0.189503
7	C4	0.27308(15)	-0.0386(3)	0.21814(11)
8	H4	0.251679	-0.085012	0.170031
9	C5	0.22035(13)	-0.0257(2)	0.27656(10)
10	H5	0.163442	-0.062747	0.268346
11	C6	0.25327(11)	0.0437(2)	0.34860(10)
12	C7	0.21756(11)	0.0769(2)	0.42072(10)
13	C8	0.13672(12)	0.0526(3)	0.44581(11)
14	H8	0.0926	0.000815	0.413066
15	C9	0.12307(14)	0.1065(3)	0.52003(12)
16	H9	0.069305	0.090764	0.537446
17	C10	0.18894(14)	0.1842(3)	0.56913(11)
18	H10	0.177871	0.221989	0.618536
19	C11	0.26986(13)	0.2067(2)	0.54658(10)
20	H11	0.313905	0.255862	0.58019
21	C12	0.28336(11)	0.1533(2)	0.47180(10)
22	C13	0.43984(11)	0.2294(2)	0.47134(10)
23	H13A	0.431394	0.338219	0.502507
24	H13B	0.476208	0.264281	0.431513
25	C14	0.48488(11)	0.0810(2)	0.52273(10)
26	H14A	0.533756	0.135854	0.552894
27	H14B	0.445936	0.036138	0.55875
28	N1	0.64295(9)	-0.16804(19)	0.56566(8)

29	C1	0.66020(11)	-0.1006(2)	0.64082(10)
30	C2	0.60721(13)	-0.0884(3)	0.70043(11)
31	H2	0.550487	-0.127219	0.693425
32	C3	0.64161(14)	-0.0170(3)	0.77007(11)
33	H3	0.607016	-0.005483	0.810497
34	C4	0.72692(15)	0.0386(3)	0.78186(11)
35	H4	0.748321	0.085012	0.829969
36	C5	0.77965(13)	0.0257(2)	0.72344(10)
37	H5	0.836558	0.062747	0.731654
38	C6	0.74673(11)	-0.0437(2)	0.65140(10)
39	C7	0.78244(11)	-0.0769(2)	0.57928(10)
40	C8	0.86328(12)	-0.0526(3)	0.55419(11)
41	H8	0.9074	-0.000815	0.586934
42	C9	0.87693(14)	-0.1065(3)	0.47997(12)
43	H9	0.930695	-0.090764	0.462554
44	C10	0.81106(14)	-0.1842(3)	0.43087(11)
45	H10	0.822129	-0.221989	0.381464
46	C11	0.73014(13)	-0.2067(2)	0.45342(10)
47	H11	0.686095	-0.255862	0.41981
48	C12	0.71664(11)	-0.1533(2)	0.52820(10)
49	C13	0.56016(11)	-0.2294(2)	0.52866(10)
50	H13A	0.568606	-0.338219	0.497493
51	H13B	0.523792	-0.264281	0.568487
52	C14	0.51512(11)	-0.0810(2)	0.47727(10)
53	H14A	0.466244	-0.135854	0.447106
54	H14B	0.554064	-0.036138	0.44125
55	N2	0.42728(12)	0.5941(3)	0.32971(12)
56	N3	0.34524(12)	0.7015(2)	0.53804(10)
57	N4	-0.05648(12)	0.4089(3)	0.40106(11)
58	N5	0.01679(12)	0.3285(3)	0.19761(11)
59	C15	0.35692(13)	0.5772(2)	0.33904(11)
60	C16	0.26836(11)	0.5509(2)	0.35146(10)
61	C17	0.24022(11)	0.5883(2)	0.42388(10)
62	C18	0.15574(11)	0.5575(2)	0.43716(10)
63	H18	0.137248	0.583125	0.485471
64	C19	0.09919(11)	0.4883(2)	0.37813(10)
65	C20	0.12663(11)	0.4533(2)	0.30500(10)
66	C21	0.21105(12)	0.4841(2)	0.29197(11)
67	H21	0.229334	0.460011	0.24344
68	C22	0.29880(13)	0.6543(3)	0.48707(11)
69	C23	0.01231(13)	0.4464(3)	0.39154(11)
70	C24	0.06643(13)	0.3830(3)	0.24429(11)