Supporting Information

Syntheses of multi-resonance frameworks towards narrowband organic light-emitting diodes

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Table S1. Conditions used to synthesise the compounds shown in Fig. 1

Compound	Condition	Solvent	Yield	Ref
DOBNA	t-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	62%	1
DABNA-1	t-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	31%	2
DABNA-2	t-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	32%	2
DtBuCzB	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	26%	3
ADBNA-Me-Mes	n-BuLi, BBr_3, $NEtiPr_2$, Mes-MgBr	^{t}Bu-benzene	29%	4
ADBNA-Me-Tip	n-BuLi, BBr_3, $NEtiPr_2$, Tip-MgBr	^{t}Bu-benzene	15%	4
BBCz-DB	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	36%	5
BBCz-R/DBN-ICZ	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	5%	5,6
BBCz-Y- II/DBN-ICz	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	7%	5,6
IDID 2BN	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	39%	7
DBTN-2	t-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	5%	8
2Br	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	38%	9
2TBr	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	40%	9
m-DBCz	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	13%	10
TMlnBN	n-BuLi, BBr_3, $NEtiPr_2$	^{t}Bu-benzene	9%	11

Table S2. Conditions used to synthesise the compounds shown in Fig. 2

Compound	Condition	Solvent	Yield	Ref
B2	BI_3	O-DCB	76%	12
B3	BI_3	1,2,4-Trichlorobenzene	45%	12
ν-DABNA	BBr_3	O-DCB	36%	13
V-DANBA-Mes	BBr_3	O-DCB	44%	14
Δ-DABNA-TB	BBr_3	O-DCB	15%	15
ν-DABNA-O2-TB	BBr_3	O-DCB	37%	15
CzB2-M/TB	BBr_3	MCB	72%	16
CzDABNA-M/TB	BBr_3	Tol	63%	16
CzB4	BI_3	O-DCB	76%	17
CzB6	BI_3	O-DCB	69%	17
CzB8	BI_3	O-DCB	75%	17
ω-DABNA	BBr_3	O-DCB	23%	18
B4N6	BBr_3	1,2,4-Trichlorobenzene	71%	19
m[B-N]N1	BBr_3	MCB	91%	20
m[B-N]N2	BBr_3	MCB	92%	20

Table S3. Conditions used to synthesise the compounds shown in Fig. 3

Compound	Condition A	Solvent	Yield	Ref
QAO/QAD	$(COCl)_2$, $FeCl_3$	DCM	39%	21
	$SOCl_2$, $AlCl_3$	DCM	60%	22
QA-2	$(COCl)_2$, $AlCl_3$	DCM	13%	23
Hel-DiDiKTa	$SOCl_2$, $AlCl_3$	DCM	60%	24
DOBDiKTa	$SOCl_2$, $SnCl_2$	DCM	51%	25

Table S4. Conditions used to synthesise the compounds shown in Fig. 4

Compound	Condition	Solvent	Yield	Ref
SFQ	DDQ	Dioxane	46%	26
SOQ	DDQ	Dioxane	41%	26
SSQ	DDQ	Dioxane	47%	26
SSeQ	DDQ	Dioxane	50%	26
SS-DAO	DDQ	DCM/H_2O/Dioxane	63%	27
TCZBAO	DDQ	DCM/H_2O/Dioxane	57%	28
h-BNCO-1	DDQ, O_2	DMSO	5%	29

Table S5. Conditions used to synthesise the compounds shown in Fig. 5

Compound	Condition	Solvent	Yield	Ref
QP3O	H_2O_2	HOAc	91%	30
PTZBN3	H_2O_2	HOAc	11%	31
tP	H_2O_2	HOAc/$CHCl_3$	80%	32
tPD	H_2O_2	HOAc/$CHCl_3$	82%	32

Table S6. Conditions used to synthesise the compounds shown in Fig. 6

Compound	Condition	Solvent	Yield	Ref
tBCzP2PO	n-BuLi, $PhPCl_2$	Et_2O	60%	33

References

1. H. Hirai, K. Nakajima, S. Nakatsuka, K. Shiren, J. Ni, S. Nomura, T. Ikuta and T. Hatakeyama, Angew. Chem., Int. Ed. Engl., 2015, 54, 13581-13585.
2. T. Hatakeyama, K. Shiren, K. Nakajima, S. Nomura, S. Nakatsuka, K. Kinoshita, J. Ni, Y. Ono and T. Ikuta, Adv. Mater., 2016, 28, 2777-2781.
3. Y. Xu, Z. Cheng, Z. Li, B. Liang, J. Wang, J. Wei, Z. Zhang and Y. Wang, *Adv. Opt. Mater.*, 2020, **8**, e1902142.
4. S. Oda, B. Kawakami, R. Kawasumi, R. Okita and T. Hatakeyama, *Org. Lett.*, 2019, **21**, 9311-9314.

5. M. Yang, I. S. Park and T. Yasuda, J. Am. Chem. Soc., 2020, 142, 19468-19472.
6. Y. Zhang, J. Wei, L. Wang, T. Huang, G. Meng, X. Wang, X. Zeng, M. Du, T. Fan, C. Yin, D. Zhang and L. Duan, Adv. Mater., 2023, 35, e2209396.
7. T. Fan, S. Zhu, X. Cao, X. Liang, M. Du, Y. Zhang, R. Liu, D. Zhang and L. Duan, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202313254.
8. X.-C. Fan, K. Wang, Y.-Z. Shi, Y.-C. Cheng, Y.-T. Lee, J. Yu, X.-K. Chen, C. Adachi and X.-H. Zhang, *Nat. Photonics.*, 2023, **17**, 280-285.
9. Y. Zhang, D. Zhang, T. Huang, A. J. Gillett, Y. Liu, D. Hu, L. Cui, Z. Bin, G. Li, J. Wei and L. Duan, *Angew. Chem., Int. Ed. Engl.*, 2021, **60**, 20498-20503.
10. X. Cai, Y. Pu, C. Li, Z. Wang and Y. Wang, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202304104.
11. C.-Z. Du, Y. Lv, H. Dai, X. Hong, J. Zhou, J.-K. Li, R.-R. Gao, D. Zhang, L. Duan and X.-Y. Wang, *J.Mater.C.C.*, 2023, **11**, 2469-2474.
12. K. Matsui, S. Oda, K. Yoshiura, K. Nakajima, N. Yasuda and T. Hatakeyama, *J. Am. Chem. Soc.*, 2018, **140**, 1195-1198.
13. Y. Kondo, K. Yoshiura, S. Kitera, H. Nishi, S. Oda, H. Gotoh, Y. Sasada, M. Yanai and T. Hatakeyama, *Nat. Photonics.*, 2019, **13**, 678-682.
14. S. Oda, B. Kawakami, Y. Yamasaki, R. Matsumoto, M. Yoshioka, D. Fukushima, S. Nakatsuka and T. Hatakeyama, *J. Am. Chem. Soc.*, 2022, **144**, 106-112.
15. M. Hayakawa, X. Tang, Y. Ueda, H. Eguchi, M. Kondo, S. Oda, X. C. Fan, G. N. Iswara Lestanto, C. Adachi and T. Hatakeyama, *J. Am. Chem. Soc.*, 2024, **146**, 18331-18340.
16. S. Oda, W. Kumano, T. Hama, R. Kawasumi, K. Yoshiura and T. Hatakeyama, *Angew. Chem., Int. Ed. Engl.*, 2021, **60**, 2882-2886.
17. Y. Sano, T. Shintani, M. Hayakawa, S. Oda, M. Kondo, T. Matsushita and T. Hatakeyama, *J. Am. Chem. Soc.*, 2023, **145**, 11504-11511.
18. S. Uemura, S. Oda, M. Hayakawa, R. Kawasumi, N. Ikeda, Y. T. Lee, C. Y. Chan, Y. Tsuchiya, C. Adachi and T. Hatakeyama, *J. Am. Chem. Soc.*, 2023, **145**, 1505-1511.
19. X. C. Fan, F. Huang, H. Wu, H. Wang, Y. C. Cheng, J. Yu, K. Wang and X. H. Zhang, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202305580.
20. G. Meng, H. Dai, T. Huang, J. Wei, J. Zhou, X. Li, X. Wang, X. Hong, C. Yin, X. Zeng, Y. Zhang, D. Yang, D. Ma, G. Li, D. Zhang and L. Duan, *Angew. Chem., Int. Ed. Engl.*, 2022, **61**, e202207293.
21. Y. Yuan, X. Tang, X. Y. Du, Y. Hu, Y. J. Yu, Z. Q. Jiang, L. S. Liao and S. T. Lee, *Adv. Opt. Mater.*, 2019, **7**, e1801536.
22. X. Li, Y. Z. Shi, K. Wang, M. Zhang, C. J. Zheng, D. M. Sun, G. L. Dai, X. C. Fan, D. Q. Wang, W. Liu, Y. Q. Li, J. Yu, X. M. Ou, C. Adachi and X. H. Zhang, *ACS Appl. Mater. Interfaces*, 2019, **11**, 13472-13480.
23. H. Min, I. S. Park and T. Yasuda, *Angew. Chem., Int. Ed. Engl.*, 2021, **60**, 7643-7648.
24. J. M. dos Santos, D. Sun, J. M. Moreno-Naranjo, D. Hall, F. Zinna, S. T. J. Ryan, W. Shi, T. Matulaitis, D. B. Cordes, A. M. Z. Slawin, D. Beljonne, S. L. Warriner, Y. Olivier, M. J. Fuchter and E. Zysman-Colman, *J.Mater.C.C.*, 2022, **10**, 4861-4870.
25. S. Wu, L. Zhang, J. Wang, A. Kumar Gupta, I. D. W. Samuel and E. Zysman-Colman, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202305182.
26. Y. J. Yu, Z. Q. Feng, X. Y. Meng, L. Chen, F. M. Liu, S. Y. Yang, D. Y. Zhou, L. S. Liao and Z. Q. Jiang, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202310047.
27. L. Liang, C. Qu, X. Fan, K. Ye, Y. Zhang, Z. Zhang, L. Duan and Y. Wang, *Angew. Chem., Int. Ed. Engl.*, 2024, **63**, e202316710.

28. Z. Yang, G. X. Yang, S. Jiang, M. Li, W. Qiu, X. Peng, C. Shen, Y. Gan, K. Liu, D. Li and S. J. Su, *Adv. Opt. Mater.*, 2023, **12**, 2301711.
29. Y. C. Cheng, X. Tang, K. Wang, X. Xiong, X. C. Fan, S. Luo, R. Walia, Y. Xie, T. Zhang, D. Zhang, J. Yu, X. K. Chen, C. Adachi and X. H. Zhang, *Nat. Commun.*, 2024, **15**, 731.
30. X. Wu, B.-K. Su, D.-G. Chen, D. Liu, C.-C. Wu, Z.-X. Huang, T.-C. Lin, C.-H. Wu, M. Zhu, E. Y. Li, W.-Y. Hung, W. Zhu and P.-T. Chou, *Nat. Photonics.*, 2021, **15**, 780-786.
31. T. Hua, J. Miao, H. Xia, Z. Huang, X. Cao, N. Li and C. Yang, *Adv. Funct. Mater.*, 2022, **32**, e2201032.
32. Jiang, Y. Yu, D. Li, Z. Chen, Y. He, M. Li, G. X. Yang, W. Qiu, Z. Yang, Y. Gan, J. Lin, Y. Ma and S. J. Su, *Angew. Chem., Int. Ed. Engl.*, 2023, **62**, e202218892.
33. P. Ma, Y. Chen, Y. Man, Q. Qi, Y. Guo, H. Wang, Z. Li, P. Chang, C. Qu, C. Han and H. Xu, *Angew. Chem., Int. Ed. Engl.*, 2024, **63**, e202316479.