

Electronic Supplementary Information (ESI)

Triphenylamine Derivatives: Different Molecular Packing, and the Corresponding Mechanoluminescent or Mechanochromism Property

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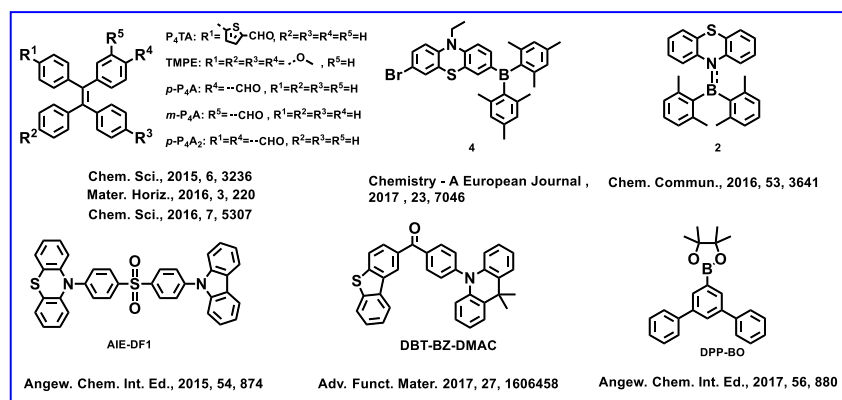
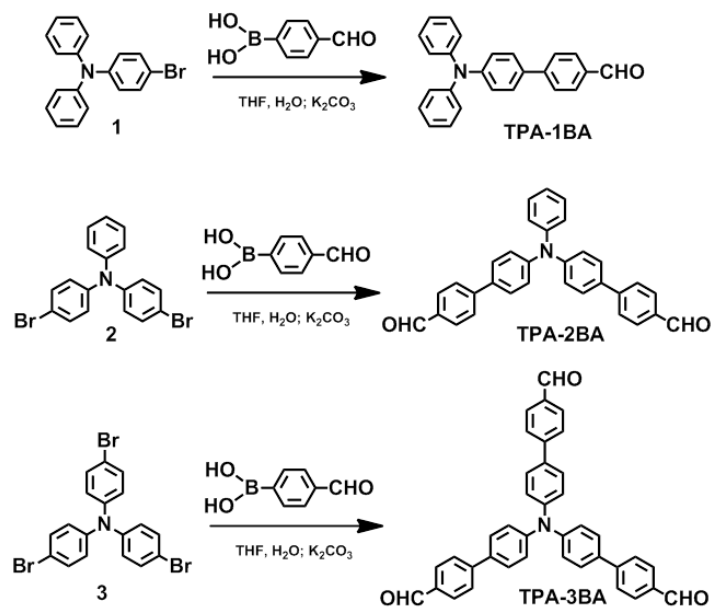


Chart S1. Chemical structures of molecules with AIE effect and ML character reported so far.



Scheme S1. Syntheses of TPA-1BA, TPA-2BA and TPA-3BA.

¹H-NMR
TPA-1BA

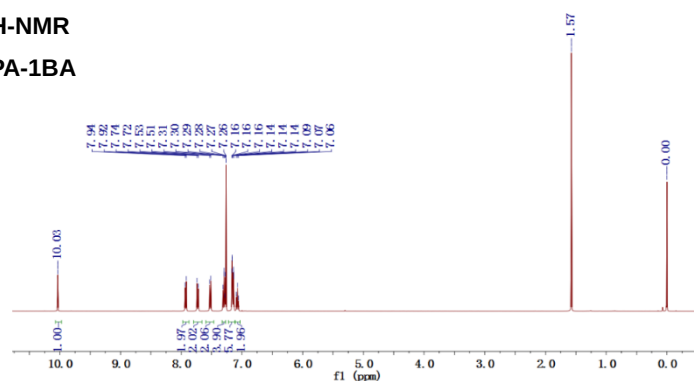


Figure S1. The ¹H NMR spectrum of TPA-1BA.

¹³C-NMR
TPA-1BA

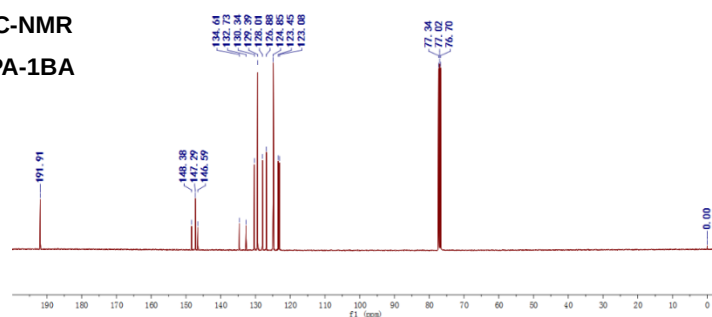


Figure S2. The ¹³C NMR spectrum of TPA-1BA.

¹H-NMR
TPA-2BA

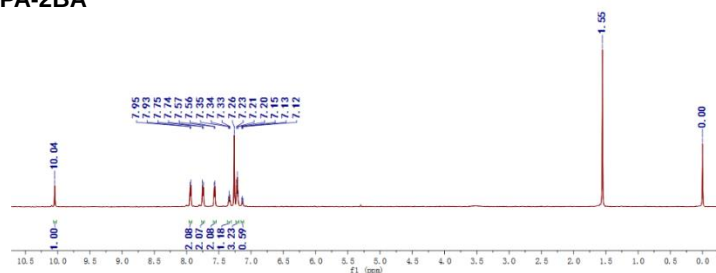


Figure S3. The ¹H NMR spectrum of TPA-2BA.

¹³C-NMR
TPA-2BA

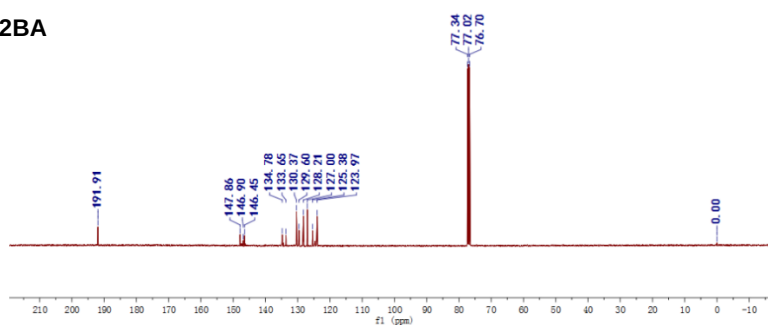


Figure S4. The ¹³C NMR spectrum of TPA-2BA.

¹H-NMR
TPA-3BA

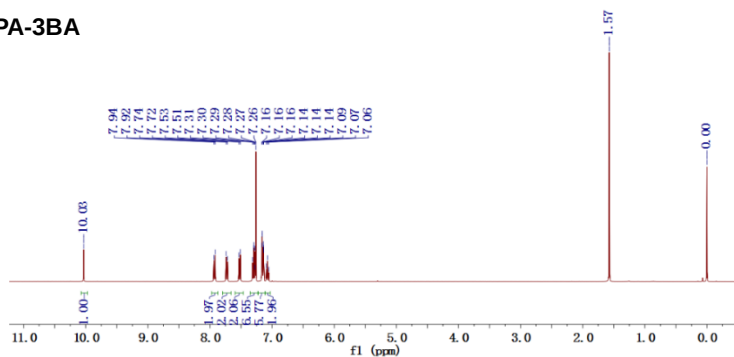


Figure S5. The ¹H NMR spectrum of TPA-3BA.

¹³C-NMR
TPA-3BA

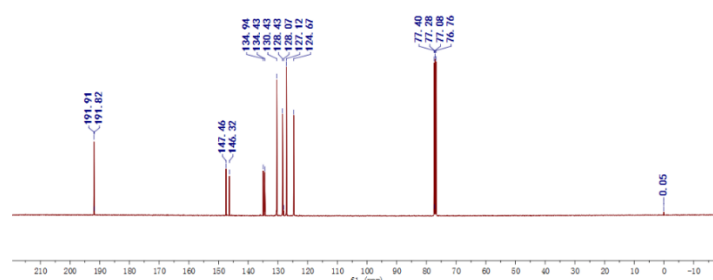


Figure S6. The ¹³C NMR spectrum of TPA-3BA.

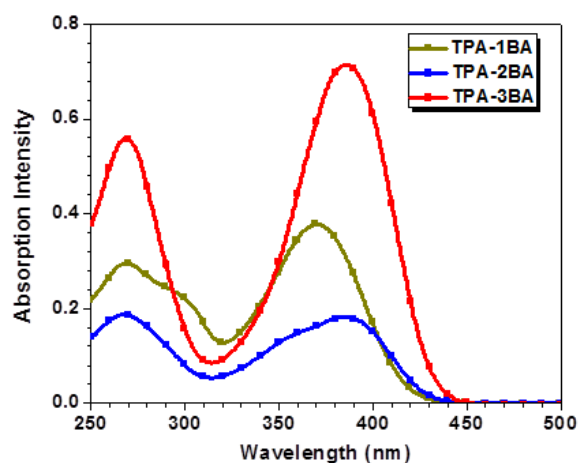


Figure S7. UV-Visible spectra of TPA-1BA, TPA-2BA and TPA-3BA in THF solution.

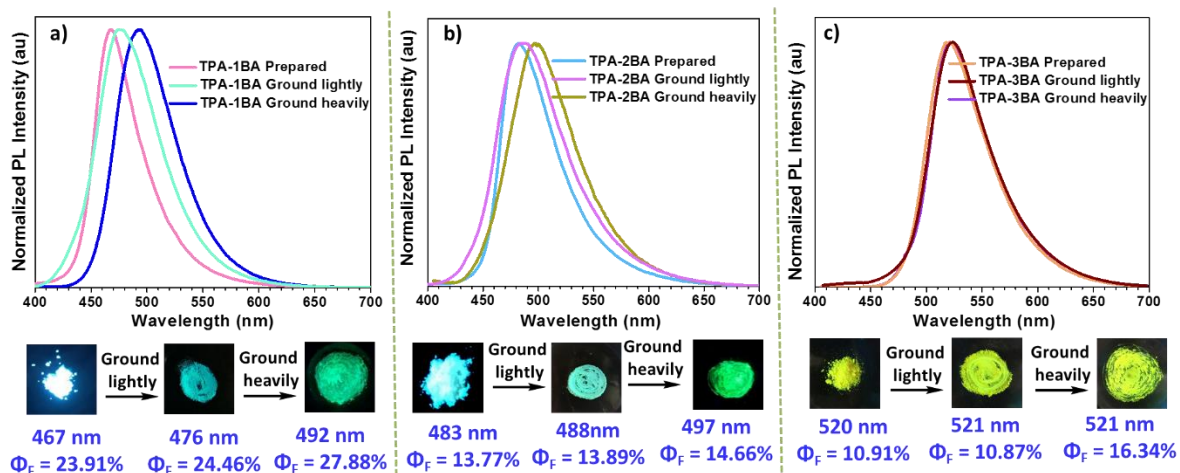


Figure S8. PL spectra of TPA-1BA (a), TPA-2BA (b) and TPA-3BA (c) before and after grinding in solid state. The inset depicts the images of TPA-1BA, TPA-2BA and TPA-3BA before and after grinding and the quantum efficiency of all compounds.

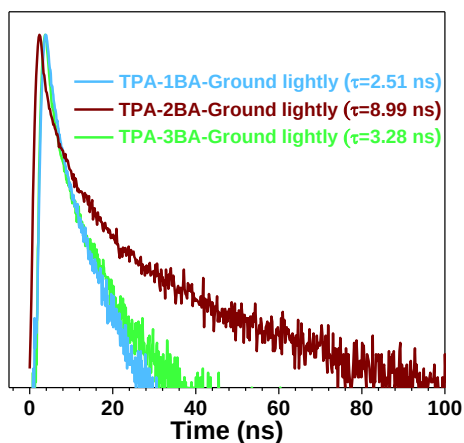


Figure S9. Emission decay of TPA-1BA-Ground lightly, TPA-2BA-Ground lightly and TPA-3BA-Ground lightly in solid state.

Table S1. Summary of crystal data and intensity collection parameters of TPA-1BA, TPA-2BA and TPA-3BA.

Compound	TPA-1BA	TPA-2BA	TPA-3BA
Empirical formula	C ₂₅ H ₁₉ N O	C ₃₂ H ₂₃ N O ₂	C ₃₉ H ₂₇ N O ₃
Formula weight	349.41	453.51	557.62
Crystal system	orthorhombic	monoclinic	monoclinic
Temp. / K	0 K	298 K	273 K
Space group	P c a 21	C 2/c	P 21/n
a / Å	15.937(5)	11.9284(13)	10.4521(18)
b / Å	18.010(6)	9.4890(11)	10.3512(18)
c / Å	13.493(4)	20.901(3)	27.549(5)
α / °	90	90	90
β / °	90	105.007(2)	99.008(3)
γ / °	90	90	90
volume / Å ³	3873(2)	2285.1(5)	2943.8(9)
Z	8	4	4
D _{calcd.} , g cm ⁻³	1.199	1.318	1.258
F(000)	1472.0	952.0	1168.0

Table S2. Summarizations of C-H $\cdots$ π interactions and C-H $\cdots$ O interactions in the TPA-1BA, TPA-2BA and TPA-3BA crystals.

Crystal	Intramolecular C-H... π	Number ^{a)}	C-H...O	Number ^{b)}
TPA-1BA _a	2.98-3.44 Å	13	2.50 Å	1
TPA-1BA _b	2.99-3.43 Å	12	2.68 Å	1
TPA-2BA	2.92-3.43 Å	9	2.68-3.42 Å	6
TPA-3BA	2.82-3.48 Å	19	2.59-3.00 Å	4

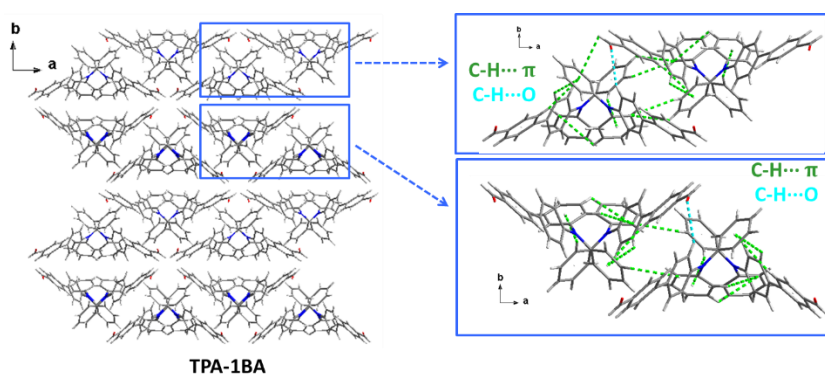


Figure S10. The C-H... π and C-H...O interactions in the TPA-1BA crystal.

Table S3. Summarization of the C-H... π and C-H...O interactions in the TPA-1BA_a crystal.

Type of Interaction	No.	d/Å
C-H ... π	1	3.33
	2	2.98
	3	3.42
	4	3.41
	5	3.21
	6	3.15
	7	3.44
	8	3.15
	9	3.42
	10	2.98
	11	3.44
	12	3.33
	13	3.21
C-H ... O	1	2.50

Table S4. Summarization of the C-H... π and C-H...O interactions in the TPA-1BA_b crystal.

Type of Interaction	No.	d/Å
C-H ... π	1	3.12
	2	3.00

	3	3.39
	4	3.43
	5	3.00
	6	3.13
	7	3.13
	8	3.12
	9	3.00
	10	3.39
	11	3.43
	12	3.00
C-H $\cdots$ O	1	2.68

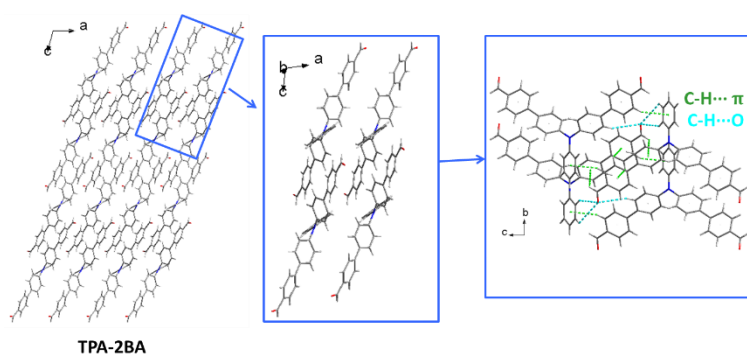


Figure S11. The C-H... π and C-H...O interactions in the TPA-2BA crystal.

Table S5. Summarization of the C-H... π and C-H...O interactions in the TPA-2BA crystal.

Type of Interaction	No.	d/Å
C-H $\cdots$ π	1	2.92
	2	3.24
	3	2.92
	4	3.43
	5	3.43
	6	2.92
	7	3.24
	8	2.92
C-H $\cdots$ O	1	3.34
	2	2.68
	3	3.42
	4	3.34
	5	2.68
	6	3.42

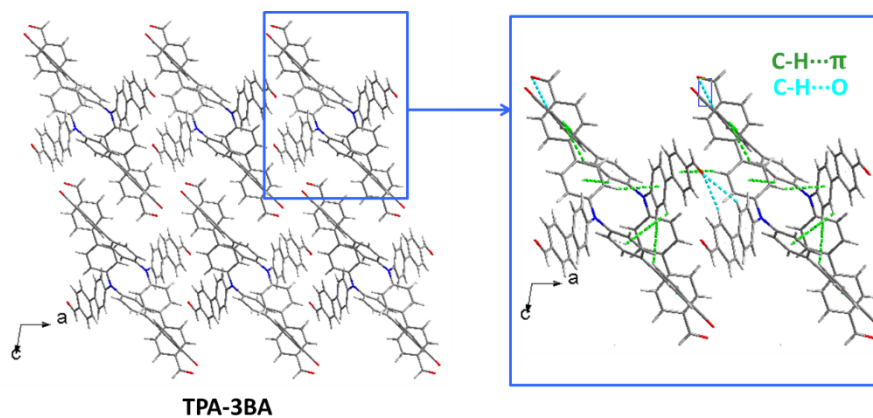


Figure S12. The C-H... π and C-H...O interactions in the TPA-2BA crystal.

Table S6. Summarization of the C-H... π and C-H...O interactions in the TPA-3BA crystal.

Type of Interaction	No.	d/Å
C-H $\cdots$ π	1	2.82
	2	3.48
	3	3.37
	4	2.92
	5	3.28
	6	3.14
	7	3.31
	8	2.84
	9	3.15
	10	2.82
	11	3.48
	12	3.37
	13	2.92
	14	3.28
	15	3.14
	16	3.31
	17	2.84
	18	3.15
	19	3.45
C-H $\cdots$ O	1	2.59
	2	2.82
	3	3.00
	4	3.00

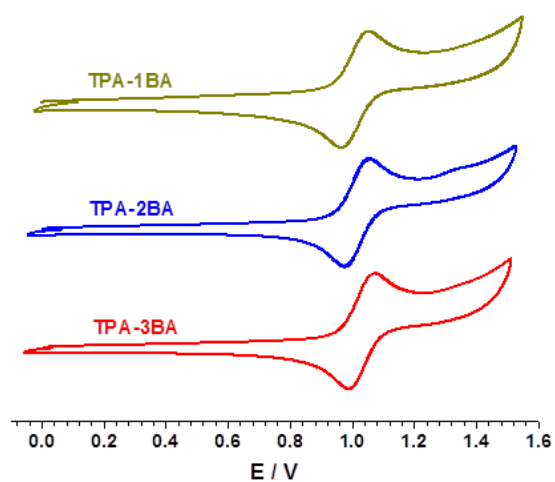


Figure S13. Cyclic voltammograms of compounds TPA-1BA, TPA-2BA and TPA-3BA.

The evaluations of k_r and k_{nr} were calculated by:

$$K_r = \Phi_F / \tau \quad (S1)$$

$$k_{nr} = k_r / \Phi_F - k_r \quad (S2)$$