Supporting Information

A triphenylamine derivative and its Cd(II) complex with high-contrast mechanochromic luminescence and vapochromism

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Figure S1 Molecular packing modes of HL·2CH₃CN and complex 1.



Figure S2 Fluorescence decay curves (excited at 371.8 nm): (a) $HL.2CH_3CN$ in different states, (b) Fit results of original sample monitored at 464 nm, (c) Fit results of ground sample of $HL.2CH_3CN$ monitored at 520 nm, (d) Fit results of HL-HCI monitored at 594 nm, (e) Fit results of $HL-HCI-NH_3$ monitored at 494 nm.



Figure S3 Fluorescence decay curves (excited at 371.8 nm): (a) **1** in different states, (b) Fit results of original sample monitored at 490 nm, (c) Fit results of ground sample of **1** monitored at 572 nm, (d) Fit results of **1-HCl** monitored at 587 nm, (e) Fit results of **1-HCl-NH₃** monitored at 503 nm.



Figure S4 CIE diagrams of HL \cdot 2CH₃CN and complex 1 with different treatments.



Figure S5 TGA curves of HL· 2CH₃CN in different states.



Figure S6 DSC curves of $HL \cdot 2CH_3CN$ (a) and complex 1 (b) in different states.



Figure S7 UV–Vis absorption spectra of HL·2CH₃CN (a) and complex 1 (b) in different states.



Figure S8 XPS spectra of HL· 2CH₃CN and HL-HCl.



Figure S9 XPS spectra of complex 1 and 1-HCl.

Table S1 Dihedral angles between different planes in $HL \cdot 2CH_3CN$ and complex 1.A/BB/CB/DC/D

HL·2CH ₃ C	O1-containing L	48.76	70.17	64.92	76.75
Ν	O3-containing L	47.10	71.03	55.92	80.41
Complex 1		12.05	79.76	60.49	83.40

 Table S2 Crystal data and structure refinement parameters of HL·2CH₃CN and complex 1.

Compound	HL·2CH ₃ CN	Complex 1
Empirical formula	$C_{60}H_{54}N_{10}O_4$	C ₂₆ H ₂₁ Cd _{0.5} ClN ₃ O ₂
Formula weight	975.10	499.11
Temperature/K	99.99(10)	100.00(1)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	11.5136(5)	7.2058(2)
b/Å	14.4562(5)	7.7740(3)
c/Å	16.3680(6)	20.4876(7)
α/°	75.824(3)	86.501(3)
β/°	85.556(3)	89.897(3)
γ/°	89.480(3)	83.117(3)
Volume/Å ³	2633.30(18)	1137.27(7)
Z	2	2
$\rho_{calc}(g \text{ cm}^{-3})$	1.230	1.458
μ/mm_{-1}	0.636	5.358
F(000)	1024.0	510.0
Radiation	CuKa ($\lambda = 1.54184$)	CuK α (λ = 1.54184)
2θ range for data	7.33 to 155.736	8.648 to 153.166
collection/°		
Index ranges	$-14 \le h \le 11, -18 \le k \le$	$-28 \le h \le 8, -9 \le k \le 9, -$
	$18, -20 \le 1 \le 20$	$25 \le 1 \le 25$
Reflections collected	32913	11748
R_{int}/R_{sigma}	0.0666/0.0553	0.0738/0.0623
Data/restraints/parameters	10507/0/673	4460/6/297
Goodness-of-fit on F ²	1.249	1.158
Final R indexes [I>=2σ	$R_1 = 0.0727, wR_2 =$	$R_1 = 0.0481, wR_2 =$
(I)]	0.1925	0.1288
Final R indexes [all data]	$R_1 = 0.0949, wR_2 =$	$R_1 = 0.0551, wR_2 =$
	0.2034	0.1306
Largest diff. peak/hole / e Å ⁻³	0.49/-0.29	0.93/-1.21
CCDC number	2099606	2099607