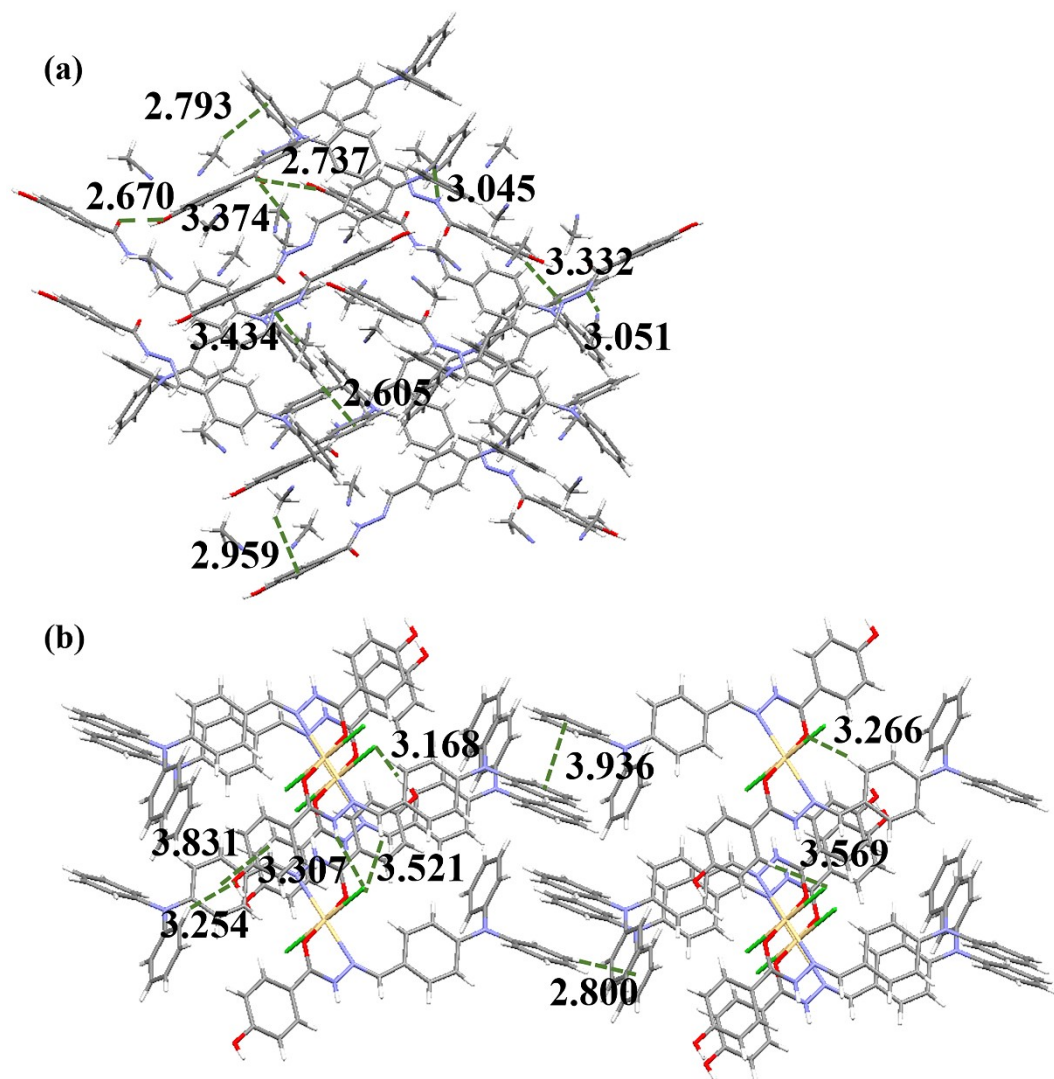# Supporting Information

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

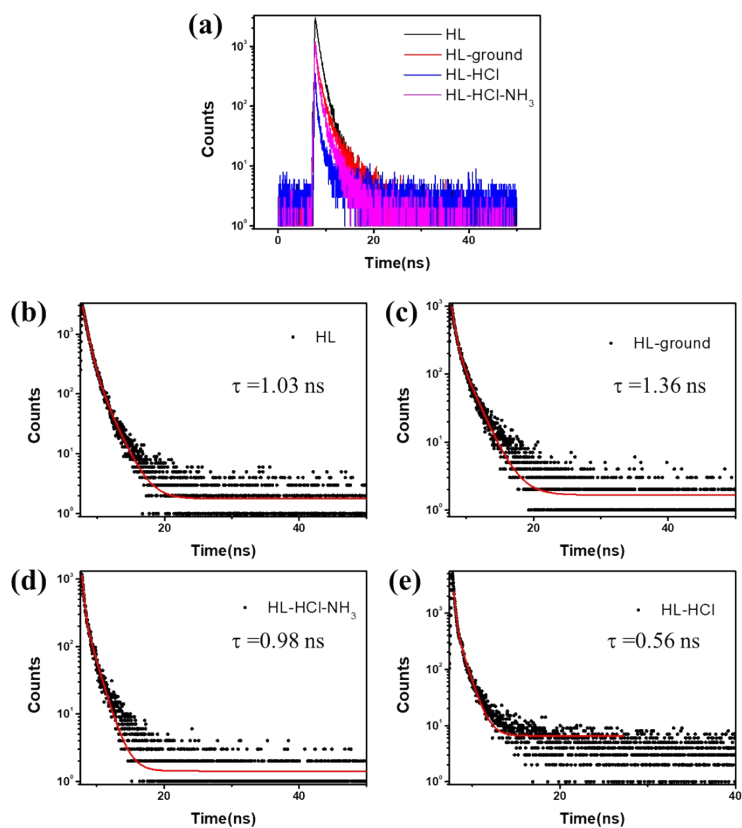Qiong-Fang Liang, Han-Wen Zheng, Dong-Dong Yang, Xiang-Jun Zheng*

Contents

(a)

(b)

Figure S1 Molecular packing modes of **HL**·2CH$_3$CN and complex **1**.

Figure S2 Fluorescence decay curves (excited at 371.8 nm): (a) **HL·2CH$_3$CN** in different states, (b) Fit results of original sample monitored at 464 nm, (c) Fit results of ground sample of **HL·2CH$_3$CN** monitored at 520 nm, (d) Fit results of **HL-HCl** monitored at 594 nm, (e) Fit results of **HL-HCl-NH$_3$** monitored at 494 nm.
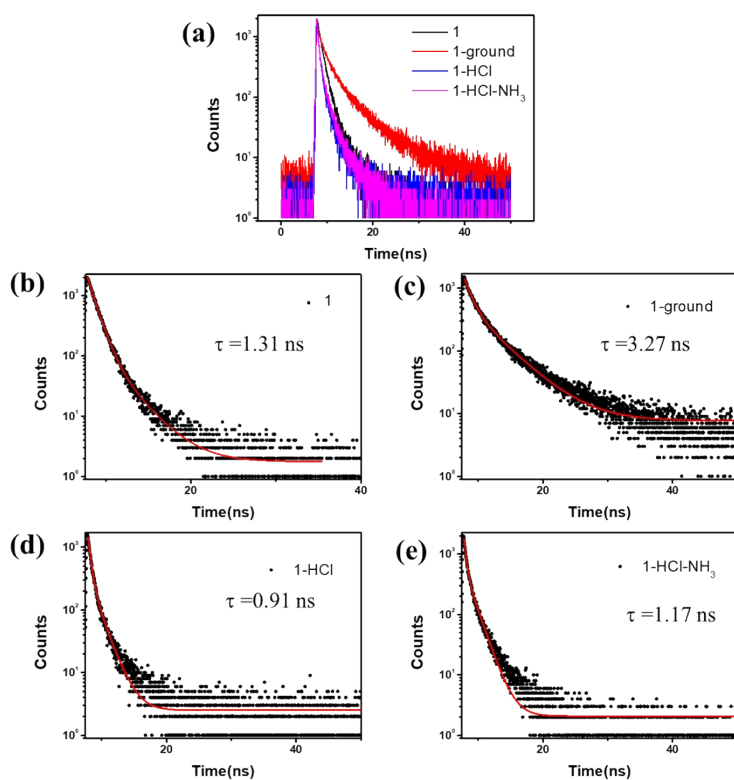
Figure S3 Fluorescence decay curves (excited at 371.8 nm): (a) **1** in different states, (b) Fit results of original sample monitored at 490 nm, (c) Fit results of ground sample of **1** monitored at 572 nm, (d) Fit results of **1-HCl** monitored at 587 nm, (e) Fit results of **1-HCl-NH₃** monitored at 503 nm.
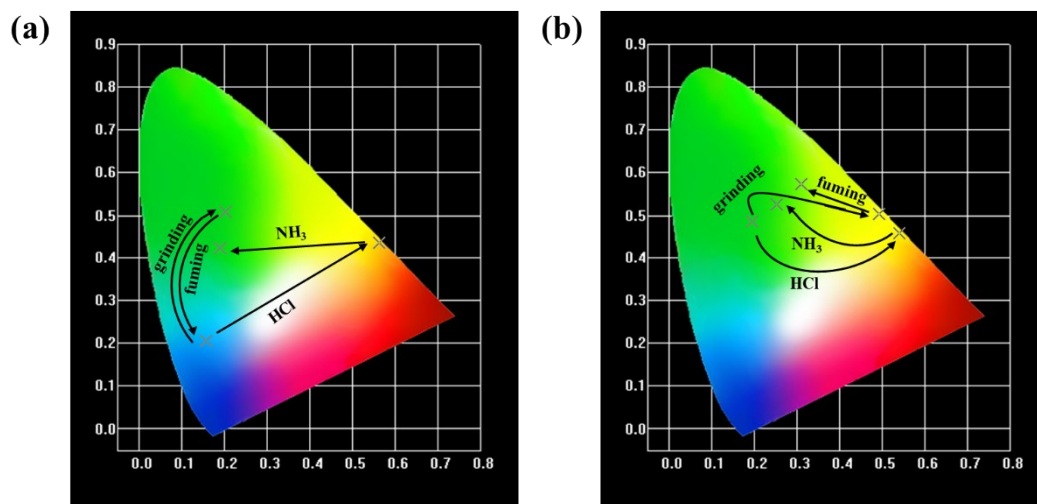
Figure S4 CIE diagrams of **HL**· 2CH₃CN and complex **1** with different treatments.
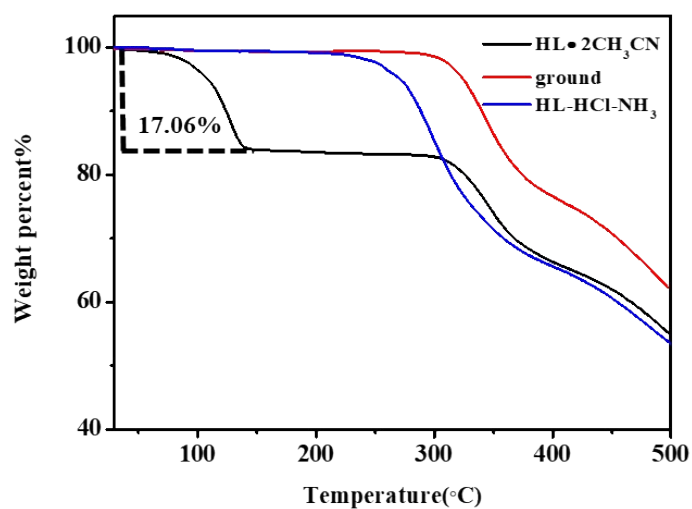
Figure S5 TGA curves of **HL**· 2CH₃CN in different states.
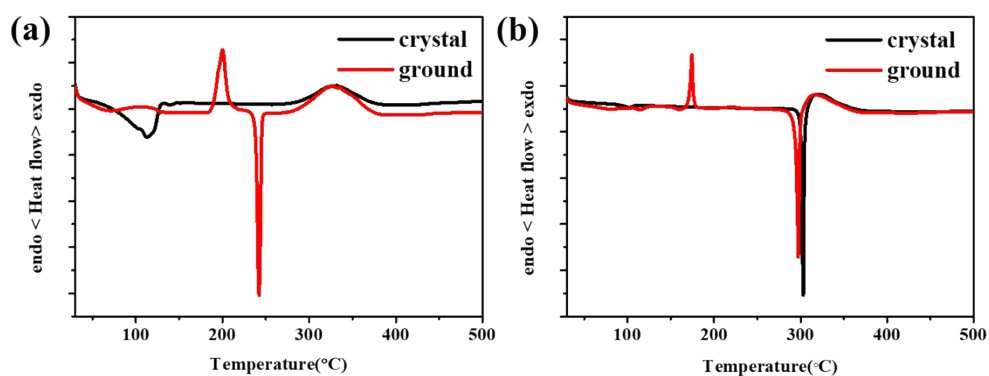
Figure S6 DSC curves of **HL**·2CH$_3$CN (a) and complex **1** (b) in different states.
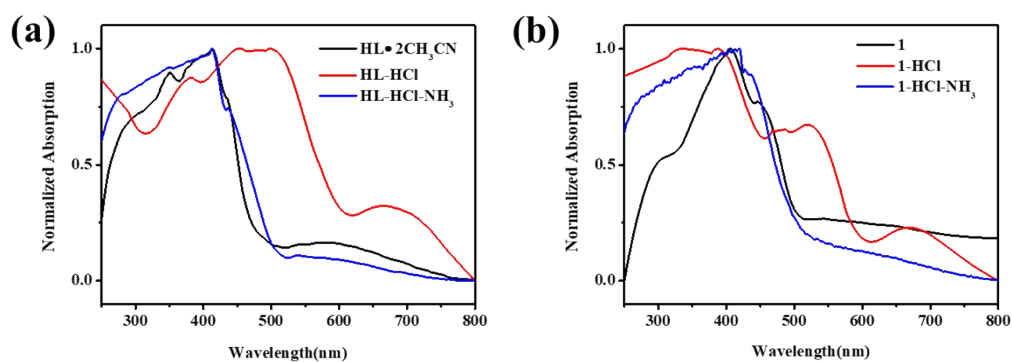
Figure S7 UV–Vis absorption spectra of **HL**·2CH$_3$CN (a) and complex **1** (b) in different states.
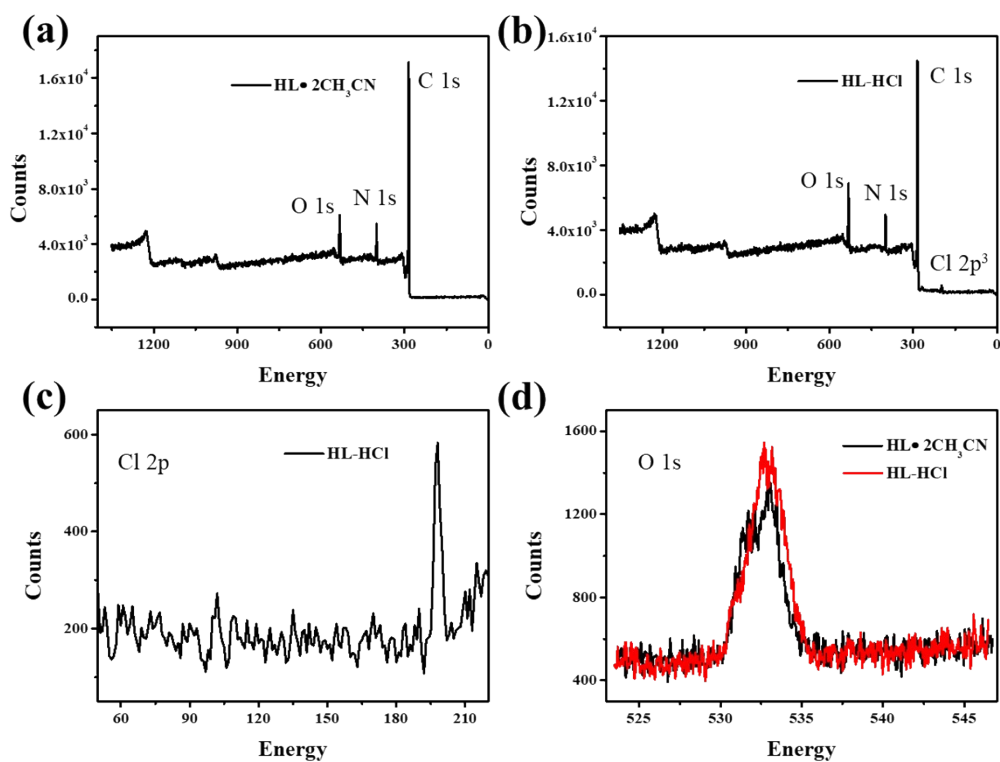
Figure S8 XPS spectra of **HL**· 2CH$_3$CN and **HL-HCl**.
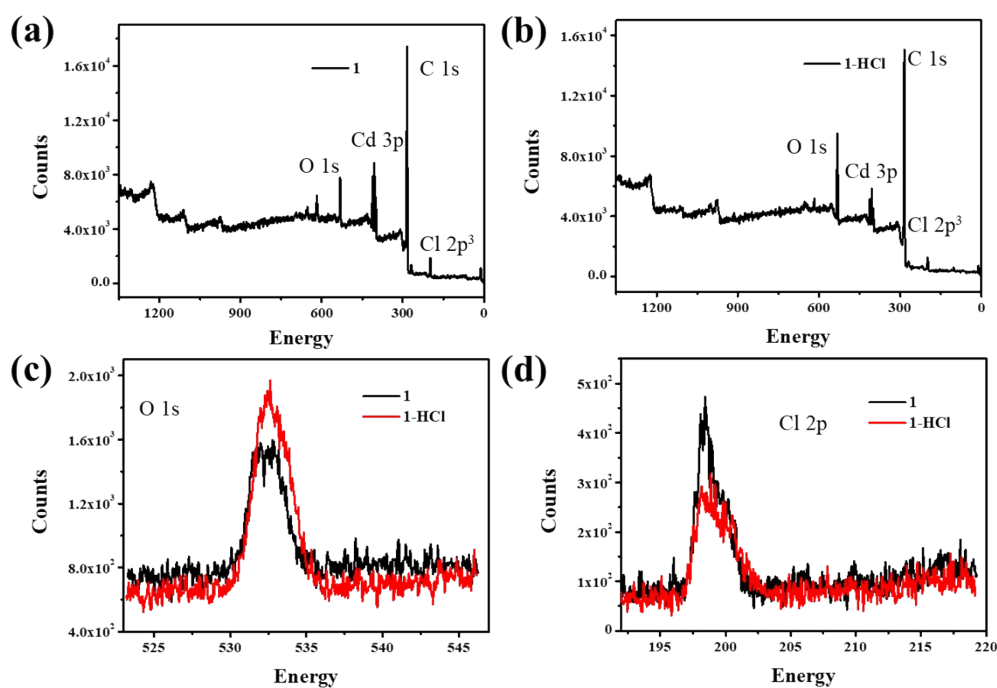
Figure S9 XPS spectra of complex **1** and **1-HCl**.

Table S1 Dihedral angles between different planes in **HL·2CH$_3$CN** and complex **1**.

	A/B	B/C	B/D	C/D

HL·2CH₃C N	O1-containing L	48.76	70.17	64.92	76.75
	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·2CH₃CN	Complex 1
Empirical formula	$C_{60}H_{54}N_{10}O_4$	$C_{26}H_{21}Cd_{0.5}ClN_3O_2$
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/Å³	2633.30(18)	1137.27(7)
Z	2	2
ρ_{calc}(g cm⁻³)	1.230	1.458
μ/mm₋₁	0.636	5.358
F(000)	1024.0	510.0
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range for data collection/°	7.33 to 155.736	8.648 to 153.166
Index ranges	-14 ≤ h ≤ 11, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20	-28≤ h ≤ 8, -9 ≤ k ≤ 9, -25 ≤ l ≤ 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 (I)]	$R_1 = 0.0727$, $wR_2 = 0.1925$	$R_1 = 0.0481$, $wR_2 = 0.1288$
Final R indexes [all data]	$R_1 = 0.0949$, $wR_2 = 0.2034$	$R_1 = 0.0551$, $wR_2 = 0.1306$
Largest diff. peak/hole / e Å⁻³	0.49/-0.29	0.93/-1.21
CCDC number	2099606	2099607