

Table 1 Crystal data and structure refinement for compounds **1**.

Compound	<b>1</b>
Chemical Formula	$[\text{Cd}(\text{C}_8\text{H}_6\text{O}_3\text{Cl})_2(\text{C}_{10}\text{H}_8\text{N}_2)]_n$
Empirical Formula	$\text{C}_{26}\text{H}_{20}\text{CdCl}_2\text{N}_2\text{O}_6$
Formula mass	639.75
Crystal system	Monoclinic
Space group	$C2/c$
$a$ (Å)	22.930(5)
$b$ (Å)	11.750(2)
$c$ (Å)	9.6800(19)
$\alpha$ (°)	90.00
$\beta$ (°)	98.82(3)
$\gamma$ (°)	90.00
$V$ (Å <sup>3</sup> )	2577.2(9)
$D_{\text{calc}}$ (g.cm <sup>-3</sup> )	1.649
$Z$	4
$F(000)$	1280
Limiting indices	$-26 \leq h \leq 29$ ; $-14 \leq k \leq 15$ ; $-12 \leq l \leq 12$
Goodness-of-fit on $F^2$	1.088
Collected reflections	10153
Independent reflections ( $R_{\text{int}}$ )	2940
Observed reflections ( $I > 2\sigma(I)$ )	2894
Final $R$ factors ( $I > 2\sigma(I)$ )	$R_1^{[a]} = 0.0268$ ; $wR_2^{[b]} = 0.0672$
Final $R$ factors (all data)	$R_1 = 0.0277$ ; $wR_2 = 0.0677$
Largest diff. map peak and hole eÅ <sup>-3</sup>	0.477 and -0.359

$$^{[a]} R_1 = \sum \left| |F_o| - |F_c| \right| / \sum |F_o| \quad . \quad ^{[b]} wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$$

Table 2 Parameters of hydrogen bonds and aromatic-aromatic interactions for compound **1**.

D-H...Cg	d(D-H) (Å)	d (H...Cg) (Å)	d (D...Cg) (Å)	H-Prep (Å)
C9-H9...Cg(1)A	0.9301(2)	3.0501(7)	3.7101(9)	2.9915(3)
C2-H2...Cg(2)B	0.9301(3)	3.185	3.7785(11)	2.9821(10)
Cg(I) -> Cg(J)	d <sub>c-c</sub> (Å)	dihedral angels (°)		
Cg(1) -> Cg(1) <sup>i</sup>	3.5104(5)	0.647		

[a] A, -x, y, 1/2-z; B, -x, -y, -z. [b] i, 3/2+x, 1/2-y, 1-z; ii, -x, y, 1/2-z. Definition of rings: Cg(1): C(1)-C(2)-C(3)-C(4)-C(5)-C(6); Cg(2): N(2)-C(12)-C(13)-C(14)-C(13)<sup>ii</sup>-C(14)<sup>ii</sup>.

Table 3 The assignments of FTIR spectra of all lignads and compounds **1** (cm<sup>-1</sup>).

Compounds Assignments	<b>1</b>	<b>bipy</b>	<b>PCPA</b>
$\nu$ (=C-H)	3068w	3068w	3013w
$\nu_{as}$ (-CH <sub>3</sub> )			
$\nu_{as}$ (-CH <sub>2</sub> -)	2936w		2916w
$\nu$ (Aromatic respiration)	1588s	1598s 1531m	1584m 1490s
$\nu_{as}$ (COO-)	1491s		1736s
$\nu_s$ (COO-)	1420m		
$\nu$ (C-N)	1282m	1222m	
$\nu$ (C-O)	1256m		1274m
$\nu_s$ (Ar-O-R)	1223m		1235m
$\gamma$ (=C-H)	830m	810m	821m
$\nu$ (C-Cl)	730w		707w

Table 4 The luminescent excitation and emission peaks of PCPA, 4,4'-bipy, compound **1**.

	$\lambda_{ex}$ (nm)	$\lambda_{em}$ (nm)
PCPA	296	313s, 371w
4,4'-bipy	369	459s, 496s
Compound <b>1</b>	378	459s, 496s

s: strong ; m: middle ; w: weak .