

## 含 2-苯基吡啶配体的中性铱配合物的合成,晶体结构及发光性质

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**摘要:** 本文合成了一种中性的铱配合物 $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCO})]$ ,并通过红外、核磁、电喷雾离子质谱和元素分析等对其进行了表征。通过 X 射线衍射确定了该配合物的晶体结构,该配合物晶体属于单斜晶系,空间群为  $P2_1/c$ 。其中  $a=0.994\,47(4)\text{ nm}$ ,  $b=1.480\,82(6)\text{ nm}$ ,  $c=2.247\,13(11)\text{ nm}$ ,  $\beta=101.183(2)^\circ$ ,  $V=3.246\,4(2)\text{ nm}^3$ ,  $Z=4$ ,  $D_c=1.647\text{ g}\cdot\text{cm}^{-3}$ ,  $F(000)=1\,592$ ,  $R_1=0.032\,8$ ,  $wR_2=0.098\,7$  ( $I>2\sigma(I)$ )。光致发光光谱表明,该配合物在二氯甲烷、氯仿和 DMF 中的最大发射波长分别为 485, 484 和 515 nm,即在二氯甲烷和氯仿中发蓝绿光,在 DMF 中发绿光。在强极性溶剂中,化合物的磷光最大发射波长发生了红移。

**关键词:** 中性铱配合物; 晶体结构; 磷光; 蓝绿光

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### Synthesis, Crystal Structure and Photoluminescence Properties of a Neutral Iridium(III) Complex Based on 2-Phenylpyridine Ligand

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**Abstract:** A neutral Iridium(III) complex  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCO})]$  has been synthesized and characterized by IR,  $^1\text{H}$  NMR, ESI mass spectra and elemental analysis. The crystal structure of the complex has been determined by X-ray analysis. The compound crystallizes in monoclinic, space group  $P2_1/c$  with  $a=0.994\,47(4)\text{ nm}$ ,  $b=1.480\,82(6)\text{ nm}$ ,  $c=2.247\,13(11)\text{ nm}$ ,  $\beta=101.183(2)^\circ$ ,  $V=3.246\,4(2)\text{ nm}^3$ ,  $Z=4$ ,  $D_c=1.647\text{ g}\cdot\text{cm}^{-3}$ ,  $F(000)=1\,592$ ,  $R_1=0.032\,8$  and  $wR_2=0.098\,7$  ( $I>2\sigma(I)$ ). The photoluminescence (PL) spectra of the complex in dichloromethane, chloroform and dimethylformamide (DMF) show emission maxima at 485, 484 and 515 nm, respectively, corresponding to blue-green light-emitting in dichloromethane and chloroform, green light-emitting in DMF. The results show that the PL maxima have red shifted in strong polar solvent. CCDC: 738942.

**Key words:** neutral iridium(III) complex; crystal structure; photoluminescence spectra; blue-green light emitting

## 0 Introduction

Iridium(III) cyclometalated complexes are attracting widespread interest because of their unique photo-physical properties and applications in organic light-emitting diodes (OLEDs)<sup>[1-13]</sup>. Several groups have used

extensively neutral iridium cyclometalated complexes in OLEDs and obtained up to 19% external quantum efficiencies<sup>[14-15]</sup>. The use of neutral iridium complexes, however, requires a complicated multilayered structure for charge injection, transport, and light emission<sup>[16-17]</sup>. For practical OLEDs applications, there have been

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continuous efforts to develop cyclometalated Ir(III) complexes with finely tuned phosphorescent emissions<sup>[18-23]</sup>. To date, the color tuning of phenylpyridine-containing cyclometalated Ir(III) complexes have mostly been done by altering the electronic structures of the phenylpyridine-based monoanionic bidentate cyclometalating ligand (C<sup>-</sup>N)<sup>[24-30]</sup>. Increasing the  $\pi$ -conjugation length or introducing fused heteroaromatic rings into the cyclometalating ligand cause a red shift in the emission<sup>[24-26,29]</sup>, whereas lowering the highest occupied molecular orbital (HOMO) by adding an electron-withdrawing group or raising the triplet state energy by use of a ligand with a strong ligand result in a blue shift in the emission<sup>[27-28,31]</sup>. Hence, in theory, the color of the emission from cyclometalated Ir(III) complexes can be tuned through the design and synthesis of novel cyclometalating ligands. Herein, we report the preparation and crystal structure of a neutral Ir(III) complex [Ir(ppy)<sub>2</sub>(PPh<sub>3</sub>)(NCO)] (**1**, Fig.1) (ppy=2-phenylpyridine, PPh<sub>3</sub>=triphenylphosphine) with a strong-field ligand NCO<sup>-</sup>. Photophysical properties and other characteristics of the complex are also investigated.

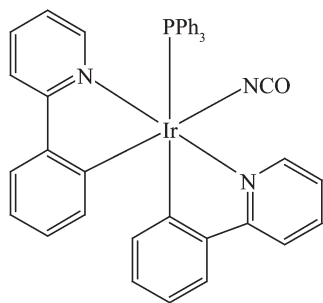


Fig.1 Chemical structure of complex **1**

## 1 Experimental

### 1.1 Materials and general method

All chemicals used were of analytical grade. Solvents were purified by conventional methods. <sup>1</sup>H NMR spectra were performed on a Bruker Avance 300 Hz Ultra shield spectrometer and reported as parts per million (ppm) from tetramethylsilane (TMS). IR spectra were recorded with a Thermo Nicolet FTIR-380 instrument (KBr discs) in 4 000~400 cm<sup>-1</sup> region. The C, H and N elemental analyses were carried out on a Thermo Finnigan Flash 1112A elemental analyzer.

Electrospray ionization (ESI) mass spectra were carried out with a Thermo Finnigan LCQADVANTAGE MAX mass spectrometer. Thermogravimetric analyses (TGA) were performed on a NETZSCH STA 449C thermal analyzer under nitrogen atmosphere at a heating rate of 10 °C·min<sup>-1</sup>. Absorption spectra were recorded on Perkin Elmer Lambda 35 ultraviolet spectrophotometer at room temperature. Photoluminescence (PL) analyses were performed on a Varian Cary Eclipse spectrofluorometer, at the highest spectral resolution, using an excitation wavelength of 360 nm. Spectra were corrected after measurement using the emission calibration obtained from measuring a calibrated lamp spectrum. PL quantum yields (PLQYs) were measured by a relative method using 1 µg·mL<sup>-1</sup> quinine sulfate in 1 N sulfuric acid as a standard<sup>[32]</sup>.

### 1.2 Synthesis of **1**

Sodium cyanate (0.021 g, 0.325 mmol) was added to a solution of [Ir(ppy)<sub>2</sub>(PPh<sub>3</sub>)Cl]<sup>[33]</sup> (0.051 g, 0.065 mmol) in chloroform (30 mL) under nitrogen. The mixture was refluxed with stirring for 24 h and then the unreacted sodium cyanate was removed by filtration. Evaporation under reduced pressure led to the crude product. Yellow block crystals of **1**, which were suitable for X-ray crystal structure analysis, were obtained by recrystallization from chloroform/hexane (1:3 V/V) in a yield of 0.032 5 g (64%). Anal.Calc(%) for **1** (C<sub>41</sub>H<sub>31</sub>IrN<sub>3</sub>OP, 804.90): C, 61.18; H, 3.88; N, 5.22. Found(%): C, 61.09; H, 3.95; N, 5.23. IR (KBr, cm<sup>-1</sup>):  $\nu$ (C=C, C=N) 1 606(s), 1 581(m), 1 478(s), 1 436(m);  $\nu$ (C≡N) 2 225(s). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (ppm):  $\delta$  9.33 (d,  $J$ =5.2 Hz, 1H), 8.87 (d,  $J$ =5.1 Hz, 1H), 8.72 (t,  $J$ =6.2 Hz, 2H), 7.91 (d,  $J$ =7.3 Hz, 2H), 7.75~7.70 (m, 2H), 7.61~7.41 (m, 4H), 7.19~7.09 (m, 9H), 6.91~6.69 (m, 4H), 6.63 (t,  $J$ =7.4 Hz, 1H), 6.55 (t,  $J$ =7.5 Hz, 1H), 6.07 (d,  $J$ =7.7 Hz, 1H), 5.91 (d,  $J$ =7.9 Hz, 1H), 5.86~5.80 (m, 2H). ESI-MS:  $m/z$ =763(M-NCO)<sup>+</sup>.

### 1.3 Structure determination

A block yellow crystal with dimensions of 0.20 mm×0.15 mm×0.12 mm was selected for X-ray analysis. All diffraction data were collected on a Bruker Smart APEX II CCD diffractometer equipped with a graphite

monochromatized Mo  $K\alpha$  radiation ( $\lambda=0.071\ 073\ \text{nm}$ ) at 293 (2) K using the  $\varphi$ - $\omega$  scan mode ( $2.86^\circ<\theta<26.68^\circ$ ). Cell parameters were retrieved using SMART software. Data reduction were performed using the SAINTPLUS software. Absorption corrections were applied using SADABS. The structure of **1** ( $\text{C}_{41}\text{H}_{31}\text{IrN}_3\text{OP}$ ) was solved by the direct methods using the SHELXS program of

the SHELXTL-97 package and refined with SHELXTL. All non-hydrogen atoms were refined anisotropic thermal parameters. Hydrogen atoms were introduced in calculated positions and included in the refinement, riding on their respective parent atoms. Crystallographic data for the complex are summarized in Table 1.

CCDC: 738942.

**Table 1** Crystallographic data for the complex

Empirical formula	$\text{C}_{41}\text{H}_{31}\text{IrN}_3\text{OP}$	$D_c / (\text{g} \cdot \text{cm}^{-3})$	1.647
Formula weight	804.86	$F(000)$	1592
Temperature / K	298(2)	Absorption coefficient / $\text{mm}^{-1}$	4.201
Crystal size / mm	0.20×0.15×0.12	$\theta$ range for data collection / $^\circ$	2.86~26.68
Crystal color, shape	Yellow, block	Index range ( $h, k, l$ )	(-11/12, -17/17, -24/27)
Crystal system	Monoclinic	Reflections collected	16 188
Space group	$P2_1/c$	Independent reflections	5 899
$a / \text{nm}$	0.994 47(4)	Data / restraints / parameters	5 889 / 62 / 424
$b / \text{nm}$	1.480 82(6)	Goodness-of-fit on $F^2$	1.167
$c / \text{nm}$	2.247 13(11)	final $R_1, wR_2$ indices [ $I>2\sigma(I)$ ]	0.032 8, 0.096 2
$\beta / ^\circ$	101.183(2)	$R_1, wR_2$ indices (all data)	0.039 4, 0.098 7
$V / \text{nm}^3$	3.246 4(2)	Largest diff. peak and hole / ( $\text{e} \cdot \text{nm}^{-3}$ )	3 291 and -2 154
$Z$	4		

## 2 Results and discussion

### 2.1 Structure analysis

The selected bond lengths and bond angles are listed in Table 2. X-ray single-crystal diffraction study reveals that complex **1** crystallizes in monoclinic with space group of  $P2_1/c$ . As depicted in Fig.2, complex **1** reveals an octahedral geometry around the Ir atom with one  $\text{NCO}^-$  anion, one  $\text{PPh}_3$  ligand and two N, C-bidentate ppy ligands. In neutral  $[\text{Ir}(\text{C}^{\wedge}\text{N})_2\text{LL}']$  type complexes, the structures of  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]^{[30]}$  and  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]^{[33]}$  have been reported. Even as

above-mentioned two complexes, two ancillary ligands ( $\text{NCO}^-$  and  $\text{PPh}_3$ ) in **1** are also in the *cis* positions. However, in cationic  $[\text{Ir}(\text{C}^{\wedge}\text{N})_2\text{LL}']^+$  type complex  $\{[\text{Ir}(\text{ppy})_2(\text{PPh}_3)_2]^+\}$ , two ancillary ligands ( $\text{PPh}_3$ ) are in the *trans* positions<sup>[34]</sup> obviously because  $\text{PPh}_3$  group is too large for the *cis*- $\text{Ir}(\text{ppy})_2$  moiety to have two  $\text{PPh}_3$  in the *cis* positions. In **1**, the pyridyl rings of two ppy ligands are in the *trans* positions and the phenyl rings of two ppy ligands locate in the *cis* positions with respect to Ir(III) center.

Two Ir-C (ppy) bond lengths are obviously different in **1**. The bond length between Ir atom and C

**Table 2** Selected bond lengths (nm) and bond angles ( $^\circ$ ) of complex **1**

Ir(1)-P(1)	0.241 73(14)	Ir(1)-C(22)	0.201 6(6)	Ir(1)-N(2)	0.204 6(5)
Ir(1)-C(11)	0.204 6(6)	Ir(1)-N(1)	0.206 3(4)	Ir(1)-N(3)	0.231 4(5)
P(1)-Ir(1)-N(1)	99.77(14)	N(2)-Ir(1)-N(3)	94.96(18)	N(2)-Ir(1)-C(22)	80.2(2)
P(1)-Ir(1)-N(2)	89.75(13)	N(3)-C(41)-O(1)	156.7(8)	N(3)-Ir(1)-C(22)	171.3(2)
P(1)-Ir(1)-N(3)	89.14(12)	N(1)-Ir(1)-C(11)	79.8(2)	C(11)-Ir(1)-C(22)	86.5(2)
P(1)-Ir(1)-C(11)	175.55(16)	N(2)-Ir(1)-C(11)	91.1(2)	Ir(1)-N(3)-C(41)	133.9(5)
P(1)-Ir(1)-C(22)	98.00(16)	N(3)-Ir(1)-C(11)	86.43(19)		
N(1)-Ir(1)-N(2)	169.07(18)	N(1)-Ir(1)-C(22)	93.1(2)		

Symmetry codes:  $x, -y-1/2, z-1/2$ .

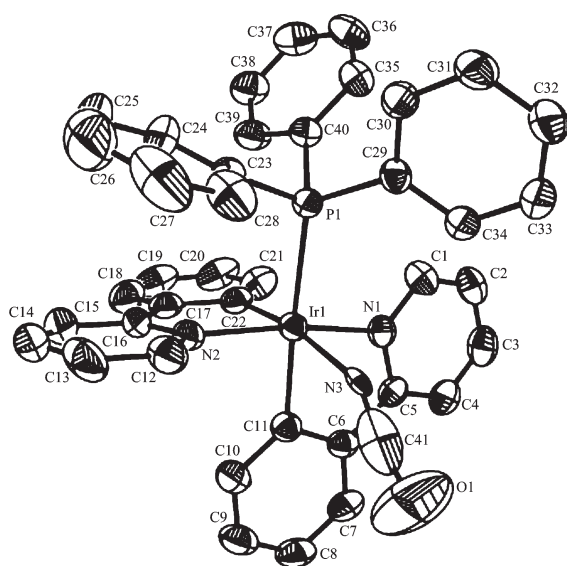


Fig.2 Molecular structure of **1** with all hydrogen atoms omitted for clarity

(ppy) atom which is in the *cis* position of  $\text{NCO}^-$  ligand with respect to the metal center (0.204 6(5) nm) is longer than that in the *trans* position of  $\text{NCO}^-$  ligand (0.201 6(6) nm). However, two Ir-C(ppy) bond lengths (0.203 1(8) nm and 0.202 4(7) nm) are slightly different in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]^{[33]}$ . This may be due to the greater *trans* effect of  $\text{NCO}^-$  in **1** compared with that of  $\text{Cl}^-$  in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]$ . As well as  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  (Ir-N(ppy)=0.205 6(3) nm and 0.206 8(3) nm)<sup>[30]</sup>, two Ir-N(ppy) bond lengths are slightly different in **1** (0.204 6(5) nm and 0.206 3(4) nm). Because two N(ppy) atoms are all in *cis* positions of  $\text{NCO}^-$  ligand with respect to the metal center. The average bond length of Ir-N(ppy) is 0.026 0 nm shorter than that of Ir-N( $\text{NCO}^-$ ) (0.233 3(4) nm), which is longer than that in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  (Ir-N( $\text{NCS}^-$ )=0.212 3(4) nm), because the coordination ability of  $\text{NCS}^-$  is stronger than that of  $\text{NCO}^-$ . Ir-P bond length in **1** (0.241 73(14) nm) is equal to that in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$ .

The bond angles about Ir atom in **1** do not indicate substantial distortion from octahedral regularity. The N3-C41-O1 bond angle of  $\text{NCO}^-$  ligand is 156.7(8)°, whereas the Ir1-N3-C41 angle is greatly bent at 133.9(5)°. These are obviously different from those in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  (N3-C39-S1=178.5(5)° and Ir1-N3-C39=172.9(4)°)<sup>[30]</sup>. In **1**,  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]$  and  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$ , two ancillary ligands are all in

the *cis* positions and one of ancillary ligands are same ( $\text{PPh}_3$ ). Different sizes of another ancillary ligands result in different steric hindrances between ancillary ligands and two ppy ligands. Two ppy groups are pushed away from the  $\text{PPh}_3$  ligand and the N1-Ir1-N2 bond angle is 169.07(18)°, which is little smaller than those in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  (169.18(14)°) and  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]$  (170.7(2)°). The N-Ir-N bond angles in three complexes decrease in the order of  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}] > [\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})] > \mathbf{1}$ . Moreover, the dihedral angle of the two ppy rings is 85.96(2)°, which is smaller than those in  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)\text{Cl}]$  (88.00(2)°) and  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  (89.25(2)°).

## 2.2 Thermal analysis

The TGA curves of **1** reveal that it is thermally stable up to 250 °C, above which  $\text{NCO}^-$  anion was removed with weight loss of 5.09 % (calcd. 5.22 %) from 250 to 320 °C. The gradual decomposition of  $\text{PPh}_3$  ligands proceeded above 500 °C for **1**, thus forming the final inorganic residue. The DSC curves of **1** reveal that there was an endothermic peak from 323 to 349 °C, which shows that it was beginning of the endothermic melting at 323 °C and complete melting at 349 °C. Fig.3 shows complex **1** is stable on air.

## 2.3 UV spectra

Fig.3 shows a comparison of absorption spectra of 0.1 mmol·L<sup>-1</sup> solutions of **1** in dichloromethane, chloroform and DMF at 298 K. The absorption spectra data of **1** are summarized in Table 3. The high-energy bands at around 281 nm are assigned to the intra-ligand  $\pi-\pi^*$  transition of 2-phenylpyridine and the low-energy bands

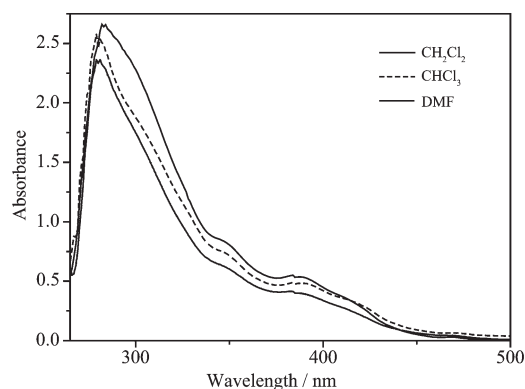


Fig.3 Absorption spectra of 0.1 mmol·L<sup>-1</sup> solutions of **1** in different solvents at 298 K

**Table 3** UV-Vis and PL spectrum data of complex **1** in different solvents at 298 K

Solvents	Abs. $\lambda_{\max}$ / nm ( $\epsilon$ / ( $\text{m}^3 \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ ))	PL $\lambda_{\max}$ / nm	PLQYs
$\text{CH}_2\text{Cl}_2$	468(0.29), 384(5.50), 349sh(8.18), 283(26.60)	485, 509	0.43
$\text{CHCl}_3$	469(0.65), 384(4.89), 279(25.79)	484	0.30
DMF	468(0.43), 383(4.15), 281(23.64)	515	0.26

at around 468 nm are categorized as metal-to-ligand charge-transfer transitions. In the spectra, the  $^1\text{MLCT}$  and  $^3\text{MLCT}$  bands are not distinct, as shown by the broad bands at around 384 nm. This is an indication of the strong-field ligands character in the MLCT states of the complex.

## 2.4 Photoluminescence

Fig.4 shows a comparison of PL spectra of 0.1  $\text{mmol} \cdot \text{L}^{-1}$  solutions of **1** in dichloromethane, chloroform and DMF at 298 K. PL spectra data of **1** in Table 3 show different curves and emission peaks, and the PL maxima have red shift in strong polar solvent. The PL maxima of **1** are 485, 484 and 515 nm, respectively; corresponding to blue-green luminescence in dichloromethane and chloroform, green luminescence in DMF. In dichloromethane, it can be clearly seen that the PL maxima blue shifts when compared with  $[\text{Ir}(\text{ppy})_2\text{Cl}]_2$ , which has an emission peak at around 512 nm<sup>[35]</sup>, and red shifts when compared with  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$ , which has an emission peak at around 477 nm<sup>[30]</sup>. The shifts in the PL spectra of **1** relative to  $[\text{Ir}(\text{ppy})_2\text{Cl}]_2$  and  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$  are consistent with the fact that the HOMO-LUMO energy gaps for **1** is larger than that of  $[\text{Ir}(\text{ppy})_2\text{Cl}]_2$  and smaller than that of  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCS})]$ . In DMF, emission peak of **1** has only one, while has two in dichloromethane and three in

chloroform. It shows that the photoluminescence color purity of **1** in DMF is better than those in dichloromethane and chloroform. The PLQYs of **1** in dichloromethane, chloroform and DMF are 0.43, 0.30 and 0.26, respectively, which are comparable with those of the related complexes.

## 3 Conclusions

In this paper, a neutral Iridium(III) complex  $[\text{Ir}(\text{ppy})_2(\text{PPh}_3)(\text{NCO})]$  was synthesized and characterized by IR,  $^1\text{H}$  NMR, ESI mass spectral, elemental analysis and X-ray crystallography. The photoluminescence (PL) spectra of **1** in dichloromethane, chloroform and dimethylformamide (DMF) show emission maxima at 485, 484 and 515 nm, respectively, corresponding to blue-green light-emitting in dichloromethane and chloroform, green light-emitting in DMF.

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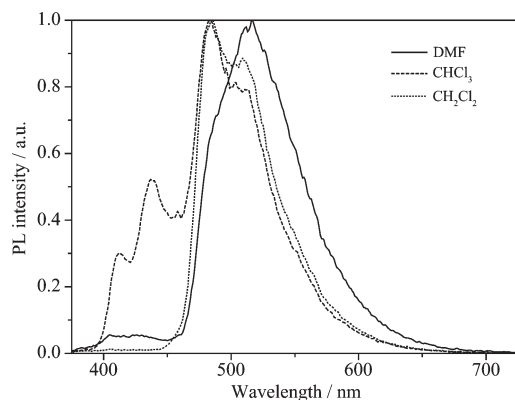


Fig.4 PL spectra of 0.1  $\text{mmol} \cdot \text{L}^{-1}$  solutions of **1** in different solvents at 298 K

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