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# Synthesis, Crystal Structure, and Photophysical Properties of Nickel Complex From Triphenylamine Schiff Base Ligand

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A novel Schiff base ligand L and its mononuclear nickel complex  $Ni(L)_2(SCN)_2$  were designed, synthesized and characterized by elemental analysis, IR spectra, MS, <sup>1</sup>H-NMR spectroscopy, and single-crystal X-ray diffraction analysis. The crystals of L and Ni  $(L)_2(SCN)_2$  belong to orthorhombic crystal system with the space group of  $P2_12_12_1$  for L and *Pbcn* for  $Ni(L)_2(SCN)_2$ , respectively. The center atom Ni(II) is coordinated with six nitrogen atoms in a distorted octahedron coordination environment. The four N atoms of them are from the two independent ligands and the other two nitrogen atoms from two SCN<sup>-</sup>. Their photophysical properties of the ligand and its Ni(II) complex were investigated and interpreted on the basis of theoretical calculations (TD-DFT).

Keywords: triphenylamine, Schiff base, crystal structure, photophysical properties

## Introduction

Triphenylamine and its derivatives have good solubility and easily film-formation, good electron-donating ability, low redox potential, high hole-transfer ability, strong fluorescence properties, and light stability, which have displayed promising properties in the development of light emission,<sup>[1,2]</sup> organic field-effect transistors (OFET), photovoltaic devices, and dye-sensitized solar cells.<sup>[3–6]</sup> Therefore, triphenylamine as a functional group has extensively been used to construct and prepare novel photoelectric materials.<sup>[7]</sup> On the other hand, Schiff base derivatives not only have novel structures, but also possess strong coordination ability as mono-, bi- and multidentate ligands, which can coordinate with various transition and rare earth metal ions to form Schiff base complexes,<sup>[8-14]</sup> which have important applications in photosensitive materials, catalytic materials, semiconductor materials, and antibacterial and antitumor uses.<sup>[15-22]</sup>

Relying on consideration previously, we designed and synthesized a novel Schiff base ligand L and its nickel complex  $Ni(L)_2(SCN)_2$ . The design strategy is based on the following: (a) triphenylamine as donor group, the C = N as the bridge and connecting with pyridine group to construct the novel D- $\pi$ -A model ligand<sup>[23,24]</sup>; (b) in order to enhance the solubility and the electron delocalizability of the molecule, ethyl oxygen was attached to the triphenylamine moiety; (c) as a result of the nickel coordinated by the ligand,<sup>[25]</sup> higher electron delocalization system forms within the functional coordination compounds.

At the present work, a novel Schiff base ligand L and its mononuclear nickel complex were synthesized. And then, their photophysical properties of them were systematically investigated both experimentally and theoretically. The synthetic procedure of Schiff base derivates are shown in Scheme 1.

## Experimental

#### Instruments and Reagents

Ni(SCN)<sub>2</sub>, 2-pyridine formaldehyde and the other reagents are analytically pure, and all will be purified before using according to the standard methods. IR spectra (4000–400 cm<sup>-1</sup>) as KBr pellets while far-IR spectra (40–400 cm<sup>-1</sup>) as nujol mull, were recorded on a Nicolet FT-IR 870 SX spectrophotometer. The <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra recorded on at 25°C using Bruker 400 Ultrashield spectrometer were reported as parts per million (ppm) from TMS ( $\delta$ ). MALDI-TOF mass spectra were recorded using Bruker Autoflex III Smartbeam. Elemental analyses were carried out on a Perkin Elmer 240 analyzer. Melting point is measured on METTLER TOLEDOFP-62 instruments. UV spectra were recorded on a SHIMADZU UV-3600 spectrophotometer. The concentration of sample solution was  $1.0 \times 10^{-5}$ mol/L.

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Sch. 1. Synthetic of the ligand L.

#### Synthesis

Synthesis of 4-ethoxy-N-(4-ethoxyphenyl)-N-(4-nitrophenyl) benzenamine (2). Added iodine benzene ether (3.72 g, 15 mmol), paranitroaniline (0.69 g, 5 mmol), anhydrous potassium carbonate (2.76 g, 20 mmol), L-proline (0.12 g), and cuprous iodide (0.10 g) were dissolved in DMSO solution and stirred for 48 h at 90°C under nitrogen. Under cooling to room temperature, the mixture solution was poured into water, and then extracted by ethyl acetate, the organic phase was dried by anhydrous magnesium sulfate, extraction filtration, the product was purified by column chromatography (silica gel, 10:1 petroleum ether/ethyl acetate) to give a solid. Yield: 64%. <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-CDCl<sub>3</sub>): 1.408–1.443 (t, 6H), 4.006–4.058 (q, 4H), 6.736–6.759 (d, 2H), 6.880–6.901 (d, 4H), 7.107–7.128 (d, 4H), 7.978–8.001 (d, 2H).

Synthesis of  $(E) -N^{1}$ - benzylidene- $N^{4}$ ,  $N^{4}$ - bis(4-ethoxyphenyl) benzene-1,4- diamine. 4-ethoxy-N-(4-ethoxyphenyl)-N-(4-nitrophenyl) benzenamine (1.00 g, 2.6 mmol) was dissolved in 8 mL ethanol solution, and refluxed, then carbon palladium



Fig. 1. Single molecular crystal structure of L.

catalyst (0.40 g) was added. Then slowly added 4 mL hydrazine hydrate (diluted with 2 mL ethanol). After 30 min, white solid appeared, and was filtered. The above solid (3.48 g, 10 mmol) and 2-pyridine formaldehyde (1.61 g, 15 mmol) were dissolved in ethanol and reflux. After 2 h, red solid precipitation appeared. Under cooling to room temperature, red crystal were separated by filtration and washed with ethanol. Yield: 91%. M. P. 147.8°C. IR (KBr, cm<sup>-1</sup>): 3035, 2978, 2907, 2866, 1626, 1565, 1504, 1479, 1335, 1245, 1046, 829. <sup>1</sup>H-NMR (400MHz, DMSO-d<sub>6</sub>) δ: 1.308–1.342 (t, 6H), 3.984–4.035 (q, 4H), 6.787-6.807 (d, 2H), 6.907-6.928 (d, 4H), 7.034-7.055 (d, 4H), 7.291–7.312 (t, 2H), 7.465–7.495 (t, 1H), 7.899–7.937 (d, 1H), 8.108-8.127 (d, 1H), 8.613 (1H), 8.678-8.689 (d, 1H). <sup>13</sup>C-NMR (100MHz, CDCl<sub>3</sub>) : 156.9, 155.4, 155.0, 149.5, 148.3, 142.8, 140.6, 136.6, 126.7, 124.6, 122.4, 121.6, 120.6, 115.3, 63.7, 14.9. Anal. Calcd. For C<sub>28</sub>H<sub>27</sub>N<sub>3</sub>O<sub>2</sub>: C, 76.85; H, 6.17; N, 9.607; Found: C, 76.68; H, 6.17; N, 9.58. MS: m/z: 438.58([M<sup>+</sup>]).

Synthesis of  $Ni(L)_2(SCN)_2$ . The ligand L (0.44 g, 1 mmol) was dissolved in methanol and stirred until clear solution appeared, and then  $Ni(SCN)_2$  (0.087 g, 0.5 mmol) was added, the mixture solution was refluxed for 4 h. Under cooling to room temperature, the precipitate was washed with distilled water and methanol. The





**Fig. 3.** (Top) Single molecular crystal structure of  $Ni(L)_2(SCN)_2$  (The solvent molecule  $H_2O$  was omitted) and (bottom) coordination environment of Ni with atom numbering scheme.

crystals were obtained by slow evaporation from acetone. Yield: 86%. M. P. >300°C. IR (KBr, cm<sup>-1</sup>): 3035, 2978, 2907, 2866, 2084, 1596, 1566, 1502, 1475, 1320, 1245, 10465, 829. FT-IR: 524, 417, 321.  $C_{58}H_{54}N_8O_4S_2Ni$ : Anal. Calcd. C, 66.34%; H, 5.15%; N, 10.68%. Found: C, 66.09%; H, 5.14%; N, 10.63%.

**Table 1.** Crystal data and structure refinement for the ligand and the complex

	L	$[Ni(L)_2(SCN)_2] \bullet H_2C$
Chemical formula Formula weight Crystal system Space group	$\begin{array}{c} C_{28}H_{27}N_3O_2\\ 437.53\\ Orthorhombic\\ P2_12_12_1 \end{array}$	$\begin{array}{c} C_{116}H_{110}N_{16}Ni_{2}O_{9}\ S_{2}\\ 2117.86\\ Orthorhombic\\ Pbcn \end{array}$
a (nm)	0.98761(15)	2.4128(5)
b (nm)	1.27433(19)	1.5869(5)
c (nm)	1.9430(3)	2.9819(5)
$V (nm^3)$ Z	2.4454(6) 4	2.9819(3) 11.417(5) 4
$D_{c} (g \cdot cm^{-3})$	1.188	1.232
$\mu (mm^{-1})$	0.076	0.465
F(000)	928	4440
$\theta$ rang (°)	1.91–24.99	1.37–25.10
Reflections collected	11515	52253
Reflections unique	4204	10170
Parameters	307	673
Max, min $\Delta \rho$ (e Å <sup>-3</sup> )	0.513, -0.364	0.629, -0.472
R <sub>1</sub> , wR <sub>2</sub> [I $\geq 2\sigma$ (I)]	0.0690, 0.1863	0.0748, 0.1553
R <sub>1</sub> , wR <sub>2</sub> [all data]	0.1096, 0.2251	0.2171, 0.1887
GOF	1.033	1.077

Table 2. Selected bond lengths (Å) and angles (°) of L

N(1)-C(17)	1.388(5)	C(3)-O(1)-C(1)	118.9(3)
N(1)-C(6)	1.432(5)	C(17)-N(1)-C(6)	120.9(3)
N(1)-C(14)	1.442(5)	C(17)-N(1)-C(14)	121.7(3)
O(1)-C(1)	1.423(6)	C(6)-N(1)-C(14)	116.8(3)
C(3)-O(1)	1.355(5)	N(3)-C(24)-C(25)	118.5(3)
C(20)-N(3)	1.440(6)	C(24)-N(3)-C(20)	114.6(3)
N(3)-C(24)	1.369(3)	C(25)-N(2)-C(29)	116.2(6)
C(24)-C(25)	1.453(6)	C(25)-N(2)	1.327(7)

#### X-Ray Crystallography

The X-ray diffraction measurements were performed on a Bruker SMART CCD area detector using graphite monochromated Mo-K<sub> $\alpha$ </sub> radiation ( $\lambda = 0.71069$  Å) at 298 (2) K. Intensity data were collected in the variable  $\omega$ -scan mode. The structures were solved by direct methods and difference Fourier syntheses. The non-hydrogen atoms were refined anisotropically and hydrogen atoms were introduced geometrically. Calculations were performed with SHELXTL-97 program package.<sup>[26]</sup>

#### **Computational Details**

Optimizations were carried out with B3LYP [LANL2DZ] without any symmetry restraints, and the TD-DFT {B3LYP [LANL2DZ]} calculations were performed on the optimized structure. All calculations, including optimizations and TD-DFT, were performed with the G03 software.<sup>[27]</sup> Geometry optimization of the singlet ground state and the TD-DFT calculation of the lowest 25 singlet-singlet excitation energies were calculated with a basis set composed of 6-31G for C, H, N, and O atoms and the Lanl2dz basis set for the Ni atom was download from the EMSL basis set library. The lowest 25-spin allowed singlet-singlet transitions, up to energy of about 5 eV, were taken into account in the calculation of the absorption spectra.

## **Results and Discussion**

## Structural Studies

The molecular structure of L and Ni(L)<sub>2</sub>(SCN)<sub>2</sub> are shown in Figures 1–4, respectively. Selected bond lengths and angles are summarized in Tables 1–3, respectively.

Table	3.	Selected	bond	lengths	(Å)	and	angles	(°)	of	Ni
(L) <sub>2</sub> (S	CN	)2								

N(2)-Ni(1)	2.113(5)	N(7)-Ni(1)-N(2)	91.6(2)
N(4)-Ni(1)	2.136(4)	N(2)-Ni(1)-N(4)	78.0(2)
N(7)-Ni(1)	2.005(6)	N(7)-Ni(1)-N(4)	168.1(2)
C(26)-N(2)	1.320(7)	C(26)-N(2)-Ni(1)	113.9(4)
C(25)-C(26)	1.462(8)	C(25)-N(4)-Ni(1)	111.7(4)
C(25)-N(4)	1.256(6)	N(2)-C(26)-C(25)	114.7(6)



Fig. 4. 1-D chain structure of Ni(L)<sub>2</sub>(SCN)<sub>2</sub>.



Fig. 5. Linear absorption spectra of the ligand L and the complex Ni(L)<sub>2</sub>(SCN)<sub>2</sub> (c =  $1.0 \times 10^{-5}$ mol/L).

Structure of L. As shown in Figure 1, the pyridine ring and the benzene ring display an almost co-planar configuration with dihedral angle of 6.44°. The bond lengths of L, such as C(20)-N(3) (1.440 (6) Å), N(3) = C(24) (1.369 (3) Å), and C (24)-C(25) (1.453 (6) Å), revealed that there is a highly  $\pi$ -electron delocalized system within the ligand molecule. The onedimensional chain structure of L is shown in Figure 2, it can be seen that the adjacent molecules are stacked through C(2)-H(2A)...O(2) (H...O is 2.6635 Å and the angle is 165.62°) (symmetry codes: x, +y-1, +z) hydrogen bond interactions.

Structure of Ni(L)<sub>2</sub>(SCN)<sub>2</sub>. In the asymmetric unit of the molecular structure (shown in Figure 3) contains two independent molecules. The bond lengths and angles in the two Schiff base ligands are similar for each other. It can be seen that the nickel atom is in a distorted octahedral coordination, and the nickel was coordinated by two Schiff base ligands and two SCN<sup>-</sup> ions. The bond distance Ni(1)-N(2) (2.113 (5) Å), Ni(1)-N(4) (2.136 (4) Å), and Ni(1)-N(7) (2.005 (6) Å) are very similar. This distorted octahedral coordination geometry is fairly regular with the six bond angles close to 90° around the metal center. The bond lengths of Ni(L)<sub>2</sub>(SCN)<sub>2</sub>, such as C(22)-N(4) (1.414 (6) Å), N(4) = C(25) (1.256 (6) Å), and C (25)-C(26) (1.462 (8) Å), revealed that there is a highly  $\pi$ -electron delocalized within the molecule compared with L. On the other hand, the dihedral angle between the pyridine ring

and the benzene ring is  $51.17^{\circ}$ , which is larger than that of L. The one-dimensional chain structure forms from the interactions of Ni(L)<sub>2</sub>(SCN)<sub>2</sub> molecules, as shown in Figure 4. As shown that the adjacent molecules are stacked through C(2)-H(2)...S(1) (symmetry codes: x - 1/2, +y - 1/2, -z + 1/2+1) (H...S is 2.965 Å and the angle is 130.23°) hydrogen bond interactions.



**Fig. 6.** Molecular orbital energy diagram for L and Ni  $(L)_2(SCN)_2$ .

Table 4. Calculated leaner absorption properties (nm), excitation energy (eV), oscillator strengths, and major contribution for L and Ni(L)<sub>2</sub>(SCN)<sub>2</sub>

$\Delta E_1{}^{aa}$	$\lambda (nm)^{bb}$	Oscillator strengths	Nature of the transition
2.996	413	0.785	116(HOMO)→
			117(LUMO)(0.65)
4.209	294	0.063	$116(HOMO) \rightarrow$
0 700	450	0.014	121(LUMO+5)(0.60)
2.703	458	0.014	$264(HOMO-6) \rightarrow$
1 222	202	0.002	2/1(LUMO)(0.54)
7.223	293	0.002	$209(1101010-1) \rightarrow 277(LUMO+6)(0.52)$
	$\Delta E_1^{aa}$ 2.996 4.209 2.703 4.223	$\begin{array}{c} \Delta E_1^{aa} \ \lambda \ (nm)^{bb} \\ \hline 2.996 \ 413 \\ 4.209 \ 294 \\ 2.703 \ 458 \\ 4.223 \ 293 \end{array}$	$\Delta E_1^{aa}$ $\lambda (nm)^{bb}$ Oscillator strengths2.9964130.7854.2092940.0632.7034580.0144.2232930.002

<sup>a</sup>The energy gap of the single-photon absorption band.

<sup>b</sup>Peak position of the linear absorption band.

#### Linear Absorption Spectra and TD-DFT

The linear absorption spectra of L and Ni(L)<sub>2</sub>(SCN)<sub>2</sub> in four different solvents are shown in Figure 5. It can be seen that the linear absorption spectra of L features an intense absorption at 410 nm, which originates from  $\pi \rightarrow \pi^*$  transition or intramolecular charge transfer (ICT) transition, while the high-energy band was assigned to the  $\pi \rightarrow \pi^*$  transition of the triphenylamine moiety. The high-energy band of the complex Ni(L)<sub>2</sub>(SCN)<sub>2</sub> is similar to the ligand L, while the low-energy band was tentatively assigned to the LMCT transitions between the ligand  $\pi^*$  and the Ni(II)  $d\pi$  orbitals.

TD-DFT computational studies were performed to elucidate the electronic structures of the ground state of L and Ni  $(L)_2(SCN)_2$ . The schematic representation of the molecular orbitals of L and Ni $(L)_2(SCN)_2$  were exhibited in Figure 6, and the energies and compositions of some frontier orbitals were listed in Table 4.

The band originates from a HOMO $\rightarrow$ LUMO for L transition was assigned to  $\pi \rightarrow \pi^*$  transition. The transition at 294 nm correspond to the HOMO $\rightarrow$ LUMO+5 for L, which can be assigned to  $\pi_{\text{triphenylamine}} \rightarrow \pi^*$  triphenylamine transition. The low-energy band calculated at 458 nm (f = 0.014) of Ni (L)<sub>2</sub>(SCN)<sub>2</sub>. This band mainly originates from transitions of HOMO-6 $\rightarrow$ LUMO, which can be assigned to a LMCT transition due to the ligand characteristic HOMO and the metal ions center characteristic LUOMO. The high-energy band calculated at 293 nm of Ni(L)<sub>2</sub>(SCN)<sub>2</sub> is similar to the ligand L. This band mainly originates from transitions of HOMO- $1\rightarrow$ LUMO+6, which can be assigned to  $\pi_{\text{triphenylamine}} \rightarrow \pi^*$ triphenylamine transition. The results are well consistent with that from the experiments.

#### Conclusion

A novel ligand L and its mononuclear nickel complex Ni  $(L)_2(SCN)_2$  have been synthesized and confirmed by a singlecrystal X-ray diffraction analysis. The photophysical properties of them were investigated and interpreted on the basis of theoretical calculations (TD-DFT). TD-DFT calculations suggested that the high-energy transitions were mainly  $\pi_{\text{triphenylamine}} \rightarrow \pi^*$  triphenylamine transition, while the lowenergy transition was attributed to  $\pi \rightarrow \pi^*$  transition for L and LMCT transition for Ni(L)<sub>2</sub>(SCN)<sub>2</sub>.

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