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1-(对甲苯基)-2-(三对甲苯基-5-亚磷酰基)乙醛的汞(Ⅱ)配合物的 X 射线晶体学、光谱表征和理论计算研究

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摘要：通过 2-溴-1-(对甲苯基)乙醛与三(对甲苯基)膦的反应制备 α-磷配体：1-(对甲苯基)-2-(三对甲苯基-5-亚磷酰基)乙醛(L)。氯化镉和溴化汞与 L 分别反应，生成配合物[Cd(L)Cl_2]$_2$ (**C1**)和[Hg(L)(μ_2-Br)Br]$_2$ (**C2**)。用 IR 和 NMR(^{1}H，^{13}C，^{31}P)对配合物进行了表征。通过单晶 X 射线衍射测定了 **C2** 的结构，并在 B3LYP/6-31G* 水平对 **C2** 的结构进行了 DFT 计算研究，以揭示 **C2** 的复合反应位点与 Schiff 碱等亲核基团的相互作用。

关键词：磷配体；汞(Ⅱ)配合物；三(对甲苯基)膦
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X-ray Crystallography, Spectral Characterization and Computational Studies of Mercury(Ⅱ) Complex with 1-(*p*-Tolyl)-2-(tri-*p*-tolyl-λ^5-phosphanylidene)ethan-1-one

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Abstract: The α-phosphorus ligand 1-(*p*-tolyl)-2-(tri-*p*-tolyl-λ^5-phosphanylidene)ethan-1-one (L) was prepared by the reaction of 2-bromo-1-(*p*-tolyl)ethan-1-one with tri(*p*-tolyl) phosphine. The reactions of L with cadmium chloride and mercury bromide resulted in [Cd(L)Cl_2]$_2$ (**C1**) and [Hg(L)(μ_2-Br)Br]$_2$ (**C2**), respectively. The complexes were characterized by IR and NMR (^{1}H, ^{13}C, ^{31}P). The structure of **C2** was detected by single crystal X-ray diffraction and its DFT computational studies at B3LYP/6-31G* level were also performed to reveal the interaction between the reaction site of complex **C2** and nucleophilic groups such as Schiff base. CCDC: 1437693, **C2**.

Keywords: phosphorus ligand; mercury(Ⅱ) halide complex; tri(*p*-tolyl) phosphine

0 Introduction

Ylides play an important role in the production of the chemical compounds, because ylides are a fundamental part of the structure of compounds which contain biological, pharmaceutical and industrial

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properties[1-3]. In ylides, carbanion directly attaches to one heteroatom with positive charge. Phosphorous ylides are formed when phosphorus enters to the structure of ylide. Because of resonance forms production, presence of carbonyl groups in adjacency of methylene carbon will lead to the higher stability of ylides. In addition to the biological, pharmaceutical and industrial applications[4-6], phosphorous ylides can coordinate with metal ether by the oxygen of carbonyl group or by methine carbon.

These compounds as ambidentate ligands hold substantial place in the organometallic chemistry. Each year considerable numbers of papers are published in this regard[7-9]. Although these complexes have some catalytic, biologic and pharmaceutical properties, their main importance is about their theoretical aspects, especially the ability of having comprehensive study on the competition of connection of hard oxygen or soft carbon in order to coordination to the hard, soft metal and transition metal centers. The comprehensive study of these complexes is so important, because there is flexibility in the structure of these compounds where R_1 to R_5 can be changed selectively[10].

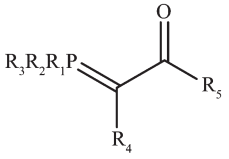


Fig.1　Structure of phosphorous ylide

In this paper, the preparation of mercury(Ⅱ) and cadmium(Ⅱ) complexes with 1-(*p*-tolyl)-2-(tri-*p*-tolyl-λ^5-phosphanylidene)ethan-1-one (L)[11] will be discussed. The crystals of $[Hg(L)(\mu_2\text{-Br})Br]_2$ (**C2**) were obtained from the reaction between ligand L and $HgBr_2$, and the crystal was characterized by X-ray crystallography and IR, ^1H NMR, ^{31}P NMR, ^{13}C NMR spectroscopic methods. Since mercury(Ⅱ) and cadmium(Ⅱ) are soft Lewis acid, their attachment to phosphorous ylide is from soft side which is methine carbon and can be confirmed by analytical methods. Since mercury is a transition metal and has full d orbitals with large atomic radius, it is highly reactive with ylides especially phosphorous ylides to form organometallic complexes[12-13]. Theoretical calculations will determine the active site of complex **C2** to bond with Schiff base. There are numerous reports about biological activities in ligands and metal complexes[9-10,13]. Therefore, the titled compounds also can be a good candidate for biological research.

1　Experimental

1.1　Material and methods

Petroleum benzene was distilled over sodium pieces prior to use. Ligand L was synthesized according to the reported method[11]. All other solvents were purchased from Merck Company and used without further purification. The ^1H, ^{31}P, ^{13}C NMR spectra were recorded at 400.13, 161.98, and 100.62 MHz, respectively on BRUKER spectrometer (Germany) in $CDCl_3$ solvent. Solid state IR spectra in the region of 500~4 000 cm^{-1} using KBr pellets were obtained on a FT-IR Nexus 670 spectrophotometer. Melting points were determined on a digital melting point apparatus (Electrothermal 9100) and remained uncorrected.

1.1.1　Synthesis of $[Cd(L)Cl_2]_2$ (**C1**)

Methanol solution (10 mL) of $CdCl_2$ (924 mg, 0.5 mmol) was added to a solution of ligand L (218 mg, 0.5 mmol) in the same solvent, and the mixture was stirred for 18 h. The pale-yellow precipitate was filtered off, washed with petroleum benzene (2×20 mL), and dried. Yield: 83%. m.p. 182~184 ℃. FT-IR (KBr, cm^{-1}): 1 631 (CO), 815 (P^+-C). ^1H NMR (DMSO-d_6): δ 2.14 (s, 24H, CH_3), 4.78 (d, $^2J_{PH}$=10.44 Hz, 2H, CH), 7.49~8.26 (m, 32H, 8Ph). ^{13}C NMR (DMSO-d_6): δ 20.25 (CH_3), 69.28 (CH), 128.75 (d, $^1J_{P\text{-}C}$=128.87 Hz, PPh_3(i)), 129.98 (COPh)(m)), 130.22 (d, $^3J_{P\text{-}C}$=15.29 Hz, PPh_3)(m)), 130.91 (COPh)(o)), 132.20 (d, $^2J_{P\text{-}C}$=18.11 Hz, PPh_3)(o)), 132.85 (d, $^3J_{P\text{-}C}$=15.29 Hz, COPh)(i)), 134.95 (s, PPh_3)(p)), 143.60 (COPh)(p)), 196.88 (s, CO). ^{31}P NMR (DMSO-d_6): δ 30.38.

1.1.2　Synthesis of $[Hg(L)(\mu_2\text{-Br})Br]_2$ (**C2**)

Methanol solution (10 mL) of $HgBr_2$ (181 mg, 0.5 mmol) was added to a solution of ligand L (218 mg, 0.5 mmol) in methanol (15 mL) and the mixture was stirred for 24 h. The white precipitate was filtered off, washed with petroleum benzene (2×15 mL), and dried.

To get the crystals of complex **C2**, ligand L 0.25 mmol (109 mg) in methanol (6 mL) were added dropwise to a solution of $HgBr_2$ (0.25 mmol, 90 mg) in the same solvent (2 mL). After standing for several days without stirring at room temperature, colorless crystals were obtained. Yield: 80%. m.p. 206~208 ℃. FT-IR (KBr, cm^{-1}): 1 626 (CO), 811 (P^+-C). ^1H NMR ($CDCl_3$): δ 2.41 (s, 24H, CH_3), 5.30 (d, J=12.41 Hz, 2H, CH), 7.25~8.02 (m, 32H, 8Ph). ^{13}C NMR ($CDCl_3$): δ 21.63 (CH_3), 67.09 (CH), 127.55 (d, $^1J_{P-C}$=124.87 Hz, PPh_3)(i)), 128.70 (COPh)(m)), 129.25 (d, $^3J_{P-C}$=12.58 Hz, PPh_3)(m)), 129.76 (COPh)(o)), 131.25 (d, $^2J_{P-C}$=13.68 Hz, PPh_3)(o)), 132.18 (d, $^3J_{P-C}$=10.36 Hz, COPh)(i)), 133.74 (s, PPh_3)(p)), 142.42 (COPh)(p)), 193.26 (CO). ^{31}P NMR ($CDCl_3$): δ 30.72.

1.2 Determination of the crystal structure of C2

The crystallographic measurement of **C2** was performed on a Xcalibur R κ-geometry automated four-circle diffractometer equipped with a ruby CCD camera and graphite-monochromatized Mo $K\alpha$ radiation (λ= 0.071 073 nm). The data were collected at 90(2) K by using the Oxford-Cryosystems cooler. Data were corrected for Lorentz and polarization effects. Data collection, cell refinement, data reduction, and analysis were carried out with Xcalibur PX software, CrysAlisPro[14]. Because **C2** was isomorphous with $Hg_2I_4((p\text{-tolyl})_3PCHC(O)\text{-}C_6H_4Cl)_2$[15], the refinement of its structure was started by using the coordinates of non-H atoms taken from iodide derivative (Cambridge Structural Database (CSD, Version 5.35[16]). The structure was refined by a full-matrix least-squares technique with SHELXL-2013[17] and anisotropic thermal parameters for non-H atoms. All H atoms were included from geometry and were refined using a riding model, with C-H bond length of 0.095~0.100 nm, and with $U_{iso}(H)=1.2U_{eq}(C)$ for CH, $1.5U_{eq}(C)$ for CH_3, respectively. The figures were drawn with the Diamond program[18]. Details of the conditions for the data collection and the structures refinements are given in Table 1.

CCDC: 1437693, **C2**.

Table 1 Crystal data and structure refinement for complex C2

Chemical formula	$C_{60}H_{58}Br_4Hg_2O_2P_2$	Z	2
M_r	1 593.82	Crystal size / mm	0.30×0.27×0.21
Crystal system	Monoclinic	μ / mm^{-1}	8.31
Space group	$P2_1/c$	Measured, independent, observed [$I>2\sigma(I)$] reflection	21 419, 8 434, 7 453
a / nm	1.178 9(2)	R_{int}	0.022
b / nm	1.078 3(2)	R_1, wR_2	0.023, 0.046
c / nm	2.244 7(4)	S	1.10
β / (°)	95.63(2)	Parameter	320
V / nm^3	2.839 7(9)	Restraint	0
D_c / ($g\cdot cm^{-3}$)	1.864	$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$ / ($e\cdot nm^{-3}$)	690, −650

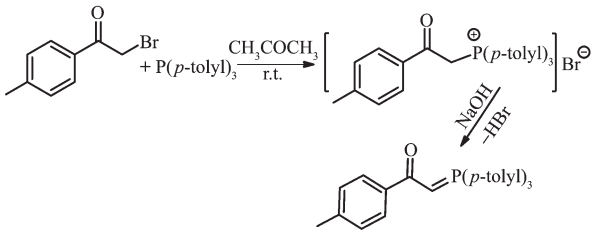
1.3 Computational methods

Density functional theory (DFT)[19] calculations were accomplished using the GAMESS program package[20]. In the case of complex **C2**, the X-ray structure was considered as starting points for the geometrical investigations. The calculations were based on the B3LYP/6-31G* level of theory[21] for all atoms to provide the most stable structure.

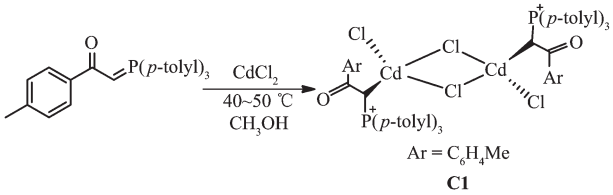
2 Results and discussion

2.1 Synthesis

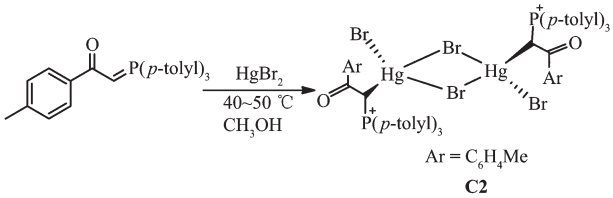
The reaction of tri-*p*-tolylphosphine with 2-bromo-1-(*p*-tolyl)ethanone at room temperature for 4 h (1:1 molar ratio) in acetone gave white solid of phosphonium salt in high yield. Further treatment with aqueous NaOH solution led to elimination of HBr, giving the free ligand L[11] (Scheme 1). Hg (Ⅱ) and Cd (Ⅱ) ions reacted with L (1∶1 molar ratio) to produce complexes **C1** and **C2** (Scheme 2 and 3). By reviewing complex **C1** spectroscopic data, investigating other similar compounds of Cd(Ⅱ)[22-23] and also considering that Cd and Hg share similar properties, the structure of complex **C1** might be similar to **C2** or other mercury halide-bridged dimeric complexes with phosphorous



Scheme 1　Synthetic route for ligand L



Scheme 2　Synthetic route for **C1**



Scheme 3　Synthetic route for **C2**

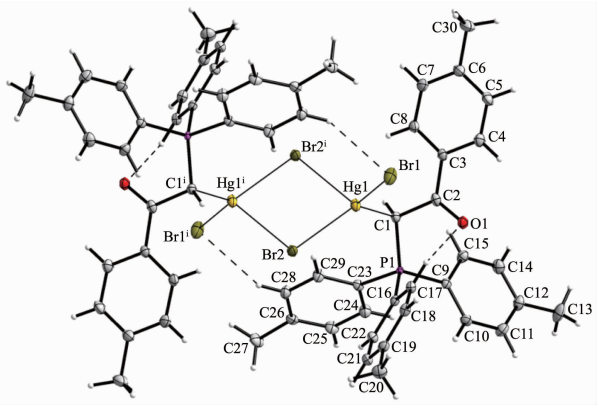
ylides[15,24-25].

2.2　Spectroscopic data

The infrared spectra of complexes **C1** and **C2** in the solid-state showed ν_{CO} in the range of 1 631 and 1 626 cm^{-1}, indicating coordination of L through carbon at higher wave numbers with respect to the free L in 1 599 cm^{-1} [11]. The expected spectra of ^{31}P and CH proton of **C1** and **C2** were shifted downfield as a consequence of C-coordination character of free L (CH in 4.36, ^{31}P in 12.98)[11]. The ^{13}C NMR shifts of CO group in **C1** and **C2** were higher than 191.34 noted for the same carbon in free L, indicating lower shielding of CO group carbon in the complexes.

2.3　X-ray crystallography

The X-ray crystallography analysis for crystal of complex **C2** revealed that **C2** crystalize in monoclinic systems. The molecular structure is shown in Fig.2, relevant bond distances and angles are given in Table 2, and also geometry of hydrogen bonds in complex **C2** is presented in Table 3. The X-ray analysis reveals that Br1 is more strongly bounded to Hg atom (Hg-Br1 0.254 77(5) nm) than Br2 (Hg-Br2 0.267 49(5) nm). This state demonstrates terminal bond is stronger



Displacement ellipsoids are drawn at the 50% probability level; Dashed line: C–H···O contacts; Symmetry codes: ^{i} $-x$, $-y+1$, $-z$

Fig.2　X-ray structure of **C2** showing atom-numbering scheme

Table 2　Comparison between experimental and calculated values of bond lengths (nm) and bond angles (°) for complex C2

	Experimental	Calculated
Hg1-C1	0.226 6(2)	0.226 587
Hg1-Br1	0.254 77(5)	0.254 763
Hg1-Br2	0.267 49(5)	0.267 495
Hg1-Br2^{i}	0.285 32(5)	0.285 328
P1-C1	0.178 2(2)	0.178 215
O1-C2	0.123 1(3)	0.123 015
C1-C2	0.148 9(3)	0.148 953
C1-Hg1-Br1	116.68(6)	116.68253
C1-Hg1-Br2	126.06(6)	126.05168
Br1-Hg1-Br2	108.250(16)	108.25162
C1-Hg1-Br2^{i}	98.91(6)	98.90585
Br1-Hg1-Br2^{i}	117.084(12)	117.08083
Br2-Hg1-Br2^{i}	85.139(17)	85.13681
Hg1-Br2-Hg1^{i}	94.859(17)	94.86319
C1-P1-C9	112.67(11)	112.68022
C2-C1-P1	111.56(16)	111.53454

Symmetry codes: ^{i} $-x$, $-y+1$, $-z$

than bridge bond. Compared to Hg-Br distances found in similar Hg(Ⅱ)-Br complexes[26-28], Hg-Br bonds in **C2** are relatively stronger. The Hg(Ⅱ) in **C2** is sp^3 hybridization and has a tetrahedral coordination. The C1-Hg1-Br bond angles (116.68(6)°, 126.06(6)°, 98.91(6)) and Br-Hg1-Br bond angles (108.250(16)°, 117.084(12)°, 85.139(17)°) indicate a relatively symmetric tetragonal environment around Hg (Ⅱ) ion. The comparison of

Table 3 Comparison between experimental and calculated values of hydrogen bond parameters for complex C2

D–H···A	Method	*d*(D-H) / nm	*d*(H···A) / nm	*d*(D···A) / nm	∠DHA / (°)
C17–H17···O1	experimental	0.095	0.237	0.311 8	136
	calculated	0.095	0.237	0.318 3	135.6
C28–H28···Br1^{i}	experimental	0.095	0.280	0.367 7	154
	calculated	0.095	0.280	0.367 7	153.5
C27–H27···O1^{ii}		0.098	0.256	0.316 4	120
C5–H5···Cg1^{iii}		0.095	0.278	0.367 5	157
C7–H7···Cg2^{iv}		0.095	0.272	0.361 7	158
C25–H25···Cg3^{v}		0.095	0.271	0.345 1	136

Symmetry codes: ^{i} $-x$, $-y+1$, $-z$; ^{ii} x, $-y+1/2$, $z-1/2$; ^{iii} $x+1$, $y+1/2$, $z+1/2$; ^{iv} x, $y+1$, z; ^{v} $x+1$, $-y+1$, $-z$; Cg1, Cg2, Cg3 are the centroids of C9~C15, C16~C22 and C3~C8 ring, respectively.

bond angles between Br2-Hg1-Br2^{i} (85.139(17)°) and Hg1-Br2-Hg1^{i} (94.859(17)°) shows a little distortion in center of molecule. This distortion must be attributed to the use of Hg (Ⅱ) orbitals with high s orbital character for bonding to ylidic carbon and the steric effects of phosphine group causing the C1-Hg-Br2 angle to be larger. Since the stabilized resonance structure for the parent ylides is destroyed by the complex formation, P1-C1 bond length in complex **C2** (0.178 2(2) nm) is significantly longer than the corresponding distances found in the similar non-complexed phosphorus ylides[29-30]. One interesting point in this crystal is unusual hydrogen bonds like C28–H28···Br1^{i} (H28···Br1^{i} 0.280 nm) and C17–H17···O1 (H17···O1 0.237 nm) that all together stabilizes the crystal packing.

2.4 DFT calculations

The single point (SP) structure of complex C2 calculated at B3LYP/6-31G* level of DFT method is showed in Fig.3. It should be mentioned that the corresponding distances in SP structure are equal to the experimental values, due to the freezing of non-hydrogen atoms in the research. According to the results, the total energy and dipole moment of complex **C2** is –439 099.94 eV and 0.000 0 Debye which seems to be thermodynamically most stable structure (Fig.2). Since complex C2 has a crystalline nature and its X-ray diffraction data are available and due to the fact that the X-ray is not able to identify the position of hydrogen atoms positions, all atoms except hydrogen atoms in this research were frozen.

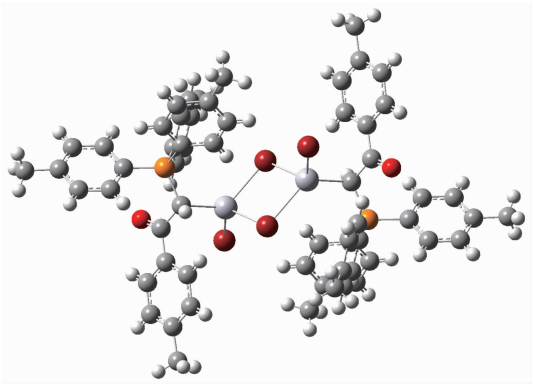
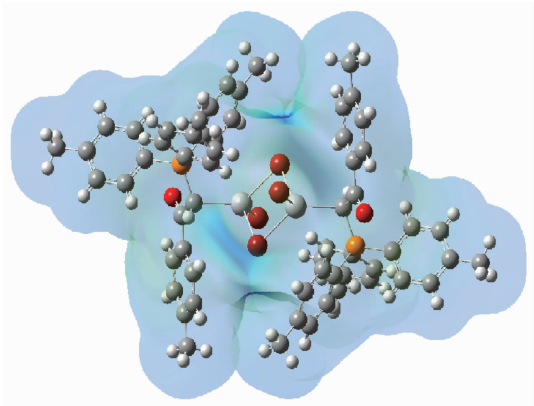


Fig.3 Calculated molecular structure of complex **C2**

The SP calculation was just performed to obtain the correct position of hydrogen atoms.

Moreover, determination of the stable configurations of single complex **C2** was accomplished regarding the molecular electrostatic potential (MEP) plot of single complex **C2** which is represented in Fig.4. As



Color range: blue, more positive than 0.441 a.u.; green, 0.441~0 a.u.; yellow, 0~–0.441 a.u.; red, less than –0.441 a.u.

Fig.4 Calculated electrostatic potentials on the molecular surfaces of a single **C2** molecule

shown in Fig.4, the more partial positive charge around the Hg atoms in structure are reactive sites toward interactions with other ylides or Schiff bases which are powerful than ylide L. The possibility of a strong ligand molecule approaching the outer surface of the complex is provided, then ligand L and its bonds to Hg atoms is removed. The obtained structural results by experimental methods confirmed the MEP analysis. This finding will help us to increase our knowledge about formed interactions nature between the studied complex and ligands.

The surfaces are defined by the 0.000 4 electrons/b3 contour of electronic density. Furthermore, since the charge distribution on the structure plays an important role in creating inter and intra-molecular interactions, it was attempted to calculate the quantitative values of atomic charges (Fig.5). Based on the results, the charge on Hg atoms is about 60.292 showing very low electron density caused by the adjacent bromide atoms which attract the electrons of mercury. The negative charge of bridged bromide is −17.961 and for terminal bromide is −11.727, which demonstrates that terminal bonds are polar than bridged bonds. So, terminal bonds are expected to be stronger than bridged bonds, which is confirmed by X-ray data.

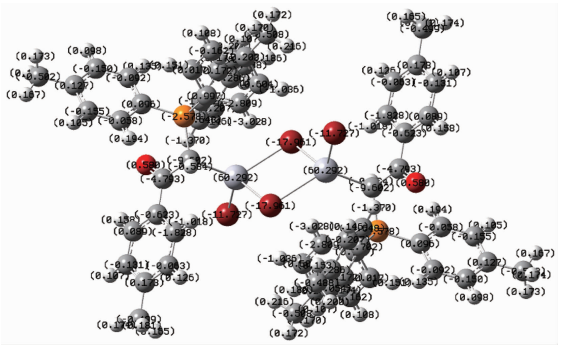


Fig.5 Charge atomic distribution of complex **C2**

Comparison between the experimental and calculated bond lengths and bond angles for complex **C2** is presented in Table 2. The calculated structure of **C2** in the gas-phase is in accordance with the structure observed by X-ray crystallography. A comparison between the experimental and calculated hydrogen bonds for complex **C2** shows that the calculated structure of **C2** in the gas-phase resembles the structure observed by X-ray crystallography (Table 3).

3 Conclusions

The present study describes the coordination chemistry and spectral characterization of mercury(Ⅱ) and cadmium(Ⅱ) complexes with ylide ligand (**C1** and **C2**). On the basis of spectroscopic data, it is proposed that L herein exhibits monodentate C-coordination to the metal center. In addition, X-ray crystallography studies confirm the trans-like dimeric structure for complex **C2** with L. Computational studies at B3LYP/6-31G* level of DFT theory were used to appoint **C2** reactive sites.

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