Coordination chemistry of organometallic polydentate ligand. Reactive chemistry of the tridentate ligand *trans*-$Fe(Ph_2PQu\text{-}P)_2(CO)_3$ [Ph_2PQu = 2-diphenyl-phosphino-4-methylquinoline] and molecular structure of $[Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgI]^+[HgI_3]^-$

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Reaction of a new type of bidentate ligand PhPQu [PhPQu = 2-diphenylphosphino-4-methylquinoline] with $Fe(CO)_5$ in butanol gave *trans*-Fe(PhPQu-P)$(CO)_3$ (1). Compound 1, which can act as a neutral tridentate organometallic ligand, was reacted with Ⅰ B, Ⅱ B metal compounds and a rhodium complex to give six binuclear complexes with Fe—M bonds, $Fe(CO)_3(\mu\text{-}Ph_2PQu)MX_n$ (2—7) [M = Zn(Ⅱ), Cd(Ⅱ), Hg(Ⅱ), Cu(Ⅰ), Ag(Ⅰ), Rh(Ⅰ)], and an ion-pair complex $[Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgI][HgI_3]^-$ (8). The structure of 8 was determined by X-ray crystallography. Complex 8 crystallizes in the space group *P*-1 with $a = 1.0758(3)$, $b = 1.6210(4)$, $c = 1.7155(4)$ nm; $\alpha = 75.60(2)$, $\beta = 71.81(2)$, $\gamma = 81.78(2)°$ and $Z = 2$ and its structure was refined to give agreement factors of $R = 0.050$ and $R_w = 0.057$. The Fe—Hg bond distance is 0.2536 nm.

Keywords 2-Diphenylphosphino-4-methylquinoline, *trans*-Fe(PhPQu-P)$(CO)_3$, neutral tridentate organometallic ligand, Ⅰ B and Ⅱ B metal compounds, rhodium complex

Introduction

Some neutral organometallic complexes can act as Lewis bases, but the formation of donor-acceptor bonds between this kind of complex and Lewis acidic metal compounds has not been recognized until the 1970s.[1,2] Nowell firstly confirmed the presence of a Co→Hg bond in $CpCo(CO)_2 \cdot HgCl_2$ by X-ray crystallography.[3] Then a series of investigations were concentrated on this area. For instance, in the 1980s, Pomeroy and co-workers systematically investigated the reaction of neutral metal carbonyl complexes as metal ligands, and some binuclear complexes containing donor-acceptor bonds were obtained.[4] Recently, we have shown that *trans*-M$(Ph_2Ppy\text{-}P)_2(CO)_3$ [M = Fe, Ru; Ph_2Ppy = 2-(diphenylphosphino)pyridine] can act as a neutral organometallic tridentate ligand in reactions with many main group and transition metal compounds to give binuclear complexes with M→M bonds. Moreover, it has also been found that these binuclear complexes possess very interesting catalytic behavior.[5] In order to inspect the effect of different ligants on their reactivities and structures of the products here we report a new neutral organometallic tridentate ligand, *trans*-Fe$(Ph_2PQu)_2(CO)_3$ [Ph_2PQu = 2-diphenylphosphino-4-methyl-quinoline], and its reactivity.

Experimental

All reactions were performed under a nitrogen atmosphere with the use of standard Schlenk techniques. Solvents were purified by standard methods, and 2-chloro-4-methyl-quinoline[6] and $[RhCl(CO)_2]_2$[7] were prepared by literature methods.

Infrared spectra were recorded on a WFD-14 spectrometer as KBr discs. The $^{31}P\{^1H\}$ NMR spectra were

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* Received November 30, 1999; accepted March 31, 2000.
Project supported by the National Natural Science Foundation of China (No. 29672078).

Corresponding author's Email: *zzhang@public1.tpt.tj.cn* recorded on a JEOL FX-90Q spectrometer at 36.19 MHz using 85% H_3PO_4 as external standard and $CDCl_3$ as solvent. FD-MS spectra were acquired with a Hitachi M-80 spectrometer.

Preparation of 2-diphenylphosphino-4-methyl quinoline With stirring, a solution of 2-chloro-4-methylquinoline (8.9 g, 0.05 mol) in tetrahydrofuran (20 mL) was added slowly to a solution of Ph_2PLi (0.1 mol) in tetrahydrofuran (80 mL) at 0℃. The resulting mixture was stirred for 3 h at room temperature, and methanol (15 mL) was added to give a pink solution. The solvent was then removed and the residue was washed with dichloromethane. After dichloromethane was removed by evaporation, a pale-yellow oily residue remained. To the residue methanol (15 mL) was added and a white crystalline solid appeared after cooling at 0℃ overnight. The solid was collected by filtration and washed with methanol. Yield: 24.7 g (79.1%). mp: 100—102℃. $^{31}P\{^1H\}$ NMR: −3.23. Anal. $C_{22}H_{18}NP$. Calcd.: C, 80.72; H, 5.50; N, 4.28. Found: C, 80.81; H, 5.76; N, 4.22.

Preparation of trans-$Fe(CO)_3(Ph_2PQu)_2$, **1** To an *n*-butanol solution (20 mL) of sodium hydroxide (0.14 g, 3.5 mmol), $Fe(CO)_5$ (0.33 mL, 2.5 mmol) was added. The mixture was stirred for 0.5 h, and 2-diphenylphosphino-4-methylquinoline (1.25 g, 4 mmol) was added. After being refluxed for 2.5 h, the mixture was cooled to room temperature, upon which a large amount of yellow precipitate was formed. The precipitate was collected by filtration, washed with methanol and recrystallized from CH_2Cl_2/CH_3OH to give an orange solid. Yield: 0.82 g (64.5%). mp 220—224℃. FD-MS, *m/z*: 794(M^+). Anal. $C_{47}H_{36}FeN_2O_3P_2$. Calcd.: C, 71.03; H, 4.53; N, 3.53. Found: C, 70.87; H, 4.28; N, 3.18.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2ZnCl_2$, **2** A solution of $ZnCl_2$(0.08 g, 0.6 mmol) in diethyl ether (5 mL) was added to a solution of **1** (0.48 g, 0.6 mmol) in dichloromethane (20 mL). The mixture was stirred for 4 h at room temperature, and a pale-yellow solution was formed. The solvent was removed *in vacuo* and the residue was recrystallized from CH_2Cl_2/Et_2O, and washed with benzene and diethyl ether to give a pale-yellow solid. Yield: 0.22 g (39.4%). mp 140—142℃. Anal. $C_{47}H_{36}Cl_2FeN_2O_3P_2Zn$. Calcd.: C, 60.64; H, 3.87; N, 3.01. Found: C, 61.02; H, 3.73; N, 3.29.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2CdCl_2$, **3** A finely-ground powder of $CdCl_2$ (0.3 g, 1.64 mmol) was added to a solution of **1** (0.5 g, 0.63 mmol) in dichloromethane (30 mL). The mixture was stirred for 12 h at room temperature. The unreacted $CdCl_2$ was filtered off, the solvent was evaporated and the residue was recrystallized from CH_2Cl_2/Et_2O to give a yellow solid. Yield: 0.28 g (45.5%). mp 162℃ (dec.). Anal. $C_{47}H_{36}CdCl_2FeN_2O_3P_2$. Calcd.: C, 57.71; H, 3.68; N, 2.86. Found: C, 57.37; H, 3.54; N, 2.98.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgCl_2$, **4** $HgCl_2$ (0.1 g, 0.37 mmol) in a 1:2 (*V*: *V*) 2-butanone/benzene mixture (15 mL) was added with stirring to a solution of **1** (0.25 g, 0.31 mmol) in the same solvent (20 mL). The color of the solution changed from orange to pale-yellow. After stirring for 45 min at room temperature, the solvent was removed *in vacuo*, and the residue was recrystallized from CH_2Cl_2/Et_2O to give a pale-yellow solid. Yield: 0.28 g (84.8%). mp 176℃ (dec.). Anal. $C_{47}H_{36}Cl_2FeHgN_2O_3P_2$. Calcd.: C, 52.93; H, 3.38; N, 2.63. Found: C, 52.72; H, 3.37; N, 2.64. FD-MS, *m/z*: 794.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2CuCl$, **5** CuCl (0.1 g, 1 mmol) was added to a stirred solution of **1** (0.5 g, 0.63 mmol) in dichloromethane. The color of the solution changed from orange to dark-red rapidly. After 40 min, the unreacted CuCl was filtered off, the volume of the solution was reduced and diethyl ether was added to give a precipitate, which was recrystallized from CH_2Cl_2/Et_2O to afford a yellow solid. Yield: 0.43 g (76.4%). mp 146℃(dec.). Anal. $C_{47}H_{36}ClCuFeN_2O_3P_2$. Calcd.: C, 63.16; H, 4.03; N, 3.14. Found: C, 62.73; H, 3.90; N, 2.77.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2AgClO_4$, **6** A solution of $AgClO_4$(0.1 g, 0.48 mmol) in dichloromethane (10 mL) was added to a solution of **1** (0.4 g, 0.5 mmol) in the same solvent (15 mL). The mixture was stirred for 3 h at room temperature. After removing the solvent in vacuum, the residue was recrystallized twice from CH_2Cl_2/Et_2O to give a pale-yellow solid. Yield: 0.32 g (66.6%). mp 156℃(dec.). Anal. $C_{47}H_{36}AgClFeN_2O_7P_2$. Calcd.: C, 56.32; H, 3.59; N, 2.80. Found: C, 56.61; H, 4.00; N, 2.77.

Preparation of $Fe(CO)_3(\mu\text{-}Ph_2PQu)_2Rh(CO)Cl$, **7** A solution of $[Rh(CO)_2Cl]_2$ (0.06 g, 0.3 mmol) in dichloromethane (10 mL) was added to a solution of **1** (0.24 g, 0.3 mmol) in dichloromethane (15 mL). The mixture was stirred for 1 h at room temperature, a red solution was formed. The volume of the solution was reduced to 5 mL, diethyl ether was added and a red-brown precipitate appeared. The precipitate was washed with acetone to give a red-brown solid. Yield: 0.16 g (62.0%). mp 177—179℃. Anal. $C_{48}H_{36}Cl_2FeN_2O_4P_2Rh$. Calcd.: C, 59.98; H, 3.75; N, 2.92. Found: C, 58.75; H, 4.19; N, 3.25.

From the acetone filtrate, another product, $Rh_2(\mu\text{-}CO)Cl_2(\mu\text{-}Ph_2PQu)_2$, **9**, was isolated as a red-brown solid. Anal. $C_{45}H_{36}Cl_2N_2OP_2Rh_2$. Calcd.: C, 56.31; H, 3.75; N, 2.92. Found: C, 55.50; H, 4.33; N, 2.70. FD-MS *m/z* (relative intensity): 956 (M^+, 100).

Preparation of $[Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgI]^+[HgI_3]^-\cdot 0.5EtO$, **8** The red solid HgI_2 (0.59 g, 1 mmol) was added to a stirred solution of **1** (0.40 g, 0.5 mmol) in dichloromethane, and the stirring was continued for 4 h at room temperature. The unreacted HgI_2 was filtered off and the solvent was evaporated. The residue was recrystallized twice from CH_2Cl_2/Et_2O to give an orange crystalline solid. Yield: 0.64 g (73.6%). mp 180℃(dec.). Anal. $C_{49}H_{41}FeHg_2I_4N_2O_{3.5}P_2$. Calcd.: C, 33.80; H, 2.36; N, 1.60. Found: C, 33.42; H, 2.35; N, 1.49. FD-MS *m/z* (relative intensity): 1120(40), 794(100).

IR and $^{31}P\{^1H\}$ NMR data of compounds **1**—**9** are summarized in Table 1.

Table 1 Spectroscopic data, IR and $^{31}P\{^1H\}$NMR, of complexes **1**—**9**

Complex	ν(CO), cm^{-1}	$^{31}P\{^1H\}$NMR, δ (^2J(M-P), Hz)
1 *trans*-$Fe(CO)_3(Ph_2PQu)_2$	1978w, 1895s, 1864s	84.00
2 $Fe(CO)_3(Ph_2PQu)_2ZnCl_2$	2000w, 1985s, 1965s	81.98
3 $Fe(CO)_3(Ph_2PQu)_2CdCl_2$	2000w, 1966s, 1942s	84.90
4 $Fe(CO)_3(Ph_2PQu)_2HgCl_2$	2000w, 1985s, 1962s	72.29 (^2J(Hg-P), 228.90)
5 $Fe(CO)_3(Ph_2PQu)_2CuCl$	1985m, 1910s, sh, 1885s	87.34
6 $Fe(CO)_3(Ph_2PQu)_2AgClO_4$	1988m, 1925s, 1900s	85.34
7 $Fe(CO)_3(Ph_2PQu)_2Rh(CO)Cl$	2050m, 1995s, 1990s, 1980s	32.64 (^2J(Rh-P), 131.7)
8 $[Fe(CO)_3(Ph_2PQu)_2HgI]^+[HgI_3]^-$	2040m, 1995s	70.54 (^2J(Hg-P), 204.65)
9 $Rh_2(\mu\text{-}CO)Cl_2(\mu\text{-}Ph_2PQu)_2$	1810s	40.23^a

[a] ^1J(Rh-P) = 142.74 Hz; ^1J(Rh-Rh) = 13.84 Hz; ^2J(Rh-P) = 9.88 Hz; ^3J(P-P) = 19.2 Hz.

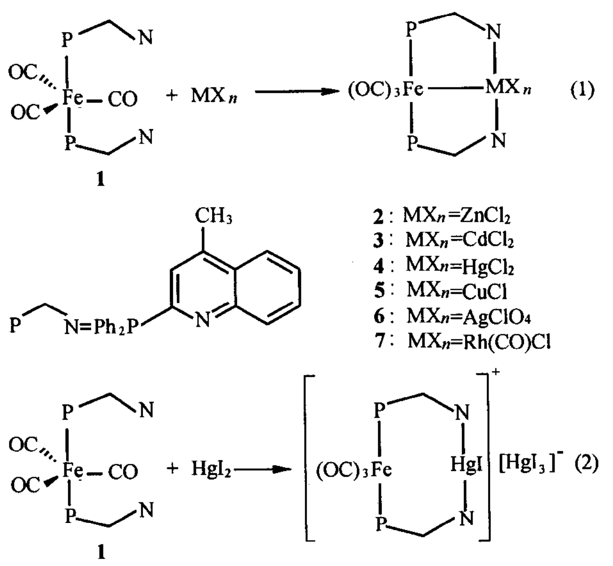
X-ray analysis of complex $\mathbf{8}\cdot 0.5Et_2O$ Crystals of $\mathbf{8}\cdot 0.5Et_2O$ suitable for X-ray crystallography were grown from CH_2Cl_2/Et_2O. A pale-yellow crystal with a suitable size (0.3 × 0.2 × 0.3 mm) was used to collect 7907 independent reflections on an Enraf-Nonius CAD4 Diffractometer with Mo-K_α graphite monochromated radiation ($\lambda = 0.071073$ nm) in the range $2 < \theta < 23°$. The measurements were carried out at room temperature (23 ± 1℃) by the ω-2θ scan technique. 3816 reflections with $I \geqslant 3\sigma(I)$ were considered to be observed and used to the structure analysis. Loreutz-polarization corrections and an empirical absorption correction were applied to the data. The structure was solved by direct methods (MULTAN82). The positions of the Hg, Fe and I atoms were found from an E-map. The coordinates of the non-hydrogen atoms were obtained through several difference-Fourier syntheses. The atomic coordinates and anisotropic thermal parameters of the non-hydrogen atoms were refined using a full-matrix least-squares procedure. The final unweighted and weighted agreement factors were $R = 0.050$ and $R_\omega = 0.057$. The highest peak in the final difference Fourier map was of height 8.8 e/nm.^{3} All calculations were performed on a PDP-11/44 computer with the program pactage SDP-PLUS.

Results and discussion

Synthetic studies

The compound *trans*-$Fe(CO)_3(Ph_2PQu)_2$, **1**, was synthesized by the previously-described method for the preparation of compounds of the type *trans*-Fe(CO)$_3$(phosphine)$_2$.[8]

Eq. 1 and 2 illustrate the synthesis of the title compounds, the complexes Fe(CO)$_3$(μ-Ph$_2$PQu)$_2$MX$_n$ [MX$_n$ = ZnCl$_2$, CdCl$_2$, HgCl$_2$, CuCl, AgClO$_4$, Rh(CO)Cl], **2**—**7**, and the complex [Fe(CO)$_3$(μ-Ph$_2$PQu)$_2$HgI]$^+$[HgI$_3$]$^-$, **8**.



All complexes except **5** are air-stable solids. **5** decomposes gradually in air.

Reaction of **1** with ZnCl$_2$ or CdCl$_2$ was difficult, due to the contamination of the product **2** or **3** by the starting material **1**. The following equilibrium may be present in these reactions (Eq. 3), because the carbonyl stretching region of **2** and **3** in dichloromethane solution contain peaks at 1864 and 1895 cm^{-1}, suggesting the presence of the starting material, **1**. Further purification of **2** and **3** was therefore performed by washing the products with large quantities of benzene to remove the more soluble **1**.

$$\mathrm{Fe(CO)_3(\mu\text{-}Ph_2PQu)_2\ (\mathbf{2}\ or\ \mathbf{3})} \rightleftharpoons \mathrm{Fe(CO)_3(Ph_2PQu)_2\ (\mathbf{1})\ +\ MCl_2} \qquad (3)$$

Reactions of **1** with HgX$_2$ (X = Cl, I) were easily carried out in solution, but the constitutions of the products are different. The reaction of **1** with HgCl$_2$ gave only a 1:1 adduct. Different ratios of **1**:HgCl$_2$ (2:1, 1:1, 1:2, or 1:3) yielded the same 1:1 complexes. However, for HgI$_2$, only 1:2 adduct was isolated even though different ratios of reactants were used. The reactivities of **1** above mentioned differed from those of Fe(CO)$_3$(Ph-Ppy)$_2$.[5b] Particularly, the reaction of the latter with HgI$_2$ afforded a non-ion pair complex Fe(CO)$_3$(μ-Ph-Ppy)$_2$HgI$_2$.[5b]

Treatment of **1** with [Rh(CO)$_2$Cl]$_2$ in dichloromethane solution, followed by precipitation with diethyl ether, yielded a red-brown solid. The solid was washed with acetone and the desired product Fe(CO)$_3$(μ-Ph$_2$PQu)$_2$Rh(CO)Cl (**7**) was obtained. Another red-brown solid was isolated out from acetone solution, which was identified as Rh$_2$(μ-CO)(μ-Ph$_2$PQu)$_2$Cl$_2$, **9**, by ^{31}P{^{1}H} NMR spectroscopy and elemental analysis.

Spectroscopic properties

Complex **1** exhibits three infrared carbonyl stretching bands at 1978, 1895, and 1864 cm^{-1}, comparable with those observed in the known complexes *trans*-Fe(CO)$_3$(PR$_3$)$_2$.[9] This suggests that the molecule of **1** have a trigonal bipyramidal coordination about the iron atom with the Ph$_2$PQu ligands at the axial positions.

For the complexes **2**—**8**, the carbonyl stretching frequencies are about 20—130 cm^{-1} higher than those observed in the starting complex **1**, consistent with both a change in stereochemistry and a decrease in the electron density on the iron atom in complexes **2**—**8**, in which the iron atom is bonded to a second metal atom, M, the iron atom donates electrons to M which has a high oxidation state, causing the electron density on the iron atom to decrease. Thus the σ-donating ability of the carbonyl ligands to the iron atom increases, while the back-donating ability of the dπ electrons of the iron atom to the empty 2pπ^* orbitals on the carbonyl ligands decreases. These two factors are responsible for the higher carbonyl absorption frequencies in these binuclear complexes.

The formation of a donor-acceptor bond between the iron atom and the second metal atom M in the binuclear complexes **2**—**8** also leads to a configurational rearrangement from trigonal bipyramid to octahedron, consistent with the fact that large structural re-organizations are expected to occur in most basic transition metal complexes when they interact with an acidic acceptor. But for most main-group bases, only small structural reorganizations are found.[10]

Interestingly, the IR spectra of the Fe/Hg complexes **4** and **8** are distinctly different, the carbonyl absorption frequencies of **4** being lower than those of **8**. The known complexes $L_2(CO)_3Fe \cdot nHgX_2$[11,12] (L = phosphine, phosphite; X = Cl, Br, I) have two types of structures: (a) $Fe \rightarrow HgX_2$ and (b) $[Fe\text{-}Hg\text{-}X]^+ X^-$ or $[Fe\text{-}Hg\text{-}X]^+ [HgX]^-$. For compounds with the same ligand L, the former (a) is expected to have a lower conductivity and lower carbonyl absorption frequencies than the latter (b). Thus, compound **4**, which has much lower carbonyl stretching frequencies, is expected to have the structure $Fe \rightarrow HgCl_2$, while **8** should have the structure $[Fe\text{-}Hg\text{-}I]^+ [HgI_3]^-$. The crystallographic study of **8** has confirmed these assignments.

The $^{31}P\{^1H\}$ NMR spectra of **2**—**8** (except **7**) show a singlet, suggesting that the phosphorus atoms have identical chemical environments. For the two mercury derivatives, the observed ^2J (P-Hg) values of 228.90 and 204.65 Hz are comparable with those in known FeHg complexes.[13,14] The spectrum of complex **7** shows a doublet with identical intensity. ^2J(Rh-P) is 131.7 Hz, indicating the existence of a Fe—Rh bond.

Molecular structure of complex **8**

Complex **8** is an ion-pair complex and consists of two parts: a positive ion (A) and a negative ion (B), plus one-half of a diethyl ether solvate molecule. The experimental data of the X-ray diffraction study are given in Table 2, while selected bond distances and angles are listed in Table 3.

Fig. 1 gives a PLUTO projection of $[Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgI]^+$ (A). The iron atom has a distorted octahedral configuration and the mercury atom has a linear coordination which is slightly distorted because of the two weak interactions with the quinoline nitrogens.

The $(CO)_3FeHg$ group is nearly planar, and the atoms of two quinoline rings, C(11)—C(20) and C(41)—C(50), are nearly coplanar. The two phosphorus atoms are *trans* to each other, and the O(2)C(2)-Fe(1)Hg(1) group is linear, nearly bisecting the angle C(1)Fe(1)C(3). Because of the presence of the Fe—Hg bond, the angle C(1)Fe(1)C(3) is increased to 155.6(5)°. The Fe(1)Hg(1)I(1) angle is 159.58 (4)°, deviating significantly from linearity.

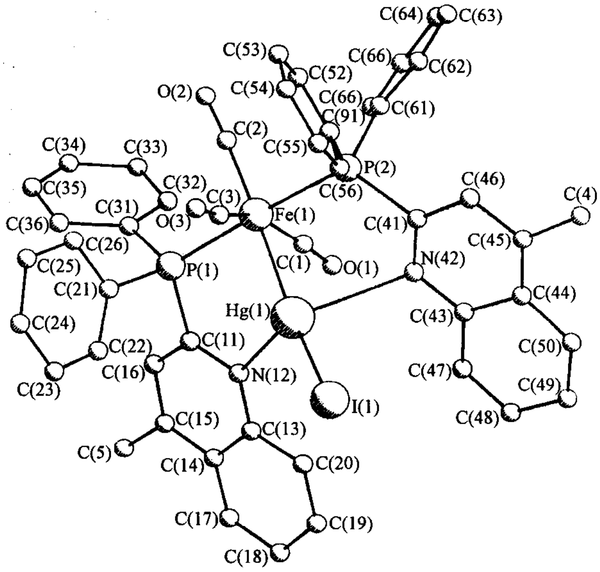


Fig. 1 PLUTO projection of A, the $[Fe(CO)_3(\mu\text{-}Ph_2PQu)_2HgI]^+$ ion in compound **8**.

Table 2 Experimental details of the X-ray diffraction analysis of **8**

formula	$C_{49}H_{41}FeHg_2I_4N_2O_{3.5}P_2$
fw	1739.8
color	yellow
space group	*P*-1
cryst syst	triclinic
a, nm	1.0758(3)
b, nm	1.6210(4)
c, nm	1.7155(4)
α, deg	75.60(2)
β, deg	71.81(2)
γ, deg	81.78(2)
Z	2
d_{calcd}, g/cm^3	2.150
cryst. size, mm	0.3×0.2×0.3
μ, cm^{-1}	81.59
final *R*	0.050
final R_w	0.057
no. of unique reflections	7907
no. of observed reflections	3816

The Fe—Hg distance is 0.2536(1) nm, which is shorter than that in most complexes containing a Fe—Hg bond.[5b] The N—Hg distances are 0.2613(7) and 0.2706(6) nm, respectively, comparable to those found in pyridine derivatives.[15] In B, the $[HgI_3]^-$ anion, the three iodine atoms are arranged in an equilateral triangle, with the mercury atom located at its center. The average I—Hg distance is 0.2661(2) nm, slightly longer than that in A.

Table 3 Selected bond distances (nm) and angles (deg) in **8**

Bond distances			
Hg(1)—I(1)	0.2609(7)	Fe(1)—C(1)	0.1760(1)
Hg(1)—Fe(1)	0.2536(1)	Fe(1)—C(2)	0.1800(1)
Hg(1)—N(12)	0.2613(7)	Fe(1)—C(3)	0.1790(1)
Hg(1)—N(42)	0.2706(6)	Fe(1)—P(1)	0.2256(3)
Hg(2)—I(2)	0.2653(2)	Fe(1)—P(2)	0.2270(2)
Hg(2)—I(3)	0.2658(2)	P(1)—C(11)	0.1820(9)
Hg(2)—I(4)	0.2673(1)	P(1)—C(21)	0.1810(2)
C(11)—C(12)	0.1334(9)	P(1)—C(31)	0.1810(2)
C(13)—N(12)	0.1370(2)	P(2)—C(41)	0.1835(9)
C(41)—N(42)	0.1300(1)	P(2)—C(51)	0.1846(9)
C(44)—C(45)	0.1550(1)	P(2)—C(61)	0.1805(8)
C(43)—N(42)	0.1350(1)	O(1)—C(1)	0.1160(1)
C(5)—C(15)	0.1510(1)	O(2)—C(2)	0.1090(1)
O(3)—C(3)	0.1140(1)		
Bond angles			
I(1)-Hg(1)-Fe(1)	159.58(4)	Hg(1)-Fe(1)-P(1)	87.07(7)
I(1)-Hg(1)-N(12)	110.4(2)	Hg(1)-Fe(1)-P(2)	89.92(8)
I(1)-Hg(1)-N(42)	95.1(2)	Hg(1)-Fe(1)-C(1)	78.7(4)
N(12)-Hg(1)-Fe(1)	88.4(2)	Hg(1)-Fe(1)-C(2)	174.5(4)
N(42)-Hg(1)-Fe(1)	84.1(2)	Hg(1)-Fe(1)-C(3)	77.0(3)
N(12)-Hg(1)-N(42)	114.5(3)	P(1)-Fe(1)-P(2)	175.9(1)
I(2)-Hg(2)-I(3)	120.20(4)	P(1)-Fe(1)-C(1)	87.1(3)
I(2)-Hg(2)-I(4)	120.88(4)	P(1)-Fe(1)-C(2)	93.5(3)
I(3)-Hg(2)-I(4)	118.67(4)	P(1)-Fe(1)-C(3)	91.6(3)
Fe(1)-P(1)-C(11)	115.4(3)	P(2)-Fe(1)-C(1)	89.6(3)
Fe(1)-P(1)-C(21)	114.3(3)	P(2)-Fe(1)-C(2)	89.7(3)
Fe(1)-P(1)-C(31)	114.7(4)	P(2)-Fe(1)-C(3)	90.4(3)
Fe(1)-P(2)-C(41)	115.7(4)	C(1)-Fe(1)-C(2)	106.9(5)
Fe(1)-P(2)-C(51)	111.1(3)	C(1)-Fe(1)-C(3)	155.6(5)
Fe(1)-P(2)-C(61)	115.4(3)	C(2)-Fe(1)-C(3)	97.5(6)
Fe(1)-C(1)-C(1)	177.9(9)	Fe(1)-C(3)-O(3)	172(2)
Fe(1)-C(2)-C(2)	176(1)	Fe(1)-Fe(41)-N(42)	115.5(7)

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(E9911167 JIANG, X.H.; LING, J.)