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# Synthesis, spectroscopic and X-ray structural studies of mercury(II) halide complexes of 4-methoxybenzoylmethylenetriphenylphosphorane

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## Abstract

The reactions of the title ylide {$(C_6H_5)_3PCHCOC_6H_4OCH_3$} (MBPPY) with mercury(II) chloride and mercury(II) bromide in equimolar ratios using methanol as the solvent produces crystals of $[(MBPPY) \cdot HgCl_2]_2$ (**1**) and $[(MBPPY) \cdot HgBr_2]_2$ (**2**), respectively. Single crystal X-ray analyses reveal the presence of centrosymmetric dimeric structures containing the ylide and $HgX_2$ (X = Cl or Br) in both cases. The IR and NMR data of the product $[(MBPPY) \cdot HgI_2]_2$ (**3**), formed by the reaction of mercury(II) iodide with the same ylide, are similar to those of **1** and **2**. Analytical data indicate a 1:1 stoichiometry between the ylide and Hg(II) halide in each of the three products.

*Keywords:* Phosphorus ylide; Mercury(II) halide complexes; X-ray Crystal structure; Triphenylphosphine

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## 1. Introduction

The organometallic chemistry of phosphorous ylides $R_3P = C (R') (R'')$ (R, R′, R″ = alkyl or aryl groups) has undergone a great growth in the last few years, mainly due to their interesting application as reactants in organometallic and metal-mediated organic synthesis [1–4]. On the whole, the α-keto-stabilized phosphorous ylides $R_3P = C(R')COR''$ show interesting properties such as high stability (which allows them to be easily handled in air) and ambidentate character as ligands (*C*- versus *O*-coordination). This ambidentate character can be rationalized in terms of the resonance forms **A**–**C**, together with the isomeric form **D** (Scheme 1). Form **B** would account for *C*-coordination to a metal (M = metal) (which is presented as **G**) while isomers **C** and **D** would explain *O*-coordination (which are presented as *cisoid*, form **F**, and *transoid*, form **E**, respectively).

In the compounds reported to date, the chemical behavior of the α-keto phosphorous ylides has been clearly dominated by the *C*-coordinated form [5–8], and very few examples of *O*-coordinated ylides are known [9–13]. Some of these examples contain the ylide *O*-coordinated to a hard, very oxophilic metal center, as Sn(IV) [9,10] or group 4 metals with a high oxidation number [11]. Only W(0) complexes of the type $W(CO)_5L$ (L = ylide) [12] and Pd(II) complexes of the stoichiometry $[Pd(C_6F_5)L_2)(APPY)](ClO_4)$ [13] [APPY = $Ph_3CCOMe$; L = $PPh_3$, $PBu_3$; $L_2$ = bipy] contain stable ylides *O*-linked to a soft metal center. Other attempts to obtain this kind of *O*-coordination to “classical” soft metals such as Pd(II), Pt(II) or Hg(II) [6,14,15] invariably gave *C*-coordination. In this study, we describe the preparation, spectroscopic characterization (IR and NMR) of complexes of mercury(II) with the title ylide. By a comparison of the data collected and single crystal X-ray diffraction of **1** and **2**, it demonstrates *C*-coordination of the ylide to the metal.

## 2. Experimental

### 2.1. Materials

Mercury halides, 4-methoxyacetophenone and triphenylphosphine were purchased from Merck. The ligand

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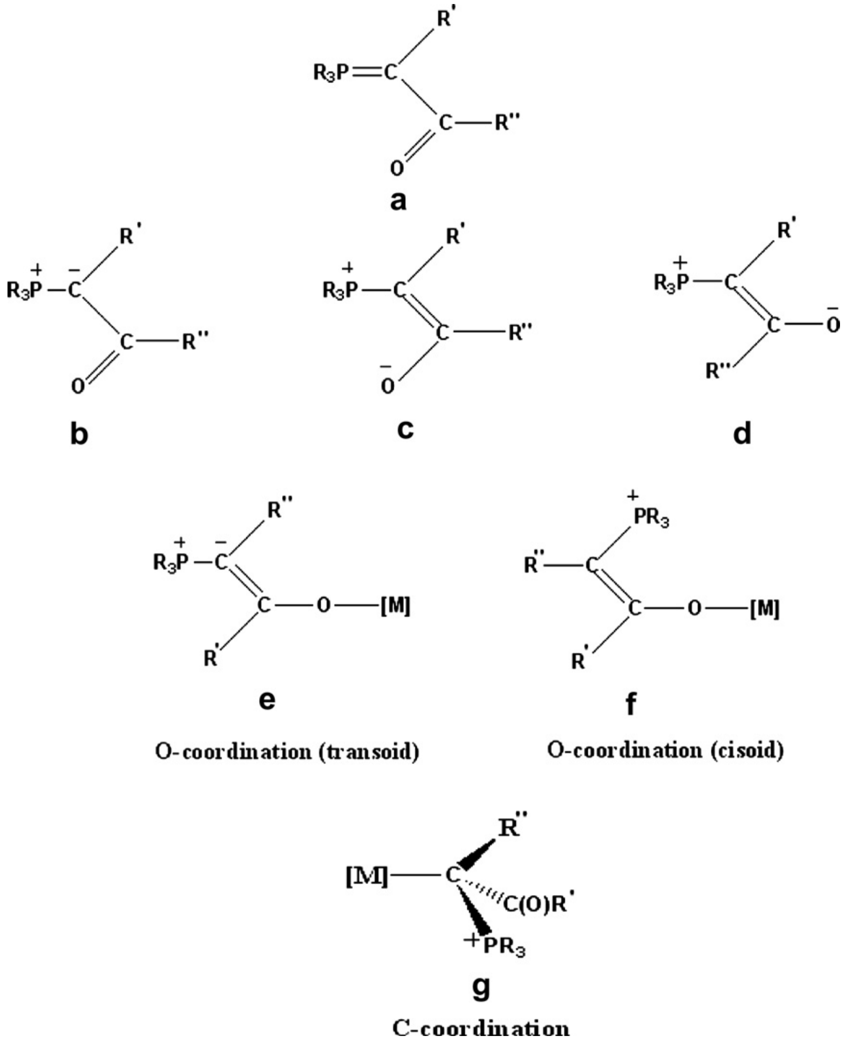


Scheme 1.

was synthesised by the reaction of triphenylphosphine with a chloroform solution of 2-bromo-4′-methoxyacetophenone and dehydrogenated by NaOH [16]. All solvents were dried by the reported methods [17].

### 2.2. Physical measurements

Melting points were measured on a SMPI apparatus. Elemental analysis for C, H and N were performed using a Perkin–Elmer 2400 series analyzer. Fourier transform IR spectra were recorded on a Shimadzu 435-U-04 spectrophotometer and samples were prepared as KBr pellets. $^{1}H$, $^{13}C$ and $^{31}P$ spectra were recorded on a 200 MHz Bruker spectrometer in DMSO-$d_6$ or $CDCl_3$ solution at 25 °C.

The single crystal X-ray diffraction analysis was performed on a STOE IPDS-II two circle diffractometer at 298 K, using graphite monochromated Mo K$\alpha$ radiation ($\lambda = 0.7107$ nm). A suitable crystal, grown from a methanol-diethylether solution, was mounted on a glass fiber. The data collection was performed at room temperature using the $\omega$-scan technique and using the STOE X-AREA software package [18]. The crystal structure was solved by direct methods and refined by full-matrix least-squares on $F^2$ by SHELX [19] and using the X-STEP32[11] crystallographic software package [20]. All non-hydrogen atoms were refined anisotropically using reflections $I > 2\sigma(I)$. Hydrogen atoms were inserted at calculated positions using a riding mode with fixed thermal parameters. Data collection and refinement parameters are given in Table 1. ORTEP views of the X-ray crystal structures of the two complexes are shown in Figs. 1 and 2. Selected bond lengths (Å) and bond angles (°) for complexes **1** and **2** are given in Table 2.

### 2.3. Synthesis of MBPPY

To a chloroform solution (25 ml) of triphenylphosphine (0.131 g, 0.5 mmol) was added 2-bromo-4′-methoxyacetophenone (0.114 g, 0.5 mmol) and the resulting mixture was stirred for 12 h. The solution was filtered off, the precipitate washed with diethelyether and dried. Further treatment with aqueous NaOH solution (0.5 M) led to elimination of HBr, giving the free ligand MBPPY. M.p: 153–158 °C. *Anal.* Calc. for $C_{27}H_{23}O_2P$: C, 67.24; H, 4.84. Found: C, 66.05; H, 4.88%.

Table 1
Crystal data and refinement details for [MBPPY · $HgCl_2]_2$ (**1**) and [MBPPY · $HgBr_2]_2 \cdot 2(C_2H_5)_2O$ (**2**)

| Compound | **1** | **2** |
|---|---|---|
| Empirical formula | $C_{54}H_{46}Cl_4Hg_2O_4P_2$ | $C_{62}H_{66}Br_4Hg_2O_6P_2$ |
| Formula weight | 363.83 | 1689.87 |
| Crystal system | triclinic | triclinic |
| Space group | $P\bar{1}$ | $P\bar{1}$ |
| Crystal size (mm) | 0.2 × 0.13 × 0.08 | 0.2 × 0.15 × 0.05 |
| $a$ (Å) | 10.3360(12) | 11.181(6) |
| $b$ (Å) | 13.7444(16) | 13.095(8) |
| $c$ (Å) | 19.657(2) | 13.124(8) |
| $\alpha$ (°) | 101.406(9) | 115.88(4) |
| $\beta$ (°) | 91.117(9) | 110.37(5) |
| $\gamma$ (°) | 108.725(9) | 91.13(5) |
| $V$ (Å$^3$) | 2582.2(5) | 186.8(16) |
| Temperature (K) | 293(2) | 293(2) |
| $Z$ | 2 | 1 |
| Calculated density (Mg/m$^3$) | 1.754 | 1.768 |
| $F$(000) | 1320 | 816 |
| Reflections collected | 23521 | 16157 |
| $\theta_{max}$ (°) | 1.6–26.80 | 1.77–28.22 |
| Final $R$ indices [$I > 2\sigma(I)$] | | |
| $R_1$ | 0.0335 | 0.0832 |
| $wR_2$ | 0.0559 | 0.1915 |
| $R$ indices (all data) | | |
| $R_1$ | 0.0460 | 0.1105 |
| $wR_2$ | 0.0593 | 0.2092 |
| Goodness-of-fit on $F^2$ | 1.134 | 1.235 |

$R_1 = \sum\|F_o| - |F_c\|/\sum|F_o|$ for reflections with $I > 2\sigma I$.
$wR_2 = [\sum w(|F_o^2| - |F_c^2|)^2/\sum|F_o^2|^2]^{1/2}$.

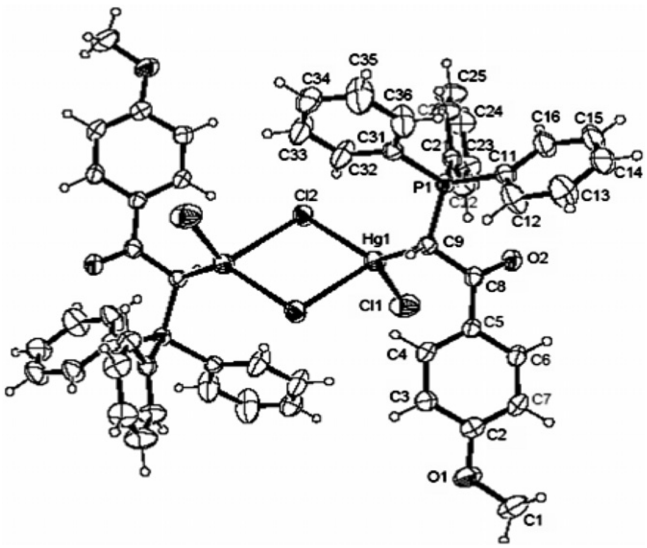


Fig. 1. ORTEP view of the X-ray crystal structure of [MBPPY · $HgCl_2]_2$.

## 2.4. Synthesis of the complexes

### 2.4.1. [MBPPY · $HgCl_2]_2$ (**1**)

To a methanolic solution (5 ml) of MBPPY (0.102 g, 0.25 mmol) was added mercury(II) chloride (0.067 g, 0.25 mmol). The mixture was stirred for 4 h. The white solid product was separated by filtration and washed with dietyl ether. Yield: 92.0%, m.p. 256–259 °C. *Anal.* Calc. for

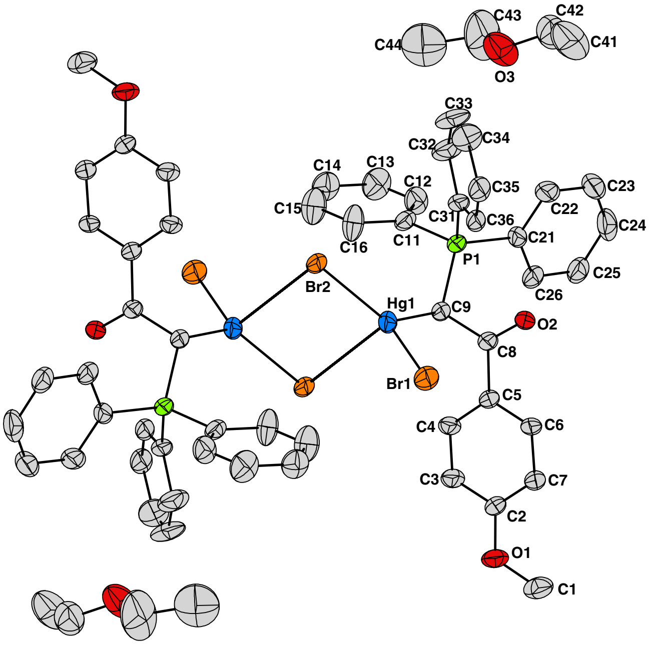


Fig. 2. ORTEP view of the X-ray crystal structure of [MBPPY · $HgBr_2]_2 \cdot 2(C_2H_5)_2O$.

Table 2
Selected bond lengths (Å) and angles (°) for the structures of **1** and **2**

| | **1** | **2** |
|---|---|---|
| *Bond distances* | | |
| Hg (1)–C(9) | 2.215(4) | 2.218(11) |
| Hg(1)–Cl(1) | 2.418(14) | 2.559(2) |
| Hg(1)–Cl(2) | 2.504(11) | 2.603(3) |
| Hg(1)–Cl(2)#1 | 2.884(12) | 3.022(2) |
| C(8)–O(2) | 1.219(5) | 1.251(13) |
| C(8)–C(9) | 1.498(5) | 1.470(16) |
| C(11)–P(1) | 1.789(4) | 1.796(13) |
| C(21)–P(1) | 1.806(4) | 1.806(11) |
| C(31)–P(1) | 1.801(4) | 1.800(12) |
| C(5)–C(8) | 1.486(6) | 1.528(14) |
| C(9)–P(1) | 1.785(4) | 1.827(11) |
| *Bond angles* | | |
| Hg(1)–Cl(2)–Hg(1)#1 | 96.10(4) | 90.16(7) |
| C(9)–Hg(1)–Cl(1) | 119.34(10) | 113.2(3) |
| C(9)–Hg(1)–Cl(2) | 129.16(10) | 132.9(3) |
| Cl(1)–Hg(1)–Cl(2) | 106.59(5) | 107.67(7) |
| C(9)–Hg(1)–Cl(2)#1 | 98.17(11) | 99.8(3) |
| Cl(1)–Hg(1)–Cl(2) | 110.86(5) | 106.36(7) |
| Cl(2)–Hg(1)–Cl(2)#1 | 83.90(4) | 89.84(7) |
| C(8)–C(9)–Hg(1) | 104.9(2) | 104.8(7) |
| P(1)–C(9)–Hg(1) | 113.00(19) | 114.3(5) |
| C(8)–C(9)–P(1) | 112.4(3) | 111.2(7) |
| C(9)–C(8)–C(5) | 119.5(3) | 118.8(9) |
| O(2)–C(8)–C(5) | 121.3(3) | 119.9(10) |
| C(11)–P(1)–C(9) | 110.80(19) | 105.5(5) |
| C(31)–P(1)–C(9) | 107.86(1) | 113.8(6) |
| C(21)–P(1)–C(9) | 113.00(18) | 112.4(5) |
| C(11)–P(1)–C(31) | 107.62(19) | 107.7(6) |
| C(11)–P(1)–C(21) | 109.33(19) | 108.6(6) |
| C(31)–P(1)–C(21) | 108.05(18) | 108.6(6) |
| O(2)–C(8)–C(9) | 119.2(4) | 121.2(10) |

$C_{54}H_{46}O_4P_2Hg_2Cl_4$: C, 47.3; H, 3.6. Found: C, 48.80; H, 3.41%.

#### 2.4.2. *[MBPPY · HgBr$_2$]$_2$ (**2**)*

To a methanolic solution (5 ml) of MBPPY (0.102 g, 0.25 mmol) was added mercury(II) bromide (0.091 g, 0.25 mmol). The mixture was stirred for 4 h. The solvent was then removed in vacuo. The white product obtained was washed with ice-cold methanol and dried in vacuum. Yield: 87.2%, m.p. 203–205 °C. *Anal.* Calc. for $C_{54}H_{46}O_4P_2Hg_2Br_4$: C, 40.66; H, 3.11. Found: C, 40.73; H, 2.88%.

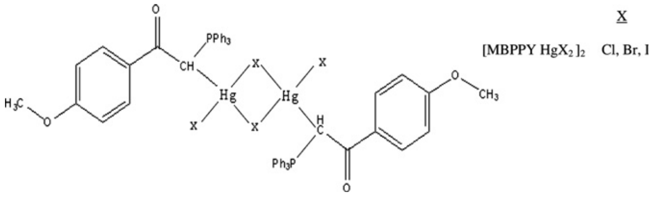
#### 2.4.3. *[MBPPY · HgI$_2$]$_2$ (**3**)*

To a methanolic solution (5 ml) of MBPPY (0.102 g, 0.25 mmol) was added mercury(II) iodide (0.113 g, 0.25 mmol). The mixture was stirred for 12 h. On concentration by removing the solvent by vacuum, a pale yellow precipitate was obtained. The products were washed with benzene and dried in vacuo. Yield: 81%, m.p. 242–245 °C. *Anal.* Calc. for $C_{54}H_{46}O_4P_2Hg_2I_4$: C, 37.49; H, 2.67. Found: C, 36.80; H, 2.64%.

## 3. Results and discussion

### 3.1. Synthesis

The ligand was synthesised by treating 2-bromo-4′-methoxyacetophenone (prepared by reacting 4-methoxyacetophenone with bromide in glacial acetic acid) with triphenylphosphine and removal of the proton from the phosphonium salt. Reactions of $HgX_2$ with the ylide in a 1:1 stoichiometry afforded the *C*-coordinated complexes with a halo-bridged dimeric structure:



### 3.2. Infra-red spectra

The $\nu$(CO) band, which is sensitive to complexation, occurs at 1601 cm$^{-1}$ in the parent ylide, as in the case of other resonance stabilized ylides [21]. Coordination of the ylide through *C*-coordination causes an increase in $\nu$(CO) while for *O*-coordination a lowering of $\nu$(CO) is expected. The IR absorption bands observed for the three complexes at 1630, 1626 and 1620 cm$^{-1}$ indicate coordination of the ylide thorough carbon. The $\nu(P^+–C^-)$ which is also diagnostic of the coordination occurs at 837 cm$^{-1}$ in $(C_6H_5)_3P^+–C–H_2$ and at 878 cm$^{-1}$ in $(C_6H_5)_3PCHCOC_6H_5$ [22]. These assignments were confirmed by comparing the IR spectra of the corresponding $^{13}C$ substituted ylides. In the present study, the $\nu(P^+–C^-)$ values for all three complexes were shifted to lower frequencies and were observed at 825, 820 and 812 cm$^{-1}$ for **1**, **2** and **3**, respectively, suggesting some removal of electron density from the P–C bond.

### 3.3. NMR spectral data

#### 3.3.1. *$^1$H NMR spectra*

The chemical shifts corresponding to the protons of the ligand and the complexes are listed in Table 3. The signals due to methine protons, when recorded in $CDCl_3$, were either broad or unobserved probably due to the very low solubility of all the complexes in $CDCl_3$. Similar behaviour was observed earlier in the case of ylide complexes of platinium(II) chloride [23]. However, a sharp doublet for the above proton was obtained in DMSO-$d_6$ for each of the three complexes in the same region. This indicates that the complexes do not react with DMSO-$d_6$. The appearance of a sharp doublet signal and expected downfield shift for the CH proton show the coordination of carbon through the methine group.

#### 3.3.2. *$^{31}$P NMR spectra*

The proton decoupled $^{31}$P NMR spectra show only one sharp singlet between $\delta$ 22.65–24.58 ppm for the complexes (Table 3). Chemical shift values for the complexes appear to be downfield by about $\delta$ 8–10 ppm with respect to the parent ylide ($\delta$ 14.061 ppm), indicating coordination of the ylide has occurred. The appearance of single signals for the PCH group in each of the $^{31}$P and $^1$H NMR spectra indicates the presence of only one isomer for all the three complexes, as expected for *C*-coordination. It must be noted that *O*-coordination of the ylide generally leads to the formation of *cis* and *trans* isomers, giving rise to two different signals in $^{31}$P and $^1$H NMR spectra [24].

#### 3.3.3. *$^{13}$CNMR*

The $^{13}$CNMR data of the complexes and the title ylide are listed in Table 3, along with possible assignments. The most interesting aspect of the $^{13}$CNMR spectra of the complexes is the upfield shift of the signals due to the ylidic carbon. Such an upfield shift observed in $PdCl(\eta^3–2–XC_3H_4)\ (C_6H_5)_3PCHCOR$ ($X = H$, $CH_3$; $R = CH_3$, $C_6H_5$) was attributed to the change in hybridization of the ylidic carbon [25]. Similar upfield shifts of 2–3 ppm with reference to the parent ylide were also observed in the case of $[(C_6H_5)_3PC_5H_4HgI_2]_2$ [23]. The $^{13}$C shifts of the CO group in the complexes are around 189 ppm, relative to 184.265 ppm noted for the same carbon in the parent ylide, indicating much lower shielding of the carbon of the CO group in these complexes. No coupling to Hg was observed at room temperature in the $^1$H, $^{13}$C and $^{31}$P NMR spectra for all these complexes. Failure to observe satellites in the above spectra was previously noted in the ylide complexes of Hg(II) [26] and Ag(I) [27], which had been explained by fast exchange of the ylide with the metal.

Table 3
$^{1}H$, $^{13}C$ and $^{31}P$ NMR data of MBPPY and its complexes with mercury (II) halides

| Compound | $^{1}H$ chemical shifts ($\delta$ ppm) | $^{13}C$ chemical shifts ($\delta$ ppm) | $^{31}P$ chemical shifts ($\delta$ ppm) |
|---|---|---|---|
| MBPPY | 3.79 (3H, $OCH_3$)<br>4.25 (1H, d ($J = 15.68$ Hz), CH)<br>6.80–8.21 (19H, m, $C_6H_5$) | 55.08 (s, $OCH_3$)<br>49.21 (d, ($J = 119.24$ Hz), CH)<br>126.77 (d, ($J = 74.8$ Hz), $PPh_3$(*i*))<br>128.70 (d, ($J = 12.4$ Hz), $PPh_3$(*m*))<br>131.89 (s, $PPh_3$(p))<br>133.98 (d, ($J = 10.2$ Hz), $PPh_3$(*o*))<br>160.65 (s, CO. Ph (*i*))<br>184.26 (s, CO) | 14.06 (s) |
| MBPPY · $HgCl_2$ | 3.83 (3H, $OCH_3$)<br>5.43 (1H, d, CH)<br>6.81–8.20 (19H, m, $C_6H_5$) | 123.46 (d, ($J = 88.58$ Hz), $PPh_3$(*i*))<br>129.32 (d, ($J = 12.61$ Hz), $PPh_3$(*m*))<br>131.89 (s, $PPh_3$ (p))<br>133.29 (d, ($J = 8.22$ Hz), $PPh_3$(*o*))<br>162.58 (s, CO. Ph (*i*))<br>189.76 (s, CO) | 24.58 (s) |
| MBPPY · $HgBr_2$ | 3.81 (3H, $OCH_3$)<br>5.45 (1H, d, CH)<br>6.90–8.30 (19H, m, $C_6H_5$) | 123.51 (d, ($J = 89.12$ Hz), $PPh_3$(*i*))<br>129.37 (d, ($J = 12.7$ Hz), $PPh_3$ (*m*))<br>130.41 (s, $PPh_3$(p))<br>133.34 (d, ($J = 9.57$ Hz), $PPh_3$(*o*))<br>162.58 (s, CO. Ph (*i*))<br>190.56 (s, CO) | 23.58 (s) |
| MBPPY · $HgI_2$ | 3.82 (3H, $OCH_3$) 22.67 (s)<br>5.25 (1H, d ($J = 6.98$ Hz), CH)<br>6.85–8.20 (19H, m, $C_6H_5$) | 123.76 (d, ($J = 90.22$ Hz), $PPh_3$(*i*))<br>129.45 (d, ($J = 12.79$ Hz), $PPh_3$(*m*))<br>130.21 (s, $PPh_3$ (p))<br>133.31 (d, ($J = 9.68$ Hz), $PPh_3$(*o*))<br>162.43 (s, CO. Ph (*i*))<br>188.71 (s, CO) | 22.65 (s) |

s = singlet, d = double, m = multiplet, *o = ortho, m = meta, p = para, i = ipso.*

### *3.4. Crystal structure*

The solid state structures of complexes **1** and **2** have been established by single crystal X-ray analysis, which revealed triclinic units. The molecular structures are shown in Figs. 1 and 2, and selected interatomic parameters are collected in Table 2.

The dimeric structure adopted by complexes **1**, **2** and **3** is in contrast to the *O*-coordinated trinuclear mercury(II) complex of the phosphorus ylide $Ph_3PCHCOPh$ [28], but is similar to the structure of *trans*-di-μ-iododiiodobis(triphenylphosphoniumcyclopentadienylide) dimercury(II) reported by Baenziger et al. [29] and the *C*-coordinated dinuclear mercury(II) halide complexes of $Ph_3CHCOPh$ (BPPY) [30]. The *C*-coordination of MBPPY is in stark contrast to the *O*-coordination of the phosphorus ylide, $Ph_3PC(COMe)(COPh)$ (ABPPY), to a Hg(II) centre [31]. The difference in coordination mode between ABPPY and MBPPY to Hg(II) can be rationalized in terms of the electronic properties and steric requirements of the ylides. The nucleophilicity of the carbanion in ABPPY is less than for MBPPY; this is due to the additional delocalization of the ylide electron density in ABPPY which is facilitated by the second carbonyl group. This will reduce the ability of ABPPY to bind via the ylidic carbon. Belluco et al. have studied steric influences on the coordination modes of ylide molecules to Pt(II) systems [32]. These authors concluded that the preferred coordination mode is via the ylidic carbon, but that steric hindrance around the metal centre or the ylidic carbon will necessitate *O*-coordination. Indeed, this trend is reflected here, both BPPY and MBPPY are slightly less sterically demanding than ABPPY, and both are *C*-coordinated to Hg(II).

The Hg(II) centre forms four close contacts with $sp^3$ hybridization and has a 4-coordinate environment with one short Hg–X bond, one Hg–C bond and two asymmetric bridging Hg–X bonds at distances of 2.504(11) and 2.884(12) Å in **1** and 2.603(3) and 3.022(2) Å in **2**.

The significant shortening of the Hg–C bond length, 2.215(4) Å **1** and 2.218(11) Å **2** compared to analogous distances in $[(C_6H_5)_3PCHCOC_6H_5HgI_2]_2$ [30] and in $[(C_5H_4P(C_6H_5)_3HgI_2]_2$ [33] (2.312(13) and 2.292(8) Å, respectively) must be attributed to the use of mercury orbitals with high s character for bonding to the ylidic carbon. The use of non-equivalent hybrid orbitals with high s character to bond to low electronegative atoms was proposed by Bent in the concept of isovalent hybridization to account for the variation in bond lengths and bond angles around a central atom [34].

The terminal Hg–Cl bond length, 2.418(14) Å **1** is comparable to 2.400 Å observed in the case of $Hg_2Cl_5N_2C_{11}H_{12}$, which has a tetrahedral coordination environment around mercury with a bridging structure [35]. The two bridged Hg–Cl bonds fall within the range 2.620–3.080 Å reported for other structures [36] containing chloro bridged mercury.

The angles around mercury vary from 83.90(4)° to 129.16(10)° for the chloride and 89.84(7)° to 132.9(3)° for the bromide, a very distorted tetrahedral environment. This distortion must be due to the higher s character of the $sp^3$ hybrid mercury orbitals involved in the above bonds and the formation of a strong halogen bridge between the Hg atoms which requires the internal XHgX angle to be considerably smaller.

The stabilized resonance structure for the title ylide is destroyed by the complexes formation. Thus, the C(8)–C(9) bond length (1.498(5) Å, **1** and 1.470(16) Å, **2**) is significantly longer than the corresponding bond found in a similar uncomplexed phosphorane (1.407(8) Å) [37]. On the other hand, the bond length of P(1)–C(9) in the similar ylide is 1.706 Å [24] which shows that the above bond is considerably elongated to 1.785(4) Å and 1.827(11) Å in complexes **1** and **2**, respectively. The plane defined by the two mercury atoms and the two bridging halogens is perfectly planar in both structures. The internuclear distances between mercury atoms were found to be 3.901(7) Å and 3.994(8) Å in structures **1** and **2**, respectively. These distances are much longer than the sum of Van der Waals radii (1.5 Å) of the two mercury atoms [38] indicating the absence of significant bonding interactions between the mercury atoms in the molecular structures. The adaptation of dimeric structures in Hg(II) ylide complexes may be explained by both the preference of Hg(II) to four coordination and the stability of the 18 electron configuration around Hg(II).

## 4. Conclusions

The present study describes the synthesis and characterization of a series of mercury ylide complexes. On the basis of the physico-chemical and spectroscopic data we propose that MBPPY herein exhibits monodentate *C*-coordination to the metal center, which is further confirmed by the X-ray crystal structures of the complexes.

## 5. Supplementary material

CCDC 622081 and 620129 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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## References

[1] Y. Shen, Acc. Chem. Res. 31 (1998) 584.

[2] C. Puke, G. Erker, N.C. Aust, E.U. Wurthweine, R. Frohich, J. Am. Chem. Soc. 120 (1998) 4863.

[3] O.I. Kolodiazhnyi, Russ. Chem. Rev. 66 (1997) 225.

[4] D.E.C. Cobridge, Phosphorus an Outline of Chemistry, Biochemistry and Uses, 5th ed., Elsevier, Amsterdam, 1995.

[5] H. Nishiyama, K. Itoh, Y. Ishii, J. Organomet. Chem. 87 (1975) 129.

[6] J. Vicent, M.T. Chicote, J. Fernandez-Baeza, J. Organomet. Chem. 364 (1989) 407.

[7] M. Onishi, Y. Ohama, K. Hiraki, H. Shintani, Polyhedron 1 (1982) 539.

[8] J. Vicent, M.T. Chicote, M.C. Lagunas, P.G. Jones, J. Chem. Soc., Dalton Trans. (1991) 2579.

[9] J. Buckle, P.G. Harrison, T.J. King, J.A. Richards, J. Chem. Soc., Chem. Commun. (1972) 1104.

[10] J. Buckle, P.G. Harrison, J. Organomet. Chem. 49 (1973) C17.

[11] J.A. Albanese, D.A. Staley, A.L. Rheingold, J.L. Burmeister, Inorg. Chem. 29 (1990) 2209.

[12] I. Kawafune, G. Matsubayashi, Inorg. Chim. Acta 70 (1983) 1.

[13] R. Uson, J. Fornies, R. Navarro, P. Espinet, C.J. Mendivil, Organomet. Chem. 290 (1985) 125.

[14] J.L. Burmeister, J.L. Silver, E.T. Weleski, E.E. Schweizer, C.M. Kopay, Synth. Inorg. Met. Org. Chem. 3 (1973) 339.

[15] M.L. Illingsworth, J.A. Teagle, J.L. Burmeister, W.C. Fultz, A.I. Rheingold, Organometallics 2 (1983) 1364.

[16] F. Ramirez, S. Dershowitz, J. Org. Chem. 22 (1957) 41.

[17] A.J. Gordon, R.A. Ford, The Chemist's Companion – A Handbook of Practical Data, Techniques and References, Wiley-Interscience, New York, 1972, p. 438.

[18] Stoe & Cie, X-AREA, version 1.30: Program for the Acquisition and Analysis of Data, Stoe & Cie GmbH, Darmatadt, Germany, 2005.

[19] G.M. Sheldrick, SHELX97. Program for Crystal Structure Solution and Refinement, University of Göttingen, Germany, 1997.

[20] Stoe & Cie, X-STEP32, Version 1.07b: Crystallographic Package, Stoe & Cie GmbH, Darmatadt, Germany, 2005.

[21] J. Vicente, M.T. Chicoto, M.C. Lagunas, P.G. Jones, J. Chem. Soc., Dalton Trans. (1991) 2579.

[22] W. Luttke, K. Wilhelm, Angew. Chem., Int. Ed. Engl. 4 (1965) 875.

[23] J.A. Teagle, J.L. Burmieister, Inorg. Chim. Acta 118 (1986) 65.

[24] R. Uson, J. Fornies, R. Navarro, P. Espinet, C. Mendivil, J. Organomet. Chem. 290 (1985) 125.

[25] G. Facchin, R. Bertani, M. Calligaris, G. Nardin, M. Mari, J. Chem. Soc., Dalton Trans. (1987) 1381.

[26] N.I. Holy, N.C. Baenziger, R.M. Flynn, D.C. Swenson, J. Am. Chem. Soc. 98 (1976) 7823.

[27] J. Vicente, M.T. Chicote, J. Fernandez-Baeza, J. Martin, I. Saura-Hamas, J. Iurpin, P.G. Jones, J. Organomet. Chem. 331 (1987) 409.

[28] M. Kalyanasundari, K. Panchanatheswaram, W.T. Robinson, Bull. Chem. Soc. Jpn. 72 (1999) 33.

[29] N.C. Baenziger, R.M. Flyuu, D.C. Swenson, Acta Crystallogr., Sect. B 34 (1978) 2300.

[30] M. Kalyanasundari, K. Panchanatheswaran, W.T. Robinson, H. Wen, J. Organomet. Chem. 491 (1995) 103.

[31] P. Laavanya, U. Venkatasubramanian, K. Panchanatheswaran, J.A. Krause Baure, Chem. Commun. (2001) 1660.

[32] U. Belluco, R.A. Michelin, R. Bertini, G. Facchin, G. Pace, L. Zanotto, M. Mozzon, M. Furlan, E. Zangrando, Inorg. Chim. Acta (1996) 355.

[33] N.I. Holy, N.C. Baenziger, R.M. Flynn, D.C. Swenson, J. Am. Chem. Soc. 98 (1976) 7823.

[34] H.A. Bent, Chem. Rev. 61 (1961) 75.

[35] A. Albinati, S.V. Meille, F. Cariati, G. Marcotrigiano, L. Menabue, G.C. Pellacani, Inorg. Chim. Acta 38 (1984) 221.

[36] N.A. Bell, S.J. Coles, M.B. Hursthouse, M.E. Light, K.A. Malik, R. Mansor, Polyhedron 19 (2000) 1719.

[37] M. Kalyanasundari, K. Panchanatheswaran, V. Parthasarathi, W.T. Robinson, H. Wen, Acta Crystallogr. 50 (1994) 1738.

[38] J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, 2nd ed., Harper Int. Ed., New York, 1978, p. 233.