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## Key indicators

Single-crystal synchrotron study
$T=150 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.005 \AA$
$R$ factor $=0.032$
$w R$ factor $=0.068$
Data-to-parameter ratio $=25.4$

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

# trans-( $\mu$-5,5'-Diethynyl-2,2'-bipyridine)bis[phenylbis(triethylphosphine)platinum(II)] 

The title compound, $\left[\mathrm{Pt}_{2}\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2}\left(\mathrm{C}_{14} \mathrm{H}_{6} \mathrm{~N}_{2}\right)\left(\mathrm{C}_{6} \mathrm{H}_{15} \mathrm{P}\right)_{4}\right]$, is a dinuclear $\mathrm{Pt}^{\mathrm{II}}$ di-yne complex that exhibits $\pi$-conjugation along the molecular backbone. It is used as a model complex for rigid-rod platinum poly-yne polymers of which it is a precursor. Such compounds are of interest because of the extended $\pi$-conjugation through the aromatic/heteroaromatic spacer group in the backbone. The asymmetric unit contains two half molecules of the title compound, each lying on a crystallographic centre of symmetry situated at the mid-point of the central $\mathrm{C}-\mathrm{C}$ bond of the bipyridine unit.

## Comment

In this paper, we report the structural characterization of the title compound, (I), which is a dinuclear platinum(II) di-yne species, trans $-\left[(\mathrm{Ph})\left(\mathrm{PEt}_{3}\right)_{2} \mathrm{Pt}-\mathrm{C} \equiv \mathrm{C}-R-\mathrm{C} \equiv \mathrm{C}-\mathrm{Pt}\left(\mathrm{PEt}_{3}\right)_{2^{-}}\right.$ (Ph)] ( $R=2,2^{\prime}$-bipyridine-5,5'-diyl). Such organoplatinum species form the building blocks for rigid-rod platinum polyynes of general formula trans- $\left[\mathrm{Pt}\left(\mathrm{P} X_{3}\right)_{2}-\mathrm{C} \equiv \mathrm{C}-R-\mathrm{C} \equiv\right.$ $\mathrm{C}-$ ] ( $X=$ tertiary phosphines and $R=$ aromatic/heteroaromatic spacer group). Platinum(II) poly-ynes are of immense current interest due to $\pi$-electron conjugation along the rigid backbone of the organometallic polymer. These materials possess a wide variety of interesting properties useful for application in modern technology. For example, incorporating platinum into the polymer backbone introduces strong spinorbit coupling and phosphorescence can be readily observed (Wittmann et al., 1994; Beljonne et al., 1996; Younus et al., 1998; Chawdhury et al., 1998, 1999). Platinum(II) poly-ynes provide model systems for the study of some of the basic photophysical properties that occur in conjugated organic and organometallic polymers (Khan, Al-Mandhary, Al-Suti, Hisahm et al., 2002; Khan, Al-Mandhary, Al-Suti, Feeder et al., 2002; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Mahon et al., 2003; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Male et al., 2003), are used in optoelectronic devices such as light emitting diodes (LEDs), lasers, photocells and field-effect transistors (FETs) (Wilson et al., 2000; Wilson, Chawdhury et al., 2001; Wilson, Dhoot et al., 2001). Group 10 metal poly-ynes also show interesting alignment and liquid crystal properties, one-dimensional conductivity and non-linear optical (NLO) properties (Takahashi et al., 1984; Wilson et al., 2003).


Precursors to these species, such as the title compound, (I), are utilized as models in the study of the molecular and electronic

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Figure 1
View of molecule 1 of (I) ( $50 \%$ probability displacement ellipsoids). The suffix $A$ denotes symmetry position $1-x, 1-y,-z$.


Figure 2
View of molecule 2 of (I) ( $50 \%$ probability displacement ellipsoids). The suffix $A$ denotes symmetry position $1-x, 2-y,-z$.
properties and structure-property relationships in the metal poly-ynes.

The asymmetric unit of the triclinic unit cell of (I) contains two structurally similar half molecules of the title compound, each sitting on a centre of symmetry corresponding to the midpoint of the central $\mathrm{C}-\mathrm{C}$ bond of the bipyridine ligand. The bipyridine ligands are orientated in the trans configuration with respect to the N atoms, as would be expected to minimize $\mathrm{H} \cdots \mathrm{H}$ contacts. The same configuration is observed in the trimethylsilyl-substituted derivative (Khan et al., 2004); the bond parameters are also similar to those found in this derivative. The platinum centres exhibit the expected squareplanar geometry and the bond parameters are similar to those reported in related platinum di-yne complexes (Khan, AlMandhary, Al-Suti, Hisahm et al., 2002; Khan, Al-Mandhary, Al-Suti, Feeder et al., 2002; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Mahon et al., 2003; Khan, Al-Mandhary, AlSuti, Raithby, Ahrens, Male et al., 2003). The platinum square plane makes dihedral angles of $79.3(1)^{\circ}$ with the adjacent pyridine ring [73.4 (1) ${ }^{\circ}$ in molecule 2], and $88.6(1)^{\circ}$ with the
terminal phenyl ring [83.1 (1) ${ }^{\circ}$ in molecule 2]. The two pyridine rings in each independent molecule are precisely coplanar by crystallographic symmetry. There are no significant short intermolecular contacts within the structure.

## Experimental

The title compound was synthesized according to the procedure of Khan, Al-Mandhary, Al-Suti, Hisahm et al. (2002). To a stirred solution of trans-[(PEt $\left.)_{2}(\mathrm{Ph}) \mathrm{PtCl}\right](0.543 \mathrm{~g}, 1.0 \mathrm{mmol})$ and $5,5^{\prime}-$ bisethynyl-2, $2^{\prime}$-bipyridine ( $0.102 \mathrm{~g}, 0.50 \mathrm{mmol}$ ) in $\mathrm{CH}_{2} \mathrm{Cl}_{2} /{ }^{i} \mathrm{Pr}_{2} \mathrm{NH}$ ( $50 \mathrm{ml}, 1: 1 \mathrm{v} / \mathrm{v}$ ) under nitrogen was added a catalytic amount (approximately 5 mg ) of CuI. The yellow solution was stirred at room temperature for 15 h , after which all volatile components were removed under reduced pressure. The residue was dissolved in $\mathrm{CH}_{2} \mathrm{Cl}_{2}$ and passed through a silica column, eluting with hexane$\mathrm{CH}_{2} \mathrm{Cl}_{2}(1: 1 \mathrm{v} / \mathrm{v})$. Removal of the solvents in vacuo gave the title complex as a pale-yellow solid ( $0.43 \mathrm{~g}, 70 \%$ ). Further purification was accomplished by triturating the complex in methanol.

## Crystal data

$\left[\mathrm{Pt}_{2}\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2}\left(\mathrm{C}_{14} \mathrm{H}_{6} \mathrm{~N}_{2}\right)\left(\mathrm{C}_{6} \mathrm{H}_{15} \mathrm{P}\right)_{4}\right]$
$M_{r}=1219.19$
Triclinic, $P \overline{1}$
$a=9.2651$ (7) $\AA$
$b=16.6840(14) \AA$
$c=16.8258(14) \AA$
$\alpha=92.130$ (2) ${ }^{\circ}$
$\beta=90.032(2)^{\circ}$
$\gamma=94.958(2)^{\circ}$
$V=2589.4$ (4) $\AA^{3}$
$Z=2$

## Data collection

Bruker AXS SMART 1K CCD
diffractometer
Narrow frame $\omega$ scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
$T_{\min }=0.895, T_{\max }=0.946$
25942 measured reflections

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.032$
$w R\left(F^{2}\right)=0.068$
$S=1.00$
13587 reflections
535 parameters
$D_{x}=1.564 \mathrm{Mg} \mathrm{m}^{-3}$
Synchrotron radiation, $\lambda=0.6941 \AA$
Cell parameters from 25942
reflections
$\theta=21.7-29.3^{\circ}$
$\mu=5.55 \mathrm{~mm}^{-1}$
$T=150(2) \mathrm{K}$
Block, yellow
$0.02 \times 0.01 \times 0.01 \mathrm{~mm}$

13587 independent reflections
11103 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.024$
$\theta_{\text {max }}=29.3^{\circ}$
$h=-12 \rightarrow 12$
$k=-23 \rightarrow 23$
$l=-23 \rightarrow 23$

H -atom parameters constrained
$w=1 /\left[\sigma^{2}\left(F_{o}^{2}\right)+(0.04 P)^{2}\right]$
where $P=\left(F_{o}{ }^{2}+2 F_{c}{ }^{2}\right) / 3$
$(\Delta / \sigma)_{\max }=0.004$
$\Delta \rho_{\text {max }}=1.63 \mathrm{e}_{\AA^{-3}}$
$\Delta \rho_{\min }=-1.86 \mathrm{e}^{\AA^{-3}}$

Aromatic, methylene and methyl H atoms were constrained as riding atoms, fixed to the parent atoms with distances of $0.95,0.99$ and $0.98 \AA$, respectively. The isotropic displacement parameters were fixed to $120 \%$ of those of the parent atoms for aromatic and methylene H atoms and $150 \%$ for methyl H atoms. The high residual electron density peaks were located close to the positions of the two unique Pt atoms.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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