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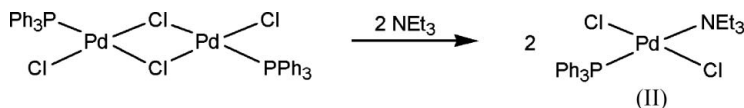
## Key indicators

Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma$ (C–C) = 0.009 Å  
*R* factor = 0.052  
*wR* factor = 0.106  
Data-to-parameter ratio = 16.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*trans*-Dichloro(triethylamine- $\kappa$ N)(triphenylphosphine- $\kappa$ P)palladium(II)The Pd atom in the title compound, *trans*-[PdCl<sub>2</sub>(C<sub>6</sub>H<sub>15</sub>N)-(C<sub>18</sub>H<sub>15</sub>P)], is in an approximately square-planar environment, coordinated by one triethylamine, one triphenylphosphine and two *trans* Cl ligands.

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## Comment

The chemistry of palladium(II) complexes containing nitrogen donor ligands continues to be of interest, in part due to the role of such compounds in C–N bond formation (Hartwig, 1998; Müller & Beller, 1998). In this work, we report the synthesis and structural characterization of the first palladium–tertiary amine complex containing a *trans*-dichloro-(triphenylphosphine) structural unit.A one-pot reaction of  $[\{\text{Pd}(\mu\text{-Cl})\text{Cl}(\text{PPh}_3)\}_2]$  and  $\text{RNNNH}\text{R}$  ( $\text{R} = 3,5$ -dimethylphenyl) with excess  $\text{NEt}_3$ , for deprotonation of the triazene ligand, yielded not only the new  $\text{Pd}^{\text{II}}$  triazene-bridged complex,  $[(\text{PPh}_3)\text{ClPd}(\mu\text{-RNNNR})_2\text{PdCl}(\text{PPh}_3)]$ , (I), but also a by-product, *viz.* *trans*-[PdCl<sub>2</sub>[N(C<sub>2</sub>H<sub>5</sub>)<sub>3</sub>]{P(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>}], (II) (Harding & Harding, 2006). Subsequently, a rational synthesis of (II) was devised (see scheme) and the compound was studied by single-crystal X-ray crystallography.Complex (II) consists of a  $\text{Pd}^{\text{II}}$  metal centre bound to one triethylamine, one triphenylphosphine and two *trans* Cl ligands (Fig. 1). The Pd–Cl and Pd–P bond distances (Table 1) are in good agreement with other structurally related compounds, such as *trans*-[PdCl<sub>2</sub>(NHCy<sub>2</sub>)(PPh<sub>3</sub>)] (Cy is cyclohexyl; Parvez *et al.*, 2004), *trans*-[PdCl<sub>2</sub>(MeNHCH<sub>2</sub>Ph)(PPh<sub>3</sub>)] (Jones *et al.*, 2000) and *trans*-[PdCl<sub>2</sub>(indoline- $\kappa$ N)(PPh<sub>3</sub>)] (Chen *et al.*, 1997). In contrast, the Pd–N bond distance is 2.236 (4) Å, far longer than that observed in palladium(II) complexes with secondary amines (Pd–N = 2.121–2.166 Å; Parvez *et al.*, 2004; Jones *et al.*, 2000; Chen *et al.*, 1997; Albinati *et al.*, 1992). The coordination of palladium has an approximately square-planar geometry (Table 1).

## Experimental

 $\text{NEt}_3$  (40  $\mu\text{l}$ , 0.29 mmol) was added to a yellow suspension of  $[\{\text{Pd}(\mu\text{-Cl})\text{Cl}(\text{PPh}_3)\}_2]$  (0.0910 g, 0.1 mmol) in  $\text{CH}_2\text{Cl}_2$  (10 ml). The resulting clear orange solution was stirred for 15 min, then *n*-hexane (15 ml) was added. The solvent was removed *in vacuo* until an orange solid started to precipitate. The mixture was stored at 253 K overnight,

yielding an orange solid (0.0670 g, 62%). Suitable orange plate-shaped crystals were obtained by allowing *n*-hexane to diffuse into a concentrated solution of the complex in CH<sub>2</sub>Cl<sub>2</sub> at 253 K.

#### Crystal data

[PdCl<sub>2</sub>(C<sub>6</sub>H<sub>15</sub>N)(C<sub>18</sub>H<sub>15</sub>P)]  
*M<sub>r</sub>* = 540.76  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 16.6260 (14) Å  
*b* = 10.7341 (9) Å  
*c* = 14.9916 (13) Å  
 $\beta$  = 113.628 (2)°  
*V* = 2451.2 (4) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.465 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 1.05 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Plate, orange  
 0.21 × 0.20 × 0.01 mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1997)  
*T<sub>min</sub>* = 0.804, *T<sub>max</sub>* = 0.990

17249 measured reflections  
 4312 independent reflections  
 3639 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.045  
 $\theta_{\max}$  = 25.0°

#### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.052  
 $wR$  (*F*<sup>2</sup>) = 0.106  
*S* = 1.17  
 4312 reflections  
 265 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 1.5049P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.59 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.78 \text{ e \AA}^{-3}$

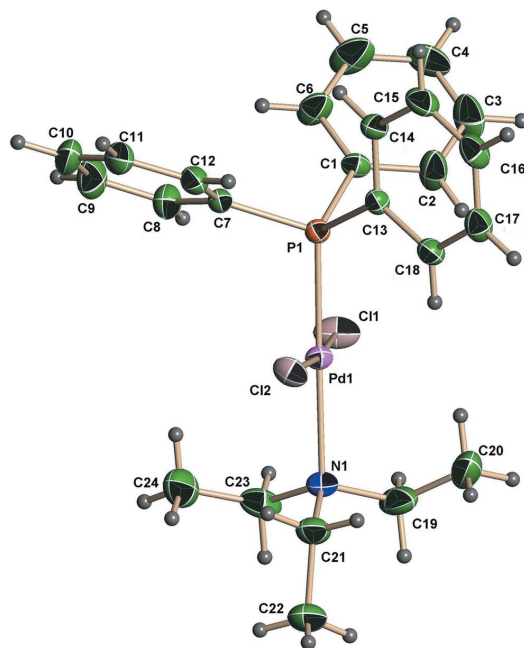
**Table 1**

Selected geometric parameters (Å, °).

Pd1—N1	2.236 (4)	Pd1—Cl2	2.2957 (12)
Pd1—P1	2.2459 (12)	Pd1—Cl1	2.2979 (14)
N1—Pd1—P1	178.30 (11)	N1—Pd1—Cl1	90.91 (11)
N1—Pd1—Cl2	93.80 (11)	P1—Pd1—Cl1	90.53 (5)
P1—Pd1—Cl2	84.83 (4)	Cl2—Pd1—Cl1	173.33 (6)

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95–0.98 Å and with *U<sub>iso</sub>*(H) values set equal to 1.2 times *U<sub>eq</sub>* of the carrier atom for *sp*<sup>2</sup> H atoms and methylene CH<sub>2</sub> groups, and to 1.5 times *U<sub>eq</sub>* of the carrier atom for the methyl H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XSEHELL (Bruker, 1997); software used to prepare material for publication: XSEHELL.



**Figure 1**

The molecular structure of (II), showing 50% probability displacement ellipsoids.

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