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Dichloro(4,4′-dinonyl-2,2′-bipyridine-κ^2N,N')platinum(II)

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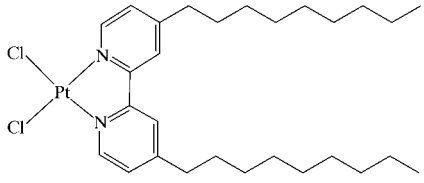
The title compound, $[PtCl_2(C_{28}H_{44}N_2)]$, is a new square-planar Pt^{II} complex containing a bipyridine moiety with two long alkyl-chain substituents. The complex forms a segregated packing structure made up of the alkyl-chain layers and paired coordination sites.

Comment

The introduction of long alkyl chains to various chemical systems is an important strategy for the construction of self-assembled nanostructures. Some approaches to the construction and control of supramolecular systems based on Pt complexes have been reported recently (Neve *et al.*, 1997; Wang *et al.*, 2000; Kimizuka *et al.*, 2000). We report here the crystal structure of the title novel Pt complex containing bipyridine with two long alkyl chains, $[PtCl_2(dnbpy)]$ (dnbpy is 4,4′-dinonyl-2,2′-bipyridine), (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The two alkyl chains are extended out of the coordination plane and are ordered almost parallel to the *bc* plane to make an alkyl-chain layer, as shown in Fig. 2. Between the alkyl-chain layers, square-planar coordination sites are paired, forming a face-to-face arrangement related to the inversion centre. As shown in Fig. 3, the coordination planes are connected mainly *via* the π–π interactions of the bipyridine ligands; the interplanar distance is 3.39 (3) Å. The Pt atoms are thus separated from each other, indicating no interaction [Pt···Pt = 5.3688 (5) Å].

The stacking features of (I) are different from those observed for both forms of the parent complex, $[PtCl_2(bpy)]$ (bpy is 2,2′-bipyridine), namely the red form containing a Pt···Pt linear chain (Connick *et al.*, 1996; Osborn & Rodger, 1974) and the yellow form containing an infinite π–π stack (Herber *et al.*, 1994). The arrangement for (I) is similar to those observed for $[PtCl_2(bu_2bpy)]$ (bu_2bpy is 4,4′-di-*tert*-butyl-2,2′-bipyridine), which has bulky substituents (Achor & Catalano, 1997), and $[PtCl_2(i\text{-}biq)]$ (i-biq is 3,3′-biisoquinoline), which has an extended π-system (Kato *et al.*, 1996), although both of these compounds form columnar stacks.

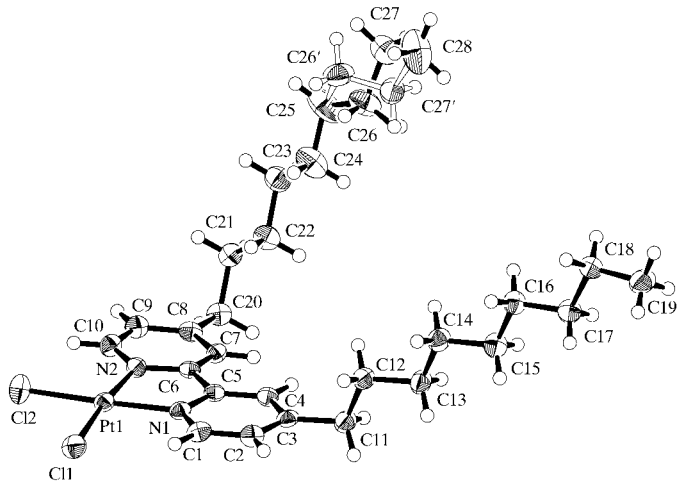


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The disordered atoms C26′ and C27′ are drawn with open bonds.

The segregated packing of the paired coordination sites and the alkyl-chain layers strongly reflects the amphiphilic nature of (I). A similar layer structure was also reported for the crystals of [Pt(*L*)Cl] {H*L* is 4′-[4-(dodecyloxy)phenyl]-6′-phenyl-2,2′-bipyridine}, although this dagger-shaped complex takes a different arrangement from (I), having an in-plane alkyl chain (Neve *et al.*, 1997).

The crystal structure of (I) suggests that the complex is appropriate for self-assembled systems on two-dimensional surfaces.

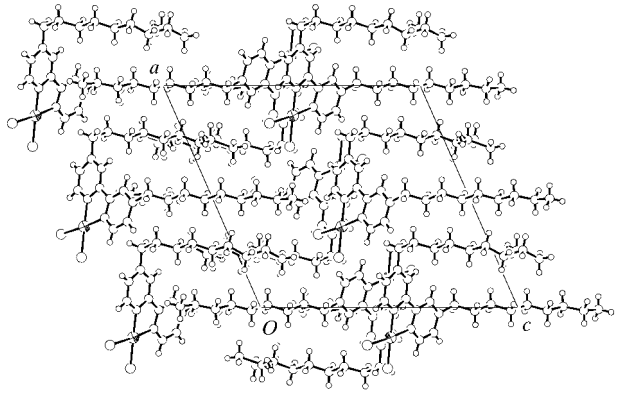


Figure 2
The packing structure of (I), viewed down the *b* axis.

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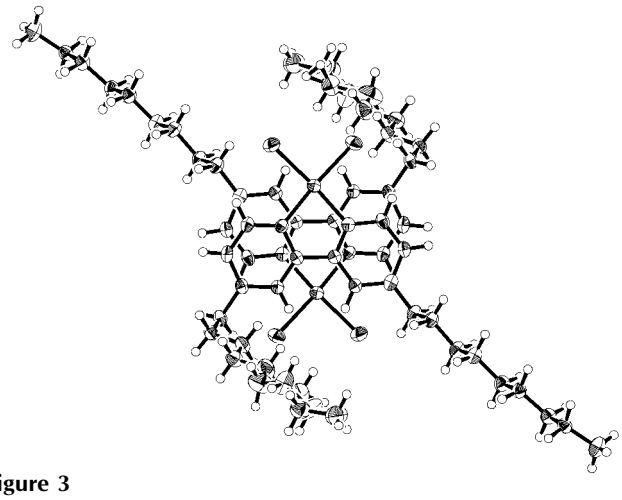

Figure 3
The face-to-face arrangement of the paired $[PtCl_2(dnbpy)]$ complexes in the structure of (I).

Experimental

The dnbpy ligand was purchased from Aldrich. An acidic aqueous solution (20 ml) of $K_2[PtCl_4]$ (103 mg, 0.25 mmol) and dnbpy (102 mg, 0.25 mmol) was heated at 343 K for 24 h, producing a yellow product, (I) (yield 158 mg, 94%). Recrystallization from *N*,*N*-dimethylformamide gave yellow plate-shaped crystals. Analysis calculated for $C_{28}H_{44}Cl_2N_2Pt$: C 49.85, H 6.57, N 4.15%; found: C 49.90, H 6.45, N 4.30%. Spectroscopic analysis, ^{1}H NMR ($CDCl_3$, δ): 0.88 (*s*, 3H, CH_3), 1.28 (*br*, 12H, CH_2), 1.74 (*br*, 12H, CH_2), 2.79 (*t*, 2H, CH_2), 7.25 (*d*, 1H, bpy), 7.84 (*s*, 1H, bpy), 9.35 (*d*, 1H, bpy).

Crystal data

$[PtCl_2(C_{28}H_{44}N_2)]$
M_r = 674.66
Monoclinic, $P2_1/a$
a = 16.663 (2) Å
b = 10.6209 (5) Å
c = 17.652 (2) Å
β = 113.725 (4)°
V = 2860.0 (4) Å^3
Z = 4
D_x = 1.567 Mg m^{-3}
D_m = 1.52 (1) Mg m^{-3}
D_m measured by flotation in hexane/CCl_4 at 294 K
Mo $K\alpha$ radiation
Cell parameters from 8757 reflections
θ = 3.0–27.5°
μ = 5.09 mm^{-1}
T = 173.2 K
Plate, yellow
0.64 × 0.47 × 0.11 mm

Data collection

Rigaku/MSC Mercury CCD area-detector diffractometer
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.126, T_{max} = 0.695
22 444 measured reflections
6472 independent reflections
5860 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°
$h = -20 \rightarrow 21$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 22$

Refinement

Refinement on F^2
$R(F)$ = 0.040
$wR(F^2)$ = 0.084
S = 1.15
6472 reflections
319 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0220P)^2 + 9.2477P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.009$
$\Delta\rho_{max}$ = 3.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—Cl1	2.301 (1)	Pt1—N1	2.012 (4)
Pt1—Cl2	2.293 (2)	Pt1—N2	2.012 (4)
Cl1—Pt1—Cl2	89.64 (5)	Cl2—Pt1—N1	175.4 (1)
Cl1—Pt1—N1	94.9 (1)	Cl2—Pt1—N2	94.9 (1)
Cl1—Pt1—N2	174.8 (1)	N1—Pt1—N2	80.6 (2)

In the course of the refinement, one of the alkyl chains showed extraordinarily large displacement parameters for two atoms, *viz*. C26 and C27. These atoms were thus assigned two disordered positions. After refinement of the restrained occupancies, the final occupancies were fixed at 0.64 for C26 and C27, and at 0.36 for C26′ and C27′, so that these atoms had similar U_{eq} values. H atoms were treated as riding, with C—H distances in the range 0.93–0.99 Å.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku Corporation, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 2000); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: OB1092). Services for accessing these data are described at the back of the journal.

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