Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

4,4′-Dinonyl-2,2′-bipyridine

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Received 16 May 2005
Accepted 18 May 2005
Online 28 May 2005

Key indicators

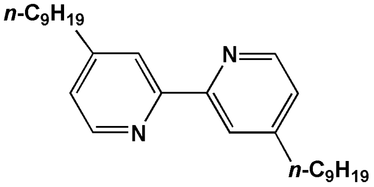
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.061
wR factor = 0.154
Data-to-parameter ratio = 21.5

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

The title compound, $C_{28}H_{44}N_2$, is one of the precursors of the amphiphilic heteroleptic ruthenium(II) sensitizer for DSC (dye-sensitized solar cells), and its molecule has a crystallographically imposed centre of symmetry. A segregated packing structure between the alkyl chain layers and pyridine rings is observed.

Comment

Ruthenium complexes containing 2,2′-bipyridine-4,4′-dicarboxylic acid (H_2dcbpy) have received much attention as photosensitizers for DSC (dye-sensitized solar cells) (Grätzel, 2003). The photovoltaic characterization of the amphiphilic heteroleptic ruthenium(II) complex containing 4,4′-dinonyl-2,2′-bipyridine (dnbpy), (I), as a ligand was recently reported as a new development for dyes applied to the solar cell (Nazeeruddin *et al.*, 2004). In our previous papers, the molecular structures of the dcbpy^{2-} ligand and the precursor complex of these dyes were reported (Fujihara, Kobayashi, Iwai & Nagasawa, 2004; Fujihara, Kobayashi & Nagasawa, 2004). As a part of a systematic investigation of the properties of these dyes, we report here the structure of the title compound, (I).



(I)

The molecule of (I) has a crystallographically imposed centre of symmetry (Fig. 1). Selected bond lengths and angles are given in Table 1. The C5—N1—C1 angle of 116.86 (12)° in the pyridine ring is similar to those for other pyridines [for example, 116.97 (13)° in dcbpy^{2-} (Fujihara, Kobayashi & Nagasawa, 2004)]. The alkyl chains are extended away from the pyridine ring and ordered across the *bc* plane to produce an alkyl chain layer (Fig. 2). The dihedral angle between the pyridine ring and the plane through the alkyl chain atoms (C6/C14) is 70.8 (1)°. An overlapped arrangement of parallel pyridine rings in neighbouring molecules with an interplanar distance of 3.54 (1) Å is observed in the crystal structure, as shown in Fig. 2. This finding suggests the existence of π–π stacking interactions between the pyridine rings in the crystal structure. The segregated packing consists of alkyl chain layers and pyridine rings as a result of the amphiphilic nature of dnbpy. A similar layered structure was also observed in a

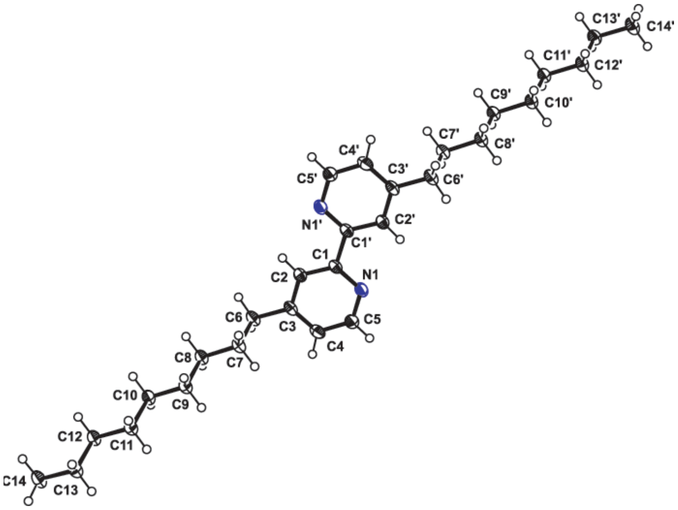


Figure 1
View of (I), with 50% probability displacement ellipsoids and the atom-numbering scheme. Atoms labelled with a prime are at the symmetry position ($-x$, $2 - y$, $-z$).

square-planar complex with Pt^{II}, *viz.* $PtCl_2(dnbpy)_2$ (Kato & Ikemori, 2003).

Experimental

Crystals of (I) suitable for X-ray diffraction were obtained from solutions in chloroform of a commercially available sample (Aldrich) by slow evaporation at 298 K.

Crystal data

$C_{28}H_{44}N_2$
$M_r = 408.65$
Monoclinic, $P2_1/n$
$a = 5.5952$ (5) Å
$b = 7.1862$ (6) Å
$c = 30.882$ (3) Å
$\beta = 94.108$ (2)°
$V = 1238.52$ (18) Å^3
$Z = 2$

$D_x = 1.096$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2439 reflections
$\theta = 2.6$–27.7°
$\mu = 0.06$ mm^{-1}
$T = 173$ (2) K
Plate, colourless
0.45 × 0.42 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.962$, $T_{max} = 0.993$
8628 measured reflections

2949 independent reflections
2465 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.0°$
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 7$
$l = -31 \rightarrow 40$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.154$
$S = 1.10$
2949 reflections
137 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.4019P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

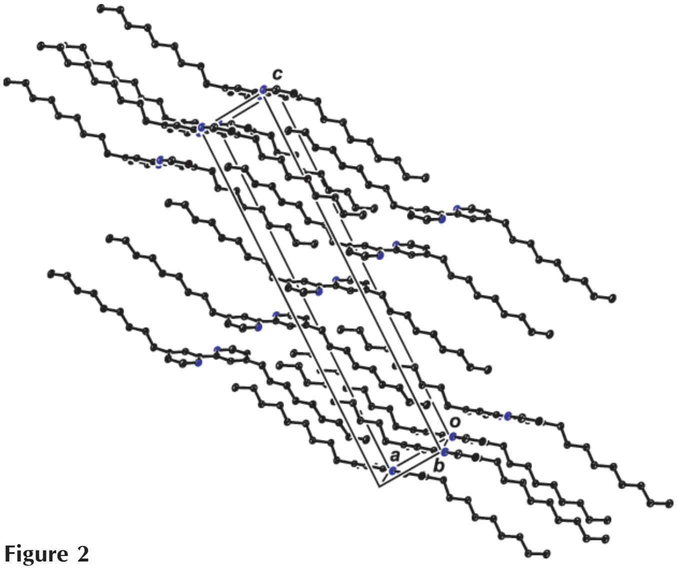


Figure 2
A molecular packing diagram of (I). H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.340 (2)	C3—C4	1.386 (2)
C1—C2	1.3924 (19)	C4—C5	1.384 (2)
C1—C1^i	1.494 (3)	C5—N1	1.3372 (19)
C2—C3	1.392 (2)		
N1—C1—C2	122.93 (13)	C5—C4—C3	119.41 (14)
C1—C2—C3	119.74 (14)	N1—C5—C4	123.91 (15)
C4—C3—C2	117.13 (13)	C5—N1—C1	116.86 (12)

Symmetry code: (i) $-x$, $-y + 2$, $-z$.

The H atoms were placed in calculated positions, with C—H = 0.98 (for CH_3), 0.99 (for CH_2) or 0.95 Å (for pyridine), and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms ($1.5U_{eq}$ for methyl H atoms).

Data collection: *SMART-W2K/NT* (Bruker, 2003); cell refinement: *SAINT-W2K/NT* (Bruker, 2003); data reduction: *SAINT-W2K/NT*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 2003); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL-NT*.

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