Crystal structure of bis(pentane-2,4-dionato-κ^2O,O')platinum(II), $Pt(C_5H_7O_2)_2$

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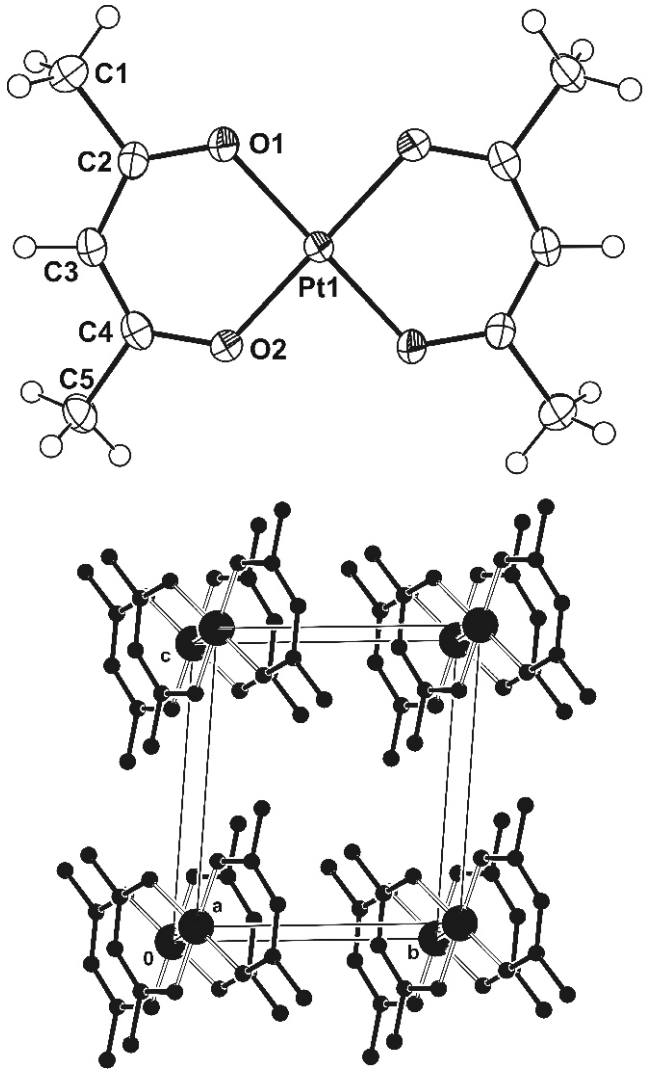

Abstract

$C_{10}H_{14}O_4Pt$, triclinic, $P\bar{1}$ (no. 2), a = 5.7236(7) Å, b = 7.0751(9) Å, c = 7.942(1) Å, α = 81.001(2)°, β = 70.010(2)°, γ = 66.231(2)°, V = 276.5 Å^3, Z = 1, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.070, T = 200 K.

Source of material

The title compound bis(pentane-2,4-dionato-κ^2O,O')platinum(II) was purchased from Aldrich chemicals and used as received. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a mixture of MeOH and CH_3CN solution.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with d(C—H) = 0.95 Å (CH) or 0.98 Å (CH_3) and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). The highest peak (1.79 e·Å^{-3}) and the deepest hole (-1.71 e·Å^{-3}) in the difference Fourier map are located 1.04 Å and 0.99 Å from the Pt1 atom, respectively.

Discussion

In the title complex, the Pt(II) ion is four-coordinated by O atoms from two chelating pentane-2,4-dionate (acetylacetonate, acac) anionic ligands in a slightly distorted square-planar manner (figure, top). The Pt atom is located on an inversion center, and therefore the asymmetric unit contains one half of the complex and the PtO_4 moiety is exactly planar. The O1–Pt1–O2 chelate angle of 96.0(2)° contributes the distortion of square. The Pt—O and O—C bond lengths are almost equivalent (d(Pt—O) = 1.981(5) Å and 1.982(5) Å; d(O—C) = 1.291(9) Å and 1.290(9) Å. On the basis of the bond lengths d(C2—C3) = 1.39(1)Å and d(C3—C4) = 1.38(1) Å, the negative charge of the anionic ligand appears to be delocalized over the five atoms O1, C2, C3, C4 and O2. In the crystal structure, the acac ligand is coordinated to the Pt atom nearly symmetrical, to form a practically planar six-membered ring (Pt1-O2) with a maximum deviation of 0.006(3) Å from least-squares plane. The planar complexes are stacked in columns parallel to the (110) plane (figure, bottom).

Table 1. Data collection and handling.

Crystal:	yellow plate, size 0.07 × 0.13 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	126.76 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	52.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1691, 1036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1035
$N(param)_{refined}$:	72
Programs:	SHELXS-97, SHELXL-97[1], ORTEP-3 [2], PLATON [3]

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	2*i*	0.4226	0.3589	–0.3804	0.055
H(1B)	2*i*	0.6108	0.3484	–0.2667	0.055
H(1C)	2*i*	0.3305	0.5389	–0.2448	0.055
H(3)	2*i*	0.3793	0.3589	0.0726	0.033
H(5A)	2*i*	0.0773	0.1656	0.4815	0.051
H(5B)	2*i*	0.1934	0.3418	0.3940	0.051
H(5C)	2*i*	0.3931	0.1049	0.3875	0.051

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	1*a*	0	0	0	0.0293(2)	0.0292(3)	0.0190(2)	–0.0176(2)	–0.0094(1)	0.0023(2)
O(1)	2*i*	0.180(1)	0.1735(8)	–0.1687(6)	0.040(3)	0.025(3)	0.023(2)	–0.019(2)	–0.012(2)	0.000(2)
O(2)	2*i*	0.058(1)	0.0591(8)	0.2152(6)	0.036(2)	0.032(3)	0.023(2)	–0.021(2)	–0.013(2)	0.006(2)
C(1)	2*i*	0.425(2)	0.390(1)	–0.265(1)	0.045(4)	0.045(5)	0.028(4)	–0.029(4)	–0.011(3)	0.007(3)
C(2)	2*i*	0.287(1)	0.275(1)	–0.117(1)	0.030(3)	0.024(4)	0.033(4)	–0.015(3)	–0.013(3)	0.003(3)
C(3)	2*i*	0.291(1)	0.278(1)	0.056(1)	0.035(3)	0.027(4)	0.031(4)	–0.018(3)	–0.014(3)	–0.002(3)
C(4)	2*i*	0.184(1)	0.178(1)	0.207(1)	0.028(3)	0.034(5)	0.027(4)	–0.013(3)	–0.010(3)	–0.007(3)
C(5)	2*i*	0.215(2)	0.199(1)	0.383(1)	0.044(4)	0.046(5)	0.027(4)	–0.028(4)	–0.013(3)	–0.003(3)

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