# Crystal structure of dichlorobis(3,5-dimethylisoxazolato)palladium(II), $PdCl_2(C_5H_7NO)_2$

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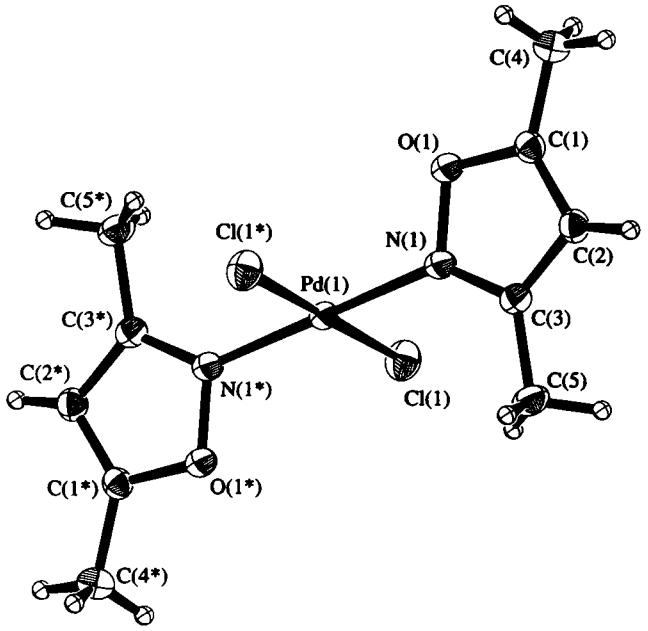


## Abstract

$C_{10}H_{14}Cl_2N_2O_2Pd$, triclinic, $P\bar{1}$ (no. 2), $a = 7.543(2)$ Å, $b = 8.629(3)$ Å, $c = 6.161(2)$ Å, $\alpha = 109.38(2)°$, $\beta = 108.03(2)°$, $\gamma = 101.89(3)°$, $V = 337.8$ Å$^3$, $Z = 1$, $R_{gt}(F) = 0.032$, $wR_{obs}(F) = 0.036$, $T = 296$ K.

## Source of material

The Pd complex was prepared by mixing a two molar excess of 3,5-dimethyl-isoxazole and $PdCl_2$ in distilled water at 300 K for 24 h [1]. Transparent yellow crystals of the product were obtained by slow recrystallization from acetone at room temperature. The crystals decompose in the range 220-225 °C.

## Experimental details

In the final refinement all non-hydrogen atoms were modelled anisotropically using teXsan [2] and absorption corrected data [3]. The coordinates of the ring hydrogen atom (H1) were refined, while the methyl hydrogen atoms were refined as two rigid groups.

## Discussion

The discovery of the effects of *cis*-platinum has attracted a significant attention to coordination chemistry in search for complexes with medicinal potential. This preparative and structural study has been undertaken due to the potential bio-activity of palladium and platinum isoxazole complexes [4,5]. It is of particular interest that the complexes exhibit a higher bio-activity than the respective parent isoxazole derivatives alone [4-6].

This report unambiguously characterizes the Pd(II) complex with two coordinated chlorine atoms and two isoxazole ligands. The structure (40 % probability ellipsoids) shows the Cl1, Cl1*, N1, N1* and Pd1 atoms in the same plane, as required by symmetry constraints. While the dihedral angle between the two least-square planes defined by the atoms Pd1–Cl1–N1–Cl1*–N1* and O1–N1–C1–C2–C3 is 107.8(1)°. The molecule is located on the center of symmetry and the coordinates of the atoms with asterisks are equal to $-x,-y,-z$ with respect to the corresponding unique atom coordinates at $x,y,z$. The palladium atom is in a slightly distorted square planar environment with the respective coordination bond angles, Cl1–Pd1–N1 and Cl1*–Pd1–N1, equal to 89.7(1)° and 90.3(1)°. Two chlorine atoms coordinate to the metal center in a *trans*-configuration and with a bonding distance $d$(Cl1—Pd1) = 2.293(1) Å. The two *trans* mono-dentate isoxazole ligands coordinate through their nitrogen atoms, and the N1—Pd1 bonding distance is equal to 1.993(3) Å. All the other bond distances and bond angles are in the normal range.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | yellow, plate-like, size 0.050 × 0.200 × 0.250 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.7107 Å) |
| $\mu$: | 35.21 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku AFC7R, $\omega/2\theta$ |
| $2\theta_{max}$: | 62° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1979, 1857 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 3\,\sigma(I_{obs})$, 1690 |
| $N(param)_{refined}$: | 79 |
| Programs: | teXsan [2], ORTEP-II [7] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 2*i* | 0.6570 | 0.3800 | 0.6930 | 0.059 |
| H(2) | 2*i* | 0.7172 | 0.6216 | 1.1601 | 0.078 |
| H(3) | 2*i* | 0.6490 | 0.4944 | 1.2701 | 0.078 |
| H(4) | 2*i* | 0.8722 | 0.6023 | 1.3741 | 0.078 |
| H(5) | 2*i* | 0.6292 | 0.0734 | 0.3402 | 0.091 |
| H(6) | 2*i* | 0.8558 | 0.1102 | 0.4548 | 0.091 |
| H(7) | 2*i* | 0.7100 | −0.0495 | 0.4464 | 0.091 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Pd(1) | 1*a* | 0 | 0 | 0 | 0.0361(2) | 0.0338(2) | 0.0265(2) | 0.0139(2) | 0.0124(1) | 0.0127(1) |
| Cl(1) | 2*i* | 0.6946(2) | −0.2139(1) | 0.8222(2) | 0.0422(5) | 0.0458(5) | 0.0527(6) | 0.0079(4) | 0.0122(5) | 0.0212(5) |
| O(1) | 2*i* | 0.8715(4) | 0.2993(3) | 1.1333(4) | 0.047(1) | 0.041(1) | 0.029(1) | 0.019(1) | 0.014(1) | 0.013(1) |
| N(1) | 2*i* | 0.8687(5) | 0.1659(4) | 0.9260(5) | 0.043(2) | 0.037(2) | 0.029(1) | 0.016(1) | 0.014(1) | 0.012(1) |
| C(1) | 2*i* | 0.7781(5) | 0.3983(5) | 1.0456(7) | 0.032(2) | 0.036(2) | 0.038(2) | 0.012(1) | 0.015(1) | 0.016(1) |
| C(2) | 2*i* | 0.7195(6) | 0.3345(5) | 0.7938(7) | 0.038(2) | 0.042(2) | 0.038(2) | 0.017(2) | 0.015(2) | 0.020(2) |
| C(3) | 2*i* | 0.7784(5) | 0.1869(5) | 0.7248(6) | 0.032(2) | 0.037(2) | 0.032(2) | 0.009(1) | 0.015(1) | 0.014(1) |
| C(4) | 2*i* | 0.7594(7) | 0.5443(5) | 1.2375(8) | 0.053(2) | 0.042(2) | 0.044(2) | 0.020(2) | 0.021(2) | 0.012(2) |
| C(5) | 2*i* | 0.7480(6) | 0.0632(6) | 0.4697(7) | 0.051(2) | 0.052(2) | 0.030(2) | 0.016(2) | 0.017(2) | 0.013(2) |

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