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Crystal structure of *trans*-dichlorido-(1,3-dimesityl-1*H*-imidazol-2(3*H*)-ylidene)-(5-methyl-3,4-dihydro-2*H*-pyrrole- κ *N*)palladium(II), $C_{25}H_{31}Cl_2N_3OPd$

Table 1: Data collection and handling.

Crystal:	Yellow prisma
Size:	0.18 × 0.13 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.95 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω
θ_{max} , completeness:	25.0°, 97%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	39904, 4516, 0.050
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 3679
$N(param)_{refined}$:	297
Programs:	Bruker [1], SHELX [2]

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Abstract

$C_{25}H_{31}Cl_2N_3OPd$, orthorhombic, *Pbca* (no. 61), $a = 9.4083(4)$ Å, $b = 17.1334(8)$ Å, $c = 31.9251(14)$ Å, $V = 5146.2(4)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0600$, $wR_{ref}(F^2) = 0.1232$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title complex was easily obtained by our very recent reported method [3]. Single crystals were grown in a mixture of ethyl acetate and petroleum ether.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Pd1	0.79736(4)	0.49971(2)	0.64596(2)	0.03921(17)
Cl1	0.94877(17)	0.57707(10)	0.60706(5)	0.0639(4)
Cl2	0.65567(15)	0.42889(8)	0.69055(5)	0.0523(4)
N1	0.5803(5)	0.5282(3)	0.58179(15)	0.0536(13)
N2	0.5327(5)	0.5986(2)	0.63581(15)	0.0469(12)
N3	0.9718(5)	0.4373(3)	0.66681(14)	0.0479(11)
O1	1.1510(5)	0.3526(3)	0.66404(14)	0.0750(13)
C1	0.6275(5)	0.5471(3)	0.62058(17)	0.0394(12)
C2	0.4576(8)	0.5688(4)	0.5729(2)	0.083(2)
H2	0.4060	0.5666	0.5481	0.099*
C3	0.4264(7)	0.6120(4)	0.6065(2)	0.077(2)
H3	0.3483	0.6448	0.6096	0.093*
C4	0.5381(6)	0.6341(3)	0.67653(19)	0.0469(14)
C5	0.4510(6)	0.6057(3)	0.7083(2)	0.0538(15)
C6	0.4666(6)	0.6378(3)	0.7478(2)	0.0580(16)
H6	0.4099	0.6192	0.7694	0.070*
C7	0.5636(6)	0.6966(3)	0.75627(19)	0.0538(15)
C8	0.6436(6)	0.7256(3)	0.72302(19)	0.0526(15)
H8	0.7071	0.7662	0.7281	0.063*
C9	0.6321(6)	0.6962(3)	0.68249(18)	0.0461(13)
C10	0.3398(7)	0.5435(4)	0.7006(2)	0.074(2)
H10A	0.2991	0.5276	0.7268	0.111*
H10B	0.3832	0.4993	0.6873	0.111*
H10C	0.2665	0.5640	0.6828	0.111*
C11	0.5822(8)	0.7287(4)	0.7998(2)	0.080(2)
H11A	0.5260	0.6988	0.8191	0.120*
H11B	0.5519	0.7822	0.8004	0.120*
H11C	0.6805	0.7256	0.8076	0.120*
C12	0.7161(7)	0.7304(4)	0.64717(19)	0.0636(18)
H12A	0.7568	0.7791	0.6559	0.095*
H12B	0.6547	0.7390	0.6236	0.095*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H12C	0.7906	0.6950	0.6394	0.095*
C13	0.6476(6)	0.4714(3)	0.55509(18)	0.0487(14)
C14	0.7399(7)	0.4959(4)	0.52394(19)	0.0571(16)
C15	0.8086(7)	0.4405(4)	0.50041(19)	0.0565(16)
H15	0.8714	0.4562	0.4795	0.068*
C16	0.7861(7)	0.3611(4)	0.5072(2)	0.0566(16)
C17	0.6884(7)	0.3396(4)	0.5367(2)	0.0593(17)
H17	0.6698	0.2868	0.5404	0.071*
C18	0.6150(6)	0.3934(3)	0.56165(18)	0.0533(15)
C19	0.5070(7)	0.3668(4)	0.5928(2)	0.0698(19)
H19A	0.5317	0.3862	0.6201	0.105*
H19B	0.5048	0.3108	0.5934	0.105*
H19C	0.4151	0.3863	0.5850	0.105*
C20	0.7599(9)	0.5821(4)	0.5145(2)	0.074(2)
H20A	0.8320	0.5883	0.4935	0.110*
H20B	0.7883	0.6088	0.5396	0.110*
H20C	0.6720	0.6037	0.5045	0.110*
C21	0.8627(9)	0.3012(4)	0.4811(2)	0.089(2)
H21A	0.9304	0.2739	0.4982	0.134*
H21B	0.9113	0.3268	0.4585	0.134*
H21C	0.7952	0.2647	0.4699	0.134*
C22	1.0134(6)	0.4276(4)	0.71026(18)	0.0556(15)
H22A	0.9351	0.4075	0.7269	0.067*
H22B	1.0451	0.4767	0.7222	0.067*
C23	1.1343(6)	0.3691(4)	0.70834(19)	0.0559(15)
H23A	1.2207	0.3912	0.7199	0.067*
H23B	1.1106	0.3221	0.7237	0.067*
C24	1.0513(6)	0.3933(4)	0.64425(18)	0.0557(16)
C25	1.0491(8)	0.3828(5)	0.59802(19)	0.083(2)
H25A	0.9560	0.3949	0.5875	0.124*
H25B	1.0722	0.3297	0.5913	0.124*
H25C	1.1176	0.4170	0.5854	0.124*

Experimental details

Hydrogen atoms were introduced using the HFIX command in the SHELXL7 program [2]. Vinylic and aromatic C—H distances were restrained to 0.93 Å with U_{iso} values to be $1.2U_{eq}(C)$ [1, 4].

Comment

N-heterocyclic carbene (NHC)-palladium(II) complexes have been good catalyst for the Suzuki-Miyaura coupling of aryl chlorides with arylboronic acids under mild conditions [5–9]. However, to the best of our knowledge, no manuscript was reported on the NHC-Pd(II) complexes catalyzed selective mono-Suzuki-Miyaura coupling of dichlorobenzenes with arylboronic acids till our recent paper was published [3]. In our recent paper, the title product, showed efficient catalytic activity for the highly selective mono-Suzuki-Miyaura coupling of dichlorobenzenes with arylboronic acids. The crystal structure of the title compound is of interest to investigate the structure-activity relationship of such complexes.

The Pd center in the title compound shows slightly distorted square-planar geometry with four ligands. The bond lengths around the Pd center ranges in the normal ones [10]. For example, the bond length of Pd(1)—C(1) is 1.967(5) Å; Pd(1)—N(3) is 2.069(4) Å; Pd(1)—Cl(1) is 2.3084(16) Å and Pd(1)—Cl(2) is 2.2970(15) Å. The bond angles around the Pd center are shown as the following: C(1)—Pd(1)—N(3) = 172.0(2)°; C(1)—Pd(1)—Cl(2) = 90.10(16)°; N(3)—Pd(1)—Cl(2) = 89.32(13)°; C(1)—Pd(1)—Cl(1) = 92.45(16)°; N(3)—Pd(1)—Cl(1) = 88.87(13)°; Cl(2)—Pd(1)—Cl(1) = 174.23(6)°.

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