Crystal structure of dichlorobis((S,E)-N-((furan-2-yl)methylene)-1-phenylethanamine)palladium(II), PdCl$_2$(C$_{13}$H$_{13}$NO)$_2$

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Abstract

C$_{76}$H$_{75}$Cl$_2$N$_2$O$_3$Pd, orthorhombic, P2$_1$2$_1$2$_1$ (no. 19), a = 12.196(2) Å, b = 14.143(3) Å, c = 14.479(3) Å, V = 2497.5 Å$^3$, Z = 4, R$_{gt}$(F) = 0.033, wR$_{gt}$(F$^2$) = 0.069, T = 113 K.

Source of material

PdCl$_2$ (88 mg, 0.5 mmol) was added to a stirred solution of (S,E)-N-((furan-2-yl)methylene)-1-phenylethanamine (199 mg, 1 mmol) in methanol (20 ml). The mixture was stirred at room temperature for 30 min and filtrated. The residue was dissolved in dichloromethane. The solution was allowed to stand by slow evaporation at room temperature. The orange crystals were obtained one week later in a yield of 80 % based on the initial PdCl$_2$ input.

Discussion

The title crystal structure consists of [PdCl$_2$(C$_{13}$H$_{13}$NO)$_2$] molecules. One of the furanyl ring and C5 disordered maybe caused by the stronger molecular temperature vibration. The Pd atoms are square-planar coordinated by two nitrogen atoms from two (S,E)-N-((furan-2-yl)methylene)-1-phenylethanamine ligands. The Pd1—N2 distance (2.015(2) Å) is almost as long as the Pd1—N1 distance (2.009(2) Å), being shorter than those (2.200(6) Å) in the complex [FePd(C$_5$H$_5$)(C$_{16}$H$_{18}$NO)Cl(PPh$_3$)]. H$_2$O [1]. The molecules are assembled by π−π stacking interactions between the phenyl rings and furanyl rings of (R,E)-N-((furan-2-yl)methylene)-1-phenylethanamine ligands of neighbouring molecules, with the mean interplanar distances of 3.702 Å between the two neighboring phenyl rings and 3.369 Å between the two neighboring furanyl rings.

Table 1. Data collection and handling.

| Crystal: | orange block, size 0.14 × 0.14 × 0.16 mm |
| Wavelength: | Mo K$_\alpha$ radiation (0.71073 Å) |
| μ: | 9.83 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku Saturn, ω |
| 2θ$_{max}$: | 55.76° |
| N(hkl)$_{measured}$, N(hkl)$_{unique}$: | 20769, 5935 |
| Criterion for I$_{obs}$. N(hkl)$_{gt}$: | I$_{obs} > 2σ$(I$_{obs}$), 5376 |
| Programs: | SHELX90 [2], SHELXS-97 [3], SHELXL-97 [4], SHELXTL [5] |

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

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* Correspondence author (e-mail: chem8000@163.com)
Table 3. Atomic coordinates and displacement parameters (in Å²).

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