Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Di-μ-acetato-$\kappa^4O:O'$-bis[2-(5-phenylisoxazolin-3-yl)phenyl-κ^2C^1,N]-dipalladium(II)

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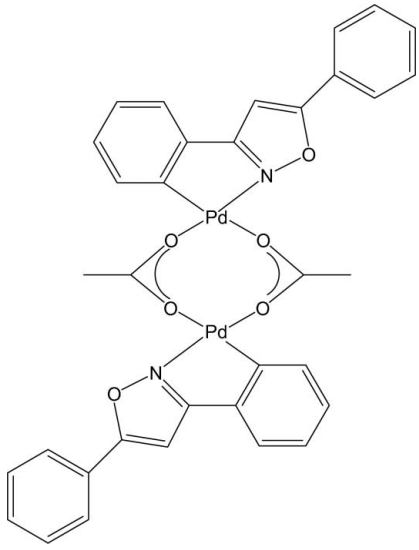
Received 22 March 2008; accepted 12 May 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.049; wR factor = 0.143; data-to-parameter ratio = 15.3.

The title compound, $[Pd_2(C_{15}H_{10}NO)_2(C_2H_3O_2)_2]$, crystallized from a dichloromethane/*n*-hexane solution with two crystallographically independent dimeric molecules in the asymmetric unit. Each molecule may be described as a dimer with an *anti* configuration and the cyclometallated fragments in the characteristic open-book disposition, linked by two bridging acetate ligands.

Related literature

For a related palladacycle bridged by acetate ligands, see: Schultz *et al.* (2004). For related literature, see: Dupont *et al.* (2005).



Experimental

Crystal data

$[Pd_2(C_{15}H_{10}NO)_2(C_2H_3O_2)_2]$
M_r = 771.37
Monoclinic, $P2_1/c$
a = 14.8160 (6) Å
b = 24.2339 (10) Å
c = 19.6397 (8) Å
β = 103.233 (1)°
V = 6864.4 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 298 (2) K
0.28 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.750, T_{max} = 0.854
80599 measured reflections
12098 independent reflections
8103 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 1.09
12098 reflections
793 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2003); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by NSFC (No. 20372042), the Doctoral Program of MOE (No. 20050422010 and 20050422011), Shandong Scientific Plan (032090105), and the Science Foundation of Shandong (Y2006B18).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2190).

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