Crystal data for di-μ-chloro-bis(2-methylallyl-3-norbornyl)palladium(II), (C_{11}H_{17}PdCl)₂, By G. TIEGHI and M. ZOCCHI, Istituto di Chimica Industriale del Politecnico, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

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The crystal data of di-μ-chloro-bis(2-methylallyl-3-norbornyl)palladium(II), (C_{11}H_{17}PdCl)₂, have been determined from its X-ray powder diffraction pattern: triclinic unit cell, a = 11.217 (4), b = 7.518 (2), c = 6.633 (2) Å, α = 89.98 (2), β = 104.23 (2), γ = 100.13 (2)°.

Introduction

In the course of our X-ray diffraction studies on catalysis, the crystal structures of some binuclear allylic complexes of Ni and Pd have been determined (Zocchi & Tieghi, 1975). Following these studies, we considered the binuclear chloro-bridged palladium complex di-μ-chloro-bis(allyl-3-norbornyl)palladium(II) and its methyl derivative di-μ-chloro-bis(2-methylallyl-3-norbornyl)palladium(II).

While the crystal structure of the former complex was easily determined (Zocchi & Tieghi, 1978) (space group P\textoverline{1}, a = 11.057 (2), b = 7.346 (1), c = 6.533 (1) Å, α = 80.54 (1), β = 104.52 (1), γ = 94.65 (1)°), for the latter no single crystals suitable for X-ray analysis were obtained. However, a comparison of the X-ray powder patterns showed that the two complexes are isostructural; on the basis of this finding we obtained the results presented in this communication.

Origin of specimens

Crystalline specimens of (C_{11}H_{17}PdCl)₂ were obtained from benzene solutions at 50°C by reaction of norbornene with \( π \)-methallyl palladium chloride (Gallazzi, Hanlon, Vitulli & Porri, 1971).

Crystal geometry

The powder patterns (Cu Kα radiation, λ = 1.5418 Å) were obtained with a Philips PW 1050 counter diffractometer equipped with a graphite monochromator and a pulse-height analyser. The unit-cell parameters, refined by means of a least-squares method, are as follows: a = 11.217 (4), b = 7.518 (2), c = 6.633 (2) Å, α = 89.98 (2), β = 104.23 (2), γ = 100.13 (2)°; \( U = 533.3 \) Å³; \( D_x = 1.811 \) g cm⁻³.

Comparison with other results

The fact that the two crystals are isostructural shows that the methyl substitution in the hydrocarbon ligand does not alter the crystal packing significantly; indeed the calculated densities are almost identical in the two cases.

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References

