The Molecular Structure of Acetylacetonato(cyclo-octa-2,4-dienyl)palladium

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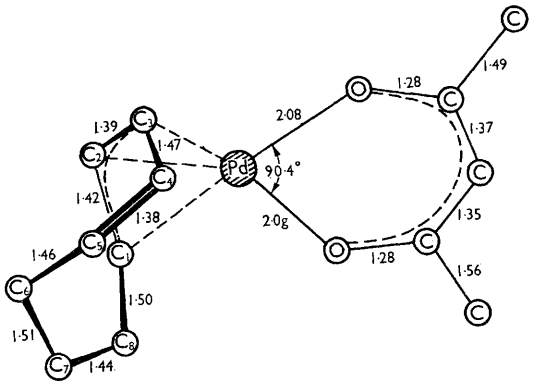
ACETYLACETONATO(CYCLO-OCTA-2,4-DIENYL)PALLADIUM,[1] $C_8H_{11}Pd(MeCO{\cdot}CH{\cdot}COMe)$, crystallizes in the triclinic space-group $P\bar{1}$ with $a = 7{\cdot}07$, $b = 9{\cdot}92$, $c = 9{\cdot}89$ Å, $\alpha = 94{\cdot}8$, $\beta = 86{\cdot}8$, $\gamma = 109{\cdot}8°$, $Z = 2$. A three-dimensional *X*-ray structural analysis of the complex, using conventional Patterson and Fourier techniques and two cycles of full-matrix refinement of positional and anisotropic thermal parameters, has converged the discrepancy index, R_1, to its present value of 7·08% for 1758 independent visually-estimated reflexions. Estimated standard deviations are ~0·02 Å for Pd–O and Pd–C, and ~0·03 Å for C–O and C–C vectors. The figure shows the essential geometry of a molecule viewed down "*a*"

The tendency for palladium to form π-allyl complexes rather than linking directly to a 1,3-diene has been well documented[1,2]; the present

[1] S. D. Robinson and B. L. Shaw, *J. Chem. Soc.*, **1964**, 5002.
[2] S. D. Robinson and B. L. Shaw, *J. Chem. Soc.*, **1963**, 4806.

structural analysis indicates that π-allyl formation is also preferred when larger conjugated systems



are attached to a palladium atom. Only three atoms of the cyclo-octadienyl ligand are involved in the metal–ligand bonding. The π-allyl carbon atoms C-1, C-2, and C-3 are distant 2·11, 2·10, and 2·12 Å from the metal, whereas the remaining two atoms of the conjugated dienyl system are 2·91 (C-4) and 3·93 Å (C-5) from the palladium. The angle at the vertex of the π-allyl group (C-1–C-2–C-3) is 119·0°. The plane of the π-allyl group makes a dihedral angle (ϕ) of 121·4° with the plane defined by the palladium and two oxygen atoms. Similar dihedral angles have been noted in π-allylpalladium chloride[3] (ϕ = 111·5°) π-allylpalladium acetate[4] (ϕ_1 = 110, ϕ_2 = 125°) and in the *endo*- and *exo*-isomers of 1-ethoxytetraphenylcyclobutenylpalladium chloride[5] (ϕ = 95° for each isomer).

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[3] A. E. Smith, *Acta Cryst.*, 1965, **18**, 331.
[4] M. R. Churchill and R. Mason, *Nature*, 1964, **204**, 777.
[5] L. F. Dahl and W. E. Oberhansli, *Inorg. Chem.*, 1965, **4**, 629.