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Unusual condensation of acetone giving η^3-allyl ligand in the $[Pd(\eta^3\text{-}C_6H_9O)(\mu\text{-}Cl)]_2$ complex

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1. Experimental single-crystal X-ray diffraction data were acquired on a Bruker SMART APEX2 automated diffractometer (λMoKα, graphite monochromator, ω–ϕ scanning). The data were indexed and integrated using the SAINT program. A correction for absorption based on equivalent reflectance measurements (SADABS) was applied. The structures were solved by the direct method followed by Fourier difference synthesis calculations. All non-hydrogen atoms were refined in anisotropic approximation. All hydrogen atoms of CH and CH_2 groups were refined using the rider model with thermal parameters U_{iso} = 1.2 U_{equiv} (U_{iso}) of the corresponding non-hydrogen atom (1.5U_{iso} for CH_3 groups).

All the calculations were performed using the SHELXTL program. The structure was solved and refined using the OLEX2 software complex.

2. IR spectra were recorded by the ATR method using the Pike attachment. FT–IR spectra were measured using a JASCO FT/IR-6600 spectrometer on an ATR PRO ONE Technologies attachment with a diamond crystal PKS-D1F by the ATR method in the range of 4000–250 cm^{-1}.

3. IR spectrum of the $[Pd(\eta^3\text{-}C_6H_9O)(\mu\text{-}Cl)]_2$ complex.