Electronic Supplementary Material (ESI) for Dalton Transactions

Mono N,C,N'-Pincer Complexes of Titanium, Vanadium and Niobium. Synthesis, Structure and catalytic activity in olefin polymerization.

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Supporting Information

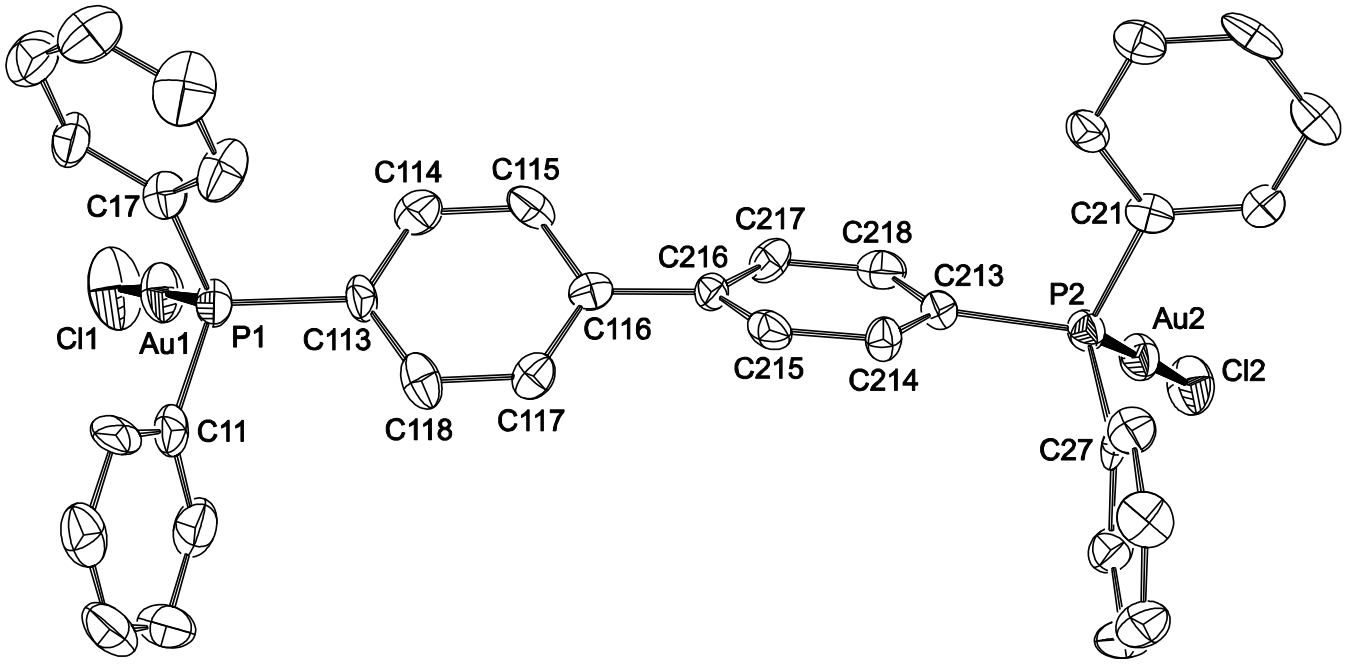

Figure S1. Displacement ellipsoid plot (50% probability) of **2** in the crystal. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å), bond angles (°) and torsion angles (°): Au(1)–Cl(1) 2.292(3), Au(1)–P(1) 2.228(2), Au(2)–Cl(2) 2.285(2), Au(2)–P(2) 2.229(2), Cl(1)–Au(1)–P(1) 177.11(9), Cl(2)–Au(2)–P(2) 178.96(8), C(117)–C(116)–C(216)–C(217) 135.9(8), C(115)–C(116)–C(216)–C(215) 143.7(8).

X-ray crystal structure determination of 2. $C_{36}H_{28}Au_2Cl_2P_2$ + disordered solvent, Fw = 987.36 [*], colourless plate, 0.15 x 0.15 x 0.03 mm^3, monoclinic, $P2_1/c$ (no. 14), a = 17.3144(4), b = 11.9885(3), c = 17.2423(5) Å, β = 103.3920(12)°, V = 3481.73(16) $Å^3$, Z = 4, D_x = 1.884 g/cm^3[*], μ = 8.69 mm^{-1}[*]. 28598 Reflections were measured on a Nonius KappaCCD diffractometer with rotating anode (graphite monochromator, λ = 0.71073 Å) up to a resolution of $(\sin \theta/\lambda)_{max}$ = 0.56 $Å^{-1}$ at a temperature of 150(2) K. Intensity integration was performed with HKL2000[501]. The SADABS program[502] was used for absorption correction and scaling based on multiple measured reflections (0.50-0.77 correction range). 5174 Reflections were unique (R_{int} = 0.076), of which 3697 were observed [I>2σ(I)]. The structure was solved with automated Patterson methods using the program DIRDIF-99[503]. The structure was refined with SHELXL-97[504] against F^2 of all reflections. Non hydrogen atoms were refined with anisotropic

displacement parameters. Hydrogen atoms were introduced in calculated positions and refined with a riding model. The crystal structure contains voids (365 $Å^3$ / unit cell) filled with disordered solvent molecules. Their contribution to the structure factors was secured by back-Fourier transformation with the SQUEEZE routine of PLATON[505] resulting in 69 electrons / unit cell. 379 Parameters were refined with no restraints. R1/wR2 [$I > 2\sigma(I)$]: 0.0381 / 0.0683. R1/wR2 [all refl.]: 0.0689 / 0.0743. S = 1.010. Residual electron density between -0.88 and 1.19 e/$Å^3$. Geometry calculations and checking for higher symmetry was performed with the PLATON program[505].

[*] Derived values do not contain the contribution of the disordered solvent.

References

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