Phosphido Pincer Complexes of Platinum: Synthesis, Structure and Reactivity

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I. Experimental details for crystal structure determination

Spatial refinement details.

Refinement of $F_2$ against ALL reflections. The weighted R-factor ($wR$) and goodness of fit (S) are based on $F_2$, conventional R-factors (R) are based on F, with F set to zero for negative $F_2$. The threshold expression of $F_2 > 2 \sqrt{ \langle F_2 \rangle}$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F_2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystals for X-ray analysis of complex 1 were obtained via vapor diffusion of petroleum ether into a THF solution. Single crystals of 3 were obtained via slow evaporation of a petroleum ether solution of the complex. X-ray diffraction studies were carried out in the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer.
**Figure S1.** ORTEP diagram of complex 1 [iPr-PPP]PtCl with thermal ellipsoids drawn at 30% probability level. The crystal structure of 1 contains two independent molecules in the asymmetric unit. Hydrogen atoms are omitted for clarity.
Table S1. Crystal data and structure refinement for 1 [iPr-PPP]-Pt(Cl).

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Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 1 [Pr-PPP]-Pt(Cl). U(eq) is defined as one third of the trace of the orthogonalized U_ij tensor.

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Table S3. Bond lengths [Å] and angles [°] for 1 [Pr-PPP]-Pt(Cl).

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Symmetry transformations used to generate equivalent atoms:
Table S4. Anisotropic displacement parameters (Å² x 10³) for 1 [Pr-PPP]-Pt(Cl). The anisotropic displacement factor exponent takes the form: -2π²[ h^2 U11 + ... + 2 h k a^* b^* U12 ]

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Figure S2. ORTEP diagram of complex 3 [{Pr-PPP}PtCH₃ with thermal ellipsoids drawn at 30% probability level. The crystal structure of 3 contains two independent molecules in the asymmetric unit. Hydrogen atoms are omitted for clarity.
Table S6. Crystal data and structure refinement for 3 \( ^{1} \text{Pr-PPP}\)-Pt(CH\(_3\))

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S-25
Table S7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [bPr-PPP]-Pt(CH₃) (3). $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

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Symmetry transformations used to generate equivalent atoms:
Table S9. Anisotropic displacement parameters (Å² x 10³) for 3[Pr-PPP]-Pt(CH₃). The anisotropic displacement factor exponent takes the form: -2π² [ h² a*²U₁₁ + ... + 2 h k a* b* U₁₂ ]

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Figure S3. Emission spectrum of 1 in the SO$_2$ free form (black trace) and in the SO$_2$ bound form (grey trace). 1 concentration = 1 µM; [SO$_2$] = 90 mM. All time traces were measured at room temperature and in benzene.
Figure S4. Emission spectrum of 1 in the NO free form (black trace) and in the NO bound form (grey trace). 1 concentration = 1 µM; [NO] = 230 µM. All time traces were measured at room temperature and in benzene.
Figure S5. $^{31}$P-NMR of 1 in the NO free form (lower spectrum) and in the NO bound form. The spectra were measured at room temperature, C$_6$D$_6$. [NO] = 300 µM.