Crystal Structure of Bis(diphenylphosphino)ethane Bis(2-selenopyridinato)platinum(II)

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The chemistry of platinum-group organochalcogenolates has attracted considerable attention in recent years due to their diverse structural possibilities and relevance in materials science.¹⁻³ Mononuclear *cis* complexes, [M(ER)₂L₂], are useful precursors for the synthesis of bi- and poly-nuclear

complexes.^{2,3} These complexes are usually derived from simple organochalcogenolate ions. Internally functionalized organochalcogenolates, such as 2-selenopyridinate, would provide additional donor sites and, consequently, may result in a new structural motif.⁵ The structure of one such complex [Pt(Sepy)₂(dppe)] is reported herein.

A schematic diagram of [Pt(Sepy)₂(dppe)] is shown in Fig. 1. Thermal ellipsoids of [Pt(Sepy)₂(dppe)] are shown in Fig. 2. Crystal and experimental data are listed in Table 1. The fractional atomic coordinates and equivalent thermal parameters for all of the refined atoms are given in Table 2. The platinum atom exists in a square-planar geometry defined by two *cis* selenium atoms derived from the 2-selenopyridinate ion and two phosphorus atoms of the chelating dppe ligand. Heavier atoms are all in a plane, whereas two carbon atoms of the dppe ligand are out of plane by the same extent on either side (± 0.37 Å). The Pt-Se distances of 2.4335(13) Å and 2.4980(14) Å are clearly not equivalent. The distances can be compared with the M-Se distances reported for [Pt(SePh)₂(dppe)]² and [Pd(SePh)₂(dppe)].³ The Pt-P^{2,3}, Pt-Se² and P-C^{2,3} are in good agreement with those reported earlier. The P-Pt-P (85.3(9)°) and Se-Pt-Se (81.52(5)°) angles are significantly reduced from the normal bond angles of 90°. The latter angle is usually acute; the E-M-E angles (E = S or Se; M

Fig. 1 Schematic diagram of [Pt(Sepy)₂(dppe)].

Fig. 2 ORTEP with numbering scheme of [Pt(Sepy)₂(dppe)] at 50% probability.

Table 1 Crystal and structure refinement data

Formula:	C ₃₆ H ₃₆ N ₂ P ₂ Se ₂ Pt
Formula weight	= 911.62
Crystal system:	monoclinic
Space group:	C2 = c
a =	37.398(5) Å
b =	8.907(5) Å
c =	23.887(5) Å
β =	122.835(5)°
V =	6686(4) Å ³
D _x =	1.811 Mg/m ³
R1 =	0.0789
No. of reflections used =	5624
Measurement:	Rigaku AFC7S
Program system:	teXsan
Structure determination:	SHELXS-97
Refinement:	full-matrix

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Table 2 Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$)

Atom	x	y	z	U_{eq}
Pt1	0.141964(11)	0.19948(4)	0.330946(17)	0.0403(2)
Se1	0.14408(3)	0.42305(12)	0.26967(5)	0.0481(3)
Se2	0.13397(5)	0.39429(13)	0.39481(6)	0.0605(4)
P4	0.14284(7)	-0.0187(3)	0.38085(11)	0.0435(5)
P5	0.14920(7)	0.0548(3)	0.26078(11)	0.0445(5)
N1	0.1277(4)	0.1792(11)	0.4750(6)	0.067(3)
N2	0.0522(4)	0.3795(16)	0.1989(7)	0.087(3)
C1	0.1394(3)	-0.1380(11)	0.2710(5)	0.052(2)
C2	0.1596(4)	-0.1647(11)	0.3458(5)	0.053(2)
C3	0.1146(3)	0.0936(12)	0.1736(5)	0.052(2)
C4	0.1287(5)	0.1759(15)	0.1389(6)	0.069(3)
C5	0.0996(6)	0.2099(15)	0.0711(7)	0.082(4)
C6	0.0572(6)	0.172(2)	0.0409(7)	0.093(5)
C7	0.0432(5)	0.097(2)	0.0746(8)	0.096(5)
C8	0.0713(4)	0.0600(17)	0.1412(6)	0.073(3)
C9	0.2034(3)	0.0509(10)	0.2794(5)	0.047(2)
C10	0.2135(4)	-0.0319(16)	0.2407(6)	0.067(3)
C11	0.2557(4)	-0.0405(18)	0.2577(8)	0.085(4)
C12	0.2864(4)	0.0366(17)	0.3120(7)	0.074(3)
C13	0.2770(4)	0.1194(16)	0.3508(7)	0.074(3)
C14	0.2347(4)	0.1216(17)	0.3336(6)	0.069(3)
C15	0.1817(3)	-0.0510(12)	0.4695(5)	0.053(2)
C16	0.1778(5)	-0.1671(17)	0.5029(8)	0.086(5)
C17	0.2088(7)	-0.197(2)	0.5685(9)	0.106(6)
C18	0.2449(5)	-0.1067(19)	0.6009(7)	0.086(4)
C19	0.2487(5)	0.004(2)	0.5651(8)	0.096(5)
C20	0.2182(4)	0.0367(15)	0.5008(7)	0.072(3)
C21	0.0909(3)	-0.0788(12)	0.3600(5)	0.053(2)
C22	0.0813(4)	-0.2301(15)	0.3575(8)	0.075(4)
C23	0.0404(5)	-0.271(2)	0.3420(10)	0.094(5)
C24	0.0117(4)	-0.1687(19)	0.3320(9)	0.091(5)
C25	0.0213(4)	-0.0189(17)	0.3344(8)	0.082(4)
C26	0.0598(3)	0.0305(14)	0.3467(6)	0.063(3)
C27	0.1256(4)	0.3246(12)	0.4629(5)	0.051(2)
C28	0.1173(4)	0.4246(13)	0.4966(6)	0.060(3)
C29	0.1099(4)	0.3822(15)	0.5438(5)	0.064(3)
C30	0.1122(5)	0.230(2)	0.5573(8)	0.085(4)
C31	0.1212(6)	0.135(2)	0.5225(8)	0.091(4)
C32	0.0853(3)	0.4491(12)	0.1991(4)	0.049(2)
C33	0.0794(3)	0.5440(14)	0.1528(5)	0.057(3)
C34	0.0404(5)	0.5620(19)	0.1014(6)	0.082(4)
C35	0.0055(4)	0.4939(19)	0.0946(7)	0.086(4)
C36	0.0119(4)	0.3978(17)	0.1443(8)	0.081(4)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a}_i \cdot \mathbf{a}_j).$$

= Pd or Pt) in $[\text{Pd}(\text{SePh})_2(\text{dppe})]$,³ $[\text{Pd}(\text{SC}_6\text{F}_5)_2(\text{dppe})]$,³ and $[\text{Pt}(\text{SePh})_2(\text{dppe})]$ ² are 99.11(4)°, 100.84(4)° and 90.70(3)°, respectively. The individual pyridyl rings are planar and inclined to one another by 85.4(8)° and are 89.3(6)° to the platinum coordination plane.

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