Crystal structure of chlorido(phenylselenolato)bis(triphenylphosphine)-platinum(II)–benzene (1:1), $\text{Pt}(\text{C}_6\text{H}_5\text{Se})(\text{C}_{18}\text{H}_{15}\text{P})_2\text{Cl} \cdot \text{C}_6\text{H}_6$

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Abstract

$\text{C}_{48}\text{H}_{41}\text{ClP}_2\text{PtSe}$, triclinic, $P\bar{1}$ (no. 2), $a = 10.1598(2)$ Å, $b = 13.8660(5)$ Å, $c = 14.7308(3)$ Å, $\alpha = 79.595(1)^\circ$, $\beta = 86.006(2)^\circ$, $\gamma = 87.997(2)^\circ$, $V = 2035.6$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.029$, $wR_{\text{ref}}(F^2) = 0.070$, $T = 150$ K.

Source of material

The reaction of $[\text{Pt}(\text{SePh})_2(\text{PPh}_3)_2]$ [1,2] with $[\text{PdCl}_2(\text{NCPh})_2]$ in molar ratio 1:1 in benzene yielded a mixture of products. A small amount of yellow crystals of $[\text{PtCl}(\text{SePh})(\text{PPh}_3)_2] \cdot \text{C}_6\text{H}_6$ was obtained after recrystallization of the hexane precipitate from benzene.

Discussion

The crystal lattice is built up of discrete mononuclear platinum complexes and benzene solvent molecules. The platinum atom shows a slightly distorted square-planar coordination [the sum of the bond angles is $359.9(1)^\circ$]. The Pt—P distances [2.316(1) Å and 2.324(1) Å] are quite normal for single bonds. The Pt—Cl bond length is 2.356(1) Å and can be compared to the Pt—Cl bond length of 2.300(1) Å in *trans*- $[\text{PtCl}_2(\text{PPh}_3)_2]$ [3] as well as to those of 2.333(2) Å and 2.356(2) Å in *cis*- $[\text{PtCl}_2(\text{PPh}_3)_2]$ [4]. The Pt—Se distance is 2.4215(5) Å. It is slightly shorter than the corresponding bonds in *cis*- $[\text{Pt}(\text{SePh})_2(\text{PPh}_3)_2]$ [2.4885(3) Å and

2.4506(3) Å] and *trans*- $[\text{Pt}(\text{SePh})_2(\text{PPh}_3)_2]$ [2.4525(5) Å and 2.4548(5) Å] [1,2]. These values are consistent with the relative *trans*-influences of Cl^- , PhSe^- , and PPh_3 .

Table 1. Data collection and handling.

Crystal:	yellow plate, size $0.07 \times 0.12 \times 0.15$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	45.18 cm^{-1}
Diffractometer, scan mode:	Nonius Kappa CCD, φ/ω with κ offsets
$2\theta_{\text{max}}$:	49.98°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	26579, 6720
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 6113
$N(\text{param})_{\text{refined}}$:	479
Programs:	SHELXS-97 [5], SHELXL-97 [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2)	2i	0.6269	0.9304	0.6310	0.048
H(3)	2i	0.5578	1.0822	0.5490	0.060
H(4)	2i	0.7150	1.2044	0.4921	0.074
H(5)	2i	0.9318	1.1748	0.5251	0.085
H(6)	2i	1.0060	1.0211	0.6042	0.035
H(12)	2i	0.7166	0.8318	0.5258	0.047
H(13)	2i	0.7237	0.9057	0.3706	0.065
H(14)	2i	0.7993	0.8167	0.2560	0.058
H(15)	2i	0.8573	0.6514	0.2969	0.049
H(16)	2i	0.8529	0.5774	0.4519	0.037
H(22)	2i	0.8897	0.4370	0.6644	0.035
H(23)	2i	0.7930	0.2855	0.6685	0.043
H(24)	2i	0.5721	0.2793	0.6377	0.044
H(25)	2i	0.4486	0.4237	0.5975	0.039
H(26)	2i	0.5439	0.5752	0.5923	0.031
H(32)	2i	1.0506	0.6383	0.5163	0.034
H(33)	2i	1.2676	0.6014	0.5546	0.043
H(34)	2i	1.3163	0.5554	0.7095	0.049
H(35)	2i	1.1447	0.5427	0.8252	0.052
H(36)	2i	0.9293	0.5848	0.7882	0.042
H(42)	2i	0.8663	0.8731	0.9046	0.041
H(43)	2i	0.9710	1.0162	0.9171	0.051
H(44)	2i	0.8695	1.1695	0.8705	0.055
H(45)	2i	0.6630	1.1794	0.8100	0.048
H(46)	2i	0.5585	1.0365	0.7937	0.036
H(52)	2i	0.4427	0.8261	0.6983	0.035
H(53)	2i	0.2271	0.8804	0.6722	0.042
H(54)	2i	0.1057	0.9587	0.7799	0.045
H(55)	2i	0.1975	0.9752	0.9165	0.049

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Table 2. Continued.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(56)	2i	0.4094	0.9140	0.9467	0.041
H(62)	2i	0.6598	0.6217	0.9271	0.043
H(63)	2i	0.6550	0.5356	1.0800	0.054
H(64)	2i	0.6167	0.6185	1.2029	0.059
H(65)	2i	0.5911	0.7880	1.1760	0.057
H(66)	2i	0.5992	0.8760	1.0245	0.045

Table 2. Continued.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(101)	2i	0.3657	0.6306	0.0033	0.070
H(102)	2i	0.2579	0.5899	0.1482	0.075
H(103)	2i	0.0331	0.6205	0.1670	0.070
H(104)	2i	−0.0858	0.6903	0.0406	0.064
H(105)	2i	0.0257	0.7308	−0.1032	0.067
H(106)	2i	0.2496	0.7026	−0.1214	0.064

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Pt(1)	2i	0.70324(2)	0.73416(1)	0.73221(1)	0.0214(1)	0.0245(1)	0.0225(1)	0.00020(6)	0.00251(6)	−0.00423(6)
Se(2)	2i	0.89127(4)	0.83805(3)	0.68387(3)	0.0275(3)	0.0327(3)	0.0372(3)	−0.0038(2)	0.0065(2)	−0.0101(2)
Cl(1)	2i	0.5281(1)	0.62576(8)	0.78017(8)	0.0268(6)	0.0345(6)	0.0340(6)	−0.0112(4)	0.0107(4)	−0.0129(5)
P(2)	2i	0.6204(1)	0.82589(8)	0.84158(7)	0.0220(6)	0.0269(6)	0.0196(5)	0.0024(4)	0.0012(4)	−0.0042(4)
P(1)	2i	0.7954(1)	0.64220(8)	0.62641(7)	0.0215(6)	0.0223(6)	0.0205(5)	0.0019(4)	0.0007(4)	−0.0040(4)
C(1)	2i	0.8210(5)	0.9609(4)	0.6267(3)	0.044(3)	0.036(3)	0.033(3)	−0.003(2)	0.013(2)	−0.017(2)
C(2)	2i	0.6898(5)	0.9797(4)	0.6092(3)	0.046(3)	0.042(3)	0.033(3)	−0.004(2)	0.008(2)	−0.015(2)
C(3)	2i	0.6484(7)	1.0701(4)	0.5600(3)	0.085(4)	0.032(3)	0.030(3)	−0.002(3)	0.011(3)	−0.008(2)
C(4)	2i	0.7415(8)	1.1432(4)	0.5269(4)	0.101(6)	0.036(3)	0.046(3)	0.005(3)	0.014(3)	−0.011(3)
C(5)	2i	0.8698(8)	1.1245(5)	0.5455(5)	0.101(6)	0.037(3)	0.071(5)	−0.007(3)	0.039(4)	−0.013(3)
C(6)	2i	0.9151(5)	1.0331(3)	0.5940(3)	0.031(3)	0.019(2)	0.036(2)	−0.009(2)	0.015(2)	−0.007(2)
C(11)	2i	0.7906(4)	0.6984(3)	0.5052(3)	0.022(2)	0.027(2)	0.025(2)	−0.003(2)	−0.002(2)	−0.004(2)
C(12)	2i	0.7481(5)	0.7954(4)	0.4796(3)	0.058(3)	0.029(3)	0.032(3)	0.002(2)	−0.010(2)	−0.005(2)
C(13)	2i	0.7513(6)	0.8391(4)	0.3874(4)	0.084(5)	0.036(3)	0.041(3)	0.000(3)	−0.018(3)	0.004(3)
C(14)	2i	0.7946(6)	0.7860(4)	0.3192(4)	0.062(4)	0.053(4)	0.028(3)	−0.013(3)	−0.010(2)	0.005(2)
C(15)	2i	0.8308(5)	0.6886(4)	0.3436(3)	0.043(3)	0.057(4)	0.022(2)	−0.002(2)	−0.001(2)	−0.005(2)
C(16)	2i	0.8285(4)	0.6447(4)	0.4357(3)	0.032(3)	0.033(3)	0.029(2)	0.005(2)	−0.002(2)	−0.009(2)
C(21)	2i	0.7264(4)	0.5214(3)	0.6285(3)	0.030(2)	0.022(2)	0.015(2)	−0.002(2)	0.005(2)	−0.004(2)
C(22)	2i	0.7999(5)	0.4346(3)	0.6509(3)	0.033(3)	0.028(2)	0.026(2)	0.005(2)	−0.000(2)	−0.004(2)
C(23)	2i	0.7424(5)	0.3445(3)	0.6536(3)	0.054(3)	0.026(3)	0.027(2)	0.002(2)	0.000(2)	−0.003(2)
C(24)	2i	0.6117(5)	0.3409(4)	0.6347(3)	0.050(3)	0.033(3)	0.027(2)	−0.015(2)	0.008(2)	−0.007(2)
C(25)	2i	0.5382(5)	0.4267(4)	0.6114(3)	0.034(3)	0.037(3)	0.027(2)	−0.006(2)	0.004(2)	−0.008(2)
C(26)	2i	0.5947(4)	0.5165(3)	0.6083(3)	0.026(2)	0.031(2)	0.022(2)	−0.001(2)	0.001(2)	−0.007(2)
C(31)	2i	0.9683(4)	0.6154(3)	0.6483(3)	0.026(2)	0.022(2)	0.028(2)	0.003(2)	−0.004(2)	−0.007(2)
C(32)	2i	1.0698(4)	0.6199(3)	0.5793(3)	0.024(3)	0.031(3)	0.030(2)	0.001(2)	0.001(2)	−0.004(2)
C(33)	2i	1.1988(5)	0.5976(3)	0.6021(3)	0.028(3)	0.034(3)	0.044(3)	0.002(2)	0.003(2)	−0.007(2)
C(34)	2i	1.2278(5)	0.5699(4)	0.6937(4)	0.025(3)	0.047(3)	0.054(3)	0.007(2)	−0.011(2)	−0.017(3)
C(35)	2i	1.1258(5)	0.5637(4)	0.7624(4)	0.040(3)	0.055(3)	0.037(3)	0.013(2)	−0.016(2)	−0.011(2)
C(36)	2i	0.9977(5)	0.5875(4)	0.7405(3)	0.032(3)	0.046(3)	0.028(2)	0.009(2)	−0.004(2)	−0.012(2)
C(41)	2i	0.7003(4)	0.9397(3)	0.8494(3)	0.024(2)	0.030(2)	0.023(2)	0.002(2)	0.003(2)	−0.009(2)
C(42)	2i	0.8244(5)	0.9350(4)	0.8852(3)	0.029(3)	0.040(3)	0.035(3)	0.006(2)	0.000(2)	−0.017(2)
C(43)	2i	0.8865(5)	1.0200(4)	0.8927(4)	0.025(3)	0.058(4)	0.048(3)	−0.001(2)	0.002(2)	−0.025(3)
C(44)	2i	0.8264(5)	1.1114(4)	0.8647(4)	0.044(3)	0.046(3)	0.053(3)	−0.015(2)	0.015(3)	−0.023(3)
C(45)	2i	0.7045(5)	1.1172(4)	0.8288(4)	0.043(3)	0.033(3)	0.043(3)	−0.002(2)	0.008(2)	−0.009(2)
C(46)	2i	0.6417(5)	1.0320(3)	0.8200(3)	0.032(3)	0.029(3)	0.028(2)	0.002(2)	0.002(2)	−0.003(2)
C(51)	2i	0.4491(4)	0.8645(3)	0.8253(3)	0.023(2)	0.026(2)	0.024(2)	0.001(2)	−0.000(2)	−0.001(2)
C(52)	2i	0.3927(4)	0.8555(3)	0.7434(3)	0.026(3)	0.037(3)	0.024(2)	0.003(2)	0.002(2)	−0.004(2)
C(53)	2i	0.2651(5)	0.8887(4)	0.7273(3)	0.031(3)	0.046(3)	0.026(2)	0.002(2)	−0.005(2)	−0.002(2)
C(54)	2i	0.1926(5)	0.9343(4)	0.7916(3)	0.022(3)	0.049(3)	0.037(3)	0.009(2)	0.001(2)	0.004(2)
C(55)	2i	0.2470(5)	0.9440(4)	0.8725(3)	0.031(3)	0.054(3)	0.038(3)	0.010(2)	0.004(2)	−0.016(2)
C(56)	2i	0.3737(4)	0.9084(4)	0.8900(3)	0.027(3)	0.046(3)	0.030(2)	0.005(2)	−0.003(2)	−0.010(2)
C(61)	2i	0.6258(4)	0.7578(3)	0.9607(3)	0.022(2)	0.037(3)	0.022(2)	0.005(2)	−0.003(2)	−0.004(2)
C(62)	2i	0.6449(5)	0.6560(4)	0.9774(3)	0.033(3)	0.040(3)	0.032(3)	0.002(2)	−0.002(2)	−0.003(2)
C(63)	2i	0.6420(5)	0.6048(4)	1.0685(4)	0.042(3)	0.046(3)	0.041(3)	0.006(2)	−0.004(2)	0.011(2)
C(64)	2i	0.6206(6)	0.6540(5)	1.1412(4)	0.050(4)	0.065(4)	0.026(3)	0.008(3)	0.000(2)	0.007(3)
C(65)	2i	0.6047(5)	0.7542(5)	1.1253(3)	0.045(3)	0.072(4)	0.024(3)	0.015(3)	−0.002(2)	−0.009(3)
C(66)	2i	0.6085(5)	0.8065(4)	1.0351(3)	0.039(3)	0.046(3)	0.026(2)	0.010(2)	−0.001(2)	−0.004(2)
C(101)	2i	0.2735(6)	0.6431(5)	0.0114(5)	0.039(4)	0.071(4)	0.072(4)	−0.002(3)	−0.001(3)	−0.032(4)
C(102)	2i	0.2101(7)	0.6190(5)	0.0966(4)	0.068(5)	0.073(5)	0.045(3)	0.008(3)	−0.013(3)	−0.007(3)
C(103)	2i	0.0772(6)	0.6369(5)	0.1075(4)	0.064(4)	0.058(4)	0.047(3)	−0.005(3)	0.017(3)	0.000(3)
C(104)	2i	0.0066(6)	0.6784(4)	0.0332(4)	0.039(3)	0.055(4)	0.070(4)	0.000(3)	0.002(3)	−0.022(3)
C(105)	2i	0.0728(7)	0.7020(4)	−0.0512(4)	0.070(5)	0.051(4)	0.047(3)	0.009(3)	−0.012(3)	−0.006(3)
C(106)	2i	0.2050(6)	0.6851(4)	−0.0621(4)	0.060(4)	0.045(3)	0.052(4)	−0.015(3)	0.016(3)	−0.009(3)

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