Crystal Structures of [Ag(bpy)(PPh₃)]X (1: X = PF₆, 2: X = ClO₄) Complexes

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The title complexes, [Ag(bpy)(PPh₃)]X (1: X = PF₆, 2: X = ClO₄), contain a bidentate 2,2'-bipyridine (bpy) ligand and a monodentate triphenylphosphine (PPh₃) ligand, which were determined by the X-ray diffraction method. The coordination geometry of the Ag atom is distorted trigonal with two N atoms from 2,2'-bipyridine and one P atom from triphenylphosphine (PPh₃).

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Depending on the ligands involved, silver(I) complexes can show a wide variety of structures.¹⁻⁵ Bipyridine (bpy) ligands have been widely applied in coordination chemistry because of their versatile coordination modes, such as chelating^{1,2} and bridging.^{3,4} Therefore, in order to develop new silver complexes, the title complexes, [Ag(bpy)(PPh₃)]X (1: X = PF₆, 2: X = ClO₄) (Fig. 1), have been synthesized and structurally investigated.

The title complexes could be easily synthesized by the reaction of 0.2 mmol AgPF₆ and AgClO₄ for **1** and **2**, respectively, with 0.2 mmol PPh₃, and 0.2 mmol bpy in CH₃OH/CH₂Cl₂ (1:1 v/v). Slow evaporation of the solvent at 0°C, gave colorless crystals of the title compound suitable for X-ray analysis. Single crystals were grown from their appropriate solvent systems under favorable conditions. White single crystals with dimensions of (0.5 × 0.3 × 0.25 for **1**, and 0.4 × 0.4 × 0.3 for **2**) mm³ were chosen for X-ray diffraction studies. The determination of unit-cell parameters and data collections were performed with Mo K_α radiation (λ = 0.7107 Å) at 295 K on a Rigaku AFC7R diffractometer. The structure was solved by heavy-atom methods and expanded using Fourier techniques, and refined by full-matrix least-squares methods on *F* with anisotropic thermal parameters for non-hydrogen atoms. Hydrogen atoms were added at the calculated positions and fixed in the refinements. All of the calculations were carried out using the teXsan crystallographic software package.⁶ The crystal and experimental data are given in Table 1.

The crystals of **1** and **2** contain an [Ag(bpy)(PPh₃)] cation and

a corresponding anion in the asymmetric unit. These structures are isostructures. ORTEP diagrams of **1** and **2** are shown in Figs. 2 and 3, respectively. Two N atoms of the bpy ligand and one P atom of the PPh₃ ligand are coordinated to the Ag(I) atom. The bpy ligand chelates the silver(I) atom to form a five-member ring with a N(1)-Ag(1)-N(2) angle of 73.0(1)° for **1** and 73.0(1)° for **2**. The angles P(1)-Ag(1)-N(1) = 149.66(9), and

Table 1 Crystal and experimental data

	1	2
Empirical formula	C ₂₈ H ₂₃ AgN ₂ P ₂ F ₆	C ₂₈ H ₂₃ AgClN ₂ O ₄ P
Formula weight	671.31	625.80
Crystal color, habit	Colorless, prismatic	Colorless, prismatic
Crystal system	triclinic	triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i>	11.150(1)Å	11.178(2)Å
<i>b</i>	12.119(1)Å	11.958(1)Å
<i>c</i>	11.005(1)Å	10.759(2)Å
α	107.518(8)°	106.45(1)°
β	107.087(8)°	107.49(2)°
γ	80.96(1)°	80.70(1)°
<i>V</i>	1351.6(3)Å ³	1311.0(4)Å ³
<i>Z</i>	2	2
<i>D</i> _x	1.649 g cm ⁻³	1.585 g cm ⁻³
<i>F</i> (0 0 0)	672.00	632.00
μ	9.248 cm ⁻¹	9.669 cm ⁻¹
<i>R</i> (<i>F</i>)	0.043	0.068
<i>wR</i> (<i>F</i>)	0.078	0.096
No. of reflection used (all data)	6505	6331
Diffractometer	Rigaku AFC7R	Rigaku AFC7R
Program system	teXsan	teXsan
Structure determination	Dirdif92 patty	Dirdif92 patty
Refinement: full matrix least-squares	SHELXL-97	SHELXL-97

The X-ray crystallographic file, in CIF format, has been deposited with the Cambridge Crystallographic Data Center, CCDC No. 286188 for **1** and CCDC No. 286256 for **2**. Copy of this information may be obtained free of charge from the Cambridge Crystallographic Data Center, 12, Union Road, Cambridge, CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk/conts/retrieving.html).

Fig. 1 Chemical structures of the complexes [Ag(bpy)(PPh₃)]X (1: X = PF₆, 2: X = ClO₄).

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Fig. 2 ORTEP structure of **1** with atom labeling, shown with 30% probability displacement ellipsoids.

$\text{P(1)-Ag(1)-N(2)} = 134.34(8)^\circ$ for **1** and $\text{P(1)-Ag(1)-N(1)} = 153.5(1)^\circ$, and $\text{P(1)-Ag(1)-N(2)} = 130.82(9)^\circ$ for **2** are slightly different from those of a regular trigonal, and are in good agreement with the corresponding angles in related complexes.^{1,2} The Ag(1)-P(1) [2.3382(9) Å] and Ag-N [2.251(3) and 2.312(3) Å] bond distances for **1** and the Ag(1)-P(1) [2.332(1) Å] and Ag-N [2.236(3) and 2.316(4) Å] for **2** are in good agreement with the corresponding distances in related complexes.^{1,2}

Fig. 3 ORTEP structure of **2** with atom labeling, shown with 30% probability displacement ellipsoids.

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