# Crystal structure of bromo-(1,10-phenathroline-*N*,*N'*)(triphenylphosphine) silver(I) dihydrate, $Ag(Phen)(PPh_3)Br \cdot 2H_2O$

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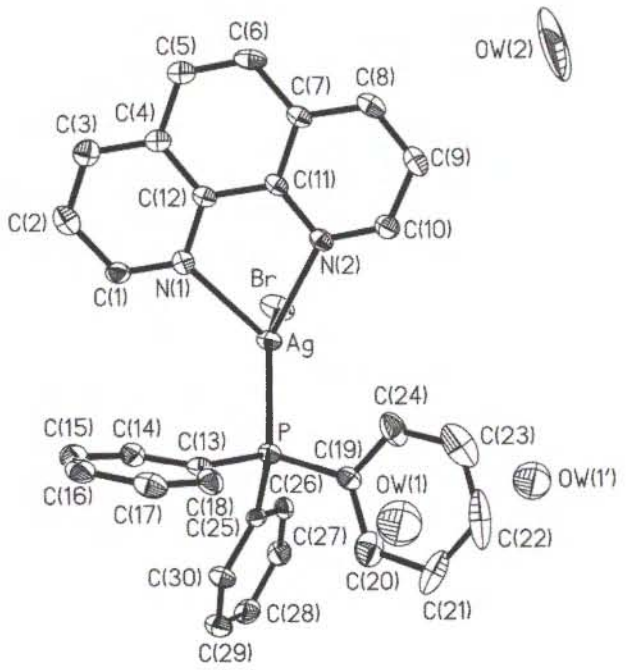


## Abstract

$C_{30}H_{27}AgBrN_2O_2P$, monoclinic, $P12_1/c1$ (No. 14), $a = 16.806(4)$ Å, $b = 9.488(3)$ Å, $c = 19.898(7)$ Å, $\beta = 107.96(2)°$, $V = 3018.3$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.068$, $wR(F^2) = 0.180$, $T = 293$ K.

## Source of material

The title compound was prepared under the reaction of AgBr, $PPh_3$ and Phen with the molar ratio of 1:1:2 in DMF solution at room temperature. The colourless columnar prism crystals were obtained by slowly evaporating the solvent.

## Discussion

Recently, we synthesized some group IB metal compounds, $[CuX(PPh_3)(C_9H_7N)]_2$ (X = Br, I) [1, 2], [CuI($PPh_3$)(Phen)](**II**) [3], that may be used as reactants for synthesis of Mo(W)-Cu-S clusters. Here we report a new Ag(I) complex: [AgBr($PPh_3$)(Phen)] (**I**) with the Ag atom coordinated to one P atom from triphenylphosphine, two N atoms from phenanthroline and one Br atom. The complex (**I**) can be regarded as being analogous to (**II**) with its Cu atom replaced by Ag atom, and iodine atom replaced by Br atom. The bond lengths Ag–P (2.375(3) Å), Ag–N (2.376(8) Å) and Ag–Br (2.6164(15) Å) are larger than the corresponding bond lenghths in (**II**). The longer Ag–N distances in (**I**) make the angle N1–Ag–N2 much smaller than N1–Cu–N2 in (**II**).

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colourless prism, size 0.2 × 0.2 × 0.5 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| μ: | 20.72 cm$^{-1}$ |
| Diffractometer, scan mode: | Siemens P4, θ/2θ |
| $2\theta_{max}$: | 50.04° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 6679, 5315 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2613 |
| $N(param)_{refined}$: | 335 |
| Programs: | SHELXS-86 [4], SHELXL-93 [5], XP [6] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | Occ. | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|---|
| Ow(1) | 4*e* | 0.62(2) | 0.099(1) | 0.404(2) | 0.091(1) | 0.146(8) |
| Ow(1') | 4*e* | 0.38 | −0.028(1) | 0.493(3) | 0.101(1) | 0.10(1) |
| H(1) | 4*e* | | 0.4961(6) | 0.121(1) | 0.4659(5) | 0.072(7) |
| H(2) | 4*e* | | 0.6156(7) | 0.227(1) | 0.5412(5) | 0.072 |
| H(3) | 4*e* | | 0.6017(6) | 0.424(1) | 0.6070(5) | 0.072 |
| H(5) | 4*e* | | 0.5074(7) | 0.591(1) | 0.6381(5) | 0.072 |
| H(6) | 4*e* | | 0.3756(7) | 0.670(1) | 0.6278(5) | 0.072 |
| H(8) | 4*e* | | 0.2196(7) | 0.636(1) | 0.5778(5) | 0.072 |
| H(9) | 4*e* | | 0.1073(7) | 0.508(1) | 0.5067(6) | 0.072 |
| H(10) | 4*e* | | 0.1334(7) | 0.304(1) | 0.4532(5) | 0.072 |
| H(14) | 4*e* | | 0.4331(6) | −0.008(1) | 0.3468(5) | 0.072 |
| H(15) | 4*e* | | 0.5335(7) | 0.093(1) | 0.3070(6) | 0.072 |
| H(16) | 4*e* | | 0.4998(8) | 0.251(1) | 0.2193(7) | 0.072 |
| H(17) | 4*e* | | 0.3612(8) | 0.308(1) | 0.1634(6) | 0.072 |
| H(18) | 4*e* | | 0.2592(7) | 0.207(1) | 0.2052(5) | 0.072 |
| H(20) | 4*e* | | 0.1441(7) | −0.070(1) | 0.1873(7) | 0.072 |
| H(21) | 4*e* | | 0.0128(8) | −0.001(2) | 0.1140(8) | 0.072 |
| H(22) | 4*e* | | −0.054(1) | 0.176(2) | 0.155(1) | 0.072 |
| H(23) | 4*e* | | 0.014(1) | 0.294(2) | 0.262(1) | 0.072 |
| H(24) | 4*e* | | 0.1473(8) | 0.228(1) | 0.3265(7) | 0.072 |
| H(26) | 4*e* | | 0.2125(5) | −0.218(1) | 0.3851(5) | 0.072 |
| H(27) | 4*e* | | 0.2051(6) | −0.458(1) | 0.3692(6) | 0.072 |
| H(28) | 4*e* | | 0.2443(7) | −0.555(1) | 0.2762(7) | 0.072 |
| H(29) | 4*e* | | 0.2948(7) | −0.417(1) | 0.2041(6) | 0.072 |
| H(30) | 4*e* | | 0.3075(6) | −0.175(1) | 0.2266(5) | 0.072 |

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**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Ag | 4*e* | 0.29211(5) | 0.09756(8) | 0.43950(4) | 0.0675(5) | 0.0463(5) | 0.0467(4) | –0.0056(4) | 0.0256(4) | –0.0100(4) |
| Br | 4*e* | 0.29707(9) | –0.0533(1) | 0.55081(6) | 0.139(1) | 0.0561(8) | 0.0648(8) | 0.0091(7) | 0.0501(8) | 0.0114(6) |
| P | 4*e* | 0.2597(2) | 0.0185(3) | 0.3208(1) | 0.054(2) | 0.041(1) | 0.040(1) | –0.002(1) | 0.020(1) | –0.002(1) |
| Ow(2) | 4*e* | 0.0349(9) | 0.753(2) | 0.537(1) | 0.17(1) | 0.22(2) | 0.60(4) | 0.15(1) | 0.17(2) | 0.07(2) |
| N(1) | 4*e* | 0.4143(5) | 0.2343(8) | 0.4902(4) | 0.047(5) | 0.039(5) | 0.048(5) | 0.003(4) | 0.019(4) | 0.010(4) |
| N(2) | 4*e* | 0.2540(5) | 0.3154(8) | 0.4816(4) | 0.056(5) | 0.033(4) | 0.054(5) | 0.005(4) | 0.025(4) | 0.001(4) |
| C(1) | 4*e* | 0.4897(6) | 0.196(1) | 0.4940(5) | 0.059(7) | 0.058(7) | 0.044(6) | –0.006(6) | 0.020(5) | –0.009(5) |
| C(2) | 4*e* | 0.5630(7) | 0.261(1) | 0.5386(5) | 0.071(7) | 0.066(7) | 0.057(6) | 0.017(6) | 0.030(6) | 0.019(6) |
| C(3) | 4*e* | 0.5551(6) | 0.377(1) | 0.5782(5) | 0.059(7) | 0.067(8) | 0.044(6) | 0.003(6) | 0.010(5) | 0.010(6) |
| C(4) | 4*e* | 0.4732(6) | 0.4217(9) | 0.5730(4) | 0.064(7) | 0.038(6) | 0.036(5) | –0.004(5) | 0.017(5) | 0.007(4) |
| C(5) | 4*e* | 0.4612(7) | 0.543(1) | 0.6095(5) | 0.069(7) | 0.047(6) | 0.049(6) | –0.005(6) | 0.018(5) | –0.003(5) |
| C(6) | 4*e* | 0.3827(7) | 0.590(1) | 0.6035(5) | 0.103(9) | 0.041(6) | 0.042(6) | –0.009(7) | 0.033(6) | –0.006(5) |
| C(7) | 4*e* | 0.3111(6) | 0.516(1) | 0.5595(5) | 0.062(7) | 0.038(5) | 0.052(6) | 0.007(5) | 0.023(5) | –0.003(5) |
| C(8) | 4*e* | 0.2289(7) | 0.557(1) | 0.5537(5) | 0.085(8) | 0.052(7) | 0.063(7) | 0.006(6) | 0.042(6) | –0.004(5) |
| C(9) | 4*e* | 0.1620(7) | 0.480(1) | 0.5123(6) | 0.065(8) | 0.062(8) | 0.086(8) | 0.015(6) | 0.041(7) | 0.005(7) |
| C(10) | 4*e* | 0.1787(7) | 0.358(1) | 0.4789(5) | 0.060(7) | 0.051(6) | 0.061(6) | –0.001(5) | 0.025(5) | –0.004(5) |
| C(11) | 4*e* | 0.3213(6) | 0.3935(9) | 0.5227(4) | 0.056(6) | 0.035(5) | 0.040(5) | 0.006(5) | 0.025(4) | 0.005(4) |
| C(12) | 4*e* | 0.4048(6) | 0.3493(9) | 0.5283(4) | 0.057(6) | 0.035(5) | 0.036(5) | 0.001(5) | 0.021(5) | 0.004(4) |
| C(13) | 4*e* | 0.3352(6) | 0.0878(9) | 0.2805(4) | 0.063(6) | 0.033(5) | 0.032(5) | –0.006(5) | 0.019(4) | 0.000(4) |
| C(14) | 4*e* | 0.4173(6) | 0.057(1) | 0.3097(5) | 0.057(7) | 0.056(7) | 0.050(6) | 0.003(5) | 0.020(5) | –0.001(5) |
| C(15) | 4*e* | 0.4777(7) | 0.118(1) | 0.2860(6) | 0.065(7) | 0.061(8) | 0.072(7) | –0.011(6) | 0.029(6) | –0.014(7) |
| C(16) | 4*e* | 0.4577(8) | 0.210(1) | 0.2339(7) | 0.080(9) | 0.053(7) | 0.089(9) | –0.031(7) | 0.051(7) | –0.032(7) |
| C(17) | 4*e* | 0.3758(8) | 0.245(1) | 0.2010(6) | 0.098(9) | 0.037(6) | 0.067(7) | –0.011(6) | 0.043(7) | –0.004(5) |
| C(18) | 4*e* | 0.3150(7) | 0.183(1) | 0.2261(5) | 0.064(7) | 0.044(6) | 0.073(7) | 0.003(5) | 0.030(6) | –0.006(6) |
| C(19) | 4*e* | 0.1587(6) | 0.070(1) | 0.2659(5) | 0.058(6) | 0.050(6) | 0.045(6) | 0.005(5) | 0.022(5) | 0.001(5) |
| C(20) | 4*e* | 0.1172(7) | 0.004(1) | 0.2015(7) | 0.078(9) | 0.063(8) | 0.12(1) | 0.010(7) | 0.021(8) | 0.013(8) |
| C(21) | 4*e* | 0.0379(8) | 0.043(2) | 0.1571(8) | 0.051(8) | 0.13(1) | 0.12(1) | –0.017(9) | –0.016(8) | 0.04(1) |
| C(22) | 4*e* | 0.000(1) | 0.149(2) | 0.181(1) | 0.06(1) | 0.17(2) | 0.22(2) | 0.05(1) | 0.07(1) | 0.11(2) |
| C(23) | 4*e* | 0.041(1) | 0.221(2) | 0.247(1) | 0.15(2) | 0.12(2) | 0.15(2) | 0.05(1) | 0.10(2) | 0.03(1) |
| C(24) | 4*e* | 0.1198(8) | 0.179(1) | 0.2854(7) | 0.084(9) | 0.10(1) | 0.077(8) | 0.046(8) | 0.032(7) | 0.019(8) |
| C(25) | 4*e* | 0.2609(5) | –0.1726(9) | 0.3083(4) | 0.040(5) | 0.036(5) | 0.037(5) | –0.001(4) | 0.008(4) | –0.005(4) |
| C(26) | 4*e* | 0.2302(5) | –0.258(1) | 0.3494(5) | 0.040(5) | 0.050(6) | 0.048(6) | –0.001(5) | 0.018(5) | 0.001(5) |
| C(27) | 4*e* | 0.2246(6) | –0.400(1) | 0.3397(6) | 0.063(7) | 0.053(7) | 0.077(8) | –0.011(6) | 0.025(6) | –0.001(6) |
| C(28) | 4*e* | 0.2490(7) | –0.459(1) | 0.2839(7) | 0.067(8) | 0.048(7) | 0.097(9) | –0.008(6) | 0.013(7) | –0.020(7) |
| C(29) | 4*e* | 0.2792(7) | –0.377(1) | 0.2410(6) | 0.081(8) | 0.058(8) | 0.063(7) | –0.006(6) | 0.032(6) | –0.013(6) |
| C(30) | 4*e* | 0.2858(6) | –0.232(1) | 0.2545(5) | 0.073(7) | 0.048(6) | 0.045(6) | 0.001(5) | 0.027(5) | –0.001(5) |

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