

# Bis(quinolin-8-ol)silver(I) 2-hydroxy-3,5-dinitrobenzoate

Chun-Lan Zhang<sup>a</sup> and Fang-Fang Jian<sup>b\*</sup>

<sup>a</sup>Microscale Science Institute, Biology Department, Weifang University, Weifang 261061, People's Republic of China, and <sup>b</sup>Microscale Science Institute, Weifang University, Weifang 261061, People's Republic of China

Correspondence e-mail: ffjian2008@163.com

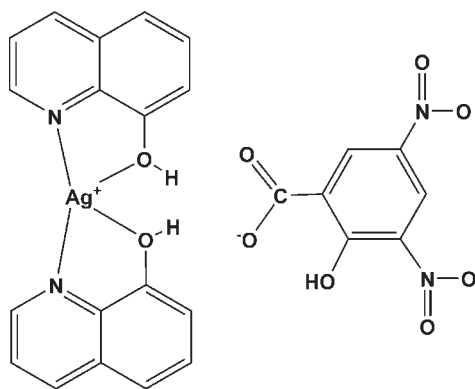
Received 29 October 2009; accepted 2 November 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.057; data-to-parameter ratio = 13.0.

The title compound,  $[\text{Ag}(\text{C}_9\text{H}_7\text{NO})_2](\text{C}_7\text{H}_3\text{N}_2\text{O}_7)$ , was prepared from 3,5-dinitrosalicylic acid (DNS), quinolin-8-ol and  $\text{AgNO}_3$ . The  $\text{Ag}^{\text{I}}$  atom is coordinated by two N atoms and two O atoms from two quinolin-8-ols in a roughly planar [maximum deviation = 0.223 (2) Å] environment. The two quinolin-8-ol ligands are bent slightly with respect to each other, making a dihedral angle of 9.55 (9)°. The DNS anion interacts with the silver complex through O—H...O hydrogen bonds

## Related literature

For related structures, see: Smith & Thomasson (1999); Smith *et al.* (2001); Wu *et al.* (2006).



## Experimental

### Crystal data

|  |                                   |
|--|-----------------------------------|
| $[\text{Ag}(\text{C}_9\text{H}_7\text{NO})_2](\text{C}_7\text{H}_3\text{N}_2\text{O}_7)$ | $V = 1139.3$ (4) Å <sup>3</sup>   |
| $M_r = 625.30$   | $Z = 2$                           |
| Monoclinic, $P2_1$   | Mo $K\alpha$ radiation            |
| $a = 9.0154$ (18) Å  | $\mu = 0.95$ mm <sup>-1</sup>     |
| $b = 7.6122$ (15) Å  | $T = 293$ K                       |
| $c = 17.138$ (3) Å   | $0.20 \times 0.15 \times 0.11$ mm |
| $\beta = 104.38$ (3)°  |                                   |

### Data collection

|   |  |
|---|--|
| Bruker SMART CCD area-detector diffractometer | 4602 independent reflections           |
| Absorption correction: none                   | 4356 reflections with $I > 2\sigma(I)$ |
| 10841 measured reflections                    | $R_{\text{int}} = 0.022$               |

### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | H-atom parameters constrained                       |
| $wR(F^2) = 0.057$               | $\Delta\rho_{\text{max}} = 0.70$ e Å <sup>-3</sup>  |
| $S = 1.09$                      | $\Delta\rho_{\text{min}} = -0.30$ e Å <sup>-3</sup> |
| 4602 reflections                | Absolute structure: Flack (1983),                   |
| 353 parameters                  | 1770 Friedel pairs                                  |
| 1 restraint                     | Flack parameter: 0.006 (18)                         |

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------|-------|-------------|-------------|---------------|
| O1—H1A...O8   | 1.00  | 1.60        | 2.602 (3)   | 175           |
| O2—H2A...O9   | 0.77  | 1.88        | 2.636 (3)   | 168           |
| O3—H3B...O9   | 0.82  | 1.74        | 2.483 (3)   | 150           |

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2508).

## References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Smith, G. & Thomasson, J. H. (1999). *Aust. J. Chem.* **52**, 317–324.
- Smith, G., Wermuth, U. D. & White, J. M. (2001). *Aust. J. Chem.* **54**, 171–175.
- Wu, H., Dong, X.-W., Liu, H.-Y. & Ma, J.-F. (2006). *Acta Cryst.* **E62**, m281–m282.

**supplementary materials**

*Acta Cryst.* (2009). E65, m1521 [ doi:10.1107/S1600536809045905 ]

## Bis(quinolin-8-ol)silver(I) 2-hydroxy-3,5-dinitrobenzoate

C.-L. Zhang and F.-F. Jian

### Comment

Quinolin-8-ol [quinolin-8-ol (oxine)] is well known as a particularly versatile ligand for use in metal complex chemistry (G. Smith, *et al.*, 2001). It is also known that most of  $\text{Ag}^{\text{I}}$  in biological systems is not in the form of free  $\text{Ag}^{\text{I}}$  ions, but is coordinated by the abundance of biological ligands (Wu, *et al.*, 2006). As part of our search for new biologically active compounds the title compound has been synthesized and we report its crystal structure here.

#### Scheme I

The  $\text{Ag}^{\text{I}}$  atom is coordinated by two N atoms and two O atoms from two quinolin-8-ols in a roughly planar environment with the largest deviation from the mean plane of the non H atoms being 0.223 (2) Å at C14 (Fig. 1). However, the two quinolin-8-ols are slightly bent with respect to each other making a dihedral angle of 9.55 (9)°. In the DNS anion, the  $\text{NO}_2$  and  $\text{CO}_2$  groups are twisted with respect to the phenyl ring making dihedral angles of 29.5 (1)° for C21, N4, O6, O7, 10.7 (2)° for C19, N3, O4, O5 and 10.0 (2)° for C23, C25, O8, O9. All of the bond lengths and bond angles are in normal ranges (Smith, *et al.*, 1999; Smith, *et al.*, 2001; Wu, *et al.*, 2006).

There are O—H...O hydrogen-bond interactions between two quinolin-8-ol and DNS which stabilize the crystal structure (Table 1, Fig. 1).

### Experimental

The title compound(I) was prepared by the process as following: A mixture of 3,5-Dinitrosalicylic acid (0.01 mol), salt of quinolin-8-ol and sulfuric acid (0.02 mol) was stirred in distilled water (30 ml) for 3 h to obtain yellow deposit. A mixture of the deposit and  $\text{AgNO}_3$  (0.01 mol) was stirred in ethanol (20 ml) at 353 K for 5 h, then afford the title compound (yield 83%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

### Refinement

H atoms were included in calculated positions, with C—H distances constrained to 0.93 Å (aromatic CH) and O—H distances constrained to 0.86 Å and with  $U_{\text{iso}}=1.2-1.5U_{\text{eq}}$ .

## Figures

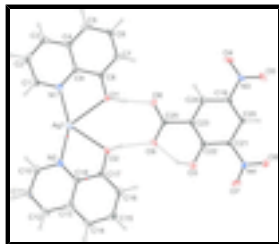


Fig. 1. The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

## Bis(quinolin-8-ol)silver(I) 2-hydroxy-3,5-dinitrobenzoate

### Crystal data

$[\text{Ag}(\text{C}_9\text{H}_7\text{NO})_2](\text{C}_7\text{H}_3\text{N}_2\text{O}_7)$

$M_r = 625.30$

Monoclinic,  $P2_1$

Hall symbol: P 2yb

$a = 9.0154 (18) \text{ \AA}$

$b = 7.6122 (15) \text{ \AA}$

$c = 17.138 (3) \text{ \AA}$

$\beta = 104.38 (3)^\circ$

$V = 1139.3 (4) \text{ \AA}^3$

$Z = 2$

$F_{000} = 628$

$D_x = 1.823 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4356 reflections

$\theta = 3.6\text{--}27.6^\circ$

$\mu = 0.95 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, yellow

$0.20 \times 0.15 \times 0.11 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293 \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: none

10841 measured reflections

4602 independent reflections

4356 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\text{max}} = 27.6^\circ$

$\theta_{\text{min}} = 3.6^\circ$

$h = -11 \rightarrow 11$

$k = -9 \rightarrow 8$

$l = -22 \rightarrow 22$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.057$

$S = 1.09$

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.3633P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$

|  |  |
|--|--|
| 4602 reflections   | $\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$       |
| 353 parameters   | Extinction correction: none                          |
| 1 restraint  | Absolute structure: Flack (1983), 1770 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.006 (18)                          |
| Secondary atom site location: difference Fourier map           |  |

### Special details

**Geometry.** 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.

**Refinement.** 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  $F^2 > \sigma(F^2)$  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.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|      | $x$           | $y$         | $z$           | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|-------------|---------------|----------------------------------|
| Ag1  | 0.062198 (19) | 0.74284 (3) | 0.668865 (11) | 0.01870 (6)                      |
| O1   | -0.0991 (2)   | 0.4624 (3)  | 0.64039 (12)  | 0.0199 (4)                       |
| H1AA | -0.0950       | 0.3450      | 0.6670        | 0.030*                           |
| O2   | 0.1744 (2)    | 0.5065 (3)  | 0.77201 (12)  | 0.0217 (4)                       |
| H2AA | 0.1409        | 0.4170      | 0.7790        | 0.033*                           |
| N1   | -0.1155 (2)   | 0.7669 (4)  | 0.55612 (13)  | 0.0174 (5)                       |
| N2   | 0.2684 (3)    | 0.8371 (3)  | 0.75436 (14)  | 0.0163 (5)                       |
| C1   | -0.1281 (3)   | 0.9178 (4)  | 0.51463 (19)  | 0.0223 (6)                       |
| H1A  | -0.0613       | 1.0090      | 0.5354        | 0.027*                           |
| C2   | -0.2364 (4)   | 0.9449 (4)  | 0.44186 (18)  | 0.0246 (6)                       |
| H2A  | -0.2410       | 1.0519      | 0.4152        | 0.030*                           |
| C3   | -0.3353 (3)   | 0.8132 (4)  | 0.41024 (19)  | 0.0211 (6)                       |
| H3A  | -0.4080       | 0.8297      | 0.3618        | 0.025*                           |
| C4   | -0.3269 (3)   | 0.6506 (4)  | 0.45167 (18)  | 0.0170 (6)                       |
| C5   | -0.4267 (3)   | 0.5080 (4)  | 0.42261 (17)  | 0.0209 (6)                       |
| H5A  | -0.5013       | 0.5186      | 0.3744        | 0.025*                           |
| C6   | -0.4132 (3)   | 0.3552 (4)  | 0.46543 (18)  | 0.0214 (6)                       |
| H6A  | -0.4774       | 0.2614      | 0.4454        | 0.026*                           |
| C7   | -0.3036 (3)   | 0.3371 (4)  | 0.53957 (17)  | 0.0187 (6)                       |
| H7A  | -0.2977       | 0.2327      | 0.5683        | 0.022*                           |
| C8   | -0.2059 (3)   | 0.4719 (4)  | 0.56950 (16)  | 0.0149 (5)                       |
| C9   | -0.2140 (3)   | 0.6332 (4)  | 0.52566 (16)  | 0.0141 (5)                       |
| C10  | 0.3161 (3)    | 0.9992 (4)  | 0.74638 (17)  | 0.0187 (6)                       |
| H10A | 0.2572        | 1.0697      | 0.7061        | 0.022*                           |
| C11  | 0.4512 (3)    | 1.0703 (4)  | 0.79573 (19)  | 0.0222 (6)                       |
| H11A | 0.4807        | 1.1847      | 0.7878        | 0.027*                           |
| C12  | 0.5375 (3)    | 0.9694 (4)  | 0.85498 (18)  | 0.0210 (6)                       |

## supplementary materials

|      |             |             |              |            |
|------|-------------|-------------|--------------|------------|
| H12A | 0.6277      | 1.0140      | 0.8878       | 0.025*     |
| C13  | 0.4907 (3)  | 0.7962 (4)  | 0.86706 (17) | 0.0172 (6) |
| C14  | 0.5745 (3)  | 0.6843 (4)  | 0.92847 (17) | 0.0199 (6) |
| H14A | 0.6655      | 0.7235      | 0.9626       | 0.024*     |
| C15  | 0.5225 (3)  | 0.5197 (4)  | 0.93780 (17) | 0.0206 (6) |
| H15A | 0.5776      | 0.4479      | 0.9788       | 0.025*     |
| C16  | 0.3864 (3)  | 0.4567 (4)  | 0.88625 (17) | 0.0177 (6) |
| H16A | 0.3520      | 0.3443      | 0.8937       | 0.021*     |
| C17  | 0.3044 (3)  | 0.5596 (4)  | 0.82523 (16) | 0.0144 (5) |
| C18  | 0.3541 (2)  | 0.7342 (6)  | 0.81437 (14) | 0.0140 (4) |
| O3   | 0.1402 (2)  | -0.0140 (3) | 0.92529 (13) | 0.0260 (5) |
| H3B  | 0.1405      | 0.0793      | 0.9015       | 0.039*     |
| O4   | -0.4152 (2) | -0.3754 (3) | 0.69128 (14) | 0.0284 (5) |
| O5   | -0.3271 (2) | -0.5962 (3) | 0.76855 (13) | 0.0273 (5) |
| O6   | 0.1239 (2)  | -0.5246 (3) | 0.98348 (12) | 0.0211 (4) |
| O7   | 0.1678 (2)  | -0.2656 (4) | 1.03550 (11) | 0.0289 (4) |
| O8   | -0.0981 (2) | 0.1498 (3)  | 0.70194 (12) | 0.0242 (5) |
| O9   | 0.0667 (2)  | 0.2136 (3)  | 0.81890 (12) | 0.0198 (5) |
| N3   | -0.3217 (2) | -0.4436 (3) | 0.74770 (14) | 0.0173 (5) |
| N4   | 0.1088 (2)  | -0.3646 (3) | 0.98082 (14) | 0.0151 (5) |
| C19  | -0.1971 (3) | -0.3338 (4) | 0.79249 (18) | 0.0131 (6) |
| C20  | -0.1028 (3) | -0.3990 (3) | 0.86303 (16) | 0.0128 (5) |
| H20A | -0.1152     | -0.5127     | 0.8803       | 0.015*     |
| C21  | 0.0095 (3)  | -0.2909 (3) | 0.90660 (15) | 0.0118 (6) |
| C22  | 0.0328 (3)  | -0.1188 (4) | 0.88193 (16) | 0.0131 (5) |
| C23  | -0.0605 (3) | -0.0602 (3) | 0.80700 (16) | 0.0130 (5) |
| C24  | -0.1769 (3) | -0.1677 (4) | 0.76339 (18) | 0.0137 (6) |
| H24A | -0.2405     | -0.1286     | 0.7152       | 0.016*     |
| C25  | -0.0306 (3) | 0.1145 (4)  | 0.77252 (16) | 0.0150 (5) |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|---------------|--------------|--------------|
| Ag1 | 0.01624 (8) | 0.01725 (9) | 0.01946 (9) | -0.00342 (12) | -0.00152 (6) | 0.00022 (11) |
| O1  | 0.0213 (10) | 0.0127 (9)  | 0.0199 (10) | -0.0063 (8)   | -0.0062 (8)  | 0.0045 (7)   |
| O2  | 0.0185 (9)  | 0.0169 (10) | 0.0244 (11) | -0.0079 (8)   | -0.0046 (8)  | 0.0028 (8)   |
| N1  | 0.0194 (9)  | 0.0143 (15) | 0.0179 (10) | -0.0003 (11)  | 0.0034 (8)   | 0.0009 (10)  |
| N2  | 0.0138 (10) | 0.0164 (12) | 0.0191 (12) | -0.0018 (9)   | 0.0047 (9)   | 0.0005 (9)   |
| C1  | 0.0256 (14) | 0.0145 (13) | 0.0262 (16) | -0.0040 (13)  | 0.0053 (12)  | 0.0045 (11)  |
| C2  | 0.0331 (16) | 0.0181 (15) | 0.0238 (16) | 0.0071 (14)   | 0.0092 (13)  | 0.0106 (12)  |
| C3  | 0.0216 (13) | 0.0248 (14) | 0.0156 (15) | 0.0061 (12)   | 0.0021 (11)  | 0.0024 (11)  |
| C4  | 0.0139 (12) | 0.0219 (15) | 0.0152 (14) | 0.0027 (11)   | 0.0036 (10)  | 0.0011 (12)  |
| C5  | 0.0161 (13) | 0.0293 (16) | 0.0149 (14) | 0.0008 (13)   | -0.0007 (10) | -0.0035 (12) |
| C6  | 0.0154 (13) | 0.0245 (15) | 0.0215 (15) | -0.0088 (12)  | -0.0008 (10) | -0.0052 (12) |
| C7  | 0.0181 (13) | 0.0179 (15) | 0.0188 (14) | -0.0042 (11)  | 0.0023 (10)  | 0.0014 (11)  |
| C8  | 0.0142 (12) | 0.0145 (13) | 0.0143 (13) | 0.0003 (11)   | 0.0002 (10)  | 0.0000 (10)  |
| C9  | 0.0142 (12) | 0.0143 (13) | 0.0135 (13) | -0.0007 (11)  | 0.0030 (9)   | 0.0009 (10)  |
| C10 | 0.0208 (13) | 0.0172 (14) | 0.0199 (15) | -0.0023 (12)  | 0.0082 (11)  | 0.0027 (11)  |

|     |             |             |             |              |             |              |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C11 | 0.0261 (14) | 0.0167 (14) | 0.0257 (16) | -0.0085 (13) | 0.0098 (12) | -0.0039 (12) |
| C12 | 0.0182 (13) | 0.0228 (15) | 0.0231 (15) | -0.0110 (12) | 0.0071 (11) | -0.0096 (12) |
| C13 | 0.0141 (11) | 0.0225 (15) | 0.0162 (13) | -0.0030 (10) | 0.0064 (10) | -0.0058 (10) |
| C14 | 0.0112 (11) | 0.0293 (15) | 0.0177 (14) | -0.0033 (11) | 0.0005 (10) | -0.0069 (10) |
| C15 | 0.0138 (12) | 0.0278 (16) | 0.0181 (14) | 0.0033 (12)  | 0.0000 (10) | 0.0019 (11)  |
| C16 | 0.0162 (12) | 0.0153 (13) | 0.0207 (14) | -0.0018 (11) | 0.0032 (10) | -0.0002 (10) |
| C17 | 0.0111 (11) | 0.0143 (13) | 0.0172 (14) | -0.0019 (11) | 0.0028 (10) | -0.0028 (10) |
| C18 | 0.0113 (9)  | 0.0151 (11) | 0.0166 (11) | 0.0013 (17)  | 0.0052 (8)  | 0.0003 (15)  |
| O3  | 0.0224 (10) | 0.0222 (11) | 0.0283 (12) | -0.0065 (9)  | -0.0032 (9) | 0.0033 (9)   |
| O4  | 0.0209 (10) | 0.0281 (12) | 0.0268 (12) | -0.0043 (9)  | -0.0115 (8) | -0.0011 (9)  |
| O5  | 0.0294 (11) | 0.0195 (11) | 0.0293 (12) | -0.0131 (10) | 0.0006 (9)  | 0.0017 (9)   |
| O6  | 0.0213 (10) | 0.0160 (10) | 0.0235 (11) | 0.0028 (8)   | 0.0008 (8)  | 0.0058 (8)   |
| O7  | 0.0344 (9)  | 0.0225 (10) | 0.0200 (9)  | 0.0054 (15)  | -0.0118 (7) | -0.0024 (13) |
| O8  | 0.0317 (11) | 0.0166 (11) | 0.0195 (11) | -0.0060 (9)  | -0.0027 (8) | 0.0065 (8)   |
| O9  | 0.0211 (8)  | 0.0132 (14) | 0.0224 (9)  | -0.0063 (9)  | 0.0004 (7)  | 0.0004 (8)   |
| N3  | 0.0140 (10) | 0.0190 (12) | 0.0169 (12) | -0.0061 (10) | 0.0004 (9)  | -0.0041 (9)  |
| N4  | 0.0115 (10) | 0.0166 (12) | 0.0153 (11) | 0.0017 (9)   | -0.0004 (8) | 0.0023 (9)   |
| C19 | 0.0078 (11) | 0.0166 (13) | 0.0139 (14) | -0.0039 (10) | 0.0007 (10) | -0.0040 (11) |
| C20 | 0.0160 (12) | 0.0084 (12) | 0.0140 (13) | -0.0004 (10) | 0.0034 (9)  | 0.0006 (9)   |
| C21 | 0.0095 (9)  | 0.0131 (18) | 0.0109 (11) | 0.0044 (10)  | -0.0009 (8) | 0.0026 (9)   |
| C22 | 0.0084 (11) | 0.0151 (14) | 0.0147 (13) | -0.0009 (10) | 0.0011 (9)  | -0.0027 (10) |
| C23 | 0.0130 (11) | 0.0110 (13) | 0.0139 (12) | -0.0003 (11) | 0.0013 (9)  | -0.0003 (10) |
| C24 | 0.0122 (12) | 0.0145 (14) | 0.0142 (14) | 0.0023 (11)  | 0.0028 (10) | 0.0010 (11)  |
| C25 | 0.0151 (12) | 0.0110 (12) | 0.0182 (14) | 0.0005 (11)  | 0.0030 (10) | 0.0009 (10)  |

*Geometric parameters (Å, °)*

|         |           |          |           |
|---------|-----------|----------|-----------|
| Ag1—N2  | 2.183 (2) | C12—C13  | 1.415 (4) |
| Ag1—N1  | 2.190 (2) | C12—H12A | 0.9300    |
| Ag1—O2  | 2.549 (2) | C13—C18  | 1.415 (4) |
| Ag1—O1  | 2.561 (2) | C13—C14  | 1.417 (4) |
| O1—C8   | 1.352 (3) | C14—C15  | 1.361 (4) |
| O1—H1AA | 0.9999    | C14—H14A | 0.9300    |
| O2—C17  | 1.355 (3) | C15—C16  | 1.406 (4) |
| O2—H2AA | 0.7666    | C15—H15A | 0.9300    |
| N1—C1   | 1.341 (4) | C16—C17  | 1.367 (4) |
| N1—C9   | 1.366 (4) | C16—H16A | 0.9300    |
| N2—C10  | 1.325 (4) | C17—C18  | 1.430 (5) |
| N2—C18  | 1.368 (4) | O3—C22   | 1.330 (3) |
| C1—C2   | 1.395 (4) | O3—H3B   | 0.8193    |
| C1—H1A  | 0.9300    | O4—N3    | 1.229 (3) |
| C2—C3   | 1.361 (5) | O5—N3    | 1.220 (3) |
| C2—H2A  | 0.9300    | O6—N4    | 1.225 (3) |
| C3—C4   | 1.420 (4) | O7—N4    | 1.217 (3) |
| C3—H3A  | 0.9300    | O8—C25   | 1.241 (3) |
| C4—C5   | 1.419 (4) | O9—C25   | 1.274 (3) |
| C4—C9   | 1.422 (4) | N3—C19   | 1.457 (3) |
| C5—C6   | 1.364 (4) | N4—C21   | 1.472 (3) |
| C5—H5A  | 0.9300    | C19—C20  | 1.386 (4) |

## supplementary materials

---

|             |             |              |           |
|-------------|-------------|--------------|-----------|
| C6—C7       | 1.409 (4)   | C19—C24      | 1.387 (4) |
| C6—H6A      | 0.9300      | C20—C21      | 1.373 (4) |
| C7—C8       | 1.366 (4)   | C20—H20A     | 0.9300    |
| C7—H7A      | 0.9300      | C21—C22      | 1.409 (4) |
| C8—C9       | 1.432 (4)   | C22—C23      | 1.421 (4) |
| C10—C11     | 1.407 (4)   | C23—C24      | 1.393 (4) |
| C10—H10A    | 0.9300      | C23—C25      | 1.507 (4) |
| C11—C12     | 1.354 (4)   | C24—H24A     | 0.9300    |
| C11—H11A    | 0.9300      |              |           |
| N2—Ag1—N1   | 151.54 (9)  | C10—C11—H11A | 120.6     |
| N2—Ag1—O2   | 68.97 (8)   | C11—C12—C13  | 120.1 (3) |
| N1—Ag1—O2   | 138.45 (9)  | C11—C12—H12A | 119.9     |
| N2—Ag1—O1   | 138.63 (8)  | C13—C12—H12A | 119.9     |
| N1—Ag1—O1   | 69.23 (8)   | C18—C13—C12  | 117.5 (3) |
| O2—Ag1—O1   | 69.67 (6)   | C18—C13—C14  | 119.5 (3) |
| C8—O1—Ag1   | 111.74 (16) | C12—C13—C14  | 123.0 (3) |
| C8—O1—H1AA  | 113.3       | C15—C14—C13  | 120.3 (2) |
| Ag1—O1—H1AA | 134.7       | C15—C14—H14A | 119.8     |
| C17—O2—Ag1  | 112.59 (16) | C13—C14—H14A | 119.8     |
| C17—O2—H2AA | 117.9       | C14—C15—C16  | 120.8 (3) |
| Ag1—O2—H2AA | 129.2       | C14—C15—H15A | 119.6     |
| C1—N1—C9    | 118.3 (2)   | C16—C15—H15A | 119.6     |
| C1—N1—Ag1   | 119.1 (2)   | C17—C16—C15  | 120.5 (3) |
| C9—N1—Ag1   | 122.58 (19) | C17—C16—H16A | 119.7     |
| C10—N2—C18  | 118.3 (3)   | C15—C16—H16A | 119.7     |
| C10—N2—Ag1  | 118.73 (19) | O2—C17—C16   | 123.9 (3) |
| C18—N2—Ag1  | 123.0 (2)   | O2—C17—C18   | 115.9 (2) |
| N1—C1—C2    | 123.3 (3)   | C16—C17—C18  | 120.3 (2) |
| N1—C1—H1A   | 118.4       | N2—C18—C13   | 121.9 (3) |
| C2—C1—H1A   | 118.4       | N2—C18—C17   | 119.6 (2) |
| C3—C2—C1    | 119.4 (3)   | C13—C18—C17  | 118.6 (3) |
| C3—C2—H2A   | 120.3       | C22—O3—H3B   | 109.5     |
| C1—C2—H2A   | 120.3       | O5—N3—O4     | 124.3 (2) |
| C2—C3—C4    | 119.6 (3)   | O5—N3—C19    | 118.3 (2) |
| C2—C3—H3A   | 120.2       | O4—N3—C19    | 117.4 (2) |
| C4—C3—H3A   | 120.2       | O7—N4—O6     | 124.3 (2) |
| C5—C4—C3    | 122.8 (3)   | O7—N4—C21    | 119.0 (2) |
| C5—C4—C9    | 119.6 (3)   | O6—N4—C21    | 116.7 (2) |
| C3—C4—C9    | 117.7 (3)   | C20—C19—C24  | 122.2 (3) |
| C6—C5—C4    | 119.9 (3)   | C20—C19—N3   | 118.7 (3) |
| C6—C5—H5A   | 120.0       | C24—C19—N3   | 119.1 (3) |
| C4—C5—H5A   | 120.0       | C21—C20—C19  | 118.0 (2) |
| C5—C6—C7    | 121.2 (3)   | C21—C20—H20A | 121.0     |
| C5—C6—H6A   | 119.4       | C19—C20—H20A | 121.0     |
| C7—C6—H6A   | 119.4       | C20—C21—C22  | 122.6 (2) |
| C8—C7—C6    | 120.5 (3)   | C20—C21—N4   | 116.7 (2) |
| C8—C7—H7A   | 119.8       | C22—C21—N4   | 120.7 (2) |
| C6—C7—H7A   | 119.8       | O3—C22—C21   | 122.2 (2) |
| O1—C8—C7    | 123.1 (2)   | O3—C22—C23   | 120.1 (3) |



|              |           |              |           |
|--------------|-----------|--------------|-----------|
| O1—C8—C9     | 116.7 (2) | C21—C22—C23  | 117.7 (2) |
| C7—C8—C9     | 120.2 (2) | C24—C23—C22  | 119.9 (3) |
| N1—C9—C4     | 121.7 (2) | C24—C23—C25  | 119.5 (2) |
| N1—C9—C8     | 119.7 (2) | C22—C23—C25  | 120.5 (2) |
| C4—C9—C8     | 118.6 (2) | C19—C24—C23  | 119.4 (3) |
| N2—C10—C11   | 123.4 (3) | C19—C24—H24A | 120.3     |
| N2—C10—H10A  | 118.3     | C23—C24—H24A | 120.3     |
| C11—C10—H10A | 118.3     | O8—C25—O9    | 125.1 (3) |
| C12—C11—C10  | 118.9 (3) | O8—C25—C23   | 118.7 (2) |
| C12—C11—H11A | 120.6     | O9—C25—C23   | 116.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------|------------|--------------|--------------|----------------|
| O1—H1AA...O8   | 1.00       | 1.60         | 2.602 (3)    | 175            |
| O2—H2AA...O9   | 0.77       | 1.88         | 2.636 (3)    | 168            |
| O3—H3B...O9    | 0.82       | 1.74         | 2.483 (3)    | 150            |

Fig. 1

