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# Bis($\mu_2$-3,5-diisopropyl-4*H*-1,2,4-triazole-$\kappa^2N^1$:$N^2$)bis[(nitrato-$\kappa O$)silver(I)]

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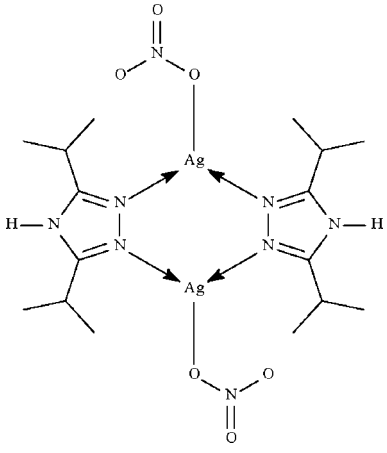
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.018 Å; disorder in main residue; $R$ factor = 0.078; $wR$ factor = 0.240; data-to-parameter ratio = 14.1.

The neutral *N*-heterocycle in the title centrosymmetric dinuclear compound, $[Ag_2(NO_3)_2(C_8H_{15}N_3)_2]$, bridges two metal atoms through its imino N atoms. The N—Ag—N skeleton is bent [N—Ag—N = 127.2 (3)°]; as one of two O atoms of the nitrate anion is nearly coplanar with this N—Ag—N skeleton [Ag—O = 2.63 (1) Å], the coordination geometry around the $Ag^I$ atom is regarded as trigonal-planar. One of the two isopropyl groups is disordered over two positions in respect of the methyl groups in a 1:1 ratio. In the crystal structure, intermolecular N—H···O hydrogen bonding is observed between the nitrate groups and triazole ligands.

## Related literature

For the background to such silver–triazole compounds, see: Yang *et al.* (2007).




## Experimental

### Crystal data

$[Ag_2(NO_3)_2(C_8H_{15}N_3)_2]$
$M_r$ = 646.22
Monoclinic, $P2_1/n$
$a$ = 5.791 (1) Å
$b$ = 14.541 (1) Å
$c$ = 14.578 (1) Å
$\beta$ = 99.523 (2)°
$V$ = 1210.6 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.66 mm$^{-1}$
$T$ = 293 K
0.41 × 0.17 × 0.13 mm

### Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.670, $T_{max}$ = 1.000
(expected range = 0.540–0.805)
5562 measured reflections
2124 independent reflections
1389 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.063

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.240
$S$ = 1.08
2124 reflections
151 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.96 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···O1$^{i}$ | 0.89 | 2.06 | 2.93 (1) | 167 |

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the Education Department of Zhengzhou University, China and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2560).

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# supporting information

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## Bis($\mu_2$-3,5-diisopropyl-4*H*-1,2,4-triazole-$\kappa^2N^1$:$N^2$)bis[(nitrato-$\kappa O$)silver(I)]

**Zhao-Yang Wang, Ying-Li Wang, Guang Yang and Seik Weng Ng**

### S1. Experimental

An acetonitrile solution (2 ml) of 3,5-diisopropyl-1*H*-1,2,4-triazole (0.1 mmol, 15 mg) was mixed with a acetoninitrile solution (1 ml) of silver nitrate (0.1 mmol, 17 mg). Ether was allowed to diffuse into the resulting solution. Colorless crystals were formed after a week in 50% yield. Calc. for $C_{16}H_{30}N_8Ag_2O_6$: C 29.7; H 4.6, N, 17.3%. Found: C 29.7, H 4.7, N, 17.6%.

### S2. Refinement

The H atoms were placed in calculated positions [C—H 0.96–0.98 Å; $U$(H) = 1.2–1.5$U_{eq}$(C)]. The amino H-atom was similarly treated [N–H 0.89 Å].

One of the two isopropyl groups is disordered over two positions in the methyl groups only; the disorder was assumed to be 1:1. The C–C distances were restrained to 1.54±0.01 Å, and the 1,3-related C···C distances to 2.51±0.01 Å. The temperature factors of the primed atoms were restrained to those of the unprimed ones; the anisotropic temperature factors were restrained to be nearly isotropic.

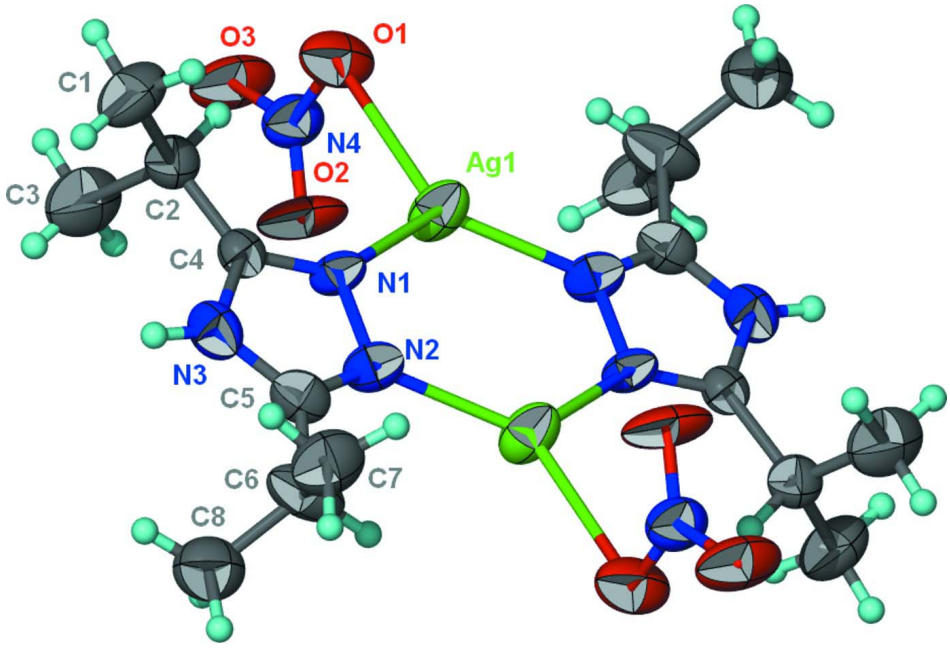


**Figure 1**

Thermal ellipsoid plot of $[Ag(C_8H_{15}N_3)(NO_3)]_2$; ellipsoids are drawn at the 50% probability level. The disorder is not shown.

**Bis($\mu_2$-3,5-diisopropyl-4*H*-1,2,4-triazole-$\kappa^2N^1$:$N^2$)bis[(nitrato-$\kappa O$)silver(I)]**

*Crystal data*

$[Ag_2(NO_3)_2(C_8H_{15}N_3)_2]$
$M_r$ = 646.22
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 5.791 (1) Å
$b$ = 14.541 (1) Å
$c$ = 14.578 (1) Å
$\beta$ = 99.523 (2)°
$V$ = 1210.6 (2) Å$^3$
$Z$ = 2
$F(000)$ = 648
$D_x$ = 1.773 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1859 reflections
$\theta$ = 2.8–21.8°
$\mu$ = 1.66 mm$^{-1}$
$T$ = 293 K
Prism, colorless
0.41 × 0.17 × 0.13 mm

*Data collection*

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.670, $T_{max}$ = 1.000
5562 measured reflections
2124 independent reflections
1389 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.063
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.0°
$h$ = −6→6
$k$ = −9→17
$l$ = −17→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.240
$S$ = 1.08
2124 reflections
151 parameters
18 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1131P)^2 + 8.3674P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.91 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.96 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Ag1 | 0.6205 (2) | 0.57863 (7) | 0.43648 (7) | 0.0682 (5) | |
| O1 | 0.8666 (17) | 0.6779 (7) | 0.3367 (8) | 0.080 (3) | |
| O2 | 1.0702 (19) | 0.5875 (8) | 0.4336 (8) | 0.094 (4) | |
| O3 | 1.2426 (18) | 0.6792 (9) | 0.3497 (8) | 0.096 (4) | |
| N1 | 0.5362 (17) | 0.4427 (6) | 0.3705 (6) | 0.047 (2) | |
| N2 | 0.4403 (17) | 0.3760 (7) | 0.4232 (7) | 0.054 (3) | |
| N3 | 0.5156 (19) | 0.3113 (7) | 0.2993 (8) | 0.061 (3) | |
| H3 | 0.5270 | 0.2681 | 0.2570 | 0.074* | |
| N4 | 1.061 (2) | 0.6493 (8) | 0.3760 (8) | 0.067 (3) | |
| C1 | 0.547 (3) | 0.4325 (13) | 0.1257 (10) | 0.087 (5) | |
| H1A | 0.3891 | 0.4523 | 0.1263 | 0.130* | |
| H1B | 0.5473 | 0.3686 | 0.1093 | 0.130* | |
| H1C | 0.6133 | 0.4680 | 0.0809 | 0.130* | |

| | | | | | |
|---|---|---|---|---|---|
| C2 | 0.692 (2) | 0.4463 (9) | 0.2217 (9) | 0.058 (3) | |
| H2 | 0.6933 | 0.5126 | 0.2339 | 0.070* | |
| C3 | 0.946 (3) | 0.4169 (15) | 0.2284 (14) | 0.104 (6) | |
| H3A | 1.0273 | 0.4274 | 0.2904 | 0.155* | |
| H3B | 1.0189 | 0.4520 | 0.1852 | 0.155* | |
| H3C | 0.9529 | 0.3527 | 0.2137 | 0.155* | |
| C4 | 0.5824 (19) | 0.4017 (7) | 0.2966 (8) | 0.044 (3) | |
| C5 | 0.429 (2) | 0.3010 (8) | 0.3788 (9) | 0.055 (3) | |
| C6 | 0.342 (2) | 0.2139 (8) | 0.4109 (12) | 0.085 (5) | |
| H6 | 0.3262 | 0.2233 | 0.4761 | 0.102* | 0.50 |
| H6′ | 0.3460 | 0.1810 | 0.3525 | 0.102* | 0.50 |
| C7 | 0.097 (3) | 0.192 (2) | 0.359 (2) | 0.087 (8) | 0.50 |
| H7A | 0.0448 | 0.1347 | 0.3805 | 0.131* | 0.50 |
| H7B | 0.1006 | 0.1882 | 0.2934 | 0.131* | 0.50 |
| H7C | −0.0092 | 0.2401 | 0.3700 | 0.131* | 0.50 |
| C8 | 0.503 (4) | 0.1308 (18) | 0.409 (3) | 0.089 (7) | 0.50 |
| H8A | 0.4306 | 0.0774 | 0.4308 | 0.134* | 0.50 |
| H8B | 0.6496 | 0.1423 | 0.4490 | 0.134* | 0.50 |
| H8C | 0.5300 | 0.1205 | 0.3468 | 0.134* | 0.50 |
| C7′ | 0.083 (2) | 0.203 (2) | 0.408 (2) | 0.087 (8) | 0.50 |
| H7′1 | 0.0510 | 0.1425 | 0.4297 | 0.131* | 0.50 |
| H7′2 | 0.0038 | 0.2097 | 0.3446 | 0.131* | 0.50 |
| H7′3 | 0.0273 | 0.2484 | 0.4461 | 0.131* | 0.50 |
| C8′ | 0.490 (4) | 0.144 (2) | 0.471 (2) | 0.089 (7) | 0.50 |
| H8′1 | 0.3938 | 0.0928 | 0.4820 | 0.134* | 0.50 |
| H8′2 | 0.5548 | 0.1720 | 0.5292 | 0.134* | 0.50 |
| H8′3 | 0.6138 | 0.1236 | 0.4399 | 0.134* | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.0868 (9) | 0.0610 (7) | 0.0623 (7) | −0.0294 (6) | 0.0285 (5) | −0.0052 (5) |
| O1 | 0.051 (6) | 0.080 (7) | 0.107 (8) | 0.001 (5) | 0.007 (5) | 0.031 (6) |
| O2 | 0.078 (7) | 0.108 (9) | 0.091 (7) | −0.021 (6) | 0.003 (6) | 0.066 (7) |
| O3 | 0.064 (6) | 0.119 (9) | 0.104 (8) | −0.015 (6) | 0.016 (6) | 0.057 (7) |
| N1 | 0.063 (6) | 0.039 (5) | 0.039 (5) | −0.016 (4) | 0.009 (4) | 0.003 (4) |
| N2 | 0.054 (6) | 0.052 (6) | 0.055 (6) | −0.018 (5) | 0.009 (5) | 0.007 (5) |
| N3 | 0.066 (7) | 0.050 (6) | 0.067 (7) | 0.004 (5) | 0.008 (6) | −0.009 (5) |
| N4 | 0.056 (7) | 0.075 (8) | 0.070 (7) | −0.001 (6) | 0.016 (6) | 0.018 (6) |
| C1 | 0.083 (10) | 0.123 (14) | 0.055 (8) | −0.004 (10) | 0.013 (7) | 0.012 (9) |
| C2 | 0.059 (8) | 0.059 (8) | 0.055 (7) | 0.004 (6) | 0.008 (6) | 0.001 (6) |
| C3 | 0.056 (9) | 0.146 (18) | 0.112 (14) | 0.007 (10) | 0.027 (9) | 0.040 (13) |
| C4 | 0.038 (6) | 0.044 (6) | 0.048 (6) | 0.002 (4) | 0.004 (5) | −0.001 (5) |
| C5 | 0.050 (7) | 0.043 (7) | 0.071 (8) | −0.010 (5) | 0.005 (6) | 0.001 (6) |
| C6 | 0.077 (10) | 0.044 (7) | 0.131 (14) | −0.003 (7) | 0.011 (9) | 0.021 (9) |
| C7 | 0.080 (9) | 0.093 (10) | 0.090 (12) | −0.017 (8) | 0.020 (8) | 0.011 (9) |
| C8 | 0.083 (10) | 0.087 (10) | 0.098 (12) | 0.002 (8) | 0.016 (9) | 0.014 (9) |
| C7′ | 0.080 (9) | 0.093 (10) | 0.090 (12) | −0.017 (8) | 0.020 (8) | 0.011 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8′ | 0.083 (10) | 0.087 (10) | 0.098 (12) | 0.002 (8) | 0.016 (9) | 0.014 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ag1—N1 | 2.218 (9) | C3—H3B | 0.9600 |
| Ag1—N2$^{i}$ | 2.232 (10) | C3—H3C | 0.9600 |
| Ag1—O2 | 2.615 (11) | C5—C6 | 1.469 (16) |
| Ag1—O1 | 2.630 (10) | C6—C7′ | 1.505 (10) |
| O1—N4 | 1.245 (14) | C6—C8′ | 1.508 (10) |
| O2—N4 | 1.224 (14) | C6—C7 | 1.529 (10) |
| O3—N4 | 1.258 (14) | C6—C8 | 1.529 (10) |
| N1—C4 | 1.297 (14) | C6—H6 | 0.9800 |
| N1—N2 | 1.407 (12) | C6—H6′ | 0.9800 |
| N2—C5 | 1.264 (15) | C7—H7A | 0.9600 |
| N2—Ag1$^{i}$ | 2.232 (10) | C7—H7B | 0.9600 |
| N3—C5 | 1.342 (17) | C7—H7C | 0.9600 |
| N3—C4 | 1.373 (15) | C8—H8A | 0.9600 |
| N3—H3 | 0.8900 | C8—H8B | 0.9600 |
| C1—C2 | 1.520 (19) | C8—H8C | 0.9600 |
| C1—H1A | 0.9600 | C7′—H7′1 | 0.9600 |
| C1—H1B | 0.9600 | C7′—H7′2 | 0.9600 |
| C1—H1C | 0.9600 | C7′—H7′3 | 0.9600 |
| C2—C4 | 1.498 (18) | C8′—H8′1 | 0.9600 |
| C2—C3 | 1.52 (2) | C8′—H8′2 | 0.9600 |
| C2—H2 | 0.9800 | C8′—H8′3 | 0.9600 |
| C3—H3A | 0.9600 | | |

| | | | |
|---|---|---|---|
| N1—Ag1—N2$^{i}$ | 127.2 (3) | N1—C4—C2 | 125.2 (10) |
| N1—Ag1—O2 | 100.7 (4) | N3—C4—C2 | 126.2 (11) |
| N2$^{i}$—Ag1—O2 | 108.0 (4) | N2—C5—N3 | 110.6 (11) |
| N1—Ag1—O1 | 110.5 (4) | N2—C5—C6 | 124.8 (13) |
| N2$^{i}$—Ag1—O1 | 121.8 (4) | N3—C5—C6 | 124.6 (13) |
| O2—Ag1—O1 | 48.0 (3) | C5—C6—C7′ | 118.6 (15) |
| N4—O1—Ag1 | 95.3 (7) | C5—C6—C8′ | 124.9 (15) |
| N4—O2—Ag1 | 96.6 (8) | C7′—C6—C8′ | 114.3 (10) |
| C4—N1—N2 | 106.9 (9) | C5—C6—C7 | 111.1 (17) |
| C4—N1—Ag1 | 135.2 (7) | C5—C6—C8 | 115.7 (17) |
| N2—N1—Ag1 | 117.1 (7) | C7′—C6—C8 | 121 (2) |
| C5—N2—N1 | 107.8 (10) | C7—C6—C8 | 110.4 (10) |
| C5—N2—Ag1$^{i}$ | 136.3 (9) | C5—C6—H6 | 106.3 |
| N1—N2—Ag1$^{i}$ | 115.6 (7) | C7—C6—H6 | 106.3 |
| C5—N3—C4 | 106.1 (10) | C8—C6—H6 | 106.3 |
| C5—N3—H3 | 126.9 | C6—C7—H7A | 109.5 |
| C4—N3—H3 | 126.9 | C6—C7—H7B | 109.5 |
| O2—N4—O1 | 119.8 (11) | H7A—C7—H7B | 109.5 |
| O2—N4—O3 | 121.1 (12) | C6—C7—H7C | 109.5 |
| O1—N4—O3 | 118.8 (11) | H7A—C7—H7C | 109.5 |
| C2—C1—H1A | 109.5 | H7B—C7—H7C | 109.5 |

| | | | |
|---|---|---|---|
| C2—C1—H1B | 109.5 | C6—C8—H8A | 109.5 |
| H1A—C1—H1B | 109.5 | C6—C8—H8B | 109.5 |
| C2—C1—H1C | 109.5 | H8A—C8—H8B | 109.5 |
| H1A—C1—H1C | 109.5 | C6—C8—H8C | 109.5 |
| H1B—C1—H1C | 109.5 | H8A—C8—H8C | 109.5 |
| C4—C2—C1 | 112.3 (11) | H8B—C8—H8C | 109.5 |
| C4—C2—C3 | 110.7 (11) | C6—C7′—H7′1 | 109.5 |
| C1—C2—C3 | 113.7 (13) | C6—C7′—H7′2 | 109.5 |
| C4—C2—H2 | 106.6 | H7′1—C7′—H7′2 | 109.5 |
| C1—C2—H2 | 106.6 | C6—C7′—H7′3 | 109.5 |
| C3—C2—H2 | 106.6 | H7′1—C7′—H7′3 | 109.5 |
| C2—C3—H3A | 109.5 | H7′2—C7′—H7′3 | 109.5 |
| C2—C3—H3B | 109.5 | C6—C8′—H8′1 | 109.5 |
| H3A—C3—H3B | 109.5 | C6—C8′—H8′2 | 109.5 |
| C2—C3—H3C | 109.5 | H8′1—C8′—H8′2 | 109.5 |
| H3A—C3—H3C | 109.5 | C6—C8′—H8′3 | 109.5 |
| H3B—C3—H3C | 109.5 | H8′1—C8′—H8′3 | 109.5 |
| N1—C4—N3 | 108.5 (10) | H8′2—C8′—H8′3 | 109.5 |

| | | | |
|---|---|---|---|
| N1—Ag1—O1—N4 | −89.2 (9) | N2—N1—C4—C2 | −178.6 (10) |
| N2$^{i}$—Ag1—O1—N4 | 82.9 (9) | Ag1—N1—C4—C2 | −9.6 (18) |
| O2—Ag1—O1—N4 | −3.1 (8) | C5—N3—C4—N1 | −0.4 (13) |
| N1—Ag1—O2—N4 | 111.2 (9) | C5—N3—C4—C2 | 179.2 (11) |
| N2$^{i}$—Ag1—O2—N4 | −113.7 (9) | C1—C2—C4—N1 | −126.3 (14) |
| O1—Ag1—O2—N4 | 3.2 (8) | C3—C2—C4—N1 | 105.4 (15) |
| N2$^{i}$—Ag1—N1—C4 | −170.4 (10) | C1—C2—C4—N3 | 54.0 (16) |
| O2—Ag1—N1—C4 | −47.8 (11) | C3—C2—C4—N3 | −74.2 (17) |
| O1—Ag1—N1—C4 | 1.2 (12) | N1—N2—C5—N3 | 1.1 (14) |
| N2$^{i}$—Ag1—N1—N2 | −2.1 (11) | Ag1$^{i}$—N2—C5—N3 | −171.8 (9) |
| O2—Ag1—N1—N2 | 120.4 (8) | N1—N2—C5—C6 | 179.2 (11) |
| O1—Ag1—N1—N2 | 169.4 (7) | Ag1$^{i}$—N2—C5—C6 | 6 (2) |
| C4—N1—N2—C5 | −1.3 (13) | C4—N3—C5—N2 | −0.4 (14) |
| Ag1—N1—N2—C5 | −172.7 (8) | C4—N3—C5—C6 | −178.5 (11) |
| C4—N1—N2—Ag1$^{i}$ | 173.2 (7) | N2—C5—C6—C7′ | 74 (3) |
| Ag1—N1—N2—Ag1$^{i}$ | 1.9 (10) | N3—C5—C6—C7′ | −108 (2) |
| Ag1—O2—N4—O1 | −5.8 (14) | N2—C5—C6—C8′ | −88 (3) |
| Ag1—O2—N4—O3 | −179.6 (12) | N3—C5—C6—C8′ | 90 (3) |
| Ag1—O1—N4—O2 | 5.8 (14) | N2—C5—C6—C7 | 104 (2) |
| Ag1—O1—N4—O3 | 179.7 (12) | N3—C5—C6—C7 | −78 (2) |
| N2—N1—C4—N3 | 1.0 (12) | N2—C5—C6—C8 | −128.8 (19) |
| Ag1—N1—C4—N3 | 170.1 (8) | N3—C5—C6—C8 | 49 (2) |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| N3—H3···O1$^{ii}$ | 0.89 | 2.06 | 2.93 (1) | 167 |

Symmetry code: (ii) $-x+3/2, y-1/2, -z+1/2$.