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Bis(μ_2-3,5-diisopropyl-4*H*-1,2,4-triazole-κ^2N^1:N^2)bis[(nitrato-κO)silver(I)]

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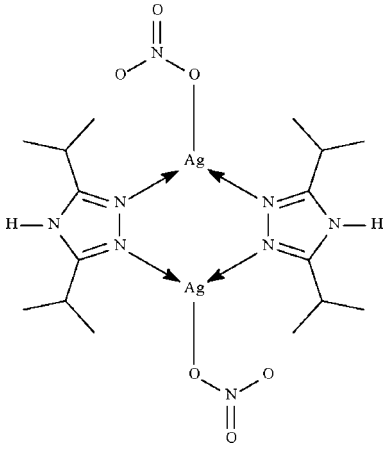
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.018 Å; disorder in main residue; R factor = 0.078; wR factor = 0.240; data-to-parameter ratio = 14.1.

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
β = 99.523 (2)°
V = 1210.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 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).

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

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Westrip, S. P. (2009). *publCIF*. In preparation.
Yang, G., Wang, Y.-L., Li, J.-P., Zhu, Y., Wang, S.-M., Hou, H.-W., Fan, Y.-T. & Ng, S. W. (2007). *Eur. J. Inorg. Chem.* pp. 714–719.

supplementary materials

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Bis(μ$_2$-3,5-diisopropyl-4*H*-1,2,4-triazole-κ^2N^1:N^2)bis[(nitrato-κO)silver(I)]

Z.-Y. Wang, Y.-L. Wang, G. Yang and S. W. Ng

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%.

Refinement

The H atoms were placed in calculated positions [C—H 0.96–0.98 Å; U(H) = 1.2–1.5U_{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.

Figures

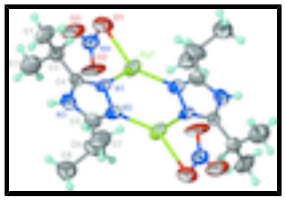

Fig. 1. Thermal ellipsoid plot of $[Ag(C_8H_{15}N_3)(NO_3)]_2$; ellipsoids are drawn at the 50% probability level. The disorder is not shown.

Bis(μ$_2$-3,5-diisopropyl-4*H*-1,2,4-triazole- κ^2N^1:N^2)bis[(nitrato-κ*O*)silver(I)]

Crystal data

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

$Z = 2$

Data collection

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

Refinement

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

	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, °)

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 codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

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 codes: (ii) −*x*+3/2, *y*−1/2, −*z*+1/2.

Fig. 1