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(2-Amino-3,5-dimethylbenzenesulfonato-κN)bis(3-methylisoquinoline-κN)silver(I)

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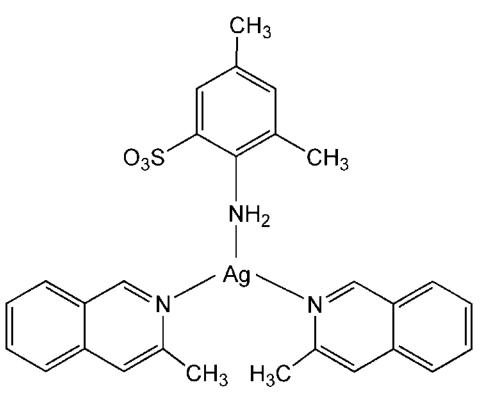
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.006 Å; R factor = 0.036; wR factor = 0.116; data-to-parameter ratio = 16.2.

The title compound, $[Ag(C_8H_{10}NO_3S)(C_{10}H_9N)_2]$, has a mononuclear structure in which the Ag^+ cation is three-coordinated by two N atoms from two different 3-methylisoquinoline molecules and one N atom from a 2-amino-3,5-dimethylbenzenesulfonate anion in a highly distorted trigonal–planar AgN_3 arrangement.

Related literature

For the structure of the related compound, Ag(L)(bipy), where L = 2-amino-3,5-dimethylbenzenesulfonate and bipy = 2,2′-bipyridine, see Liu *et al.* (2006).



Experimental

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{10}H_9N)_2]$
M_r = 594.47
Monoclinic, $P2_1/n$
a = 11.910 (2) Å
b = 11.199 (2) Å
c = 19.507 (4) Å
β = 92.05 (3)°
V = 2600.4 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 292 (2) K
0.24 × 0.23 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) T_{min} = 0.884, T_{max} = 0.908
20026 measured reflections
5336 independent reflections
2764 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.116
S = 0.91
5336 reflections
329 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.248 (3)	Ag1—N3	2.308 (3)
Ag1—N2	2.290 (3)		
N1—Ag1—N2	122.95 (12)	N2—Ag1—N3	114.36 (11)
N1—Ag1—N3	121.97 (12)		

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2426).

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supplementary materials

Acta Cryst. (2007). E**63**, m1806 [**doi:10.1107/S1600536807025275**]

(2-Amino-3,5-dimethylbenzenesulfonato-*κN*)bis(3-methylisoquinoline-*κN*)silver(I)

Y.-J. Li, S.-P. Shangguan and X.-W. Dong

Comment

In this paper, the structure of the title compound, (I) (Fig. 1), containing two 3-methylisoquinoline molecules and 2-amino-3,5-dimethylbenzenesulfonate (*L*) anion is described.

In (I), two 3-methylisoquinoline molecules and one *L* anion are coordinated to the metal, resulting in a highly distorted trigonal planar coordination geometry for Ag (Table 1). Atoms Ag1, N1, N2 and N3 are almost coplanar and the bond-angle sum about Ag is 359.36°. The Ag—N_L distances are longer than the Ag—$N_{3\text{-methylisoquinoline}}$ distance. The distances are similar to the equivalent values in related compounds (Liu *et al.*, 2006). In (I), the coordination ability of the amine group of *L* is evidently stronger than that of sulfonate group and the latter group does not coordinate to the Ag ion. The dihedral angle between the two quinoline rings of the different two coordinated 3-methylisoquinoline molecules is 96.3°.

Experimental

An aqueous solution (10 ml) of 2-amino-3,5-dimethylbenzenesulfonic acid (0.101 g, 0.5 mmol) was added to solid Ag_2CO_3 (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO_2 was given off; 3-methylisoquinoline (0.0715 g, 0.5 mmol) in methanol (5 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH_3 (14 *M*). Colourless prisms of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H)= 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

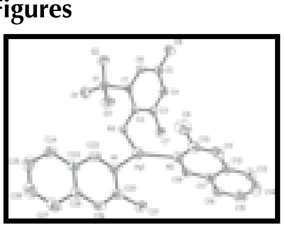


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids. All H atoms are omitted for clarty.

(2-Amino-3,5-dimethylbenzenesulfonato-κ*N*)bis(3-methylisoquinoline- κ*N*)silver(I)

Crystal data

$[Ag(C_8H_{10}NO_3S)(C_{10}H_9N)_2]$	F_{000} = 1216

$M_r = 594.47$	$D_x = 1.518$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9129 reflections
$a = 11.910$ (2) Å	$\theta = 2.0–27.5°$
$b = 11.199$ (2) Å	$\mu = 0.89$ mm^{-1}
$c = 19.507$ (4) Å	$T = 292$ (2) K
$\beta = 92.05$ (3)°	Prism, colorless
$V = 2600.4$ (9) Å^3	0.24 × 0.23 × 0.11 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID CCD diffractometer	5336 independent reflections
Radiation source: fine-focus sealed tube	2764 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5°$
$T = 292(2)$ K	$\theta_{min} = 2.0°$
ω scans	$h = -15\rightarrow15$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13\rightarrow14$
$T_{min} = 0.884$, $T_{max} = 0.908$	$l = -25\rightarrow25$
20026 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.91$	$(\Delta/\sigma)_{max} < 0.001$
5336 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
329 parameters	$\Delta\rho_{min} = -0.82$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.42331 (3)	0.17081 (3)	0.26819 (2)	0.07452 (17)
C1	0.3582 (3)	0.5198 (3)	0.24067 (18)	0.0391 (8)
C2	0.3483 (3)	0.4187 (3)	0.1985 (2)	0.0414 (9)
C3	0.3905 (3)	0.4228 (3)	0.1326 (2)	0.0461 (9)
C4	0.4351 (3)	0.5290 (3)	0.1093 (2)	0.0520 (10)
H4	0.4612	0.5320	0.0650	0.062*
C5	0.4422 (3)	0.6309 (3)	0.1495 (2)	0.0511 (10)
C6	0.4057 (3)	0.6233 (3)	0.2151 (2)	0.0470 (9)
H6	0.4129	0.6896	0.2436	0.056*
C7	0.3857 (4)	0.3133 (3)	0.0872 (2)	0.0614 (11)
H7A	0.4235	0.2482	0.1102	0.092*
H7B	0.4220	0.3301	0.0451	0.092*
H7C	0.3088	0.2920	0.0773	0.092*
C8	0.4894 (4)	0.7462 (4)	0.1215 (3)	0.0763 (14)
H8A	0.4412	0.7748	0.0846	0.114*
H8B	0.5631	0.7318	0.1049	0.114*
H8C	0.4939	0.8050	0.1574	0.114*
C9	0.6794 (5)	0.2767 (5)	0.2884 (3)	0.1042 (19)
H9A	0.6424	0.2412	0.3263	0.156*
H9B	0.6383	0.3460	0.2730	0.156*
H9C	0.7543	0.2997	0.3027	0.156*
C10	0.6844 (4)	0.1878 (4)	0.2307 (2)	0.0629 (12)
C11	0.7789 (4)	0.1545 (4)	0.2013 (3)	0.0698 (13)
H11	0.8474	0.1808	0.2200	0.084*
C12	0.7782 (4)	0.0813 (4)	0.1434 (3)	0.0643 (12)
C13	0.8747 (4)	0.0459 (5)	0.1080 (4)	0.0984 (19)
H13	0.9457	0.0695	0.1241	0.118*
C14	0.8638 (6)	−0.0210 (6)	0.0518 (4)	0.126 (3)
H14	0.9285	−0.0447	0.0302	0.151*
C15	0.7613 (7)	−0.0569 (5)	0.0239 (3)	0.109 (2)
H15	0.7574	−0.1014	−0.0163	0.130*
C16	0.6657 (4)	−0.0263 (4)	0.0560 (3)	0.0763 (14)
H16	0.5960	−0.0502	0.0380	0.092*
C17	0.6731 (3)	0.0414 (3)	0.1164 (2)	0.0523 (10)
C18	0.5794 (3)	0.0753 (3)	0.1530 (2)	0.0537 (10)
H18	0.5098	0.0459	0.1379	0.064*
C20	0.4270 (3)	−0.0291 (3)	0.3849 (2)	0.0481 (9)
C21	0.4904 (4)	−0.0917 (4)	0.3305 (2)	0.0635 (12)
H21A	0.4494	−0.0855	0.2874	0.095*
H21B	0.4995	−0.1743	0.3425	0.095*
H21C	0.5629	−0.0553	0.3267	0.095*
C22	0.3471 (4)	0.1490 (3)	0.4187 (2)	0.0559 (11)

H22	0.3320	0.2292	0.4103	0.067*
C23	0.3106 (3)	0.0997 (3)	0.4802 (2)	0.0498 (10)
C24	0.2469 (4)	0.1652 (4)	0.5271 (2)	0.0677 (12)
H24	0.2317	0.2456	0.5191	0.081*
C25	0.2085 (4)	0.1114 (5)	0.5832 (3)	0.0791 (14)
H25	0.1654	0.1543	0.6135	0.095*
C26	0.2328 (4)	−0.0089 (5)	0.5963 (2)	0.0806 (15)
H26	0.2062	−0.0445	0.6356	0.097*
C27	0.2939 (4)	−0.0739 (4)	0.5532 (2)	0.0705 (13)
H27	0.3092	−0.1536	0.5631	0.085*
C28	0.3351 (3)	−0.0214 (3)	0.4927 (2)	0.0515 (10)
C19	0.3956 (3)	−0.0829 (3)	0.4434 (2)	0.0550 (11)
H29	0.4145	−0.1625	0.4510	0.066*
N1	0.4015 (3)	0.0891 (3)	0.37210 (18)	0.0530 (8)
N2	0.5818 (3)	0.1448 (3)	0.20680 (19)	0.0561 (9)
N3	0.3002 (3)	0.3120 (2)	0.22318 (17)	0.0499 (8)
H3A	0.2599	0.2781	0.1885	0.060*
H3B	0.2519	0.3316	0.2558	0.060*
O2	0.3372 (2)	0.6325 (2)	0.35541 (14)	0.0552 (7)
O1	0.1868 (2)	0.5006 (3)	0.31586 (15)	0.0659 (8)
O3	0.3625 (3)	0.4186 (2)	0.35988 (15)	0.0671 (8)
S1	0.30740 (8)	0.51752 (8)	0.32519 (5)	0.0474 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0839 (3)	0.0711 (3)	0.0698 (3)	0.01131 (19)	0.01920 (19)	0.02028 (19)
C1	0.039 (2)	0.0351 (19)	0.043 (2)	0.0060 (17)	0.0023 (16)	0.0016 (16)
C2	0.0348 (19)	0.037 (2)	0.052 (3)	0.0032 (17)	0.0011 (17)	0.0043 (17)
C3	0.045 (2)	0.046 (2)	0.047 (2)	0.0069 (18)	−0.0003 (18)	−0.0002 (18)
C4	0.054 (2)	0.053 (2)	0.050 (3)	0.005 (2)	0.0113 (19)	0.0100 (19)
C5	0.055 (2)	0.041 (2)	0.058 (3)	0.0003 (19)	0.011 (2)	0.0087 (18)
C6	0.048 (2)	0.0374 (19)	0.056 (3)	−0.0028 (18)	0.0034 (19)	−0.0006 (17)
C7	0.079 (3)	0.052 (2)	0.053 (3)	0.007 (2)	0.007 (2)	−0.005 (2)
C8	0.091 (3)	0.055 (3)	0.085 (4)	−0.013 (3)	0.027 (3)	0.015 (2)
C9	0.146 (5)	0.103 (4)	0.063 (4)	−0.022 (4)	−0.003 (4)	−0.013 (3)
C10	0.078 (3)	0.066 (3)	0.045 (3)	−0.010 (2)	−0.004 (2)	0.013 (2)
C11	0.058 (3)	0.079 (3)	0.071 (4)	−0.016 (2)	−0.013 (3)	0.016 (3)
C12	0.053 (3)	0.063 (3)	0.078 (4)	−0.002 (2)	0.014 (2)	0.022 (2)
C13	0.068 (4)	0.089 (4)	0.140 (6)	−0.005 (3)	0.036 (4)	0.020 (4)
C14	0.119 (6)	0.099 (5)	0.167 (8)	−0.009 (4)	0.098 (6)	−0.004 (5)
C15	0.153 (6)	0.077 (4)	0.100 (5)	−0.026 (4)	0.068 (5)	−0.014 (3)
C16	0.097 (4)	0.062 (3)	0.072 (4)	−0.018 (3)	0.019 (3)	0.003 (2)
C17	0.056 (3)	0.047 (2)	0.054 (3)	−0.006 (2)	0.008 (2)	0.0132 (19)
C18	0.050 (2)	0.050 (2)	0.061 (3)	−0.007 (2)	0.001 (2)	0.014 (2)
C20	0.049 (2)	0.042 (2)	0.052 (3)	−0.0017 (18)	−0.0103 (19)	−0.0013 (18)
C21	0.069 (3)	0.057 (3)	0.065 (3)	0.004 (2)	0.004 (2)	−0.010 (2)
C22	0.068 (3)	0.037 (2)	0.062 (3)	0.003 (2)	0.002 (2)	−0.0028 (19)

C23	0.058 (2)	0.044 (2)	0.048 (3)	−0.0058 (19)	−0.004 (2)	−0.0032 (18)
C24	0.082 (3)	0.060 (3)	0.061 (3)	−0.002 (2)	0.002 (3)	−0.016 (2)
C25	0.082 (3)	0.097 (4)	0.058 (3)	−0.011 (3)	0.010 (3)	−0.026 (3)
C26	0.095 (4)	0.099 (4)	0.048 (3)	−0.031 (3)	0.012 (3)	−0.007 (3)
C27	0.088 (3)	0.066 (3)	0.056 (3)	−0.019 (3)	−0.003 (3)	0.012 (2)
C28	0.056 (2)	0.050 (2)	0.048 (3)	−0.011 (2)	−0.009 (2)	0.0019 (19)
C19	0.065 (3)	0.038 (2)	0.061 (3)	−0.001 (2)	−0.009 (2)	0.0051 (19)
N1	0.059 (2)	0.0428 (19)	0.057 (2)	−0.0004 (16)	0.0009 (17)	0.0055 (16)
N2	0.061 (2)	0.055 (2)	0.052 (2)	−0.0063 (17)	0.0078 (18)	0.0112 (17)
N3	0.0541 (19)	0.0354 (17)	0.061 (2)	−0.0047 (15)	0.0097 (16)	−0.0041 (14)
O2	0.0776 (18)	0.0400 (13)	0.0480 (17)	0.0021 (13)	0.0024 (14)	−0.0054 (12)
O1	0.0560 (18)	0.0773 (19)	0.065 (2)	−0.0087 (15)	0.0135 (14)	−0.0032 (16)
O3	0.101 (2)	0.0428 (15)	0.0568 (19)	0.0097 (15)	−0.0058 (17)	0.0105 (13)
S1	0.0577 (6)	0.0395 (5)	0.0451 (6)	0.0009 (5)	0.0034 (5)	0.0025 (4)

Geometric parameters (Å, °)

Ag1—N1	2.248 (3)	C14—H14	0.9300
Ag1—N2	2.290 (3)	C15—C16	1.363 (7)
Ag1—N3	2.308 (3)	C15—H15	0.9300
C1—C6	1.390 (5)	C16—C17	1.401 (6)
C1—C2	1.402 (5)	C16—H16	0.9300
C1—S1	1.777 (4)	C17—C18	1.398 (5)
C2—C3	1.397 (5)	C18—N2	1.306 (5)
C2—N3	1.417 (4)	C18—H18	0.9300
C3—C4	1.386 (5)	C20—C19	1.354 (5)
C3—C7	1.513 (5)	C20—N1	1.378 (5)
C4—C5	1.385 (5)	C20—C21	1.500 (5)
C4—H4	0.9300	C21—H21A	0.9600
C5—C6	1.369 (5)	C21—H21B	0.9600
C5—C8	1.518 (5)	C21—H21C	0.9600
C6—H6	0.9300	C22—N1	1.318 (5)
C7—H7A	0.9600	C22—C23	1.404 (5)
C7—H7B	0.9600	C22—H22	0.9300
C7—H7C	0.9600	C23—C28	1.406 (5)
C8—H8A	0.9600	C23—C24	1.414 (6)
C8—H8B	0.9600	C24—C25	1.344 (6)
C8—H8C	0.9600	C24—H24	0.9300
C9—C10	1.505 (6)	C25—C26	1.399 (7)
C9—H9A	0.9600	C25—H25	0.9300
C9—H9B	0.9600	C26—C27	1.346 (6)
C9—H9C	0.9600	C26—H26	0.9300
C10—C11	1.336 (6)	C27—C28	1.422 (6)
C10—N2	1.379 (5)	C27—H27	0.9300
C11—C12	1.396 (7)	C28—C19	1.403 (6)
C11—H11	0.9300	C19—H29	0.9300
C12—C17	1.413 (6)	N3—H3A	0.9000
C12—C13	1.418 (7)	N3—H3B	0.9000
C13—C14	1.331 (9)	O2—S1	1.455 (3)

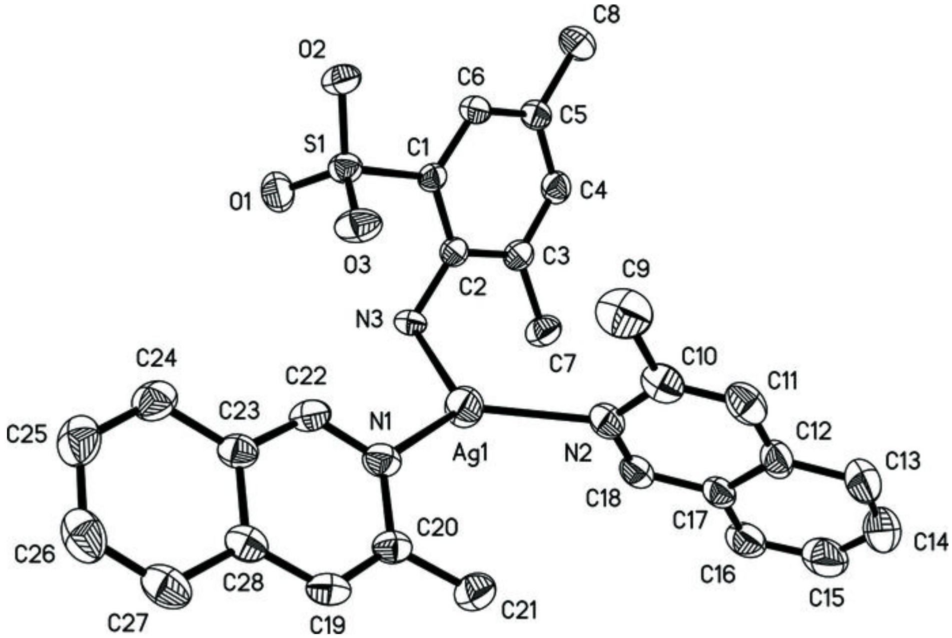
C13—H13	0.9300	O1—S1	1.454 (3)
C14—C15	1.378 (9)	O3—S1	1.443 (3)
N1—Ag1—N2	122.95 (12)	C17—C16—H16	120.2
N1—Ag1—N3	121.97 (12)	C18—C17—C16	123.3 (4)
N2—Ag1—N3	114.36 (11)	C18—C17—C12	115.9 (4)
C6—C1—C2	119.3 (3)	C16—C17—C12	120.8 (4)
C6—C1—S1	120.1 (3)	N2—C18—C17	125.2 (4)
C2—C1—S1	120.6 (3)	N2—C18—H18	117.4
C3—C2—C1	119.2 (3)	C17—C18—H18	117.4
C3—C2—N3	120.3 (3)	C19—C20—N1	121.0 (4)
C1—C2—N3	120.5 (3)	C19—C20—C21	123.4 (4)
C4—C3—C2	119.0 (3)	N1—C20—C21	115.7 (4)
C4—C3—C7	120.7 (4)	C20—C21—H21A	109.5
C2—C3—C7	120.3 (3)	C20—C21—H21B	109.5
C5—C4—C3	122.5 (4)	H21A—C21—H21B	109.5
C5—C4—H4	118.7	C20—C21—H21C	109.5
C3—C4—H4	118.7	H21A—C21—H21C	109.5
C6—C5—C4	117.5 (4)	H21B—C21—H21C	109.5
C6—C5—C8	121.6 (4)	N1—C22—C23	124.3 (3)
C4—C5—C8	120.9 (4)	N1—C22—H22	117.8
C5—C6—C1	122.3 (4)	C23—C22—H22	117.8
C5—C6—H6	118.8	C22—C23—C28	117.3 (4)
C1—C6—H6	118.8	C22—C23—C24	122.6 (4)
C3—C7—H7A	109.5	C28—C23—C24	120.1 (4)
C3—C7—H7B	109.5	C25—C24—C23	120.0 (4)
H7A—C7—H7B	109.5	C25—C24—H24	120.0
C3—C7—H7C	109.5	C23—C24—H24	120.0
H7A—C7—H7C	109.5	C24—C25—C26	120.4 (4)
H7B—C7—H7C	109.5	C24—C25—H25	119.8
C5—C8—H8A	109.5	C26—C25—H25	119.8
C5—C8—H8B	109.5	C27—C26—C25	121.3 (5)
H8A—C8—H8B	109.5	C27—C26—H26	119.3
C5—C8—H8C	109.5	C25—C26—H26	119.3
H8A—C8—H8C	109.5	C26—C27—C28	120.4 (4)
H8B—C8—H8C	109.5	C26—C27—H27	119.8
C10—C9—H9A	109.5	C28—C27—H27	119.8
C10—C9—H9B	109.5	C19—C28—C23	117.6 (4)
H9A—C9—H9B	109.5	C19—C28—C27	124.6 (4)
C10—C9—H9C	109.5	C23—C28—C27	117.8 (4)
H9A—C9—H9C	109.5	C20—C19—C28	121.6 (4)
H9B—C9—H9C	109.5	C20—C19—H29	119.2
C11—C10—N2	120.5 (4)	C28—C19—H29	119.2
C11—C10—C9	124.3 (5)	C22—N1—C20	118.3 (3)
N2—C10—C9	115.2 (5)	C22—N1—Ag1	119.3 (3)
C10—C11—C12	122.1 (4)	C20—N1—Ag1	121.5 (3)
C10—C11—H11	118.9	C18—N2—C10	118.3 (4)
C12—C11—H11	118.9	C18—N2—Ag1	120.1 (3)
C11—C12—C17	117.8 (4)	C10—N2—Ag1	121.0 (3)
C11—C12—C13	125.2 (5)	C2—N3—Ag1	116.6 (2)

C17—C12—C13	117.0 (5)	C2—N3—H3A	108.1
C14—C13—C12	120.1 (6)	Ag1—N3—H3A	108.1
C14—C13—H13	119.9	C2—N3—H3B	108.1
C12—C13—H13	119.9	Ag1—N3—H3B	108.1
C13—C14—C15	123.2 (6)	H3A—N3—H3B	107.3
C13—C14—H14	118.4	O3—S1—O1	112.91 (18)
C15—C14—H14	118.4	O3—S1—O2	112.90 (17)
C16—C15—C14	119.3 (6)	O1—S1—O2	113.05 (17)
C16—C15—H15	120.4	O3—S1—C1	106.36 (17)
C14—C15—H15	120.4	O1—S1—C1	104.68 (17)
C15—C16—C17	119.6 (5)	O2—S1—C1	106.09 (16)
C15—C16—H16	120.2		

C6—C1—C2—C3	2.5 (5)	C22—C23—C28—C19	1.0 (5)
S1—C1—C2—C3	−179.1 (3)	C24—C23—C28—C19	178.1 (4)
C6—C1—C2—N3	−180.0 (3)	C22—C23—C28—C27	−177.0 (4)
S1—C1—C2—N3	−1.6 (4)	C24—C23—C28—C27	0.1 (6)
C1—C2—C3—C4	−3.8 (5)	C26—C27—C28—C19	−177.4 (4)
N3—C2—C3—C4	178.7 (3)	C26—C27—C28—C23	0.5 (6)
C1—C2—C3—C7	177.3 (3)	N1—C20—C19—C28	0.6 (6)
N3—C2—C3—C7	−0.3 (5)	C21—C20—C19—C28	−179.3 (4)
C2—C3—C4—C5	1.8 (6)	C23—C28—C19—C20	−1.6 (6)
C7—C3—C4—C5	−179.3 (4)	C27—C28—C19—C20	176.2 (4)
C3—C4—C5—C6	1.5 (6)	C23—C22—N1—C20	−1.7 (6)
C3—C4—C5—C8	−178.8 (4)	C23—C22—N1—Ag1	167.9 (3)
C4—C5—C6—C1	−2.9 (6)	C19—C20—N1—C22	1.0 (6)
C8—C5—C6—C1	177.4 (4)	C21—C20—N1—C22	−179.1 (4)
C2—C1—C6—C5	0.9 (6)	C19—C20—N1—Ag1	−168.4 (3)
S1—C1—C6—C5	−177.5 (3)	C21—C20—N1—Ag1	11.5 (4)
N2—C10—C11—C12	3.8 (7)	N2—Ag1—N1—C22	144.2 (3)
C9—C10—C11—C12	−173.2 (4)	N3—Ag1—N1—C22	−25.6 (3)
C10—C11—C12—C17	−0.6 (7)	N2—Ag1—N1—C20	−46.5 (3)
C10—C11—C12—C13	177.6 (5)	N3—Ag1—N1—C20	143.7 (3)
C11—C12—C13—C14	−177.7 (5)	C17—C18—N2—C10	−1.0 (6)
C17—C12—C13—C14	0.5 (8)	C17—C18—N2—Ag1	−172.1 (3)
C12—C13—C14—C15	1.6 (10)	C11—C10—N2—C18	−3.0 (6)
C13—C14—C15—C16	−2.1 (10)	C9—C10—N2—C18	174.2 (4)
C14—C15—C16—C17	0.3 (8)	C11—C10—N2—Ag1	168.0 (3)
C15—C16—C17—C18	−179.1 (4)	C9—C10—N2—Ag1	−14.7 (5)
C15—C16—C17—C12	1.8 (7)	N1—Ag1—N2—C18	106.7 (3)
C11—C12—C17—C18	−3.0 (6)	N3—Ag1—N2—C18	−82.8 (3)
C13—C12—C17—C18	178.7 (4)	N1—Ag1—N2—C10	−64.1 (3)
C11—C12—C17—C16	176.1 (4)	N3—Ag1—N2—C10	106.4 (3)
C13—C12—C17—C16	−2.2 (6)	C3—C2—N3—Ag1	82.7 (4)
C16—C17—C18—N2	−175.2 (4)	C1—C2—N3—Ag1	−94.8 (3)
C12—C17—C18—N2	3.9 (6)	N1—Ag1—N3—C2	128.7 (3)
N1—C22—C23—C28	0.7 (6)	N2—Ag1—N3—C2	−41.9 (3)
N1—C22—C23—C24	−176.3 (4)	C6—C1—S1—O3	−125.5 (3)
C22—C23—C24—C25	176.0 (4)	C2—C1—S1—O3	56.1 (3)
C28—C23—C24—C25	−0.9 (6)	C6—C1—S1—O1	114.7 (3)

C23—C24—C25—C26	1.2 (7)	C2—C1—S1—O1	−63.7 (3)
C24—C25—C26—C27	−0.7 (8)	C6—C1—S1—O2	−5.1 (3)
C25—C26—C27—C28	−0.2 (7)	C2—C1—S1—O2	176.5 (3)

Fig. 1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