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Bis[μ-4-methyl-2-(2-pyridylmethylsulfanyl)pyrimidine-κN^1]bis[(trifluoromethanesulfonato-κO)silver(I)]

Huan-Huan Wang, Chao-Yan Zhang, Yue Cui, Qian Gao and Ya-Bo Xie*

College of Environmental and Energy Engineering, Beijing University of Technology, Beijing 100124, People's Republic of China
Correspondence e-mail: xieyabo@bjut.edu.cn

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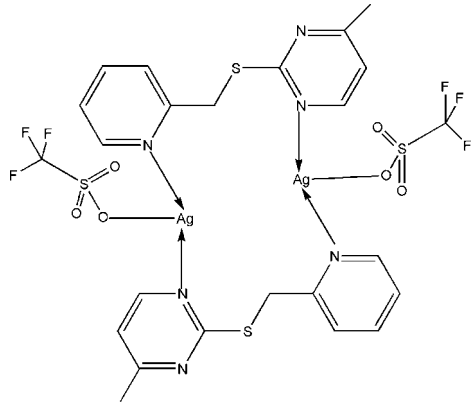
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.044; wR factor = 0.138; data-to-parameter ratio = 17.0.

In the centrosymmetric dinuclear title complex, $[Ag_2(CF_3SO_3)_2(C_{11}H_{11}N_3S)_2]$, the Ag^I atom is coordinated by two N atoms from two 4-methyl-2-(2-pyridylmethylsulfanyl)-pyrimidine ligands and one O atom from a trifluoromethanesulfonate anion in a distorted T-type coordination geometry. The ligand adopts a bidentate bridging coordination mode through one pyridyl N atom and one pyrimidine N atom. In the crystal structure, π–π interactions are present between adjacent pyrimidine rings, with a centroid-to-centroid distance of 3.875 (7) Å.

Related literature

For the architectures of metal complexes, see: Hamblin *et al.* (2002). For a related structure, see: Xie *et al.* (2006).



Experimental

Crystal data

$[Ag_2(CF_3O_3S)_2(C_{11}H_{11}N_3S)_2]$
M_r = 948.50
Triclinic, $P\overline{1}$
a = 8.9999 (18) Å
b = 9.1087 (18) Å
c = 10.937 (2) Å
α = 75.07 (3)°
β = 88.59 (3)°
γ = 68.97 (3)°
V = 806.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 293 K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.800, T_{max} = 0.860
8621 measured reflections
3681 independent reflections
3007 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.138
S = 0.97
3681 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—N1	2.150 (4)	Ag1—O5	2.700 (4)
Ag1—N3^{i}	2.161 (3)		

Symmetry code: (i) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2366).

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supplementary materials

Acta Cryst. (2010). E**66**, m1496 [**doi:10.1107/S1600536810043631**]

Bis[μ-4-methyl-2-(2-pyridylmethylsulfanyl)pyrimidine-κN^1]bis[(trifluoromethanesulfonato-κO)silver(I)]

H.-H. Wang, C.-Y. Zhang, Y. Cui, Q. Gao and Y.-B. Xie

Comment

The coordination geometry of metal ions and the nature of ligands decide the generation of coordination architectures (Hamblin *et al.*, 2002). In previous studies, much attention has been paid to the use of flexible bridging ligands because of their conformational freedom and flexible properties (Xie *et al.*, 2006). As part of our investigation of flexible ligands and their complexes, the crystal structure of a silver(I) complex with a flexible thioether ligand, the title compound, is reported here.

In the binuclear structure of the title complex (Fig. 1), the Ag^I atom is coordinated by two N atoms from two 4-methyl-2-(2-pyridylmethylsulfanyl)pyrimidine ligands and one O atom from a trifluoromethanesulfonate anion (Table 1), displaying a slightly distorted T-type coordination geometry. The ligand adopts a bidentate bridging coordination mode through two N atoms. The dihedral angle between the pyrimidine ring and pyridine ring is 82.67 (3)°. The two pyrimidine rings are nearly parallel, and so are the two pyridine rings. In the crystal structure, π–π interactions between adjacent pyrimidine rings are present, with a centroid–centroid distance of 3.875 (7) Å.

Experimental

A solution of $AgSO_3CF_3$ (0.04 mmol) in acetone (4 ml) was carefully layered on top of a mixture of chloroform (2 ml) and acetone (2 ml), which was carefully layered on top of a solution of 4-methyl-2-(2-pyridylmethylsulfanyl)pyrimidine (0.04 mmol) in chloroform (4 ml) in a test tube. After 2 weeks at room temperature, colourless prism single crystals appeared.

Refinement

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C).

Figures

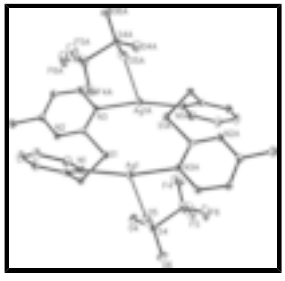


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (A) -*x* + 1, -*y* + 1, -*z*.]

Bis[μ-4-methyl-2-(2-pyridylmethylsulfanyl)pyrimidine- κN^1]bis[(trifluoromethanesulfonato-κ*O*)silver(I)]

Crystal data

$[Ag_2(CF_3O_3S)_2(C_{11}H_{11}N_3S)_2]$	$Z = 1$
$M_r = 948.50$	$F(000) = 468$
Triclinic, $P\overline{1}$	$D_x = 1.953$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.9999$ (18) Å	Cell parameters from 3696 reflections
$b = 9.1087$ (18) Å	$\theta = 3.1$–$27.5°$
$c = 10.937$ (2) Å	$\mu = 1.56$ mm^{-1}
$\alpha = 75.07$ (3)°	$T = 293$ K
$\beta = 88.59$ (3)°	Prism, colourless
$\gamma = 68.97$ (3)°	0.15 × 0.12 × 0.10 mm
$V = 806.3$ (3) Å^3	

Data collection

Bruker APEX CCD diffractometer	3681 independent reflections
Radiation source: fine-focus sealed tube	3007 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.028$
φ and ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -11 \rightarrow 11$
$T_{min} = 0.800$, $T_{max} = 0.860$	$k = -11 \rightarrow 11$
8621 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.138$	H-atom parameters constrained
$S = 0.97$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3681 reflections	$(\Delta/\sigma)_{max} = 0.001$
217 parameters	$\Delta\rho_{max} = 0.72$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.41$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.76401 (4)	0.50847 (4)	0.08737 (3)	0.04428 (16)

S1	0.60205 (13)	0.26916 (13)	0.01310 (10)	0.0376 (3)
N1	0.7984 (4)	0.2971 (4)	0.2435 (3)	0.0379 (8)
N2	0.5373 (4)	0.0216 (4)	0.1602 (3)	0.0348 (7)
N3	0.3225 (4)	0.2503 (4)	0.0425 (3)	0.0318 (7)
C1	0.8050 (6)	0.3150 (6)	0.3602 (4)	0.0463 (11)
H1A	0.8072	0.4131	0.3690	0.056*
C2	0.8086 (6)	0.1969 (6)	0.4671 (5)	0.0526 (12)
H2A	0.8122	0.2143	0.5470	0.063*
C3	0.8067 (7)	0.0511 (6)	0.4541 (5)	0.0540 (12)
H3A	0.8082	−0.0316	0.5253	0.065*
C4	0.8026 (5)	0.0294 (5)	0.3361 (5)	0.0440 (10)
H4A	0.8026	−0.0689	0.3261	0.053*
C5	0.7986 (5)	0.1535 (5)	0.2314 (4)	0.0340 (8)
C6	0.7891 (5)	0.1365 (5)	0.1003 (4)	0.0357 (9)
H6A	0.8038	0.0243	0.1048	0.043*
H6B	0.8751	0.1606	0.0551	0.043*
C7	0.4768 (5)	0.1670 (5)	0.0809 (4)	0.0314 (8)
C8	0.4366 (5)	−0.0528 (5)	0.2077 (4)	0.0374 (9)
C9	0.2748 (5)	0.0237 (5)	0.1742 (5)	0.0420 (10)
H9A	0.2036	−0.0269	0.2068	0.050*
C10	0.2224 (5)	0.1756 (5)	0.0921 (5)	0.0420 (10)
H10A	0.1136	0.2291	0.0697	0.050*
C11	0.5077 (6)	−0.2182 (6)	0.2968 (5)	0.0533 (12)
H11A	0.6214	−0.2489	0.3064	0.080*
H11B	0.4831	−0.2954	0.2638	0.080*
H11C	0.4645	−0.2171	0.3779	0.080*
S4	0.93636 (13)	0.38405 (13)	−0.22242 (10)	0.0377 (3)
F4	0.6405 (4)	0.5740 (6)	−0.2672 (5)	0.1020 (14)
F5	0.7551 (7)	0.5239 (5)	−0.4298 (4)	0.130 (2)
F6	0.8009 (6)	0.6879 (4)	−0.3447 (5)	0.1096 (16)
O4	0.8891 (5)	0.2489 (4)	−0.2085 (4)	0.0680 (11)
O5	0.9355 (5)	0.4366 (5)	−0.1096 (3)	0.0722 (12)
O6	1.0735 (5)	0.3760 (5)	−0.2887 (5)	0.0839 (15)
C24	0.7756 (8)	0.5505 (7)	−0.3235 (5)	0.0635 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0506 (2)	0.0315 (2)	0.0441 (2)	−0.01457 (15)	−0.00205 (16)	0.00090 (15)
S1	0.0406 (6)	0.0352 (5)	0.0372 (6)	−0.0193 (4)	0.0008 (4)	−0.0018 (4)
N1	0.0400 (19)	0.0379 (19)	0.0376 (19)	−0.0195 (16)	0.0016 (15)	−0.0051 (15)
N2	0.0354 (17)	0.0285 (16)	0.0391 (19)	−0.0131 (14)	−0.0017 (15)	−0.0044 (14)
N3	0.0337 (17)	0.0267 (16)	0.0347 (17)	−0.0119 (13)	0.0004 (14)	−0.0065 (13)
C1	0.062 (3)	0.041 (2)	0.044 (3)	−0.028 (2)	0.003 (2)	−0.011 (2)
C2	0.067 (3)	0.052 (3)	0.044 (3)	−0.029 (2)	−0.001 (2)	−0.011 (2)
C3	0.076 (3)	0.044 (3)	0.040 (3)	−0.030 (3)	−0.001 (2)	0.005 (2)
C4	0.045 (2)	0.033 (2)	0.055 (3)	−0.0189 (19)	−0.004 (2)	−0.006 (2)
C5	0.0302 (19)	0.0310 (19)	0.039 (2)	−0.0112 (16)	0.0035 (17)	−0.0058 (17)

C6	0.030 (2)	0.036 (2)	0.043 (2)	−0.0138 (16)	0.0022 (17)	−0.0113 (18)
C7	0.035 (2)	0.0287 (19)	0.033 (2)	−0.0123 (16)	0.0003 (16)	−0.0118 (16)
C8	0.048 (2)	0.0286 (19)	0.038 (2)	−0.0159 (18)	0.0007 (19)	−0.0090 (17)
C9	0.041 (2)	0.037 (2)	0.052 (3)	−0.0249 (19)	0.001 (2)	−0.004 (2)
C10	0.030 (2)	0.038 (2)	0.055 (3)	−0.0130 (17)	−0.0072 (19)	−0.007 (2)
C11	0.053 (3)	0.040 (2)	0.059 (3)	−0.019 (2)	−0.002 (2)	0.003 (2)
S4	0.0418 (6)	0.0342 (5)	0.0405 (6)	−0.0173 (4)	0.0089 (5)	−0.0110 (4)
F4	0.053 (2)	0.114 (3)	0.111 (3)	0.003 (2)	−0.013 (2)	−0.029 (3)
F5	0.206 (6)	0.096 (3)	0.053 (2)	−0.003 (4)	−0.048 (3)	−0.029 (2)
F6	0.160 (4)	0.0394 (19)	0.110 (3)	−0.030 (2)	−0.016 (3)	0.005 (2)
O4	0.073 (3)	0.0426 (19)	0.096 (3)	−0.0370 (19)	0.015 (2)	−0.009 (2)
O5	0.079 (3)	0.071 (3)	0.050 (2)	0.002 (2)	−0.015 (2)	−0.029 (2)
O6	0.072 (3)	0.068 (3)	0.121 (4)	−0.036 (2)	0.055 (3)	−0.030 (3)
C24	0.092 (4)	0.046 (3)	0.040 (3)	−0.010 (3)	−0.010 (3)	−0.011 (2)

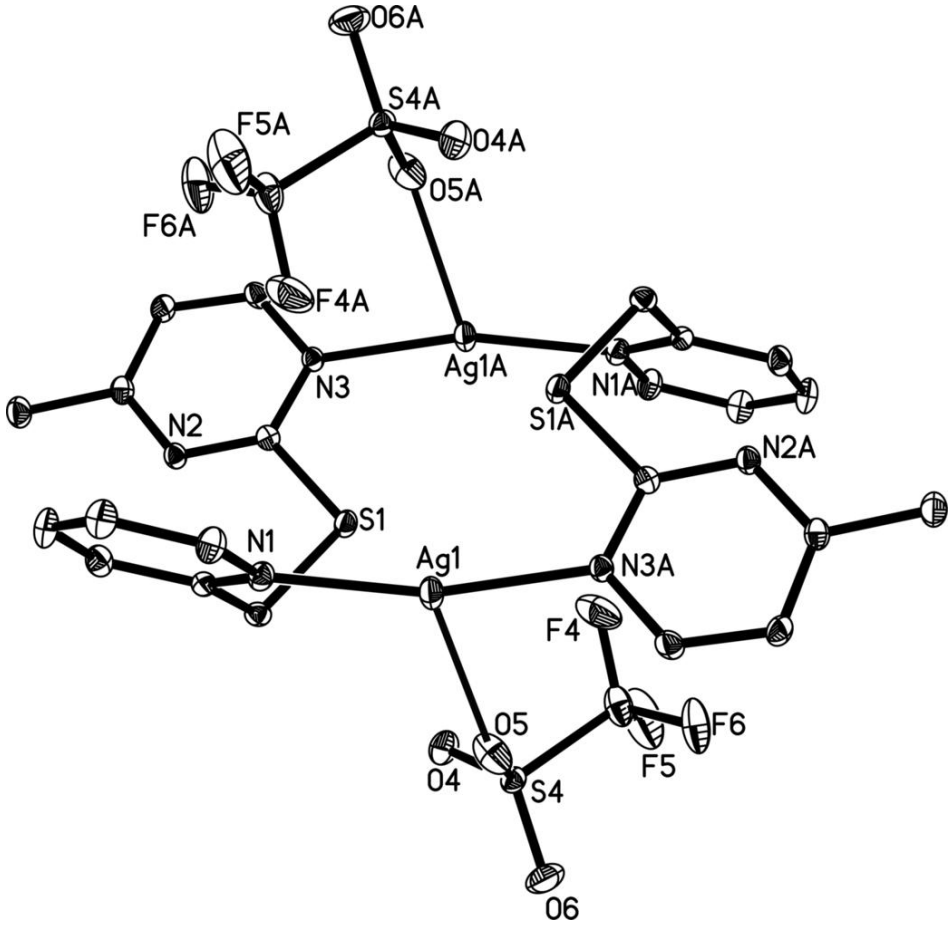
Geometric parameters (Å, °)

Ag1—N1	2.150 (4)	C4—H4A	0.9300
Ag1—N3^{i}	2.161 (3)	C5—C6	1.488 (6)
Ag1—O5	2.700 (4)	C6—H6A	0.9700
S1—C7	1.744 (4)	C6—H6B	0.9700
S1—C6	1.797 (4)	C8—C9	1.381 (6)
N1—C1	1.333 (6)	C8—C11	1.488 (6)
N1—C5	1.347 (5)	C9—C10	1.362 (6)
N2—C7	1.311 (5)	C9—H9A	0.9300
N2—C8	1.337 (5)	C10—H10A	0.9300
N3—C7	1.337 (5)	C11—H11A	0.9600
N3—C10	1.340 (5)	C11—H11B	0.9600
N3—Ag1^{i}	2.161 (3)	C11—H11C	0.9600
C1—C2	1.362 (7)	S4—O6	1.404 (4)
C1—H1A	0.9300	S4—O4	1.412 (3)
C2—C3	1.378 (7)	S4—O5	1.433 (4)
C2—H2A	0.9300	S4—C24	1.804 (6)
C3—C4	1.358 (7)	F4—C24	1.323 (8)
C3—H3A	0.9300	F5—C24	1.278 (6)
C4—C5	1.377 (6)	F6—C24	1.313 (7)
N1—Ag1—N3^{i}	164.97 (13)	N2—C7—N3	126.4 (4)
N1—Ag1—O5	112.81 (13)	N2—C7—S1	119.9 (3)
N3^{i}—Ag1—O5	81.84 (13)	N3—C7—S1	113.7 (3)
C7—S1—C6	100.93 (19)	N2—C8—C9	120.3 (4)
C1—N1—C5	118.1 (4)	N2—C8—C11	116.8 (4)
C1—N1—Ag1	117.2 (3)	C9—C8—C11	122.9 (4)
C5—N1—Ag1	124.4 (3)	C10—C9—C8	118.0 (4)
C7—N2—C8	117.6 (3)	C10—C9—H9A	121.0
C7—N3—C10	115.5 (3)	C8—C9—H9A	121.0
C7—N3—Ag1^{i}	123.1 (3)	N3—C10—C9	122.2 (4)
C10—N3—Ag1^{i}	121.4 (3)	N3—C10—H10A	118.9
N1—C1—C2	123.3 (4)	C9—C10—H10A	118.9

N1—C1—H1A	118.4	C8—C11—H11A	109.5
C2—C1—H1A	118.4	C8—C11—H11B	109.5
C1—C2—C3	118.3 (5)	H11A—C11—H11B	109.5
C1—C2—H2A	120.8	C8—C11—H11C	109.5
C3—C2—H2A	120.8	H11A—C11—H11C	109.5
C4—C3—C2	119.3 (5)	H11B—C11—H11C	109.5
C4—C3—H3A	120.4	O6—S4—O4	115.1 (3)
C2—C3—H3A	120.4	O6—S4—O5	113.5 (3)
C3—C4—C5	119.8 (4)	O4—S4—O5	115.0 (3)
C3—C4—H4A	120.1	O6—S4—C24	105.0 (3)
C5—C4—H4A	120.1	O4—S4—C24	103.5 (3)
N1—C5—C4	121.2 (4)	O5—S4—C24	102.9 (2)
N1—C5—C6	117.4 (4)	S4—O5—Ag1	144.3 (3)
C4—C5—C6	121.4 (4)	F5—C24—F6	108.9 (5)
C5—C6—S1	112.7 (3)	F5—C24—F4	108.0 (6)
C5—C6—H6A	109.0	F6—C24—F4	106.2 (5)
S1—C6—H6A	109.0	F5—C24—S4	112.2 (4)
C5—C6—H6B	109.0	F6—C24—S4	111.1 (5)
S1—C6—H6B	109.0	F4—C24—S4	110.1 (4)
H6A—C6—H6B	107.8		
$N3^{i}$—Ag1—N1—C1	−51.9 (6)	C6—S1—C7—N2	−7.9 (4)
O5—Ag1—N1—C1	141.6 (3)	C6—S1—C7—N3	172.8 (3)
$N3^{i}$—Ag1—N1—C5	121.5 (5)	C7—N2—C8—C9	−0.7 (6)
O5—Ag1—N1—C5	−45.0 (4)	C7—N2—C8—C11	179.6 (4)
C5—N1—C1—C2	−1.4 (7)	N2—C8—C9—C10	0.1 (7)
Ag1—N1—C1—C2	172.5 (4)	C11—C8—C9—C10	179.8 (4)
N1—C1—C2—C3	0.6 (8)	C7—N3—C10—C9	−1.2 (6)
C1—C2—C3—C4	0.5 (8)	$Ag1^{i}$—N3—C10—C9	−179.9 (4)
C2—C3—C4—C5	−0.8 (8)	C8—C9—C10—N3	0.9 (7)
C1—N1—C5—C4	1.1 (6)	O6—S4—O5—Ag1	177.9 (4)
Ag1—N1—C5—C4	−172.3 (3)	O4—S4—O5—Ag1	−46.7 (5)
C1—N1—C5—C6	179.2 (4)	C24—S4—O5—Ag1	65.0 (5)
Ag1—N1—C5—C6	5.8 (5)	N1—Ag1—O5—S4	85.8 (4)
C3—C4—C5—N1	0.0 (7)	$N3^{i}$—Ag1—O5—S4	−90.7 (4)
C3—C4—C5—C6	−178.1 (4)	O6—S4—C24—F5	62.5 (6)
N1—C5—C6—S1	−65.9 (4)	O4—S4—C24—F5	−58.5 (6)
C4—C5—C6—S1	112.3 (4)	O5—S4—C24—F5	−178.5 (5)
C7—S1—C6—C5	−76.0 (3)	O6—S4—C24—F6	−59.7 (5)
C8—N2—C7—N3	0.5 (6)	O4—S4—C24—F6	179.3 (4)
C8—N2—C7—S1	−178.8 (3)	O5—S4—C24—F6	59.2 (5)
C10—N3—C7—N2	0.5 (6)	O6—S4—C24—F4	−177.1 (4)
$Ag1^{i}$—N3—C7—N2	179.2 (3)	O4—S4—C24—F4	61.8 (4)
C10—N3—C7—S1	179.7 (3)	O5—S4—C24—F4	−58.2 (5)
$Ag1^{i}$—N3—C7—S1	−1.6 (4)		

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

Fig. 1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S4A
F5A
O4A
O5A
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N2
S1A
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N1
Ag1
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F4
O5
F6
O4
F5
S4
O6