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catena-Poly[silver(I)-μ-2-phenylimidazolato-κ^2N:N']

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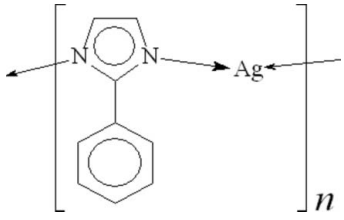
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.041; wR factor = 0.068; data-to-parameter ratio = 18.0.

The asymmetric unit of the title compound, $[Ag(C_9H_7N_2)]_n$, contains two independent Ag^I ions and two 2-phenylimidazolate (L) ligands. Each Ag^I centre is linearly coordinated by two N atoms [Ag—N 2.092 (3)–2.097 (3) Å]. Ligands L bridge Ag^I ions into polymeric chains parallel to the c axis, with Ag···Ag separations of 6.232 (2) and 6.254 (2) Å. No interactions between the Ag centres from neighbouring chains are observed.

Related literature

For related polymeric crystal structures, see: Liu & Zhu (2005); Mukhopadhyay & Pal (2006); Huang *et al.* (2006).



Experimental

Crystal data

$[Ag(C_9H_7N_2)]$
M_r = 251.04
Monoclinic, $P2_1$
a = 10.091 (2) Å
b = 6.9995 (14) Å
c = 12.470 (3) Å
β = 101.59 (3)°
V = 862.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.28 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Bruker, 1998)
T_{min} = 0.924, T_{max} = 1.000
(expected range = 0.586–0.634)
9131 measured reflections
3905 independent reflections
3209 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.068
S = 1.00
3905 reflections
217 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 1770 Friedel pairs
Flack parameter: −0.01 (4)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: CV2336).

References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Huang, X.-C., Zhang, J.-P. & Chen, X.-M. (2006). *Cryst. Growth Des.* **6**, 1194–1198.
Liu, X.-Y. & Zhu, H.-L. (2005). *Synth. React. Inorg. Met.-Org. Nano-Metal Chem.* **35**, 155–159.
Mukhopadhyay, A. & Pal, S. (2006). *Eur. J. Inorg. Chem.* pp. 4879–4887.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

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supplementary materials

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catena-Poly[silver(I)-μ-2-phenylimidazolato-κ^2N:N']

Q. Gao, J.-B. Feng, C.-Y. Zhang and Y.-B. Xie

Comment

The crystal structures of silver(I) imidazolate, catena-poly[(m/^{2}-2-imidazolato-N,N')-silver(I)] (Huang et al., 2006) and silver(I) methylimidazolate, catena-poly[(m/^{2}-2-methylimidazolato-N,N')-silver(I)] (Liu & Zhu, 2005) have been reported recently. Both complexes take a one-dimensional ligand-bridged-Ag(I) chain structure, which is further extended to form a three-dimensional framework through Ag—Ag interactions. On the other hand, for the 2-phenylimidazolate ligand, only one metal complex was documented (Mukhopadhyay & Pal, 2006). Herein, we report the structure of silver(I) 2-phenylimidazolate, $[Ag_2(C_9H_7N_2)_2]_n$ (I), which has also a one-dimensional ligand-bridged chain structure, however, without Ag—Ag interactions that may be attributed to the bulky substituent 2-phenylimidazolate, which isolates the chains.

As shown in Figure 1, (I) has a one-dimensional chain structure, in which there exist two crystallographically independent Ag(I) ions Ag1 and Ag2 and two 2-phenylimidazolate ligands with similar coordination environments, respectively. Each Ag(I) center linearly coordinates to two N atoms from two ligands with the N—Ag—N angles of 176.40 (15) and 173.72 (19) ° for Ag1 and Ag2, respectively. Simultaneously, each 2-phenylimidazolate group bridges two Ag(I) ions to form a one-dimensional chain related by a 2_1 axis, with the Ag—Ag separations of 6.232 (2) [Ag1—Ag2] and 6.254 (2) Å [Ag1—Ag2B]. The dihedral angles between benzene ring and imidazole ring are 31.1 (2) ° for [ring C4—C9 and C1—C3—N1—N2] and 37.6 (2) ° for [ring C13—C18 and C10—C11—N3—N4], respectively. In the crystal, these chains are packed parallel along the c direction and without Ag—Ag or other weak interactions (Figure 2).

Experimental

A mixture of 2-phenylimidazole (43 mg, 0.3 mmol) and $AgNO_3$ (51 mg, 0.3 mmol) was dissolved in 10 ml of ammonium hydroxide (20%). The resulted solution was filtered and filtrate was allowed to stand for 15 days in the dark. Colourless crystals of (I) were collected, in about 30% yield.

Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

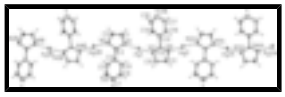

Fig. 1. A portion of polymeric one-dimensional chain structure of (I), showing the atomic numbering and 30% probabilty displacement ellipsoids [symmetry codes: (A) x, y, 1 + z; (B) x, y, z − 1].

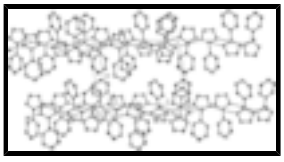

Fig. 2. A portion of crystal packing viewed approximately down the *b* axis. H atoms omitted for clarity.

catena-Poly[(m/^{2}-2-phenylimidazolato-N,_N_')-silver(I)]

Crystal data

$[Ag(C_9H_7N_2)]$	F_{000} = 488
M_r = 251.04	D_x = 1.933 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 8115 reflections
a = 10.091 (2) Å	θ = 3.3–27.5º
b = 6.9995 (14) Å	μ = 2.28 mm^{-1}
c = 12.470 (3) Å	T = 293 (2) K
β = 101.59 (3)º	Block, colourless
V = 862.8 (3) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3905 independent reflections
Radiation source: fine-focus sealed tube	3209 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 293(2) K	θ_{max} = 27.5º
φ and ω scan	θ_{min} = 3.3º
Absorption correction: multi-scan SADABS (Bruker, 1998)	h = −13→13
T_{min} = 0.924, T_{max} = 1.000	k = −9→9
9131 measured reflections	l = −16→16

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.015P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.068	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
3905 reflections	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
217 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983)

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Flack parameter: −0.01 (4)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	1.01351 (4)	0.61504 (6)	0.37721 (2)	0.04521 (13)
Ag2	1.04157 (4)	0.63552 (5)	0.88088 (2)	0.05074 (14)
N1	1.0799 (4)	0.6277 (9)	0.2284 (2)	0.0429 (9)
N2	1.0931 (4)	0.6167 (9)	0.0521 (3)	0.0420 (10)
N3	0.9598 (4)	0.5982 (8)	0.5304 (2)	0.0422 (11)
N4	0.9737 (4)	0.6318 (10)	0.7105 (3)	0.0447 (10)
C1	1.2115 (5)	0.5983 (12)	0.2218 (3)	0.0536 (16)
H1A	1.2835	0.5844	0.2809	0.064*
C2	1.2200 (5)	0.5929 (10)	0.1145 (4)	0.0518 (16)
H2A	1.2989	0.5757	0.0879	0.062*
C3	1.0099 (4)	0.6291 (18)	0.1249 (3)	0.0335 (11)
C4	0.8623 (5)	0.6610 (9)	0.0921 (3)	0.0357 (14)
C5	0.7890 (5)	0.5820 (8)	−0.0049 (3)	0.0424 (13)
H5A	0.8331	0.5050	−0.0475	0.051*
C6	0.6528 (5)	0.6166 (11)	−0.0384 (4)	0.0596 (14)
H6A	0.6062	0.5673	−0.1046	0.071*
C7	0.5846 (6)	0.7250 (9)	0.0265 (5)	0.0701 (19)
H7A	0.4924	0.7476	0.0041	0.084*
C8	0.6537 (6)	0.7985 (8)	0.1235 (5)	0.0546 (15)
H8A	0.6080	0.8691	0.1678	0.065*
C9	0.7912 (6)	0.7680 (7)	0.1555 (4)	0.0454 (14)
H9A	0.8372	0.8203	0.2210	0.055*
C10	0.8325 (5)	0.5729 (9)	0.5531 (4)	0.0505 (18)
H10A	0.7538	0.5457	0.5024	0.061*
C11	0.8428 (5)	0.5950 (12)	0.6630 (4)	0.0554 (17)
H11A	0.7715	0.5864	0.6998	0.067*
C12	1.0415 (4)	0.628 (2)	0.6275 (3)	0.0359 (9)
C13	1.1888 (5)	0.6649 (9)	0.6416 (3)	0.0393 (14)
C14	1.2641 (6)	0.5643 (8)	0.5782 (4)	0.0543 (16)
H14A	1.2222	0.4726	0.5288	0.065*

C15	1.4013 (6)	0.6000 (11)	0.5883 (4)	0.0703 (17)
H15A	1.4513	0.5322	0.5460	0.084*
C16	1.4629 (7)	0.7352 (11)	0.6606 (6)	0.081 (2)
H16A	1.5544	0.7602	0.6653	0.098*
C17	1.3931 (7)	0.8356 (9)	0.7269 (5)	0.0691 (18)
H17A	1.4367	0.9251	0.7769	0.083*
C18	1.2549 (6)	0.7987 (8)	0.7164 (4)	0.0509 (14)
H18A	1.2060	0.8648	0.7603	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0583 (2)	0.0590 (3)	0.01865 (16)	−0.0022 (4)	0.00847 (14)	−0.0002 (2)
Ag2	0.0724 (3)	0.0617 (4)	0.02221 (18)	0.0098 (4)	0.01922 (15)	0.0024 (3)
N1	0.053 (2)	0.058 (3)	0.0187 (16)	−0.003 (5)	0.0101 (15)	−0.003 (3)
N2	0.056 (2)	0.049 (3)	0.0236 (17)	0.005 (4)	0.0143 (15)	−0.004 (3)
N3	0.054 (2)	0.054 (3)	0.0194 (17)	−0.002 (3)	0.0085 (15)	−0.003 (2)
N4	0.055 (2)	0.059 (3)	0.0235 (17)	0.012 (5)	0.0160 (16)	0.005 (3)
C1	0.047 (3)	0.080 (5)	0.032 (2)	0.015 (4)	0.004 (2)	0.009 (4)
C2	0.053 (3)	0.059 (5)	0.048 (3)	0.013 (4)	0.022 (2)	0.006 (3)
C3	0.047 (3)	0.035 (3)	0.0197 (19)	−0.018 (6)	0.0108 (16)	−0.008 (4)
C4	0.047 (3)	0.038 (4)	0.024 (2)	−0.005 (3)	0.0117 (19)	0.004 (3)
C5	0.054 (3)	0.043 (4)	0.032 (2)	−0.003 (3)	0.013 (2)	−0.005 (3)
C6	0.060 (3)	0.070 (4)	0.043 (3)	−0.022 (5)	−0.003 (2)	−0.003 (4)
C7	0.041 (4)	0.087 (5)	0.081 (5)	−0.010 (3)	0.011 (3)	0.016 (4)
C8	0.048 (4)	0.060 (4)	0.057 (4)	0.005 (3)	0.017 (3)	0.001 (3)
C9	0.053 (4)	0.049 (3)	0.036 (3)	−0.004 (3)	0.012 (3)	−0.003 (3)
C10	0.047 (3)	0.067 (6)	0.037 (3)	−0.003 (3)	0.006 (2)	0.002 (3)
C11	0.055 (3)	0.075 (5)	0.041 (3)	0.013 (4)	0.023 (2)	0.012 (4)
C12	0.050 (3)	0.039 (3)	0.0212 (19)	−0.002 (5)	0.0126 (16)	0.000 (4)
C13	0.052 (3)	0.046 (4)	0.020 (2)	0.008 (3)	0.0083 (19)	0.005 (3)
C14	0.057 (4)	0.063 (4)	0.043 (3)	0.007 (3)	0.007 (3)	−0.012 (3)
C15	0.060 (4)	0.085 (5)	0.070 (4)	0.017 (5)	0.023 (3)	−0.007 (4)
C16	0.047 (4)	0.103 (6)	0.090 (5)	0.003 (4)	0.005 (4)	0.001 (5)
C17	0.063 (5)	0.074 (5)	0.061 (4)	−0.003 (4)	−0.010 (4)	−0.009 (3)
C18	0.062 (4)	0.056 (4)	0.034 (3)	0.007 (3)	0.007 (3)	−0.003 (3)

Geometric parameters (Å, °)

Ag1—N1	2.097 (3)	C6—H6A	0.9300
Ag1—N3	2.092 (3)	C7—C8	1.370 (8)
Ag2—N2^{i}	2.097 (3)	C7—H7A	0.9300
Ag2—N4	2.097 (3)	C8—C9	1.381 (7)
N1—C3	1.342 (4)	C8—H8A	0.9300
N1—C1	1.363 (5)	C9—H9A	0.9300
N2—C3	1.358 (5)	C10—C11	1.362 (6)
N2—C2	1.368 (6)	C10—H10A	0.9300
N2—Ag2^{ii}	2.097 (3)	C11—H11A	0.9300

N3—C12	1.338 (5)	C12—C13	1.484 (6)
N3—C10	1.381 (6)	C13—C14	1.393 (6)
N4—C12	1.351 (4)	C13—C18	1.394 (7)
N4—C11	1.359 (6)	C14—C15	1.387 (7)
C1—C2	1.358 (6)	C14—H14A	0.9300
C1—H1A	0.9300	C15—C16	1.367 (9)
C2—H2A	0.9300	C15—H15A	0.9300
C3—C4	1.480 (7)	C16—C17	1.381 (9)
C4—C9	1.388 (7)	C16—H16A	0.9300
C4—C5	1.399 (6)	C17—C18	1.399 (8)
C5—C6	1.375 (7)	C17—H17A	0.9300
C5—H5A	0.9300	C18—H18A	0.9300
C6—C7	1.388 (8)		
N3—Ag1—N1	176.40 (15)	C6—C7—H7A	120.1
N4—Ag2—N2^{i}	173.72 (19)	C7—C8—C9	120.0 (5)
C3—N1—C1	105.9 (3)	C7—C8—H8A	120.0
C3—N1—Ag1	130.7 (3)	C9—C8—H8A	120.0
C1—N1—Ag1	122.4 (3)	C8—C9—C4	121.5 (5)
C3—N2—C2	105.1 (3)	C8—C9—H9A	119.2
C3—N2—Ag2^{ii}	128.1 (3)	C4—C9—H9A	119.2
C2—N2—Ag2^{ii}	126.8 (3)	C11—C10—N3	107.8 (4)
C12—N3—C10	105.4 (3)	C11—C10—H10A	126.1
C12—N3—Ag1	126.3 (3)	N3—C10—H10A	126.1
C10—N3—Ag1	128.1 (3)	N4—C11—C10	109.3 (4)
C12—N4—C11	105.1 (4)	N4—C11—H11A	125.3
C12—N4—Ag2	131.6 (3)	C10—C11—H11A	125.3
C11—N4—Ag2	122.3 (3)	N3—C12—N4	112.4 (4)
C2—C1—N1	108.6 (4)	N3—C12—C13	123.7 (3)
C2—C1—H1A	125.7	N4—C12—C13	123.8 (4)
N1—C1—H1A	125.7	C14—C13—C18	118.6 (5)
C1—C2—N2	108.7 (4)	C14—C13—C12	119.6 (6)
C1—C2—H2A	125.7	C18—C13—C12	121.8 (6)
N2—C2—H2A	125.7	C15—C14—C13	120.3 (5)
N1—C3—N2	111.5 (4)	C15—C14—H14A	119.8
N1—C3—C4	125.0 (4)	C13—C14—H14A	119.8
N2—C3—C4	123.3 (4)	C16—C15—C14	119.9 (6)
C9—C4—C5	117.5 (5)	C16—C15—H15A	120.1
C9—C4—C3	122.0 (5)	C14—C15—H15A	120.1
C5—C4—C3	120.4 (5)	C15—C16—C17	121.8 (6)
C6—C5—C4	121.0 (5)	C15—C16—H16A	119.1
C6—C5—H5A	119.5	C17—C16—H16A	119.1
C4—C5—H5A	119.5	C16—C17—C18	118.0 (6)
C5—C6—C7	120.1 (5)	C16—C17—H17A	121.0
C5—C6—H6A	119.9	C18—C17—H17A	121.0
C7—C6—H6A	119.9	C13—C18—C17	121.3 (5)
C8—C7—C6	119.8 (5)	C13—C18—H18A	119.3
C8—C7—H7A	120.1	C17—C18—H18A	119.3
C3—N1—C1—C2	3.3 (10)	C12—N3—C10—C11	1.8 (10)

Ag1—N1—C1—C2	172.7 (5)	Ag1—N3—C10—C11	−172.3 (5)
N1—C1—C2—N2	−0.6 (9)	C12—N4—C11—C10	−0.9 (11)
C3—N2—C2—C1	−2.2 (10)	Ag2—N4—C11—C10	−170.7 (4)
Ag2^{ii}—N2—C2—C1	176.6 (5)	N3—C10—C11—N4	−0.6 (10)
C1—N1—C3—N2	−4.8 (12)	C10—N3—C12—N4	−2.5 (12)
Ag1—N1—C3—N2	−173.1 (5)	Ag1—N3—C12—N4	171.8 (6)
C1—N1—C3—C4	−178.6 (10)	C10—N3—C12—C13	−179.3 (11)
Ag1—N1—C3—C4	13.2 (16)	Ag1—N3—C12—C13	−5.0 (17)
C2—N2—C3—N1	4.4 (11)	C11—N4—C12—N3	2.1 (13)
Ag2^{ii}—N2—C3—N1	−174.4 (5)	Ag2—N4—C12—N3	170.6 (6)
C2—N2—C3—C4	178.3 (9)	C11—N4—C12—C13	178.9 (11)
Ag2^{ii}—N2—C3—C4	−0.5 (15)	Ag2—N4—C12—C13	−12.6 (18)
N1—C3—C4—C9	27.6 (14)	N3—C12—C13—C14	−39.2 (16)
N2—C3—C4—C9	−145.5 (9)	N4—C12—C13—C14	144.4 (10)
N1—C3—C4—C5	−152.0 (9)	N3—C12—C13—C18	140.4 (10)
N2—C3—C4—C5	34.9 (13)	N4—C12—C13—C18	−36.1 (16)
C9—C4—C5—C6	2.8 (8)	C18—C13—C14—C15	−1.2 (8)
C3—C4—C5—C6	−177.5 (7)	C12—C13—C14—C15	178.4 (7)
C4—C5—C6—C7	−2.6 (9)	C13—C14—C15—C16	−0.2 (9)
C5—C6—C7—C8	0.5 (10)	C14—C15—C16—C17	1.6 (10)
C6—C7—C8—C9	1.3 (9)	C15—C16—C17—C18	−1.5 (10)
C7—C8—C9—C4	−1.0 (9)	C14—C13—C18—C17	1.4 (8)
C5—C4—C9—C8	−1.1 (8)	C12—C13—C18—C17	−178.2 (7)
C3—C4—C9—C8	179.3 (6)	C16—C17—C18—C13	0.0 (9)

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

Fig. 1

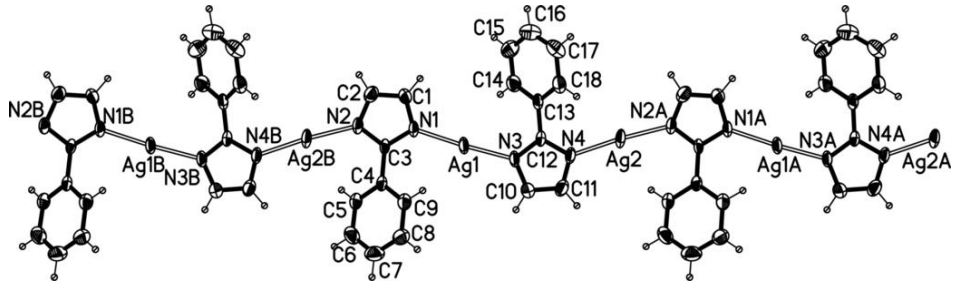
C16
C15
C17
C14
C18
C13
C2
C1
N2
N1
N3
N4
C12
C3
C4
C10
C11
C5
C9
C8
C6
C7
N2B
N1B
Ag1B
N3B
N4B
Ag2B
Ag1
Ag2
N2A
N1A
N3A
N4A
Ag1A
Ag2A

Fig. 2