addenda and errata

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Poly[bis(μ -hemihydrogen 2-phenylquinoline-4-carboxylato- $\kappa^2 N$,O)silver(I)]. Corrigendum

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The affiliation of one of the authors in the paper by Zhang, Wei & Li [*Acta Cryst.* (2009), E**65**, m223] is corrected.

In the paper by Zhang, Wei & Li [*Acta Cryst.* (2009), E65, m223], the affiliation of the second author was given incorrectly. The correct address is given here.

V = 2429.5 (3) Å³

Mo $K\alpha$ radiation $\mu = 0.87 \text{ mm}^{-1}$

 $0.20 \times 0.15 \times 0.15 \text{ mm}$

9257 measured reflections

2791 independent reflections

2550 reflections with $I > 2\sigma(I)$

T = 293 (2) K

 $R_{\rm int} = 0.020$

Z = 4

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Poly[bis(*µ*-hemihydrogen 2-phenylquinoline-4-carboxylato- $\kappa^2 N.O$)silver(I)]

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.003 Å; R factor = 0.029: wR factor = 0.067: data-to-parameter ratio = 15.8.

In the title compound, $[Ag(C_{16}H_{10.5}NO_2)_2]$, the Ag^I cation (site symmetry 2) is coordinated by two N atoms in a nearlinear AgN₂ arrangement. Two carboxylate O atoms from two additional 2-phenylquinoline-4-carboxylate ligands form long Ag–O bonds [2.6585 (17) Å], resulting in a distorted squareplanar arrangement. The bridging ligands result in infinite corrugated sheets propagating in (010). An O-H···O hydrogen bond, disordered about a twofold axis, completes the structure.

Related literature

For the related coordination polymers containing Mn^{II}, Co^{II} and Cu^{II}, see: Xiao et al. (2005); Xie et al. (2005) and Xie et al. (2006), respectively.



Experimental

Crystal data

$[Ag(C_{16}H_{10.5}NO_2)_2]$
$M_r = 605.38$
Monoclinic, $C2/c$
a = 7.2163 (6) Å
b = 20.5060 (17) Å
c = 16.5632 (12) Å
$\beta = 97.585 \ (3)^{\circ}$

Data collection

Bruker SMART CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2001) $T_{\min} = 0.877, T_{\max} = 1.00$ (expected range = 0.769–0.877)

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	177 parameters
$wR(F^2) = 0.067$	H-atom parameters constrained
S = 1.10	$\Delta \rho_{\rm max} = 0.66 \text{ e } \text{\AA}^{-3}$
2791 reflections	$\Delta \rho_{\rm min} = -0.33 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ag1-N1	2.2413 (15)	
N1-Ag1-N1 ⁱ	177.38 (8)	
Symmetry code: (i) $-x$	$z + 1, y, -z - \frac{1}{2}$	

Table 2

Hydrogen-bond geometry (Å, °).

	• • •	·		
$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
O1-H1O···O1 ⁱⁱ	0.82	1.68	2.470 (3)	162
Summature and a (ii)				

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2825).

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supplementary materials

Acta Cryst. (2009). E65, m223 [doi:10.1107/S1600536809001184]

Poly[bis(#-hemihydrogen 2-phenylquinoline-4-carboxylato- $\kappa^2 N$,O)silver(I)]

X. Zhang, P. Wei and B. Li

Experimental

A mixture of silver nitrate (0.5 mmol) and 2-phenyl-4-quinolinecarboxylic acid (0.5 mmol) in H₂O (8 ml) and ethanol (8 ml) was sealed in a 25 ml Teflon-lined stainless steel autoclave and kept at 413 K for three days. Orange prisms of (I) were obtained after cooling to room temperature with a yield of 27%. Anal. Calc. for $C_{32}H_{21}AgN_2O_4$: C 63.43, H 3.47, N 4.63%; Found: C 63.41, H 3.32, N 4.59%.

Refinement

The H atoms were placed in calculated positions (C—H = 0.93 Å, O—H = 0.82Å) and refined as riding with and $U_{iso}(H) = 1.2U_{eq}(carruer)$.

Figures



Fig. 1. A view of the structure of (I), expanded to show the Ag—N bonds, showing 30% probability displacement ellipsoids. Symmetry code: I: 1-x, y, -z-1/2.



Fig. 2. Part of a polymeric sheet in (I).

Poly[bis(μ -hemihydrogen 2-phenylquinoline-4-carboxylato- $\kappa^2 N$,O)silver(I)]

 $F_{000} = 1224$

 $\lambda = 0.71073 \text{ Å}$

 $\theta = 2.3 - 27.5^{\circ}$

 $\mu = 0.87 \text{ mm}^{-1}$

T = 293 (2) K

Prism, orange

 $0.20\times0.15\times0.15~mm$

 $D_{\rm x} = 1.655 {\rm Mg m}^{-3}$ Mo Kα radiation

Cell parameters from 3290 reflections

Crystal data

 $[Ag(C_{16}H_{10.5}NO_2)_2]$ $M_r = 605.38$ Monoclinic, C2/c Hall symbol: -C 2yc a = 7.2163 (6) Å *b* = 20.5060 (17) Å c = 16.5632 (12) Å $\beta = 97.585 (3)^{\circ}$ V = 2429.5 (3) Å³ Z = 4

Data collection

Bruker SMART CCD diffractometer	2791 independent reflections
Radiation source: fine-focus sealed tube	2550 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.020$
T = 293(2) K	$\theta_{\text{max}} = 27.5^{\circ}$
ω scans	$\theta_{\min} = 2.3^{\circ}$
Absorption correction: Multi-scan (SADABS; Bruker, 2001)	$h = -9 \rightarrow 9$
$T_{\min} = 0.877, \ T_{\max} = 1.00$	$k = -25 \rightarrow 26$
9257 measured reflections	$l = -21 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 1.551P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{\rm max} < 0.001$
2791 reflections	$\Delta \rho_{max} = 0.66 \text{ e } \text{\AA}^{-3}$
177 parameters	$\Delta \rho_{min} = -0.33 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct	Extinction correction: none

methods

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.

 $U_{\rm iso}*/U_{\rm eq}$ Occ. (<1) \boldsymbol{Z} х y 0.5000 0.03976 (9) Ag1 0.224313 (10) -0.2500N1 0.4524(2)0.22681 (7) -0.11903(9)0.0305 (3) 01 0.4807 (3) 0.16931 (8) 0.17478 (8) 0.0506 (4) H1O 0.50 0.4750 0.1750 0.2234 0.061* 02 0.6459(3) 0.26118 (9) 0.18437 (10) 0.0555 (4) C1 0.4841(3)0.28414 (9) -0.07613(11)0.0323(4)C2 0.4827(4)0.34294 (10) -0.12074(13)0.0468(5)H2A 0.056* 0.4619 0.3417 -0.1773C3 0.5113(4)0.40127 (11) -0.08202(16)0.0562(7)H3A 0.5094 0.4396 -0.11210.067* C4 0.5437 (4) 0.40349 (11) 0.00334 (16) 0.0546 (6) H4A 0.5627 0.4436 0.0294 0.065* C5 0.5477 (3) 0.34808 (11) 0.04857 (13) 0.0446 (5) 0.054* H5A 0.5712 0.3506 0.1051 C6 0.5165 (3) 0.28627 (9) 0.01036(11) 0.0317 (4) C7 0.5077 (3) 0.22584 (9) 0.05293 (11) 0.0313 (4) C8 0.4621 (3) 0.17105 (10) 0.00812 (11) 0.0344 (4) H8A 0.0348 0.041* 0.4467 0.1319 C9 0.4376 (3) 0.17227 (9) -0.07805(10)0.0302 (4) C10 0.3928 (3) 0.11103 (9) -0.12467 (11) 0.0331 (4) C11 0.2740(3) 0.11181 (10) -0.19829(12)0.0379 (4) H11A 0.2219 0.1510 -0.21850.045* C12 0.2330 (3) 0.05444 (12) -0.24147 (13) 0.0476 (5) H12A 0.057* 0.1558 0.0555 -0.2911C13 0.3063 (4) -0.00390(12)-0.21119 (15) 0.0570(7) H13A 0.2773 -0.0424-0.2399 0.068* C14 0.4230 (4) -0.00520(11)-0.13802(15)0.0593 (7) H14A -0.04460.071* 0.4731 -0.1177C15 0.4659 (4) 0.05159 (11) -0.09489(12)0.0463 (5) H15A 0.5442 0.0502 -0.04560.056* C16 0.5497 (3) 0.22006 (10) 0.14510(11) 0.0356 (4)

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

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05874 (17)	0.04506 (14)	0.01656 (11)	0.000	0.00894 (9)	0.000
N1	0.0388 (9)	0.0352 (8)	0.0176 (7)	0.0017 (7)	0.0040 (6)	0.0002 (6)
01	0.0877 (12)	0.0478 (8)	0.0152 (6)	-0.0092 (8)	0.0029 (7)	-0.0008 (6)
02	0.0607 (11)	0.0753 (11)	0.0275 (8)	-0.0222 (9)	-0.0048 (7)	-0.0068 (7)
C1	0.0384 (10)	0.0364 (10)	0.0232 (9)	0.0005 (8)	0.0081 (8)	-0.0004 (7)
C2	0.0718 (16)	0.0412 (11)	0.0289 (10)	0.0025 (11)	0.0122 (10)	0.0043 (8)
C3	0.085 (2)	0.0358 (11)	0.0494 (14)	-0.0001 (11)	0.0162 (13)	0.0038 (10)
C4	0.0766 (18)	0.0373 (11)	0.0498 (14)	-0.0021 (11)	0.0084 (12)	-0.0110 (10)
C5	0.0549 (14)	0.0462 (12)	0.0330 (11)	0.0004 (10)	0.0066 (10)	-0.0110 (9)
C6	0.0331 (10)	0.0391 (10)	0.0236 (9)	0.0001 (8)	0.0060 (7)	-0.0047 (7)
C7	0.0313 (10)	0.0447 (10)	0.0179 (8)	0.0001 (8)	0.0036 (7)	-0.0016 (7)
C8	0.0485 (12)	0.0369 (9)	0.0179 (8)	-0.0024 (9)	0.0046 (8)	0.0019 (7)
C9	0.0364 (10)	0.0368 (9)	0.0176 (8)	0.0005 (8)	0.0039 (7)	0.0010 (7)
C10	0.0457 (12)	0.0347 (9)	0.0194 (8)	-0.0039 (8)	0.0066 (8)	0.0005 (7)
C11	0.0447 (12)	0.0434 (11)	0.0252 (9)	-0.0031 (9)	0.0035 (8)	0.0000 (8)
C12	0.0557 (14)	0.0549 (13)	0.0309 (10)	-0.0146 (11)	0.0007 (10)	-0.0074 (9)
C13	0.088 (2)	0.0440 (12)	0.0401 (12)	-0.0171 (12)	0.0113 (12)	-0.0106 (10)
C14	0.101 (2)	0.0359 (11)	0.0414 (13)	0.0018 (12)	0.0110 (13)	0.0044 (9)
C15	0.0723 (16)	0.0412 (11)	0.0243 (10)	0.0009 (10)	0.0023 (10)	0.0027 (8)
C16	0.0385 (11)	0.0488 (11)	0.0193 (8)	0.0033 (9)	0.0031 (8)	-0.0040 (8)

Geometric parameters (Å, °)

Ag1—N1	2.2413 (15)	C5—H5A	0.9300
Ag1—N1 ⁱ	2.2413 (15)	C6—C7	1.431 (3)
Ag1—O2 ⁱⁱ	2.6585 (17)	С7—С8	1.363 (3)
Ag1—O2 ⁱⁱⁱ	2.6585 (17)	C7—C16	1.521 (2)
N1—C9	1.320 (2)	С8—С9	1.415 (2)
N1—C1	1.377 (2)	C8—H8A	0.9300
O1—C16	1.280 (2)	C9—C10	1.487 (3)
01—H10	0.8200	C10—C15	1.392 (3)
O2—C16	1.223 (3)	C10—C11	1.395 (3)
O2—Ag1 ⁱⁱⁱ	2.6585 (17)	C11—C12	1.388 (3)
C1—C2	1.414 (3)	C11—H11A	0.9300
C1—C6	1.421 (3)	C12—C13	1.376 (4)
C2—C3	1.360 (3)	C12—H12A	0.9300
C2—H2A	0.9300	C13—C14	1.382 (4)
C3—C4	1.403 (4)	C13—H13A	0.9300
С3—НЗА	0.9300	C14—C15	1.380 (3)
C4—C5	1.359 (3)	C14—H14A	0.9300
C4—H4A	0.9300	C15—H15A	0.9300
C5—C6	1.421 (3)		
N1—Ag1—N1 ⁱ	177.38 (8)	C8—C7—C16	118.96 (17)

N1—Ag1—O2 ⁱⁱ	97.54 (6)	C6—C7—C16	123.08 (16)
N1 ⁱ —Ag1—O2 ⁱⁱ	82.16 (6)	C7—C8—C9	121.59 (18)
N1—Ag1—O2 ⁱⁱⁱ	82.16 (6)	С7—С8—Н8А	119.2
N1 ⁱ —Ag1—O2 ⁱⁱⁱ	97.54 (6)	С9—С8—Н8А	119.2
O2 ⁱⁱ —Ag1—O2 ⁱⁱⁱ	167.15 (8)	N1—C9—C8	121.72 (17)
C9—N1—C1	118.51 (16)	N1—C9—C10	118.39 (15)
C9—N1—Ag1	120.76 (12)	C8—C9—C10	119.90 (16)
C1—N1—Ag1	118.86 (11)	C15—C10—C11	118.69 (18)
C16—O1—H1O	109.5	C15—C10—C9	120.59 (18)
C16—O2—Ag1 ⁱⁱⁱ	137.88 (16)	C11—C10—C9	120.70 (17)
N1—C1—C2	117.98 (17)	C12-C11-C10	120.3 (2)
N1—C1—C6	122.71 (17)	C12-C11-H11A	119.8
C2—C1—C6	119.30 (17)	C10-C11-H11A	119.8
C3—C2—C1	120.9 (2)	C13—C12—C11	120.3 (2)
С3—С2—Н2А	119.6	C13—C12—H12A	119.9
C1—C2—H2A	119.6	C11—C12—H12A	119.9
C2—C3—C4	119.9 (2)	C12—C13—C14	119.8 (2)
С2—С3—НЗА	120.0	С12—С13—Н13А	120.1
С4—С3—НЗА	120.0	C14—C13—H13A	120.1
C5—C4—C3	121.1 (2)	C15-C14-C13	120.5 (2)
C5—C4—H4A	119.4	C15-C14-H14A	119.8
C3—C4—H4A	119.4	C13—C14—H14A	119.8
C4—C5—C6	120.6 (2)	C14—C15—C10	120.5 (2)
С4—С5—Н5А	119.7	C14—C15—H15A	119.8
С6—С5—Н5А	119.7	C10-C15-H15A	119.8
C5—C6—C1	118.14 (18)	O2—C16—O1	125.35 (19)
C5—C6—C7	124.57 (18)	O2—C16—C7	120.26 (18)
C1—C6—C7	117.24 (16)	O1—C16—C7	114.37 (17)
C8—C7—C6	117.95 (17)		

Symmetry codes: (i) -x+1, y, -z-1/2; (ii) x-1/2, -y+1/2, z-1/2; (iii) -x+3/2, -y+1/2, -z.

Hydrogen-bond geometry (Å, °)				
D—H···A	D—H	$H \cdots A$	$D \cdots A$	D—H···A
O1—H1O···O1 ^{iv}	0.82	1.68	2.470 (3)	162
Symmetry codes: (iv) $-x+1$, y , $-z+1/2$.				



Fig. 1



