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Bis(8-hydroxy-1-methylquinolin-1-ium) bis(1,2-dicyanoethene-1,2-dithiolato)-nickelate(II) dihydrate

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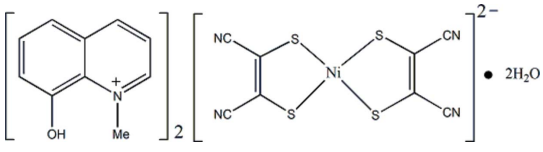
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.097; data-to-parameter ratio = 13.6.

In the title ion-pair complex, $(C_{10}H_{10}NO)_2[Ni(C_4N_2S_2)_2]\cdot 2H_2O$, the anion has crystallographically imposed centre of symmetry. The Ni^{II} atom exhibits a slightly distorted square-planar coordination geometry. In the crystal, the water molecule links anions and cations into a three-dimensional network *via* O—H···N, O—H···S and O—H···O hydrogen bonds. The structure is further stabilized by weak S···π contacts [S···centroid = 3.8047 (9) Å] and π–π stacking interactions [centriod–centroid distance = 3.8653 (7) Å].

Related literature

For background to the properties and applications of bis-1,2-dithiolene metal complexes, see: Brammer (2004); Hill *et al.* (2005); Robin & Fromm (2006); Carlucci *et al.* (2003). For details of square-planar 1,2-dithiolene metal complexes, see: Robertson & Cronin (2002); Coomber *et al.* (1996); Ni *et al.* (2005); Duan *et al.* (2010).



Experimental

Crystal data

$(C_{10}H_{10}NO)_2[Ni(C_4N_2S_2)_2]\cdot 2H_2O$
M_r = 695.50
Triclinic, $P\overline{1}$
a = 8.786 (2) Å
b = 9.277 (2) Å
c = 9.667 (2) Å
α = 82.064 (4)°
β = 78.058 (4)°
γ = 83.324 (4)°
V = 760.4 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 291 K
0.35 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.796, T_{max} = 0.865
3798 measured reflections
2679 independent reflections
2179 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.097
S = 1.00
2679 reflections
197 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···O2	0.98	1.66	2.639 (3)	180
O2—H2B···S2	0.85	2.64	3.224 (3)	128
O2—H2B···N2^{i}	0.85	2.51	2.948 (3)	113

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: RZ2659).

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Bis(8-hydroxy-1-methylquinolin-1-ium) bis(1,2-dicyanoethene-1,2-dithiolato)nickelate(II) dihydrate

Zhi-Heng Guan, Zhang Jiang and Fang-Ming Wang

S1. Comment

During the past few years, bis-1,2-dithiolene complexes of transition metals have been widely studied for their novel properties and applications in the areas of conducting and magnetic materials, dyes, non-linear optics, catalysis and others, due to their extended electronically delocalized core comprising the central metal, four sulphur atoms and the C═C units (Brammer, 2004; Hill *et al.*, 2005; Robin & Fromm, 2006; Carlucci *et al.*, 2003). Among them, maleonitriledithiolate (mnt^{2-}) transition metal complexes are typical examples of bis-1,2-dithiolene complexes used as building blocks for magnetic and conducting molecular materials (Robertson & Cronin, 2002; Coomber *et al.*, 1996; Ni *et al.*, 2005; Duan *et al.*, 2010). To gain more insight into how the substituted groups affects the stacking mode of the $Ni(mnt)_2^{2-}$ anion, we herein present the crystal structure of a new $Ni(mnt)_2^{2-}$ salt containing the 1-methyl-8-hydroxyl-quinolinium $(MeHoQl)^+$ cation.

As shown in Fig. 1, the title salt consists of one $(MeHoQl)^+$ cation, half of a $Ni(mnt)_2^{2-}$ anion and one water molecule in the asymmetric unit. The anion possesses crystallographically imposed inversion centre and exhibits a slightly distorted square-planar coordination geometry. The crystal structure is stabilized by O–H···N, O–H···S and O–H···O hydrogen bonds (Table 1) involving the water molecule, linking cations and anions into a three-dimensional network. Anions and cation further interact through weak S···π contacts ($S2\cdots Cg1^{i}$ = 3.8047 (9) Å) and π–π stacking interactions ($Cg1\cdots Cg2^{ii}$ = 3.8653 (7) Å; Cg1 and Cg2 are the centroids of the N1/C1–C4/C9 and C4–C9 rings, respectively; symmetry codes: (i) x, y, z-1; (ii) -x, -y, 1-z).

S2. Experimental

The title compound was prepared by the direct reaction of equimolar mixture of $NiCl_2.6H_2O$, sodium maleonitriledithiolate and 1-methyl-8-hydroxyl-quinolinium iodide in water/ethanol (1:1 *v*/*v*). Red-brown block-like single crystals were obtained by slow evaporation of a CH_3CN solution at room temperature for about two weeks.

S3. Refinement

The hydroxy H atom was located in a difference Fourier map and refined as riding with O–H = 0.98 Å and free isotropic displacement parameter. All other H atoms were fixed geometrically and treated as riding with C—H = 0.96 Å, O–H = 0.85 Å and with U_{iso} (H) = 1.2U_{eq}(C) or 1.5U_{eq}(C, O) for methyl and water H atoms.

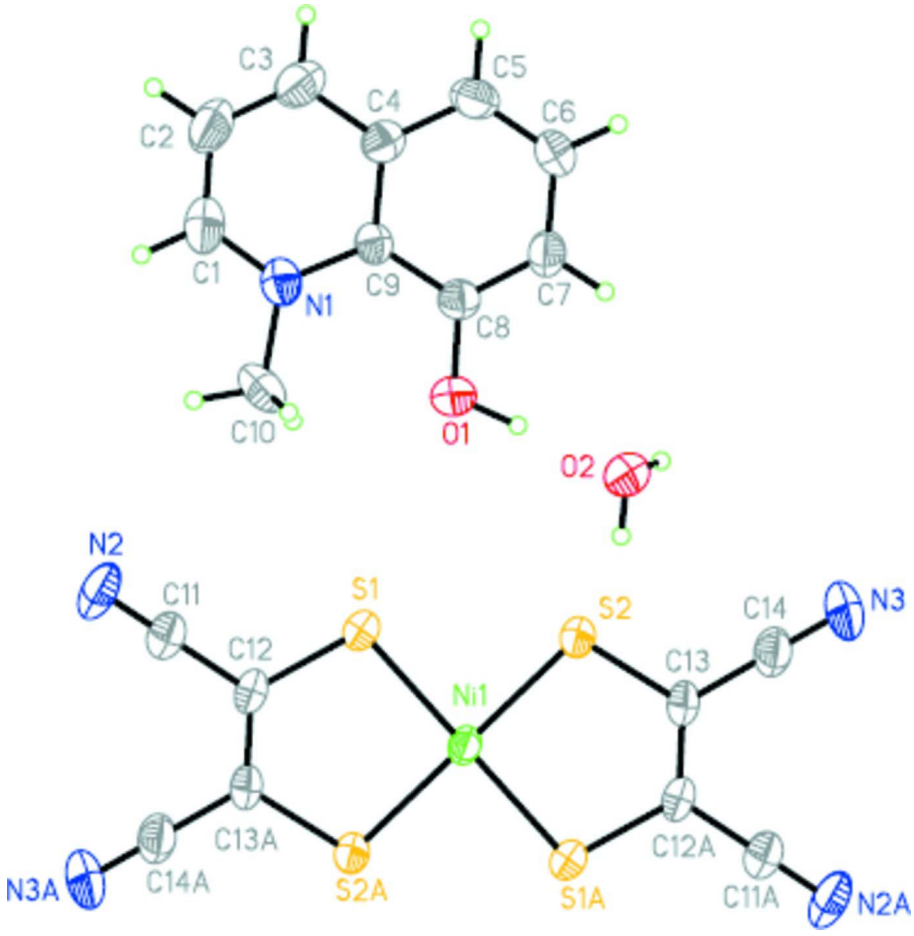

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids. Atoms labeled with the suffix A are generated by the symmetry operator (1 - *x*, -*y*, 2 - *z*).

Bis(8-hydroxy-1-methylquinolin-1-ium) bis(1,2-dicyanoethene-1,2-dithiolato)nickelate(II) dihydrate

Crystal data

$(C_{10}H_{10}NO)_2[Ni(C_4N_2S_2)_2]\cdot 2H_2O$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.786\ (2)$ Å
$b = 9.277\ (2)$ Å
$c = 9.667\ (2)$ Å
$\alpha = 82.064\ (4)°$
$\beta = 78.058\ (4)°$
$\gamma = 83.324\ (4)°$
$V = 760.4\ (3)$ Å^3
$Z = 1$
$F(000) = 358$
$D_x = 1.519$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1684 reflections
$\theta = 2.4–24.2°$
$\mu = 0.96$ mm^{-1}
$T = 291$ K
Block, red-brown
0.35 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.796, T_{max} = 0.865
3798 measured reflections
2679 independent reflections
2179 reflections with $I > 2\sigma(I)$

R_{int} = 0.057
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −10→9
k = −11→10
l = −11→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.097
S = 1.00
2679 reflections
197 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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}
C1	0.1931 (4)	−0.1818 (4)	0.2692 (4)	0.0795 (10)
H1A	0.2548	−0.2742	0.2672	0.095*
C2	0.0785 (4)	−0.1531 (4)	0.1891 (4)	0.0880 (12)
H2A	0.0584	−0.2267	0.1362	0.106*
C3	−0.0068 (4)	−0.0222 (4)	0.1882 (4)	0.0806 (10)
H3A	−0.0890	−0.0007	0.1347	0.097*
C4	0.0262 (3)	0.0846 (3)	0.2640 (3)	0.0593 (8)
C5	−0.0561 (4)	0.2226 (4)	0.2571 (4)	0.0722 (9)
H5A	−0.1334	0.2450	0.1983	0.087*
C6	−0.0264 (4)	0.3248 (3)	0.3313 (4)	0.0724 (9)
H6A	−0.0808	0.4207	0.3252	0.087*
C7	0.0860 (3)	0.2922 (3)	0.4167 (3)	0.0648 (8)
H7A	0.1040	0.3660	0.4704	0.078*
C8	0.1707 (3)	0.1592 (3)	0.4260 (3)	0.0551 (7)
C9	0.1429 (3)	0.0509 (3)	0.3479 (3)	0.0499 (7)
C10	0.3498 (4)	−0.1336 (3)	0.4296 (4)	0.0816 (10)
H10A	0.3917	−0.2316	0.4143	0.122*
H10B	0.4315	−0.0692	0.3997	0.122*
H10C	0.3070	−0.1299	0.5289	0.122*

C11	0.5319 (4)	−0.3805 (3)	0.7603 (3)	0.0642 (8)
C12	0.5454 (3)	−0.2796 (3)	0.8553 (3)	0.0529 (7)
C13	0.3540 (3)	0.3089 (3)	1.0562 (3)	0.0533 (7)
C14	0.2600 (4)	0.4443 (3)	1.0453 (4)	0.0684 (9)
N1	0.2236 (3)	−0.0862 (3)	0.3466 (3)	0.0615 (7)
N2	0.5227 (4)	−0.4590 (3)	0.6826 (3)	0.0914 (10)
N3	0.1864 (4)	0.5531 (3)	1.0351 (4)	0.1009 (11)
Ni1	0.5000	0.0000	1.0000	0.04543 (18)
O1	0.2796 (2)	0.1319 (2)	0.5071 (2)	0.0766 (6)
H1W	0.2823	0.2143	0.5595	0.108 (13)*
O2	0.2867 (2)	0.3545 (2)	0.6480 (2)	0.0839 (7)
H2B	0.3566	0.3340	0.6984	0.126*
H2C	0.3081	0.4295	0.5889	0.126*
S1	0.42937 (9)	−0.11519 (8)	0.84759 (9)	0.0614 (2)
S2	0.33291 (10)	0.17888 (8)	0.95058 (9)	0.0642 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.082 (2)	0.059 (2)	0.094 (3)	−0.0075 (17)	0.002 (2)	−0.0232 (19)
C2	0.091 (3)	0.085 (3)	0.096 (3)	−0.014 (2)	−0.013 (2)	−0.044 (2)
C3	0.074 (2)	0.097 (3)	0.079 (3)	−0.014 (2)	−0.0163 (18)	−0.030 (2)
C4	0.0545 (17)	0.068 (2)	0.0558 (18)	−0.0078 (14)	−0.0072 (14)	−0.0133 (15)
C5	0.064 (2)	0.079 (2)	0.076 (2)	0.0047 (17)	−0.0257 (17)	−0.0060 (18)
C6	0.070 (2)	0.0572 (19)	0.091 (3)	0.0102 (15)	−0.0244 (19)	−0.0137 (18)
C7	0.0657 (19)	0.0527 (18)	0.078 (2)	0.0002 (15)	−0.0132 (17)	−0.0211 (16)
C8	0.0519 (17)	0.0595 (18)	0.0540 (18)	−0.0054 (14)	−0.0105 (14)	−0.0065 (14)
C9	0.0463 (15)	0.0481 (16)	0.0521 (17)	−0.0034 (12)	−0.0023 (13)	−0.0064 (13)
C10	0.070 (2)	0.066 (2)	0.102 (3)	0.0150 (16)	−0.0217 (19)	0.0055 (19)
C11	0.077 (2)	0.0518 (17)	0.068 (2)	−0.0134 (15)	−0.0130 (16)	−0.0142 (16)
C12	0.0634 (17)	0.0405 (15)	0.0569 (18)	−0.0102 (12)	−0.0069 (14)	−0.0161 (13)
C13	0.0656 (18)	0.0344 (14)	0.0603 (18)	−0.0057 (12)	−0.0091 (15)	−0.0109 (13)
C14	0.088 (2)	0.0467 (18)	0.073 (2)	−0.0078 (16)	−0.0168 (18)	−0.0117 (16)
N1	0.0581 (15)	0.0531 (15)	0.0690 (17)	−0.0041 (12)	−0.0024 (13)	−0.0080 (13)
N2	0.127 (3)	0.0699 (19)	0.091 (2)	−0.0243 (17)	−0.0265 (18)	−0.0361 (17)
N3	0.125 (3)	0.0481 (17)	0.131 (3)	0.0179 (17)	−0.039 (2)	−0.0167 (18)
Ni1	0.0547 (3)	0.0370 (3)	0.0474 (3)	−0.0059 (2)	−0.0121 (2)	−0.0100 (2)
O1	0.0821 (15)	0.0746 (15)	0.0849 (16)	0.0071 (11)	−0.0431 (13)	−0.0210 (13)
O2	0.0993 (17)	0.0704 (14)	0.0964 (18)	−0.0024 (12)	−0.0490 (14)	−0.0184 (13)
S1	0.0712 (5)	0.0514 (4)	0.0716 (5)	−0.0004 (3)	−0.0299 (4)	−0.0223 (4)
S2	0.0840 (6)	0.0460 (4)	0.0722 (5)	0.0070 (4)	−0.0361 (4)	−0.0195 (4)

Geometric parameters (Å, º)

C1—N1	1.319 (4)	C10—H10A	0.9599
C1—C2	1.374 (5)	C10—H10B	0.9599
C1—H1A	0.9600	C10—H10C	0.9600
C2—C3	1.351 (5)	C11—N2	1.135 (3)

C2—H2A	0.9599	C11—C12	1.430 (4)
C3—C4	1.399 (4)	C12—C13^{i}	1.334 (4)
C3—H3A	0.9600	C12—S1	1.735 (3)
C4—C5	1.396 (4)	C13—C12^{i}	1.334 (4)
C4—C9	1.416 (4)	C13—C14	1.424 (4)
C5—C6	1.343 (4)	C13—S2	1.733 (3)
C5—H5A	0.9600	C14—N3	1.138 (4)
C6—C7	1.395 (4)	Ni1—S2^{i}	2.1546 (8)
C6—H6A	0.9600	Ni1—S2	2.1546 (8)
C7—C8	1.366 (4)	Ni1—S1	2.1599 (7)
C7—H7A	0.9600	Ni1—S1^{i}	2.1599 (7)
C8—O1	1.340 (3)	O1—H1W	0.9789
C8—C9	1.408 (4)	O2—H2B	0.8500
C9—N1	1.383 (4)	O2—H2C	0.8500
C10—N1	1.492 (4)		

N1—C1—C2	122.5 (3)	N1—C10—H10A	110.0
N1—C1—H1A	118.7	N1—C10—H10B	109.5
C2—C1—H1A	118.8	H10A—C10—H10B	109.5
C3—C2—C1	119.4 (3)	N1—C10—H10C	108.9
C3—C2—H2A	120.7	H10A—C10—H10C	109.5
C1—C2—H2A	119.8	H10B—C10—H10C	109.5
C2—C3—C4	119.9 (3)	N2—C11—C12	178.7 (4)
C2—C3—H3A	120.7	C13^{i}—C12—C11	121.4 (3)
C4—C3—H3A	119.4	C13^{i}—C12—S1	121.27 (19)
C5—C4—C3	120.0 (3)	C11—C12—S1	117.3 (2)
C5—C4—C9	120.6 (3)	C12^{i}—C13—C14	122.4 (2)
C3—C4—C9	119.4 (3)	C12^{i}—C13—S2	119.9 (2)
C6—C5—C4	120.2 (3)	C14—C13—S2	117.7 (2)
C6—C5—H5A	119.9	N3—C14—C13	179.1 (4)
C4—C5—H5A	119.9	C1—N1—C9	121.0 (3)
C5—C6—C7	119.8 (3)	C1—N1—C10	116.5 (3)
C5—C6—H6A	120.6	C9—N1—C10	122.6 (3)
C7—C6—H6A	119.6	S2^{i}—Ni1—S2	180.00 (4)
C8—C7—C6	122.2 (3)	S2^{i}—Ni1—S1	91.80 (3)
C8—C7—H7A	119.3	S2—Ni1—S1	88.20 (3)
C6—C7—H7A	118.6	S2^{i}—Ni1—S1^{i}	88.20 (3)
O1—C8—C7	120.8 (3)	S2—Ni1—S1^{i}	91.80 (3)
O1—C8—C9	120.2 (3)	S1—Ni1—S1^{i}	180.000 (1)
C7—C8—C9	119.0 (3)	C8—O1—H1W	111.5
N1—C9—C8	124.1 (3)	H2B—O2—H2C	109.5
N1—C9—C4	117.7 (3)	C12—S1—Ni1	103.10 (10)
C8—C9—C4	118.2 (3)	C13—S2—Ni1	103.92 (10)

N1—C1—C2—C3	0.2 (6)	C5—C4—C9—C8	1.4 (4)
C1—C2—C3—C4	2.5 (6)	C3—C4—C9—C8	−178.3 (2)
C2—C3—C4—C5	176.5 (3)	C2—C1—N1—C9	−1.6 (5)
C2—C3—C4—C9	−3.7 (5)	C2—C1—N1—C10	179.2 (3)

C3—C4—C5—C6	179.0 (3)	C8—C9—N1—C1	−179.0 (3)
C9—C4—C5—C6	−0.7 (5)	C4—C9—N1—C1	0.3 (4)
C4—C5—C6—C7	−0.7 (5)	C8—C9—N1—C10	0.2 (4)
C5—C6—C7—C8	1.3 (5)	C4—C9—N1—C10	179.5 (3)
C6—C7—C8—O1	178.9 (3)	C13^{i}—C12—S1—Ni1	1.1 (3)
C6—C7—C8—C9	−0.6 (5)	C11—C12—S1—Ni1	−177.2 (2)
O1—C8—C9—N1	−0.9 (4)	S2^{i}—Ni1—S1—C12	0.20 (10)
C7—C8—C9—N1	178.6 (3)	S2—Ni1—S1—C12	−179.80 (10)
O1—C8—C9—C4	179.8 (3)	C12^{i}—C13—S2—Ni1	−2.0 (3)
C7—C8—C9—C4	−0.7 (4)	C14—C13—S2—Ni1	178.6 (2)
C5—C4—C9—N1	−178.0 (2)	S1—Ni1—S2—C13	−178.97 (10)
C3—C4—C9—N1	2.3 (4)	S1^{i}—Ni1—S2—C13	1.03 (10)

Symmetry code: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···O2	0.98	1.66	2.639 (3)	180
O2—H2*B*···S2	0.85	2.64	3.224 (3)	128
O2—H2*B*···N2^{ii}	0.85	2.51	2.948 (3)	113

Symmetry code: (ii) *x*, *y*+1, *z*.