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Hexakis(1*H*-imidazole-κN^3)copper(II) dichloride tetrahydrate

Yu-Min Yang, Tao-Tao Zhu, Peng-Cheng Lu and Chang-Hong Liu*

Jiangsu Province Key Laboratory of Neuroregeneration, Nantong University, Nantong 226001, People's Republic of China, and State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: changhong_liu2223@yahoo.com.cn

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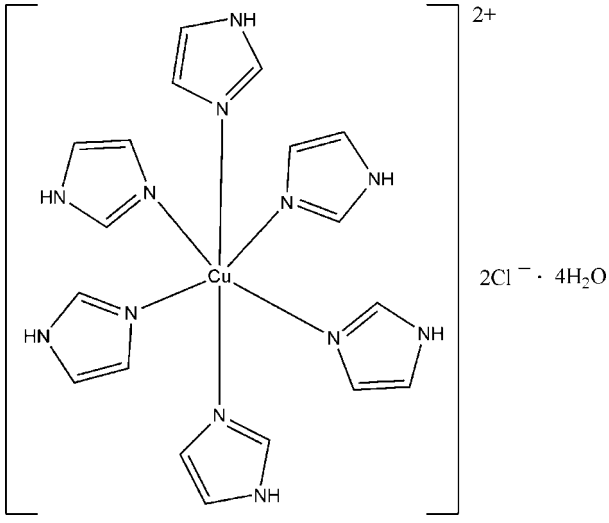
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.150; data-to-parameter ratio = 14.7.

The centrosymmetric title complex, $[Cu(C_3H_4N_2)_6]Cl_2\cdot 4H_2O$, has a distorted octahedral coordination geometry. There is extensive hydrogen bonding involving the cations, anions and water molecules.

Related literature

For related literature, see: Liu & Zhu (2005); Liu *et al.* (1999); Yang *et al.* (2000, 2001); Zhu *et al.* (1998, 2000, 2003); Zhu, Bu *et al.* (1999); Zhu, Hang *et al.* (1999); Zhu, Tong *et al.* (1999); Zhu, Zheng *et al.* (1999).



Experimental

Crystal data

$[Cu(C_3H_4N_2)_6]Cl_2\cdot 4H_2O$
M_r = 615.00
Triclinic, $P\overline{1}$
a = 8.783 (4) Å
b = 9.064 (4) Å
c = 10.576 (5) Å
α = 75.156 (5)°
β = 83.105 (6)°
γ = 61.848 (5)°
V = 717.6 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 298 (2) K
0.42 × 0.35 × 0.21 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.680, T_{max} = 0.819
3756 measured reflections
2498 independent reflections
2190 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.150
S = 1.06
2498 reflections
170 parameters
48 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2D···Cl1	0.90	2.28	3.165 (4)	169
O2—H2C···O1^{i}	0.88	1.87	2.743 (5)	179
O1—H1C···O1^{ii}	0.91	2.31	2.805 (7)	113
O1—H1B···Cl1^{iii}	0.91	2.31	3.201 (4)	168
N6—H6A···Cl1^{i}	0.86	2.58	3.383 (4)	156
N4—H4A···Cl1^{iv}	0.86	2.36	3.214 (3)	170
N2—H2A···Cl1^{v}	0.86	2.50	3.320 (4)	161

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $x-1, y, z-1$; (v) $-x, -y+1, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: CF2104).

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supplementary materials

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Hexakis(1*H*-imidazole-κN^3)copper(II) dichloride tetrahydrate

Y.-M. Yang, T.-T. Zhu, P.-C. Lu and C.-H. Liu

Comment

Organic compounds containing an imidazole group are widespread in nature. In recent years, many transition metal complexes with imidazole molecules or anions, or their analogues, were reported. They include complexes of copper(II) (Zhu *et al.*, 2000, 1998; Zhu, Hang *et al.*, 1999; Zhu, Tong *et al.*, 1999; Zhu, Bu *et al.*, 1999; Liu *et al.*, 1999), silver(I) (Yang *et al.*, 2000; Liu *et al.*, 2005), zinc(II) (Zhu, Zheng *et al.*, 1999), iron(II) (Yang *et al.*, 2001*a*), manganese(II) (Yang *et al.*, 2001*b*) and cobalt(II) (Zhu *et al.*, 2003). We report here the crystal structure of the title copper(II) complex, (I).

The title complex is a mononuclear copper(II) complex, similar to the cobalt(II) complex reported by Zhu *et al.* (2003). The asymmetric unit consists of half the complex dication, a chloride anion and two water molecules; the cation is centrosymmetric. In the cation, the central copper(II) atom is coordinated by six nitrogen atoms from six imidazole ligands, forming a slightly distorted octahedral geometry around the metal. The average Mn—N bond length is 2.168 (3) Å. The dihedral angles between pairs of imidazole rings in the asymmetric unit are 89.3 (3), 85.0 (3) and 84.4 (3)°, the ligands being almost perpendicular to one another.

All the non-coordinated nitrogen atoms in imidazole ligands, the water molecules and chloride anions participate in the stabilization of the crystal structure by the formation of hydrogen bonds, which form a hydrophilic chain along the *a* axis, these chains being connected in a two-dimensional layer in the *ab* plane.

Experimental

In a similar procedure to that of Zhu *et al.* (2003) the title complex was prepared as follows. $CuCl_2·6H_2O$ and six equivalents of imidazole were dissoved in water, with stirring for a few minutes to obtain a clear pale-pink solution. After allowing the resulting solution to stand in air for 3 days, dark blue crystals were formed. These crystals were isolated, washed with water three times and dried in a vacuum desiccator using $CaCl_2$ (yield 56%).

Refinement

C– and N-bound H atoms were included in the riding model approximation with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*). H atoms of water were located in a difference map and refined as riding in their as-found relative positions, with U_{iso}(H) = 1.5U_{eq}(O).

Figures

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. [Symmetry code for unlabelled atoms: −*x*, −*y*, −*z*.]

Hexakis(1*H*-imidazole-κN^3)copper(II) dichloride tetrahydrate

Crystal data

$[Cu(C_3H_4N_2)_6]Cl_2·4H_2O$	$Z = 1$
$M_r = 615.00$	$F_{000} = 319$
Triclinic, $P\overline{1}$	$D_x = 1.423$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.783$ (4) Å	Cell parameters from 718 reflections
$b = 9.064$ (4) Å	$\theta = 3.4$–26.1º
$c = 10.576$ (5) Å	$\mu = 0.99$ mm^{-1}
$\alpha = 75.156$ (5)º	$T = 298$ (2) K
$\beta = 83.105$ (6)º	Prism, dark blue
$\gamma = 61.848$ (5)º	0.42 × 0.35 × 0.21 mm
$V = 717.6$ (5) Å^3	

Data collection

Bruker APEX area-detector diffractometer	2498 independent reflections
Radiation source: fine-focus sealed tube	2190 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 9$
$T_{min} = 0.680$, $T_{max} = 0.819$	$k = -10 \rightarrow 6$
3756 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.150$	$w = 1/[\sigma^2(F_o^2) + (0.0908P)^2 + 0.8952P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.005$
2498 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
170 parameters	$\Delta\rho_{min} = -0.87$ e Å^{-3}
48 restraints	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.049 (6)

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}
Cu1	0.0000	0.0000	0.0000	0.0332 (2)
Cl1	0.69768 (12)	0.79338 (11)	0.50423 (8)	0.0418 (3)
O1	0.0404 (4)	0.8257 (5)	0.5269 (4)	0.0714 (10)
O2	0.6643 (5)	0.4581 (5)	0.5131 (5)	0.0899 (13)
N1	−0.1959 (3)	0.1465 (4)	0.1260 (3)	0.0319 (6)
N2	−0.3870 (4)	0.2053 (5)	0.2829 (3)	0.0519 (9)
H2A	−0.4461	0.1902	0.3514	0.062*
N3	−0.0032 (4)	0.2346 (3)	−0.1173 (3)	0.0332 (6)
N4	−0.0732 (5)	0.4703 (4)	−0.2703 (3)	0.0504 (8)
H4A	−0.1235	0.5506	−0.3377	0.061*
N5	0.2019 (4)	−0.0357 (4)	0.1215 (3)	0.0332 (6)
N6	0.3312 (5)	−0.0241 (5)	0.2801 (3)	0.0539 (9)
H6A	0.3452	0.0026	0.3487	0.065*
C1	−0.2612 (5)	0.0824 (5)	0.2301 (3)	0.0410 (8)
H1A	−0.2245	−0.0346	0.2633	0.049*
C2	−0.4041 (6)	0.3573 (6)	0.2089 (5)	0.0577 (11)
H2B	−0.4817	0.4658	0.2219	0.069*
C3	−0.2864 (5)	0.3210 (5)	0.1122 (4)	0.0448 (9)
H3	−0.2693	0.4021	0.0463	0.054*
C4	−0.0987 (5)	0.3335 (5)	−0.2216 (4)	0.0414 (8)
H4B	−0.1750	0.3103	−0.2569	0.050*
C5	0.0465 (7)	0.4602 (6)	−0.1943 (5)	0.0612 (12)
H5	0.0907	0.5378	−0.2052	0.073*
C6	0.0887 (6)	0.3155 (5)	−0.0997 (4)	0.0471 (9)
H6B	0.1678	0.2764	−0.0329	0.057*
C7	0.1798 (5)	0.0280 (5)	0.2244 (3)	0.0421 (8)
H7	0.0730	0.0999	0.2547	0.051*
C8	0.4565 (6)	−0.1244 (7)	0.2111 (5)	0.0621 (12)
H8	0.5745	−0.1782	0.2276	0.075*
C9	0.3774 (5)	−0.1326 (5)	0.1113 (4)	0.0483 (10)
H9	0.4332	−0.1937	0.0471	0.058*
H2C	0.7583	0.3668	0.5013	0.058*
H2D	0.6872	0.5439	0.5168	0.058*

H1B	−0.0523	0.8161	0.5077	0.058*
H1C	0.0580	0.8951	0.4535	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0342 (4)	0.0354 (4)	0.0281 (4)	−0.0153 (3)	−0.0008 (2)	−0.0049 (2)
Cl1	0.0435 (5)	0.0408 (5)	0.0364 (5)	−0.0184 (4)	−0.0006 (4)	−0.0030 (4)
O1	0.060 (2)	0.078 (2)	0.089 (3)	−0.0377 (18)	0.0101 (18)	−0.032 (2)
O2	0.066 (2)	0.060 (2)	0.149 (4)	−0.0246 (18)	−0.017 (2)	−0.032 (2)
N1	0.0310 (14)	0.0371 (15)	0.0268 (14)	−0.0147 (12)	0.0018 (11)	−0.0087 (11)
N2	0.0462 (19)	0.070 (2)	0.0433 (19)	−0.0285 (18)	0.0206 (15)	−0.0249 (17)
N3	0.0340 (14)	0.0312 (14)	0.0311 (15)	−0.0142 (12)	0.0022 (11)	−0.0044 (11)
N4	0.056 (2)	0.0385 (17)	0.0444 (19)	−0.0190 (16)	−0.0075 (15)	0.0091 (14)
N5	0.0336 (14)	0.0370 (15)	0.0293 (14)	−0.0173 (12)	−0.0038 (11)	−0.0043 (12)
N6	0.063 (2)	0.078 (3)	0.0386 (18)	−0.042 (2)	−0.0065 (16)	−0.0184 (17)
C1	0.044 (2)	0.049 (2)	0.0308 (18)	−0.0229 (17)	0.0067 (15)	−0.0102 (16)
C2	0.049 (2)	0.051 (2)	0.062 (3)	−0.011 (2)	0.014 (2)	−0.025 (2)
C3	0.048 (2)	0.0379 (19)	0.041 (2)	−0.0154 (17)	0.0072 (17)	−0.0102 (16)
C4	0.042 (2)	0.0377 (19)	0.0373 (19)	−0.0174 (16)	−0.0045 (15)	0.0026 (15)
C5	0.081 (3)	0.047 (2)	0.063 (3)	−0.040 (2)	−0.008 (2)	0.002 (2)
C6	0.057 (2)	0.044 (2)	0.044 (2)	−0.0297 (19)	−0.0087 (18)	0.0009 (17)
C7	0.048 (2)	0.049 (2)	0.0325 (19)	−0.0238 (18)	−0.0025 (15)	−0.0122 (16)
C8	0.043 (2)	0.092 (4)	0.058 (3)	−0.032 (2)	−0.010 (2)	−0.020 (3)
C9	0.0352 (19)	0.062 (3)	0.046 (2)	−0.0175 (18)	−0.0042 (16)	−0.0167 (19)

Geometric parameters (Å, °)

Cu1—N3^{i}	2.159 (3)	N4—H4A	0.860
Cu1—N3	2.159 (3)	N5—C7	1.312 (5)
Cu1—N5	2.167 (3)	N5—C9	1.375 (5)
Cu1—N5^{i}	2.167 (3)	N6—C8	1.331 (6)
Cu1—N1	2.168 (3)	N6—C7	1.338 (5)
Cu1—N1^{i}	2.168 (3)	N6—H6A	0.860
O1—H1B	0.9101	C1—H1A	0.930
O1—H1C	0.9139	C2—C3	1.349 (6)
O2—H2C	0.8751	C2—H2B	0.930
O2—H2D	0.9011	C3—H3	0.930
N1—C1	1.309 (5)	C4—H4B	0.930
N1—C3	1.371 (5)	C5—C6	1.348 (6)
N2—C1	1.335 (5)	C5—H5	0.930
N2—C2	1.347 (6)	C6—H6B	0.930
N2—H2A	0.860	C7—H7	0.930
N3—C4	1.315 (5)	C8—C9	1.367 (6)
N3—C6	1.375 (5)	C8—H8	0.930
N4—C4	1.327 (5)	C9—H9	0.930
N4—C5	1.354 (6)		
N3^{i}—Cu1—N3	180	C9—N5—Cu1	128.2 (2)

$N3^{i}$—Cu1—N5	89.82 (11)	C8—N6—C7	108.4 (3)
N3—Cu1—N5	90.18 (11)	C8—N6—H6A	125.8
$N3^{i}$—Cu1—$N5^{i}$	90.18 (11)	C7—N6—H6A	125.8
N3—Cu1—$N5^{i}$	89.82 (11)	N1—C1—N2	111.8 (4)
N5—Cu1—$N5^{i}$	180	N1—C1—H1A	124.1
$N3^{i}$—Cu1—N1	90.37 (11)	N2—C1—H1A	124.1
N3—Cu1—N1	89.63 (11)	N2—C2—C3	106.4 (4)
N5—Cu1—N1	90.61 (11)	N2—C2—H2B	126.8
$N5^{i}$—Cu1—N1	89.39 (11)	C3—C2—H2B	126.8
$N3^{i}$—Cu1—$N1^{i}$	89.63 (11)	C2—C3—N1	109.6 (4)
N3—Cu1—$N1^{i}$	90.37 (11)	C2—C3—H3	125.2
N5—Cu1—$N1^{i}$	89.39 (11)	N1—C3—H3	125.2
$N5^{i}$—Cu1—$N1^{i}$	90.61 (11)	N3—C4—N4	111.8 (3)
N1—Cu1—$N1^{i}$	180	N3—C4—H4B	124.1
H1B—O1—H1C	104.9	N4—C4—H4B	124.1
H2C—O2—H2D	111.6	C6—C5—N4	106.4 (4)
C1—N1—C3	104.9 (3)	C6—C5—H5	126.8
C1—N1—Cu1	125.6 (3)	N4—C5—H5	126.8
C3—N1—Cu1	129.4 (2)	C5—C6—N3	109.4 (4)
C1—N2—C2	107.3 (3)	C5—C6—H6B	125.3
C1—N2—H2A	126.4	N3—C6—H6B	125.3
C2—N2—H2A	126.4	N5—C7—N6	111.0 (3)
C4—N3—C6	104.9 (3)	N5—C7—H7	124.5
C4—N3—Cu1	126.5 (3)	N6—C7—H7	124.5
C6—N3—Cu1	128.6 (2)	N6—C8—C9	106.4 (4)
C4—N4—C5	107.4 (3)	N6—C8—H8	126.8
C4—N4—H4A	126.3	C9—C8—H8	126.8
C5—N4—H4A	126.3	C8—C9—N5	108.8 (4)
C7—N5—C9	105.5 (3)	C8—C9—H9	125.6
C7—N5—Cu1	126.3 (2)	N5—C9—H9	125.6
$N3^{i}$—Cu1—N1—C1	1.5 (3)	N3—Cu1—N5—C9	−95.5 (3)
N3—Cu1—N1—C1	−178.5 (3)	$N5^{i}$—Cu1—N5—C9	−51 (8)
N5—Cu1—N1—C1	−88.3 (3)	N1—Cu1—N5—C9	174.9 (3)
$N5^{i}$—Cu1—N1—C1	91.7 (3)	$N1^{i}$—Cu1—N5—C9	−5.1 (3)
$N1^{i}$—Cu1—N1—C1	119.8 (3)	C3—N1—C1—N2	−0.1 (4)
$N3^{i}$—Cu1—N1—C3	−173.6 (3)	Cu1—N1—C1—N2	−176.1 (2)
N3—Cu1—N1—C3	6.4 (3)	C2—N2—C1—N1	0.0 (5)
N5—Cu1—N1—C3	96.6 (3)	C1—N2—C2—C3	0.0 (5)
$N5^{i}$—Cu1—N1—C3	−83.4 (3)	N2—C2—C3—N1	0.0 (5)
$N1^{i}$—Cu1—N1—C3	−55.2 (3)	C1—N1—C3—C2	0.1 (5)
$N3^{i}$—Cu1—N3—C4	57 (100)	Cu1—N1—C3—C2	175.9 (3)
N5—Cu1—N3—C4	177.5 (3)	C6—N3—C4—N4	0.0 (4)
$N5^{i}$—Cu1—N3—C4	−2.5 (3)	Cu1—N3—C4—N4	178.8 (2)
N1—Cu1—N3—C4	−91.9 (3)	C5—N4—C4—N3	0.4 (5)

N1^{i}—Cu1—N3—C4	88.1 (3)	C4—N4—C5—C6	−0.6 (5)
N3^{i}—Cu1—N3—C6	−125 (100)	N4—C5—C6—N3	0.5 (5)
N5—Cu1—N3—C6	−4.0 (3)	C4—N3—C6—C5	−0.3 (5)
N5^{i}—Cu1—N3—C6	176.0 (3)	Cu1—N3—C6—C5	−179.1 (3)
N1—Cu1—N3—C6	86.7 (3)	C9—N5—C7—N6	−0.4 (4)
N1^{i}—Cu1—N3—C6	−93.3 (3)	Cu1—N5—C7—N6	177.6 (2)
N3^{i}—Cu1—N5—C7	−93.0 (3)	C8—N6—C7—N5	0.3 (5)
N3—Cu1—N5—C7	87.0 (3)	C7—N6—C8—C9	−0.1 (5)
N5^{i}—Cu1—N5—C7	131 (8)	N6—C8—C9—N5	−0.2 (5)
N1—Cu1—N5—C7	−2.6 (3)	C7—N5—C9—C8	0.3 (5)
N1^{i}—Cu1—N5—C7	177.4 (3)	Cu1—N5—C9—C8	−177.6 (3)
N3^{i}—Cu1—N5—C9	84.5 (3)		

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2D···Cl1	0.90	2.28	3.165 (4)	169
O2—H2C···O1^{ii}	0.88	1.87	2.743 (5)	179
O1—H1C···O1^{iii}	0.91	2.31	2.805 (7)	113
O1—H1B···Cl1^{iv}	0.91	2.31	3.201 (4)	168
N6—H6A···Cl1^{ii}	0.86	2.58	3.383 (4)	156
N4—H4A···Cl1^{v}	0.86	2.36	3.214 (3)	170
N2—H2A···Cl1^{vi}	0.86	2.50	3.320 (4)	161

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+2, −*z*+1; (iv) *x*−1, *y*, *z*; (v) *x*−1, *y*, *z*−1; (vi) −*x*, −*y*+1, −*z*+1.

Fig. 1