Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chlorobenzohydrazide

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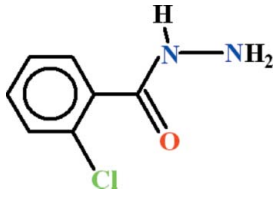
Received 15 February 2012; accepted 23 March 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; R factor = 0.083; wR factor = 0.217; data-to-parameter ratio = 14.6.

The asymmetric unit of the the title compound, $C_7H_7ClN_2O$, contains two molecules in which the chlorophenyl and the formic hydrazide units are almost planar (r.m.s. deviations of 0.0081 and 0.0100 Å, respectively, in one molecule and 0.0069 and 0.0150 Å in the other) and are oriented with respect to each other at dihedral angles of 56.8 (2) and 56.9 (2)°. In the crystal, the molecules are consolidated in the form of polymeric chains extending along [010]. $R_3^3(10)$ ring motifs exist due to N—H···O and N—H···N hydrogen bonds.

Related literature

For a related structure, see: Zareef *et al.* (2006). For graph-set notation, see: Bernstein *et al.* (1995). For the synthetic method, see: Moise *et al.* (2009).



Experimental

Crystal data

$C_7H_7ClN_2O$
M_r = 170.60
Monoclinic, $P2_1/c$
a = 25.7589 (16) Å
b = 4.9618 (3) Å
c = 12.9205 (8) Å
β = 103.648 (3)°
V = 1604.75 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 296 K
0.34 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.979, T_{max} = 0.988
11488 measured reflections
3091 independent reflections
2089 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.217
S = 1.08
3091 reflections
211 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.05	2.825 (5)	149
N2—H2A···N2^{ii}	0.89 (6)	2.27 (6)	3.151 (7)	172 (5)
N3—H3A···O2^{iii}	0.86	2.10	2.812 (5)	140
N4—H4B···N4^{iv}	0.80 (6)	2.40 (6)	3.155 (6)	158 (5)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. The authors also acknowledge the technical support provided by Syed Muhammad Hussain Rizvi of Bana International, Karachi, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2284).

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supplementary materials

Acta Cryst. (2012). E**68**, o1254 [doi:10.1107/S1600536812012640]

2-Chlorobenzohydrazide

Shakeel Ahmad, Abdul Jabbar, Muhammad Tahir Hussain and M. Nawaz Tahir

Comment

The title compound (I), (Fig. 1) has been synthesized as a precursor for the preparation of various substituted triazole derivatives.

We have reported the crystal structures of *N*-2-bromobenzoylhydrazide (Zareef *et al.*, 2006), which is related to (I).

In (I), two molecules are present in the asymmetric unit, which differ slightly from each other geometrically. In one molecule, the chlorophenyl group A (C1–C6/Cl1) and the formic hydrazide moiety B (O1/C7/N1/N2) are planar with r. m. s. deviations of 0.0081Å and 0.0100 Å, respectively. The dihedral angle between A/B is 56.8 (2)°. In second molecule, the chlorophenyl group C (C8–C13/Cl2) and the formic hydrazide moiety D (O2/C14/N3/N4) are also planar with r. m. s. deviation of 0.0069Å and 0.0150 Å, respectively and the dihedral angle between C/D is 56.89 (20)°. Each molecule is connected to symmetry related neighbors through classical intermolecular H–bonding of the N—H···O or N—H···N type (Table 1, Fig. 2) with $R_3^3(10)$ ring motifs (Bernstein *et al.*, 1995) to generate one-dimensional polymeric chains along the [0 1 0] direction.

Experimental

2-Chlorobenzoic acid (3.44 g, 22 mmol) was converted to methyl 2-chlorobenzoate by refluxing in methanol (20 ml) in the presence of a catalytic amount of sulfuric acid. This ester was converted into the title compound, 2-chlorobenzoyl-hydrazide, by refluxing with hydrazine hydrate (80 %, 10 ml) in dry methanol using the literature procedure (Moise *et al.*, 2009). M.p. 379-380K.

Refinement

The coordinates of the H-atoms of the NH_2 groups were refined. The remaining H atoms were positioned geometrically with (N–H = 0.86 and C–H = 0.93 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C, N)$, where $x = 1.2$ for all H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

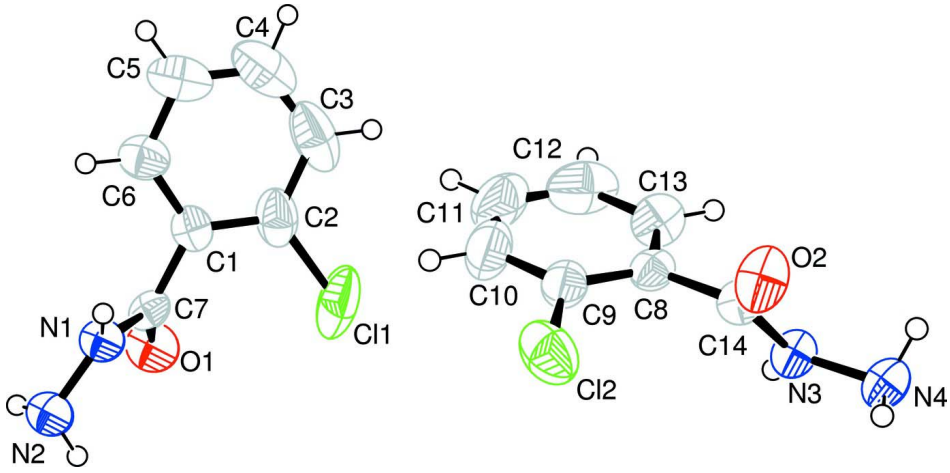

Figure 1

View of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown as small circles of arbitrary radii.

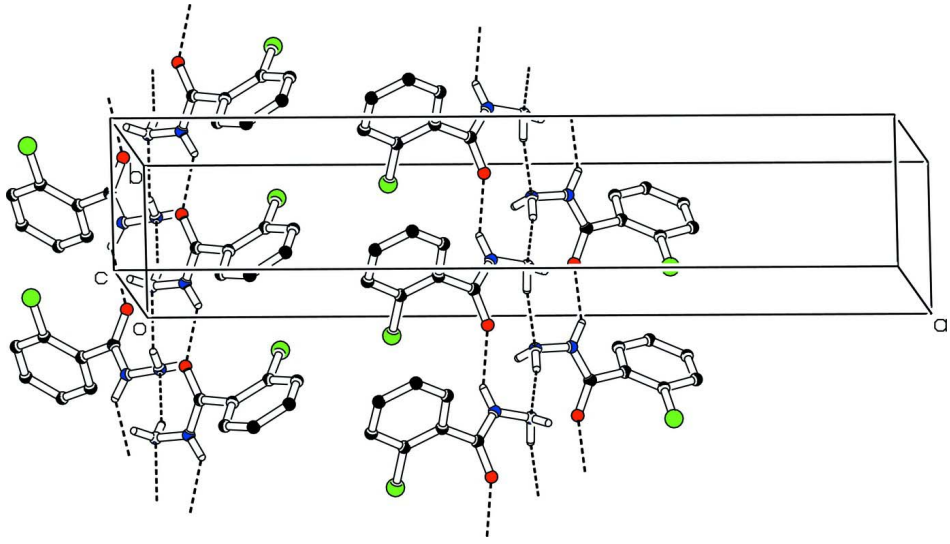

Figure 2

Partial packing diagram (*PLATON*; Spek, 2009) which shows that the molecules form polymeric chains extending along the [0 1 0] direction forming $R_3^3(10)$ ring motifs.

2-Chlorobenzohydrazide

Crystal data

$C_7H_7ClN_2O$
$M_r = 170.60$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 25.7589$ (16) Å
$b = 4.9618$ (3) Å
$c = 12.9205$ (8) Å
$\beta = 103.648$ (3)°
$V = 1604.75$ (17) Å^3
$Z = 8$

$F(000) = 704$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2089 reflections
$\theta = 0.8$–$26.0°$
$\mu = 0.42$ mm^{-1}
$T = 296$ K
Needle, colorless
0.34 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.6 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.979, T_{max} = 0.988
11488 measured reflections
3091 independent reflections
2089 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.0°, θ_{min} = 0.8°
h = −31→31
k = −6→5
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.217
S = 1.08
3091 reflections
211 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 4.8436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}
Cl1	0.32498 (8)	−0.2330 (4)	0.33851 (15)	0.1011 (8)
O1	0.45056 (16)	−0.1875 (7)	0.4080 (3)	0.0622 (15)
N1	0.45512 (15)	0.2531 (8)	0.3704 (3)	0.0425 (12)
N2	0.49903 (18)	0.2265 (9)	0.3247 (4)	0.0481 (16)
C1	0.39139 (18)	0.1163 (10)	0.4673 (4)	0.0432 (17)
C2	0.3415 (2)	0.0002 (13)	0.4426 (4)	0.067 (2)
C3	0.3025 (3)	0.0750 (18)	0.4998 (7)	0.093 (3)
C4	0.3167 (3)	0.256 (2)	0.5818 (7)	0.102 (4)
C5	0.3654 (3)	0.3692 (15)	0.6064 (5)	0.080 (3)
C6	0.4023 (2)	0.3033 (11)	0.5501 (4)	0.0570 (17)
C7	0.43389 (18)	0.0452 (9)	0.4120 (3)	0.0397 (16)
Cl2	0.16784 (6)	0.7856 (3)	−0.01597 (14)	0.0751 (6)
O2	0.04466 (14)	0.6942 (7)	−0.0529 (3)	0.0583 (11)
N3	0.04524 (14)	0.2531 (7)	−0.0886 (3)	0.0399 (12)
N4	−0.00065 (18)	0.2615 (9)	−0.1749 (3)	0.0461 (14)
C8	0.10837 (18)	0.4182 (10)	0.0635 (3)	0.0422 (16)

C9	0.15626 (19)	0.5612 (12)	0.0799 (4)	0.0546 (19)
C10	0.1956 (2)	0.5229 (16)	0.1706 (6)	0.081 (3)
C11	0.1879 (3)	0.348 (2)	0.2458 (6)	0.094 (3)
C12	0.1414 (3)	0.2024 (17)	0.2324 (5)	0.089 (3)
C13	0.1015 (2)	0.2401 (12)	0.1409 (4)	0.0598 (19)
C14	0.06346 (18)	0.4680 (9)	−0.0317 (3)	0.0388 (16)
H1	0.44118	0.41011	0.37190	0.0512*
H2A	0.496 (2)	0.082 (12)	0.283 (4)	0.0577*
H2B	0.523 (2)	0.180 (13)	0.366 (4)	0.0577*
H3	0.26820	0.00263	0.48178	0.1112*
H4	0.29213	0.30088	0.62131	0.1223*
H5	0.37401	0.49282	0.66193	0.0959*
H6	0.43564	0.38561	0.56747	0.0681*
H3A	0.06170	0.10231	−0.07305	0.0475*
H4A	−0.026 (2)	0.298 (11)	−0.141 (4)	0.0556*
H4B	0.006 (2)	0.363 (12)	−0.218 (4)	0.0556*
H10	0.22764	0.61712	0.18040	0.0978*
H11	0.21460	0.32500	0.30771	0.1128*
H12	0.13680	0.08032	0.28412	0.1061*
H13	0.06966	0.14431	0.13169	0.0717*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0933 (12)	0.1012 (16)	0.0900 (12)	−0.0555 (11)	−0.0160 (9)	0.0057 (11)
O1	0.083 (3)	0.0225 (19)	0.088 (3)	−0.0036 (18)	0.034 (2)	−0.0005 (19)
N1	0.055 (2)	0.021 (2)	0.055 (2)	−0.0018 (17)	0.0199 (19)	−0.0024 (18)
N2	0.057 (3)	0.032 (2)	0.060 (3)	−0.002 (2)	0.023 (2)	−0.002 (2)
C1	0.046 (3)	0.034 (3)	0.050 (3)	−0.002 (2)	0.012 (2)	0.013 (2)
C2	0.054 (3)	0.076 (5)	0.067 (3)	−0.018 (3)	0.006 (3)	0.022 (3)
C3	0.053 (3)	0.115 (7)	0.112 (6)	−0.008 (4)	0.023 (4)	0.046 (5)
C4	0.080 (5)	0.129 (8)	0.112 (6)	0.017 (5)	0.052 (5)	0.015 (6)
C5	0.095 (5)	0.082 (5)	0.073 (4)	0.020 (4)	0.042 (4)	0.005 (4)
C6	0.066 (3)	0.048 (3)	0.062 (3)	0.004 (3)	0.025 (3)	0.002 (3)
C7	0.055 (3)	0.022 (3)	0.041 (2)	−0.005 (2)	0.009 (2)	−0.003 (2)
Cl2	0.0653 (9)	0.0623 (10)	0.1057 (12)	−0.0121 (8)	0.0360 (8)	−0.0044 (9)
O2	0.067 (2)	0.0225 (19)	0.075 (2)	0.0001 (16)	−0.0040 (18)	0.0014 (17)
N3	0.049 (2)	0.019 (2)	0.048 (2)	0.0053 (16)	0.0041 (16)	−0.0001 (17)
N4	0.056 (2)	0.034 (3)	0.044 (2)	−0.001 (2)	0.0032 (19)	−0.0001 (19)
C8	0.046 (3)	0.037 (3)	0.042 (2)	0.008 (2)	0.007 (2)	−0.006 (2)
C9	0.046 (3)	0.055 (4)	0.060 (3)	0.009 (2)	0.007 (2)	−0.019 (3)
C10	0.055 (3)	0.094 (6)	0.084 (5)	0.005 (4)	−0.006 (3)	−0.032 (4)
C11	0.079 (5)	0.126 (7)	0.061 (4)	0.036 (5)	−0.017 (4)	−0.020 (5)
C12	0.112 (6)	0.096 (6)	0.056 (4)	0.051 (5)	0.017 (4)	0.020 (4)
C13	0.070 (3)	0.051 (4)	0.056 (3)	0.007 (3)	0.010 (3)	0.010 (3)
C14	0.049 (3)	0.024 (3)	0.044 (2)	−0.002 (2)	0.012 (2)	0.002 (2)

Geometric parameters (Å, º)

Cl1—C2	1.749 (6)	C3—C4	1.371 (13)
Cl2—C9	1.743 (6)	C4—C5	1.342 (11)
O1—C7	1.237 (6)	C5—C6	1.366 (9)
O2—C14	1.228 (6)	C3—H3	0.9300
N1—N2	1.400 (6)	C4—H4	0.9300
N1—C7	1.338 (6)	C5—H5	0.9300
N1—H1	0.8600	C6—H6	0.9300
N2—H2A	0.89 (6)	C8—C14	1.497 (6)
N2—H2B	0.75 (5)	C8—C9	1.395 (7)
N3—C14	1.317 (6)	C8—C13	1.377 (7)
N3—N4	1.421 (6)	C9—C10	1.370 (9)
N3—H3A	0.8600	C10—C11	1.352 (11)
N4—H4A	0.89 (5)	C11—C12	1.374 (12)
N4—H4B	0.80 (6)	C12—C13	1.384 (9)
C1—C2	1.375 (7)	C10—H10	0.9300
C1—C7	1.484 (7)	C11—H11	0.9300
C1—C6	1.394 (7)	C12—H12	0.9300
C2—C3	1.430 (10)	C13—H13	0.9300
N2—N1—C7	123.0 (4)	C5—C4—H4	119.00
C7—N1—H1	118.00	C3—C4—H4	119.00
N2—N1—H1	119.00	C6—C5—H5	120.00
N1—N2—H2B	110 (4)	C4—C5—H5	120.00
H2A—N2—H2B	97 (6)	C1—C6—H6	119.00
N1—N2—H2A	112 (3)	C5—C6—H6	119.00
N4—N3—C14	122.3 (4)	C9—C8—C13	118.5 (4)
C14—N3—H3A	119.00	C13—C8—C14	119.7 (4)
N4—N3—H3A	119.00	C9—C8—C14	121.7 (4)
N3—N4—H4B	107 (4)	Cl2—C9—C10	118.7 (4)
H4A—N4—H4B	121 (5)	C8—C9—C10	120.6 (5)
N3—N4—H4A	101 (3)	Cl2—C9—C8	120.7 (4)
C6—C1—C7	119.3 (4)	C9—C10—C11	120.0 (6)
C2—C1—C7	122.9 (5)	C10—C11—C12	121.2 (7)
C2—C1—C6	117.7 (5)	C11—C12—C13	119.1 (7)
Cl1—C2—C3	119.8 (5)	C8—C13—C12	120.7 (5)
Cl1—C2—C1	120.0 (4)	O2—C14—C8	121.5 (4)
C1—C2—C3	120.2 (6)	N3—C14—C8	115.4 (4)
C2—C3—C4	118.5 (7)	O2—C14—N3	123.1 (4)
C3—C4—C5	121.4 (8)	C9—C10—H10	120.00
C4—C5—C6	120.2 (7)	C11—C10—H10	120.00
C1—C6—C5	121.9 (5)	C10—C11—H11	120.00
O1—C7—C1	123.0 (4)	C12—C11—H11	119.00
N1—C7—C1	115.3 (4)	C11—C12—H12	120.00
O1—C7—N1	121.6 (4)	C13—C12—H12	120.00
C4—C3—H3	121.00	C8—C13—H13	120.00
C2—C3—H3	121.00	C12—C13—H13	120.00
N2—N1—C7—O1	−3.4 (7)	C3—C4—C5—C6	−0.6 (13)

N2—N1—C7—C1	173.6 (4)	C4—C5—C6—C1	−0.9 (10)
N4—N3—C14—O2	−5.1 (7)	C13—C8—C9—Cl2	179.0 (4)
N4—N3—C14—C8	173.5 (4)	C13—C8—C9—C10	0.6 (8)
C7—C1—C2—Cl1	−2.5 (7)	C14—C8—C9—Cl2	−5.3 (7)
C7—C1—C2—C3	179.2 (6)	C14—C8—C9—C10	176.3 (5)
C2—C1—C6—C5	0.7 (8)	C9—C8—C13—C12	−0.5 (8)
C7—C1—C6—C5	−177.6 (5)	C14—C8—C13—C12	−176.3 (5)
C2—C1—C7—O1	−57.1 (7)	C9—C8—C14—O2	−54.9 (7)
C2—C1—C7—N1	125.9 (5)	C9—C8—C14—N3	126.5 (5)
C6—C1—C7—O1	121.1 (5)	C13—C8—C14—O2	120.7 (5)
C6—C1—C7—N1	−55.9 (6)	C13—C8—C14—N3	−57.9 (6)
C6—C1—C2—C3	1.0 (9)	Cl2—C9—C10—C11	−179.3 (6)
C6—C1—C2—Cl1	179.2 (4)	C8—C9—C10—C11	−0.9 (10)
C1—C2—C3—C4	−2.5 (11)	C9—C10—C11—C12	1.2 (12)
Cl1—C2—C3—C4	179.3 (7)	C10—C11—C12—C13	−1.2 (12)
C2—C3—C4—C5	2.3 (13)	C11—C12—C13—C8	0.8 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.05	2.825 (5)	149
N2—H2*A*···N2^{ii}	0.89 (6)	2.27 (6)	3.151 (7)	172 (5)
N3—H3*A*···O2^{iii}	0.86	2.10	2.812 (5)	140
N4—H4*B*···N4^{iv}	0.80 (6)	2.40 (6)	3.155 (6)	158 (5)

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