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2-(3-Methyl-2-oxo-1,2-dihydroquinoxalin-1-yl)-acetic acid dihydrate

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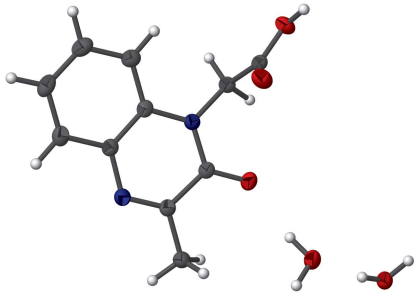
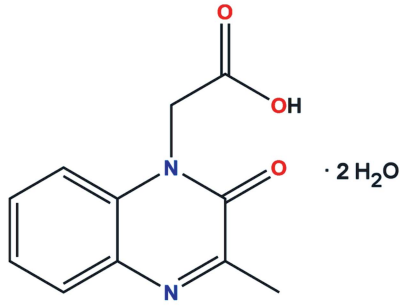
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{11}H_{10}N_2O_3\cdot 2H_2O$, the constituent atoms of the dihydroquinoxaline moiety deviate from the mean plane of the unit by +0.0572 (8) to −0.0874 (8) Å while the acetic acid substituent is nearly orthogonal to this plane. The crystal packing consists of corrugated layers constructed by O—H···O, O—H···N and C—H···O hydrogen bonds, which also involve the lattice water molecules. O—H···O hydrogen bonds and π–π stacking interactions hold these layers together.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives have attracted interest because of their biological and pharmacological activities (Ramli *et al.*, 2014; Ramli & Essassi, 2015). As a continuation of our work on the synthesis of 3-methylquinoxalin-2-one derivatives in order to evaluate their pharmacological activities (Ramli *et al.* 2010*a*,*b*, 2011, 2013, 2017, 2018; Caleb *et al.*, 2016; Missioui *et al.*, 2017), the title compound (Fig. 1) was synthesized and its crystal structure is reported here.

The dihydroquinoxaline portion of the molecule is not completely planar, as can be seen from the displacements [+0.0572 (8) (N2) to −0.0874 (8) Å (C9)] from the mean plane (r.m.s. deviation = 0.0411 Å) of the bicyclic unit. In addition, a puckering analysis of the heterocyclic ring gave the parameters Q = 0.0893 (11) Å. θ = 72.7 (7)° and φ = 205.6 (8)°. The N2/C10/C11 unit is inclined to the mean plane of the dihydroquinoxaline portion by 82.91 (8)° while the C11/O2/O3 unit is rotated from the N2/C10/C11 unit by 8.4 (2)°.

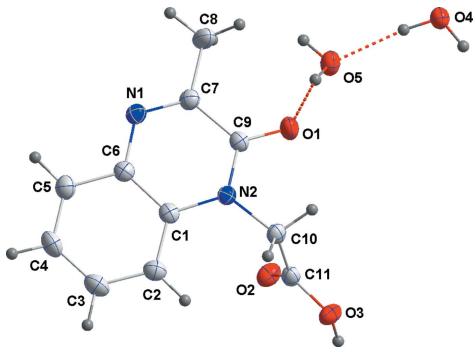


Figure 1
The asymmetric unit of the title compound with labelling scheme and 50% probability ellipsoids. The O—H···O hydrogen bonds (Table 1) involving the lattice water molecules are shown as dashed lines.

In the crystal, the main molecule, together with the lattice water molecules, form zigzag chains along the *b*-axis direction through O3—H3*A*···O4 and O4—H4*B*···N1 hydrogen bonds (Table 1 and Fig. 2). The chains are connected into corrugated layers parallel to the bc plane by O5—H5*B*···O1 hydrogen bonds and the layers are then associated through inversion-related pairs of O5—H5*A*···O2 hydrogen bonds and head-to-tail π–π stacking interactions between inversion-related dihydroquinoxaline moieties [centroid–centroid distance = 3.5295 (7) Å; dihedral angle = 3.33 (5)°; symmetry code 1 − *x*, 1 − *y*, 2 − *z*; Table 1 and Fig. 3].

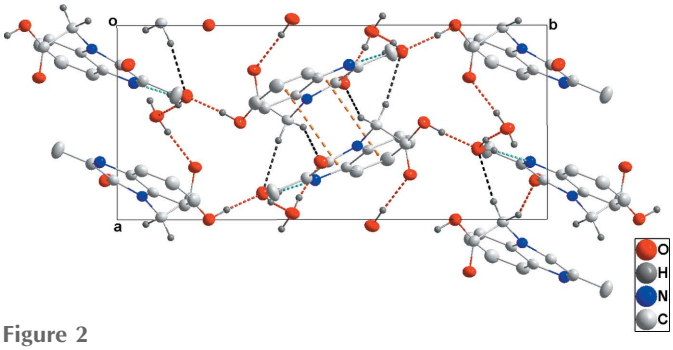


Figure 2
Packing diagram of the title compound viewed along the *c* axis with intermolecular interactions shown as in Fig. 2.

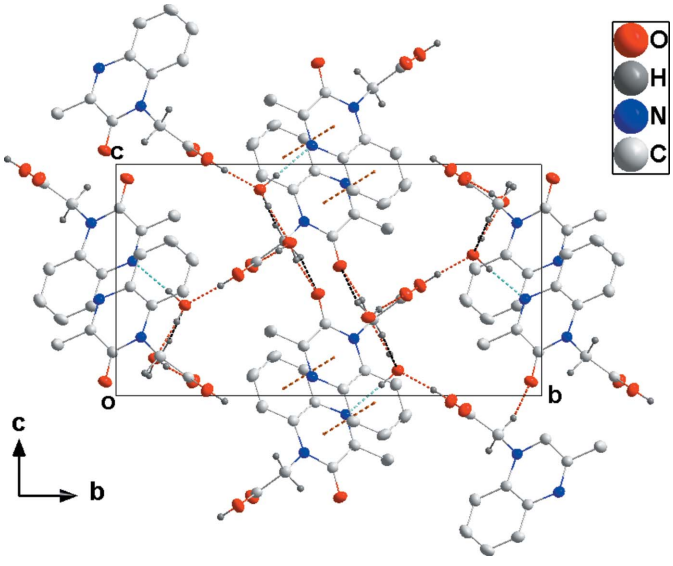


Figure 3
Packing diagram of the title compound viewed along the *a* axis with O—H···O, O—H···N and C—H···O hydrogen bonds (Table 1) shown, respectively, as red, light-blue and black dashed lines. The π–π stacking interactions are shown as orange dashed lines

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O4^{i}	0.87	1.67	2.5400 (12)	176
C10—H10*A*···O1^{ii}	0.986 (15)	2.334 (15)	3.2524 (14)	154.7 (11)
C10—H10*B*···O4^{ii}	0.989 (15)	2.369 (15)	3.3520 (14)	172.1 (12)
O4—H4*A*···O5	0.87	1.83	2.6966 (11)	171
O4—H4*B*···N1^{iii}	0.87	1.97	2.8344 (13)	171
O5—H5*A*···O2^{iv}	0.87	1.96	2.8287 (12)	175
O5—H5*B*···O1	0.87	1.96	2.8177 (11)	170

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{10}N_2O_3{\cdot}2H_2O$
M_r	254.24
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, *b*, *c* (Å)	7.7306 (5), 16.8048 (11), 9.3113 (6)
β (°)	102.001 (2)
V (Å^3)	1183.20 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.97
Crystal size (mm)	0.21 × 0.15 × 0.08
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.86, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9051, 2359, 2163
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.031, 0.082, 1.02
No. of reflections	2359
No. of parameters	200
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

1 g of ethyl 2- (3-methyl-2-oxoquinoxalin-1(2*H*)-yl) acetate in 15 ml of a mixture of H_2O/EtOH (50:50 *v*/*v*) and 5 ml of 10% NaOH were stirred at room temperature for 1 h. After completion of the reaction (monitored by TLC), the medium

was acidified with HCl (3 *M*). The precipitate obtained was crystallized from ethanol to afford colourless crystals in 55% yield.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180882 [https://doi.org/10.1107/S2414314618008829]

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Crystal data

$C_{11}H_{10}N_2O_3·2H_2O$
M_r = 254.24
Monoclinic, $P2_1/n$
a = 7.7306 (5) Å
b = 16.8048 (11) Å
c = 9.3113 (6) Å
β = 102.001 (2)°
V = 1183.20 (13) Å^3
Z = 4
$F(000)$ = 536
D_x = 1.427 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 7699 reflections
θ = 5.3–74.5°
μ = 0.97 mm^{-1}
T = 150 K
Block, colourless
0.21 × 0.15 × 0.08 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.86, T_{max} = 0.93
9051 measured reflections
2359 independent reflections
2163 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 74.5°, θ_{min} = 5.3°
h = −9→9
k = −18→21
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.02
2359 reflections
200 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.3842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL2018* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0073 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The C-bound H atoms were located in a difference Fourier map and refined freely. As independent refinement of the H atoms attached to oxygen gave unsatisfactory geometries, particularly for H3A, the positions of these atoms were idealized and they were included as riding contributions with U_{iso}(H) = 1.5 U_{eq}(O).
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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to oxygen were placed in locations derived from a difference map, their coordinates were adjusted to give O—H = 0.87 Å and were included as riding contributions.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.29637 (11)	0.52589 (5)	0.56060 (9)	0.0275 (2)
O2	0.23074 (10)	0.31882 (5)	0.56225 (9)	0.0284 (2)
O3	0.49925 (11)	0.28631 (5)	0.52405 (9)	0.0275 (2)
H3A	0.449130	0.245199	0.475735	0.041*
N1	0.20378 (12)	0.53983 (6)	0.91754 (10)	0.0229 (2)
N2	0.37927 (11)	0.44157 (5)	0.75315 (10)	0.0198 (2)
C1	0.35985 (13)	0.41602 (6)	0.89191 (12)	0.0201 (2)
C2	0.42554 (15)	0.34290 (7)	0.95184 (13)	0.0258 (3)
H2	0.487 (2)	0.3067 (10)	0.8985 (18)	0.038 (4)*
C3	0.39994 (17)	0.32121 (8)	1.08882 (14)	0.0308 (3)
H3	0.443 (2)	0.2703 (10)	1.1277 (17)	0.038 (4)*
C4	0.31163 (17)	0.37105 (8)	1.16941 (13)	0.0307 (3)
H4	0.297 (2)	0.3572 (10)	1.2651 (19)	0.040 (4)*
C5	0.24815 (15)	0.44351 (7)	1.11188 (13)	0.0262 (3)
H5	0.188 (2)	0.4802 (9)	1.1667 (16)	0.033 (4)*
C6	0.27024 (14)	0.46666 (6)	0.97219 (12)	0.0209 (2)
C7	0.21326 (15)	0.55956 (7)	0.78503 (12)	0.0227 (2)
C8	0.1406 (2)	0.63718 (8)	0.72178 (14)	0.0340 (3)
H8A	0.226 (2)	0.6636 (11)	0.672 (2)	0.052 (5)*
H8B	0.029 (2)	0.6263 (10)	0.6467 (19)	0.044 (4)*
H8C	0.109 (3)	0.6704 (12)	0.798 (2)	0.058 (5)*
C9	0.29624 (14)	0.50840 (6)	0.68914 (12)	0.0209 (2)
C10	0.48739 (14)	0.39698 (7)	0.67001 (12)	0.0217 (2)
H10A	0.5238 (19)	0.4329 (9)	0.5980 (16)	0.028 (3)*
H10B	0.592 (2)	0.3753 (9)	0.7384 (16)	0.031 (4)*
C11	0.38939 (14)	0.32998 (7)	0.58021 (11)	0.0214 (2)
O4	0.13522 (11)	0.66176 (5)	0.10852 (9)	0.0262 (2)
H4A	0.091253	0.642524	0.180009	0.039*
H4B	0.144293	0.623447	0.047672	0.039*
O5	0.03254 (10)	0.59251 (5)	0.33839 (8)	0.0271 (2)
H5A	−0.048291	0.617676	0.373004	0.041*

H5B	0.113130	0.576940	0.412786	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0292 (4)	0.0330 (5)	0.0219 (4)	0.0051 (3)	0.0089 (3)	0.0055 (3)
O2	0.0208 (4)	0.0309 (4)	0.0330 (4)	−0.0003 (3)	0.0045 (3)	−0.0072 (4)
O3	0.0254 (4)	0.0258 (4)	0.0329 (5)	0.0021 (3)	0.0099 (3)	−0.0062 (3)
N1	0.0235 (5)	0.0236 (5)	0.0208 (4)	0.0005 (4)	0.0027 (4)	−0.0018 (4)
N2	0.0186 (4)	0.0208 (4)	0.0203 (4)	−0.0003 (3)	0.0043 (3)	−0.0004 (4)
C1	0.0169 (5)	0.0222 (5)	0.0204 (5)	−0.0037 (4)	0.0015 (4)	−0.0003 (4)
C2	0.0245 (5)	0.0238 (6)	0.0282 (6)	0.0003 (4)	0.0036 (4)	0.0014 (5)
C3	0.0311 (6)	0.0279 (6)	0.0314 (6)	0.0007 (5)	0.0024 (5)	0.0082 (5)
C4	0.0323 (6)	0.0362 (7)	0.0231 (6)	−0.0028 (5)	0.0045 (5)	0.0085 (5)
C5	0.0253 (6)	0.0310 (6)	0.0219 (5)	−0.0022 (5)	0.0040 (4)	−0.0008 (5)
C6	0.0188 (5)	0.0219 (5)	0.0208 (5)	−0.0022 (4)	0.0012 (4)	−0.0009 (4)
C7	0.0235 (5)	0.0230 (5)	0.0209 (5)	0.0002 (4)	0.0028 (4)	−0.0013 (4)
C8	0.0493 (8)	0.0278 (6)	0.0250 (6)	0.0129 (6)	0.0079 (6)	0.0016 (5)
C9	0.0191 (5)	0.0221 (5)	0.0211 (5)	−0.0016 (4)	0.0036 (4)	0.0010 (4)
C10	0.0187 (5)	0.0239 (5)	0.0231 (5)	0.0015 (4)	0.0060 (4)	0.0004 (4)
C11	0.0217 (5)	0.0230 (5)	0.0196 (5)	0.0028 (4)	0.0049 (4)	0.0031 (4)
O4	0.0319 (4)	0.0259 (4)	0.0219 (4)	0.0014 (3)	0.0080 (3)	0.0012 (3)
O5	0.0235 (4)	0.0364 (5)	0.0216 (4)	0.0037 (3)	0.0051 (3)	0.0016 (3)

Geometric parameters (Å, º)

O1—C9	1.2326 (14)	C4—H4	0.950 (17)
O2—C11	1.2173 (14)	C5—C6	1.4017 (16)
O3—C11	1.3107 (13)	C5—H5	0.978 (16)
O3—H3A	0.8703	C7—C9	1.4785 (15)
N1—C7	1.2944 (15)	C7—C8	1.4919 (16)
N1—C6	1.3878 (15)	C8—H8A	0.989 (19)
N2—C9	1.3673 (14)	C8—H8B	1.011 (18)
N2—C1	1.3989 (14)	C8—H8C	0.98 (2)
N2—C10	1.4589 (14)	C10—C11	1.5092 (15)
C1—C2	1.4005 (16)	C10—H10A	0.986 (15)
C1—C6	1.4064 (16)	C10—H10B	0.989 (15)
C2—C3	1.3797 (18)	O4—H4A	0.8702
C2—H2	0.972 (16)	O4—H4B	0.8701
C3—C4	1.3941 (19)	O5—H5A	0.8700
C3—H3	0.961 (17)	O5—H5B	0.8700
C4—C5	1.3788 (18)		
C11—O3—H3A	113.3	N1—C7—C9	122.98 (10)
C7—N1—C6	119.11 (10)	N1—C7—C8	120.60 (10)
C9—N2—C1	121.59 (9)	C9—C7—C8	116.42 (10)
C9—N2—C10	117.35 (9)	C7—C8—H8A	110.1 (11)
C1—N2—C10	121.05 (9)	C7—C8—H8B	108.2 (10)

N2—C1—C2	122.52 (10)	H8A—C8—H8B	108.6 (14)
N2—C1—C6	117.68 (10)	C7—C8—H8C	110.1 (12)
C2—C1—C6	119.80 (10)	H8A—C8—H8C	112.3 (15)
C3—C2—C1	119.36 (11)	H8B—C8—H8C	107.4 (15)
C3—C2—H2	119.2 (10)	O1—C9—N2	121.60 (10)
C1—C2—H2	121.4 (10)	O1—C9—C7	122.39 (10)
C2—C3—C4	121.28 (11)	N2—C9—C7	115.96 (9)
C2—C3—H3	118.5 (9)	N2—C10—C11	113.59 (9)
C4—C3—H3	120.2 (9)	N2—C10—H10A	108.8 (8)
C5—C4—C3	119.73 (11)	C11—C10—H10A	105.1 (8)
C5—C4—H4	118.5 (10)	N2—C10—H10B	109.2 (8)
C3—C4—H4	121.7 (10)	C11—C10—H10B	109.4 (9)
C4—C5—C6	120.23 (11)	H10A—C10—H10B	110.6 (12)
C4—C5—H5	121.6 (9)	O2—C11—O3	125.23 (10)
C6—C5—H5	118.2 (9)	O2—C11—C10	124.50 (10)
N1—C6—C5	118.61 (10)	O3—C11—C10	110.27 (9)
N1—C6—C1	121.80 (10)	H4A—O4—H4B	108.7
C5—C6—C1	119.59 (10)	H5A—O5—H5B	107.6

C9—N2—C1—C2	171.99 (10)	C2—C1—C6—C5	0.25 (15)
C10—N2—C1—C2	−7.10 (15)	C6—N1—C7—C9	−1.59 (16)
C9—N2—C1—C6	−7.91 (14)	C6—N1—C7—C8	179.03 (11)
C10—N2—C1—C6	172.99 (9)	C1—N2—C9—O1	−171.44 (10)
N2—C1—C2—C3	−179.34 (10)	C10—N2—C9—O1	7.68 (15)
C6—C1—C2—C3	0.55 (16)	C1—N2—C9—C7	10.93 (14)
C1—C2—C3—C4	−0.71 (18)	C10—N2—C9—C7	−169.95 (9)
C2—C3—C4—C5	0.03 (19)	N1—C7—C9—O1	176.13 (11)
C3—C4—C5—C6	0.79 (18)	C8—C7—C9—O1	−4.46 (16)
C7—N1—C6—C5	−175.57 (10)	N1—C7—C9—N2	−6.26 (16)
C7—N1—C6—C1	5.03 (16)	C8—C7—C9—N2	173.15 (10)
C4—C5—C6—N1	179.66 (10)	C9—N2—C10—C11	−93.62 (11)
C4—C5—C6—C1	−0.93 (17)	C1—N2—C10—C11	85.51 (12)
N2—C1—C6—N1	−0.45 (15)	N2—C10—C11—O2	8.67 (16)
C2—C1—C6—N1	179.64 (10)	N2—C10—C11—O3	−171.79 (9)
N2—C1—C6—C5	−179.85 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O4^{i}	0.87	1.67	2.5400 (12)	176
C10—H10*A*···O1^{ii}	0.986 (15)	2.334 (15)	3.2524 (14)	154.7 (11)
C10—H10*B*···O4^{ii}	0.989 (15)	2.369 (15)	3.3520 (14)	172.1 (12)
O4—H4*A*···O5	0.87	1.83	2.6966 (11)	171
O4—H4*B*···N1^{iii}	0.87	1.97	2.8344 (13)	171
O5—H5*A*···O2^{iv}	0.87	1.96	2.8287 (12)	175
O5—H5*B*···O1	0.87	1.96	2.8177 (11)	170

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