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catena-Poly[[diaquacobalt(II)]-μ_3-5-aminoisophthalato-$\kappa^4O,O':O'':N$]

Yan Yang,[a,c] Ming-Hua Zeng,[b] Shu-Hua Zhang[b] and Hong Liang[a,b]*

[a]College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, People's Republic of China, [b]Department of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China, and [c]Department of Chemistry and Biology, Yulin Teachers' College, Yulin 537000, People's Republic of China
Correspondence e-mail: hliang@mailbox.gxnu.edu.cn

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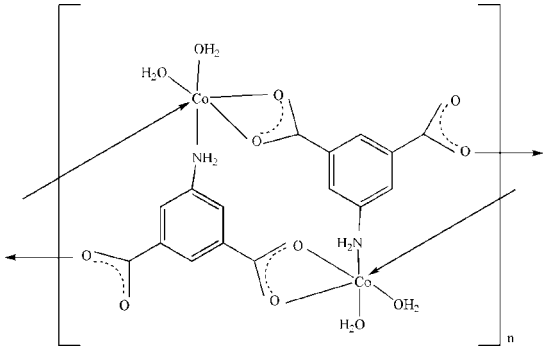
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.096; data-to-parameter ratio = 13.0.

In the title compound, $[Co(C_8H_5NO_4)(H_2O)_2]_n$, the Co^{II} atom is coordinated in a distorted octahedral fashion by three O atoms of two carboxylate groups (one in a monodentate and one in a 1,3-bidentate mode) from two 5-aminoisophthalate anions, one N atom from the third 5-aminoisophthalate anion and two aqua ligands. The complex consists of an infinite neutral railroad-like linear polymer, which is packed into a three-dimensional framework through intricate N—H···O and O—H···O hydrogen bonding.

Related literature

For related literature, see: Dobson & Gerkin (1998); Hagrman *et al.* (1999); Janiak (2003); Moulton & Zaworotko (2001); Wu *et al.* (2002).



Experimental

Crystal data

$[Co(C_8H_5NO_4)(H_2O)_2]$
M_r = 274.10
Triclinic, $P\overline{1}$
a = 6.4168 (4) Å
b = 8.0919 (4) Å
c = 10.1493 (7) Å
α = 113.184 (1)°
β = 99.946 (3)°
γ = 98.995 (2)°
V = 462.28 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.87 mm^{-1}
T = 153 (2) K
0.15 × 0.13 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.767, T_{max} = 0.835
4523 measured reflections
2110 independent reflections
1854 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.096
S = 1.01
2110 reflections
162 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1^{i}	2.0266 (18)	Co—O3^{ii}	2.0848 (18)
Co—O5	2.037 (2)	Co—N	2.109 (2)
Co—O6	2.0516 (19)	Co—O4^{ii}	2.1631 (18)
O1^{i}—Co—O5	88.76 (8)	O5—Co—N	176.15 (8)
O1^{i}—Co—O6	95.54 (8)	O6—Co—N	84.80 (9)
O5—Co—O6	91.77 (8)	O3^{ii}—Co—N	90.27 (8)
O1^{i}—Co—O3^{ii}	162.55 (8)	O1^{i}—Co—O4^{ii}	100.38 (7)
O5—Co—O3^{ii}	92.15 (8)	O5—Co—O4^{ii}	90.18 (8)
O6—Co—O3^{ii}	101.84 (8)	O6—Co—O4^{ii}	163.99 (8)
O1^{i}—Co—N	89.82 (8)	O3^{ii}—Co—O4^{ii}	62.20 (7)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O2^{iii}	0.92	2.38	3.275 (3)	165
N—H0B···O3^{iii}	0.92	2.09	2.991 (3)	165
O5—H5B···O1^{iv}	0.84 (6)	1.90 (6)	2.738 (3)	175 (5)
O5—H5A···O2^{v}	0.98 (4)	1.89 (5)	2.802 (3)	154 (4)
O6—H6B···O2^{i}	0.86 (5)	1.92 (5)	2.755 (3)	162 (4)
O6—H6A···O4^{vi}	0.97 (4)	1.87 (5)	2.791 (3)	158 (4)

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: KJ2057).

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supplementary materials

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catena-Poly[[diaquacobalt(II)]-μ_3-5-aminoisophthalato-$\kappa^4O,O':O'':N$]

Y. Yang, M.-H. Zeng, S.-H. Zhang and H. Liang

Comment

In recent years, a large number of metal-organic compounds have been prepared because of the fascinating structural and topological features of these compounds and their potential applications as functional materials, such as catalysts, optical materials and molecule-based magnets (Hagrman *et al.*, 1999; Moulton & Zaworotko, 2001; Janiak, 2003). 5-aminoisophthalic acid (AIP) (Dobson *et al.*, 1998), a polydentate organic ligand containing an amino group and two carboxyl groups, can be used as a bridging and/or terminal ligand. In this field, studies have been focused on organic-inorganic hybrid materials containing N-donor rigid heteroaromatic ligands, such as pyrazine or 4,4' –bipyridine. However, much less work has been carried out to investigate transition metal polymers containing aminobenzoic acid ligands. Using AIP, we have hydrothermally prepared the title compound, $[Co(AIP)(H_2O)_2]_n$. The title complex consists of one Co(II) cation, one 5-aminoisophthalate anion and two coordinated water molecules (Fig. 1). Each AIP ligand employs its two carboxylate groups and one amino group to coordinate to three different metal centers. Each Co^{II} center possesses a distorted six-coordinated octahedral geometry, defined by three carboxyl oxygen atoms, one from a monodentate and two from a 1,3-bidentate AIP^{2-} ligands, one nitrogen atom from the third 5-aminoisophthalate anion and two aqua ligands. The mean Co—O (carboxyl) bond distance is 2.092 (18) Å, which is slightly shorter than that in $[Co(C_8NH_5O_4)(H_2O)]_n$ (2.109 (2) Å) (Wu *et al.*, 2002). This difference is probably attributed to the different coordination modes of the ligands. The most interesting feature is that the AIP ligands link cobalt centers in different ways to produces two different subrings A and B, which are both 14-membered rings located on an inversion centre, with Co—Co distances of 7.917 (3) and 7.689 (3) Å, respectively. THe difference between the rings is that the A ring is closed by bidentate carboxylate groups and the B ring by monodentate carboxylate groups. Together they form an open railroad-like framework polymer, running in the c direction. Each linear polymer is connected into a three-dimensional supramolecular network by intermolecular hydrogen bonds among aqua ligands, the oxygen atoms of carboxylate groups and amino groups (Table 2).

Experimental

Cobalt chlorine hexahydrate (0.119 g, 0.5 mmol), and 5-aminoisophthalic acid (0.0905 g, 0.5 mmol) were dissolved in water (9 ml). The solution was placed in a 15-ml Teflon-lined, stainless-steel, Parr bomb. The bomb was heated at 433 K for 6 days. The cooled-down mixture yielded light red crystals; these were washed with water and then dried in air (yield *ca* 70%, based on Co).

Refinement

The water H atoms were located on difference Fourier maps; their coordinates and isotropic displacement parameters were refined freely. All other H atoms were positioned geometrically and refined with a riding model, with C—H distances of 0.95 (aromatic) Å, N—H distances of 0.92 Å, and with $U_{iso}(H) = 1.2U_{eq}(C \text{ \& } N)$.

Figures

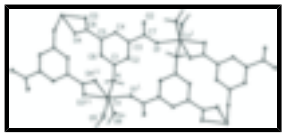

Fig. 1. A view of (I), showing 30% probability displacement ellipsoids. Symmetry codes:(i)-*x* + 1,-*y* + 1,-*z* + 2; (ii) −*x* + 1,-*y* + 1,-*z* + 1.

catena-Poly[[diaquacobalt(II)]-μ$_3$-5-aminoisophthalato- κ^4*O*,*O*':*O*'':*N*]

Crystal data

$[Co(C_8H_5NO_4)(H_2O)_2]$	$Z = 2$
$M_r = 274.10$	$F_{000} = 278$
Triclinic, $P\overline{1}$	$D_x = 1.969$ Mg m^{-3}
$a = 6.4168$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 8.0919$ (4) Å	Cell parameters from 3976 reflections
$c = 10.1493$ (7) Å	$\theta = 3.3$–27.5º
$\alpha = 113.184$ (1)º	$\mu = 1.87$ mm^{-1}
$\beta = 99.946$ (3)º	$T = 153$ (2) K
$\gamma = 98.995$ (2)º	PRISM, green
$V = 462.28$ (5) Å^3	0.15 × 0.13 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2110 independent reflections
Radiation source: Rotating Anode	1854 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 153$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.3$º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.767$, $T_{max} = 0.835$	$k = -10 \rightarrow 10$
4523 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.466P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.55$ e Å^{-3}

2110 reflections

162 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.75$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.007 (1)

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}
Co	0.20196 (5)	0.75115 (5)	0.80493 (3)	0.01298 (14)
O1	0.6666 (3)	0.2413 (3)	0.9957 (2)	0.0187 (4)
O2	0.9520 (3)	0.2510 (3)	0.8966 (2)	0.0244 (4)
O3	0.8351 (3)	0.2502 (3)	0.4037 (2)	0.0201 (4)
O4	0.5073 (3)	0.2130 (3)	0.2718 (2)	0.0187 (4)
O5	0.2461 (3)	1.0316 (3)	0.9070 (2)	0.0218 (4)
O6	−0.1152 (3)	0.7068 (3)	0.8195 (2)	0.0213 (4)
N	0.1401 (4)	0.4592 (3)	0.7069 (2)	0.0165 (4)
H0A	0.0745	0.4180	0.7659	0.020*
H0B	0.0389	0.4155	0.6172	0.020*
C1	0.3142 (4)	0.3725 (4)	0.6807 (3)	0.0166 (5)
C2	0.4366 (4)	0.3411 (4)	0.7907 (3)	0.0184 (5)
H2	0.3983	0.3718	0.8823	0.022*
C3	0.6145 (4)	0.2655 (4)	0.7693 (3)	0.0164 (5)
C4	0.6708 (4)	0.2196 (4)	0.6345 (3)	0.0171 (5)
H4	0.7907	0.1656	0.6182	0.021*
C5	0.5498 (4)	0.2536 (4)	0.5241 (3)	0.0171 (5)
C6	0.3705 (4)	0.3267 (4)	0.5456 (3)	0.0169 (5)
H6	0.2857	0.3456	0.4687	0.020*
C7	0.7566 (4)	0.2477 (3)	0.8947 (3)	0.0168 (5)
C8	0.6319 (4)	0.2345 (4)	0.3918 (3)	0.0162 (5)
H5A	0.150 (7)	1.097 (6)	0.873 (5)	0.047 (12)*
H5B	0.373 (9)	1.097 (7)	0.930 (6)	0.068 (16)*
H6A	−0.227 (7)	0.764 (6)	0.792 (5)	0.046 (11)*
H6B	−0.093 (8)	0.719 (6)	0.910 (5)	0.051 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0108 (2)	0.0199 (2)	0.0113 (2)	0.00718 (13)	0.00536 (13)	0.00760 (15)
O1	0.0169 (9)	0.0289 (10)	0.0139 (9)	0.0070 (8)	0.0050 (7)	0.0119 (8)
O2	0.0179 (10)	0.0403 (12)	0.0225 (10)	0.0142 (9)	0.0086 (8)	0.0171 (10)
O3	0.0170 (9)	0.0317 (11)	0.0153 (9)	0.0092 (8)	0.0066 (7)	0.0119 (9)
O4	0.0155 (9)	0.0282 (10)	0.0154 (9)	0.0086 (8)	0.0066 (7)	0.0101 (8)
O5	0.0183 (10)	0.0240 (10)	0.0248 (10)	0.0088 (8)	0.0079 (8)	0.0100 (9)
O6	0.0144 (9)	0.0321 (11)	0.0203 (10)	0.0091 (8)	0.0076 (8)	0.0116 (9)
N	0.0137 (10)	0.0207 (11)	0.0157 (10)	0.0061 (8)	0.0050 (8)	0.0075 (9)
C1	0.0157 (12)	0.0180 (12)	0.0171 (12)	0.0051 (10)	0.0069 (10)	0.0071 (11)
C2	0.0170 (12)	0.0230 (12)	0.0175 (12)	0.0055 (10)	0.0076 (10)	0.0096 (11)
C3	0.0167 (12)	0.0198 (12)	0.0141 (12)	0.0050 (10)	0.0056 (10)	0.0079 (11)
C4	0.0157 (12)	0.0179 (12)	0.0202 (13)	0.0071 (10)	0.0072 (10)	0.0087 (11)
C5	0.0175 (12)	0.0209 (12)	0.0135 (12)	0.0043 (10)	0.0074 (10)	0.0068 (11)
C6	0.0172 (12)	0.0197 (12)	0.0148 (12)	0.0054 (10)	0.0045 (10)	0.0080 (11)
C7	0.0194 (13)	0.0172 (12)	0.0169 (12)	0.0076 (10)	0.0069 (10)	0.0085 (11)
C8	0.0174 (12)	0.0186 (12)	0.0144 (12)	0.0064 (10)	0.0046 (10)	0.0081 (11)

Geometric parameters (Å, °)

Co—O1^{i}	2.0266 (18)	O6—H6B	0.86 (5)
Co—O5	2.037 (2)	N—C1	1.418 (3)
Co—O6	2.0516 (19)	N—H0A	0.9200
Co—O3^{ii}	2.0848 (18)	N—H0B	0.9200
Co—N	2.109 (2)	C1—C2	1.382 (4)
Co—O4^{ii}	2.1631 (18)	C1—C6	1.401 (4)
Co—C8^{ii}	2.452 (3)	C2—C3	1.387 (4)
O1—C7	1.274 (3)	C2—H2	0.9500
O1—Co^{i}	2.0266 (18)	C3—C4	1.397 (4)
O2—C7	1.246 (3)	C3—C7	1.503 (3)
O3—C8	1.270 (3)	C4—C5	1.394 (4)
O3—Co^{ii}	2.0848 (18)	C4—H4	0.9500
O4—C8	1.267 (3)	C5—C6	1.385 (4)
O4—Co^{ii}	2.1632 (18)	C5—C8	1.487 (3)
O5—H5A	0.98 (4)	C6—H6	0.9500
O5—H5B	0.84 (6)	C8—Co^{ii}	2.452 (3)
O6—H6A	0.97 (4)		
O1^{i}—Co—O5	88.76 (8)	Co—N—H0A	107.3
O1^{i}—Co—O6	95.54 (8)	C1—N—H0B	107.3
O5—Co—O6	91.77 (8)	Co—N—H0B	107.3
O1^{i}—Co—O3^{ii}	162.55 (8)	H0A—N—H0B	106.9
O5—Co—O3^{ii}	92.15 (8)	C2—C1—C6	119.4 (2)
O6—Co—O3^{ii}	101.84 (8)	C2—C1—N	120.4 (2)

O1^{i}—Co—N	89.82 (8)	C6—C1—N	120.1 (2)
O5—Co—N	176.15 (8)	C1—C2—C3	121.0 (2)
O6—Co—N	84.80 (9)	C1—C2—H2	119.5
O3^{ii}—Co—N	90.27 (8)	C3—C2—H2	119.5
O1^{i}—Co—O4^{ii}	100.38 (7)	C2—C3—C4	119.7 (2)
O5—Co—O4^{ii}	90.18 (8)	C2—C3—C7	120.1 (2)
O6—Co—O4^{ii}	163.99 (8)	C4—C3—C7	120.1 (2)
O3^{ii}—Co—O4^{ii}	62.20 (7)	C5—C4—C3	119.6 (2)
N—Co—O4^{ii}	93.60 (8)	C5—C4—H4	120.2
O1^{i}—Co—C8^{ii}	131.37 (8)	C3—C4—H4	120.2
O5—Co—C8^{ii}	92.79 (8)	C6—C5—C4	120.3 (2)
O6—Co—C8^{ii}	132.92 (9)	C6—C5—C8	120.0 (2)
O3^{ii}—Co—C8^{ii}	31.18 (8)	C4—C5—C8	119.2 (2)
N—Co—C8^{ii}	90.83 (8)	C5—C6—C1	120.0 (2)
O4^{ii}—Co—C8^{ii}	31.08 (8)	C5—C6—H6	120.0
C7—O1—Co^{i}	130.14 (17)	C1—C6—H6	120.0
C8—O3—Co^{ii}	90.60 (15)	O2—C7—O1	125.6 (2)
C8—O4—Co^{ii}	87.15 (15)	O2—C7—C3	118.7 (2)
Co—O5—H5A	123 (3)	O1—C7—C3	115.7 (2)
Co—O5—H5B	117 (4)	O4—C8—O3	119.8 (2)
H5A—O5—H5B	106 (4)	O4—C8—C5	121.9 (2)
Co—O6—H6A	128 (3)	O3—C8—C5	118.2 (2)
Co—O6—H6B	99 (3)	O4—C8—Co^{ii}	61.77 (13)
H6A—O6—H6B	114 (4)	O3—C8—Co^{ii}	58.23 (13)
C1—N—Co	120.08 (17)	C5—C8—Co^{ii}	171.81 (19)
C1—N—H0A	107.3		
O1^{i}—Co—N—C1	−74.77 (19)	C2—C1—C6—C5	−1.1 (4)
O6—Co—N—C1	−170.35 (19)	N—C1—C6—C5	175.6 (2)
O3^{ii}—Co—N—C1	87.78 (19)	Co^{i}—O1—C7—O2	3.9 (4)
O4^{ii}—Co—N—C1	25.62 (19)	Co^{i}—O1—C7—C3	−171.81 (17)
C8^{ii}—Co—N—C1	56.61 (19)	C2—C3—C7—O2	−152.1 (3)
Co—N—C1—C2	86.4 (3)	C4—C3—C7—O2	22.9 (4)
Co—N—C1—C6	−90.3 (3)	C2—C3—C7—O1	23.9 (4)
C6—C1—C2—C3	0.2 (4)	C4—C3—C7—O1	−161.1 (2)
N—C1—C2—C3	−176.5 (2)	Co^{ii}—O4—C8—O3	−4.7 (2)
C1—C2—C3—C4	−0.2 (4)	Co^{ii}—O4—C8—C5	171.5 (2)
C1—C2—C3—C7	174.8 (2)	Co^{ii}—O3—C8—O4	4.8 (3)
C2—C3—C4—C5	1.2 (4)	Co^{ii}—O3—C8—C5	−171.5 (2)
C7—C3—C4—C5	−173.8 (2)	C6—C5—C8—O4	−27.7 (4)
C3—C4—C5—C6	−2.2 (4)	C4—C5—C8—O4	160.3 (2)
C3—C4—C5—C8	169.8 (2)	C6—C5—C8—O3	148.5 (3)
C4—C5—C6—C1	2.1 (4)	C4—C5—C8—O3	−23.4 (4)
C8—C5—C6—C1	−169.8 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0A···O2^{iii}	0.92	2.38	3.275 (3)	165
N—H0B···O3^{iii}	0.92	2.09	2.991 (3)	165
O5—H5B···O1^{iv}	0.84 (6)	1.90 (6)	2.738 (3)	175 (5)
O5—H5A···O2^{v}	0.98 (4)	1.89 (5)	2.802 (3)	154 (4)
O6—H6B···O2^{i}	0.86 (5)	1.92 (5)	2.755 (3)	162 (4)
O6—H6A···O4^{vi}	0.97 (4)	1.87 (5)	2.791 (3)	158 (4)

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

Fig. 1