

Hexaaquacobalt(II) 2,2'-[naphthalene-1,8-diylbis(oxy)]diacetate dihydrate

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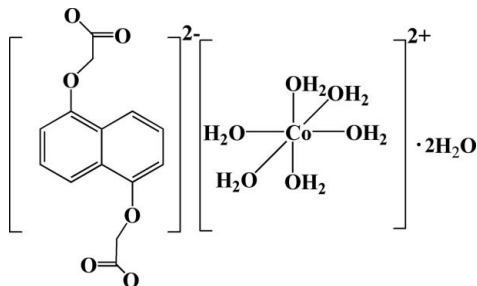
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 10.4.

In the title compound, $[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{14}\text{H}_{10}\text{O}_6)\cdot 2\text{H}_2\text{O}$, the 2,2'-[naphthalene-1,8-diylbis(oxy)]diacetate dianion L is not coordinated to the Co^{II} ion. The asymmetric unit contains half of the L dianion, half of a $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$ cation (both molecules being completed by inversion symmetry), and one water molecule. The crystal packing features $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding between the carboxylate groups, the aqua ligands and the hydrate water molecules.

Related literature

In recent years, metal complexes have been synthesized with potential applications in molecular sorption, electrical conductivity, catalysis, magnetism, non-linear optics and molecular sensing, see: James (2003); Murray *et al.* (2009); Karmakar *et al.* (2009); Kurmoo (2009); Bradshaw *et al.* (2005). The 5-carboxymethoxy-naphthalene-1-yl(oxy)-acetate ligand can provide a dominant packing feature and it often controls the supramolecular assembly, see: Desiraju (2007). For Cd complexes with different co-ligands, see: Deka *et al.* (2011); Li *et al.* (2012) and for Zn complexes, see: Mondal *et al.* (2008).



Experimental

Crystal data

$[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{14}\text{H}_{10}\text{O}_6)\cdot 2\text{H}_2\text{O}$	$\gamma = 64.911$ (8) $^\circ$
$M_r = 477.28$	$V = 486.8$ (3) Å ³
Triclinic, $P\bar{1}$	$Z = 1$
$a = 6.377$ (2) Å	Mo $K\alpha$ radiation
$b = 6.642$ (2) Å	$\mu = 0.95$ mm ⁻¹
$c = 12.979$ (5) Å	$T = 293$ K
$\alpha = 79.669$ (10) $^\circ$	$0.30 \times 0.28 \times 0.25$ mm
$\beta = 79.963$ (11) $^\circ$	

Data collection

Siemens CCD area-detector diffractometer	3126 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	1678 independent reflections
$T_{\min} = 0.731$, $T_{\max} = 1.000$	1605 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$\Delta\rho_{\text{max}} = 0.37$ e Å ⁻³
$S = 1.09$	$\Delta\rho_{\text{min}} = -0.48$ e Å ⁻³
1678 reflections	
161 parameters	
12 restraints	

Table 1

Selected bond lengths (Å).

Co1—O4	2.056 (2)	Co1—O6	2.093 (2)
Co1—O5	2.0792 (17)		

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O6—H6C \cdots O7 ⁱ	0.96 (2)	1.76 (3)	2.723 (3)	174 (3)
O6—H6D \cdots O7 ⁱⁱ	0.93 (2)	1.83 (3)	2.751 (3)	171 (3)
O5—H5A \cdots O2 ⁱⁱⁱ	0.93 (3)	1.96 (3)	2.850 (3)	159 (2)
O5—H5B \cdots O3 ^{iv}	0.94 (3)	1.87 (2)	2.783 (3)	165 (2)
O7—H7A \cdots O3 ^v	0.92 (2)	1.82 (3)	2.736 (3)	171 (3)
O7—H7B \cdots O2 ^{vi}	0.93 (3)	1.89 (3)	2.780 (3)	158 (2)

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: VM2185).

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supplementary materials

Acta Cryst. (2013). E69, m103–m104 [doi:10.1107/S1600536813000512]

Hexaaquacobalt(II) 2,2'-[naphthalene-1,8-diylbis(oxy)]diacetate dihydrate**Hui Fang Shi, Tao Wu, Peng Gang Jiang, Zhi Hao and Miao Miao Zhang****Comment**

In recent years, metal complexes have been synthesized with potential applications in molecular sorption, electrical conductivity, catalysis, magnetism, nonlinear optics, and molecular sensing (James, 2003; Murray *et al.*, 2009; Kurmoo, 2009; Karmakar *et al.*, 2009; Bradshaw *et al.*, 2005). The *LH2* ligand (5-carboxymethoxy-naphthalen-1-yl-oxy)-acetic acid has received our attention because it can provide a dominant packing feature and it often controls the supramolecular assembly (Desiraju *et al.*, 2007). At present, many of its metal complexes have already been reported, but most are focused on Cd complexes (Deka *et al.*, 2011; Li *et al.*, 2012) and Zn complexes (Li *et al.*, 2012) with different co-ligands such as 2,2-bipyridine or 1,10-phenanthroline (phen). In the present paper, we hydrothermally synthesized a novel coordination complex constructed by Co^{II}, *L* and water molecules and determined its crystal structure (Fig. 1).

The asymmetric unit of the complex consists of a half ligand *L*, a half Co^{II} ion complexed with three water molecules and one additional water molecule. The Co^{II} center is octahedrally coordinated by six water molecules. The two carboxylate arms of the *LH2* ligand lie in the same plane as the naphthalene ring. The hydrogen atoms of the water molecular and the oxygen atoms which are coordinated by Co^{II} are involved in hydrogen bonding with the oxygen atoms of the carboxylate group (Table 2, Fig. 2). In this case a sheet-like structure is formed.

Experimental

The ligand *LH2* was synthesized according to the procedure published by Mondal *et al.* (2008).

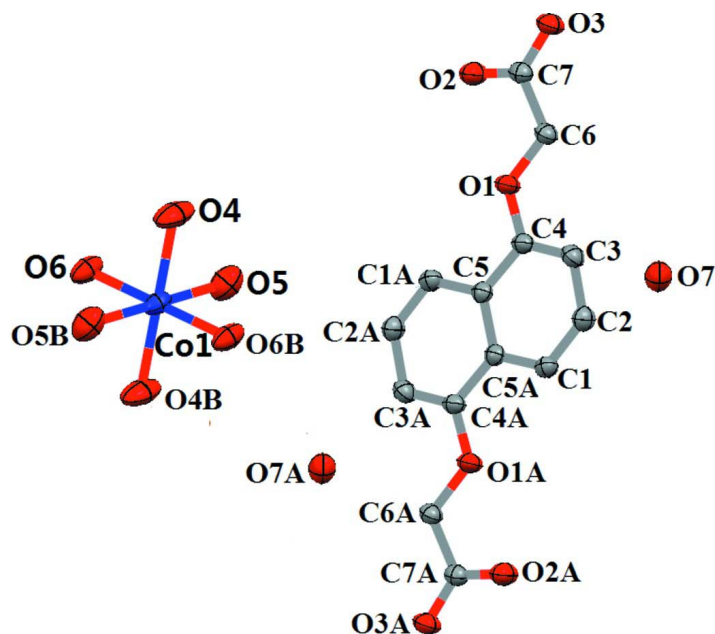
A mixture of Co(NO₃)₂·6H₂O (0.05 mmol, 0.015 g), *L* (0.05 mmol, 0.013 g), water (1 ml) and DMF (1 ml) was heated at 393 K in a Teflon-lined autoclave for three days, followed by slow cooling to room temperature. The resulting pink block crystals were filtered off and washed with distilled water.

Refinement

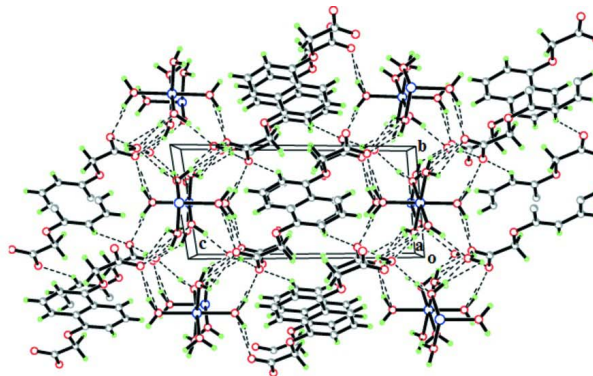
The H atoms on the ligands were positioned geometrically and refined as riding [C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. Hydrogen atoms of the water molecules were located in the Fourier difference maps and refined with restraints for the O–H distances and H–O–H angles.

Computing details

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).


Figure 1

The molecular structure of (I), with the atomic numbering scheme and displacement ellipsoids at the 50% probability level (H atoms omitted for clarity) [symmetry codes: (A) $-x + 1, -y + 1, -z + 1$, (B) $-x, -y + 1, -z$].


Figure 2

Three dimensional supramolecular architecture constructed by intermolecular hydrogen bonds. The dotted lines indicate the hydrogen bonds.

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Crystal data

$[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{14}\text{H}_{10}\text{O}_6) \cdot 2\text{H}_2\text{O}$

$M_r = 477.28$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.377\ (2)\ \text{\AA}$

$b = 6.642\ (2)\ \text{\AA}$

$c = 12.979\ (5)\ \text{\AA}$

$\alpha = 79.669\ (10)^\circ$

$\beta = 79.963\ (11)^\circ$

$\gamma = 64.911\ (8)^\circ$

$V = 486.8\ (3)\ \text{\AA}^3$

$Z = 1$

$F(000) = 249$

$D_x = 1.628\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1414 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 0.95\ \text{mm}^{-1}$

$T = 293$ K
Block, pink

$0.30 \times 0.28 \times 0.25$ mm

Data collection

Siemens CCD area-detector diffractometer	3126 measured reflections
Radiation source: fine-focus sealed tube	1678 independent reflections
Graphite monochromator	1605 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.018$
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 3.4^\circ$
$T_{\text{min}} = 0.731$, $T_{\text{max}} = 1.000$	$h = -7 \rightarrow 7$
	$k = -7 \rightarrow 7$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.1833P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
1678 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
161 parameters	$\Delta\rho_{\text{max}} = 0.37 \text{ e } \text{\AA}^{-3}$
12 restraints	$\Delta\rho_{\text{min}} = -0.48 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.7658 (2)	0.7636 (3)	0.38143 (11)	0.0299 (3)
O2	0.9252 (3)	0.9376 (3)	0.20485 (12)	0.0374 (4)
O3	1.0787 (3)	1.1022 (3)	0.28675 (12)	0.0331 (4)
C5	0.5504 (3)	0.5494 (3)	0.45495 (15)	0.0222 (4)
C4	0.6759 (3)	0.6729 (3)	0.47211 (15)	0.0239 (4)
C3	0.6996 (3)	0.6953 (3)	0.57172 (16)	0.0275 (4)
H3	0.7826	0.7752	0.5816	0.033*
C2	0.5966 (3)	0.5961 (4)	0.65934 (16)	0.0282 (4)
H2	0.6115	0.6131	0.7269	0.034*
C1	0.4761 (3)	0.4762 (3)	0.64724 (15)	0.0257 (4)
H1	0.4113	0.4111	0.7062	0.031*
C6	0.8919 (3)	0.8899 (3)	0.39326 (15)	0.0254 (4)
H6A	1.0262	0.7948	0.4304	0.031*
H6B	0.7933	1.0118	0.4343	0.031*

C7	0.9709 (3)	0.9827 (3)	0.28607 (16)	0.0255 (4)
Co1	0.0000	0.5000	0.0000	0.03054 (16)
O7	0.5069 (3)	1.0109 (3)	0.83972 (12)	0.0387 (4)
O5	0.0045 (3)	0.5054 (3)	0.15926 (12)	0.0407 (4)
O6	0.3582 (3)	0.3007 (3)	-0.00989 (14)	0.0504 (5)
H6C	0.403 (6)	0.199 (5)	0.0532 (16)	0.075 (10)*
H6D	0.411 (6)	0.214 (5)	-0.0654 (18)	0.087 (12)*
H5A	-0.021 (6)	0.630 (4)	0.191 (2)	0.076 (10)*
H5B	0.013 (5)	0.385 (4)	0.211 (2)	0.067 (9)*
H7A	0.638 (3)	0.982 (5)	0.7915 (19)	0.062 (9)*
H7B	0.380 (4)	1.029 (6)	0.807 (2)	0.085 (11)*
O4	0.0880 (5)	0.7707 (3)	-0.03180 (15)	0.0629 (6)
H4A	0.2060	0.7419	-0.0738	0.094*
H4B	-0.043 (5)	0.897 (9)	-0.061 (4)	0.27 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0387 (8)	0.0372 (9)	0.0246 (7)	-0.0275 (7)	-0.0017 (6)	-0.0010 (6)
O2	0.0532 (9)	0.0444 (10)	0.0277 (8)	-0.0338 (8)	-0.0041 (7)	-0.0010 (7)
O3	0.0386 (8)	0.0346 (9)	0.0351 (8)	-0.0253 (7)	-0.0006 (6)	-0.0033 (6)
C5	0.0206 (8)	0.0211 (10)	0.0238 (9)	-0.0079 (7)	-0.0025 (7)	-0.0012 (7)
C4	0.0240 (9)	0.0241 (10)	0.0250 (10)	-0.0128 (8)	-0.0005 (7)	-0.0005 (8)
C3	0.0293 (10)	0.0295 (11)	0.0299 (11)	-0.0170 (8)	-0.0041 (8)	-0.0044 (8)
C2	0.0337 (10)	0.0323 (11)	0.0223 (10)	-0.0157 (9)	-0.0039 (8)	-0.0049 (8)
C1	0.0270 (9)	0.0288 (11)	0.0229 (10)	-0.0143 (8)	-0.0006 (7)	-0.0014 (8)
C6	0.0285 (9)	0.0254 (10)	0.0274 (10)	-0.0160 (8)	-0.0027 (8)	-0.0027 (8)
C7	0.0260 (9)	0.0231 (10)	0.0284 (11)	-0.0117 (8)	-0.0013 (8)	-0.0023 (8)
Co1	0.0457 (3)	0.0224 (2)	0.0229 (2)	-0.01429 (18)	-0.00138 (17)	-0.00230 (16)
O7	0.0332 (8)	0.0466 (10)	0.0329 (9)	-0.0127 (7)	-0.0026 (7)	-0.0068 (7)
O5	0.0655 (11)	0.0304 (9)	0.0257 (8)	-0.0194 (8)	-0.0046 (7)	-0.0026 (7)
O6	0.0605 (11)	0.0451 (11)	0.0359 (10)	-0.0118 (9)	-0.0026 (8)	-0.0085 (8)
O4	0.1209 (18)	0.0469 (12)	0.0407 (10)	-0.0550 (13)	-0.0101 (11)	0.0015 (9)

Geometric parameters (\AA , $^\circ$)

O1—C4	1.371 (2)	C6—H6B	0.9700
O1—C6	1.427 (2)	Co1—O4	2.056 (2)
O2—C7	1.257 (3)	Co1—O4 ⁱⁱ	2.056 (2)
O3—C7	1.253 (3)	Co1—O5 ⁱⁱ	2.0792 (17)
C5—C1 ⁱ	1.414 (3)	Co1—O5	2.0792 (17)
C5—C5 ⁱ	1.425 (4)	Co1—O6	2.093 (2)
C5—C4	1.431 (3)	Co1—O6 ⁱⁱ	2.093 (2)
C4—C3	1.368 (3)	O7—H7A	0.921 (17)
C3—C2	1.413 (3)	O7—H7B	0.932 (17)
C3—H3	0.9300	O5—H5A	0.931 (17)
C2—C1	1.362 (3)	O5—H5B	0.933 (17)
C2—H2	0.9300	O6—H6C	0.962 (17)
C1—C5 ⁱ	1.414 (3)	O6—H6D	0.929 (18)
C1—H1	0.9300	O4—H4A	0.8200

C6—C7	1.510 (3)	O4—H4B	0.97 (2)
C6—H6A	0.9700		
C4—O1—C6	116.91 (15)	O4—Co1—O4 ⁱⁱ	180.0
C1 ⁱ —C5—C5 ⁱ	119.8 (2)	O4—Co1—O5 ⁱⁱ	91.63 (7)
C1 ⁱ —C5—C4	122.26 (18)	O4 ⁱⁱ —Co1—O5 ⁱⁱ	88.37 (7)
C5 ⁱ —C5—C4	117.9 (2)	O4—Co1—O5	88.37 (7)
C3—C4—O1	124.53 (18)	O4 ⁱⁱ —Co1—O5	91.63 (7)
C3—C4—C5	121.27 (18)	O5 ⁱⁱ —Co1—O5	180.00 (11)
O1—C4—C5	114.19 (17)	O4—Co1—O6	86.53 (10)
C4—C3—C2	119.38 (19)	O4 ⁱⁱ —Co1—O6	93.47 (10)
C4—C3—H3	120.3	O5 ⁱⁱ —Co1—O6	91.34 (7)
C2—C3—H3	120.3	O5—Co1—O6	88.66 (7)
C1—C2—C3	121.62 (18)	O4—Co1—O6 ⁱⁱ	93.47 (10)
C1—C2—H2	119.2	O4 ⁱⁱ —Co1—O6 ⁱⁱ	86.53 (10)
C3—C2—H2	119.2	O5 ⁱⁱ —Co1—O6 ⁱⁱ	88.66 (7)
C2—C1—C5 ⁱ	119.98 (18)	O5—Co1—O6 ⁱⁱ	91.34 (7)
C2—C1—H1	120.0	O6—Co1—O6 ⁱⁱ	180.00 (7)
C5 ⁱ —C1—H1	120.0	H7A—O7—H7B	110 (2)
O1—C6—C7	109.63 (16)	Co1—O5—H5A	126.3 (19)
O1—C6—H6A	109.7	Co1—O5—H5B	123.8 (18)
C7—C6—H6A	109.7	H5A—O5—H5B	109 (2)
O1—C6—H6B	109.7	Co1—O6—H6C	112.4 (19)
C7—C6—H6B	109.7	Co1—O6—H6D	113 (2)
H6A—C6—H6B	108.2	H6C—O6—H6D	107 (2)
O3—C7—O2	125.29 (19)	Co1—O4—H4A	109.5
O3—C7—C6	115.32 (17)	Co1—O4—H4B	107 (4)
O2—C7—C6	119.39 (18)	H4A—O4—H4B	111.3

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O6—H6C...O7 ⁱ	0.96 (2)	1.76 (3)	2.723 (3)	174 (3)
O6—H6D...O7 ⁱⁱⁱ	0.93 (2)	1.83 (3)	2.751 (3)	171 (3)
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O5—H5B...O3 ^v	0.94 (3)	1.87 (2)	2.783 (3)	165 (2)
O7—H7A...O3 ^{vi}	0.92 (2)	1.82 (3)	2.736 (3)	171 (3)
O7—H7B...O2 ^{vii}	0.93 (3)	1.89 (3)	2.780 (3)	158 (2)

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