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## Structure Reports

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# *trans,trans,trans*-Diaquabis(nicotinamide- $\kappa$ N)bis(2-nitrobenzoato- $\kappa$ O)-copper(II)

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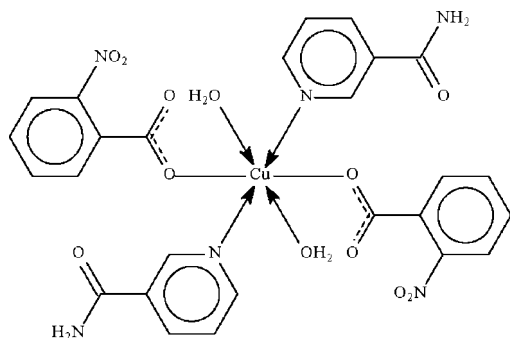
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 Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.111; data-to-parameter ratio = 10.9.

The water-coordinated metal atom in the title compound,  $[\text{Cu}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$ , lies on a center of inversion in an all-*trans* octahedral environment with slight distortions. The molecule interacts with adjacent molecules through  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming a layered network parallel to (010).

## Related literature

There are recent examples of diaquadi(arylcarboxylato)-di(nicotinamide)metal(II) compounds, see: Hökelek & Necefoğlu (2007*a,b*); Hökelek *et al.* (2007); Koksharova *et al.* (2006); Şahin *et al.* (2007*a, b*); Stachova *et al.* (2006); Çaylak *et al.* (2007); Zhang *et al.* (2009).



## Experimental

## Crystal data

 $[\text{Cu}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$ 
 $M_r = 676.05$ 

 Monoclinic,  $P2_1/n$ 
 $a = 7.9582$  (3) Å

 $b = 18.7044$  (6) Å

 $c = 9.8573$  (2) Å

 $\beta = 104.012$  (2)°

 $V = 1423.63$  (8) Å<sup>3</sup>
 $Z = 2$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.84$  mm<sup>-1</sup>
 $T = 295$  K

 $0.45 \times 0.20 \times 0.16$  mm

## Data collection

 Bruker SMART area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.557$ ,  $T_{\max} = 0.877$ 

 7295 measured reflections  
 2507 independent reflections  
 2069 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.111$   
 $S = 1.12$   
 2507 reflections  
 229 parameters  
 4 restraints

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.46$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Cu1—O1	1.995 (2)	Cu1—O1w	2.537 (3)
Cu1—N2	2.006 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H11 $\cdots$ O2 <sup>i</sup>	0.85 (4)	1.92 (2)	2.726 (4)	159 (4)
O1w—H12 $\cdots$ O5 <sup>ii</sup>	0.85 (4)	2.11 (2)	2.934 (2)	165 (3)
N3—H32 $\cdots$ O2 <sup>iii</sup>	0.85 (4)	2.15 (2)	2.929 (4)	152 (4)
N3—H31 $\cdots$ O5 <sup>iv</sup>	0.85 (4)	2.11 (2)	2.926 (4)	161 (4)

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

We thank the Foundation of Jiangsu Provincial Key Program of Physical Chemistry in Yangzhou University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2894).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m427-m428 [ doi:10.1107/S1600536809007995 ]

***trans,trans,trans*-Diaquabis(nicotinamide- $\kappa$ N)bis(2-nitrobenzoato- $\kappa$ O)copper(II)**

**K.-L. Zhang, Q.-L. Xie and S. W. Ng**

**Experimental**

A water/methanol (1:1 *v/v*) solution (3 ml) of copper nitrate trihydrate (0.174 g, 0.6 mmol) was added to a water/methanol (1:1 *v/v*) solution (3 ml) of 2-nitrobenzoic acid (0.100 g, 0.6 mmol), sodium hydroxide (0.024 g 0.6 mmol) and nicotinamide (0.073 g, 0.6 mmol). Blue block were obtained after several days (yield: 40%). CH&N elemental analysis: calc. for C<sub>26</sub>H<sub>24</sub>CuN<sub>6</sub>O<sub>12</sub>: C 46.19, H 3.59, N 12.43%; found: C 46.37, H 3.41, N 12.60%.

**Refinement**

Carbon-bound H atoms were placed in calculated positions and were allowed to ride on the parent atoms. The oxygen-bound ones were located in a difference Fourier map, and were refined with distance restraints N–H, O–H = 0.85±0.01 Å; an additional H··H 1.39 + 0.01 Å restraint was used. Their displacement parameters were freely refined.

**Figures**

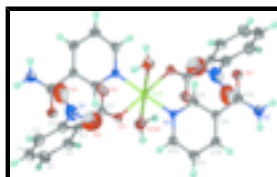


Fig. 1. Thermal ellipsoid plot of Cu(H<sub>2</sub>O)<sub>2</sub>(C<sub>7</sub>H<sub>4</sub>NO<sub>4</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radii.

***trans,trans,trans*-Diaquabis(nicotinamide-  $\kappa$ N)bis(2-nitrobenzoato- $\kappa$ O)copper(II)**

*Crystal data*

[Cu(C<sub>7</sub>H<sub>4</sub>NO<sub>4</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

*M<sub>r</sub>* = 676.05

Monoclinic, *P*2<sub>1</sub>/*n*

Hall symbol: -*P* 2<sub>1</sub>/*n*

*a* = 7.9582 (3) Å

*b* = 18.7044 (6) Å

*c* = 9.8573 (2) Å

$\beta$  = 104.012 (2)°

*V* = 1423.63 (8) Å<sup>3</sup>

*Z* = 2

*F*<sub>000</sub> = 694

*D<sub>x</sub>* = 1.577 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation

$\lambda$  = 0.71073 Å

Cell parameters from 3858 reflections

$\theta$  = 2.2–25.0°

$\mu$  = 0.84 mm<sup>-1</sup>

*T* = 295 K

Block, blue

0.45 × 0.20 × 0.16 mm

## Data collection

Bruker SMART area-detector diffractometer	2507 independent reflections
Radiation source: medium-focus sealed tube	2069 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.036$
$T = 295$ K	$\theta_{\text{max}} = 25.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.557$ , $T_{\text{max}} = 0.877$	$k = -14 \rightarrow 22$
7295 measured reflections	$l = -11 \rightarrow 11$

## Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 1.8061P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
2507 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
229 parameters	$\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$
4 restraints	$\Delta\rho_{\text{min}} = -0.46 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.5000	0.5000	0.5000	0.02960 (19)
O1	0.6141 (3)	0.41263 (12)	0.4483 (2)	0.0329 (5)
O2	0.3896 (3)	0.37179 (15)	0.2856 (3)	0.0531 (7)
O3	0.3215 (5)	0.2416 (3)	0.0916 (5)	0.1123 (16)
O4	0.3942 (5)	0.2153 (2)	0.3108 (5)	0.1137 (16)
O5	0.0632 (4)	0.49124 (18)	0.8331 (3)	0.0642 (9)
O1W	0.8082 (4)	0.54476 (16)	0.5876 (3)	0.0493 (7)
H11	0.772 (6)	0.5753 (19)	0.637 (4)	0.067 (15)*
H12	0.883 (5)	0.522 (2)	0.647 (4)	0.073 (16)*
N1	0.4256 (5)	0.2375 (2)	0.2043 (5)	0.0624 (10)
N2	0.4917 (3)	0.45491 (14)	0.6829 (3)	0.0290 (6)
N3	0.1614 (5)	0.4274 (2)	1.0283 (3)	0.0539 (9)
H31	0.081 (4)	0.442 (2)	1.065 (4)	0.069 (14)*
H32	0.241 (4)	0.403 (2)	1.082 (4)	0.075 (16)*
C1	0.6639 (4)	0.32322 (17)	0.2924 (3)	0.0297 (7)

C2	0.6033 (5)	0.26281 (19)	0.2137 (4)	0.0372 (8)
C3	0.7038 (6)	0.2231 (2)	0.1461 (4)	0.0496 (10)
H3	0.6578	0.1835	0.0929	0.057 (12)*
C4	0.8740 (6)	0.2428 (2)	0.1585 (4)	0.0552 (11)
H4	0.9433	0.2170	0.1125	0.065 (13)*
C5	0.9406 (5)	0.3009 (2)	0.2392 (4)	0.0503 (10)
H5	1.0561	0.3135	0.2495	0.067 (14)*
C6	0.8366 (4)	0.3409 (2)	0.3053 (4)	0.0395 (8)
H6	0.8834	0.3801	0.3591	0.038 (10)*
C7	0.5449 (4)	0.37176 (17)	0.3480 (3)	0.0289 (7)
C8	0.3508 (4)	0.46333 (17)	0.7327 (3)	0.0306 (7)
H8	0.2571	0.4882	0.6785	0.029 (9)*
C9	0.3378 (4)	0.43678 (18)	0.8613 (3)	0.0304 (7)
C10	0.4781 (5)	0.3999 (2)	0.9403 (4)	0.0434 (9)
H10	0.4747	0.3819	1.0276	0.048 (11)*
C11	0.6240 (5)	0.3899 (2)	0.8889 (4)	0.0461 (10)
H11A	0.7186	0.3644	0.9402	0.062 (13)*
C12	0.6259 (4)	0.41833 (19)	0.7608 (4)	0.0364 (8)
H12A	0.7241	0.4120	0.7268	0.032 (9)*
C13	0.1760 (5)	0.4530 (2)	0.9067 (4)	0.0419 (9)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0375 (3)	0.0296 (3)	0.0256 (3)	0.0041 (3)	0.0153 (2)	0.0014 (2)
O1	0.0378 (13)	0.0332 (12)	0.0292 (12)	0.0057 (10)	0.0110 (10)	-0.0034 (10)
O2	0.0318 (14)	0.0677 (19)	0.0557 (17)	0.0093 (13)	0.0028 (12)	-0.0203 (14)
O3	0.061 (2)	0.178 (5)	0.091 (3)	-0.027 (3)	0.006 (2)	-0.071 (3)
O4	0.094 (3)	0.118 (4)	0.140 (4)	-0.030 (3)	0.049 (3)	0.048 (3)
O5	0.0489 (16)	0.107 (3)	0.0436 (15)	0.0375 (17)	0.0254 (13)	0.0285 (16)
O1W	0.0454 (16)	0.0586 (19)	0.0407 (16)	0.0032 (14)	0.0045 (13)	-0.0056 (14)
N1	0.060 (2)	0.051 (2)	0.079 (3)	-0.0141 (19)	0.023 (2)	-0.022 (2)
N2	0.0302 (14)	0.0338 (15)	0.0250 (14)	0.0037 (12)	0.0104 (11)	-0.0004 (12)
N3	0.046 (2)	0.084 (3)	0.039 (2)	0.020 (2)	0.0237 (17)	0.0225 (18)
C1	0.0332 (18)	0.0310 (17)	0.0259 (17)	0.0033 (14)	0.0089 (14)	0.0021 (14)
C2	0.040 (2)	0.0354 (19)	0.037 (2)	0.0021 (16)	0.0110 (16)	0.0003 (16)
C3	0.066 (3)	0.037 (2)	0.046 (2)	0.007 (2)	0.014 (2)	-0.0094 (18)
C4	0.069 (3)	0.054 (3)	0.050 (3)	0.025 (2)	0.027 (2)	0.003 (2)
C5	0.041 (2)	0.052 (2)	0.062 (3)	0.0077 (19)	0.0224 (19)	0.005 (2)
C6	0.036 (2)	0.037 (2)	0.045 (2)	0.0019 (16)	0.0094 (16)	-0.0030 (17)
C7	0.0341 (18)	0.0287 (17)	0.0254 (17)	0.0025 (14)	0.0104 (14)	0.0028 (14)
C8	0.0326 (18)	0.0327 (18)	0.0270 (17)	0.0055 (15)	0.0082 (14)	0.0006 (14)
C9	0.0335 (18)	0.0333 (18)	0.0269 (17)	0.0033 (14)	0.0123 (14)	0.0022 (14)
C10	0.050 (2)	0.054 (2)	0.0303 (18)	0.0127 (19)	0.0168 (17)	0.0124 (17)
C11	0.043 (2)	0.056 (2)	0.042 (2)	0.0189 (19)	0.0159 (18)	0.0153 (18)
C12	0.0342 (19)	0.041 (2)	0.038 (2)	0.0087 (16)	0.0168 (16)	0.0057 (16)
C13	0.042 (2)	0.053 (2)	0.0347 (19)	0.0079 (18)	0.0167 (17)	0.0081 (17)

## supplementary materials

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### Geometric parameters (Å, °)

Cu1—O1 <sup>i</sup>	1.995 (2)	C1—C6	1.389 (5)
Cu1—O1	1.995 (2)	C1—C7	1.507 (4)
Cu1—N2 <sup>i</sup>	2.006 (3)	C2—C3	1.377 (5)
Cu1—N2	2.006 (3)	C3—C4	1.380 (6)
Cu1—O1 <sub>w</sub>	2.537 (3)	C3—H3	0.9300
O1—C7	1.266 (4)	C4—C5	1.375 (6)
O2—C7	1.240 (4)	C4—H4	0.9300
O3—N1	1.216 (5)	C5—C6	1.389 (5)
O4—N1	1.210 (5)	C5—H5	0.9300
O5—C13	1.237 (4)	C6—H6	0.9300
O1 <sub>w</sub> —H11	0.85 (4)	C8—C9	1.389 (4)
O1 <sub>w</sub> —H12	0.85 (4)	C8—H8	0.9300
N1—C2	1.472 (5)	C9—C10	1.381 (5)
N2—C8	1.337 (4)	C9—C13	1.493 (5)
N2—C12	1.342 (4)	C10—C11	1.387 (5)
N3—C13	1.322 (5)	C10—H10	0.9300
N3—H31	0.85 (4)	C11—C12	1.374 (5)
N3—H32	0.85 (4)	C11—H11A	0.9300
C1—C2	1.389 (5)	C12—H12A	0.9300
O1 <sup>i</sup> —Cu1—O1	180.000 (1)	C4—C3—H3	120.5
O1 <sup>i</sup> —Cu1—N2 <sup>i</sup>	90.07 (10)	C5—C4—C3	119.7 (4)
O1—Cu1—N2 <sup>i</sup>	89.93 (10)	C5—C4—H4	120.1
O1 <sup>i</sup> —Cu1—N2	89.93 (10)	C3—C4—H4	120.1
O1—Cu1—N2	90.07 (10)	C4—C5—C6	120.4 (4)
N2 <sup>i</sup> —Cu1—N2	180.00 (14)	C4—C5—H5	119.8
O1 <sup>i</sup> —Cu1—O1 <sub>w</sub>	96.04 (9)	C6—C5—H5	119.8
O1—Cu1—O1 <sub>w</sub>	83.96 (9)	C5—C6—C1	121.2 (4)
N2 <sup>i</sup> —Cu1—O1 <sub>w</sub>	85.84 (10)	C5—C6—H6	119.4
N2—Cu1—O1 <sub>w</sub>	94.16 (10)	C1—C6—H6	119.4
C7—O1—Cu1	123.7 (2)	O2—C7—O1	125.5 (3)
Cu1—O1 <sub>w</sub> —H11	89 (3)	O2—C7—C1	117.3 (3)
Cu1—O1 <sub>w</sub> —H12	122 (3)	O1—C7—C1	117.1 (3)
H11—O1 <sub>w</sub> —H12	103 (4)	N2—C8—C9	123.2 (3)
O4—N1—O3	125.1 (4)	N2—C8—H8	118.4
O4—N1—C2	116.9 (4)	C9—C8—H8	118.4
O3—N1—C2	117.9 (4)	C10—C9—C8	117.7 (3)
C8—N2—C12	118.1 (3)	C10—C9—C13	124.8 (3)
C8—N2—Cu1	119.6 (2)	C8—C9—C13	117.5 (3)
C12—N2—Cu1	122.3 (2)	C9—C10—C11	119.7 (3)
C13—N3—H31	120 (3)	C9—C10—H10	120.2
C13—N3—H32	123 (3)	C11—C10—H10	120.2
H31—N3—H32	115 (4)	C12—C11—C10	118.7 (3)
C2—C1—C6	116.5 (3)	C12—C11—H11A	120.7
C2—C1—C7	122.0 (3)	C10—C11—H11A	120.7

C6—C1—C7	121.2 (3)	N2—C12—C11	122.6 (3)
C3—C2—C1	123.1 (3)	N2—C12—H12A	118.7
C3—C2—N1	117.2 (3)	C11—C12—H12A	118.7
C1—C2—N1	119.7 (3)	O5—C13—N3	122.1 (3)
C2—C3—C4	119.0 (4)	O5—C13—C9	119.9 (3)
C2—C3—H3	120.5	N3—C13—C9	118.0 (3)
N2 <sup>i</sup> —Cu1—O1—C7	-65.5 (2)	C2—C1—C6—C5	1.7 (5)
N2—Cu1—O1—C7	114.5 (2)	C7—C1—C6—C5	-171.9 (3)
O1W—Cu1—O1—C7	-151.3 (2)	Cu1—O1—C7—O2	-14.1 (5)
O1 <sup>i</sup> —Cu1—N2—C8	40.3 (2)	Cu1—O1—C7—C1	160.6 (2)
O1—Cu1—N2—C8	-139.7 (2)	C2—C1—C7—O2	-24.1 (5)
O1W—Cu1—N2—C8	136.3 (2)	C6—C1—C7—O2	149.2 (3)
O1 <sup>i</sup> —Cu1—N2—C12	-137.2 (3)	C2—C1—C7—O1	160.7 (3)
O1—Cu1—N2—C12	42.8 (3)	C6—C1—C7—O1	-26.0 (4)
O1W—Cu1—N2—C12	-41.1 (3)	C12—N2—C8—C9	0.7 (5)
C6—C1—C2—C3	-2.6 (5)	Cu1—N2—C8—C9	-176.9 (2)
C7—C1—C2—C3	171.0 (3)	N2—C8—C9—C10	-0.1 (5)
C6—C1—C2—N1	175.3 (3)	N2—C8—C9—C13	177.3 (3)
C7—C1—C2—N1	-11.1 (5)	C8—C9—C10—C11	-0.8 (6)
O4—N1—C2—C3	111.8 (5)	C13—C9—C10—C11	-178.0 (4)
O3—N1—C2—C3	-69.5 (5)	C9—C10—C11—C12	1.2 (6)
O4—N1—C2—C1	-66.2 (5)	C8—N2—C12—C11	-0.4 (5)
O3—N1—C2—C1	112.5 (4)	Cu1—N2—C12—C11	177.2 (3)
C1—C2—C3—C4	1.3 (6)	C10—C11—C12—N2	-0.6 (6)
N1—C2—C3—C4	-176.6 (4)	C10—C9—C13—O5	174.3 (4)
C2—C3—C4—C5	0.9 (6)	C8—C9—C13—O5	-2.9 (5)
C3—C4—C5—C6	-1.6 (6)	C10—C9—C13—N3	-3.5 (6)
C4—C5—C6—C1	0.3 (6)	C8—C9—C13—N3	179.3 (4)

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

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1w—H11 $\cdots$ O2 <sup>i</sup>	0.85 (4)	1.92 (2)	2.726 (4)	159 (4)
O1w—H12 $\cdots$ O5 <sup>ii</sup>	0.85 (4)	2.11 (2)	2.934 (2)	165 (3)
N3—H32 $\cdots$ O2 <sup>iii</sup>	0.85 (4)	2.15 (2)	2.929 (4)	152 (4)
N3—H31 $\cdots$ O5 <sup>iv</sup>	0.85 (4)	2.11 (2)	2.926 (4)	161 (4)

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

