Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquamanganese(II) tetraaquabis(2-aminopyrazine-κN^4)manganese(II) disulfate dihydrate

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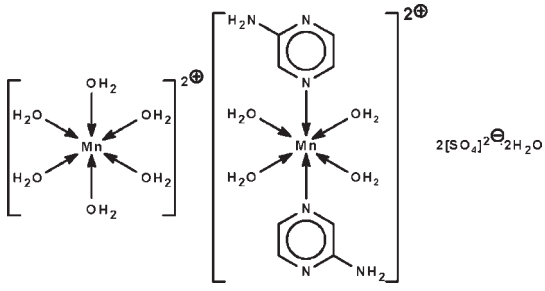
Received 27 October 2009; accepted 29 October 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.129; data-to-parameter ratio = 13.7.

The reaction of manganese(II) sulfate and 2-aminopyrazine affords the title salt, $[Mn(H_2O)_6][Mn(C_4H_5N_3)_2(H_2O)_4](SO_4)_2{\cdot}2H_2O$. The metal atoms in the tetraaqua-coordinated and hexaaqua-coordinated cations lie on centers of inversion in octahedral geometries. The cations, anions and solvent water molecules are linked by O—H···O, N—H···O and O—H···N hydrogen bonds into a three-dimensional network.

Related literature

For the isostructural cobalt(II) analog, see: Kang *et al.* (2009).



Experimental

Crystal data

$[Mn(H_2O)_6][Mn(C_4H_5N_3)_2(H_2O)_4](SO_4)_2{\cdot}2H_2O$
M_r = 708.43
Triclinic, $P\overline{1}$
a = 6.6242 (3) Å
b = 8.4639 (4) Å
c = 13.2719 (8) Å
α = 75.654 (2)°
β = 78.364 (2)°
γ = 78.834 (2)°
V = 697.95 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 K
0.38 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.670, T_{max} = 0.821
6866 measured reflections
3159 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.129
S = 1.15
3159 reflections
231 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O1	0.84 (1)	1.95 (2)	2.779 (3)	167 (4)
O1w—H1w2···N2^{i}	0.85 (1)	1.94 (1)	2.792 (3)	176 (5)
O2w—H2w1···O3	0.85 (1)	1.95 (1)	2.775 (3)	166 (4)
O2w—H2w2···O1^{ii}	0.85 (1)	1.92 (1)	2.770 (3)	172 (4)
O3w—H3w1···O2	0.85 (1)	1.90 (1)	2.744 (4)	170 (5)
O3w—H3w2···O6w	0.85 (1)	1.88 (1)	2.728 (4)	175 (4)
O4w—H4w1···O6w^{iii}	0.85 (1)	1.96 (2)	2.780 (4)	162 (5)
O4w—H4w2···O2^{iii}	0.85 (1)	1.92 (2)	2.744 (4)	164 (5)
O5w—H5w1···O3^{iv}	0.84 (1)	2.00 (2)	2.813 (3)	159 (5)
O5w—H5w2···O4^{v}	0.85 (1)	1.88 (1)	2.726 (4)	177 (6)
O6w—H6w1···O3^{i}	0.85 (1)	1.95 (2)	2.783 (3)	167 (6)
O6w—H6w2···O4^{iv}	0.85 (1)	1.87 (1)	2.709 (4)	172 (6)
N3—H3n2···O1^{vi}	0.85 (1)	2.18 (1)	3.026 (4)	172 (5)

Symmetry codes: (i) $x, y-1, z$; (ii) $x+1, y, z$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+2$; (v) $-x, -y+1, -z+2$; (vi) $-x+1, -y+3, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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 Natural Science Foundation of Heilongjiang Province (No. B200501), Heilongjiang University, China, and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2658).

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supporting information

Acta Cryst. (2009). E**65**, m1504 [doi:10.1107/S1600536809045322]

Hexaaquamanganese(II) tetraaquabis(2-aminopyrazine-κN^4)manganese(II) disulfate dihydrate

Li-Hua Huo, Shan Gao and Seik Weng Ng

S1. Experimental

To an aqueous solution of 3-aminopyrazine (0.19 g, 2 mmol) was added manganese(II) sulfate tetrahydrate (0.45 g, 2 mmol). Colorless crystals of the salt separated from the solution after a few days. CH&N elemental analysis. Calc. for $C_8H_{34}N_6O_{20}S_2Mn_2$: C 13.56, H 4.84, N 11.86%; found: C 13.52, H 4.80, N 11.85%.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C). The amino and water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H = O–H = 0.85±0.01 Å; their temperature factors were refined.

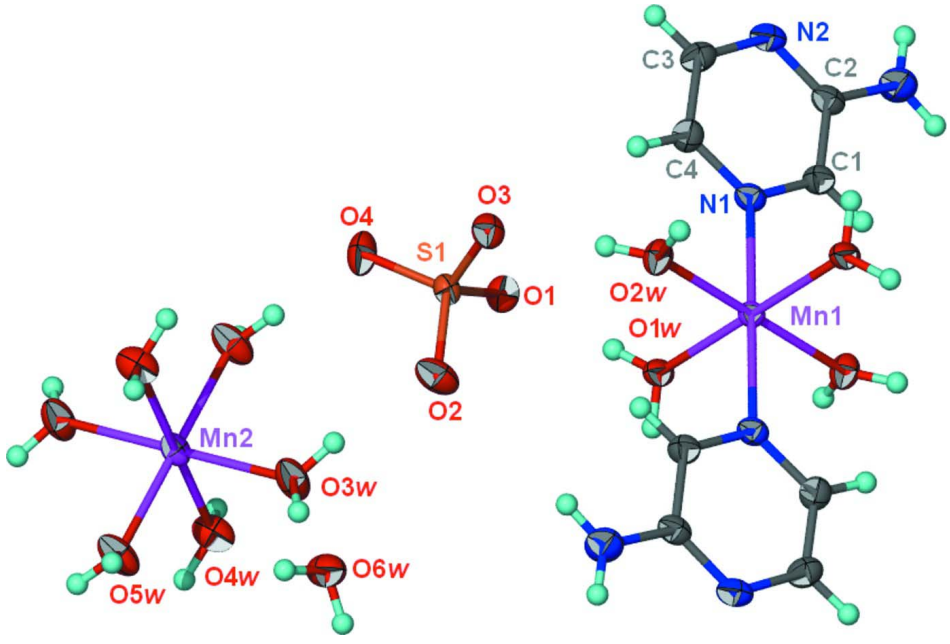

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[Mn(H_2O)_6]$ $[Mn(H_2O)_4(C_4H_5N_3)_2]$ $2[SO_4]\cdot 2H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Hexaaquamanganese(II) tetraaquabis(2-aminopyrazine-κN^4)manganese(II) disulfate dihydrate

Crystal data

$[Mn(H_2O)_6][Mn(C_4H_5N_3)_2(H_2O)_4](SO_4)_2\cdot 2H_2O$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$b = 8.4639$ (4) Å
$c = 13.2719$ (8) Å
$\alpha = 75.654$ (2)°
$\beta = 78.364$ (2)°
$\gamma = 78.834$ (2)°
$V = 697.95$ (6) Å^3
$Z = 1$
$F(000) = 366$
$D_x = 1.685$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6492 reflections
$\theta = 3.2$–$27.5°$
$\mu = 1.14$ mm^{-1}
$T = 293$ K
Prism, colorless
0.38 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.670$, $T_{max} = 0.821$
6866 measured reflections
3159 independent reflections
2874 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -8\rightarrow 8$
$k = -10\rightarrow 10$
$l = -17\rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.129$
$S = 1.15$
3159 reflections
231 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 1.1503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	1.0000	1.0000	0.5000	0.02349 (17)
Mn2	0.0000	0.5000	1.0000	0.02867 (18)
S1	0.47994 (10)	0.88750 (9)	0.80279 (5)	0.02457 (18)
O1	0.4091 (3)	0.9828 (3)	0.70435 (17)	0.0322 (5)
O2	0.5386 (4)	0.7129 (3)	0.7978 (2)	0.0444 (6)
O3	0.6644 (3)	0.9501 (3)	0.81657 (17)	0.0318 (5)
O4	0.3121 (4)	0.9084 (4)	0.89137 (19)	0.0441 (6)
O1W	0.7084 (4)	0.9110 (3)	0.53580 (19)	0.0335 (5)
O2W	1.0209 (4)	0.9617 (3)	0.66525 (17)	0.0345 (5)
O3W	0.2937 (4)	0.4732 (3)	0.8939 (2)	0.0471 (7)
O4W	−0.1480 (4)	0.4748 (3)	0.8707 (2)	0.0429 (6)
O5W	0.0400 (4)	0.2353 (3)	1.0577 (2)	0.0456 (6)

O6W	0.6189 (4)	0.2200 (3)	0.9081 (2)	0.0399 (6)
N1	0.8363 (4)	1.2689 (3)	0.4980 (2)	0.0301 (5)
N2	0.7098 (4)	1.6040 (3)	0.4930 (2)	0.0344 (6)
N3	0.7810 (6)	1.6587 (4)	0.3104 (3)	0.0482 (8)
C1	0.8414 (5)	1.3800 (4)	0.4078 (3)	0.0334 (7)
H1	0.8899	1.3447	0.3450	0.040*
C2	0.7760 (5)	1.5496 (4)	0.4039 (3)	0.0325 (6)
C3	0.7019 (5)	1.4892 (4)	0.5836 (3)	0.0376 (7)
H3	0.6532	1.5237	0.6466	0.045*
C4	0.7623 (5)	1.3238 (4)	0.5874 (3)	0.0348 (7)
H4	0.7522	1.2491	0.6521	0.042*
H1W1	0.614 (5)	0.948 (5)	0.581 (3)	0.048 (12)*
H1W2	0.715 (7)	0.817 (3)	0.521 (4)	0.053 (13)*
H2W1	0.919 (4)	0.972 (5)	0.714 (2)	0.028 (9)*
H2W2	1.135 (4)	0.967 (5)	0.683 (3)	0.044 (11)*
H3W1	0.357 (7)	0.556 (4)	0.866 (4)	0.066 (15)*
H3W2	0.391 (5)	0.392 (3)	0.901 (3)	0.039 (11)*
H4W1	−0.195 (8)	0.386 (4)	0.876 (4)	0.073 (17)*
H4W2	−0.247 (5)	0.554 (4)	0.859 (4)	0.063 (15)*
H5W1	0.126 (6)	0.160 (4)	1.089 (3)	0.059 (14)*
H5W2	−0.072 (5)	0.194 (7)	1.074 (5)	0.081 (18)*
H6W1	0.624 (9)	0.148 (5)	0.873 (4)	0.079 (18)*
H6W2	0.641 (9)	0.170 (6)	0.9698 (19)	0.072 (17)*
H3N1	0.831 (7)	1.629 (6)	0.252 (2)	0.062 (15)*
H3N2	0.738 (8)	1.7613 (19)	0.308 (4)	0.060 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0217 (3)	0.0225 (3)	0.0255 (3)	−0.0022 (2)	−0.0054 (2)	−0.0034 (2)
Mn2	0.0218 (3)	0.0271 (3)	0.0341 (3)	−0.0032 (2)	−0.0067 (2)	0.0002 (2)
S1	0.0209 (3)	0.0257 (3)	0.0260 (3)	−0.0046 (3)	−0.0066 (2)	−0.0004 (3)
O1	0.0289 (11)	0.0353 (12)	0.0302 (11)	−0.0007 (9)	−0.0115 (9)	−0.0009 (9)
O2	0.0423 (14)	0.0252 (11)	0.0645 (17)	−0.0035 (10)	−0.0175 (12)	−0.0014 (11)
O3	0.0224 (10)	0.0385 (12)	0.0356 (11)	−0.0062 (9)	−0.0079 (8)	−0.0062 (9)
O4	0.0313 (12)	0.0672 (17)	0.0317 (12)	−0.0132 (12)	0.0012 (10)	−0.0078 (11)
O1W	0.0277 (11)	0.0325 (12)	0.0423 (13)	−0.0092 (9)	0.0038 (9)	−0.0157 (10)
O2W	0.0258 (11)	0.0521 (14)	0.0264 (10)	−0.0058 (10)	−0.0080 (9)	−0.0068 (10)
O3W	0.0281 (12)	0.0356 (14)	0.0671 (18)	−0.0064 (11)	0.0055 (12)	−0.0012 (12)
O4W	0.0395 (14)	0.0380 (14)	0.0542 (15)	−0.0039 (11)	−0.0212 (12)	−0.0059 (12)
O5W	0.0318 (13)	0.0320 (12)	0.0679 (17)	−0.0074 (10)	−0.0194 (12)	0.0096 (12)
O6W	0.0477 (14)	0.0317 (12)	0.0413 (14)	−0.0016 (11)	−0.0131 (11)	−0.0086 (10)
N1	0.0269 (12)	0.0226 (12)	0.0390 (14)	−0.0011 (10)	−0.0063 (10)	−0.0044 (10)
N2	0.0293 (13)	0.0255 (12)	0.0498 (16)	−0.0013 (10)	−0.0095 (12)	−0.0109 (11)
N3	0.063 (2)	0.0285 (15)	0.0451 (18)	0.0031 (15)	−0.0061 (16)	−0.0039 (13)
C1	0.0347 (16)	0.0256 (15)	0.0380 (16)	0.0001 (12)	−0.0061 (13)	−0.0069 (12)
C2	0.0289 (15)	0.0238 (14)	0.0435 (17)	−0.0014 (12)	−0.0071 (13)	−0.0060 (12)
C3	0.0337 (16)	0.0391 (18)	0.0425 (18)	0.0019 (14)	−0.0073 (14)	−0.0182 (14)

C4	0.0318 (16)	0.0335 (16)	0.0352 (16)	0.0037 (13)	−0.0075 (13)	−0.0051 (13)

Geometric parameters (Å, º)

Mn1—O1W	2.131 (2)	O3W—H3W1	0.849 (10)
Mn1—O1W^{i}	2.131 (2)	O3W—H3W2	0.849 (10)
Mn1—O2W^{i}	2.165 (2)	O4W—H4W1	0.848 (10)
Mn1—O2W	2.165 (2)	O4W—H4W2	0.850 (10)
Mn1—N1	2.320 (2)	O5W—H5W1	0.849 (10)
Mn1—N1^{i}	2.320 (2)	O5W—H5W2	0.850 (10)
Mn2—O3W	2.168 (3)	O6W—H6W1	0.850 (10)
Mn2—O3W^{ii}	2.168 (3)	O6W—H6W2	0.850 (10)
Mn2—O4W	2.212 (3)	N1—C1	1.325 (4)
Mn2—O4W^{ii}	2.212 (3)	N1—C4	1.347 (4)
Mn2—O5W^{ii}	2.163 (2)	N2—C2	1.337 (4)
Mn2—O5W	2.163 (2)	N2—C3	1.344 (5)
S1—O4	1.466 (2)	N3—C2	1.350 (5)
S1—O2	1.468 (3)	N3—H3N1	0.855 (10)
S1—O1	1.468 (2)	N3—H3N2	0.854 (10)
S1—O3	1.482 (2)	C1—C2	1.408 (4)
O1W—H1W1	0.844 (10)	C1—H1	0.9300
O1W—H1W2	0.851 (10)	C3—C4	1.371 (5)
O2W—H2W1	0.846 (10)	C3—H3	0.9300
O2W—H2W2	0.852 (10)	C4—H4	0.9300
O1W—Mn1—O1W^{i}	180.000 (1)	Mn1—O1W—H1W1	118 (3)
O1W—Mn1—O2W^{i}	87.90 (9)	Mn1—O1W—H1W2	114 (3)
O1W^{i}—Mn1—O2W^{i}	92.10 (9)	H1W1—O1W—H1W2	123 (4)
O1W—Mn1—O2W	92.10 (9)	Mn1—O2W—H2W1	125 (3)
O1W^{i}—Mn1—O2W	87.90 (9)	Mn1—O2W—H2W2	120 (3)
O2W^{i}—Mn1—O2W	180.000 (1)	H2W1—O2W—H2W2	112 (4)
O1W—Mn1—N1	91.71 (9)	Mn2—O3W—H3W1	120 (4)
O1W^{i}—Mn1—N1	88.29 (9)	Mn2—O3W—H3W2	126 (3)
O2W^{i}—Mn1—N1	89.32 (10)	H3W1—O3W—H3W2	104 (4)
O2W—Mn1—N1	90.68 (10)	Mn2—O4W—H4W1	119 (4)
O1W—Mn1—N1^{i}	88.29 (9)	Mn2—O4W—H4W2	110 (3)
O1W^{i}—Mn1—N1^{i}	91.71 (9)	H4W1—O4W—H4W2	107 (5)
O2W^{i}—Mn1—N1^{i}	90.68 (10)	Mn2—O5W—H5W1	139 (3)
O2W—Mn1—N1^{i}	89.32 (10)	Mn2—O5W—H5W2	115 (4)
N1—Mn1—N1^{i}	180.000 (1)	H5W1—O5W—H5W2	103 (5)
O5W^{ii}—Mn2—O5W	180.000 (1)	H6W1—O6W—H6W2	108 (5)
O5W^{ii}—Mn2—O3W	90.64 (10)	C1—N1—C4	117.4 (3)
O5W—Mn2—O3W	89.36 (10)	C1—N1—Mn1	119.9 (2)
O5W^{ii}—Mn2—O3W^{ii}	89.36 (10)	C4—N1—Mn1	121.9 (2)
O5W—Mn2—O3W^{ii}	90.64 (10)	C2—N2—C3	116.8 (3)
O3W—Mn2—O3W^{ii}	180.000 (1)	C2—N3—H3N1	122 (3)
O5W^{ii}—Mn2—O4W	89.84 (10)	C2—N3—H3N2	121 (3)
O5W—Mn2—O4W	90.16 (10)	H3N1—N3—H3N2	117 (5)

O3W—Mn2—O4W	86.45 (11)	N1—C1—C2	122.2 (3)
O3W^{ii}—Mn2—O4W	93.55 (11)	N1—C1—H1	118.9
O5W^{ii}—Mn2—O4W^{ii}	90.16 (10)	C2—C1—H1	118.9
O5W—Mn2—O4W^{ii}	89.84 (10)	N2—C2—N3	119.4 (3)
O3W—Mn2—O4W^{ii}	93.55 (11)	N2—C2—C1	120.2 (3)
O3W^{ii}—Mn2—O4W^{ii}	86.45 (11)	N3—C2—C1	120.4 (3)
O4W—Mn2—O4W^{ii}	180.000 (1)	N2—C3—C4	123.1 (3)
O4—S1—O2	110.85 (17)	N2—C3—H3	118.4
O4—S1—O1	109.03 (14)	C4—C3—H3	118.4
O2—S1—O1	109.60 (15)	N1—C4—C3	120.3 (3)
O4—S1—O3	109.10 (14)	N1—C4—H4	119.9
O2—S1—O3	109.02 (14)	C3—C4—H4	119.9
O1—S1—O3	109.22 (13)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O1	0.84 (1)	1.95 (2)	2.779 (3)	167 (4)
O1w—H1w2···N2^{iii}	0.85 (1)	1.94 (1)	2.792 (3)	176 (5)
O2w—H2w1···O3	0.85 (1)	1.95 (1)	2.775 (3)	166 (4)
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O4w—H4w1···O6w^{v}	0.85 (1)	1.96 (2)	2.780 (4)	162 (5)
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O5w—H5w1···O3^{vi}	0.84 (1)	2.00 (2)	2.813 (3)	159 (5)
O5w—H5w2···O4^{ii}	0.85 (1)	1.88 (1)	2.726 (4)	177 (6)
O6w—H6w1···O3^{iii}	0.85 (1)	1.95 (2)	2.783 (3)	167 (6)
O6w—H6w2···O4^{vi}	0.85 (1)	1.87 (1)	2.709 (4)	172 (6)
N3—H3n2···O1^{vii}	0.85 (1)	2.18 (1)	3.026 (4)	172 (5)

Symmetry codes: (ii) −*x*, −*y*+1, −*z*+2; (iii) *x*, *y*−1, *z*; (iv) *x*+1, *y*, *z*; (v) *x*−1, *y*, *z*; (vi) −*x*+1, −*y*+1, −*z*+2; (vii) −*x*+1, −*y*+3, −*z*+1.