inorganic compounds

Redetermination of synthetic warwickite, $Mg_3TiO_2(BO_3)_2$

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Single crystals of warwickite, trimagnesium titanium(IV) dioxide bis(borate), $Mg_3TiO_2(BO_3)_2$, were prepared by slow cooling of the melt. The title compound is isotypic with $Co_3TiO_2(BO_3)_2$. In contrast to the previous refinement of warwickite [Moore & Araki (1974). *Am. Mineral.* **59**, 985–1004], that reported only isotropic atomic displacement parameters for all atoms, anisotropic displacement parameters of all atoms were refined during the current redetermination. All atoms are situated on special positions (site symmetry .*m*.). One of the two Mg sites is statistically disordered with Ti atoms (ratio 1:1), while the other is fully occupied by Mg atoms. The occupancy ratio of the Mg and Ti atoms is similar to that reported in the previous study. Metal atoms (*M*) at the Ti/Mg and Mg sites are coordinated by six O atoms in form of distorted octahedra. Four edge-sharing MO_6 octahedra form M_4O_{18} units, which are connected by common corners into layers parallel to (010). Adjacent layers are linked along [010] into a framework structure by sharing common edges. The B atoms are located in the triangular prismatic tunnels of the framework.

Related literature

For the structure determination of natural warwickite, $Mg_3TiO_2(BO_3)_2$, see: Takéuchi *et al.* (1950); Moore & Araki (1974). For the synthesis and crystal structure analysis of $Co_3MO_2(BO_3)_2$ (*M* = Ti, Zr), see: Utzolino & Bluhm (1995). For the synthesis of $Mg_5TiO_4(BO_3)_2$ and $Mg_3ZrO_2(BO_3)_2$, see: Konijnendijk & Blasse (1985). For the structure of $Mg_5TiO_4(BO_3)_2$, see: Kawano & Yamane (2010). For bond-valence-sum calculations, see: Brown & Altermatt (1985). For bond-valence parameters, see: Brese & O'Keeffe (1991). For structure standardization, see: Gelato & Parthé (1987).

Experimental

Crystal data

$Mg_3TiO_2(BO_3)_2$	V = 270.86 (3) $Å^3$
M_r = 270.45	Z = 2
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
a = 9.3013 (5) Å	μ = 1.94 mm^{-1}
b = 3.10080 (14) Å	T = 293 K
c = 9.3914 (6) Å	$0.17 \times 0.17 \times 0.12$ mm

Data collection

Rigaku R-AXIS RAPID II diffractometer	2510 measured reflections
Absorption correction: numerical (*NUMABS*; Higashi, 1999)	364 independent reflections
T_{min} = 0.791, T_{max} = 0.839	348 reflections with $I > 2\sigma(I)$
	R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026	44 parameters
$wR(F^2)$ = 0.070	$\Delta\rho_{max}$ = 0.36 e $Å^{-3}$
S = 1.20	$\Delta\rho_{min}$ = −0.59 e $Å^{-3}$
364 reflections	

Table 1
Selected geometric parameters (Å, °), *M* = (Mg, Ti).

$M1–O4^i$	1.9702 (12)	$Mg2–O1$	2.1387 (19)
$M1–O4^{ii}$	1.9989 (19)	$Mg2–O2^v$	2.1522 (13)
$M1–O2$	2.0730 (18)	$B1–O3$	1.353 (3)
$M1–O1^i$	2.1565 (13)	$B1–O2$	1.393 (3)
$Mg2–O3^{iii}$	2.0043 (12)	$B1–O1$	1.395 (3)
$Mg2–O4^{iv}$	2.0698 (19)		
$O3–B1–O2$	119.1 (2)	$O2–B1–O1$	120.3 (2)
$O3–B1–O1$	120.7 (2)		

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

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2005); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *VESTA* (Momma & Izumi, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2443).

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supplementary materials

Redetermination of synthetic warwickite, $Mg_3TiO_2(BO_3)_2$

T. Kawano and H. Yamane

Comment

Crystal structure determinations of the mineral warwickite, $Mg_3TiO_2(BO_3)_2$, were reported by Takéuchi *et al.* (1950) and Moore & Araki (1974). The natural samples contained a few amount of Fe and Al. The crystal structure of synthetic $Mg_3TiO_2(BO_3)_2$ has not been analyzed up to now. We obtained single crystals of this compound during the preparation of $Mg_5TiO_4(BO_3)_2$ (Kawano & Yamane, 2010). Anisotropic atomic displacement parameters (U_{ij}) of Mg, Ti, B and O atoms were refined in the present study. Moore & Araki (1974) refined isotropic atomic displacement parameters (B_{iso}) of Mg, Ti, B and O atoms; neither U nor B-values were reported by Takéuchi *et al.* (1950).

Synthetic warwickite-type oxyborates with general composition $M^{II}_3M^{IV}O_2(BO_3)_2$ are known for $Co_3MO_2(BO_3)_2$ [M = Ti, Zr (Utzolino & Bluhm, 1995)] and $Mg_3ZrO_2(BO_3)_2$ (Konijnendijk & Blasse, 1985). However, only the crystal structures of $Co_3MO_2(BO_3)_2$ (M = Ti, Zr) were analyzed. The title compound $Mg_3TiO_2(BO_3)_2$ is isotypic with $Co_3MO_2(BO_3)_2$ [M = Ti, Zr (Utzolino & Bluhm, 1995)].

Figs. 1 and 2 show the coordination environments of the Mg, Ti, B and O atoms, and the crystal structure of $Mg_3TiO_2(BO_3)_2$, respectively. In the asymmetric unit, there is one Ti/Mg mixed site (M1) with occupancies of 0.5/0.5 and one Mg site (M2). Moore and Araki (1974) refined the site occupancy factors of Mg and Ti atoms at the M1 and M2 sites, ignoring Al and Fe atoms due to their similarities with the scattering profiles of Mg^{2+} and Ti^{4+}, respectively. Refined occupancy factors were M1 = $Mg_{0.96 (1)}/Ti_{0.04 (1)}$ and M2 = $Mg_{0.62 (2)}/Ti_{0.38 (2)}$ and an ideal formula of $Mg(Mg_{0.5}Ti_{0.5})O_2[BO_3]$ was suggested (Moore & Araki, 1974). Our refinement (M1 = Mg1 and M2 = $Mg_{0.5}/Ti_{0.5}$) is consistent with the ideal formula. Although Takéuchi *et al.* (1950) reported the atomic coordinates of natural warwickite, site occupancy factors of the M1 and M2 sites were not reported.

All atoms are at special positions (x, 1/4, z), $4c$, with site symmetries of (.m.). Mg and Ti atoms occupy six-coordinated oxygen-octahedral sites, forming layers composed of M_4O_{18} (M = Ti/Mg, Mg) units. The layers are connected by edge-sharing O4 atoms of $(Ti1/Mg1)O_6$ and $Mg2O_6$ octahedra into a three-dimensional framework. B1 atoms are located in triangular prismatic tunnels of the framework.

Bond valence sums (BVS; Brown & Altermatt, 1985) of the Mg, Ti and B atoms were calculated with the bond valence parameters of 1.693 Å for Mg^{2+}, 1.815 Å for Ti^{4+} and 1.371 Å for B^{3+} (Brese & O'Keeffe, 1991). The BVS values of the Mg2 and B1 atoms were 2.1 and 2.9, respectively. Those of the Ti1 and Mg1 atoms at the Ti1/Mg1 site were 3.22 and 2.31, respectively. The average of these value is 2.8 and close to the expected mean valence (+3) of Mg^{2+} and Ti^{4+}. The B1—O distances of 1.353 (3)–1.395 (3) Å agree well with those of isotypic $Co_3MO_2(BO_3)_2$ (M = Ti, Zr): 1.36 (2)–1.39 (2) Å (Utzolino & Bluhm, 1995).

supplementary materials

Warwickite-type $Mg_3TiO_2(BO_3)_2$ did not emit visible light under ultraviolet excitation at room temperature, while lud-wigite-type $Mg_5TiO_4(BO_3)_2$ shows broad blue emission (435 nm) attributed to charge transfer transitions between Ti^{4+} and O^{2-} (Konijnendijk & Blasse, 1985).

Experimental

Starting materials were powders of MgO (99.9%, Rare Metallic), TiO_2 (99.9%, Rare Metallic) and H_3BO_3 (99.99%, Sigma-Aldrich). MgO was heated at 1173–1273 K for 6–12 h in air before weighing. The powders were weighed with a molar ratio of MgO: TiO_2: H_3BO_3 = 5: 1: 2.7 and mixed in an agate mortar with a pestle. The mixture was pressed into a pellet, placed in a Pt boat and heated at 1623 K for 6 h in air. Heating and cooling rates were 200 and 900 K/h, respectively. About 400 mg of the sample and 100 mg of H_3BO_3 were weighed and mixed. The mixture in the Pt boat was heated at 1723 K for 3 h in air and cooled to room temperature at a cooling rate of 900 K/h. The obtained sample was crushed into fragments and a colourless and transparent single-crystal of about 0.12–0.17 mm was picked up under an optical microscope.

Refinement

The crystal structures of natural warwickites were described in the space group *Pnam* (no. 62) in the previous studies (Takéuchi *et al.*, 1950; Moore & Araki, 1974). The original single-crystal X-ray diffraction data in the present study were indexed in a different setting in space group *Pmnb* and unit-cell parameters of a = 3.10080 (14), b = 9.3013 (5) and c = 9.3914 (6) Å. Structure parameters were eventually standardized based on the standard setting of the space group *Pnma* using the *STRUCTURE TIDY* program (Gelato & Parthé, 1987). In the final refinement, site occupation factors (s.o.f.'s) of the Ti and Mg atoms at the Ti1/Mg1 and Mg2 sites were fixed to 0.5/0.5 and 1.0, respectively, since the freely refined s.o.f.'s of the Ti and Mg atoms at the Ti1/Mg1 site were close to 1/2, and the s.o.f. of the Mg atom at the Mg2 site was about 1.0. The highest peak in the difference electron density map is 0.36 Å from O2 while the deepest hole is -0.59 Å from Ti1/Mg1.

Figures

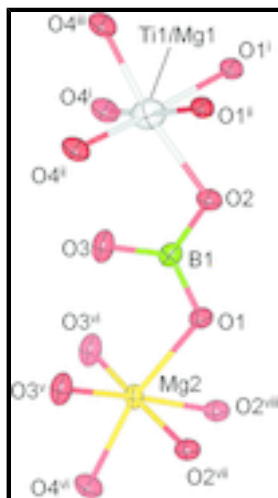Fig. 1. The atomic arrangement around Mg, Ti, B and O atoms in the structure of $Mg_3TiO_2(BO_3)_2$. Displacement ellipsoids are drawn at the 95% probability level. Symmetry codes: (i) $-x + 1/2, -y, z-1/2$; (ii) $-x + 1/2, -y + 1, z-1/2$; (iii) $x-1/2, y, -z + 1/2$; (iv) $-x, -y, -z + 1$; (v) $-x, -y + 1, -z + 1$; (vi) $x-1/2, y, -z + 3/2$; (vii) $-x + 1/2, -y + 1, z + 1/2$; (viii) $-x + 1/2, -y, z + 1/2$.
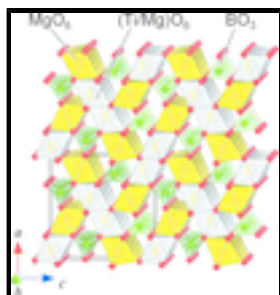
Fig. 2. The crystal structure of $Mg_3TiO_2(BO_3)_2$ in a representation using cation-centred oxygen polyhedra.

trimagnesium titanium(IV) dioxide bis(borate)

Crystal data

$Mg_3TiO_2(BO_3)_2$	$F(000) = 264$
$M_r = 270.45$	$D_x = 3.316$ Mg m^{-3}
Orthorhombic, *Pnma*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2n	Cell parameters from 2288 reflections
$a = 9.3013\ (5)$ Å	$\theta = 3.1–27.5°$
$b = 3.10080\ (14)$ Å	$\mu = 1.94$ mm^{-1}
$c = 9.3914\ (6)$ Å	$T = 293$ K
$V = 270.86\ (3)$ Å^3	Block, colourless
$Z = 2$	$0.17 \times 0.17 \times 0.12$ mm

Data collection

Rigaku R-AXIS RAPID II diffractometer	364 independent reflections
Radiation source: fine-focus sealed tube	348 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.018$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
ω scans	$h = -12 \rightarrow 11$
Absorption correction: numerical (*NUMABS*; Higashi, 1999)	$k = -3 \rightarrow 3$
$T_{min} = 0.791$, $T_{max} = 0.839$	$l = -12 \rightarrow 12$
2510 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.3981P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.070$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.20$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
364 reflections	$\Delta\rho_{min} = -0.59$ e Å^{-3}

supplementary materials

44 parameters

0 restraints

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.039 (7)

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 ($\mathring{A}^2$)

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Ti1	0.11388 (7)	0.2500	0.07167 (7)	0.0115 (3)	0.50
Mg1	0.11388 (7)	0.2500	0.07167 (7)	0.0115 (3)	0.50
Mg2	0.10160 (8)	0.2500	0.68497 (9)	0.0055 (3)	
B1	0.1708 (3)	0.2500	0.3719 (3)	0.0061 (5)	
O1	0.24045 (19)	0.2500	0.50344 (18)	0.0088 (4)	
O2	0.25030 (18)	0.2500	0.24622 (19)	0.0078 (4)	
O3	0.0255 (2)	0.2500	0.36441 (19)	0.0100 (4)	
O4	0.5095 (2)	0.2500	0.61439 (18)	0.0100 (4)	

Atomic displacement parameters ($\mathring{A}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0148 (4)	0.0079 (4)	0.0119 (4)	0.000	−0.0015 (2)	0.000
Mg1	0.0148 (4)	0.0079 (4)	0.0119 (4)	0.000	−0.0015 (2)	0.000
Mg2	0.0040 (4)	0.0045 (5)	0.0079 (4)	0.000	0.0001 (3)	0.000
B1	0.0069 (12)	0.0038 (13)	0.0077 (12)	0.000	−0.0013 (9)	0.000
O1	0.0071 (8)	0.0139 (10)	0.0054 (7)	0.000	−0.0006 (6)	0.000
O2	0.0085 (8)	0.0090 (9)	0.0058 (7)	0.000	0.0004 (6)	0.000
O3	0.0063 (9)	0.0095 (10)	0.0143 (9)	0.000	−0.0017 (7)	0.000
O4	0.0102 (9)	0.0128 (10)	0.0071 (8)	0.000	−0.0020 (6)	0.000

Geometric parameters ($\mathring{A}$, °)

Ti1—O4[i]	1.9702 (12)	Mg2—O4[x]	2.0698 (19)
Ti1—O4[ii]	1.9702 (12)	Mg2—O1	2.1387 (19)
Ti1—O4[iii]	1.9989 (19)	Mg2—O2[xi]	2.1522 (13)
Ti1—O2	2.0730 (18)	Mg2—O2[xii]	2.1522 (13)
Ti1—O1[ii]	2.1565 (13)	Mg2—Mg2[vi]	3.10080 (14)

Ti1—O1^{i}	2.1565 (13)	Mg2—Mg2^{vii}	3.10080 (14)
Ti1—Ti1^{iv}	2.9502 (11)	Mg2—Ti1^{xi}	3.2465 (9)
Ti1—Mg1^{iv}	2.9502 (11)	Mg2—Mg1^{xi}	3.2465 (9)
Ti1—Ti1^{v}	2.9502 (11)	Mg2—Ti1^{xii}	3.2465 (9)
Ti1—Mg1^{v}	2.9502 (11)	Mg2—Mg1^{xii}	3.2465 (9)
Ti1—Ti1^{vi}	3.10080 (14)	B1—O3	1.353 (3)
Ti1—Ti1^{vii}	3.10080 (14)	B1—O2	1.393 (3)
Mg2—O3^{viii}	2.0043 (12)	B1—O1	1.395 (3)
Mg2—O3^{ix}	2.0043 (12)		
O4^{i}—Ti1—O4^{ii}	103.80 (9)	Mg2—O1—Ti1^{xi}	98.20 (6)
O4^{i}—Ti1—O4^{iii}	83.98 (6)	B1—O1—Ti1^{xii}	123.71 (9)
O4^{ii}—Ti1—O4^{iii}	83.98 (6)	Mg2—O1—Ti1^{xii}	98.20 (6)
O4^{i}—Ti1—O2	101.28 (6)	Mg1^{xi}—O1—Ti1^{xii}	91.94 (7)
O4^{ii}—Ti1—O2	101.28 (6)	Ti1^{xi}—O1—Ti1^{xii}	91.94 (7)
O4^{iii}—Ti1—O2	171.31 (8)	B1—O1—Mg1^{xii}	123.71 (9)
O4^{i}—Ti1—O1^{ii}	172.87 (6)	Mg2—O1—Mg1^{xii}	98.20 (6)
O4^{ii}—Ti1—O1^{ii}	82.00 (5)	Mg1^{xi}—O1—Mg1^{xii}	91.94 (7)
O4^{iii}—Ti1—O1^{ii}	92.60 (6)	Ti1^{xi}—O1—Mg1^{xii}	91.94 (7)
O2—Ti1—O1^{ii}	81.39 (6)	B1—O2—Ti1	110.19 (15)
O4^{i}—Ti1—O1^{i}	82.00 (5)	B1—O2—Mg2^{ii}	124.49 (8)
O4^{ii}—Ti1—O1^{i}	172.87 (6)	Ti1—O2—Mg2^{ii}	100.40 (6)
O4^{iii}—Ti1—O1^{i}	92.60 (6)	B1—O2—Mg2^{i}	124.49 (8)
O2—Ti1—O1^{i}	81.39 (6)	Ti1—O2—Mg2^{i}	100.40 (6)
O1^{ii}—Ti1—O1^{i}	91.94 (7)	Mg2^{ii}—O2—Mg2^{i}	92.17 (7)
O3^{viii}—Mg2—O3^{ix}	101.34 (9)	B1—O3—Mg2^{viii}	126.96 (6)
O3^{viii}—Mg2—O4^{x}	88.08 (6)	B1—O3—Mg2^{ix}	126.96 (6)
O3^{ix}—Mg2—O4^{x}	88.08 (6)	Mg2^{viii}—O3—Mg2^{ix}	101.34 (9)
O3^{viii}—Mg2—O1	99.89 (7)	Mg1^{xii}—O4—Mg1^{xi}	103.80 (9)
O3^{ix}—Mg2—O1	99.89 (7)	Ti1^{xii}—O4—Mg1^{xi}	103.80 (9)
O4^{x}—Mg2—O1	167.30 (8)	Mg1^{xii}—O4—Ti1^{xi}	103.80 (9)
O3^{viii}—Mg2—O2^{xi}	175.34 (6)	Ti1^{xii}—O4—Ti1^{xi}	103.80 (9)
O3^{ix}—Mg2—O2^{xi}	83.24 (5)	Mg1^{xii}—O4—Mg1^{xiii}	96.02 (6)
O4^{x}—Mg2—O2^{xi}	91.24 (6)	Ti1^{xii}—O4—Mg1^{xiii}	96.02 (6)
O1—Mg2—O2^{xi}	80.01 (6)	Mg1^{xi}—O4—Mg1^{xiii}	96.02 (6)
O3^{viii}—Mg2—O2^{xii}	83.24 (5)	Ti1^{xi}—O4—Mg1^{xiii}	96.02 (6)
O3^{ix}—Mg2—O2^{xii}	175.34 (6)	Mg1^{xii}—O4—Ti1^{xiii}	96.02 (6)
O4^{x}—Mg2—O2^{xii}	91.24 (6)	Ti1^{xii}—O4—Ti1^{xiii}	96.02 (6)
O1—Mg2—O2^{xii}	80.01 (6)	Mg1^{xi}—O4—Ti1^{xiii}	96.02 (6)
O2^{xi}—Mg2—O2^{xii}	92.17 (7)	Ti1^{xi}—O4—Ti1^{xiii}	96.02 (6)
O3—B1—O2	119.1 (2)	g1^{xii}—O4—Mg2^{xiv}	115.24 (6)

O3—B1—O1	120.7 (2)	Ti1^{xii}—O4—Mg2^{xiv}	115.24 (6)
O2—B1—O1	120.3 (2)	Mg1^{xi}—O4—Mg2^{xiv}	115.24 (6)
B1—O1—Mg2	115.18 (15)	Ti1^{xi}—O4—Mg2^{xiv}	115.24 (6)
B1—O1—Mg1^{xi}	123.71 (9)	Mg1^{xiii}—O4—Mg2^{xiv}	126.50 (10)
Mg2—O1—Mg1^{xi}	98.20 (6)	Ti1^{xiii}—O4—Mg2^{xiv}	126.50 (10)
B1—O1—Ti1^{xi}	123.71 (9)		

Symmetry codes: (i) −x+1/2, −y, z−1/2; (ii) −x+1/2, −y+1, z−1/2; (iii) x−1/2, y, −z+1/2; (iv) −x, −y, −z; (v) −x, −y+1, −z; (vi) x, y+1, z; (vii) x, y−1, z; (viii) −x, −y, −z+1; (ix) −x, −y+1, −z+1; (x) x−1/2, y, −z+3/2; (xi) −x+1/2, −y+1, z+1/2; (xii) −x+1/2, −y, z+1/2; (xiii) x+1/2, y, −z+1/2; (xiv) x+1/2, y, −z+3/2.

Fig. 1

Fig. 2