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Di-μ-bromido-bis[(η^4-cycloocta-1,5-diene)iridium(I)]

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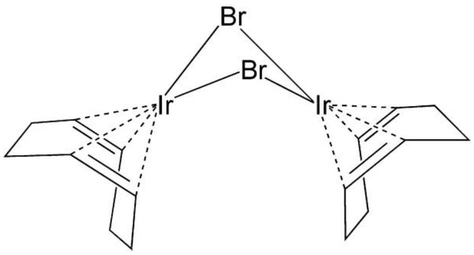
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.010 Å; R factor = 0.034; wR factor = 0.064; data-to-parameter ratio = 31.2.

The title complex, $[Ir_2(\mu\text{-}Br)_2(C_8H_{12})_2]$, displays a dinuclear structure with bridging Br atoms, generated by twofold symmetry. The coordination geometry around the Ir atom is pseudo-square-planar, involving two Br atoms and two η^2 C=C bonds. The $Ir_2(\mu\text{-}Br)_2$ core shows a bent geometry with a hinge angle of 101.58 (3)°.

Related literature

For related literature, see: Aullón *et al.* (1998); Cotton *et al.* (1986, 1999); Dorta *et al.* (1997); Pettinari *et al.* (2002); De Ridder & Imhoef (1994); Tani *et al.* (1995); Yamagata *et al.* (1997).



Experimental

Crystal data

$[Ir_2Br_2(C_8H_{12})_2]$
M_r = 760.57
Tetragonal, $P4_12_12$
a = 8.3839 (5) Å
c = 24.1471 (19) Å
V = 1697.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 20.36 mm^{-1}
T = 100 (1) K
0.19 × 0.15 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*ABSCOR*; Higashi, 1999)
T_{min} = 0.114, T_{max} = 0.431
48361 measured reflections
2840 independent reflections
2591 reflections with $I > 2\sigma(I)$
R_{int} = 0.129

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.064
S = 1.09
2840 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.33 e Å^{-3}
$\Delta\rho_{min}$ = −2.56 e Å^{-3}
Absolute structure: Flack (1983), 1112 Friedel pairs
Flack parameter: 0.02 (2)

Table 1
Selected geometric parameters (Å, °).

Ir—C5	2.105 (6)	Ir—Br	2.5293 (7)
Ir—C1	2.111 (6)	Ir—Br^i	2.5335 (7)
Ir—C6	2.121 (7)	Ir···Ir^i	2.9034 (5)
Ir—C2	2.123 (6)		
Br—Ir—Br^i	84.52 (3)	Ir—Br—Ir^i	69.987 (19)

Symmetry code: (i) $-y+1, -x+1, -z+\frac{3}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *PROCESS* in *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and local routines.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2369).

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supplementary materials

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Di-μ-bromido-bis[(η^4-cycloocta-1,5-diene)iridium(I)]

T. Yamagata, **M. Nagata**, **K. Mashima** and **K. Tani**

Comment

Crystal data for many kinds of the binuclear complexes of d^8 transition metal ions of type $[L_2M(\mu\text{-}X)]_2$ (M= Rh or Ir, X = halide) and their theoretical analysis have been reported (Aullón, *et al.*, 1998; Cotton, *et al.*, 1999). The bromide analogues are fairly rare, however. Among these complexes cyclooctadiene complexes of group 8 transition elements $[M(\mu\text{-}Cl)(cod)]_2$ (COD = *cis*,*cis*-1,5-cyclooctadiene; M = Ir^I or Rh^I) have been used as starting key complexes for various kinds of Ir^I or Rh^I complexes useful as efficient catalyst precursors. For example, we have reported the molecular structure of $[Ir(\mu\text{-}Cl)\{(R)\text{-binap}\}]_2$ (Yamagata *et al.*, 1997), which was prepared from the reaction of $[Ir(\mu\text{-}Cl)(cod)]_2$ with two equivalents of (*R*)-BINAP {(*R*)-(+)-2,2'-bis(diphenylphosphanyl)-1,1'-binaphthyl}, and its use as an efficient catalyst for asymmetric hydrogenation of prochiral imines (Tani, *et al.*, 1995). The catalytic asymmetric olefin hydroamination with $[Ir(\mu\text{-}Cl)(diphosphine)]_2$ and the structure of $[Ir(\mu\text{-}Cl)\{(R)\text{-binap}\}]_2$ have also been investigated by Togni and his co-workers (Dorta, *et al.*, 1997). Although $[Rh(\mu\text{-}Cl)(cod)]_2$ (De Ridder, *et al.*, 1994) has an almost square planar structure (the hinge angle 169.1 (3)°), $[Ir(\mu\text{-}Cl)(cod)]_2$ (Cotton, *et al.*, 1986) and $[Rh(\mu\text{-}Br)(cod)]_2$ (Pettinari, *et al.*, 2002) show bent structures; the hinge angles are 109.4 (3)° and 148.7 (3)°, respectively. Thus, it may be interest to examine the structure of $[Ir(\mu\text{-}Br)(cod)]_2$, (I), which is reported here. (I) is isostructural with $[Ir(\mu\text{-}Cl)(cod)]_2$ and $[Rh(\mu\text{-}Br)(cod)]_2$. The $Ir_2(\mu\text{-}Br)_2$ core in (I) shows a bent geometry with the hinge angles of 101.58 (3)°. The $M\cdots M$ distances of (I), $[Ir(\mu\text{-}Cl)(cod)]_2$, and $[Rh(\mu\text{-}Br)(cod)]_2$ are 2.9034 (5), 2.910 (1), and 3.565 Å, respectively. The degree of the bending is Rh < Ir and Cl < Br. These tendencies can be explained by the differences in diffuseness of the metal d orbitals and by analyzing the $<p_z{}^2/d_z{}^2>$ and $<d_z{}^2/d_z{}^2>$ overlap integrals between the Slater orbitals (EH calculations) (Aullón, *et al.*, 1998).

Experimental

To a Schlenk flask were added 2.11 g of Na_2IrBr_6 (2.94 mmol), H_2O (20 ml), isopropyl alcohol (9.0 ml) and 1,5-cyclooctadiene (2.9 ml, 24 mmol). The mixture was heated under reflux for 12 hr and then cooled to ambient temperature. The whole volume was reduced to a small volume (*ca* 3 ml) under reduced pressure. To the residue were added 20 ml of H_2O and 30 ml of toluene. The reddish organic layer was separated and the aqueous layer was extracted three times with toluene (20 ml each). The combined organic layer and the extracts were condensed to dryness. The resulting deep red solid was washed with ethanol, H_2O, and ethanol successively and dried *in vacuo* to yield $[Ir(\mu\text{-}Br)(cod)]_2$ as a deep red solid (1.28 g, 57%). Recrystallization from THF afforded (I) as an analytically pure product. mp.: 469 K (melt, decomp. in capillary). ^1H NMR (300 MHz, $CDCl_3$, 308 K, δ, p.p.m.): 4.35 (m, 8H, =C*H*), 2.20 − 2.24 (m, 8H, –C*H*H–), 1.40 − 1.50 (m, 8H, –CH*H*–). IR (Nujol, cm^{-1}): 410(w), 330(w). Analysis calculated for $C_{16}H_{24}Br_2Ir_2$: C 25.27, H 3.18%; found: C 25.22; H 2.83%.

Refinement

All H-atoms were geometrically placed (C—H = 0.95–0.99 Å) and refined as riding with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$ [or $1.5U_{\mathrm{eq}}(\mathrm{C})$ for methyl groups].

Figures

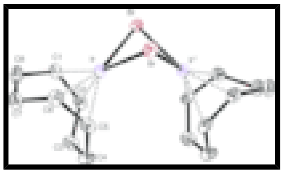

Fig. 1. The molecule structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The H-atoms have been omitted. Symmetry code: (i) $1 - y$, $1 - x$, $3/2 - z$.

Di-μ-bromido-bis[(η^4-cycloocta-1,5-diene)iridium(I)]

Crystal data

$[\mathrm{Ir_2Br_2(C_8H_{12})_2}]$
$M_r = 760.57$
Tetragonal, $P4_12_12$
Hall symbol: P 4abw 2nw
$a = 8.3839$ (5) Å
$b = 8.3839$ (5) Å
$c = 24.1471$ (19) Å
$\alpha = 90°$
$\beta = 90°$
$\gamma = 90°$
$V = 1697.3$ (2) Å^3

$Z = 4$
$F_{000} = 1376$
$D_x = 2.976$ Mg m^{-3}
Melting point: 469 K
Mo $K\alpha$ radiation
$\lambda = 0.71075$ Å
Cell parameters from 69455 reflections
$\theta = 3.4$–31.3°
$\mu = 20.36$ mm^{-1}
$T = 100$ (1) K
Block, red
0.19 × 0.15 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: normal-focus sealed tube
Monochromator: graphite
Detector resolution: 10.00 pixels mm^{-1}
$T = 100(1)$ K
ω scans
Absorption correction: numerical (ABSCOR; Higashi, 1999)
$T_{\mathrm{min}} = 0.114$, $T_{\mathrm{max}} = 0.431$
48361 measured reflections

2840 independent reflections
2591 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.129$
$\theta_{\mathrm{max}} = 31.6°$
$\theta_{\mathrm{min}} = 3.4°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 4.3085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.09$	$\Delta\rho_{max} = 1.33$ e Å^{-3}
2840 reflections	$\Delta\rho_{min} = -2.56$ e Å^{-3}
91 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1112 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (2)

Special details

Experimental. Indexing was performed from 3 oscillations which were exposed for 1.3 minutes. The camera radiuswas 127.40 mm. Readout performed in the 0.100 mm pixel mode. A total of 300 images, corresponding to 600.0 °. osillation angles, were collected with 4 different goniometer setting. Exposure time was 100 s per degree. The camera radiuswas 127.40 mm. Readout performed in the 0.100 mm pixel mode.

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. Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

− 1.1015 (0.0026) *x* + 8.0857 (0.0009) *y* + 5.5390 (0.0060) *z* = 7.6598 (0.0050)

* 0.0000 (0.0000) Ir * 0.0000 (0.0000) Br * 0.0000 (0.0000) Br_$1

Rms deviation of fitted atoms = 0.0000

8.0857 (0.0009) *x* − 1.1015 (0.0026) *y* + 5.5390 (0.0060) *z* = 7.6329 (0.0044)

Angle to previous plane (with approximate e.s.d.) = 78.42 (0.03)

* 0.0000 (0.0000) Ir_$1 * 0.0000 (0.0000) Br * 0.0000 (0.0000) Br_$1

Rms deviation of fitted atoms = 0.0000

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*	$U_{iso}*/U_{eq}$

Ir	0.71261 (3)	0.51576 (3)	0.771695 (9)	0.01892 (6)
Br	0.55064 (8)	0.55356 (8)	0.68431 (2)	0.02227 (14)
C1	0.8208 (8)	0.5503 (8)	0.8497 (2)	0.0225 (14)
H1	0.7181	0.5761	0.8637	0.027*
C2	0.8474 (9)	0.3900 (9)	0.8320 (2)	0.0233 (14)
H2	0.7609	0.3170	0.8337	0.028*
C3	1.0064 (9)	0.3299 (9)	0.8105 (3)	0.0267 (15)
H3A	1.0216	0.2178	0.8222	0.032*
H3B	1.0935	0.3942	0.8269	0.032*
C4	1.0161 (9)	0.3402 (9)	0.7468 (3)	0.0262 (15)
H4A	1.1289	0.3534	0.7356	0.031*
H4B	0.9768	0.2390	0.7306	0.031*
C5	0.9189 (8)	0.4778 (9)	0.7238 (2)	0.0232 (13)
H5	0.8512	0.4563	0.6931	0.028*
C6	0.9213 (9)	0.6350 (8)	0.7443 (3)	0.0241 (15)
H6	0.8515	0.7107	0.7279	0.029*
C7	1.0287 (9)	0.6909 (10)	0.7912 (3)	0.0289 (15)
H7A	1.0621	0.8023	0.7841	0.035*
H7B	1.1259	0.6238	0.7921	0.035*
C8	0.9438 (10)	0.6819 (9)	0.8479 (3)	0.0303 (17)
H8A	1.0241	0.6633	0.8772	0.036*
H8B	0.8910	0.7852	0.8556	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir	0.02031 (13)	0.02195 (14)	0.01450 (9)	0.00101 (10)	−0.00110 (9)	−0.00051 (9)
Br	0.0270 (4)	0.0221 (3)	0.0177 (3)	0.0016 (3)	−0.0040 (2)	0.0020 (2)
C1	0.022 (4)	0.026 (4)	0.019 (3)	−0.004 (3)	−0.002 (2)	0.004 (2)
C2	0.021 (4)	0.033 (4)	0.016 (3)	−0.002 (3)	−0.002 (2)	0.003 (2)
C3	0.025 (4)	0.033 (4)	0.023 (3)	0.003 (3)	0.000 (3)	0.009 (3)
C4	0.030 (4)	0.027 (4)	0.022 (3)	0.006 (3)	0.008 (3)	−0.001 (3)
C5	0.020 (3)	0.033 (4)	0.017 (3)	0.004 (3)	0.000 (2)	0.005 (3)
C6	0.028 (4)	0.021 (3)	0.023 (3)	−0.002 (3)	0.002 (3)	0.005 (2)
C7	0.025 (4)	0.034 (4)	0.028 (3)	−0.008 (3)	0.000 (3)	0.000 (3)
C8	0.036 (4)	0.032 (4)	0.023 (3)	−0.008 (3)	−0.008 (3)	−0.005 (3)

Geometric parameters (Å, °)

Ir—C5	2.105 (6)	C3—H3A	0.9900
Ir—C1	2.111 (6)	C3—H3B	0.9900
Ir—C6	2.121 (7)	C4—C5	1.518 (9)
Ir—C2	2.123 (6)	C4—H4A	0.9900
Ir—Br	2.5293 (7)	C4—H4B	0.9900
Ir—Br^{i}	2.5335 (7)	C5—C6	1.408 (10)
Ir—Ir^{i}	2.9034 (5)	C5—H5	0.9500
Br—Ir^{i}	2.5335 (7)	C6—C7	1.519 (10)
C1—C2	1.429 (10)	C6—H6	0.9500

C1—C8	1.511 (10)	C7—C8	1.546 (10)
C1—H1	0.9500	C7—H7A	0.9900
C2—C3	1.517 (10)	C7—H7B	0.9900
C2—H2	0.9500	C8—H8A	0.9900
C3—C4	1.542 (9)	C8—H8B	0.9900

C5—Ir—C1	99.1 (3)	C2—C3—H3A	109.3
C5—Ir—C6	38.9 (3)	C4—C3—H3A	109.3
C1—Ir—C6	81.9 (3)	C2—C3—H3B	109.3
C5—Ir—C2	82.2 (3)	C4—C3—H3B	109.3
C1—Ir—C2	39.4 (3)	H3A—C3—H3B	108.0
C6—Ir—C2	90.5 (3)	C5—C4—C3	112.3 (6)
C5—Ir—Br	90.09 (17)	C5—C4—H4A	109.1
C1—Ir—Br	163.4 (2)	C3—C4—H4A	109.1
C6—Ir—Br	97.13 (19)	C5—C4—H4B	109.1
C2—Ir—Br	156.9 (2)	C3—C4—H4B	109.1
C5—Ir—Br^{i}	157.1 (2)	H4A—C4—H4B	107.9
C1—Ir—Br^{i}	91.95 (18)	C6—C5—C4	125.1 (6)
C6—Ir—Br^{i}	163.9 (2)	C6—C5—Ir	71.1 (4)
C2—Ir—Br^{i}	94.1 (2)	C4—C5—Ir	110.8 (4)
Br—Ir—Br^{i}	84.52 (3)	C6—C5—H5	117.5
C5—Ir—Ir^{i}	104.1 (2)	C4—C5—H5	117.5
C1—Ir—Ir^{i}	134.09 (18)	Ir—C5—H5	88.1
C6—Ir—Ir^{i}	137.95 (19)	C5—C6—C7	124.0 (7)
C2—Ir—Ir^{i}	105.7 (2)	C5—C6—Ir	69.9 (4)
Br—Ir—Ir^{i}	55.074 (17)	C7—C6—Ir	113.7 (4)
Br^{i}—Ir—Ir^{i}	54.939 (16)	C5—C6—H6	118.0
Ir—Br—Ir^{i}	69.987 (19)	C7—C6—H6	118.0
C2—C1—C8	124.8 (7)	Ir—C6—H6	86.4
C2—C1—Ir	70.7 (3)	C6—C7—C8	111.8 (6)
C8—C1—Ir	111.5 (4)	C6—C7—H7A	109.3
C2—C1—H1	117.6	C8—C7—H7A	109.3
C8—C1—H1	117.6	C6—C7—H7B	109.3
Ir—C1—H1	87.7	C8—C7—H7B	109.3
C1—C2—C3	123.5 (7)	H7A—C7—H7B	107.9
C1—C2—Ir	69.8 (4)	C1—C8—C7	112.1 (6)
C3—C2—Ir	113.5 (4)	C1—C8—H8A	109.2
C1—C2—H2	118.2	C7—C8—H8A	109.2
C3—C2—H2	118.2	C1—C8—H8B	109.2
Ir—C2—H2	86.8	C7—C8—H8B	109.2
C2—C3—C4	111.6 (6)	H8A—C8—H8B	107.9

C5—Ir—Br—Ir^{i}	107.2 (2)	C3—C4—C5—C6	47.0 (10)
C1—Ir—Br—Ir^{i}	−128.8 (6)	C3—C4—C5—Ir	−34.0 (8)
C6—Ir—Br—Ir^{i}	145.6 (2)	C1—Ir—C5—C6	−64.8 (4)
C2—Ir—Br—Ir^{i}	37.3 (5)	C2—Ir—C5—C6	−100.5 (4)
Br^{i}—Ir—Br—Ir^{i}	−50.44 (3)	Br—Ir—C5—C6	101.3 (4)

C5—Ir—C1—C2	−65.7 (4)	Br^{i}—Ir—C5—C6	177.3 (4)
C6—Ir—C1—C2	−100.8 (4)	Ir^{i}—Ir—C5—C6	155.1 (3)
Br—Ir—C1—C2	171.5 (5)	C1—Ir—C5—C4	56.5 (5)
Br^{i}—Ir—C1—C2	94.1 (4)	C6—Ir—C5—C4	121.3 (7)
Ir^{i}—Ir—C1—C2	54.2 (5)	C2—Ir—C5—C4	20.8 (5)
C5—Ir—C1—C8	55.1 (6)	Br—Ir—C5—C4	−137.4 (5)
C6—Ir—C1—C8	20.1 (5)	Br^{i}—Ir—C5—C4	−61.4 (7)
C2—Ir—C1—C8	120.8 (7)	Ir^{i}—Ir—C5—C4	−83.6 (5)
Br—Ir—C1—C8	−67.7 (9)	C4—C5—C6—C7	3.1 (11)
Br^{i}—Ir—C1—C8	−145.0 (5)	Ir—C5—C6—C7	105.7 (6)
Ir^{i}—Ir—C1—C8	175.1 (4)	C4—C5—C6—Ir	−102.6 (6)
C8—C1—C2—C3	2.1 (10)	C1—Ir—C6—C5	115.5 (4)
Ir—C1—C2—C3	105.4 (6)	C2—Ir—C6—C5	76.9 (4)
C8—C1—C2—Ir	−103.3 (6)	Br—Ir—C6—C5	−81.2 (4)
C5—Ir—C2—C1	114.7 (4)	Br^{i}—Ir—C6—C5	−176.2 (5)
C6—Ir—C2—C1	76.6 (4)	Ir^{i}—Ir—C6—C5	−37.5 (5)
Br—Ir—C2—C1	−173.8 (4)	C5—Ir—C6—C7	−119.3 (7)
Br^{i}—Ir—C2—C1	−88.0 (4)	C1—Ir—C6—C7	−3.8 (6)
Ir^{i}—Ir—C2—C1	−142.7 (4)	C2—Ir—C6—C7	−42.4 (6)
C5—Ir—C2—C3	−4.1 (6)	Br—Ir—C6—C7	159.4 (5)
C1—Ir—C2—C3	−118.8 (8)	Br^{i}—Ir—C6—C7	64.5 (10)
C6—Ir—C2—C3	−42.3 (6)	Ir^{i}—Ir—C6—C7	−156.9 (4)
Br—Ir—C2—C3	67.4 (8)	C5—C6—C7—C8	−93.9 (8)
Br^{i}—Ir—C2—C3	153.1 (5)	Ir—C6—C7—C8	−12.8 (8)
Ir^{i}—Ir—C2—C3	98.4 (5)	C2—C1—C8—C7	48.2 (9)
C1—C2—C3—C4	−93.8 (8)	Ir—C1—C8—C7	−32.8 (8)
Ir—C2—C3—C4	−13.2 (8)	C6—C7—C8—C1	29.7 (9)
C2—C3—C4—C5	30.8 (9)		

Symmetry codes: (i) −*y*+1, −*x*+1, −*z*+3/2.

Fig. 1