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catena-Poly[[(5,5′-dimethyl- 2,2′-bipyridine-κ^2N,N')cadmium(II)]-di-μ-chlorido]

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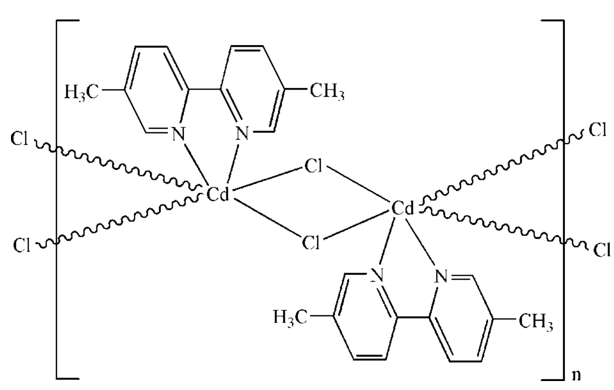
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 22.1.

The asymmetric unit of the title compound, $[CdCl_2(C_{12}H_{12}N_2)]_n$, contains one half-molecule; a twofold rotation axis passes through the Cd atom. The Cd^{II} atom is six-coordinated in a distorted octahedral configuration by two N atoms from 2,2′-bipyridine-5,5′-dimethyl and four bridging Cl atoms. The bridging function of the chloro atoms leads to a one-dimensional chain structure. There is a π–π contact between the pyridine rings [centroid–centroid distance = 3.9807 (9) Å].

Related literature

For related literature, see: Chen *et al.* (2003); Flook *et al.* (1973); Hu & Englert (2002); Janiak *et al.* (1999); Satoh *et al.* (2001); Zhou *et al.* (2003); Khalighi *et al.* (2008).



Experimental

Crystal data

$[CdCl_2(C_{12}H_{12}N_2)]$
M_r = 367.55
Monoclinic, $C2/c$
a = 20.365 (4) Å
b = 9.3135 (19) Å
c = 7.2313 (14) Å
β = 107.53 (3)°
V = 1307.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.06 mm^{-1}
T = 298 (2) K
0.20 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.666, T_{max} = 0.740
4283 measured reflections
1724 independent reflections
1585 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.089
S = 1.08
1724 reflections
78 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—Cl1^{i}	2.7668 (10)	N1—Cd1	2.355 (2)
Cl1—Cd1	2.5457 (9)		
Cl1—Cd1—Cl1^{i}	85.18 (2)	N1—Cd1—Cl1	93.57 (6)
Cl1—Cd1—Cl1^{ii}	96.22 (3)	N1^{iii}—Cd1—Cl1	159.71 (6)
Cl1^{i}—Cd1—Cl1^{ii}	177.73 (2)	N1—Cd1—Cl1^{i}	93.89 (5)
Cl1^{iii}—Cd1—Cl1	104.77 (4)	N1—Cd1—Cl1^{ii}	84.24 (5)
N1—Cd1—Cl1^{iii}	159.71 (6)	N1—Cd1—N1^{iii}	69.98 (10)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2520).

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Acta Cryst. (2008). E**64**, m1233   [doi:10.1107/S1600536808027657]

catena-Poly[[(5,5′-dimethyl- 2,2′-bipyridine-κ^2*N*,*N*′)cadmium(II)]-di-μ-chlorido]

Roya Ahmadi, Aida Khalighi, Khadijeh Kalateh, Vahid Amani and Hamid Reza Khavasi

S1. Comment

In a recent paper, we reported the synthesis and crystal structure of [Zn(5,5′-dmbpy)Cl_2], (Khalighi *et al.*, 2008) [where 5,5′-dmbpy is 5,5′-dimethyl-2,2′-bipyridine]. Several Cd^{II} polymer complexes, with formula, [Cd(N—N)(μ-Cl)$_2$]$_n$, such as [Cd(phen)(μ-Cl)$_2$]$_n$, (II) (Chen *et al.*, 2003), {[Cd(5,5′-dabpy)(μ-Cl)$_2$].2H_2O}$_n$, (III) (Janiak *et al.*, 1999) and [Cd(bipy)(μ-Cl)$_2$]$_n$, (IV) (Zhou *et al.*, 2003) [where bipy is 2,2′-bipyridine, 5,5′-dabpy is 5,5′-diamino -2,2′-bipyridine and phen is 1,10-phenanthroline] have been synthesized and characterized by single-crystal X-ray diffraction methods. There are also several Cd^{II} polymer complexes, with formula, [Cd(μ-Cl)$_2$$L_2$]$_n$, such as [Cd($\mu$-Cl)$_2$(3,5-Me$_2$py)$_2$]$_n$, (V), [Cd($\mu$-Cl)$_2$(3,5-Br$_2$py)$_2$]$_n$, (VI) and [Cd($\mu$-Cl)$_2$(3,5-Cl$_2$py)$_2$]$_n$, (VII) (Hu & Englert, 2002), [Cd(μ-Cl)$_2$(3-Mepy)$_2$]$_n$, (VIII) (Satoh, *et al.*, 2001) and [Cd(μ-Cl)$_2$(im)$_2$]$_n$, (IX) (Flook *et al.*, 1973) [where py is pyridine and im is imidazole] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound (I).

The asymmetric unit of the title compound, (I), contains one half-molecule (Fig. 1). The Cd^{II} atom is six-coordinated in a distorted octahedral configuration by two N atoms from 2,2′-bipyridine-5,5′-dimethyl and four bridging Cl atoms. The bridging function of chloro atoms leads to a one-dimensional chain structure. The Cd—Cl and Cd—N bond lengths and angles (Table 1) are within normal ranges, as in (II), (III) and (IV).

In the crystal structure, the π—π contact (Fig. 2) between the pyridine rings, Cg4···Cg4^i [symmetry code: (i) x, 1/2- y, z, where Cg4 is centroid of the ring (N1/C1/C2/C4-C6)] may stabilize the structure, with centroid-centroid distance of 3.9807 (9) Å.

S2. Experimental

For the preparation of the title compound, a solution of 5,5′-dimethyl-2,2′ -bipyridine (0.25 g, 1.33 mmol) in methanol (10 ml) was added to a solution of $CdCl_2.H_2O$ (0.27 g, 1.33 mmol) in methanol (10 ml) at room temperature. The suitable crystals for X-ray analysis were obtained by methanol diffusion to a colorless solution in DMSO. Suitable crystals were isolated after one week (yield; 0.35 g, 71.6%, m.p. < 573 K).

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C).

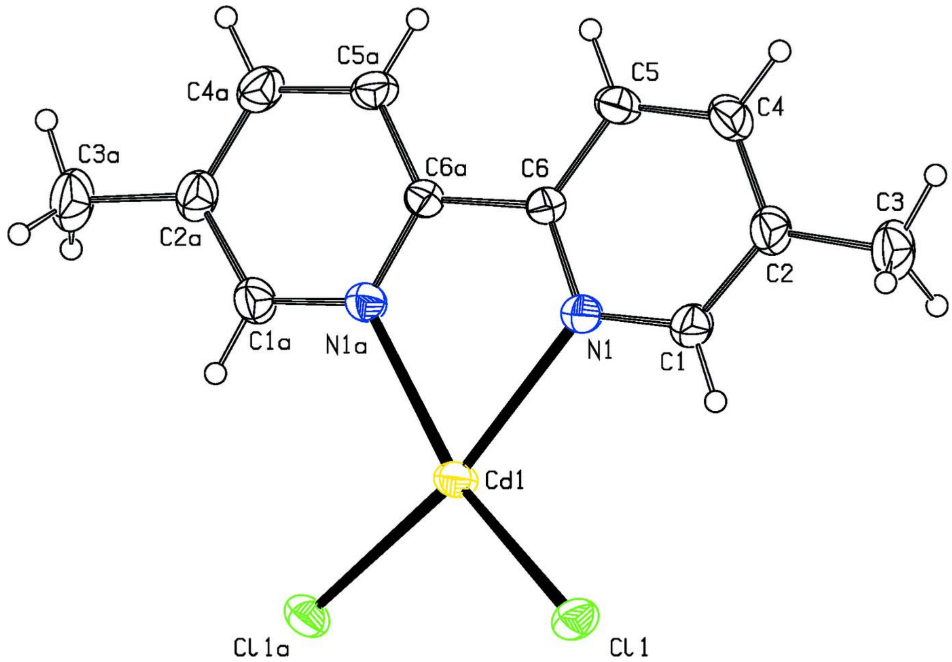

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (a) -x, y, 3/2 - z].

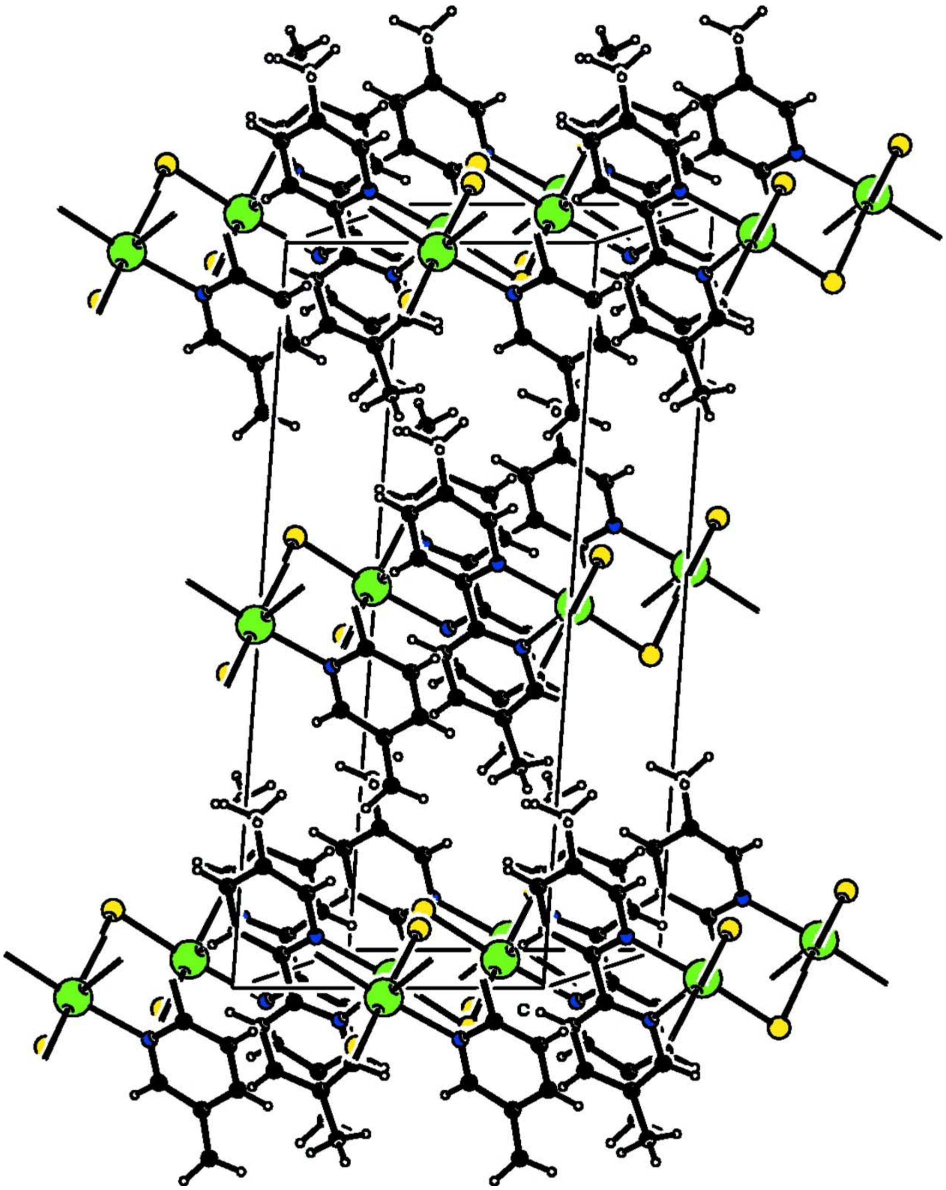

Figure 2

A packing diagram of the title compound.

catena-Poly[[(5,5′-dimethyl-2,2′-bipyridine- κ²_N_,_N′_)cadmium(II)]-di-μ-chlorido]

Crystal data

$[CdCl_2(C_{12}H_{12}N_2)]$
M_r = 367.55
Monoclinic, $C2/c$
Hall symbol: -C 2yc
a = 20.365 (4) Å
b = 9.3135 (19) Å
c = 7.2313 (14) Å
β = 107.53 (3)°
V = 1307.9 (5) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.867 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1004 reflections
θ = 4.1–29.2°
μ = 2.06 mm^{-1}
T = 298 K
Block, colorless
0.20 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.666$, $T_{max} = 0.740$
4283 measured reflections
1724 independent reflections
1585 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 29.2°$, $\theta_{min} = 4.1°$
$h = -27 \rightarrow 18$
$k = -12 \rightarrow 11$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.089$
$S = 1.08$
1724 reflections
78 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.9451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.011$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.76$ e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.58047 (2)	0.7500	0.03912 (12)
Cl1	0.07886 (4)	0.41364 (6)	0.99832 (11)	0.04502 (17)
N1	0.06292 (10)	0.7876 (2)	0.8828 (3)	0.0383 (4)
C1	0.12723 (13)	0.7815 (3)	1.0067 (4)	0.0460 (5)
H1	0.1458	0.6918	1.0488	0.055*
C2	0.16716 (14)	0.9023 (3)	1.0746 (5)	0.0480 (6)
C3	0.23917 (17)	0.8878 (5)	1.2093 (6)	0.0674 (9)
H3A	0.2665	0.8339	1.1466	0.081*
H3B	0.2381	0.8389	1.3251	0.081*
H3C	0.2589	0.9815	1.2422	0.081*
C4	0.13695 (15)	1.0347 (3)	1.0145 (4)	0.0484 (6)
H4	0.1612	1.1187	1.0594	0.058*
C5	0.07094 (15)	1.0418 (3)	0.8883 (4)	0.0435 (5)
H5	0.0504	1.1303	0.8486	0.052*
C6	0.03548 (12)	0.9157 (2)	0.8213 (4)	0.0344 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04181 (17)	0.02643 (15)	0.04102 (17)	0.000	0.00027 (11)	0.000
Cl1	0.0458 (3)	0.0370 (3)	0.0479 (3)	0.0092 (2)	0.0074 (3)	0.0073 (2)
N1	0.0373 (9)	0.0313 (9)	0.0426 (10)	0.0009 (8)	0.0064 (8)	−0.0023 (8)
C1	0.0381 (11)	0.0426 (13)	0.0501 (13)	0.0045 (10)	0.0024 (10)	−0.0068 (11)
C2	0.0364 (12)	0.0536 (16)	0.0507 (14)	−0.0035 (10)	0.0080 (11)	−0.0133 (11)
C3	0.0394 (14)	0.082 (2)	0.070 (2)	−0.0029 (15)	−0.0003 (14)	−0.0177 (18)
C4	0.0448 (13)	0.0457 (14)	0.0529 (15)	−0.0112 (11)	0.0117 (11)	−0.0135 (12)
C5	0.0487 (13)	0.0303 (10)	0.0533 (14)	−0.0046 (10)	0.0179 (12)	−0.0062 (10)
C6	0.0339 (10)	0.0296 (11)	0.0406 (11)	0.0012 (7)	0.0129 (9)	−0.0020 (8)

Geometric parameters (Å, º)

Cd1—Cl1^{i}	2.5457 (9)	C2—C3	1.502 (4)
Cd1—Cl1^{ii}	2.7668 (10)	C3—H3A	0.9600
Cd1—Cl1^{iii}	2.7668 (10)	C3—H3B	0.9600
Cl1—Cd1	2.5457 (9)	C3—H3C	0.9600
Cl1—Cd1^{ii}	2.7668 (10)	C4—C5	1.380 (4)
Cd1—N1^{i}	2.355 (2)	C4—H4	0.9300
N1—Cd1	2.355 (2)	C5—C6	1.387 (3)
C1—N1	1.347 (3)	C5—H5	0.9300
C1—C2	1.389 (4)	C6—N1	1.336 (3)
C1—H1	0.9300	C6—C6^{i}	1.501 (5)
C2—C4	1.388 (4)		
Cd1—Cl1—Cd1^{ii}	94.82 (2)	N1—C1—H1	118.3
Cl1^{i}—Cd1—Cl1^{ii}	96.22 (3)	C2—C1—H1	118.3
Cl1—Cd1—Cl1^{ii}	85.18 (2)	C4—C2—C1	116.9 (3)
Cl1^{i}—Cd1—Cl1^{iii}	85.18 (2)	C4—C2—C3	122.5 (3)
Cl1—Cd1—Cl1^{iii}	96.22 (3)	C1—C2—C3	120.6 (3)
Cl1^{ii}—Cd1—Cl1^{iii}	177.73 (2)	C2—C3—H3A	109.5
Cl1^{i}—Cd1—Cl1	104.77 (4)	C2—C3—H3B	109.5
N1—Cd1—Cl1^{i}	159.71 (6)	H3A—C3—H3B	109.5
N1^{i}—Cd1—Cl1^{i}	93.57 (6)	C2—C3—H3C	109.5
N1—Cd1—Cl1	93.57 (6)	H3A—C3—H3C	109.5
N1^{i}—Cd1—Cl1	159.71 (6)	H3B—C3—H3C	109.5
N1—Cd1—Cl1^{ii}	93.89 (5)	C5—C4—C2	120.1 (3)
N1^{i}—Cd1—Cl1^{ii}	84.24 (5)	C5—C4—H4	120.0
N1—Cd1—Cl1^{iii}	84.24 (5)	C2—C4—H4	120.0
N1^{i}—Cd1—Cl1^{iii}	93.89 (5)	C4—C5—C6	119.4 (3)
N1—Cd1—N1^{i}	69.98 (10)	C4—C5—H5	120.3
C6—N1—C1	119.0 (2)	C6—C5—H5	120.3
C6—N1—Cd1	118.31 (15)	N1—C6—C5	121.2 (2)
C1—N1—Cd1	122.49 (18)	N1—C6—C6^{i}	116.64 (13)
N1—C1—C2	123.3 (3)	C5—C6—C6^{i}	122.15 (16)

N1—C1—C2—C4	2.3 (5)	C1—N1—Cd1—N1^{i}	−176.1 (3)
N1—C1—C2—C3	−178.6 (3)	C6—N1—Cd1—Cl1^{i}	36.2 (3)
C1—C2—C4—C5	−1.9 (4)	C1—N1—Cd1—Cl1^{i}	−138.71 (19)
C3—C2—C4—C5	179.1 (3)	C6—N1—Cd1—Cl1	−168.97 (17)
C2—C4—C5—C6	−0.5 (4)	C1—N1—Cd1—Cl1	16.1 (2)
C4—C5—C6—N1	2.8 (4)	C6—N1—Cd1—Cl1^{ii}	−83.57 (18)
C4—C5—C6—C6^{i}	−177.9 (3)	C1—N1—Cd1—Cl1^{ii}	101.5 (2)
C5—C6—N1—C1	−2.5 (4)	C6—N1—Cd1—Cl1^{iii}	95.14 (18)
C6^{i}—C6—N1—C1	178.2 (3)	C1—N1—Cd1—Cl1^{iii}	−79.8 (2)
C5—C6—N1—Cd1	−177.59 (18)	Cd1^{ii}—Cl1—Cd1—N1	93.61 (5)
C6^{i}—C6—N1—Cd1	3.0 (3)	Cd1^{ii}—Cl1—Cd1—N1^{i}	58.77 (15)
C2—C1—N1—C6	−0.1 (4)	Cd1^{ii}—Cl1—Cd1—Cl1^{i}	−95.17 (2)
C2—C1—N1—Cd1	174.8 (2)	Cd1^{ii}—Cl1—Cd1—Cl1^{ii}	0.0
C6—N1—Cd1—N1^{i}	−1.14 (13)	Cd1^{ii}—Cl1—Cd1—Cl1^{iii}	178.20 (2)

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