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Bis(2-aminopyrimidine-κN^1)-dibromidozinc(II)

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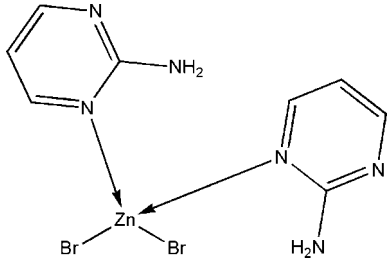
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.009 Å; R factor = 0.042; wR factor = 0.111; data-to-parameter ratio = 15.0.

The title compound, $[ZnBr_2(C_4H_5N_3)_2]$, is a mononuclear complex in which the Zn^{II} ions have distorted tetrahedral coordination geometry. The Zn^{II} ion binds to two N atoms from two different 2-aminopyrimidine ligands and two bromide ions. N—H···N hydrogen bonds link the molecules to form a one-dimensional supramolecular structure. The supramolecular chains are parallel to each other and N—H···Br hydrogen bonds link them into a two-dimensional network in the *ac* plane. Additionally, there are strong π–π interactions [centroid–centroid distance = 3.403 (3) Å].

Related literature

For related literature, see: Bourne *et al.* (2001); Etter *et al.* (1990); Lin & Zeng (2007); Pon *et al.* (1997).



Experimental

Crystal data

$[ZnBr_2(C_4H_5N_3)_2]$
M_r = 415.41
Triclinic, $P\overline{1}$
a = 6.7912 (11) Å
b = 7.2197 (12) Å
c = 15.512 (3) Å
α = 81.060 (3)°
β = 83.823 (3)°
γ = 63.132 (2)°
V = 669.61 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 7.79 mm^{-1}
T = 292 (2) K
0.20 × 0.16 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.305, T_{max} = 0.408
(expected range = 0.251–0.336)
5351 measured reflections
2342 independent reflections
1878 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.02
2342 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected bond lengths (Å).

Br1—Zn1	2.3528 (9)	N1—Zn1	2.060 (4)
Br2—Zn1	2.3593 (8)	N4—Zn1	2.056 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···Br2^{i}	0.93	2.87	3.651 (5)	142
N6—H6B···N5^{ii}	0.89	2.47	2.996 (6)	119
N3—H3A···Br2	0.75	2.74	3.480 (5)	170

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2036).

References

Bourne, S. A., Kilkenny, M. & Nassimbeni, L. R. (2001). *Dalton Trans.* pp. 1176–1179.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Lin, Z.-D. & Zeng, W. (2007). *Acta Cryst.* E**63**, m1597.
Pon, G., Willett, R. D., Prince, B. A. & Robinson, W. T. (1997). *Inorg. Chim. Acta*, **255**, 325–334.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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Bis(2-aminopyrimidine-κN^1)dibromidozinc(II)

Yang Qu, Shi Ming Zhang, Xian Zong Wu, Huan Zhang and Zhi Dong Lin

S1. Comment

Recently, the design of molecular architecture with pyrimidine and bipyrimidine has aroused interest in the fields of coordination, bioinorganic and magnetochemistry (Pon *et al.*, 1997).

In our laboratory, analogous crystals have been obtained from the interaction of zinc(II) chloride with 2-amino-pyrimidine (Lin & Zeng, 2007). As an extension of this work, we report the crystal structure of the title compound, (I), bis(2-aminopyrimidine)-zinc(II) bromide. Compound I contains discrete L_2CuBr_2 molecules (*L*: 2-aminopyrimidine). The Zn^{II} ion is coordinated by two N atoms from two different 2-aminopyrimidine ligands and two Br anions, giving distorted tetrahedral coordination geometry [mean Zn—N = 2.058 (8) Å and mean Zn—Br = 2.356 (4) Å]. The bond lengths and angles of Zn—N and Zn—Br (Table 1) are within the expected ranges (Bourne *et al.*, 2001).

In the crystal structure, N—H···N hydrogen bonds and N—H···Br hydrogen bonds (Table 2) help to establish the crystal packing. The 2-aminopyrimidine molecules form N—H···N hydrogen bonds, resulting in eight membered ring graph-set motif, $[R^2_2(8)]$ (Etter *et al.*, 1990). The N—H···N hydrogen bonds bind the neighboring 2-aminopyrimidine molecules to form a zigzag one-dimensional ribbon structure. The supramolecular ribbons are parallel to each other and N—H···Br hydrogen bonds link them into a two-dimensional network. The close distance, 3.403 (3) Å, between the centroids of two rings (N4,N5,C5,C6,C7,C8 and its symmetry equivalent at -*x*,1 - *y*,1 - *z*) indicates that there are also strong π -π interactions.

S2. Experimental

10 ml e thanol solution containing $ZnBr_2$ (0.5 mmol) and 2-aminopyrimidine (1.0 mmol) was stirred at room temperature for 12 h and then filtered. The filtrate was kept at room temperature in the dark for two weeks to give white crystals of (I). The crystals were isolated and washed three times with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$. Analysis calculated for $C_8N_6H_{10}$ Zn Br_2: C 23.13, N 20.23, H 2.43%; found: C 23.19, N 20.46,H 2.61%.

S3. Refinement

The H atoms bonded to C atoms were placed in calculated positions, and were allowed to ride on their parent C atoms, with a distance of 0.93 Å for aromatic H atoms and U_{iso}(H) = 1.2 times its parent atom. The H atoms of –NH_2 were found from residue peaks in the difference map. The H atoms of the NH_2 group were placed in geometrically calculated positions and the N—H distance restrained to 0.86 (2) Å. The isotropic displacement parameters were set equal to 1.5U_{eq}(parent N atom) for amino H atoms.

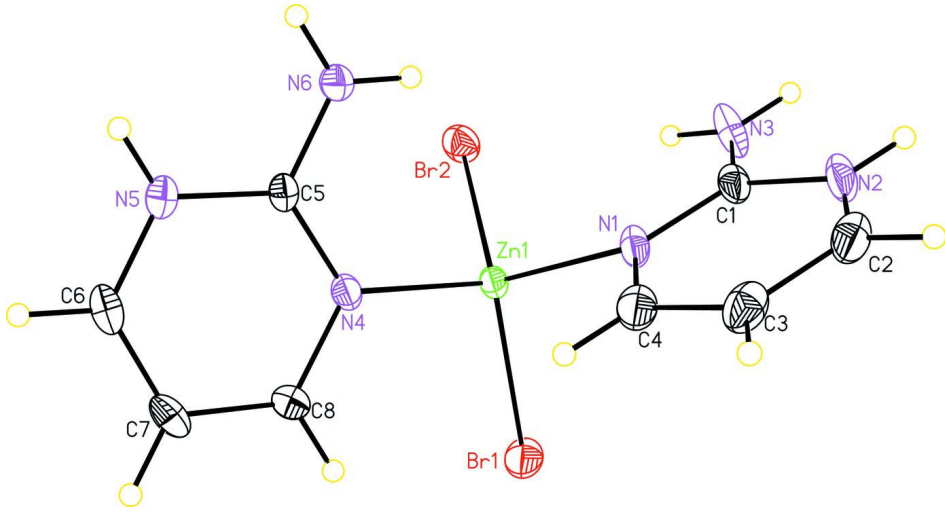

Figure 1

The molecular components of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

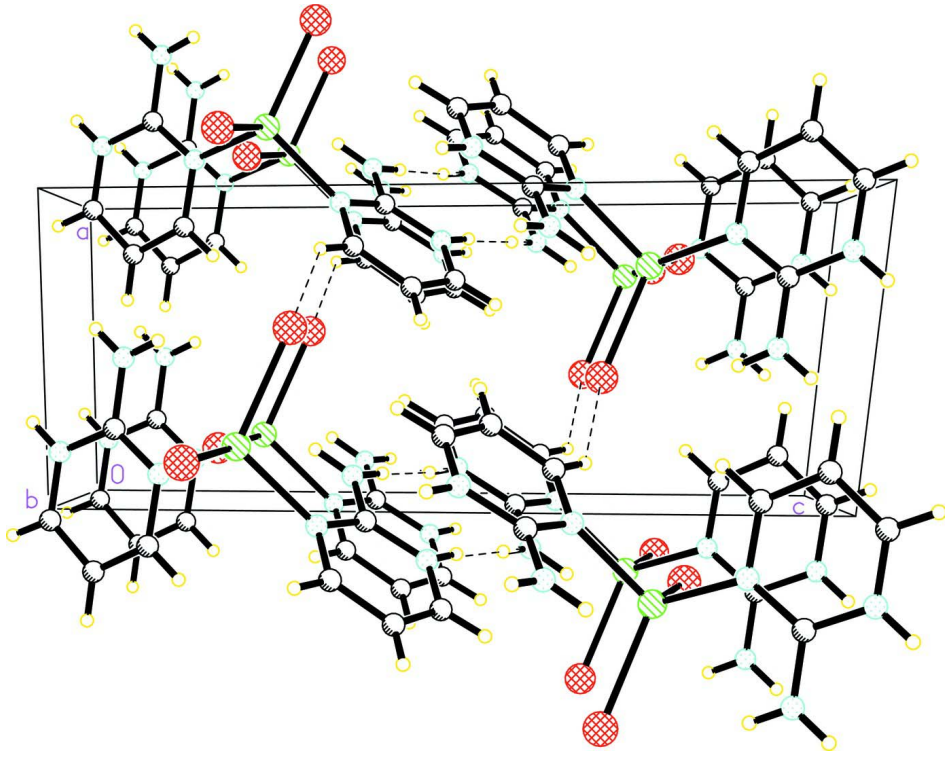

Figure 2

Crystal packing of (I) viewed along the *a* axis. The O–H···N and Br—H···N hydrogen bonding interactions are shown as dashed lines.

Bis(2-aminopyrimidine-κN^1)dibromidozinc(II)

Crystal data

$[ZnBr_2(C_4H_5N_3)_2]$
$M_r = 415.41$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.7912$ (11) Å
$b = 7.2197$ (12) Å
$c = 15.512$ (3) Å
$\alpha = 81.060$ (3)°
$\beta = 83.823$ (3)°
$\gamma = 63.132$ (2)°
$V = 669.61$ (19) Å^3
$Z = 2$
$F(000) = 400$
$D_x = 2.060$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2800 reflections
$\theta = 2.1$–$28.7°$
$\mu = 7.79$ mm^{-1}
$T = 292$ K
Block, white
0.20 × 0.16 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.305$, $T_{max} = 0.409$
5351 measured reflections
2342 independent reflections
1878 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -8 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.110$
$S = 1.02$
2342 reflections
156 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
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ 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}
Br1	0.19184 (13)	0.75744 (9)	0.20800 (4)	0.0660 (2)
Br2	0.57558 (9)	0.19239 (9)	0.31136 (4)	0.0528 (2)
C1	0.2693 (11)	0.1954 (8)	0.0989 (3)	0.0472 (14)

C2	−0.0153 (14)	0.2437 (10)	0.0194 (4)	0.0631 (18)
H2	−0.0664	0.2230	−0.0298	0.076*
C3	−0.1718 (12)	0.3635 (10)	0.0799 (4)	0.0613 (17)
H3	−0.3231	0.4171	0.0737	0.074*
C4	−0.0852 (11)	0.3955 (9)	0.1486 (4)	0.0527 (15)
H4	−0.1815	0.4767	0.1901	0.063*
C5	−0.0098 (7)	0.2696 (8)	0.4074 (3)	0.0322 (10)
C6	−0.2637 (9)	0.4775 (9)	0.5028 (3)	0.0470 (14)
H6	−0.3439	0.4925	0.5559	0.056*
C7	−0.2909 (8)	0.6530 (9)	0.4488 (4)	0.0481 (14)
H7	−0.3932	0.7848	0.4622	0.058*
C8	−0.1607 (8)	0.6272 (8)	0.3737 (3)	0.0452 (13)
H8	−0.1738	0.7449	0.3357	0.054*
N1	0.1338 (8)	0.3141 (7)	0.1588 (2)	0.0412 (10)
N2	0.1963 (11)	0.1600 (8)	0.0279 (3)	0.0594 (14)
N3	0.4858 (9)	0.1121 (9)	0.1065 (3)	0.0674 (16)
H3A	0.5101	0.1135	0.1524	0.101*
H3B	0.5506	0.1597	0.0607	0.101*
N4	−0.0134 (6)	0.4360 (6)	0.3530 (2)	0.0356 (9)
N5	−0.1293 (7)	0.2848 (7)	0.4844 (3)	0.0414 (10)
N6	0.1223 (8)	0.0761 (7)	0.3887 (3)	0.0477 (11)
H6A	0.1646	0.0802	0.3421	0.071*
H6B	0.0449	0.0026	0.3950	0.071*
Zn1	0.22458 (9)	0.41974 (8)	0.25651 (3)	0.0358 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1151 (6)	0.0446 (4)	0.0495 (4)	−0.0468 (4)	0.0003 (3)	−0.0032 (3)
Br2	0.0431 (4)	0.0522 (4)	0.0541 (4)	−0.0125 (3)	0.0026 (3)	−0.0125 (3)
C1	0.082 (5)	0.042 (3)	0.033 (3)	−0.042 (3)	0.011 (3)	−0.011 (2)
C2	0.115 (6)	0.062 (4)	0.037 (3)	−0.061 (4)	−0.013 (3)	0.002 (3)
C3	0.086 (5)	0.067 (4)	0.051 (4)	−0.051 (4)	−0.017 (3)	0.005 (3)
C4	0.081 (5)	0.050 (3)	0.040 (3)	−0.040 (3)	−0.002 (3)	−0.005 (3)
C5	0.027 (2)	0.041 (3)	0.027 (2)	−0.014 (2)	0.0021 (18)	−0.007 (2)
C6	0.042 (3)	0.068 (4)	0.038 (3)	−0.028 (3)	0.009 (2)	−0.024 (3)
C7	0.032 (3)	0.050 (3)	0.058 (3)	−0.010 (3)	0.009 (2)	−0.024 (3)
C8	0.041 (3)	0.037 (3)	0.045 (3)	−0.006 (2)	0.001 (2)	−0.007 (2)
N1	0.063 (3)	0.049 (3)	0.027 (2)	−0.037 (2)	0.0078 (19)	−0.0118 (19)
N2	0.109 (5)	0.058 (3)	0.036 (3)	−0.056 (3)	0.004 (3)	−0.015 (2)
N3	0.081 (4)	0.090 (4)	0.049 (3)	−0.049 (3)	0.023 (3)	−0.041 (3)
N4	0.036 (2)	0.038 (2)	0.030 (2)	−0.0123 (18)	0.0025 (16)	−0.0095 (18)
N5	0.040 (2)	0.056 (3)	0.030 (2)	−0.023 (2)	0.0061 (18)	−0.011 (2)
N6	0.056 (3)	0.044 (3)	0.042 (3)	−0.022 (2)	0.014 (2)	−0.011 (2)
Zn1	0.0478 (4)	0.0332 (3)	0.0277 (3)	−0.0190 (3)	0.0045 (2)	−0.0081 (2)

Geometric parameters (Å, º)

Br1—Zn1	2.3528 (9)	C5—N5	1.360 (6)
Br2—Zn1	2.3593 (8)	C6—N5	1.330 (7)
C1—N3	1.324 (8)	C6—C7	1.354 (8)
C1—N1	1.340 (7)	C6—H6	0.9300
C1—N2	1.358 (7)	C7—C8	1.368 (8)
C2—N2	1.295 (9)	C7—H7	0.9300
C2—C3	1.401 (10)	C8—N4	1.353 (6)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.368 (8)	N1—Zn1	2.060 (4)
C3—H3	0.9300	N3—H3A	0.7500
C4—N1	1.347 (8)	N3—H3B	0.9006
C4—H4	0.9300	N4—Zn1	2.056 (4)
C5—N6	1.333 (6)	N6—H6A	0.7500
C5—N4	1.348 (6)	N6—H6B	0.8901
N3—C1—N1	119.5 (5)	N4—C8—H8	119.0
N3—C1—N2	117.2 (5)	C7—C8—H8	119.0
N1—C1—N2	123.2 (6)	C1—N1—C4	117.6 (5)
N2—C2—C3	124.1 (6)	C1—N1—Zn1	126.4 (4)
N2—C2—H2	118.0	C4—N1—Zn1	115.4 (3)
C3—C2—H2	118.0	C2—N2—C1	117.5 (6)
C4—C3—C2	114.9 (7)	C1—N3—H3A	109.5
C4—C3—H3	122.5	C1—N3—H3B	111.2
C2—C3—H3	122.5	H3A—N3—H3B	120.6
N1—C4—C3	122.7 (6)	C5—N4—C8	116.8 (4)
N1—C4—H4	118.6	C5—N4—Zn1	124.1 (3)
C3—C4—H4	118.6	C8—N4—Zn1	118.1 (4)
N6—C5—N4	120.2 (4)	C6—N5—C5	116.2 (5)
N6—C5—N5	116.0 (5)	C5—N6—H6A	109.5
N4—C5—N5	123.8 (4)	C5—N6—H6B	109.0
N5—C6—C7	123.9 (5)	H6A—N6—H6B	108.2
N5—C6—H6	118.0	N4—Zn1—N1	101.97 (16)
C7—C6—H6	118.0	N4—Zn1—Br1	109.63 (11)
C6—C7—C8	116.9 (5)	N1—Zn1—Br1	109.06 (12)
C6—C7—H7	121.6	N4—Zn1—Br2	108.97 (11)
C8—C7—H7	121.6	N1—Zn1—Br2	114.70 (13)
N4—C8—C7	122.1 (5)	Br1—Zn1—Br2	112.00 (3)
N2—C2—C3—C4	2.8 (9)	C7—C8—N4—C5	3.9 (7)
C2—C3—C4—N1	−1.5 (9)	C7—C8—N4—Zn1	−164.7 (4)
N5—C6—C7—C8	−4.1 (8)	C7—C6—N5—C5	2.0 (7)
C6—C7—C8—N4	1.0 (8)	N6—C5—N5—C6	−179.1 (4)
N3—C1—N1—C4	−179.8 (5)	N4—C5—N5—C6	3.5 (7)
N2—C1—N1—C4	2.2 (8)	C5—N4—Zn1—N1	79.9 (4)
N3—C1—N1—Zn1	9.2 (7)	C8—N4—Zn1—N1	−112.3 (4)
N2—C1—N1—Zn1	−168.8 (4)	C5—N4—Zn1—Br1	−164.6 (3)

C3—C4—N1—C1	−0.8 (8)	C8—N4—Zn1—Br1	3.2 (4)
C3—C4—N1—Zn1	171.2 (5)	C5—N4—Zn1—Br2	−41.7 (4)
C3—C2—N2—C1	−1.5 (9)	C8—N4—Zn1—Br2	126.0 (3)
N3—C1—N2—C2	−179.1 (5)	C1—N1—Zn1—N4	−149.6 (4)
N1—C1—N2—C2	−1.1 (8)	C4—N1—Zn1—N4	39.2 (4)
N6—C5—N4—C8	176.3 (4)	C1—N1—Zn1—Br1	94.5 (4)
N5—C5—N4—C8	−6.3 (7)	C4—N1—Zn1—Br1	−76.7 (4)
N6—C5—N4—Zn1	−15.8 (6)	C1—N1—Zn1—Br2	−32.1 (5)
N5—C5—N4—Zn1	161.6 (3)	C4—N1—Zn1—Br2	156.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Br2^{i}	0.93	2.87	3.651 (5)	142
N6—H6*B*···N5^{ii}	0.89	2.47	2.996 (6)	119
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Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) −*x*, −*y*, −*z*+1.