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3-Allyl-1-(2-cyanobenzyl)-2-methylbenzimidazol-3-ium bromide

Xiong-Bin Xu and Qiong Ye*

Ordered Matter Science Research Center, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: yeqiong@seu.edu.cn

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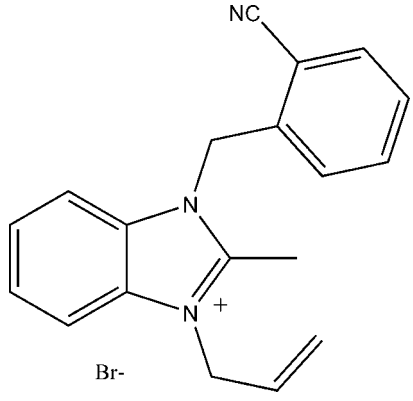
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.143; data-to-parameter ratio = 20.3.

In the title compound, $C_{19}H_{18}N_3^+\cdot Br^-$, both the allyl and cyanophenyl groups are approximately perpendicular to the central benzimidazole unit, making dihedral angles of 89.7 (2) and 85.09 (13)°, respectively. The crystal packing is dominated by C—H···Br interactions, with each anion interacting with five neighboring cations.

Related literature

For olefin–copper coordination compounds, see: Ye *et al.* (2005). For the synthesis, see: Aakeroy *et al.* (2005). For a similar structure, see: Herrmann *et al.* (1997).



Experimental

Crystal data

$C_{19}H_{18}N_3^+\cdot Br^-$
M_r = 368.27
Triclinic, $P\overline{1}$
a = 9.123 (5) Å
b = 10.100 (4) Å
c = 10.520 (4) Å
α = 98.924 (2)°
β = 108.490 (18)°
γ = 102.851 (11)°
V = 869.2 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.37 mm^{-1}
T = 293 (2) K
0.15 × 0.10 × 0.07 mm

Data collection

Rigaku Mercury2 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.872, T_{max} = 1.000
(expected range = 0.739–0.847)
9212 measured reflections
4233 independent reflections
3434 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.143
S = 0.92
4233 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 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
C13—H13A···Br1	0.93	2.91	3.738 (4)	149
C14—H14A···Br1^{i}	0.97	2.82	3.740 (3)	158
C20—H20A···Br1^{ii}	0.93	2.91	3.787 (4)	158
C29—H29A···Br1^{iii}	0.97	2.90	3.798 (3)	155
C29—H29B···Br1^{ii}	0.97	2.91	3.848 (3)	164

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by a Start-up Grant from SEU to YQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2171).

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supporting information

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3-Allyl-1-(2-cyanobenzyl)-2-methylbenzimidazol-3-ium bromide

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S1. Comment

It has been almost a century since the discovery of olefin- copper coordination compounds. We are interested in obtaining stable olefin- copper(I) coordination compounds under solvothermal conditions since these compounds display novel cluster structures and interesting physical properties such as fluorescence, SHG and ferroelectric(Ye *et al.* (2005)). The title compound (Fig 1) was synthesized as part of this project. No unexpected bond distances and angles were found in (I). Both the allyl and cyano-phenyl groups are approximately perpendicular to the central benzimidazole moiety with dihedral angles of 89.72 (23)° and 85.09 (13)° respectively such that the phenyl ring and the olefin moeity are almost parallel to one another in a conformation similar to that found by Herrmann *et al.* (1997). Thus, the molecule could adopt an end-to-head or parallel packing mode to form tight stacking. However, no π-π interactions are found. Crystal packing is dominated by C—H···Br interactions with each anion cation interacting with five neighboring cations.

S2. Experimental

2-((2-methyl-1*H*-benzo[*d*]imidazol-1-yl)methyl) benzonitrile (2.48 g) synthesized according to the procedure reported by (Aakeroy, *et al.*(2005) was dissolved in THF (30 ml) and allyl bromide;3- bromopropene (3.7 g) was added.The solution was stirred at 50° C for two days. The resulting white solid resultant was filterered out and washed twice with acetone to get 1.94 g of (I), (yield 66.7%). Colorless crystals suitable for X-ray diffraction were obtained by evaporation from methanol/water.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with U_{iso}(H) = 1.2Ueq.

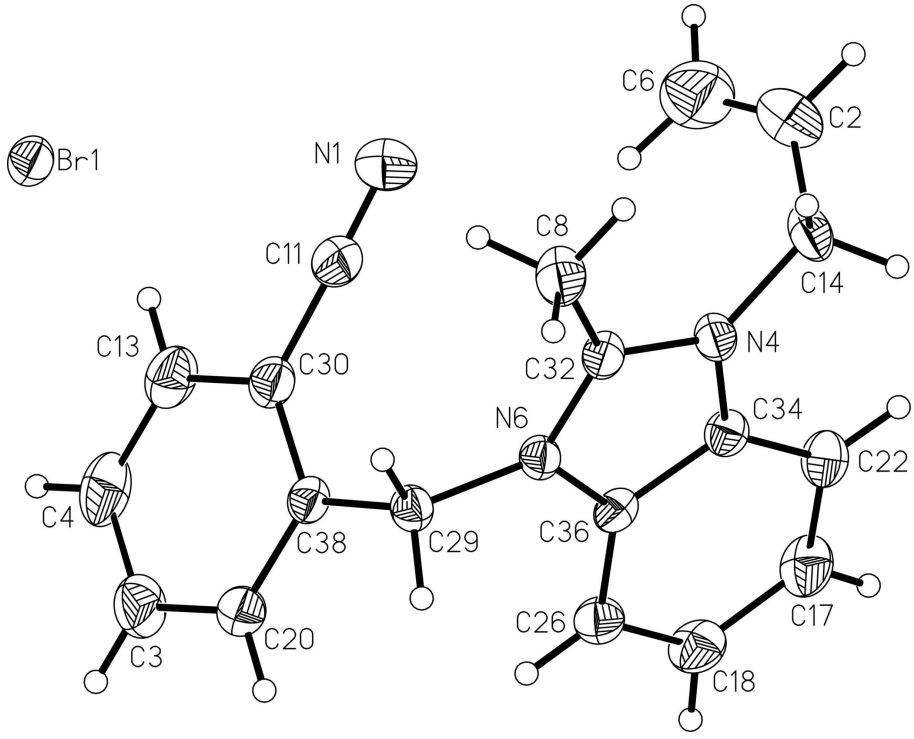

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level

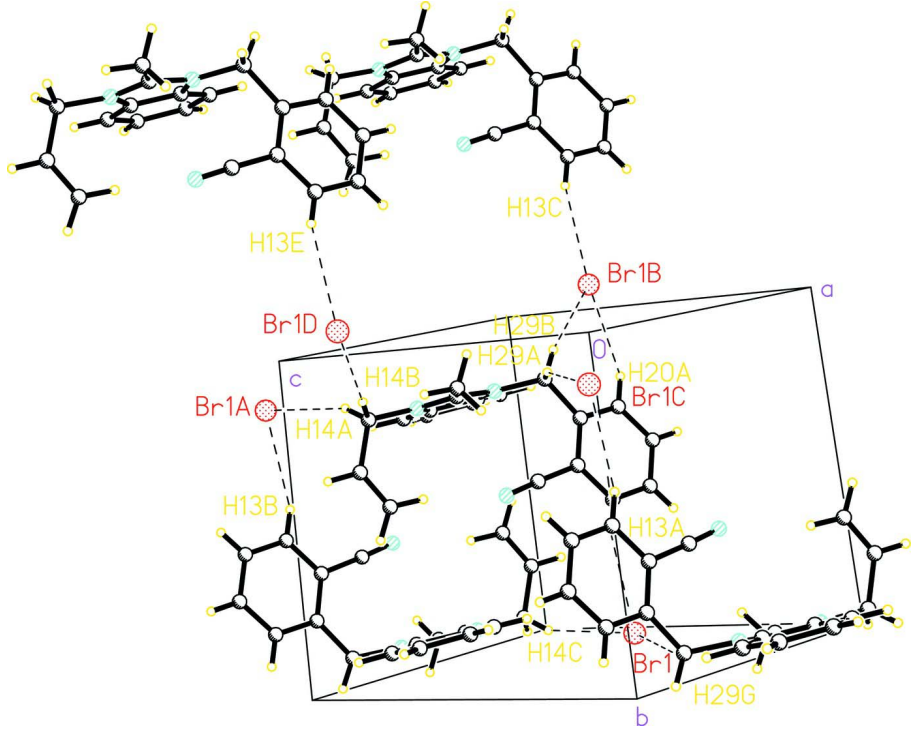

Figure 2

Packing and cell box view of the title compound.

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$\beta = 108.490$ (18)°
$\gamma = 102.851$ (11)°
$V = 869.2$ (7) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.407$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2405 reflections
$\theta = 3.2$–$28.2°$
$\mu = 2.37$ mm^{-1}
$T = 293$ K
Prism, colorless
0.15 × 0.10 × 0.07 mm

Data collection

Rigaku Mercury2 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.872$, $T_{max} = 1.000$
9212 measured reflections
4233 independent reflections
3434 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.143$
$S = 0.92$
4233 reflections
209 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.28828 (4)	0.88178 (3)	0.19130 (3)	0.04548 (14)
N1	−0.1709 (5)	0.4159 (4)	0.1763 (4)	0.0776 (11)
N4	−0.1796 (3)	0.1568 (3)	0.4110 (3)	0.0405 (6)
N6	−0.0363 (3)	0.1395 (3)	0.2796 (2)	0.0363 (5)
C2	−0.3282 (6)	0.3088 (6)	0.4888 (5)	0.0740 (12)
H2A	−0.4050	0.3187	0.5274	0.089*
C3	0.3772 (5)	0.3551 (5)	0.1240 (5)	0.0682 (11)
H3A	0.4730	0.3470	0.1146	0.082*
C4	0.3403 (5)	0.4803 (5)	0.1239 (5)	0.0705 (12)
H4A	0.4108	0.5561	0.1133	0.085*
C6	−0.2509 (8)	0.4191 (6)	0.4705 (6)	0.0950 (17)
H6A	−0.1700	0.4139	0.4312	0.114*
H6B	−0.2708	0.5071	0.4951	0.114*
C8	−0.3359 (4)	0.0951 (5)	0.1562 (4)	0.0572 (9)
H8A	−0.4256	0.0966	0.1849	0.086*
H8B	−0.3539	0.0031	0.1023	0.086*
H8C	−0.3255	0.1618	0.1015	0.086*
C11	−0.0554 (5)	0.3978 (4)	0.1660 (4)	0.0568 (9)
C13	0.1989 (6)	0.4936 (4)	0.1394 (4)	0.0619 (10)
H13A	0.1752	0.5787	0.1416	0.074*
C14	−0.3138 (4)	0.1649 (4)	0.4574 (4)	0.0530 (9)
H14A	−0.2991	0.1291	0.5396	0.064*
H14B	−0.4139	0.1050	0.3861	0.064*
C17	0.2104 (5)	0.2193 (4)	0.6974 (4)	0.0584 (9)
H17A	0.2618	0.2399	0.7929	0.070*
C18	0.3013 (4)	0.2017 (4)	0.6138 (4)	0.0562 (9)
H18A	0.4098	0.2076	0.6551	0.067*
C20	0.2714 (4)	0.2415 (4)	0.1381 (4)	0.0525 (8)
H20A	0.2975	0.1576	0.1383	0.063*
C22	0.0487 (4)	0.2073 (4)	0.6436 (3)	0.0499 (8)
H22A	−0.0116	0.2162	0.6993	0.060*
C26	0.2329 (4)	0.1757 (4)	0.4708 (3)	0.0471 (7)
H26A	0.2925	0.1642	0.4149	0.056*
C29	0.0100 (4)	0.1207 (3)	0.1566 (3)	0.0395 (6)
H29A	−0.0867	0.0945	0.0741	0.047*
H29B	0.0584	0.0444	0.1556	0.047*
C30	0.0921 (4)	0.3786 (4)	0.1518 (3)	0.0470 (7)
C32	−0.1857 (4)	0.1316 (3)	0.2799 (3)	0.0398 (6)
C34	−0.0194 (4)	0.1809 (3)	0.5002 (3)	0.0390 (6)
C36	0.0703 (3)	0.1677 (3)	0.4164 (3)	0.0375 (6)
C38	0.1274 (4)	0.2503 (3)	0.1520 (3)	0.0391 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0481 (2)	0.0486 (2)	0.0420 (2)	0.01498 (14)	0.01626 (15)	0.01637 (14)
N1	0.092 (3)	0.078 (2)	0.094 (3)	0.050 (2)	0.051 (2)	0.034 (2)
N4	0.0351 (13)	0.0511 (15)	0.0358 (13)	0.0106 (11)	0.0139 (10)	0.0129 (11)
N6	0.0338 (12)	0.0422 (13)	0.0345 (12)	0.0112 (10)	0.0135 (10)	0.0118 (10)
C2	0.062 (3)	0.086 (3)	0.079 (3)	0.025 (2)	0.034 (2)	0.011 (2)
C3	0.054 (2)	0.082 (3)	0.076 (3)	0.011 (2)	0.032 (2)	0.032 (2)
C4	0.068 (3)	0.063 (3)	0.069 (3)	−0.008 (2)	0.022 (2)	0.028 (2)
C6	0.117 (5)	0.085 (4)	0.096 (4)	0.044 (3)	0.050 (4)	0.015 (3)
C8	0.0373 (17)	0.084 (3)	0.0443 (19)	0.0105 (17)	0.0088 (14)	0.0216 (18)
C11	0.071 (2)	0.055 (2)	0.061 (2)	0.0308 (18)	0.0323 (19)	0.0238 (17)
C13	0.079 (3)	0.0445 (19)	0.062 (2)	0.0124 (18)	0.026 (2)	0.0195 (17)
C14	0.0428 (18)	0.076 (2)	0.0447 (19)	0.0134 (16)	0.0240 (15)	0.0161 (17)
C17	0.055 (2)	0.071 (2)	0.0361 (18)	0.0108 (17)	0.0047 (15)	0.0113 (16)
C18	0.0442 (19)	0.066 (2)	0.050 (2)	0.0148 (16)	0.0039 (15)	0.0172 (17)
C20	0.0500 (19)	0.059 (2)	0.057 (2)	0.0203 (16)	0.0238 (16)	0.0241 (17)
C22	0.055 (2)	0.0531 (19)	0.0370 (16)	0.0115 (15)	0.0142 (14)	0.0107 (14)
C26	0.0394 (16)	0.0554 (19)	0.0463 (18)	0.0166 (14)	0.0118 (14)	0.0158 (15)
C29	0.0415 (15)	0.0431 (16)	0.0354 (15)	0.0120 (12)	0.0161 (12)	0.0100 (12)
C30	0.0554 (19)	0.0478 (18)	0.0404 (17)	0.0164 (14)	0.0184 (15)	0.0143 (14)
C32	0.0357 (14)	0.0451 (16)	0.0380 (15)	0.0087 (12)	0.0117 (12)	0.0164 (12)
C34	0.0389 (15)	0.0416 (15)	0.0342 (15)	0.0108 (12)	0.0106 (12)	0.0102 (12)
C36	0.0364 (14)	0.0368 (14)	0.0375 (15)	0.0103 (11)	0.0089 (12)	0.0143 (12)
C38	0.0415 (15)	0.0428 (16)	0.0332 (14)	0.0121 (12)	0.0123 (12)	0.0130 (12)

Geometric parameters (Å, º)

N1—C11	1.144 (5)	C11—C30	1.451 (5)
N4—C32	1.344 (4)	C13—C30	1.393 (5)
N4—C34	1.406 (4)	C13—H13A	0.9300
N4—C14	1.468 (4)	C14—H14A	0.9700
N6—C32	1.348 (4)	C14—H14B	0.9700
N6—C36	1.400 (4)	C17—C22	1.371 (5)
N6—C29	1.482 (4)	C17—C18	1.405 (6)
C2—C6	1.256 (7)	C17—H17A	0.9300
C2—C14	1.484 (7)	C18—C26	1.389 (5)
C2—H2A	0.9300	C18—H18A	0.9300
C3—C4	1.379 (7)	C20—C38	1.388 (5)
C3—C20	1.387 (5)	C20—H20A	0.9300
C3—H3A	0.9300	C22—C34	1.392 (4)
C4—C13	1.383 (6)	C22—H22A	0.9300
C4—H4A	0.9300	C26—C36	1.389 (4)
C6—H6A	0.9600	C26—H26A	0.9300
C6—H6B	0.9600	C29—C38	1.514 (4)
C8—C32	1.484 (4)	C29—H29A	0.9700
C8—H8A	0.9600	C29—H29B	0.9700

C8—H8B	0.9600	C30—C38	1.403 (5)
C8—H8C	0.9600	C34—C36	1.391 (4)

C32—N4—C34	108.8 (3)	C22—C17—H17A	118.8
C32—N4—C14	126.9 (3)	C18—C17—H17A	118.8
C34—N4—C14	124.3 (3)	C26—C18—C17	121.6 (3)
C32—N6—C36	108.6 (2)	C26—C18—H18A	119.2
C32—N6—C29	126.6 (2)	C17—C18—H18A	119.2
C36—N6—C29	124.8 (2)	C3—C20—C38	121.4 (4)
C6—C2—C14	128.9 (5)	C3—C20—H20A	119.3
C6—C2—H2A	115.5	C38—C20—H20A	119.3
C14—C2—H2A	115.5	C17—C22—C34	115.8 (3)
C4—C3—C20	120.0 (4)	C17—C22—H22A	122.1
C4—C3—H3A	120.0	C34—C22—H22A	122.1
C20—C3—H3A	120.0	C36—C26—C18	116.0 (3)
C3—C4—C13	120.3 (3)	C36—C26—H26A	122.0
C3—C4—H4A	119.9	C18—C26—H26A	122.0
C13—C4—H4A	119.9	N6—C29—C38	113.6 (2)
C2—C6—H6A	118.5	N6—C29—H29A	108.9
C2—C6—H6B	121.6	C38—C29—H29A	108.9
H6A—C6—H6B	120.0	N6—C29—H29B	108.9
C32—C8—H8A	109.5	C38—C29—H29B	108.9
C32—C8—H8B	109.5	H29A—C29—H29B	107.7
H8A—C8—H8B	109.5	C13—C30—C38	121.1 (3)
C32—C8—H8C	109.5	C13—C30—C11	117.2 (3)
H8A—C8—H8C	109.5	C38—C30—C11	121.7 (3)
H8B—C8—H8C	109.5	N4—C32—N6	109.3 (3)
N1—C11—C30	178.4 (4)	N4—C32—C8	124.5 (3)
C4—C13—C30	119.5 (4)	N6—C32—C8	126.2 (3)
C4—C13—H13A	120.3	C36—C34—C22	122.4 (3)
C30—C13—H13A	120.3	C36—C34—N4	106.4 (3)
N4—C14—C2	113.6 (3)	C22—C34—N4	131.2 (3)
N4—C14—H14A	108.8	C26—C36—C34	121.7 (3)
C2—C14—H14A	108.8	C26—C36—N6	131.3 (3)
N4—C14—H14B	108.8	C34—C36—N6	106.9 (2)
C2—C14—H14B	108.8	C20—C38—C30	117.8 (3)
H14A—C14—H14B	107.7	C20—C38—C29	119.5 (3)
C22—C17—C18	122.4 (3)	C30—C38—C29	122.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···Br1	0.93	2.91	3.738 (4)	149
C14—H14*A*···Br1^{i}	0.97	2.82	3.740 (3)	158
C20—H20*A*···Br1^{ii}	0.93	2.91	3.787 (4)	158

C29—H29*A*···Br1^{iii}	0.97	2.90	3.798 (3)	155
C29—H29*B*···Br1^{ii}	0.97	2.91	3.848 (3)	164

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