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4-Methylpyridinium 4-hydroxybenzoate

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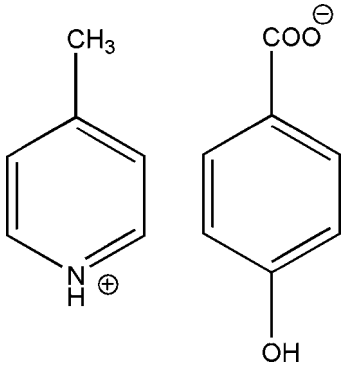
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.128; data-to-parameter ratio = 16.4.

In the crystal structure of the title salt, $C_6H_8N^+\cdot C_7H_5O_3^-$, the anions and cations are linked by classical N—H···O hydrogen bonds. The anions are connected by pairs of C—H···O hydrogen bonds into inversion dimers and further linked by classical O—H···O hydrogen bonds. Weak π–π interactions [centroid–centroid distances = 3.740 (3) and 3.855 (3) Å] also occur. The dihedral angle between the CO_2^- group and the benzene ring to which it is attached is 20.95 (8)°.

Related literature

For biological applications of picolinium-containing compounds, see: Butler & Walker (1993); Roy *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_6H_8N^+\cdot C_7H_5O_3^-$
M_r = 231.24
Monoclinic, $P2_1/c$
a = 7.479 (5) Å
b = 11.671 (4) Å
c = 13.520 (5) Å
β = 100.217 (5)°
V = 1161.4 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.983
11741 measured reflections
2564 independent reflections
1939 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.128
S = 1.06
2564 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.85	2.6707 (19)	176
N1—H1A···O3^{ii}	0.86	1.73	2.5889 (19)	173
C2—H2···O1^{iii}	0.93	2.60	3.485 (2)	160

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2392).

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supplementary materials

Acta Cryst. (2013). E**69**, o279 [doi:10.1107/S1600536813001785]

4-Methylpyridinium 4-hydroxybenzoate

S. Sudhahar, M. Krishnakumar, B. M. Sornamurthy, G. Chakkaravarthi and R. Mohankumar

Comment

Picolinium compounds are valuable intermediates in organic synthesis and they have been used widely in industrially important products and biologically active substrates as antitumor, antifungal, antibacterial, antineoplastic and antviral (Butler & Walker, 1993; Roy *et al.*, 2001) activities.

The asymmetric unit of the title salt, **I**, (Fig. 1), contains $C_6H_8N^+$ cation and $C_7H_5O_3^-$ anion. The bond lengths and angles in both anion and cation are within normal range (Allen *et al.*, 1987). The crystal structure exhibit weak intermolecular classical N—H···O, O—H···O and non–classical C—H···O interactions (Table 1 & Fig. 2). The π–π interactions are found in crystal structure: $Cg1\cdots Cg2^{iv}$ = 3.740 (3)Å; $Cg1\cdots Cg2^{v}$ = 3.855 (3)Å, where *Cg*1 and *Cg*2 are the centroids of the rings (C1–C6) and (N1/C8–C12), respectively. Symmetry codes: (iv) *x*, -*y*+1/2, *z*+1/2); (v) *x*+1, *y*, *z*;

Experimental

4-Picolinium 4-hydroxybenzoate compound was synthesized by using the starting materials of 4-picoline (1.66 g) and 4-hydroxybenzoic acid (1.12 g) in methanol and the single crystals suitable for X-ray diffraction were grown by slow evaporation.

Refinement

The H atoms were positioned geometrically with C—H = 0.93Å and 0.96Å, O—H = 0.82Å and N—H = 0.86Å, and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O) for hydroxy group, U_{iso}(H) = 1.2U_{eq}(N) for amino group, U_{iso}(H) = 1.2U_{eq}(C) for aryl H and U_{iso}(H) = 1.5U_{eq}(C) for methyl H.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

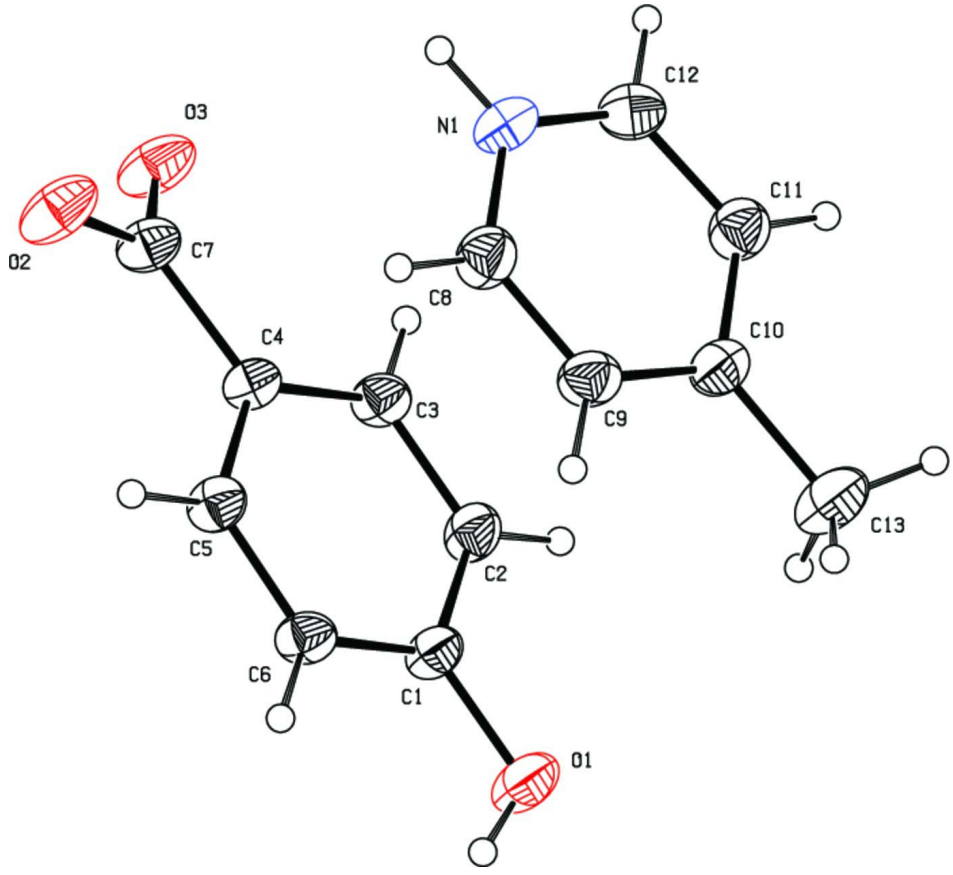

Figure 1

The molecular structure of title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

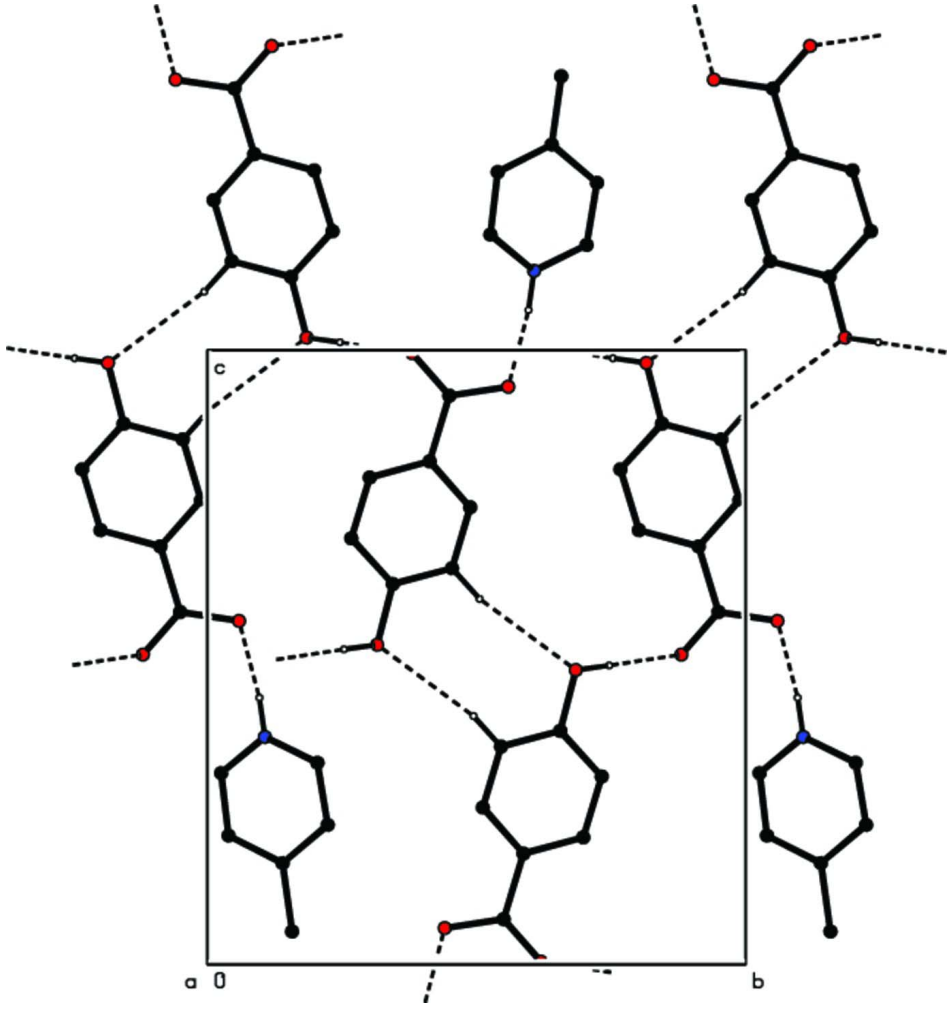

Figure 2

The crystal packing of **I**, viewed down *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

4-Methylpyridinium 4-hydroxybenzoate

Crystal data

$C_6H_8N^+·C_7H_5O_3^-$
M_r = 231.24
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.479 (5) Å
b = 11.671 (4) Å
c = 13.520 (5) Å
β = 100.217 (5)°
V = 1161.4 (10) Å^3
Z = 4

$F(000)$ = 488
D_x = 1.322 Mg m^{-3}
Melting point = 470.4–481.2 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7082 reflections
θ = 2.3–27.1°
μ = 0.10 mm^{-1}
T = 295 K
Block, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine–focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.983

11741 measured reflections
2564 independent reflections
1939 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.2°, θ_{min} = 2.3°
h = −9→9
k = −14→8
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.128
S = 1.06
2564 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
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.3003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.010 (2)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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}
O1	0.55020 (18)	0.18454 (10)	0.02055 (8)	0.0578 (4)
H1	0.5981	0.2464	0.0131	0.087*
O2	0.7215 (2)	0.11967 (10)	0.49538 (9)	0.0599 (4)
O3	0.71511 (18)	−0.05893 (9)	0.44053 (8)	0.0563 (4)
C1	0.5832 (2)	0.15548 (13)	0.11952 (11)	0.0396 (4)
C2	0.5407 (2)	0.04549 (13)	0.14510 (11)	0.0435 (4)
H2	0.4883	−0.0056	0.0955	0.052*
C3	0.5761 (2)	0.01174 (12)	0.24435 (11)	0.0394 (4)
H3	0.5492	−0.0628	0.2612	0.047*
C4	0.6512 (2)	0.08716 (12)	0.31929 (10)	0.0356 (3)
C5	0.6894 (2)	0.19833 (12)	0.29287 (11)	0.0394 (4)
H5	0.7375	0.2503	0.3427	0.047*
C6	0.6571 (2)	0.23261 (13)	0.19390 (11)	0.0397 (4)
H6	0.6846	0.3070	0.1769	0.048*
C7	0.6972 (2)	0.05049 (13)	0.42610 (11)	0.0412 (4)

N1	0.18709 (19)	0.10699 (12)	0.37067 (10)	0.0475 (4)
H1A	0.2170	0.0966	0.4344	0.057*
C8	0.2266 (2)	0.20451 (14)	0.32853 (13)	0.0490 (4)
H8	0.2872	0.2617	0.3692	0.059*
C9	0.1813 (2)	0.22368 (14)	0.22732 (12)	0.0473 (4)
H9	0.2099	0.2933	0.2005	0.057*
C10	0.0932 (2)	0.13982 (14)	0.16510 (11)	0.0446 (4)
C11	0.0517 (2)	0.03949 (14)	0.20988 (13)	0.0480 (4)
H11	−0.0091	−0.0190	0.1709	0.058*
C12	0.1000 (2)	0.02581 (14)	0.31174 (13)	0.0478 (4)
H12	0.0710	−0.0424	0.3407	0.057*
C13	0.0475 (3)	0.15746 (19)	0.05391 (14)	0.0686 (6)
H13A	0.0259	0.2374	0.0398	0.103*
H13B	−0.0596	0.1145	0.0272	0.103*
H13C	0.1469	0.1318	0.0234	0.103*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0913 (9)	0.0446 (7)	0.0328 (6)	−0.0132 (6)	−0.0014 (6)	0.0060 (5)
O2	0.1019 (10)	0.0430 (7)	0.0334 (6)	0.0124 (6)	0.0079 (6)	−0.0037 (5)
O3	0.0980 (10)	0.0342 (6)	0.0363 (6)	0.0073 (6)	0.0106 (6)	0.0038 (5)
C1	0.0502 (9)	0.0365 (8)	0.0309 (7)	0.0008 (6)	0.0040 (6)	0.0032 (6)
C2	0.0561 (9)	0.0357 (8)	0.0363 (8)	−0.0062 (7)	0.0014 (7)	−0.0028 (6)
C3	0.0509 (9)	0.0283 (7)	0.0391 (8)	−0.0019 (6)	0.0081 (7)	0.0025 (6)
C4	0.0440 (8)	0.0316 (7)	0.0320 (7)	0.0046 (6)	0.0091 (6)	0.0012 (6)
C5	0.0520 (9)	0.0325 (8)	0.0339 (8)	−0.0003 (6)	0.0085 (6)	−0.0050 (6)
C6	0.0537 (9)	0.0282 (7)	0.0383 (8)	−0.0022 (6)	0.0106 (7)	0.0016 (6)
C7	0.0554 (9)	0.0357 (8)	0.0343 (8)	0.0052 (7)	0.0123 (7)	−0.0005 (6)
N1	0.0592 (9)	0.0506 (8)	0.0323 (7)	0.0066 (6)	0.0073 (6)	0.0070 (6)
C8	0.0561 (10)	0.0450 (9)	0.0441 (9)	−0.0015 (7)	0.0036 (7)	−0.0009 (7)
C9	0.0550 (10)	0.0417 (9)	0.0454 (9)	−0.0008 (7)	0.0089 (7)	0.0087 (7)
C10	0.0468 (9)	0.0502 (10)	0.0365 (8)	0.0059 (7)	0.0068 (7)	0.0045 (7)
C11	0.0544 (10)	0.0446 (9)	0.0440 (9)	−0.0011 (7)	0.0057 (7)	−0.0018 (7)
C12	0.0563 (10)	0.0415 (9)	0.0474 (9)	0.0016 (7)	0.0138 (8)	0.0070 (7)
C13	0.0898 (15)	0.0731 (13)	0.0400 (10)	0.0027 (11)	0.0039 (9)	0.0092 (9)

Geometric parameters (Å, º)

O1—C1	1.3599 (18)	N1—C8	1.329 (2)
O1—H1	0.8200	N1—C12	1.331 (2)
O2—C7	1.2255 (19)	N1—H1A	0.8600
O3—C7	1.2953 (19)	C8—C9	1.369 (2)
C1—C2	1.381 (2)	C8—H8	0.9300
C1—C6	1.389 (2)	C9—C10	1.379 (2)
C2—C3	1.378 (2)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.379 (2)
C3—C4	1.384 (2)	C10—C13	1.496 (2)
C3—H3	0.9300	C11—C12	1.370 (2)
C4—C5	1.389 (2)	C11—H11	0.9300

C4—C7	1.487 (2)	C12—H12	0.9300
C5—C6	1.376 (2)	C13—H13A	0.9600
C5—H5	0.9300	C13—H13B	0.9600
C6—H6	0.9300	C13—H13C	0.9600
C1—O1—H1	109.5	C8—N1—H1A	120.8
O1—C1—C2	117.94 (13)	C12—N1—H1A	120.8
O1—C1—C6	122.02 (14)	N1—C8—C9	122.28 (16)
C2—C1—C6	120.05 (14)	N1—C8—H8	118.9
C3—C2—C1	119.75 (14)	C9—C8—H8	118.9
C3—C2—H2	120.1	C8—C9—C10	120.04 (15)
C1—C2—H2	120.1	C8—C9—H9	120.0
C2—C3—C4	120.93 (14)	C10—C9—H9	120.0
C2—C3—H3	119.5	C11—C10—C9	117.07 (15)
C4—C3—H3	119.5	C11—C10—C13	121.95 (16)
C3—C4—C5	118.77 (13)	C9—C10—C13	120.97 (16)
C3—C4—C7	121.46 (13)	C12—C11—C10	120.06 (16)
C5—C4—C7	119.74 (13)	C12—C11—H11	120.0
C6—C5—C4	120.85 (14)	C10—C11—H11	120.0
C6—C5—H5	119.6	N1—C12—C11	122.17 (15)
C4—C5—H5	119.6	N1—C12—H12	118.9
C5—C6—C1	119.62 (14)	C11—C12—H12	118.9
C5—C6—H6	120.2	C10—C13—H13A	109.5
C1—C6—H6	120.2	C10—C13—H13B	109.5
O2—C7—O3	122.48 (15)	H13A—C13—H13B	109.5
O2—C7—C4	122.01 (14)	C10—C13—H13C	109.5
O3—C7—C4	115.47 (13)	H13A—C13—H13C	109.5
C8—N1—C12	118.37 (14)	H13B—C13—H13C	109.5
O1—C1—C2—C3	178.41 (14)	C5—C4—C7—O2	20.1 (2)
C6—C1—C2—C3	−1.7 (2)	C3—C4—C7—O3	20.0 (2)
C1—C2—C3—C4	1.1 (2)	C5—C4—C7—O3	−157.84 (15)
C2—C3—C4—C5	0.4 (2)	C12—N1—C8—C9	−0.1 (2)
C2—C3—C4—C7	−177.46 (14)	N1—C8—C9—C10	−0.7 (3)
C3—C4—C5—C6	−1.4 (2)	C8—C9—C10—C11	1.2 (2)
C7—C4—C5—C6	176.54 (14)	C8—C9—C10—C13	−178.06 (16)
C4—C5—C6—C1	0.8 (2)	C9—C10—C11—C12	−0.9 (2)
O1—C1—C6—C5	−179.34 (14)	C13—C10—C11—C12	178.39 (17)
C2—C1—C6—C5	0.7 (2)	C8—N1—C12—C11	0.5 (2)
C3—C4—C7—O2	−162.01 (16)	C10—C11—C12—N1	0.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.85	2.6707 (19)	176
N1—H1*A*···O3^{ii}	0.86	1.73	2.5889 (19)	173
C2—H2···O1^{iii}	0.93	2.60	3.485 (2)	160

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