organic compounds

3-[(4-Amino-5-chloro-2-ethoxybenz-amido)methyl]pyrrolo[2,1-c][1,4]-oxazin-5-ium chloride monohydrate

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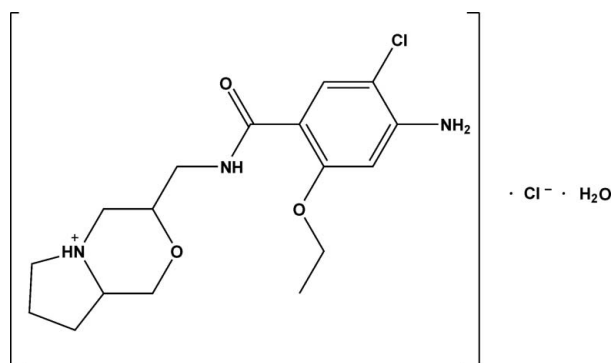Correspondence e-mail: cep02chl@yahoo.cn

The title compound, $C_{17}H_{25}ClN_3O_3{}^+ \cdot Cl^- \cdot H_2O$, is a monohydrated hydrochloride salt of a new derivative of mosapride, which is a pharmaceutical compound possessing gastrointestinal pro-kinetic activity. The chloride anion accepts hydrogen bonds from the NH group of the pyrrolooxazine fused-ring system and from the amine group, and the water molecules form hydrogen bonds that bridge between the chloride anion and the C=O bond of the amide.

Related literature

For related structures and background information concerning mosapride, see: Kakigami *et al.* (1998); Morie *et al.* (1995); Omae *et al.* (2002); Aoki *et al.* (2007).

Experimental

Crystal data

$C_{17}H_{25}ClN_3O_3{}^+ \cdot Cl^- \cdot H_2O$	$V = 1974.0\ (4)\ \text{Å}^3$
$M_r = 408.32$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.0984\ (9)\ \text{Å}$	$\mu = 0.36\ \text{mm}^{-1}$
$b = 11.1594\ (13)\ \text{Å}$	$T = 293\ (2)\ \text{K}$
$c = 21.843\ (3)\ \text{Å}$	$0.24 \times 0.20 \times 0.16$ mm

Data collection

Bruker APEX CCD diffractometer	10642 measured reflections
Absorption correction: multi-scan	3848 independent reflections
(*SADABS*; Bruker, 2000)	3188 reflections with $I > 2\sigma(I)$
$T_{min} = 0.919$, $T_{max} = 0.945$	$R_{int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	$\Delta\rho_{max} = 0.32\ \text{e Å}^{-3}$
$wR(F^2) = 0.096$	$\Delta\rho_{min} = -0.22\ \text{e Å}^{-3}$
$S = 1.06$	Absolute structure: Flack (1983),
3848 reflections	1631 Friedel pairs
261 parameters	Flack parameter: −0.02 (7)
H atoms treated by a mixture of independent and constrained refinement	

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1A⋯Cl1[i]	0.84 (4)	2.66 (4)	3.384 (3)	146 (3)
N1—H1B⋯Cl1[ii]	0.85 (3)	2.45 (3)	3.281 (3)	169 (3)
N3—H3C⋯Cl1	0.92 (3)	2.18 (3)	3.077 (3)	164 (2)
O1W—H1WA⋯Cl1[iii]	0.79 (3)	2.62 (3)	3.410 (4)	176 (3)
O1W—H1WB⋯O2	0.88 (4)	1.95 (5)	2.800 (4)	161 (4)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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 materials

3-[(4-Amino-5-chloro-2-ethoxybenzamido)methyl]pyrrolo[2,1-*c*][1,4]oxazin-5-ium chloride monohydrate

T.-F. Tong, J. Zhao, L. Cheng and Y.-H. Zhang

Comment

Mosapride citrate is a benzamide derivative that possesses a gastrointestinal prokinetic activity (Aoki *et al.* 2007). The title compound (Fig. 1) is a new mosapride derivative, and crystals of its hydrochloride salt were obtained by acidifying with hydrochloric acid then recrystallizing from methanol.

In the benzamide unit, the C=O bond distance of 1.229 (3) Å is much shorter than the C—O bond distances (1.359 (3)–1.432 (3) Å), showing it to have full double-bond character. Meanwhile, the C9—N2 distance of 1.330 (4) Å is comparable with that of C4—N1 (1.352 (4) Å), but much shorter than N2—C10 (1.441 (3) Å), N3—C13 (1.493 (4) Å), N3—C14 (1.489 (4) Å) and N3—C17 (1.492 (4) Å). Thus, the C4—N1 bond has partial double-bond character.

Experimental

A mixture of 4-amino-5-chloro-2-ethoxybenzoic acid (8.613 g, 40 mmol), (hexahydro-1*H*-pyrrolo[2,1-*c*][1,4]oxazin-3-yl)methanamine (4.8 g, 30.72 mmol) and 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (11.8 g, 61.8 mmol) in CH$_2$Cl$_2$ (60 ml) was stirred for two hours under an argon atmosphere. The products were treated with saturated NaHCO$_3$ (200 ml) and extracted with CH$_2$Cl$_2$ (3 × 300 ml), then the organic layer was dried with anhydrous MgSO$_4$ and distilled under vacuum. The white solids were collected and dried (yield 5.856 g, 54.0%). Crystals of the title compound were obtained by acidifying with hydrochloric acid then recrystallizing from methanol.

Refinement

With the exception of the central amide group, H atoms bonded to N and O atoms were located in difference Fourier maps and refined without restraint. Other H atoms were positioned geometrically and refined using a riding model with N—H = 0.86 Å, C—H = 0.93–0.97 Å and with $U_{iso}(H) = 1.2$ times $U_{eq}(C/N)$.
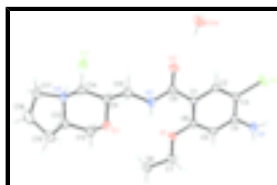
Figures

Fig. 1. Molecular structure of the title compound with 30% displacement ellipsoids for non-H atoms.

3-[(4-Amino-5-chloro-2-ethoxybenzamido)methyl]pyrrolo[2,1- *c*][1,4]oxazin-5-ium chloride monohydrate

Crystal data

$C_{17}H_{25}ClN_3O_3{}^+ \cdot Cl^- \cdot H_2O$	$F_{000} = 864$
$M_r = 408.32$	$D_x = 1.374$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 735 reflections
$a = 8.0984\ (9)$ Å	$\theta = 2.5–28.0^\circ$
$b = 11.1594\ (13)$ Å	$\mu = 0.36$ mm^{-1}
$c = 21.843\ (3)$ Å	$T = 293\ (2)$ K
$V = 1974.0\ (4)$ Å^3	Block, colourless
$Z = 4$	$0.24 \times 0.20 \times 0.16$ mm

Data collection

Bruker APEX CCD diffractometer	3848 independent reflections
Radiation source: fine-focus sealed tube	3188 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.037$
$T = 293(2)$ K	$\theta_{max} = 26.0^\circ$
φ and ω scans	$\theta_{min} = 2.6^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -9 \rightarrow 9$
$T_{min} = 0.919$, $T_{max} = 0.945$	$k = -10 \rightarrow 13$
10642 measured reflections	$l = -26 \rightarrow 25$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o{}^2) + (0.0412P)^2]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
3848 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
261 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1631 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.02 (7)

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}
C1	0.6257 (3)	0.7564 (2)	0.77046 (11)	0.0307 (6)
C2	0.4701 (4)	0.8084 (3)	0.76571 (13)	0.0364 (7)
C3	0.3807 (3)	0.8034 (3)	0.71361 (13)	0.0376 (7)
C4	0.4363 (4)	0.7438 (2)	0.66142 (12)	0.0344 (6)
C5	0.5913 (4)	0.6900 (3)	0.66594 (13)	0.0368 (7)
C6	0.6851 (3)	0.6961 (2)	0.71801 (12)	0.0323 (6)
C7	0.9124 (4)	0.5928 (3)	0.66895 (12)	0.0443 (8)
H7A	0.9261	0.6511	0.6364	0.053*
H7B	0.8429	0.5283	0.6541	0.053*
C8	1.0757 (4)	0.5452 (3)	0.68833 (13)	0.0455 (8)
H8A	1.0590	0.4780	0.7150	0.068*
H8B	1.1371	0.5201	0.6530	0.068*
H8C	1.1360	0.6065	0.7096	0.068*
C9	0.7127 (4)	0.7704 (2)	0.82975 (12)	0.0309 (6)
C10	0.9629 (4)	0.7321 (3)	0.88920 (13)	0.0452 (8)
H10A	0.8921	0.7486	0.9240	0.054*
H10B	1.0431	0.7964	0.8860	0.054*
C11	1.0507 (4)	0.6148 (3)	0.89873 (12)	0.0374 (7)
H11	0.9690	0.5504	0.9021	0.045*
C12	1.2222 (4)	0.4781 (3)	0.84947 (14)	0.0523 (10)
H12A	1.2880	0.4646	0.8130	0.063*
H12B	1.1348	0.4186	0.8502	0.063*
C13	1.3298 (4)	0.4625 (3)	0.90549 (13)	0.0408 (8)
H13	1.3596	0.3777	0.9090	0.049*
C14	1.1561 (4)	0.6167 (3)	0.95570 (11)	0.0345 (7)
H14A	1.2381	0.6798	0.9527	0.041*
H14B	1.0878	0.6323	0.9913	0.041*
C15	1.4860 (4)	0.5363 (3)	0.90920 (16)	0.0545 (9)
H15A	1.4693	0.6151	0.8916	0.065*
H15B	1.5759	0.4969	0.8878	0.065*
C16	1.5225 (5)	0.5453 (4)	0.97717 (17)	0.0689 (11)
H16A	1.6182	0.4971	0.9876	0.083*
H16B	1.5443	0.6278	0.9886	0.083*

C17	1.3705 (4)	0.4991 (3)	1.01002 (14)	0.0511 (9)
H17A	1.3891	0.4191	1.0259	0.061*
H17B	1.3406	0.5516	1.0436	0.061*
Cl1	0.92851 (11)	0.35057 (8)	0.99188 (4)	0.0554 (3)
Cl2	0.18901 (10)	0.87543 (9)	0.70977 (4)	0.0614 (3)
N1	0.3486 (4)	0.7381 (3)	0.60884 (12)	0.0482 (7)
H1A	0.266 (5)	0.780 (3)	0.5990 (16)	0.072*
H1B	0.394 (4)	0.717 (3)	0.5755 (15)	0.072*
N2	0.8652 (3)	0.7270 (2)	0.83413 (10)	0.0438 (7)
H2A	0.9079	0.6941	0.8023	0.053*
N3	1.2391 (3)	0.4983 (2)	0.96212 (11)	0.0363 (6)
O1	0.8390 (2)	0.64810 (19)	0.72151 (8)	0.0410 (5)
O2	0.6491 (3)	0.8222 (2)	0.87342 (8)	0.0453 (6)
O3	1.1512 (3)	0.59417 (19)	0.84669 (9)	0.0478 (6)
O1W	0.3524 (4)	0.8923 (3)	0.92869 (14)	0.0712 (8)
H2	0.426 (3)	0.845 (2)	0.8005 (12)	0.038 (8)*
H5	0.627 (3)	0.648 (3)	0.6312 (12)	0.043 (8)*
H3C	1.161 (3)	0.443 (2)	0.9736 (11)	0.031 (8)*
H1WA	0.368 (4)	0.954 (3)	0.9456 (15)	0.049 (12)*
H1WB	0.444 (6)	0.887 (4)	0.9073 (18)	0.103 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0306 (16)	0.0293 (15)	0.0321 (14)	−0.0011 (13)	0.0022 (12)	0.0019 (12)
C2	0.0337 (18)	0.0426 (18)	0.0329 (16)	0.0061 (14)	0.0033 (13)	−0.0059 (14)
C3	0.0220 (15)	0.0445 (18)	0.0461 (17)	0.0067 (13)	−0.0004 (13)	0.0014 (15)
C4	0.0289 (15)	0.0347 (16)	0.0395 (16)	0.0000 (14)	−0.0011 (14)	0.0037 (13)
C5	0.0427 (19)	0.0369 (17)	0.0308 (15)	−0.0003 (14)	0.0093 (14)	−0.0037 (13)
C6	0.0295 (16)	0.0310 (16)	0.0364 (15)	0.0031 (13)	0.0027 (13)	0.0048 (13)
C7	0.046 (2)	0.0475 (19)	0.0396 (17)	0.0091 (16)	0.0043 (15)	−0.0063 (15)
C8	0.0380 (19)	0.0496 (19)	0.0488 (18)	0.0063 (17)	0.0112 (16)	−0.0018 (15)
C9	0.0303 (16)	0.0275 (15)	0.0350 (15)	0.0027 (12)	0.0025 (13)	0.0008 (13)
C10	0.045 (2)	0.0479 (19)	0.0430 (18)	0.0126 (16)	−0.0087 (15)	−0.0073 (15)
C11	0.0368 (16)	0.0376 (17)	0.0380 (15)	0.0030 (15)	−0.0034 (14)	−0.0028 (14)
C12	0.052 (2)	0.063 (2)	0.0426 (18)	0.0179 (19)	−0.0069 (16)	−0.0193 (17)
C13	0.0390 (19)	0.0365 (17)	0.0468 (17)	0.0072 (15)	−0.0058 (15)	−0.0087 (14)
C14	0.0361 (16)	0.0335 (16)	0.0338 (14)	0.0030 (14)	−0.0013 (13)	−0.0051 (13)
C15	0.038 (2)	0.054 (2)	0.071 (2)	0.0050 (16)	0.0032 (18)	−0.0074 (19)
C16	0.043 (2)	0.077 (3)	0.087 (3)	−0.0011 (19)	−0.016 (2)	−0.024 (2)
C17	0.059 (2)	0.0451 (19)	0.0486 (19)	0.0065 (17)	−0.0229 (17)	−0.0012 (16)
Cl1	0.0476 (5)	0.0593 (5)	0.0594 (5)	−0.0128 (4)	−0.0147 (4)	0.0070 (4)
Cl2	0.0388 (5)	0.0819 (7)	0.0635 (5)	0.0261 (5)	−0.0107 (4)	−0.0162 (5)
N1	0.0410 (17)	0.067 (2)	0.0367 (15)	0.0077 (15)	−0.0072 (13)	−0.0028 (14)
N2	0.0434 (16)	0.0529 (16)	0.0350 (13)	0.0173 (13)	−0.0074 (12)	−0.0107 (12)
N3	0.0367 (15)	0.0338 (14)	0.0385 (14)	−0.0018 (12)	−0.0079 (11)	0.0017 (12)
O1	0.0352 (12)	0.0515 (13)	0.0364 (10)	0.0138 (10)	0.0004 (9)	−0.0086 (10)
O2	0.0358 (12)	0.0588 (15)	0.0415 (11)	0.0069 (11)	0.0012 (10)	−0.0108 (11)

O3	0.0531 (14)	0.0558 (14)	0.0346 (10)	0.0229 (12)	−0.0035 (10)	−0.0039 (10)
O1W	0.0479 (18)	0.088 (2)	0.078 (2)	0.0005 (17)	0.0099 (15)	−0.0155 (18)

Geometric parameters (Å, °)

C1—C2	1.391 (4)	C11—H11	0.980
C1—C6	1.413 (4)	C12—O3	1.419 (4)
C1—C9	1.483 (4)	C12—C13	1.512 (4)
C2—C3	1.350 (4)	C12—H12A	0.970
C2—H2	0.93 (3)	C12—H12B	0.970
C3—C4	1.394 (4)	C13—N3	1.493 (4)
C3—Cl2	1.750 (3)	C13—C15	1.511 (4)
C4—N1	1.352 (4)	C13—H13	0.980
C4—C5	1.395 (4)	C14—N3	1.489 (4)
C5—C6	1.369 (4)	C14—H14A	0.970
C5—H5	0.94 (3)	C14—H14B	0.970
C6—O1	1.359 (3)	C15—C16	1.517 (4)
C7—O1	1.432 (3)	C15—H15A	0.970
C7—C8	1.486 (4)	C15—H15B	0.970
C7—H7A	0.970	C16—C17	1.515 (5)
C7—H7B	0.970	C16—H16A	0.970
C8—H8A	0.960	C16—H16B	0.970
C8—H8B	0.960	C17—N3	1.492 (4)
C8—H8C	0.960	C17—H17A	0.970
C9—O2	1.229 (3)	C17—H17B	0.970
C9—N2	1.330 (4)	N1—H1A	0.84 (4)
C10—N2	1.441 (3)	N1—H1B	0.85 (3)
C10—C11	1.504 (4)	N2—H2A	0.860
C10—H10A	0.970	N3—H3C	0.92 (3)
C10—H10B	0.970	O1W—H1WA	0.79 (3)
C11—O3	1.417 (3)	O1W—H1WB	0.88 (4)
C11—C14	1.509 (4)		
C2—C1—C6	116.5 (3)	O3—C12—H12B	109.2
C2—C1—C9	116.8 (2)	C13—C12—H12B	109.2
C6—C1—C9	126.7 (2)	H12A—C12—H12B	107.9
C3—C2—C1	122.1 (3)	N3—C13—C15	102.8 (2)
C3—C2—H2	120.1 (17)	N3—C13—C12	110.9 (2)
C1—C2—H2	117.8 (17)	C15—C13—C12	117.6 (3)
C2—C3—C4	122.4 (3)	N3—C13—H13	108.4
C2—C3—Cl2	119.8 (2)	C15—C13—H13	108.4
C4—C3—Cl2	117.8 (2)	C12—C13—H13	108.4
N1—C4—C3	123.2 (3)	N3—C14—C11	108.7 (2)
N1—C4—C5	120.8 (3)	N3—C14—H14A	109.9
C3—C4—C5	116.0 (3)	C11—C14—H14A	109.9
C6—C5—C4	122.4 (3)	N3—C14—H14B	109.9
C6—C5—H5	122.0 (18)	C11—C14—H14B	109.9
C4—C5—H5	115.6 (18)	H14A—C14—H14B	108.3
O1—C6—C5	122.4 (2)	C13—C15—C16	104.6 (3)
O1—C6—C1	117.0 (2)	C13—C15—H15A	110.8

C5—C6—C1	120.6 (3)	C16—C15—H15A	110.8
O1—C7—C8	107.1 (2)	C13—C15—H15B	110.8
O1—C7—H7A	110.3	C16—C15—H15B	110.8
C8—C7—H7A	110.3	H15A—C15—H15B	108.9
O1—C7—H7B	110.3	C17—C16—C15	106.4 (3)
C8—C7—H7B	110.3	C17—C16—H16A	110.4
H7A—C7—H7B	108.5	C15—C16—H16A	110.4
C7—C8—H8A	109.1	C17—C16—H16B	110.4
C7—C8—H8B	109.7	C15—C16—H16B	110.4
H8A—C8—H8B	109.5	H16A—C16—H16B	108.6
C7—C8—H8C	109.7	N3—C17—C16	104.4 (3)
H8A—C8—H8C	109.5	N3—C17—H17A	110.9
H8B—C8—H8C	109.5	C16—C17—H17A	110.9
O2—C9—N2	120.3 (3)	N3—C17—H17B	110.9
O2—C9—C1	121.9 (2)	C16—C17—H17B	110.9
N2—C9—C1	117.7 (2)	H17A—C17—H17B	108.9
N2—C10—C11	109.9 (2)	C4—N1—H1A	127 (3)
N2—C10—H10A	109.7	C4—N1—H1B	121 (3)
C11—C10—H10A	109.7	H1A—N1—H1B	106 (3)
N2—C10—H10B	109.7	C9—N2—C10	123.8 (2)
C11—C10—H10B	109.7	C9—N2—H2A	118.1
H10A—C10—H10B	108.2	C10—N2—H2A	118.1
O3—C11—C10	107.6 (2)	C14—N3—C17	112.5 (2)
O3—C11—C14	109.8 (2)	C14—N3—C13	112.4 (2)
C10—C11—C14	111.7 (2)	C17—N3—C13	103.4 (2)
O3—C11—H11	109.2	C14—N3—H3C	108.4 (17)
C10—C11—H11	109.2	C17—N3—H3C	107.6 (16)
C14—C11—H11	109.2	C13—N3—H3C	112.4 (16)
O3—C12—C13	111.9 (3)	C6—O1—C7	120.4 (2)
O3—C12—H12A	109.2	C11—O3—C12	110.3 (2)
C13—C12—H12A	109.2	H1WA—O1W—H1WB	100 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Cl1[i]	0.84 (4)	2.66 (4)	3.384 (3)	146 (3)
N1—H1B···Cl1[ii]	0.85 (3)	2.45 (3)	3.281 (3)	169 (3)
N3—H3C···Cl1	0.92 (3)	2.18 (3)	3.077 (3)	164 (2)
O1W—H1WA···Cl1[iii]	0.79 (3)	2.62 (3)	3.410 (4)	176 (3)
O1W—H1WB···O2	0.88 (4)	1.95 (5)	2.800 (4)	161 (4)

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

Fig. 1