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4-Bromo-5-[(5,5-dimethyl-4,5-dihydroisoxazol-3-yl)sulfonylmethyl]-3-methyl-1-(2,2,2-trifluoroethyl)-1*H*-pyrazole

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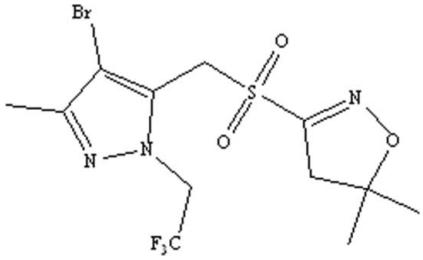
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 17.1.

In the title compound, $C_{12}H_{15}BrF_3N_3O_3S$, which has potential herbicidal activity, the molecule is twisted, as indicated by the C—S—C—C torsion angle of 67.86 (19)° for the atoms linking the ring systems. An intramolecular C—H···F short contact occurs and intermolecular C—H···O interactions link the molecules in the crystal.

Related literature

For background to pyrazoles and their pharmacological and pharmaceutical applications, see: Aiello *et al.* (2000); Hirai *et al.* (2002); Lahm *et al.* (2007); Meegalla *et al.* (2004); Ohno *et al.* (2004); Shiga *et al.* (2003); Sivaprasad *et al.* (2006); Vicentini *et al.* (2005); Waldrep *et al.* (1990). The trifluoromethyl group is present in many biologically active pharmaceutical and agrochemical compounds, presumably due to its increased lipophilicity, electronegativity and relatively small size, see: Welch (1987).



Experimental

Crystal data

$C_{12}H_{15}BrF_3N_3O_3S$
M_r = 418.24
Monoclinic, $P2_1/n$
a = 16.127 (3) Å
b = 5.4356 (11) Å
c = 19.135 (4) Å
β = 106.85 (3)°
V = 1605.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.74 mm^{-1}
T = 173 K
0.16 × 0.15 × 0.05 mm

Data collection

Rigaku MM007HF + CCD (Saturn724+) diffractometer
Absorption correction: numerical (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.668, T_{max} = 0.875
11131 measured reflections
3614 independent reflections
3353 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.14
3614 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···F2	0.99	2.44	3.229 (3)	137
C5—H5A···O1^{i}	0.99	2.30	3.131 (3)	141
C7—H7B···O2^{ii}	0.99	2.29	3.271 (3)	169

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

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); 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: HB5125).

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supporting information

Acta Cryst. (2009). E**65**, o2702–o2703 [https://doi.org/10.1107/S1600536809040380]

4-Bromo-5-[(5,5-dimethyl-4,5-dihydroisoxazol-3-yl)sulfonylmethyl]-3-methyl-1-(2,2,2-trifluoroethyl)-1*H*-pyrazole

Hong-Ju Ma, Qian-Fei Zhao, Xiang-Dong Mei and Jun Ning

S1. Comment

Pyrazole derivatives represent one of the most important classes of organic heterocyclic compounds, possessing a wide spectrum of biological activities in agrochemicals such as insecticidal (Lahm *et al.*, 2007; Meegalla *et al*., 2004; Shiga *et al.*, 2003), fungicidal (Aiello *et al.*, 2000; Sivaprasad *et al.*, 2006), herbicidal (Ohno *et al.*, 2004; Vicentini *et al.*, 2005; Waldrep *et al.*, 1990) activities. Some pyrazole derivatives are in use as herbicides such as pyrazolate, pyrazoxyfen, benzofenap, pyraflufen-ethyl, fluazolate and pyrazosulfuron-ethyl (Hirai *et al.*,2002). The trifluoromethyl moiety is particularly encountered in many biologically active pharmaceutical and agrochemical compounds presumably due to its increased lipophilicity, electronegativity and relatively small size (Welch 1987). Recently, we introduced trifluoromethyl to forming a novel title compound (I) with high herbicidal activity that has not been reported in literatures. The crystal structure of the title compound is shown in Fig. 1.

S2. Experimental

4-Bromo-5-[(5,5-dimethyl-4,5-dihydroisoxazol-3-yl)sulfonylmethyl]-3-methyl-1-(2,2,2-trifluoroethyl)-1*H*-pyrazole (0.2 g) was dissolved in acetone (50 ml) at room temperature. Colourless crystals of the title compound (I) were obtained through slow evaporation after two weeks.

S3. Refinement

The H atoms were placed at calculated positions, with C—H=0.93–0.98 Å, and were included in the refinement in the riding model approximation with *U*iso(H) set to 1.2 - 1.5*U*eq(C).

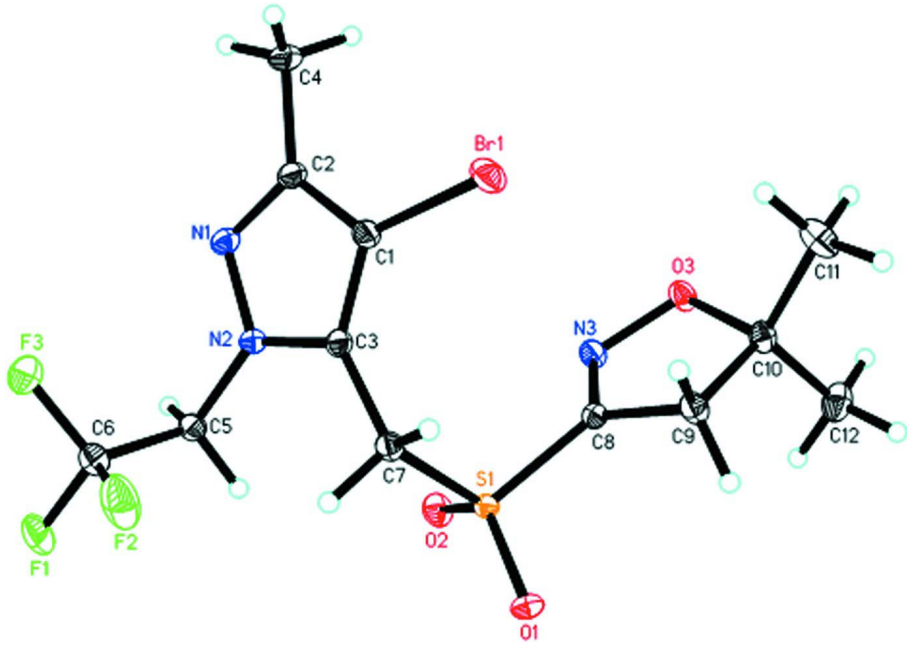

Figure 1

The molecular structure of the title compound, showing 50° probability displacement ellipsoids and the atom-numbering scheme.

4-Bromo-5-[(5,5-dimethyl-4,5-dihydroisoxazol-3-yl)sulfonylmethyl]-3-methyl-1- (2,2,2-trifluoroethyl)-1*H*-pyrazole

Crystal data

$C_{12}H_{15}BrF_3N_3O_3S$
$M_r = 418.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 16.127\ (3)$ Å
$b = 5.4356\ (11)$ Å
$c = 19.135\ (4)$ Å
$\beta = 106.85\ (3)°$
$V = 1605.3\ (6)$ Å^3
$Z = 4$
$F(000) = 840$
$D_x = 1.730$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5465 reflections
$\theta = 1.5–27.5°$
$\mu = 2.74$ mm^{-1}
$T = 173$ K
Slab, colourless
0.16 × 0.15 × 0.05 mm

Data collection

Rigaku MM007HF + CCD (Saturn724+) diffractometer
Radiation source: Rotating Anode
Confocal monochromator
Detector resolution: 28.5714 pixels mm^{-1}
ω scans at fixed $\chi = 45°$
Absorption correction: numerical (*CrystalClear*; Rigaku, 2008)
$T_{min} = 0.668$, $T_{max} = 0.875$
11131 measured reflections
3614 independent reflections
3353 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.5°$
$h = -20\rightarrow18$
$k = -7\rightarrow6$
$l = -21\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.093$
$S = 1.14$
3614 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 1.0315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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	0.445686 (15)	0.94374 (5)	0.090555 (14)	0.03063 (10)
S1	0.36847 (3)	0.46277 (11)	0.24140 (3)	0.01880 (13)
F1	0.05557 (10)	0.1917 (4)	0.03774 (10)	0.0506 (5)
F2	0.10792 (11)	0.5508 (4)	0.06883 (11)	0.0533 (5)
F3	0.09624 (11)	0.4150 (4)	−0.03880 (9)	0.0446 (5)
O1	0.34862 (11)	0.5488 (4)	0.30560 (9)	0.0302 (4)
O2	0.35701 (10)	0.2071 (3)	0.22232 (9)	0.0278 (4)
O3	0.60544 (10)	0.5023 (3)	0.23928 (9)	0.0247 (4)
N1	0.29249 (12)	0.3877 (4)	−0.01482 (10)	0.0245 (4)
N2	0.27115 (12)	0.4000 (4)	0.04901 (10)	0.0202 (4)
N3	0.52217 (12)	0.4076 (4)	0.22290 (11)	0.0218 (4)
C1	0.36847 (14)	0.6842 (4)	0.05707 (12)	0.0215 (5)
C2	0.35194 (15)	0.5606 (5)	−0.01018 (12)	0.0233 (5)
C3	0.31611 (14)	0.5796 (4)	0.09432 (12)	0.0190 (4)
C4	0.39090 (17)	0.6042 (6)	−0.07062 (14)	0.0352 (6)
H4A	0.3649	0.4916	−0.1110	0.053*
H4B	0.4535	0.5753	−0.0531	0.053*
H4C	0.3800	0.7745	−0.0876	0.053*
C5	0.20495 (14)	0.2363 (5)	0.05891 (12)	0.0235 (5)
H5A	0.2172	0.1966	0.1114	0.028*
H5B	0.2064	0.0809	0.0323	0.028*
C6	0.11590 (16)	0.3492 (5)	0.03153 (14)	0.0306 (6)
C7	0.30517 (14)	0.6434 (5)	0.16676 (12)	0.0203 (4)
H7A	0.2433	0.6247	0.1641	0.024*
H7B	0.3206	0.8188	0.1770	0.024*

C8	0.47706 (14)	0.5475 (4)	0.25141 (12)	0.0180 (4)
C9	0.52301 (14)	0.7679 (5)	0.29165 (13)	0.0242 (5)
H9A	0.5152	0.7824	0.3409	0.029*
H9B	0.5041	0.9221	0.2641	0.029*
C10	0.61659 (14)	0.6997 (4)	0.29502 (13)	0.0221 (5)
C11	0.66758 (17)	0.9027 (5)	0.27253 (17)	0.0347 (6)
H11A	0.7229	0.8370	0.2691	0.052*
H11B	0.6786	1.0347	0.3090	0.052*
H11C	0.6343	0.9682	0.2249	0.052*
C12	0.66479 (18)	0.5845 (5)	0.36726 (15)	0.0359 (6)
H12A	0.7202	0.5188	0.3643	0.054*
H12B	0.6300	0.4508	0.3786	0.054*
H12C	0.6754	0.7093	0.4058	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02683 (15)	0.02743 (17)	0.03790 (17)	−0.00740 (9)	0.00979 (11)	0.00368 (10)
S1	0.0184 (3)	0.0222 (3)	0.0175 (3)	−0.00311 (19)	0.0078 (2)	−0.0020 (2)
F1	0.0246 (8)	0.0738 (14)	0.0495 (10)	−0.0205 (8)	0.0044 (7)	0.0103 (9)
F2	0.0288 (9)	0.0612 (13)	0.0659 (13)	0.0097 (8)	0.0074 (8)	−0.0243 (10)
F3	0.0334 (9)	0.0640 (13)	0.0331 (9)	0.0067 (8)	0.0043 (7)	0.0170 (8)
O1	0.0277 (9)	0.0473 (12)	0.0192 (8)	−0.0046 (8)	0.0126 (7)	−0.0057 (8)
O2	0.0285 (9)	0.0204 (9)	0.0328 (9)	−0.0056 (7)	0.0065 (7)	0.0001 (7)
O3	0.0180 (8)	0.0272 (9)	0.0307 (9)	−0.0019 (6)	0.0098 (7)	−0.0084 (7)
N1	0.0237 (10)	0.0334 (12)	0.0174 (9)	0.0014 (8)	0.0076 (8)	−0.0002 (8)
N2	0.0185 (9)	0.0257 (10)	0.0173 (9)	−0.0007 (7)	0.0065 (7)	−0.0004 (8)
N3	0.0187 (9)	0.0221 (10)	0.0251 (10)	−0.0013 (7)	0.0070 (8)	−0.0031 (8)
C1	0.0183 (10)	0.0239 (12)	0.0220 (11)	0.0001 (8)	0.0055 (8)	0.0036 (9)
C2	0.0204 (11)	0.0320 (14)	0.0185 (11)	0.0040 (9)	0.0072 (9)	0.0041 (9)
C3	0.0180 (10)	0.0201 (11)	0.0187 (10)	0.0014 (8)	0.0047 (8)	0.0009 (8)
C4	0.0289 (13)	0.0569 (19)	0.0236 (13)	−0.0009 (12)	0.0133 (10)	0.0072 (12)
C5	0.0231 (11)	0.0254 (12)	0.0219 (11)	−0.0066 (9)	0.0066 (9)	0.0003 (9)
C6	0.0242 (12)	0.0373 (15)	0.0295 (13)	−0.0075 (11)	0.0067 (10)	0.0009 (11)
C7	0.0190 (10)	0.0207 (12)	0.0217 (11)	0.0008 (8)	0.0067 (8)	−0.0028 (9)
C8	0.0181 (10)	0.0189 (11)	0.0170 (10)	−0.0008 (8)	0.0049 (8)	−0.0015 (8)
C9	0.0199 (11)	0.0235 (12)	0.0298 (12)	−0.0028 (9)	0.0083 (9)	−0.0064 (10)
C10	0.0208 (11)	0.0183 (12)	0.0261 (12)	−0.0002 (8)	0.0053 (9)	−0.0037 (9)
C11	0.0256 (13)	0.0256 (14)	0.0546 (18)	−0.0013 (10)	0.0141 (12)	0.0048 (12)
C12	0.0350 (14)	0.0383 (16)	0.0277 (14)	0.0000 (11)	−0.0014 (11)	0.0005 (11)

Geometric parameters (Å, º)

Br1—C1	1.868 (2)	C4—H4B	0.9800
S1—O1	1.4346 (17)	C4—H4C	0.9800
S1—O2	1.4351 (18)	C5—C6	1.509 (3)
S1—C8	1.767 (2)	C5—H5A	0.9900
S1—C7	1.789 (2)	C5—H5B	0.9900

F1—C6	1.327 (3)	C7—H7A	0.9900
F2—C6	1.334 (3)	C7—H7B	0.9900
F3—C6	1.339 (3)	C8—C9	1.499 (3)
O3—N3	1.387 (2)	C9—C10	1.537 (3)
O3—C10	1.487 (3)	C9—H9A	0.9900
N1—C2	1.327 (3)	C9—H9B	0.9900
N1—N2	1.363 (3)	C10—C12	1.511 (3)
N2—C3	1.366 (3)	C10—C11	1.512 (3)
N2—C5	1.444 (3)	C11—H11A	0.9800
N3—C8	1.279 (3)	C11—H11B	0.9800
C1—C3	1.376 (3)	C11—H11C	0.9800
C1—C2	1.407 (3)	C12—H12A	0.9800
C2—C4	1.487 (3)	C12—H12B	0.9800
C3—C7	1.488 (3)	C12—H12C	0.9800
C4—H4A	0.9800		

O1—S1—O2	119.28 (11)	F1—C6—C5	110.8 (2)
O1—S1—C8	106.41 (11)	F2—C6—C5	112.2 (2)
O2—S1—C8	109.30 (10)	F3—C6—C5	112.5 (2)
O1—S1—C7	106.71 (11)	C3—C7—S1	114.91 (16)
O2—S1—C7	109.08 (11)	C3—C7—H7A	108.5
C8—S1—C7	105.17 (11)	S1—C7—H7A	108.5
N3—O3—C10	109.76 (16)	C3—C7—H7B	108.5
C2—N1—N2	105.69 (19)	S1—C7—H7B	108.5
N1—N2—C3	112.23 (19)	H7A—C7—H7B	107.5
N1—N2—C5	118.40 (19)	N3—C8—C9	115.9 (2)
C3—N2—C5	129.33 (19)	N3—C8—S1	117.85 (17)
C8—N3—O3	108.43 (18)	C9—C8—S1	126.24 (17)
C3—C1—C2	107.1 (2)	C8—C9—C10	99.33 (18)
C3—C1—Br1	125.64 (18)	C8—C9—H9A	111.9
C2—C1—Br1	127.23 (18)	C10—C9—H9A	111.9
N1—C2—C1	109.9 (2)	C8—C9—H9B	111.9
N1—C2—C4	121.4 (2)	C10—C9—H9B	111.9
C1—C2—C4	128.7 (2)	H9A—C9—H9B	109.6
N2—C3—C1	105.0 (2)	O3—C10—C12	106.28 (19)
N2—C3—C7	125.0 (2)	O3—C10—C11	106.6 (2)
C1—C3—C7	130.0 (2)	C12—C10—C11	112.6 (2)
C2—C4—H4A	109.5	O3—C10—C9	103.34 (17)
C2—C4—H4B	109.5	C12—C10—C9	112.1 (2)
H4A—C4—H4B	109.5	C11—C10—C9	114.9 (2)
C2—C4—H4C	109.5	C10—C11—H11A	109.5
H4A—C4—H4C	109.5	C10—C11—H11B	109.5
H4B—C4—H4C	109.5	H11A—C11—H11B	109.5
N2—C5—C6	111.7 (2)	C10—C11—H11C	109.5
N2—C5—H5A	109.3	H11A—C11—H11C	109.5
C6—C5—H5A	109.3	H11B—C11—H11C	109.5
N2—C5—H5B	109.3	C10—C12—H12A	109.5
C6—C5—H5B	109.3	C10—C12—H12B	109.5

H5A—C5—H5B	107.9	H12A—C12—H12B	109.5
F1—C6—F2	107.2 (2)	C10—C12—H12C	109.5
F1—C6—F3	107.2 (2)	H12A—C12—H12C	109.5
F2—C6—F3	106.7 (2)	H12B—C12—H12C	109.5
C2—N1—N2—C3	0.2 (3)	N2—C3—C7—S1	86.0 (2)
C2—N1—N2—C5	178.1 (2)	C1—C3—C7—S1	−96.3 (3)
C10—O3—N3—C8	10.9 (2)	O1—S1—C7—C3	−179.38 (16)
N2—N1—C2—C1	−0.1 (3)	O2—S1—C7—C3	−49.28 (19)
N2—N1—C2—C4	−179.6 (2)	C8—S1—C7—C3	67.86 (19)
C3—C1—C2—N1	0.0 (3)	O3—N3—C8—C9	1.1 (3)
Br1—C1—C2—N1	−179.51 (17)	O3—N3—C8—S1	−177.89 (14)
C3—C1—C2—C4	179.4 (2)	O1—S1—C8—N3	148.46 (19)
Br1—C1—C2—C4	0.0 (4)	O2—S1—C8—N3	18.4 (2)
N1—N2—C3—C1	−0.2 (3)	C7—S1—C8—N3	−98.6 (2)
C5—N2—C3—C1	−177.8 (2)	O1—S1—C8—C9	−30.4 (2)
N1—N2—C3—C7	178.0 (2)	O2—S1—C8—C9	−160.43 (19)
C5—N2—C3—C7	0.4 (4)	C7—S1—C8—C9	82.6 (2)
C2—C1—C3—N2	0.2 (2)	N3—C8—C9—C10	−11.7 (3)
Br1—C1—C3—N2	179.65 (16)	S1—C8—C9—C10	167.21 (17)
C2—C1—C3—C7	−177.9 (2)	N3—O3—C10—C12	100.6 (2)
Br1—C1—C3—C7	1.6 (4)	N3—O3—C10—C11	−139.07 (19)
N1—N2—C5—C6	−89.7 (2)	N3—O3—C10—C9	−17.6 (2)
C3—N2—C5—C6	87.8 (3)	C8—C9—C10—O3	16.2 (2)
N2—C5—C6—F1	176.9 (2)	C8—C9—C10—C12	−97.8 (2)
N2—C5—C6—F2	−63.4 (3)	C8—C9—C10—C11	131.9 (2)
N2—C5—C6—F3	56.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···F2	0.99	2.44	3.229 (3)	137
C5—H5*A*···O1^{i}	0.99	2.30	3.131 (3)	141
C7—H7*B*···O2^{ii}	0.99	2.29	3.271 (3)	169

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