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1-Bromo-4-nitro-2-(trifluoromethyl)-benzene

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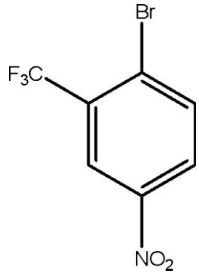
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.093; data-to-parameter ratio = 11.4.

The title compound, $C_7H_3BrNO_2$, was synthesized by the nitration of 1-bromo-2-(trifluoromethyl)benzene. In the crystal structure, there are three independent molecules, one of which lies on a crystallographic mirror plane.

Related literature

For related literature, see: Alaimo (1983).



Experimental

Crystal data

$C_7H_3BrF_3NO_2$
M_r = 270.01
Orthorhombic, *Pnma*
a = 9.775 (2) Å
b = 34.665 (7) Å
c = 12.615 (3) Å
V = 4274.8 (15) Å^3
Z = 20
Mo $K\alpha$ radiation
μ = 4.83 mm^{-1}
T = 113 (2) K
0.32 × 0.28 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: numerical (*NUMABS*; Rigaku, 2005)
T_{min} = 0.307, T_{max} = 0.644
19894 measured reflections
3814 independent reflections
3342 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.093
S = 1.23
3814 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 1999); 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: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2517).

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supplementary materials

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1-Bromo-4-nitro-2-(trifluoromethyl)benzene

Z. Shang and Y. Yu

Comment

Substituted trifluoromethylindolo[2,3-*b*]quinoxaline is useful as a immunomodulating agent (Alaimo, 1983). Herein we report the crystal structure of the starting material 1-bromo-4-nitro-2-(trifluoromethyl)benzene (Fig. 1) obtained from 1-bromo-2-(trifluoromethyl)benzene through nitration. There are two and a half molecules in the asymmetric unit. In each molecule the C—C(F_3) bond length reflects the expected lack of delocalization of electrons from the benzene ring.

Experimental

To a mixture of 1-bromo-2-(trifluoromethyl)benzene (75 g, 0.33 mol) and concentrated sulfonic acid (37 ml) was added a mixture of concentrated HNO~3 (15 mL) and concentrated H~2SO~4 (24 ml) and cooled with ice-water. The reaction mixture was stirred at room temperature for 2 h. Then the solution was poured into 500 ml ice-water and a solid appeared which was collected through filtration and recrystalized with ethnaol. 50 mg was dissolved in 20 ml me thanol and the solution was kept at room temperature for 10 d; natural evaporation gave colorless single crystals of suitable for X-ray analysis.

Refinement

H atoms were positioned geometrically, with C—H = 0.95Å refined in a riding-model approximation, with U_{iso}(H)=1.2U_{eq}.

Figures

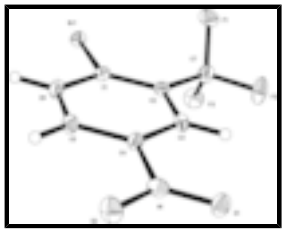

Fig. 1. The molecular structure of one of the independent molecules in the asymmetric unit drawn with 30% probability ellipsoids.

1-Bromo-4-nitro-2-(trifluoromethyl)benzene

Crystal data

$C_7H_3BrF_3NO_2$	D_x = 2.098 Mg m^{-3}
M_r = 270.01	Melting point: 167-169 K
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 7636 reflections

a = 9.775 (2) Å	θ = 2.6–25.0º
b = 34.665 (7) Å	μ = 4.83 mm^{-1}
c = 12.615 (3) Å	T = 113 (2) K
V = 4274.8 (15) $Å^3$	Platelet, colorless
Z = 20	0.32 × 0.28 × 0.10 mm
F_{000} = 2600	

Data collection

Rigaku Saturn diffractometer	3342 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	R_{int} = 0.054
Monochromator: confocal	θ_{max} = 25.0º
T = 113(2) K	θ_{min} = 1.7º
ω scans	h = −11→11
Absorption correction: numerical (NUMABS; Rigaku, 2005)	k = −41→41
T_{min} = 0.307, T_{max} = 0.644	l = −10→15
19894 measured reflections	Standard reflections: ?
3814 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 5.9058P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.23	$(\Delta/\sigma)_{max}$ = 0.002
3814 reflections	$\Delta\rho_{max}$ = 0.43 e $Å^{-3}$
334 parameters	$\Delta\rho_{min}$ = −0.60 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.71785 (6)	0.7500	0.49590 (5)	0.02333 (17)
Br2	−0.10592 (4)	0.551368 (12)	0.49280 (3)	0.02231 (14)
Br3	0.51998 (5)	0.645799 (12)	0.50253 (3)	0.02508 (14)
F1	0.5706 (3)	0.71904 (7)	0.28711 (19)	0.0329 (6)
F2	0.3915 (4)	0.7500	0.2374 (3)	0.0441 (11)
F3	0.0436 (3)	0.57794 (7)	0.27940 (19)	0.0336 (6)
F4	0.2229 (3)	0.54607 (9)	0.23590 (19)	0.0419 (8)
F5	0.0439 (3)	0.51612 (7)	0.28866 (19)	0.0343 (7)
F6	0.6698 (3)	0.61994 (8)	0.71395 (19)	0.0357 (7)
F7	0.8453 (3)	0.65256 (9)	0.76192 (19)	0.0428 (8)
F8	0.6631 (3)	0.68178 (7)	0.71057 (18)	0.0340 (6)
N1	0.1000 (5)	0.7500	0.5521 (4)	0.0237 (12)
N2	0.5125 (4)	0.54562 (10)	0.5514 (3)	0.0238 (8)
N3	1.1380 (4)	0.65554 (10)	0.4493 (3)	0.0247 (8)
O1	0.0275 (5)	0.7500	0.4712 (3)	0.0394 (12)
O2	0.0532 (5)	0.7500	0.6412 (3)	0.0401 (13)
O3	0.5832 (3)	0.54160 (9)	0.4723 (2)	0.0292 (7)
O4	0.5569 (3)	0.54644 (9)	0.6419 (2)	0.0314 (8)
O5	1.2087 (3)	0.65726 (10)	0.5286 (3)	0.0381 (9)
O6	1.1842 (3)	0.65564 (10)	0.3590 (2)	0.0371 (9)
C1	0.5243 (6)	0.7500	0.5085 (4)	0.0188 (13)
C2	0.4383 (6)	0.7500	0.4201 (4)	0.0189 (13)
C3	0.2988 (6)	0.7500	0.4362 (5)	0.0242 (15)
H3	0.2382	0.7500	0.3773	0.029*
C4	0.2480 (6)	0.7500	0.5372 (5)	0.0200 (13)
C5	0.3315 (6)	0.7500	0.6263 (4)	0.0234 (14)
H5	0.2937	0.7500	0.6957	0.028*
C6	0.4716 (6)	0.7500	0.6105 (5)	0.0219 (14)
H6	0.5318	0.7500	0.6697	0.026*
C7	0.4938 (6)	0.7500	0.3082 (5)	0.0256 (14)
C8	0.0869 (4)	0.55219 (11)	0.5058 (3)	0.0182 (9)
C9	0.1733 (4)	0.54956 (11)	0.4182 (3)	0.0205 (9)
C10	0.3136 (4)	0.54771 (11)	0.4334 (3)	0.0203 (10)
H10	0.3745	0.5457	0.3749	0.024*
C11	0.3622 (4)	0.54888 (12)	0.5362 (3)	0.0209 (9)
C12	0.2802 (4)	0.55240 (12)	0.6238 (3)	0.0225 (10)
H12	0.3181	0.5537	0.6931	0.027*
C13	0.1405 (5)	0.55405 (12)	0.6077 (3)	0.0242 (10)
H13	0.0806	0.5565	0.6667	0.029*
C14	0.1212 (4)	0.54739 (13)	0.3056 (3)	0.0260 (10)
C15	0.7127 (4)	0.64767 (12)	0.4907 (3)	0.0210 (10)
C16	0.7981 (4)	0.65073 (12)	0.5794 (3)	0.0201 (10)
C17	0.9380 (4)	0.65353 (12)	0.5639 (3)	0.0213 (10)
H17	0.9981	0.6554	0.6229	0.026*
C18	0.9892 (4)	0.65353 (12)	0.4621 (3)	0.0211 (9)

C19	0.9059 (4)	0.65096 (12)	0.3741 (3)	0.0226 (10)
H19	0.9440	0.6512	0.3048	0.027*
C20	0.7655 (4)	0.64801 (12)	0.3885 (3)	0.0225 (10)
H20	0.7061	0.6462	0.3291	0.027*
C21	0.7434 (5)	0.65155 (13)	0.6910 (3)	0.0268 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0202 (3)	0.0245 (3)	0.0253 (4)	0.000	−0.0005 (3)	0.000
Br2	0.0167 (2)	0.0241 (3)	0.0261 (3)	0.00012 (18)	0.00066 (19)	0.00021 (18)
Br3	0.0192 (3)	0.0269 (3)	0.0291 (3)	−0.00023 (18)	−0.00128 (19)	0.00139 (18)
F1	0.0358 (16)	0.0361 (15)	0.0268 (14)	0.0032 (13)	0.0095 (12)	−0.0070 (11)
F2	0.028 (2)	0.091 (3)	0.0139 (19)	0.000	−0.0012 (17)	0.000
F3	0.0398 (16)	0.0340 (15)	0.0270 (14)	0.0056 (13)	−0.0095 (12)	0.0045 (11)
F4	0.0253 (15)	0.082 (2)	0.0183 (14)	0.0028 (15)	−0.0004 (12)	−0.0042 (14)
F5	0.0393 (16)	0.0343 (16)	0.0294 (15)	−0.0051 (13)	−0.0098 (12)	−0.0076 (12)
F6	0.0423 (17)	0.0352 (16)	0.0295 (15)	−0.0059 (13)	0.0083 (13)	0.0103 (12)
F7	0.0294 (16)	0.083 (2)	0.0160 (13)	0.0012 (16)	−0.0023 (12)	−0.0010 (13)
F8	0.0410 (17)	0.0352 (16)	0.0259 (14)	0.0061 (13)	0.0098 (12)	−0.0043 (11)
N1	0.022 (3)	0.030 (3)	0.019 (3)	0.000	−0.002 (2)	0.000
N2	0.021 (2)	0.024 (2)	0.026 (2)	−0.0008 (16)	−0.0073 (18)	0.0009 (16)
N3	0.026 (2)	0.026 (2)	0.022 (2)	0.0000 (17)	0.0018 (18)	0.0019 (16)
O1	0.026 (3)	0.069 (4)	0.023 (2)	0.000	−0.007 (2)	0.000
O2	0.025 (3)	0.079 (4)	0.016 (2)	0.000	0.006 (2)	0.000
O3	0.0215 (18)	0.042 (2)	0.0239 (17)	0.0042 (15)	0.0010 (14)	−0.0009 (15)
O4	0.0261 (18)	0.045 (2)	0.0229 (17)	−0.0038 (15)	−0.0078 (14)	−0.0005 (14)
O5	0.0189 (18)	0.071 (3)	0.0250 (18)	−0.0058 (17)	−0.0026 (15)	−0.0014 (17)
O6	0.027 (2)	0.062 (2)	0.0224 (18)	−0.0043 (17)	0.0091 (15)	−0.0014 (16)
C1	0.023 (3)	0.012 (3)	0.021 (3)	0.000	−0.004 (3)	0.000
C2	0.022 (3)	0.021 (3)	0.014 (3)	0.000	0.001 (3)	0.000
C3	0.027 (4)	0.027 (4)	0.018 (3)	0.000	−0.004 (3)	0.000
C4	0.021 (3)	0.020 (3)	0.019 (3)	0.000	0.007 (3)	0.000
C5	0.028 (4)	0.030 (4)	0.013 (3)	0.000	0.001 (3)	0.000
C6	0.027 (4)	0.018 (3)	0.021 (3)	0.000	−0.001 (3)	0.000
C7	0.017 (3)	0.037 (4)	0.022 (3)	0.000	0.002 (3)	0.000
C8	0.015 (2)	0.018 (2)	0.021 (2)	−0.0001 (17)	−0.0026 (18)	−0.0025 (17)
C9	0.025 (3)	0.017 (2)	0.020 (2)	0.0034 (18)	−0.0015 (19)	−0.0004 (17)
C10	0.022 (3)	0.022 (2)	0.017 (2)	−0.0043 (19)	0.0026 (18)	0.0014 (17)
C11	0.020 (2)	0.021 (2)	0.022 (2)	0.0007 (18)	0.0051 (19)	−0.0002 (18)
C12	0.025 (3)	0.026 (3)	0.016 (2)	0.000 (2)	−0.0023 (18)	−0.0028 (18)
C13	0.027 (3)	0.025 (2)	0.021 (2)	−0.002 (2)	0.0072 (19)	−0.0026 (18)
C14	0.019 (2)	0.036 (3)	0.023 (2)	0.002 (2)	−0.002 (2)	0.000 (2)
C15	0.019 (2)	0.020 (2)	0.024 (2)	0.0037 (18)	−0.0014 (19)	0.0005 (18)
C16	0.022 (3)	0.019 (2)	0.019 (2)	−0.0017 (18)	0.0005 (19)	0.0011 (18)
C17	0.023 (3)	0.020 (2)	0.021 (2)	−0.0019 (19)	−0.0009 (19)	−0.0011 (18)
C18	0.021 (2)	0.020 (2)	0.022 (2)	−0.0031 (19)	0.002 (2)	−0.0022 (18)
C19	0.027 (3)	0.025 (2)	0.016 (2)	0.001 (2)	0.0038 (19)	0.0008 (18)

C20	0.024 (3)	0.021 (2)	0.022 (2)	0.002 (2)	−0.0046 (19)	0.0008 (18)
C21	0.025 (3)	0.036 (3)	0.019 (2)	0.003 (2)	0.000 (2)	0.003 (2)

Geometric parameters (Å, °)

Br1—C1	1.898 (6)	C4—C5	1.388 (8)
Br2—C8	1.892 (4)	C5—C6	1.385 (8)
Br3—C15	1.891 (4)	C5—H5	0.9500
F1—C7	1.336 (4)	C6—H6	0.9500
F2—C7	1.342 (7)	C7—F1^{i}	1.336 (4)
F3—C14	1.343 (5)	C8—C13	1.389 (5)
F4—C14	1.328 (5)	C8—C9	1.394 (6)
F5—C14	1.338 (5)	C9—C10	1.386 (6)
F6—C21	1.342 (5)	C9—C14	1.511 (6)
F7—C21	1.339 (5)	C10—C11	1.382 (6)
F8—C21	1.333 (5)	C10—H10	0.9500
N1—O2	1.213 (6)	C11—C12	1.370 (6)
N1—O1	1.242 (6)	C12—C13	1.382 (6)
N1—C4	1.459 (8)	C12—H12	0.9500
N2—O4	1.221 (4)	C13—H13	0.9500
N2—O3	1.222 (4)	C15—C20	1.388 (6)
N2—C11	1.486 (6)	C15—C16	1.400 (6)
N3—O5	1.217 (4)	C16—C17	1.385 (6)
N3—O6	1.225 (4)	C16—C21	1.507 (6)
N3—C18	1.466 (5)	C17—C18	1.378 (6)
C1—C6	1.387 (8)	C17—H17	0.9500
C1—C2	1.397 (8)	C18—C19	1.379 (6)
C2—C3	1.378 (8)	C19—C20	1.389 (6)
C2—C7	1.511 (8)	C19—H19	0.9500
C3—C4	1.368 (8)	C20—H20	0.9500
C3—H3	0.9500		
O2—N1—O1	123.1 (5)	C9—C10—H10	121.0
O2—N1—C4	119.5 (5)	C12—C11—C10	123.9 (4)
O1—N1—C4	117.4 (5)	C12—C11—N2	118.8 (4)
O4—N2—O3	124.4 (4)	C10—C11—N2	117.3 (4)
O4—N2—C11	118.0 (4)	C11—C12—C13	117.6 (4)
O3—N2—C11	117.6 (3)	C11—C12—H12	121.2
O5—N3—O6	123.7 (4)	C13—C12—H12	121.2
O5—N3—C18	118.4 (4)	C12—C13—C8	120.4 (4)
O6—N3—C18	117.9 (4)	C12—C13—H13	119.8
C6—C1—C2	121.2 (6)	C8—C13—H13	119.8
C6—C1—Br1	116.6 (4)	F4—C14—F5	106.8 (4)
C2—C1—Br1	122.2 (4)	F4—C14—F3	106.7 (4)
C3—C2—C1	118.5 (5)	F5—C14—F3	106.3 (3)
C3—C2—C7	119.5 (5)	F4—C14—C9	111.8 (4)
C1—C2—C7	121.9 (5)	F5—C14—C9	112.4 (4)
C4—C3—C2	119.8 (6)	F3—C14—C9	112.5 (4)
C4—C3—H3	120.1	C20—C15—C16	121.3 (4)
C2—C3—H3	120.1	C20—C15—Br3	116.4 (3)

C3—C4—C5	122.7 (6)	C16—C15—Br3	122.2 (3)
C3—C4—N1	118.7 (5)	C17—C16—C15	118.8 (4)
C5—C4—N1	118.6 (5)	C17—C16—C21	118.7 (4)
C6—C5—C4	117.7 (5)	C15—C16—C21	122.5 (4)
C6—C5—H5	121.1	C18—C17—C16	119.3 (4)
C4—C5—H5	121.1	C18—C17—H17	120.3
C5—C6—C1	120.1 (6)	C16—C17—H17	120.3
C5—C6—H6	120.0	C17—C18—C19	122.4 (4)
C1—C6—H6	120.0	C17—C18—N3	117.6 (4)
F1^{i}—C7—F1	106.9 (5)	C19—C18—N3	120.0 (4)
F1^{i}—C7—F2	106.6 (3)	C18—C19—C20	118.8 (4)
F1—C7—F2	106.6 (3)	C18—C19—H19	120.6
F1^{i}—C7—C2	112.8 (3)	C20—C19—H19	120.6
F1—C7—C2	112.8 (3)	C15—C20—C19	119.4 (4)
F2—C7—C2	110.7 (5)	C15—C20—H20	120.3
C13—C8—C9	120.5 (4)	C19—C20—H20	120.3
C13—C8—Br2	117.2 (3)	F8—C21—F7	107.1 (4)
C9—C8—Br2	122.3 (3)	F8—C21—F6	106.7 (3)
C10—C9—C8	119.6 (4)	F7—C21—F6	106.0 (3)
C10—C9—C14	117.5 (4)	F8—C21—C16	113.4 (4)
C8—C9—C14	123.0 (4)	F7—C21—C16	111.1 (4)
C11—C10—C9	117.9 (4)	F6—C21—C16	112.1 (4)
C11—C10—H10	121.0		
C6—C1—C2—C3	0.000 (1)	C10—C11—C12—C13	1.4 (7)
Br1—C1—C2—C3	180.0	N2—C11—C12—C13	−177.8 (4)
C6—C1—C2—C7	180.000 (2)	C11—C12—C13—C8	0.0 (6)
Br1—C1—C2—C7	0.000 (2)	C9—C8—C13—C12	−1.5 (6)
C1—C2—C3—C4	0.000 (1)	Br2—C8—C13—C12	176.1 (3)
C7—C2—C3—C4	180.000 (1)	C10—C9—C14—F4	−3.5 (6)
C2—C3—C4—C5	0.000 (1)	C8—C9—C14—F4	178.4 (4)
C2—C3—C4—N1	180.0	C10—C9—C14—F5	116.6 (4)
O2—N1—C4—C3	180.000 (1)	C8—C9—C14—F5	−61.6 (5)
O1—N1—C4—C3	0.000 (1)	C10—C9—C14—F3	−123.5 (4)
O2—N1—C4—C5	0.000 (1)	C8—C9—C14—F3	58.4 (5)
O1—N1—C4—C5	180.000 (1)	C20—C15—C16—C17	−1.0 (6)
C3—C4—C5—C6	0.000 (1)	Br3—C15—C16—C17	−177.4 (3)
N1—C4—C5—C6	180.000 (1)	C20—C15—C16—C21	178.3 (4)
C4—C5—C6—C1	0.000 (1)	Br3—C15—C16—C21	1.9 (6)
C2—C1—C6—C5	0.000 (1)	C15—C16—C17—C18	0.5 (6)
Br1—C1—C6—C5	180.000 (1)	C21—C16—C17—C18	−178.8 (4)
C3—C2—C7—F1^{i}	119.4 (4)	C16—C17—C18—C19	0.2 (6)
C1—C2—C7—F1^{i}	−60.6 (4)	C16—C17—C18—N3	−178.5 (4)
C3—C2—C7—F1	−119.4 (4)	O5—N3—C18—C17	−0.3 (6)
C1—C2—C7—F1	60.6 (4)	O6—N3—C18—C17	−179.8 (4)
C3—C2—C7—F2	0.000 (1)	O5—N3—C18—C19	−179.0 (4)
C1—C2—C7—F2	180.0	O6—N3—C18—C19	1.4 (6)
C13—C8—C9—C10	1.8 (6)	C17—C18—C19—C20	−0.5 (7)
Br2—C8—C9—C10	−175.7 (3)	N3—C18—C19—C20	178.2 (4)

C13—C8—C9—C14	179.9 (4)	C16—C15—C20—C19	0.8 (6)
Br2—C8—C9—C14	2.4 (6)	Br3—C15—C20—C19	177.4 (3)
C8—C9—C10—C11	−0.5 (6)	C18—C19—C20—C15	−0.1 (6)
C14—C9—C10—C11	−178.7 (4)	C17—C16—C21—F8	116.7 (4)
C9—C10—C11—C12	−1.1 (6)	C15—C16—C21—F8	−62.6 (6)
C9—C10—C11—N2	178.1 (4)	C17—C16—C21—F7	−4.0 (6)
O4—N2—C11—C12	−0.4 (6)	C15—C16—C21—F7	176.7 (4)
O3—N2—C11—C12	178.3 (4)	C17—C16—C21—F6	−122.4 (4)
O4—N2—C11—C10	−179.7 (4)	C15—C16—C21—F6	58.3 (6)
O3—N2—C11—C10	−0.9 (6)		

Symmetry codes: (i) *x*, −*y*+3/2, *z*.

Fig. 1