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A new alkaline earth metal tetrafluoroterephthalate: [Ba(tfBDC)(DMF)(EtOH)]

Daniel Smets, Miriam Sobieray and Uwe Ruschewitz*

University of Cologne, Greinstrasse 6, D-50939 Cologne, Germany. *Correspondence e-mail: uwe.ruschewitz@uni-koeln.de

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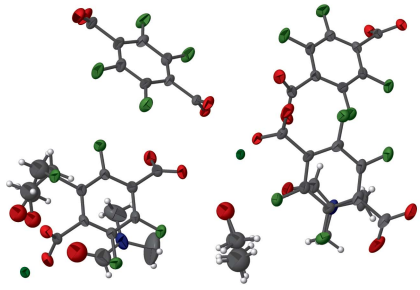
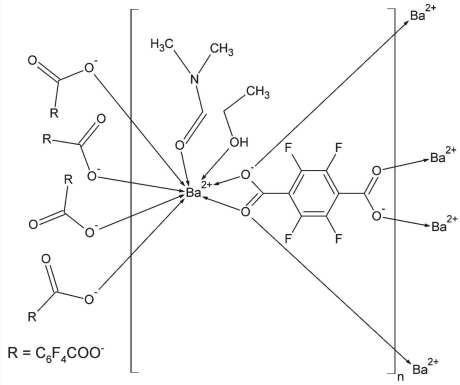
[Ba($C_8F_4O_4$)(C_3H_7NO)(C_2H_5OH)] or [Ba(tfBDC)(DMF)(EtOH)], where $tfBDC^{2-}$ = tetrafluoroterephthalate, DMF = dimethylformamide, EtOH = ethanol, systematic name poly[(dimethylformamide-1κO)(ethanol-1κO)(μ_5-2,3,5,6-tetrafluorobenzenedicarboxylato-1:2κ^2O^1;1:3$\kappa^2O^{1'}$;4κO^4;5$\kappa O^{4'}$)barium(II)], has been synthesized by a diffusion controlled synthesis from an EtOH/DMF solution. In the crystal structure two crystallographically independent Ba^{2+} cations are linked by two crystallographically distinct $tfBDC^{2-}$ anions to form a three-dimensional network structure. The coordination spheres of the first (CN = 8) and second (CN = 8) independent Ba cations are completed by the O atoms of DMF and EtOH molecules, with both EtOH molecules being disordered over two sets of sites (occupancy ratio 0.7:0.3 and 0.6:0.4, respectively).

3D view



Chemical scheme



Structure description

Despite the high interest in coordination polymers with tetrafluoroterephthalate ($tfBDC^{2-}$) as a bridging ligand, only few alkaline earth metal tetrafluoroterephthalates have been reported up to now. Only in 2014, three calcium-based tetrafluoroterephthalates were published, one of them crystallizing in the chiral space group $P4_12_12$ (Chen *et al.*, 2014). Interesting pyrotechnical effects have been observed in several alkali and alkaline earth metal tetrafluoroterephthalates, and some of their crystal structures were examined (Blair *et al.*, 2015). Ca(tfBDC)·4H_2O and Sr(tfBDC)·4H_2O were synthesized mechanochemically and their crystal structures were solved and refined from X-ray powder diffraction data (Al-Terkawi *et al.*, 2016). Here we report the first barium-containing coordination polymer with $tfBDC^{2-}$ as bridging ligand.

The asymmetric unit of [Ba(tfBDC)(DMF)(EtOH)] contains two crystallographically independent Ba^{2+} cations, two symmetry-independent $tfBDC^{2-}$ anions, two dimethylformamide (DMF) and two ethanol (EtOH) molecules. Each Ba^{2+} cation forms a BaO_8

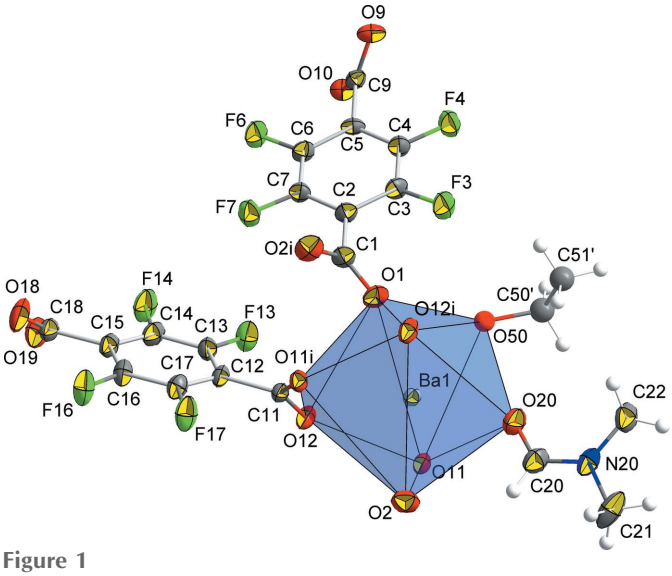


Figure 1
ORTEP plot of the coordination sphere around Ba1, drawn with displacement parameters at the 50% probability level. The BaO_8 polyhedron is highlighted in dark blue. Only one position of the disordered EtOH molecule is shown. Colour code: Ba (silver), O (red), N (dark blue), F (green), C (dark grey), H (white). [Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.]

polyhedron with six oxygen atoms stemming from five different $tfBDC^{2-}$ ligands (Figs. 1 and 2). The coordination

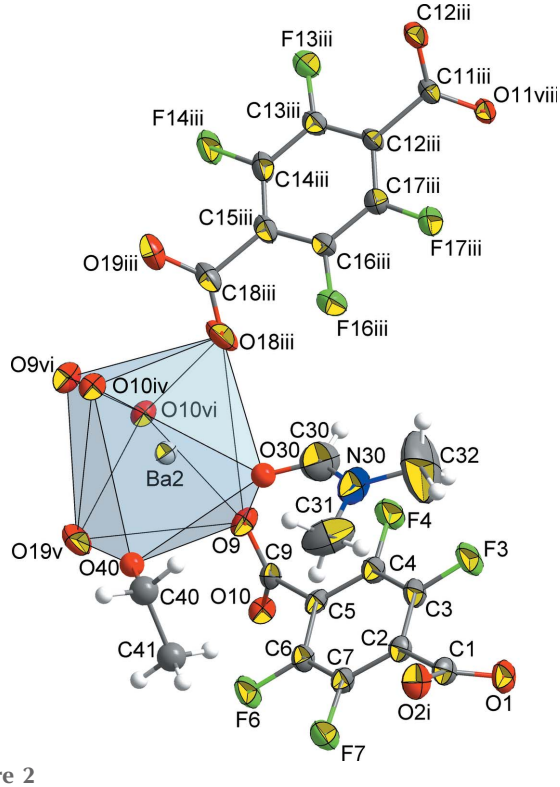


Figure 2
ORTEP plot of the coordination sphere around Ba2, drawn with displacement parameters at the 50% probability level. The BaO_8 polyhedron is highlighted in light blue. Only one position of the disordered EtOH molecule is shown. Colour code: see Fig. 1. [Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x, y+1, z$; (v) $-x, -y+1, -z+1$; (vi) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (viii) $-x+1, -y+1, -z+1$.]

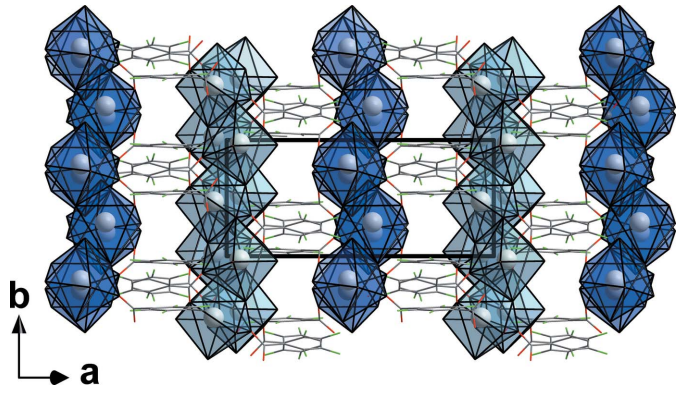


Figure 3
View along [001] highlighting the zigzag chains of connected BaO_8 polyhedra extending in the [010] direction. Only $tfbdc^{2-}$ ligands are shown and given in a wires/sticks representation. Colour code: see Fig. 1.

spheres are completed by one DMF and one EtOH molecule for each polyhedron [Ba1—O = 2.677 (4)-2.886 (3) Å; Ba2—O = 2.603 (17)-2.867 (3) Å]. The two independent EtOH molecules are each disordered over two sets of sites, and only one of the two positions is shown in the figures. The observed Ba—O distances are in good agreement with those in comparable Ba^{2+} coordination polymers (Blair *et al.*, 2015; Lo *et al.*, 1998).

The BaO_8 polyhedra are connected *via* common edges to form zigzag chains along [010]. These chains are shown in Fig. 3. Each chain contains only Ba1 or Ba2, respectively, as highlighted in Fig. 3. The Ba1—O and Ba2—O chains are very similar, but have a different orientation, as shown in Fig. 4. The arrangement of the Ba—O chains resembles the motif of a hexagonal rod packing. The $tfBDC^{2-}$ ligands interconnect these chains in the (010) plane so that a three-dimensional network structure is formed. The shortest Ba—Ba separations within the chains are Ba1—Ba1 = 4.5122 (3) Å and Ba2—Ba2 = 4.4999 (3) Å. The distances between Ba^{2+} cations of different chains exceed 9.5 Å.

Each $tfBDC^{2-}$ linker coordinates to five Ba^{2+} cations. One carboxylate group of each $tfBDC^{2-}$ linker (O19—C18—O18

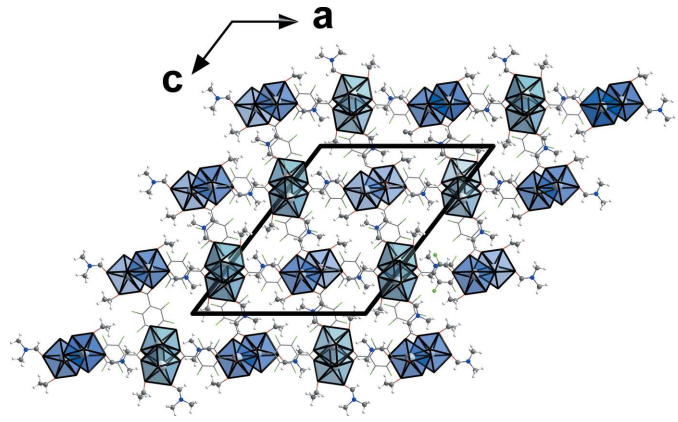


Figure 4
View along [010] in direction of the Ba–O zigzag chains. $tfbdc^{2-}$ ligands are shown in a wires/sticks representation, EtOH and DMF as ball and sticks. Colour code: see Fig. 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Ba(C_8F_4O_4)(C_3H_7NO)(C_2H_6O)]$
M_r	492.58
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	21.4745 (8), 7.4295 (2), 26.1730 (11)
β (°)	127.366 (2)
V (Å^3)	3318.8 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.47
Crystal size (mm)	0.35 × 0.2 × 0.1
Data collection	
Diffractometer	STOE *IPDS* 2T
Absorption correction	Numerical (*X-RED-32* and *X-SHAPE*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.589, 0.808
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39756, 7048, 5576
R_{int}	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.099, 1.04
No. of reflections	7048
No. of parameters	436
No. of restraints	10
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.82, −1.18

Computer programs: *X-AREA* (Stoe, 2002), *SIR92* (Altomare *et al.*, 1994), *SHELXL2013* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

and O1—C1—O2) bridges two Ba^{2+} cations in a monodentate fashion, whereas the other carboxylate groups (O11—C11—O12 and O9—C9—O10) bridge three Ba^{2+} cations in a bis-monodentate and chelating fashion. As found in many other tetrafluoroterephthalates, the $tfBDC^{2-}$ linker is not planar, with the carboxylate groups twisted out of the plane of the benzene rings (Seidel *et al.*, 2011). The respective torsion angles are 51.3 (3)° / 64.4 (2)° for linker I (C1–C9) and 35.4 (2)° / 48.8 (2)° for linker II (C11–C18). Both ethanol molecules are involved in hydrogen bonds, as indicated by the short O···O distances: O50···O1 = 2.68 (1) Å, O40′···O30 = 2.55 (3) Å, O40···O19 = 2.759 (8) Å. Since these hydrogen bonds only connect ethanol molecules to other oxygen atoms within the same BaO_8 coordination polyhedron, the three-dimensional network structure of [Ba(tfBDC)(DMF)(EtOH)] is entirely held together by coordinating bonds.

Synthesis and crystallization

In a snap-cap tube 61.4 mg (0.15 mmol, 1 eq.) $BaI_2{\cdot}H_2O$ and 35.6 mg (0.15 mmol, 1 eq.) H_2tfBDC (tetrafluoroterephthalic acid) were dissolved in 1.1 ml of a mixture of EtOH/DMF (3:1, *v*/*v*). The tube was closed with a cap and the latter was perforated once. This tube was then placed in a bigger one, which contained the same solvent mixture and an additional amount of 1.25 ml triethylamine. The bigger tube was closed with a non-perforated cap. After three weeks, rod-shaped colourless crystals were obtained, which are very sensitive, obviously due to an easy loss of solvent molecules. Therefore a single-crystal was isolated in perfluorinated oil for the diffraction experiment and cooled down to 170 K immediately.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The two crystallographically independent ethanol molecules are disordered and were refined using a split model with restraints and occupancies of 70:30 (O40/C40/C41/O40′/C40′/C41′) and 60:40 (C50/C51/C50′/C51′), respectively. The displacement parameters of the disordered atoms were refined isotropically and their bond lengths were set to ideal values by using the restraint command *DFIX*. The hydroxy H atoms of the disordered ethanol molecules could not be located in the final difference Fourier maps and were thus omitted in the final refinement.

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full crystallographic data

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A new alkaline earth metal tetrafluoroterephthalate: [Ba(tfBDC)(DMF)(EtOH)]

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Poly[(dimethylformamide-1κO)(ethanol-1κO)(μ_5-2,3,5,6-tetrafluorobenzenedicarboxylato-1:2κ^2O^1;1:3$\kappa^2O^{1'}$;4κO^4;5$\kappa O^{4'}$)barium(II)]

Crystal data

$[Ba(C_8F_4O_4)(C_3H_7NO)(C_2H_6O)]$
M_r = 492.58
Monoclinic, $P2_1/c$
a = 21.4745 (8) Å
b = 7.4295 (2) Å
c = 26.1730 (11) Å
β = 127.366 (2)°
V = 3318.8 (2) Å^3
Z = 8
$F(000)$ = 1896
D_x = 1.968 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 19777 reflections
θ = 2.0–26.8°
μ = 2.47 mm^{-1}
T = 293 K
Rod, colourless
0.35 × 0.2 × 0.1 mm

Data collection

STOE IPDS 2T diffractometer
φ and ω scans
Absorption correction: numerical (*XRED-32* and *XSHAPE*; Stoe & Cie, 2002)
T_{min} = 0.589, T_{max} = 0.808
39756 measured reflections
7048 independent reflections
5576 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 26.8°, θ_{min} = 2.0°
h = −27→27
k = −9→9
l = −33→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.04
7048 reflections
436 parameters
10 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 2.4924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ba1	0.54553 (2)	0.20736 (4)	0.73378 (2)	0.02214 (9)	
Ba2	0.04870 (2)	0.97090 (4)	0.31093 (2)	0.02406 (9)	
F3	0.35904 (18)	0.4686 (6)	0.51315 (16)	0.0507 (10)	
F4	0.23839 (19)	0.4857 (5)	0.38998 (15)	0.0469 (9)	
F6	0.06587 (17)	0.4292 (5)	0.44316 (15)	0.0426 (8)	
F7	0.18585 (18)	0.4252 (5)	0.56698 (15)	0.0433 (8)	
F13	0.27083 (19)	0.1178 (5)	0.65661 (16)	0.0445 (8)	
F14	0.14422 (18)	0.1505 (6)	0.64894 (17)	0.0505 (9)	
F16	0.2977 (2)	0.3578 (6)	0.86381 (18)	0.0506 (9)	
F17	0.42256 (19)	0.3398 (5)	0.86864 (17)	0.0475 (9)	
O1	0.4015 (2)	0.3431 (6)	0.63339 (17)	0.0402 (9)	
O2	0.6559 (2)	0.0624 (6)	0.85008 (19)	0.0424 (9)	
O9	0.0705 (2)	0.6121 (5)	0.31403 (17)	0.0341 (8)	
O10	0.0356 (2)	0.3338 (5)	0.31744 (16)	0.0291 (7)	
O11	0.53018 (19)	−0.1568 (5)	0.71318 (17)	0.0265 (7)	
O12	0.4348 (2)	0.0661 (5)	0.7489 (2)	0.0338 (8)	
O18	0.1380 (3)	0.3946 (6)	0.7816 (3)	0.0572 (12)	
O19	0.0914 (2)	0.1469 (6)	0.7214 (2)	0.0476 (10)	
O20	0.6787 (2)	0.2181 (6)	0.7461 (2)	0.0463 (10)	
O30	0.1902 (5)	0.9587 (10)	0.4261 (4)	0.095 (2)*	
O50	0.5090 (3)	0.2685 (8)	0.6153 (3)	0.0698 (14)*	
N20	0.8055 (3)	0.2099 (7)	0.7848 (3)	0.0401 (11)	
N30	0.3132 (3)	0.9290 (8)	0.5129 (3)	0.0528 (14)	
C1	0.3478 (3)	0.4508 (7)	0.6164 (2)	0.0316 (11)	
C2	0.2774 (3)	0.4472 (7)	0.5454 (2)	0.0273 (10)	
C3	0.2869 (3)	0.4590 (8)	0.4973 (2)	0.0325 (11)	
C4	0.2242 (3)	0.4672 (7)	0.4335 (2)	0.0300 (11)	
C5	0.1482 (3)	0.4571 (6)	0.4125 (2)	0.0253 (10)	
C6	0.1387 (3)	0.4392 (7)	0.4600 (2)	0.0289 (10)	
C7	0.2010 (3)	0.4382 (7)	0.5242 (2)	0.0286 (10)	
C9	0.0792 (3)	0.4689 (6)	0.3426 (2)	0.0249 (10)	
C11	0.4248 (3)	0.2118 (6)	0.7664 (2)	0.0256 (10)	
C12	0.3519 (3)	0.2282 (6)	0.7632 (3)	0.0269 (10)	
C13	0.2790 (3)	0.1794 (7)	0.7083 (3)	0.0309 (11)	
C14	0.2127 (3)	0.1936 (7)	0.7053 (3)	0.0345 (12)	
C15	0.2145 (3)	0.2545 (7)	0.7562 (3)	0.0334 (12)	
C16	0.2878 (3)	0.3020 (7)	0.8108 (3)	0.0330 (12)	
C17	0.3543 (3)	0.2916 (7)	0.8135 (3)	0.0322 (11)	
C18	0.1413 (3)	0.2670 (8)	0.7535 (3)	0.0363 (12)	
C20	0.7486 (3)	0.1856 (8)	0.7900 (3)	0.0405 (13)	
H20	0.7617	0.1416	0.8287	0.049*	
C21	0.8862 (4)	0.1656 (11)	0.8383 (4)	0.062 (2)	
H21A	0.9197	0.1913	0.8264	0.093*	
H21B	0.8897	0.0401	0.8484	0.093*	
H21C	0.9022	0.2363	0.8751	0.093*	

C22	0.7904 (4)	0.2747 (9)	0.7264 (3)	0.0477 (15)	
H22A	0.8389	0.2834	0.7321	0.072*	
H22B	0.7663	0.3913	0.7161	0.072*	
H22C	0.7560	0.1926	0.6920	0.072*	
C30	0.2595 (5)	0.9333 (13)	0.4528 (4)	0.074 (2)	
H30	0.2745	0.9152	0.4266	0.089*	
C31	0.2971 (7)	0.9511 (12)	0.5589 (5)	0.087 (3)	
H31A	0.3453	0.9446	0.6017	0.131*	
H31B	0.2625	0.8574	0.5529	0.131*	
H31C	0.2730	1.0661	0.5526	0.131*	
C32	0.3949 (6)	0.898 (2)	0.5417 (7)	0.147 (6)	
H32A	0.4252	0.9009	0.5877	0.220*	
H32B	0.4132	0.9896	0.5279	0.220*	
H32C	0.4005	0.7820	0.5286	0.220*	
O40	0.0241 (5)	0.9520 (11)	0.4043 (4)	0.069 (2)*	0.7
C40	0.0647 (8)	1.0064 (15)	0.4708 (5)	0.077 (3)*	0.7
H40A	0.0353	1.0945	0.4757	0.092*	0.7
H40B	0.1170	1.0515	0.4899	0.092*	0.7
C41	0.0660 (10)	0.8223 (17)	0.4973 (8)	0.087 (4)*	0.7
H41A	0.0918	0.8319	0.5426	0.131*	0.7
H41B	0.0939	0.7384	0.4900	0.131*	0.7
H41C	0.0133	0.7809	0.4760	0.131*	0.7
C50′	0.5375 (7)	0.2571 (14)	0.5775 (6)	0.058 (3)*	0.6
H50A	0.4951	0.2311	0.5328	0.069*	0.6
H50B	0.5774	0.1649	0.5941	0.069*	0.6
C51′	0.5713 (8)	0.4427 (15)	0.5848 (7)	0.072 (4)*	0.6
H51A	0.5919	0.4485	0.5609	0.107*	0.6
H51B	0.6126	0.4656	0.6294	0.107*	0.6
H51C	0.5309	0.5314	0.5687	0.107*	0.6
O40′	0.0662 (12)	0.969 (2)	0.4185 (9)	0.062 (5)*	0.3
C40′	0.0422 (14)	0.844 (4)	0.4449 (9)	0.076 (8)*	0.3
H40C	0.0400	0.7231	0.4300	0.091*	0.3
H40D	−0.0092	0.8756	0.4324	0.091*	0.3
C41′	0.1047 (13)	0.856 (3)	0.5193 (9)	0.044 (5)*	0.3
H41D	0.0912	0.7736	0.5395	0.067*	0.3
H41E	0.1061	0.9762	0.5333	0.067*	0.3
H41F	0.1552	0.8250	0.5309	0.067*	0.3
C50	0.5493 (10)	0.375 (2)	0.5953 (8)	0.057 (4)*	0.4
H50C	0.6043	0.3917	0.6308	0.068*	0.4
H50D	0.5248	0.4915	0.5785	0.068*	0.4
C51	0.5390 (18)	0.256 (4)	0.5426 (12)	0.113 (9)*	0.4
H51D	0.5629	0.3141	0.5256	0.170*	0.4
H51E	0.4842	0.2389	0.5088	0.170*	0.4
H51F	0.5635	0.1417	0.5605	0.170*	0.4

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01810 (14)	0.02236 (14)	0.02548 (15)	0.00131 (10)	0.01298 (12)	0.00198 (11)
Ba2	0.01982 (15)	0.02342 (15)	0.02311 (15)	−0.00225 (10)	0.01000 (12)	0.00058 (11)
F3	0.0188 (15)	0.093 (3)	0.0347 (17)	0.0036 (16)	0.0132 (14)	0.0115 (18)
F4	0.0343 (18)	0.079 (3)	0.0306 (16)	0.0061 (17)	0.0214 (15)	0.0093 (17)
F6	0.0188 (15)	0.071 (2)	0.0307 (16)	−0.0013 (15)	0.0113 (13)	0.0017 (16)
F7	0.0295 (16)	0.072 (2)	0.0278 (15)	0.0013 (16)	0.0172 (14)	0.0036 (16)
F13	0.0337 (17)	0.061 (2)	0.0418 (18)	−0.0033 (16)	0.0247 (15)	−0.0107 (17)
F14	0.0227 (16)	0.079 (3)	0.0448 (19)	−0.0064 (16)	0.0177 (15)	−0.0097 (19)
F16	0.045 (2)	0.069 (2)	0.055 (2)	−0.0086 (18)	0.0383 (18)	−0.0189 (19)
F17	0.0314 (17)	0.067 (2)	0.0470 (19)	−0.0147 (16)	0.0251 (16)	−0.0211 (18)
O1	0.0225 (19)	0.057 (3)	0.0282 (19)	0.0068 (18)	0.0089 (16)	0.0045 (18)
O2	0.034 (2)	0.048 (2)	0.032 (2)	0.0015 (18)	0.0134 (18)	0.0079 (18)
O9	0.0319 (19)	0.0285 (19)	0.0265 (18)	0.0031 (15)	0.0096 (16)	0.0035 (15)
O10	0.0300 (19)	0.0248 (17)	0.0262 (17)	−0.0022 (14)	0.0138 (16)	−0.0028 (14)
O11	0.0247 (17)	0.0253 (17)	0.0345 (18)	0.0024 (14)	0.0206 (16)	−0.0007 (15)
O12	0.0314 (19)	0.0242 (17)	0.056 (2)	0.0022 (15)	0.0316 (19)	0.0009 (17)
O18	0.054 (3)	0.048 (3)	0.102 (4)	0.004 (2)	0.064 (3)	−0.002 (3)
O19	0.031 (2)	0.060 (3)	0.057 (3)	−0.006 (2)	0.029 (2)	0.001 (2)
O20	0.031 (2)	0.053 (3)	0.059 (3)	0.0053 (19)	0.029 (2)	0.009 (2)
N20	0.028 (2)	0.040 (3)	0.053 (3)	−0.002 (2)	0.025 (2)	−0.006 (2)
N30	0.032 (3)	0.058 (3)	0.037 (3)	−0.005 (2)	0.004 (2)	0.003 (3)
C1	0.023 (3)	0.039 (3)	0.024 (2)	−0.002 (2)	0.010 (2)	0.000 (2)
C2	0.025 (3)	0.028 (3)	0.025 (2)	0.000 (2)	0.013 (2)	−0.001 (2)
C3	0.018 (2)	0.044 (3)	0.027 (2)	0.001 (2)	0.009 (2)	0.003 (2)
C4	0.025 (3)	0.040 (3)	0.024 (2)	0.002 (2)	0.013 (2)	0.002 (2)
C5	0.023 (2)	0.023 (2)	0.019 (2)	0.0008 (19)	0.007 (2)	0.0013 (18)
C6	0.020 (2)	0.033 (3)	0.026 (2)	−0.002 (2)	0.010 (2)	−0.001 (2)
C7	0.024 (2)	0.037 (3)	0.020 (2)	0.003 (2)	0.011 (2)	0.002 (2)
C9	0.022 (2)	0.025 (2)	0.023 (2)	0.0013 (19)	0.012 (2)	−0.002 (2)
C11	0.022 (2)	0.026 (2)	0.033 (3)	0.0037 (19)	0.019 (2)	0.005 (2)
C12	0.026 (2)	0.023 (2)	0.041 (3)	0.0009 (19)	0.025 (2)	0.000 (2)
C13	0.032 (3)	0.030 (3)	0.040 (3)	0.000 (2)	0.027 (2)	0.001 (2)
C14	0.022 (3)	0.036 (3)	0.043 (3)	−0.002 (2)	0.018 (2)	0.001 (2)
C15	0.029 (3)	0.028 (3)	0.052 (3)	0.000 (2)	0.029 (3)	0.004 (2)
C16	0.034 (3)	0.033 (3)	0.045 (3)	−0.004 (2)	0.030 (3)	−0.007 (2)
C17	0.027 (3)	0.033 (3)	0.038 (3)	−0.003 (2)	0.020 (2)	−0.005 (2)
C18	0.031 (3)	0.035 (3)	0.053 (3)	0.005 (2)	0.031 (3)	0.010 (3)
C20	0.031 (3)	0.039 (3)	0.049 (3)	0.000 (2)	0.022 (3)	0.000 (3)
C21	0.025 (3)	0.076 (5)	0.068 (5)	0.000 (3)	0.020 (3)	−0.024 (4)
C22	0.045 (4)	0.041 (3)	0.072 (4)	−0.003 (3)	0.044 (4)	0.002 (3)
C30	0.053 (5)	0.082 (6)	0.064 (5)	−0.011 (4)	0.023 (4)	0.007 (4)
C31	0.123 (8)	0.058 (5)	0.073 (6)	−0.012 (5)	0.056 (6)	0.001 (4)
C32	0.043 (6)	0.158 (13)	0.173 (13)	−0.012 (7)	0.031 (7)	−0.037 (11)

Geometric parameters (Å, º)

Ba1—O20	2.677 (4)	C2—C7	1.378 (7)
Ba1—O12^{i}	2.694 (4)	C2—C3	1.394 (7)
Ba1—O2	2.699 (4)	C3—C4	1.371 (7)
Ba1—O50	2.737 (5)	C4—C5	1.373 (7)
Ba1—O11	2.739 (3)	C5—C6	1.385 (7)
Ba1—O1	2.761 (4)	C5—C9	1.503 (6)
Ba1—O12	2.837 (3)	C6—C7	1.372 (7)
Ba1—O11^{i}	2.886 (3)	C9—Ba2^{vii}	3.209 (5)
Ba1—C11	3.183 (4)	C11—O11^{i}	1.243 (6)
Ba1—Ba1^{ii}	4.5122 (3)	C11—C12	1.522 (6)
Ba1—Ba1^{i}	4.5122 (3)	C12—C17	1.369 (7)
Ba2—O40′	2.603 (17)	C12—C13	1.385 (8)
Ba2—O18^{iii}	2.654 (4)	C13—C14	1.381 (7)
Ba2—O30	2.685 (8)	C14—C15	1.385 (8)
Ba2—O9	2.699 (4)	C15—C16	1.384 (8)
Ba2—O10^{iv}	2.727 (4)	C15—C18	1.532 (7)
Ba2—O19^{v}	2.728 (4)	C16—C17	1.387 (7)
Ba2—O40	2.799 (8)	C20—H20	0.9300
Ba2—O9^{vi}	2.862 (4)	C21—H21A	0.9600
Ba2—O10^{vi}	2.867 (3)	C21—H21B	0.9600
Ba2—C9^{vi}	3.209 (5)	C21—H21C	0.9600
Ba2—Ba2^{vi}	4.4999 (3)	C22—H22A	0.9600
Ba2—Ba2^{vii}	4.4999 (3)	C22—H22B	0.9600
F3—C3	1.340 (6)	C22—H22C	0.9600
F4—C4	1.352 (6)	C30—H30	0.9300
F6—C6	1.345 (6)	C31—H31A	0.9600
F7—C7	1.346 (6)	C31—H31B	0.9600
F13—C13	1.335 (6)	C31—H31C	0.9600
F14—C14	1.345 (6)	C32—H32A	0.9600
F16—C16	1.336 (6)	C32—H32B	0.9600
F17—C17	1.339 (6)	C32—H32C	0.9600
O1—C1	1.243 (6)	O40—C40	1.454 (9)
O2—C1^{ii}	1.246 (7)	C40—C41	1.526 (9)
O9—C9	1.248 (6)	C40—H40A	0.9700
O9—Ba2^{vii}	2.862 (4)	C40—H40B	0.9700
O10—C9	1.252 (6)	C41—H41A	0.9600
O10—Ba2^{viii}	2.727 (3)	C41—H41B	0.9600
O10—Ba2^{vii}	2.867 (3)	C41—H41C	0.9600
O11—C11^{ii}	1.243 (6)	C50′—C51′	1.516 (9)
O11—Ba1^{ii}	2.886 (3)	C50′—H50A	0.9700
O12—C11	1.244 (6)	C50′—H50B	0.9700
O12—Ba1^{ii}	2.694 (4)	C51′—H51A	0.9600
O18—C18	1.230 (7)	C51′—H51B	0.9600
O18—Ba2^{ix}	2.654 (4)	C51′—H51C	0.9600
O19—C18	1.248 (7)	O40′—C40′	1.430 (10)
O19—Ba2^{v}	2.728 (4)	C40′—C41′	1.558 (10)

O20—C20	1.240 (7)	C40′—H40C	0.9700
O30—C30	1.214 (10)	C40′—H40D	0.9700
O50—C50′	1.447 (8)	C41′—H41D	0.9600
O50—C50	1.481 (9)	C41′—H41E	0.9600
N20—C20	1.320 (7)	C41′—H41F	0.9600
N20—C22	1.441 (8)	C50—C51	1.535 (10)
N20—C21	1.458 (8)	C50—H50C	0.9700
N30—C30	1.267 (10)	C50—H50D	0.9700
N30—C32	1.448 (11)	C51—H51D	0.9600
N30—C31	1.448 (11)	C51—H51E	0.9600
C1—O2^{i}	1.246 (7)	C51—H51F	0.9600
C1—C2	1.526 (7)		

O20—Ba1—O12^{i}	84.46 (12)	C20—N20—C22	121.9 (5)
O20—Ba1—O2	74.51 (13)	C20—N20—C21	120.4 (6)
O12^{i}—Ba1—O2	105.31 (13)	C22—N20—C21	117.7 (5)
O20—Ba1—O50	71.47 (15)	C30—N30—C32	123.6 (9)
O12^{i}—Ba1—O50	86.25 (15)	C30—N30—C31	122.2 (8)
O2—Ba1—O50	142.71 (15)	C32—N30—C31	114.2 (9)
O20—Ba1—O11	92.61 (12)	O1—C1—O2^{i}	128.2 (5)
O12^{i}—Ba1—O11	176.68 (10)	O1—C1—C2	116.3 (5)
O2—Ba1—O11	75.31 (12)	O2^{i}—C1—C2	115.5 (5)
O50—Ba1—O11	91.34 (14)	C7—C2—C3	115.5 (4)
O20—Ba1—O1	126.98 (13)	C7—C2—C1	123.2 (4)
O12^{i}—Ba1—O1	76.67 (12)	C3—C2—C1	121.2 (4)
O2—Ba1—O1	158.26 (12)	F3—C3—C4	118.1 (5)
O50—Ba1—O1	58.39 (14)	F3—C3—C2	119.9 (4)
O11—Ba1—O1	104.00 (12)	C4—C3—C2	122.0 (5)
O20—Ba1—O12	156.67 (12)	F4—C4—C3	118.4 (4)
O12^{i}—Ba1—O12	113.66 (8)	F4—C4—C5	119.3 (4)
O2—Ba1—O12	86.11 (12)	C3—C4—C5	122.4 (5)
O50—Ba1—O12	122.10 (14)	C4—C5—C6	115.7 (4)
O11—Ba1—O12	69.58 (10)	C4—C5—C9	122.6 (4)
O1—Ba1—O12	73.64 (12)	C6—C5—C9	121.6 (4)
O20—Ba1—O11^{i}	143.49 (12)	F6—C6—C7	118.5 (4)
O12^{i}—Ba1—O11^{i}	69.47 (10)	F6—C6—C5	119.1 (4)
O2—Ba1—O11^{i}	87.86 (11)	C7—C6—C5	122.3 (5)
O50—Ba1—O11^{i}	129.03 (14)	F7—C7—C6	118.0 (4)
O11—Ba1—O11^{i}	113.85 (8)	F7—C7—C2	119.9 (4)
O1—Ba1—O11^{i}	72.39 (11)	C6—C7—C2	122.1 (5)
O12—Ba1—O11^{i}	45.42 (10)	O9—C9—O10	125.2 (4)
O20—Ba1—C11	162.04 (14)	O9—C9—C5	117.2 (4)
O12^{i}—Ba1—C11	90.82 (11)	O10—C9—C5	117.6 (4)
O2—Ba1—C11	90.16 (12)	O9—C9—Ba2^{vii}	62.8 (2)
O50—Ba1—C11	125.61 (15)	O10—C9—Ba2^{vii}	63.0 (2)
O11—Ba1—C11	92.45 (11)	C5—C9—Ba2^{vii}	170.6 (3)
O1—Ba1—C11	68.11 (12)	O11^{i}—C11—O12	125.4 (4)
O12—Ba1—C11	22.93 (11)	O11^{i}—C11—C12	117.8 (4)

O11^{i}—Ba1—C11	22.97 (11)	O12—C11—C12	116.8 (4)
O20—Ba1—Ba1^{ii}	123.72 (10)	O11^{i}—C11—Ba1	65.0 (2)
O12^{i}—Ba1—Ba1^{ii}	145.52 (7)	O12—C11—Ba1	62.7 (2)
O2—Ba1—Ba1^{ii}	69.13 (9)	C12—C11—Ba1	164.7 (3)
O50—Ba1—Ba1^{ii}	119.42 (12)	C17—C12—C13	116.5 (4)
O11—Ba1—Ba1^{ii}	37.79 (6)	C17—C12—C11	122.6 (5)
O1—Ba1—Ba1^{ii}	96.70 (9)	C13—C12—C11	120.9 (4)
O12—Ba1—Ba1^{ii}	34.29 (7)	F13—C13—C14	118.2 (5)
O11^{i}—Ba1—Ba1^{ii}	76.25 (7)	F13—C13—C12	120.8 (4)
C11—Ba1—Ba1^{ii}	56.06 (9)	C14—C13—C12	121.1 (5)
O20—Ba1—Ba1^{i}	120.38 (10)	F14—C14—C13	116.5 (5)
O12^{i}—Ba1—Ba1^{i}	36.40 (7)	F14—C14—C15	120.4 (5)
O2—Ba1—Ba1^{i}	107.49 (9)	C13—C14—C15	123.0 (5)
O50—Ba1—Ba1^{i}	102.58 (12)	C16—C15—C14	115.2 (5)
O11—Ba1—Ba1^{i}	146.72 (6)	C16—C15—C18	121.6 (5)
O1—Ba1—Ba1^{i}	61.01 (9)	C14—C15—C18	123.1 (5)
O12—Ba1—Ba1^{i}	77.45 (7)	F16—C16—C15	121.0 (4)
O11^{i}—Ba1—Ba1^{i}	35.57 (7)	F16—C16—C17	117.0 (5)
C11—Ba1—Ba1^{i}	54.87 (9)	C15—C16—C17	122.0 (5)
Ba1^{ii}—Ba1—Ba1^{i}	110.827 (11)	F17—C17—C12	120.4 (4)
O40′—Ba2—O18^{iii}	131.2 (5)	F17—C17—C16	117.4 (5)
O40′—Ba2—O30	57.6 (5)	C12—C17—C16	122.2 (5)
O18^{iii}—Ba2—O30	79.2 (2)	O18—C18—O19	128.0 (5)
O40′—Ba2—O9	93.1 (4)	O18—C18—C15	116.8 (5)
O18^{iii}—Ba2—O9	103.75 (13)	O19—C18—C15	115.2 (5)
O30—Ba2—O9	82.84 (17)	O20—C20—N20	123.6 (6)
O40′—Ba2—O10^{iv}	83.7 (4)	O20—C20—H20	118.2
O18^{iii}—Ba2—O10^{iv}	76.45 (12)	N20—C20—H20	118.2
O30—Ba2—O10^{iv}	93.01 (17)	N20—C21—H21A	109.5
O9—Ba2—O10^{iv}	175.70 (10)	N20—C21—H21B	109.5
O40′—Ba2—O19^{v}	75.1 (5)	H21A—C21—H21B	109.5
O18^{iii}—Ba2—O19^{v}	152.23 (16)	N20—C21—H21C	109.5
O30—Ba2—O19^{v}	128.43 (18)	H21A—C21—H21C	109.5
O9—Ba2—O19^{v}	80.29 (13)	H21B—C21—H21C	109.5
O10^{iv}—Ba2—O19^{v}	101.56 (12)	N20—C22—H22A	109.5
O18^{iii}—Ba2—O40	145.4 (2)	N20—C22—H22B	109.5
O30—Ba2—O40	72.7 (2)	H22A—C22—H22B	109.5
O9—Ba2—O40	92.61 (19)	N20—C22—H22C	109.5
O10^{iv}—Ba2—O40	85.06 (19)	H22A—C22—H22C	109.5
O19^{v}—Ba2—O40	59.9 (2)	H22B—C22—H22C	109.5
O40′—Ba2—O9^{vi}	132.8 (4)	O30—C30—N30	126.4 (10)
O18^{iii}—Ba2—O9^{vi}	80.44 (14)	O30—C30—H30	116.8
O30—Ba2—O9^{vi}	155.96 (17)	N30—C30—H30	116.8
O9—Ba2—O9^{vi}	114.53 (9)	N30—C31—H31A	109.5
O10^{iv}—Ba2—O9^{vi}	69.77 (10)	N30—C31—H31B	109.5
O19^{v}—Ba2—O9^{vi}	73.11 (12)	H31A—C31—H31B	109.5
O40—Ba2—O9^{vi}	120.3 (2)	N30—C31—H31C	109.5
O40′—Ba2—O10^{vi}	147.1 (4)	H31A—C31—H31C	109.5

O18^{iii}—Ba2—O10^{vi}	81.28 (14)	H31B—C31—H31C	109.5
O30—Ba2—O10^{vi}	141.53 (17)	N30—C32—H32A	109.5
O9—Ba2—O10^{vi}	70.06 (10)	N30—C32—H32B	109.5
O10^{iv}—Ba2—O10^{vi}	114.13 (8)	H32A—C32—H32B	109.5
O19^{v}—Ba2—O10^{vi}	74.28 (12)	N30—C32—H32C	109.5
O40—Ba2—O10^{vi}	133.3 (2)	H32A—C32—H32C	109.5
O9^{vi}—Ba2—O10^{vi}	45.60 (10)	H32B—C32—H32C	109.5
O40′—Ba2—C9^{vi}	143.7 (5)	C40—O40—Ba2	137.5 (7)
O18^{iii}—Ba2—C9^{vi}	81.90 (15)	O40—C40—C41	97.3 (9)
O30—Ba2—C9^{vi}	158.58 (18)	O40—C40—H40A	112.3
O9—Ba2—C9^{vi}	91.95 (11)	C41—C40—H40A	112.3
O10^{iv}—Ba2—C9^{vi}	92.33 (11)	O40—C40—H40B	112.3
O19^{v}—Ba2—C9^{vi}	70.44 (13)	C41—C40—H40B	112.3
O40—Ba2—C9^{vi}	128.4 (2)	H40A—C40—H40B	109.9
O9^{vi}—Ba2—C9^{vi}	22.82 (11)	C40—C41—H41A	109.5
O10^{vi}—Ba2—C9^{vi}	22.91 (11)	C40—C41—H41B	109.5
O40′—Ba2—Ba2^{vi}	118.1 (4)	H41A—C41—H41B	109.5
O18^{iii}—Ba2—Ba2^{vi}	65.86 (11)	C40—C41—H41C	109.5
O30—Ba2—Ba2^{vi}	123.09 (16)	H41A—C41—H41C	109.5
O9—Ba2—Ba2^{vi}	146.52 (7)	H41B—C41—H41C	109.5
O10^{iv}—Ba2—Ba2^{vi}	37.52 (7)	O50—C50′—C51′	103.3 (7)
O19^{v}—Ba2—Ba2^{vi}	95.39 (10)	O50—C50′—H50A	111.1
O40—Ba2—Ba2^{vi}	114.04 (18)	C51′—C50′—H50A	111.1
O9^{vi}—Ba2—Ba2^{vi}	34.78 (7)	O50—C50′—H50B	111.1
O10^{vi}—Ba2—Ba2^{vi}	76.78 (7)	C51′—C50′—H50B	111.1
C9^{vi}—Ba2—Ba2^{vi}	55.93 (9)	H50A—C50′—H50B	109.1
O40′—Ba2—Ba2^{vii}	117.5 (4)	C50′—C51′—H51A	109.5
O18^{iii}—Ba2—Ba2^{vii}	102.27 (11)	C50′—C51′—H51B	109.5
O30—Ba2—Ba2^{vii}	119.36 (16)	H51A—C51′—H51B	109.5
O9—Ba2—Ba2^{vii}	37.21 (7)	C50′—C51′—H51C	109.5
O10^{iv}—Ba2—Ba2^{vii}	147.07 (7)	H51A—C51′—H51C	109.5
O19^{v}—Ba2—Ba2^{vii}	64.18 (10)	H51B—C51′—H51C	109.5
O40—Ba2—Ba2^{vii}	108.93 (18)	C40′—O40′—Ba2	132.0 (14)
O9^{vi}—Ba2—Ba2^{vii}	77.53 (7)	O40′—C40′—C41′	106.2 (17)
O10^{vi}—Ba2—Ba2^{vii}	35.40 (7)	O40′—C40′—H40C	110.5
C9^{vi}—Ba2—Ba2^{vii}	55.40 (9)	C41′—C40′—H40C	110.5
Ba2^{vi}—Ba2—Ba2^{vii}	111.282 (12)	O40′—C40′—H40D	110.5
C1—O1—Ba1	146.7 (3)	C41′—C40′—H40D	110.5
C1^{ii}—O2—Ba1	132.2 (3)	H40C—C40′—H40D	108.7
C9—O9—Ba2	145.1 (3)	C40′—C41′—H41D	109.5
C9—O9—Ba2^{vii}	94.4 (3)	C40′—C41′—H41E	109.5
Ba2—O9—Ba2^{vii}	108.01 (12)	H41D—C41′—H41E	109.5
C9—O10—Ba2^{viii}	138.8 (3)	C40′—C41′—H41F	109.5
C9—O10—Ba2^{vii}	94.0 (3)	H41D—C41′—H41F	109.5
Ba2^{viii}—O10—Ba2^{vii}	107.08 (11)	H41E—C41′—H41F	109.5
C11^{ii}—O11—Ba1	136.2 (3)	O50—C50—C51	102.4 (8)
C11^{ii}—O11—Ba1^{ii}	92.1 (3)	O50—C50—H50C	111.3
Ba1—O11—Ba1^{ii}	106.64 (10)	C51—C50—H50C	111.3

C11—O12—Ba1^{ii}	147.5 (3)	O50—C50—H50D	111.3
C11—O12—Ba1	94.4 (3)	C51—C50—H50D	111.3
Ba1^{ii}—O12—Ba1	109.31 (11)	H50C—C50—H50D	109.2
C18—O18—Ba2^{ix}	141.2 (4)	C50—C51—H51D	109.5
C18—O19—Ba2^{v}	140.7 (4)	C50—C51—H51E	109.5
C20—O20—Ba1	135.2 (4)	H51D—C51—H51E	109.5
C30—O30—Ba2	143.9 (7)	C50—C51—H51F	109.5
C50′—O50—Ba1	144.7 (6)	H51D—C51—H51F	109.5
C50—O50—Ba1	131.4 (7)	H51E—C51—H51F	109.5
Ba1—O1—C1—O2^{i}	2.1 (11)	O12—C11—C12—C17	131.3 (5)
Ba1—O1—C1—C2	−178.1 (4)	Ba1—C11—C12—C17	−144.3 (11)
O1—C1—C2—C7	130.7 (6)	O11^{i}—C11—C12—C13	131.9 (5)
O2^{i}—C1—C2—C7	−49.5 (7)	O12—C11—C12—C13	−49.0 (7)
O1—C1—C2—C3	−51.4 (7)	Ba1—C11—C12—C13	35.5 (15)
O2^{i}—C1—C2—C3	128.4 (6)	C17—C12—C13—F13	179.4 (5)
C7—C2—C3—F3	179.9 (5)	C11—C12—C13—F13	−0.4 (8)
C1—C2—C3—F3	1.9 (8)	C17—C12—C13—C14	−0.4 (8)
C7—C2—C3—C4	2.2 (8)	C11—C12—C13—C14	179.8 (5)
C1—C2—C3—C4	−175.9 (5)	F13—C13—C14—F14	−2.7 (8)
F3—C3—C4—F4	−0.4 (8)	C12—C13—C14—F14	177.1 (5)
C2—C3—C4—F4	177.4 (5)	F13—C13—C14—C15	179.5 (5)
F3—C3—C4—C5	179.5 (5)	C12—C13—C14—C15	−0.7 (8)
C2—C3—C4—C5	−2.7 (9)	F14—C14—C15—C16	−177.3 (5)
F4—C4—C5—C6	−179.7 (5)	C13—C14—C15—C16	0.4 (8)
C3—C4—C5—C6	0.4 (8)	F14—C14—C15—C18	3.5 (8)
F4—C4—C5—C9	−1.0 (8)	C13—C14—C15—C18	−178.8 (5)
C3—C4—C5—C9	179.1 (5)	C14—C15—C16—F16	−178.0 (5)
C4—C5—C6—F6	179.7 (5)	C18—C15—C16—F16	1.2 (8)
C9—C5—C6—F6	1.1 (7)	C14—C15—C16—C17	1.0 (8)
C4—C5—C6—C7	2.3 (8)	C18—C15—C16—C17	−179.8 (5)
C9—C5—C6—C7	−176.4 (5)	C13—C12—C17—F17	179.2 (5)
F6—C6—C7—F7	0.7 (8)	C11—C12—C17—F17	−1.0 (8)
C5—C6—C7—F7	178.2 (5)	C13—C12—C17—C16	1.8 (8)
F6—C6—C7—C2	179.7 (5)	C11—C12—C17—C16	−178.4 (5)
C5—C6—C7—C2	−2.8 (9)	F16—C16—C17—F17	−0.6 (8)
C3—C2—C7—F7	179.5 (5)	C15—C16—C17—F17	−179.7 (5)
C1—C2—C7—F7	−2.5 (8)	F16—C16—C17—C12	176.8 (5)
C3—C2—C7—C6	0.5 (8)	C15—C16—C17—C12	−2.2 (9)
C1—C2—C7—C6	178.5 (5)	Ba2^{ix}—O18—C18—O19	5.6 (12)
Ba2—O9—C9—O10	121.2 (5)	Ba2^{ix}—O18—C18—C15	−176.2 (4)
Ba2^{vii}—O9—C9—O10	−9.5 (5)	Ba2^{v}—O19—C18—O18	−5.4 (11)
Ba2—O9—C9—C5	−59.9 (7)	Ba2^{v}—O19—C18—C15	176.4 (4)
Ba2^{vii}—O9—C9—C5	169.4 (4)	C16—C15—C18—O18	36.9 (8)
Ba2—O9—C9—Ba2^{vii}	130.7 (5)	C14—C15—C18—O18	−143.9 (6)
Ba2^{viii}—O10—C9—O9	131.3 (4)	C16—C15—C18—O19	−144.6 (6)
Ba2^{vii}—O10—C9—O9	9.4 (5)	C14—C15—C18—O19	34.5 (8)
Ba2^{viii}—O10—C9—C5	−47.6 (7)	Ba1—O20—C20—N20	−176.7 (4)

Ba2^{vii}—O10—C9—C5	−169.4 (4)	C22—N20—C20—O20	−1.0 (9)
Ba2^{viii}—O10—C9—Ba2^{vii}	121.9 (4)	C21—N20—C20—O20	−179.0 (6)
C4—C5—C9—O9	−62.6 (7)	Ba2—O30—C30—N30	−175.7 (6)
C6—C5—C9—O9	116.0 (5)	C32—N30—C30—O30	179.9 (11)
C4—C5—C9—O10	116.4 (6)	C31—N30—C30—O30	1.4 (15)
C6—C5—C9—O10	−65.1 (6)	Ba2—O40—C40—C41	−125.3 (10)
Ba1^{ii}—O12—C11—O11^{i}	119.3 (6)	C50—O50—C50′—C51′	−0.8 (14)
Ba1—O12—C11—O11^{i}	−18.1 (5)	Ba1—O50—C50′—C51′	−93.6 (11)
Ba1^{ii}—O12—C11—C12	−59.7 (8)	Ba2—O40′—C40′—C41′	149.4 (16)
Ba1—O12—C11—C12	162.8 (4)	C50′—O50—C50—C51	11.1 (17)
Ba1^{ii}—O12—C11—Ba1	137.5 (6)	Ba1—O50—C50—C51	140.7 (14)
O11^{i}—C11—C12—C17	−47.8 (7)		

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) *x*, *y*+1, *z*; (v) −*x*, −*y*+1, −*z*+1; (vi) −*x*, *y*+1/2, −*z*+1/2; (vii) −*x*, *y*−1/2, −*z*+1/2; (viii) *x*, *y*−1, *z*; (ix) *x*, −*y*+3/2, *z*+1/2.