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2-Methylimidazolium tetrakis(2-thenoyltrifluoroacetonato-κ^2O,O')neodymium(III)

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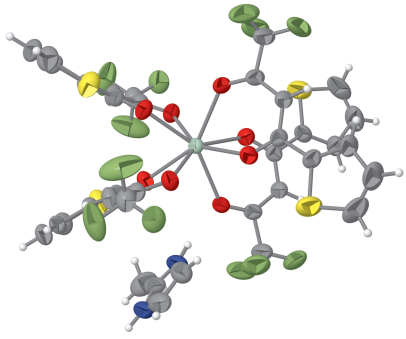
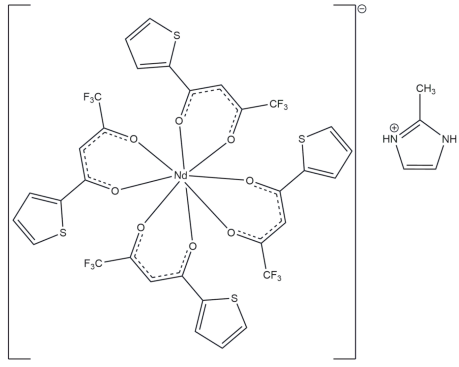
The title complex, $(C_4H_7N_2)[Nd(C_8H_4F_3O_2S)_4]$, is a salt formed *via* the acid–base reaction between 2-thenoyltrifluoroacetone (HTTA) and 2-methylimidazole (MeIm) in presence of neodymium(III) trifluoromethanesulfonate. The resulting compound features $[Nd(TTA)_4]^-$ anions with the central rare-earth metal cation placed on a twofold rotation axis, and $[MeImH]^+$ cations, disordered over an inversion centre. Cations and anions are linked through N—H···O hydrogen bonds to form zigzag chains running along [001].

3D view



Chemical scheme



Structure description

2-Thenoyltrifluoroacetone (HTTA) is a β-diketone ligand with chelating ability for rare-earth ions that can be used to produce highly luminescent complexes of Eu^{3+}, Tb^{3+} and Sm^{3+}, with high quantum yields and long luminescence lifetimes, because non-radiative decay pathways are minimized in the rigid coordination environment (Gujar *et al.*, 2019). The ligand is also able to sensitize lanthanide-centred emission *via* an efficient antenna effect. Nd^{3+} has sharp and well-defined *f*–*f* transitions, which makes it ideal for near-infrared luminescence applications. By coordinating this metal with β-diketonates like TTA^-, one can expect the development of more efficient luminescent materials, with practical applications in optoelectronics, catalysts and biomedicine (Ahmed *et al.*, 2020).

In this context, we synthesized the title compound, $[MeImH][Nd(TTA)_4]$ using MeIm (2-methylimidazole), HTTA, and neodymium(III) trifluoromethanesulfonate as starting materials. During the sonochemical reaction, an acid–base reaction occurs

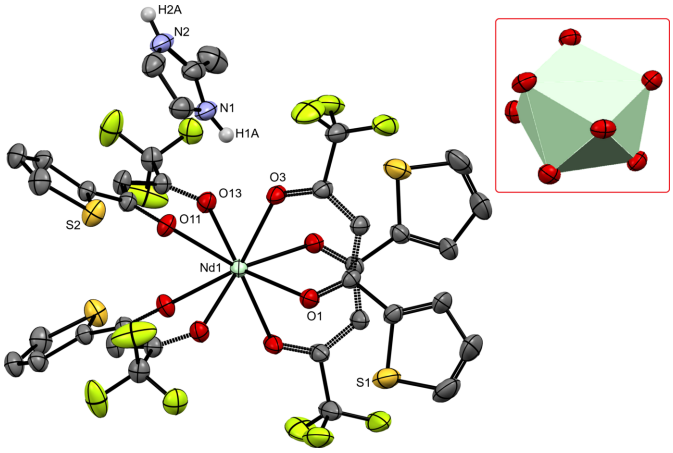


Figure 1
Structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. Only one disordered cation is shown for clarity. Non-labelled S and O atoms are generated by symmetry operation $1-x$, $y, \frac{1}{2}-z$. Only H atoms belonging to the NH groups in the cation are given. The antiprismatic coordination polyhedron around Nd1 is represented in the inset.

between MeIm (pK_b = 6.1) and HTTA (pK_a = 7.4) to form the title salt. The anion is placed on the twofold rotation axis in space group *C*2/*c*, while the cation is disordered over an inversion centre, with occupancy fixed to 1/2 in the asymmetric unit. The central ion Nd^{3+} forms a slightly distorted square-antiprismatic polyhedron with eight O atoms of the TTA^- ligands (Fig. 1). The distortion is reflected in Nd—O bond lengths in the range 2.396 (2) to 2.4758 (18) Å, which are comparable to bond lengths observed in other salts of the $[Nd(TTA)_4]^-$ anion crystallized with pyridinium (Leipoldt *et al.*, 1977), ammonium (Cary *et al.*, 2018) or a derivative of diphenyliodonium (Chen *et al.*, 1997). The anion $[Ln(TTA)_4]^-$ has also been characterized with all other lanthanides, except with *Ln* = Ho and *Ln* = Lu. The coordination geometry is systematically close to square-antiprismatic, with idealized point group D_{4d} (*e.g.* Assunção *et al.*, 2025; *Ln* = Eu). Ligands TTA^- are nearly planar: the dihedral angle between the thiophene and *β*-diketonate moieties is 13.91 (16) or 5.30 (16)°. The angle formed between the planes of the six-membered chelate rings Nd1–O1–C1–C2–C3–O3 and Nd1–O11–C11–C12–C13–O13 in the asymmetric unit is 89.45 (7)°, indicating an almost orthogonal arrangement for the independent TTA^- ligands.

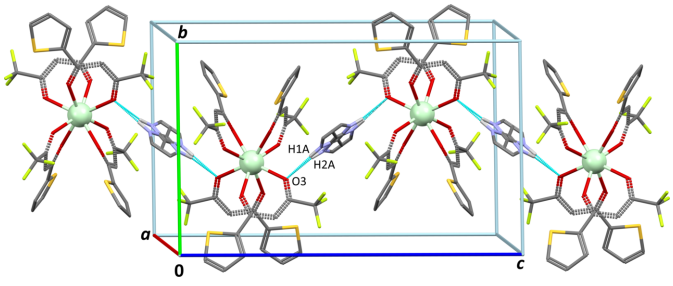


Figure 2
Part of the crystal structure, viewed nearly down [100]. One supramolecular chain is shown, with N—H···O hydrogen bonds represented as blue dashed bonds. All H atoms not involved in hydrogen-bonding have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3^{i}	0.86	2.03	2.865 (6)	163
N2—H2*A*···O3	0.86	2.06	2.904 (6)	168

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_4H_7N_2)[Nd(C_8H_4F_3O_2S)_4]$
M_r	1112.04
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	295
a, *b*, *c* (Å)	17.3191 (4), 12.6547 (2), 20.5387 (4)
β (°)	103.772 (2)
V (Å^3)	4372.01 (15)
Z	4
Radiation type	Ag *Kα*, λ = 0.56083 Å
μ (mm^{-1})	0.78
Crystal size (mm)	0.31 × 0.26 × 0.24
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Multi-scan (*X-AREA*; Stoe & Cie, 2019)
T_{min}, T_{max}	0.556, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	97427, 8697, 7163
R_{int}	0.043
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.782
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.113, 1.06
No. of reflections	8697
No. of parameters	313
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.70, −0.90

Computer programs: *X-AREA* (Stoe & Cie, 2019), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Supramolecular analysis of the title compound reveals intermolecular contacts between anions and cations, involving NH groups in the cation as donors and O3 as acceptor (Table 1 and Fig. 2). Zigzag chains alternating cations and anions are formed, running along [001]. These chains are stacked in the crystal with no significant contacts. Since cations are then sandwiched by two thiophene rings belonging to neighbouring anions along the chain, weak *π*–*π* interactions consolidate the crystal structure. In the asymmetric unit, the centroid-to-centroid separation between the thiophene ring S2 and the imidazole ring is 4.212 (6) Å, and corresponding mean planes form a dihedral angle of 23.4 (6)°.

Synthesis and crystallization

Crystals of [MeImH][Nd(TTA)$_4$] were prepared *via* a sonochemical route using an Nd^{3+}:HTTA = 1:2.5 stoichiometric

ratio, starting from 1 mmol (0.591 g) of $Nd(CF_3SO_3)_3$ dissolved in 25 ml of methanol and mixed with 25 ml of the ligand solution [2.5 mmol (0.555 g) of HTTA and 2 mmol (0.164 g) of MeIm] in deionized water. All solutions were stirred, mixed, and sonicated at room temperature using an Ultrasonic Processor equipment UP400St, applying a frequency of 24 kHz and power of 400 W with 1 pulsation per second for 20 min, until precipitation occurred. After a few hours at room temperature, the precipitate was separated from the mother liquor by centrifugation and washed with deionized water to remove soluble byproducts and/or excess of precursor materials. The dried product was kept at 343 K overnight, affording single crystals suitable for X-ray diffraction.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The cation $[MeImH]^+$ is placed close to an inversion centre, and is thus equally disordered over two positions by symmetry. The occupancy for the cation in the asymmetric unit was fixed to 1/2. All H atoms were placed in idealized positions (Sheldrick, 2015*b*).

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full crystallographic data

IUCrData (2025). **10**, x250569 [https://doi.org/10.1107/S2414314625005693]

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Crystal data

$(C_4H_7N_2)[Nd(C_8H_4F_3O_2S)_4]$
M_r = 1112.04
Monoclinic, $C2/c$
a = 17.3191 (4) Å
b = 12.6547 (2) Å
c = 20.5387 (4) Å
β = 103.772 (2)°
V = 4372.01 (15) Å^3
Z = 4
$F(000)$ = 2196
D_x = 1.689 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56083 Å
Cell parameters from 122785 reflections
θ = 1.9–29.2°
μ = 0.78 mm^{-1}
T = 295 K
Irregular, blue
0.31 × 0.26 × 0.24 mm

Data collection

Stoe Stadivari diffractometer
Radiation source: Sealed X-ray tube, Axo Astix-f Microfocus source
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2019)
T_{min} = 0.556, T_{max} = 1.000
97427 measured reflections
8697 independent reflections
7163 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.0°, θ_{min} = 1.9°
h = −27→27
k = −18→19
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.113
S = 1.06
8697 reflections
313 parameters
0 restraints
0 constraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 6.0925P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Nd1	0.500000	0.38687 (2)	0.250000	0.03908 (6)	

S1	0.36020 (8)	0.07268 (11)	0.11099 (5)	0.0853 (3)	
O1	0.41250 (13)	0.23740 (15)	0.21178 (10)	0.0508 (4)	
C1	0.39885 (15)	0.1532 (2)	0.23872 (13)	0.0435 (5)	
F1	0.3888 (2)	0.2515 (3)	0.45231 (13)	0.1088 (10)	
C2	0.41016 (19)	0.1387 (2)	0.30859 (14)	0.0508 (6)	
H2	0.400999	0.072079	0.324391	0.061*	
F2	0.51077 (18)	0.2131 (2)	0.46517 (11)	0.0966 (8)	
S2	0.32140 (5)	0.68267 (7)	0.30984 (5)	0.0663 (2)	
F3	0.4226 (3)	0.0935 (2)	0.43956 (12)	0.1309 (15)	
O3	0.45289 (13)	0.31300 (15)	0.34528 (10)	0.0519 (4)	
C3	0.43400 (18)	0.2183 (2)	0.35402 (13)	0.0499 (6)	
C4	0.4388 (3)	0.1920 (3)	0.42796 (17)	0.0738 (11)	
F4	0.71200 (14)	0.6641 (2)	0.43086 (17)	0.1057 (10)	
C5	0.36846 (18)	0.0630 (2)	0.19456 (14)	0.0508 (6)	
F5	0.73633 (12)	0.50159 (18)	0.43148 (12)	0.0720 (5)	
F6	0.74347 (15)	0.5903 (4)	0.34738 (16)	0.1279 (14)	
C6	0.3428 (3)	−0.0367 (3)	0.21092 (18)	0.0749 (11)	
H6	0.342232	−0.058169	0.254091	0.090*	
C7	0.3182 (4)	−0.0996 (3)	0.1533 (3)	0.1059 (19)	
H7	0.298623	−0.167868	0.154069	0.127*	
C8	0.3258 (3)	−0.0518 (4)	0.0976 (2)	0.0946 (15)	
H8	0.313345	−0.083671	0.055615	0.114*	
C11	0.47677 (16)	0.61847 (19)	0.33016 (14)	0.0446 (5)	
O11	0.44749 (11)	0.53626 (15)	0.30053 (10)	0.0489 (4)	
C12	0.56012 (17)	0.6335 (2)	0.35716 (17)	0.0511 (6)	
H12	0.578136	0.699386	0.374301	0.061*	
C13	0.61449 (15)	0.5539 (2)	0.35866 (14)	0.0455 (5)	
O13	0.60391 (12)	0.46054 (15)	0.33646 (10)	0.0500 (4)	
C14	0.70171 (17)	0.5786 (3)	0.39209 (18)	0.0564 (7)	
C15	0.42182 (15)	0.7013 (2)	0.34063 (13)	0.0442 (5)	
C16	0.43723 (18)	0.7944 (2)	0.37833 (15)	0.0521 (6)	
H16	0.487658	0.819560	0.398658	0.063*	
C17	0.3646 (2)	0.8451 (3)	0.38110 (18)	0.0625 (8)	
H17	0.362778	0.907832	0.404259	0.075*	
C18	0.2991 (2)	0.7944 (3)	0.3473 (2)	0.0672 (9)	
H18	0.247536	0.817743	0.344799	0.081*	
N1	0.5374 (5)	0.5365 (5)	0.5489 (3)	0.0672 (17)	0.5
H1A	0.529815	0.579440	0.579218	0.081*	0.5
N2	0.5165 (6)	0.4413 (6)	0.4631 (3)	0.0714 (19)	0.5
H2A	0.492977	0.410787	0.426307	0.086*	0.5
C21	0.4825 (6)	0.5068 (19)	0.4964 (11)	0.070 (4)	0.5
C22	0.5920 (11)	0.4282 (12)	0.4934 (7)	0.079 (4)	0.5
H22	0.627250	0.383783	0.478873	0.094*	0.5
C23	0.6100 (10)	0.4887 (11)	0.5485 (6)	0.073 (3)	0.5
H23	0.658822	0.496792	0.578961	0.087*	0.5
C24	0.3995 (9)	0.5422 (14)	0.4791 (8)	0.097 (5)	0.5
H24A	0.365313	0.483663	0.482293	0.146*	0.5
H24B	0.386518	0.569207	0.434144	0.146*	0.5

H24C	0.392314	0.596802	0.509566	0.146*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.04478 (10)	0.03509 (8)	0.03947 (9)	0.000	0.01416 (7)	0.000
S1	0.1074 (8)	0.0947 (7)	0.0497 (4)	−0.0175 (6)	0.0106 (5)	−0.0124 (4)
O1	0.0579 (11)	0.0472 (9)	0.0457 (9)	−0.0091 (8)	0.0094 (8)	−0.0007 (7)
C1	0.0419 (11)	0.0438 (11)	0.0446 (12)	−0.0046 (9)	0.0095 (9)	−0.0045 (9)
F1	0.141 (3)	0.132 (2)	0.0769 (16)	−0.033 (2)	0.0713 (18)	−0.0225 (15)
C2	0.0627 (16)	0.0455 (12)	0.0450 (13)	−0.0166 (11)	0.0146 (12)	−0.0038 (9)
F2	0.117 (2)	0.116 (2)	0.0475 (11)	−0.0292 (17)	0.0014 (12)	0.0016 (12)
S2	0.0474 (4)	0.0646 (5)	0.0862 (6)	0.0010 (3)	0.0143 (4)	−0.0178 (4)
F3	0.254 (4)	0.0848 (16)	0.0529 (13)	−0.078 (2)	0.0341 (19)	0.0033 (11)
O3	0.0697 (12)	0.0464 (9)	0.0460 (9)	−0.0154 (8)	0.0265 (9)	−0.0084 (7)
C3	0.0585 (15)	0.0526 (13)	0.0419 (12)	−0.0170 (12)	0.0185 (11)	−0.0056 (10)
C4	0.108 (3)	0.070 (2)	0.0467 (15)	−0.036 (2)	0.0250 (18)	−0.0092 (14)
F4	0.0641 (13)	0.0690 (14)	0.160 (3)	0.0003 (11)	−0.0209 (15)	−0.0394 (16)
C5	0.0529 (14)	0.0501 (13)	0.0461 (13)	−0.0021 (11)	0.0051 (11)	−0.0091 (10)
F5	0.0547 (10)	0.0712 (12)	0.0823 (14)	0.0083 (9)	0.0007 (10)	0.0047 (10)
F6	0.0552 (13)	0.243 (4)	0.0871 (19)	−0.0286 (18)	0.0194 (13)	0.047 (2)
C6	0.113 (3)	0.0473 (15)	0.0555 (17)	−0.0206 (17)	0.0030 (19)	−0.0096 (13)
C7	0.153 (5)	0.060 (2)	0.089 (3)	−0.025 (3)	−0.002 (3)	−0.023 (2)
C8	0.104 (3)	0.093 (3)	0.072 (3)	−0.003 (3)	−0.007 (2)	−0.040 (2)
C11	0.0472 (12)	0.0408 (11)	0.0480 (12)	−0.0004 (9)	0.0154 (10)	−0.0020 (9)
O11	0.0450 (9)	0.0439 (9)	0.0598 (11)	−0.0013 (7)	0.0163 (8)	−0.0127 (8)
C12	0.0442 (12)	0.0396 (11)	0.0690 (17)	−0.0025 (9)	0.0123 (12)	−0.0091 (11)
C13	0.0429 (12)	0.0436 (11)	0.0504 (13)	−0.0022 (9)	0.0117 (10)	0.0001 (9)
O13	0.0503 (10)	0.0433 (9)	0.0548 (11)	0.0033 (7)	0.0089 (8)	−0.0053 (7)
C14	0.0434 (13)	0.0528 (14)	0.0712 (19)	−0.0011 (11)	0.0100 (13)	0.0008 (13)
C15	0.0433 (12)	0.0419 (11)	0.0485 (12)	0.0015 (9)	0.0133 (10)	−0.0030 (9)
C16	0.0554 (15)	0.0487 (13)	0.0519 (14)	0.0109 (11)	0.0123 (12)	−0.0075 (11)
C17	0.0682 (19)	0.0487 (14)	0.074 (2)	0.0105 (14)	0.0232 (16)	−0.0099 (14)
C18	0.0555 (17)	0.0618 (18)	0.088 (2)	0.0146 (14)	0.0246 (17)	−0.0015 (16)
N1	0.099 (5)	0.060 (3)	0.048 (3)	−0.021 (4)	0.029 (4)	−0.013 (2)
N2	0.108 (6)	0.066 (4)	0.048 (3)	−0.035 (4)	0.033 (4)	−0.017 (3)
C21	0.095 (11)	0.070 (6)	0.048 (5)	−0.032 (10)	0.026 (9)	−0.004 (4)
C22	0.104 (10)	0.066 (5)	0.077 (8)	−0.023 (5)	0.043 (8)	−0.013 (5)
C23	0.086 (7)	0.074 (6)	0.057 (5)	−0.027 (5)	0.017 (5)	−0.004 (4)
C24	0.084 (8)	0.113 (19)	0.091 (15)	−0.030 (11)	0.016 (12)	0.023 (9)

Geometric parameters (Å, º)

Nd1—O13^{i}	2.396 (2)	C7—H7	0.9300
Nd1—O13	2.396 (2)	C8—H8	0.9300
Nd1—O1^{i}	2.4340 (19)	C11—O11	1.250 (3)
Nd1—O1	2.4340 (19)	C11—C12	1.430 (4)
Nd1—O11^{i}	2.4346 (18)	C11—C15	1.466 (3)

Nd1—O11	2.4346 (17)	C12—C13	1.374 (4)
Nd1—O3	2.4758 (18)	C12—H12	0.9300
Nd1—O3^{i}	2.4758 (18)	C13—O13	1.263 (3)
S1—C8	1.683 (5)	C13—C14	1.535 (4)
S1—C5	1.693 (3)	C15—C16	1.400 (4)
O1—C1	1.249 (3)	C16—C17	1.424 (4)
C1—C2	1.413 (4)	C16—H16	0.9300
C1—C5	1.475 (4)	C17—C18	1.345 (5)
F1—C4	1.330 (5)	C17—H17	0.9300
C2—C3	1.369 (4)	C18—H18	0.9300
C2—H2	0.9300	N1—C21	1.31 (2)
F2—C4	1.325 (5)	N1—C23	1.398 (19)
S2—C18	1.698 (4)	N1—H1A	0.8600
S2—C15	1.720 (3)	N2—C21	1.30 (2)
F3—C4	1.312 (4)	N2—C22	1.32 (2)
O3—C3	1.266 (3)	N2—H2A	0.8600
C3—C4	1.538 (4)	C21—C24	1.47 (2)
F4—C14	1.330 (4)	C22—C23	1.340 (13)
C5—C6	1.404 (4)	C22—H22	0.9300
F5—C14	1.316 (4)	C23—H23	0.9300
F6—C14	1.306 (4)	C24—H24A	0.9600
C6—C7	1.406 (5)	C24—H24B	0.9600
C6—H6	0.9300	C24—H24C	0.9600
C7—C8	1.327 (8)		

O13^{i}—Nd1—O13	134.20 (9)	C6—C7—H7	123.4
O13^{i}—Nd1—O1^{i}	147.31 (7)	C7—C8—S1	112.9 (3)
O13—Nd1—O1^{i}	76.30 (7)	C7—C8—H8	123.5
O13^{i}—Nd1—O1	76.30 (7)	S1—C8—H8	123.5
O13—Nd1—O1	147.31 (7)	O11—C11—C12	123.6 (2)
O1^{i}—Nd1—O1	78.00 (10)	O11—C11—C15	117.7 (2)
O13^{i}—Nd1—O11^{i}	70.90 (6)	C12—C11—C15	118.6 (2)
O13—Nd1—O11^{i}	73.91 (7)	C11—O11—Nd1	134.77 (17)
O1^{i}—Nd1—O11^{i}	118.29 (7)	C13—C12—C11	122.3 (2)
O1—Nd1—O11^{i}	137.14 (7)	C13—C12—H12	118.9
O13^{i}—Nd1—O11	73.91 (7)	C11—C12—H12	118.9
O13—Nd1—O11	70.90 (6)	O13—C13—C12	129.6 (3)
O1^{i}—Nd1—O11	137.15 (7)	O13—C13—C14	113.2 (2)
O1—Nd1—O11	118.28 (7)	C12—C13—C14	117.2 (2)
O11^{i}—Nd1—O11	78.11 (9)	C13—O13—Nd1	130.54 (18)
O13^{i}—Nd1—O3	113.71 (7)	F6—C14—F5	105.6 (3)
O13—Nd1—O3	83.79 (7)	F6—C14—F4	108.1 (3)
O1^{i}—Nd1—O3	75.45 (7)	F5—C14—F4	105.0 (3)
O1—Nd1—O3	70.39 (6)	F6—C14—C13	111.0 (3)
O11^{i}—Nd1—O3	148.98 (7)	F5—C14—C13	112.3 (3)
O11—Nd1—O3	74.30 (7)	F4—C14—C13	114.3 (3)
O13^{i}—Nd1—O3^{i}	83.79 (7)	C16—C15—C11	129.7 (3)
O13—Nd1—O3^{i}	113.71 (7)	C16—C15—S2	111.2 (2)

O1^{i}—Nd1—O3^{i}	70.39 (6)	C11—C15—S2	118.89 (19)
O1—Nd1—O3^{i}	75.45 (7)	C15—C16—C17	110.3 (3)
O11^{i}—Nd1—O3^{i}	74.30 (7)	C15—C16—H16	124.8
O11—Nd1—O3^{i}	148.98 (7)	C17—C16—H16	124.8
O3—Nd1—O3^{i}	135.63 (9)	C18—C17—C16	114.2 (3)
C8—S1—C5	92.2 (2)	C18—C17—H17	122.9
C1—O1—Nd1	133.56 (17)	C16—C17—H17	122.9
O1—C1—C2	124.5 (2)	C17—C18—S2	112.1 (2)
O1—C1—C5	117.7 (2)	C17—C18—H18	124.0
C2—C1—C5	117.8 (2)	S2—C18—H18	124.0
C3—C2—C1	122.9 (2)	C21—N1—C23	110.4 (10)
C3—C2—H2	118.6	C21—N1—H1A	124.8
C1—C2—H2	118.6	C23—N1—H1A	124.8
C18—S2—C15	92.21 (16)	C21—N2—C22	110.7 (9)
C3—O3—Nd1	127.90 (16)	C21—N2—H2A	124.6
O3—C3—C2	130.3 (3)	C22—N2—H2A	124.6
O3—C3—C4	112.9 (2)	N2—C21—N1	106.5 (10)
C2—C3—C4	116.8 (3)	N2—C21—C24	127.4 (17)
F3—C4—F2	107.4 (4)	N1—C21—C24	126.1 (18)
F3—C4—F1	106.5 (4)	N2—C22—C23	109.4 (17)
F2—C4—F1	106.0 (3)	N2—C22—H22	125.3
F3—C4—C3	114.9 (3)	C23—C22—H22	125.3
F2—C4—C3	110.4 (3)	C22—C23—N1	102.9 (15)
F1—C4—C3	111.2 (4)	C22—C23—H23	128.6
C6—C5—C1	129.4 (3)	N1—C23—H23	128.6
C6—C5—S1	110.7 (2)	C21—C24—H24A	109.5
C1—C5—S1	119.9 (2)	C21—C24—H24B	109.5
C5—C6—C7	110.9 (4)	H24A—C24—H24B	109.5
C5—C6—H6	124.5	C21—C24—H24C	109.5
C7—C6—H6	124.5	H24A—C24—H24C	109.5
C8—C7—C6	113.3 (4)	H24B—C24—H24C	109.5
C8—C7—H7	123.4		

Nd1—O1—C1—C2	25.1 (4)	C11—C12—C13—O13	2.6 (5)
Nd1—O1—C1—C5	−155.3 (2)	C11—C12—C13—C14	−177.1 (3)
O1—C1—C2—C3	3.2 (5)	C12—C13—O13—Nd1	23.9 (5)
C5—C1—C2—C3	−176.4 (3)	C14—C13—O13—Nd1	−156.4 (2)
Nd1—O3—C3—C2	−22.7 (5)	O13—C13—C14—F6	74.2 (4)
Nd1—O3—C3—C4	157.8 (2)	C12—C13—C14—F6	−106.0 (4)
C1—C2—C3—O3	−3.1 (6)	O13—C13—C14—F5	−43.7 (4)
C1—C2—C3—C4	176.4 (3)	C12—C13—C14—F5	136.0 (3)
O3—C3—C4—F3	−177.5 (4)	O13—C13—C14—F4	−163.1 (3)
C2—C3—C4—F3	2.9 (6)	C12—C13—C14—F4	16.6 (4)
O3—C3—C4—F2	−55.9 (4)	O11—C11—C15—C16	171.8 (3)
C2—C3—C4—F2	124.5 (3)	C12—C11—C15—C16	−5.0 (4)
O3—C3—C4—F1	61.5 (4)	O11—C11—C15—S2	−1.8 (3)
C2—C3—C4—F1	−118.1 (3)	C12—C11—C15—S2	−178.7 (2)
O1—C1—C5—C6	−174.7 (3)	C18—S2—C15—C16	−1.2 (2)

C2—C1—C5—C6	5.0 (5)	C18—S2—C15—C11	173.5 (2)
O1—C1—C5—S1	4.9 (4)	C11—C15—C16—C17	−172.8 (3)
C2—C1—C5—S1	−175.5 (2)	S2—C15—C16—C17	1.2 (3)
C8—S1—C5—C6	−1.1 (3)	C15—C16—C17—C18	−0.6 (4)
C8—S1—C5—C1	179.3 (3)	C16—C17—C18—S2	−0.3 (4)
C1—C5—C6—C7	179.9 (4)	C15—S2—C18—C17	0.9 (3)
S1—C5—C6—C7	0.3 (5)	C22—N2—C21—N1	0.3 (19)
C5—C6—C7—C8	0.9 (8)	C22—N2—C21—C24	179.8 (18)
C6—C7—C8—S1	−1.8 (8)	C23—N1—C21—N2	0.7 (18)
C5—S1—C8—C7	1.7 (5)	C23—N1—C21—C24	−178.7 (17)
C12—C11—O11—Nd1	−16.4 (4)	C21—N2—C22—C23	−1 (2)
C15—C11—O11—Nd1	166.90 (18)	N2—C22—C23—N1	1.6 (19)
O11—C11—C12—C13	−6.8 (5)	C21—N1—C23—C22	−1.5 (18)
C15—C11—C12—C13	169.9 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···F3^{ii}	0.93	2.60	3.429 (4)	149
N1—H1*A*···O3^{iii}	0.86	2.03	2.865 (6)	163
N2—H2*A*···O3	0.86	2.06	2.904 (6)	168
C24—H24*B*···S2	0.96	2.91	3.852 (15)	167

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