Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[neodymate(III)bis[μ-dimethyl(phenylsulfonyl)amidophosphato]sodium(I)bis[μ-dimethyl(phenylsulfonyl)amidophosphato]]

Olesia V. Moroz,[a] Svitlana V. Shishkina,[b] Viktor A. Trush,[a] Tetyana Yu. Sliva[a]* and Volodymyr M. Amirkhanov[a]

[a]National Taras Shevchenko University, Department of Chemistry, Volodymyrska Street 64, 01033 Kyiv, Ukraine, and [b]STC 'Institute for Single Crystals', 60 Lenina Avenue, Khar'kov 61001, Ukraine
Correspondence e-mail: tatianasliva@yahoo.com

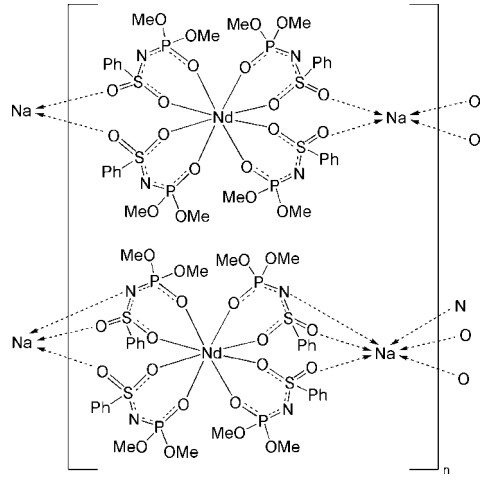
Received 6 November 2007; accepted 16 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.054; wR factor = 0.152; data-to-parameter ratio = 29.2.

The crystal structure of the title compound, $[NaNd(C_8H_{11}NO_5PS)_4]_n$, is composed of two types of crystallographically independent polymeric chains, *A* and *B*, respectively, which are formed by alternating anions and sodium cations. In both polymeric chains, Nd^{III} ions are eight-coordinated by O atoms belonging to the sulfonyl and phosphoryl groups of four bidentate chelate ligands. In chain *A*, the coordination polyhedron of the Nd^{III} ion has a conformation intermediate between bicapped trigonal-prismatic and square-antiprismatic, and the Na^{I} ion is coordinated by two N and four O atoms in a distorted octahedral geometry. In chain *B*, the coordination polyhedron of Nd is a slightly distorted square antiprism, and Na is coordinated by four O atoms in a distorted tetrahedral geometry.

Related literature

For details of the pharmacological and biological properties of sulfonylamide derivatives, see: Kishino & Saito (1979); Xu & Angell (2000). For the structural analogues of phosphorylated sulfonylamides, see: Amirkhanov *et al.* (1996); Borzechowska *et al.* (2002); Burgi & Dunitz (1994); Malandrino *et al.* (1998); Pietraszkiewicz *et al.* (2002); Skopenko *et al.* (2004); Trush *et al.* (2001). For calculation of polyhedra of lanthanide anions, see: Porai-Koshits & Aslanov (1972). For the synthesis of the ligand, see: Kirsanov (1952); Kirsanov & Shevchenko (1954).



Experimental

Crystal data

$[NaNd(C_8H_{11}NO_5PS)_4]$
M_r = 1224.10
Orthorhombic, $P2_12_12_1$
a = 20.276 (2) Å
b = 21.9129 (9) Å
c = 22.058 (2) Å
V = 9800.5 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 293 (2) K
0.5 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur-3 diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.705, T_{max} = 0.855
104650 measured reflections
34763 independent reflections
20694 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 0.90
34763 reflections
1189 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 4.50 e Å^{-3}
$\Delta\rho_{min}$ = −1.95 e Å^{-3}
Absolute structure: Flack (1983), 15958 Friedel pairs
Flack parameter: −0.063 (8)

Table 1
Selected bond lengths (Å).

Na1*A*—O10*A*^{i}	2.385 (4)	Nd1*A*—O11*A*	2.409 (4)
Na1*A*—O20*A*	2.411 (4)	Nd1*A*—O9*A*	2.478 (3)
Na1*A*—O5*A*	2.421 (4)	Nd1*A*—O1*A*	2.485 (3)
Na1*A*—O15*A*^{i}	2.433 (4)	Nd1*A*—O19*A*	2.492 (4)
Na1*A*—N3*A*^{i}	2.526 (4)	Nd1*A*—O14*A*	2.515 (4)
Na1*A*—N4*A*	2.589 (5)	Nd1*B*—O1*B*	2.368 (4)
Na1*B*—O15*B*	2.186 (5)	Nd1*B*—O16*B*	2.372 (4)
Na1*B*—O20*B*^{ii}	2.211 (5)	Nd1*B*—O11*B*	2.380 (4)
Na1*B*—O5*B*^{ii}	2.242 (5)	Nd1*B*—O6*B*	2.382 (4)
Na1*B*—O10*B*	2.261 (4)	Nd1*B*—O19*B*	2.484 (4)
Nd1*A*—O6*A*	2.362 (4)	Nd1*B*—O14*B*	2.493 (4)
Nd1*A*—O4*A*	2.375 (4)	Nd1*B*—O4*B*	2.513 (4)
Nd1*A*—O16*A*	2.406 (4)	Nd1*B*—O9*B*	2.509 (4)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*

 doi:10.1107/S1600536807060023

(Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2351).

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supplementary materials

Acta Cryst. (2007). E**63**, m3175-m3176 [**doi:10.1107/S1600536807060023**]

catena-Poly[neodymate(III)bis[μ-dimethyl(phenylsulfonyl)amidophosphato]sodium(I)bis[μ-dimethyl(phenylsulfonyl)amidophosphato]]

O. V. Moroz, S. V. Shishkina, V. A. Trush, T. Y. Sliva and V. M. Amirkhanov

Comment

It is known that sulfonylamide derivatives of a general view $RSO_2NHPO(R_1)_2$ are widely used in medicine and toxicology as bactericidal drugs (Xu & Angell, 2000); some sulfonyl phosphoramides are important pesticides (Kishino & Saito, 1979). Earlier systematically investigated by us carbacylamidophosphates and their coordination compounds (Skopenko *et al.*, 2004; Amirkhanov *et al.*, 1996) may be considered as structural analogous of phosphorylated sulfonylamides. To date the coordination chemistry of these ligands have been of great interest (Pietraszkiewicz *et al.*, 2002), however there are no reports on the crystal structure of the complexes with dimethyl(phenylsulfonyl)amidophosphate (HL). This paper is devoted to the crystal structure of tetrakis–complex of composition $\{Na[Nd(L)_4]\}_n$.

The title compound contains two independent one-dimensional polymeric chains, A and B, respectively, which are formed by $[Nd(L_4)]^-$ anions and sodium cations as the linkers (Figs. 1 and 2). The distinctions between the chains are in the different types of coordination polyhedra for Nd^{3+} and Na^+ ions.

In complex anions the neodymium atoms have eight-coordinated environment formed by oxygen atoms belonging to sulfonyl and phosphoryl groups of four bidentate chelate ligands. The coordinated residues of acido ligand (*L*) are once deprotonated by amide group. According to the geometrical standards, which are proposed by Porai-Koshits (Porai-Koshits & Aslanov, 1972) the resulting coordination polyhedra can be described as a medium conformation between bicapped trigonal prism and square antiprism for Nd1A atom and as a slightly distorted square antiprism for Nd1B atom.

The Nd—O distances (Table 1) fall in the range 2.362 (4)–2.409 (4) Å, for phosphoryl and 2.478 (3)–2.515 (4) Å for sulfonyl groups. The average Nd—O(P) bond lengths are shorter than Nd—O(S) separation that can be explained by higher affinity of phosphoryl group to lanthanide ions. The conclusion of deprotonation of amide goups can be achieved from the analysis of the O—S—N—P—O chelate fragments (Burgi & Dunitz, 1994). The bite angles around the central atom lie in the range 72.03 (13)–73.57 (11)° for Nd1A and 71.67 (12)–73.19 (13)° for Nd1B which are typical for lanthanide complexes with oxygen donor atoms chelate ligands (Malandrino *et al.*, 1998; Trush *et al.*, 2001; Borzechowska *et al.*, 2002). The metallocycles are almost flat with a deviation of the Nd atoms from the mean planes defined by the other five atoms of 0.124 (1) Å for Nd1A and 0.064 (1) Å for Nd1B.

The connection of complex anions in one-dimensional polymer structure is provided by Na ions (Fig 3). The Na polyhedron in A is a distorted octahedron and in B it can be described as a tetrahedron. The distorted octahedral environment is formed by four oxygen atoms belonging to SO groups (two from one complex anion and two from the neighbor one) and two nitrogen atoms from amide groups of different tetrakis anions. The tetrahedral environment is formed by four SO O atoms from different anions only. The Na—O, Na—N bond lengths are indicated in Table 1.

Experimental

The synthesis of HL was carried out according to the method by Kirsanov (Kirsanov, 1952; Kirsanov & Shevchenko, 1954).

$Nd(NO_3)_3 5H_2O$ (0,42 g, 1 mmol) was dissolved in acetone (10 ml) and added to 10 ml of an acetone solution of NaL (1,48 g, 4 mmol). After 20 min the precipitate of $NaNO_3$ was filtered off and *i*-PrOH (10 ml) was added to filtrate. The resulting clear solution was left at ambient temperature for crystallization in air. The crystals were separated by filtration after 48 h, washed with cool *i*–PrOH (10 ml) and finally dried in air. Yield: 85–90%. Analysis found: C 31.3, H 3.8, N 4.6, S 10.2%; $C_{32}H_{44}N_4NaNdO_{20}P_4S_4$ requires: C 31.4, H 3.6, N 4.6, S 10.5%; IR (KBr pellet, cm^{-1}): 1240, 1060 (s, SO_2) and 1170 (s, PO).

Refinement

All H atoms were placed at calculated positions and treated as riding on their parent atoms [C—H = 0.93 and 0.96 Å, and $U_{iso}(H) = 1.2$ and $1.5U_{eq}(C)$].

Figures

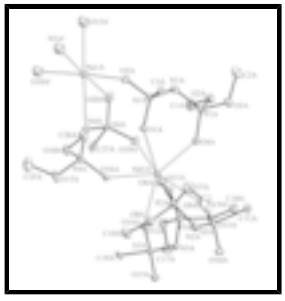

Fig. 1. A portion of polymeric chain A in the title compound, showing 30% probability displacement ellipsoids and the atomic numbering [symmetry codes: (') $-x + 1/2, -y, z - 1/2$]. H atoms and phenyl groups have been omitted for clarity.

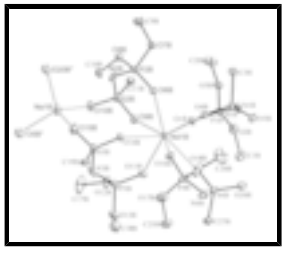

Fig. 2. A portion of polymeric chain B in the title compound, showing the 30% probability displacement ellipsoids and atomic numbering [symmetry codes: (") $-x - 1/2, -y, z - 1/2$]. H atoms and phenyl groups have been omitted for clarity.

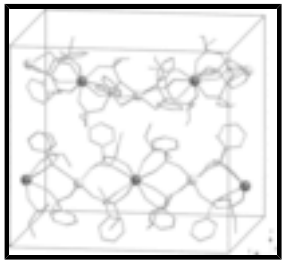

Fig. 3. A schematic view of packing diagram for $\{Na[Nd(L)_4]\}_n$ (projection along the *y* direction).

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Crystal data

$[NaNd(C_8H_{11}NO_5PS)_4]$	$F_{000} = 4952$
$M_r = 1224.10$	$D_x = 1.659$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 18882 reflections
$a = 20.276$ (2) Å	$\theta = 2.8$–35.7°
$b = 21.9129$ (9) Å	$\mu = 1.45$ mm^{-1}
$c = 22.058$ (2) Å	$T = 293$ (2) K
$V = 9800.5$ (14) Å^3	Prism, violet
$Z = 8$	0.5 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur-3 diffractometer	34763 independent reflections
Radiation source: Enhance (Mo) X-ray Source	20694 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 16.1827 pixels mm^{-1}	$\theta_{max} = 32.5^\circ$
$T = 293(2)$ K	$\theta_{min} = 2.6^\circ$
ω–scans	$h = -30 \rightarrow 30$
Absorption correction: multi-scan (Blessing, 1995)	$k = -32 \rightarrow 33$
$T_{min} = 0.705$, $T_{max} = 0.855$	$l = -32 \rightarrow 33$
104650 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0935P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.152$	$(\Delta/\sigma)_{max} = 0.078$
$S = 0.90$	$\Delta\rho_{max} = 4.50$ e Å^{-3}
34763 reflections	$\Delta\rho_{min} = -1.95$ e Å^{-3}
1189 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 15958 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.063 (8)

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}
Na1A	0.31989 (10)	−0.00395 (10)	0.00630 (8)	0.0228 (4)
Na1B	−0.25624 (12)	0.05492 (10)	0.24305 (9)	0.0308 (5)
Nd1A	0.248935 (14)	0.043855 (11)	0.255686 (10)	0.01692 (5)
Nd1B	−0.242758 (13)	−0.001980 (12)	0.493901 (11)	0.01890 (6)
S1A	0.30001 (6)	0.12309 (6)	0.11316 (6)	0.0190 (2)
P1A	0.38553 (7)	0.14088 (6)	0.21158 (6)	0.0215 (3)
S4A	0.32373 (7)	−0.05224 (6)	0.13521 (6)	0.0214 (3)
S2A	0.19740 (6)	0.12772 (6)	0.39493 (6)	0.0201 (2)
S3A	0.17303 (6)	−0.04805 (6)	0.37917 (5)	0.0179 (2)
P3A	0.30991 (6)	−0.04396 (7)	0.38386 (6)	0.0180 (2)
S3B	−0.15431 (7)	−0.01199 (7)	0.34484 (6)	0.0264 (3)
S1B	−0.33835 (7)	−0.07169 (6)	0.62316 (6)	0.0240 (3)
S4B	−0.14056 (7)	0.00743 (8)	0.63551 (7)	0.0302 (3)
P2B	−0.37113 (7)	−0.04943 (7)	0.38790 (6)	0.0213 (3)
S2B	−0.33767 (7)	0.07335 (6)	0.36820 (6)	0.0230 (3)
P2A	0.11519 (7)	0.14624 (7)	0.29394 (6)	0.0234 (3)
P4A	0.18659 (7)	−0.04864 (7)	0.13143 (6)	0.0227 (3)
P1B	−0.36680 (7)	0.05289 (7)	0.60228 (6)	0.0218 (3)
P3B	−0.12031 (7)	0.09140 (7)	0.41599 (7)	0.0267 (3)
P4B	−0.10897 (8)	−0.09204 (8)	0.55909 (7)	0.0309 (3)
O14A	0.17013 (17)	−0.01282 (17)	0.32340 (16)	0.0199 (7)
O19A	0.32611 (19)	−0.01557 (18)	0.19049 (17)	0.0232 (8)
O1A	0.25385 (18)	0.09189 (15)	0.15375 (13)	0.0192 (6)
O4A	0.33863 (18)	0.11358 (17)	0.25542 (17)	0.0216 (8)
O9A	0.24397 (19)	0.09624 (14)	0.35513 (14)	0.0200 (6)
O13A	0.35939 (18)	−0.01317 (19)	0.42924 (17)	0.0256 (8)
O11B	−0.15789 (19)	0.06905 (18)	0.46978 (18)	0.0267 (8)
O16A	0.18266 (18)	−0.02189 (19)	0.19306 (16)	0.0231 (8)
O6A	0.16206 (18)	0.11558 (18)	0.25205 (18)	0.0243 (8)
O20A	0.3783 (2)	−0.04113 (19)	0.09404 (18)	0.0292 (9)
O1B	−0.32340 (17)	0.05402 (17)	0.54805 (16)	0.0211 (7)
O11A	0.31541 (18)	−0.01940 (17)	0.32081 (16)	0.0200 (8)
O4B	−0.29617 (19)	−0.07223 (17)	0.56942 (17)	0.0236 (8)

O17A	0.1611 (2)	−0.11590 (19)	0.1343 (2)	0.0368 (11)
O5A	0.30675 (19)	0.09454 (17)	0.05458 (16)	0.0247 (8)
O2A	0.45775 (18)	0.11663 (19)	0.22033 (18)	0.0272 (8)
O15A	0.11878 (18)	−0.03708 (18)	0.42070 (16)	0.0238 (8)
O19B	−0.18847 (19)	0.02765 (19)	0.59044 (17)	0.0280 (9)
O18A	0.1364 (2)	−0.01928 (19)	0.08576 (19)	0.0310 (9)
O6B	−0.32740 (18)	−0.05602 (17)	0.44166 (16)	0.0228 (8)
O9B	−0.29341 (18)	0.07156 (17)	0.42016 (17)	0.0238 (8)
O10A	0.1876 (2)	0.09848 (18)	0.45320 (17)	0.0278 (8)
O10B	−0.3112 (2)	0.10557 (19)	0.31667 (18)	0.0298 (9)
O8A	0.04239 (19)	0.12444 (19)	0.28378 (18)	0.0287 (9)
O3B	−0.4405 (2)	0.0679 (2)	0.5854 (2)	0.0354 (10)
O2B	−0.3559 (2)	0.10833 (18)	0.64584 (18)	0.0279 (9)
O14B	−0.19272 (17)	−0.03540 (17)	0.39616 (16)	0.0235 (8)
O16B	−0.16265 (19)	−0.07776 (19)	0.51560 (17)	0.0273 (8)
O8B	−0.3681 (2)	−0.10607 (18)	0.34444 (18)	0.0282 (9)
O3A	0.3933 (2)	0.21049 (19)	0.2281 (2)	0.0315 (9)
O12A	0.3344 (2)	−0.11157 (17)	0.38361 (17)	0.0249 (8)
O7A	0.1108 (2)	0.2149 (2)	0.2746 (2)	0.0401 (11)
O15B	−0.1914 (2)	−0.0096 (2)	0.28950 (18)	0.0378 (10)
O5B	−0.3090 (2)	−0.1023 (2)	0.67577 (18)	0.0330 (10)
N3A	0.2390 (2)	−0.03994 (18)	0.41528 (16)	0.0191 (8)
O20B	−0.1689 (2)	−0.0003 (2)	0.6944 (2)	0.0469 (13)
O7B	−0.44491 (19)	−0.0548 (2)	0.41161 (19)	0.0374 (10)
O13B	−0.0474 (2)	0.1064 (2)	0.4320 (2)	0.0428 (12)
N2A	0.1294 (2)	0.1408 (2)	0.3644 (2)	0.0273 (10)
N1B	−0.3645 (2)	−0.0068 (2)	0.6408 (2)	0.0274 (10)
N1A	0.3690 (2)	0.1333 (2)	0.1413 (2)	0.0235 (9)
O12B	−0.1481 (3)	0.1555 (2)	0.3984 (2)	0.0409 (11)
N4A	0.2575 (2)	−0.04653 (19)	0.09954 (17)	0.0237 (8)
N3B	−0.1200 (2)	0.0490 (2)	0.3569 (2)	0.0319 (11)
O18B	−0.1122 (3)	−0.1594 (2)	0.5830 (2)	0.0531 (14)
C27A	0.3299 (3)	−0.1283 (2)	0.1613 (2)	0.0217 (10)
O17B	−0.0437 (2)	−0.0923 (3)	0.5218 (3)	0.0613 (16)
C3A	0.2634 (3)	0.1951 (2)	0.1001 (2)	0.0217 (10)
N2B	−0.3626 (2)	0.0090 (2)	0.3458 (2)	0.0288 (11)
C11A	0.2363 (3)	0.1988 (2)	0.4112 (2)	0.0217 (10)
C1A	0.4692 (3)	0.0509 (3)	0.2174 (3)	0.0333 (13)
H1AA	0.5153	0.0427	0.2231	0.050*
H1AB	0.4557	0.0358	0.1784	0.050*
H1AC	0.4442	0.0309	0.2485	0.050*
C5A	0.2618 (4)	0.2887 (3)	0.0448 (3)	0.0364 (15)
H5AA	0.2803	0.3147	0.0162	0.044*
C19A	0.1694 (2)	−0.1250 (2)	0.3557 (2)	0.0216 (10)
C11B	−0.4077 (3)	0.1155 (3)	0.3909 (3)	0.0253 (11)
C10A	0.0301 (3)	0.0590 (3)	0.2793 (3)	0.0359 (14)
H10A	−0.0162	0.0520	0.2735	0.054*
H10B	0.0443	0.0394	0.3160	0.054*
H10C	0.0542	0.0426	0.2456	0.054*

C28A	0.3402 (3)	−0.1406 (2)	0.2219 (3)	0.0288 (12)
H28A	0.3433	−0.1086	0.2493	0.035*
C16B	−0.4551 (3)	0.1321 (3)	0.3486 (3)	0.0287 (12)
H16A	−0.4507	0.1205	0.3082	0.034*
C4B	−0.4504 (3)	−0.1362 (3)	0.6504 (3)	0.0290 (12)
H4BA	−0.4425	−0.1257	0.6906	0.035*
C19B	−0.0907 (3)	−0.0650 (3)	0.3314 (3)	0.0290 (12)
C18A	0.3639 (3)	0.0523 (3)	0.4349 (3)	0.0374 (15)
H18A	0.3966	0.0624	0.4646	0.056*
H18B	0.3219	0.0683	0.4472	0.056*
H18C	0.3760	0.0696	0.3965	0.056*
C8A	0.2089 (3)	0.2137 (3)	0.1332 (3)	0.0272 (11)
H8AA	0.1921	0.1891	0.1639	0.033*
C10B	−0.3090 (3)	−0.1170 (3)	0.3087 (3)	0.0313 (13)
H10D	−0.3149	−0.1530	0.2846	0.047*
H10E	−0.2720	−0.1224	0.3353	0.047*
H10F	−0.3011	−0.0826	0.2827	0.047*
C12A	0.2913 (3)	0.2162 (3)	0.3778 (3)	0.0271 (12)
H12A	0.3067	0.1921	0.3461	0.033*
C15A	0.2433 (3)	0.2885 (2)	0.4717 (3)	0.0349 (13)
H15A	0.2278	0.3129	0.5031	0.042*
C6A	0.2065 (4)	0.3067 (3)	0.0757 (3)	0.0412 (16)
H6AA	0.1868	0.3440	0.0670	0.049*
C22A	0.1722 (3)	−0.2462 (3)	0.3219 (3)	0.0363 (14)
H22A	0.1734	−0.2871	0.3106	0.044*
N4B	−0.1010 (3)	−0.0482 (3)	0.6160 (3)	0.0413 (14)
C14B	−0.5162 (3)	0.1834 (3)	0.4265 (3)	0.0334 (13)
H14A	−0.5531	0.2058	0.4382	0.040*
C4A	0.2902 (3)	0.2331 (3)	0.0553 (3)	0.0329 (13)
H4AA	0.3268	0.2207	0.0331	0.040*
C12B	−0.4146 (3)	0.1326 (3)	0.4511 (3)	0.0325 (14)
H12B	−0.3832	0.1209	0.4796	0.039*
C5B	−0.5047 (3)	−0.1709 (3)	0.6350 (3)	0.0383 (15)
H5BA	−0.5330	−0.1844	0.6653	0.046*
C8B	−0.4208 (3)	−0.1306 (3)	0.5448 (3)	0.0296 (12)
H8BA	−0.3933	−0.1158	0.5144	0.036*
C16A	0.2110 (3)	0.2350 (3)	0.4578 (3)	0.0313 (13)
H16B	0.1733	0.2233	0.4788	0.038*
C13B	−0.4696 (3)	0.1681 (3)	0.4689 (3)	0.0377 (15)
H13A	−0.4741	0.1809	0.5089	0.045*
C26A	0.1342 (3)	0.0468 (3)	0.0749 (3)	0.0320 (13)
H26A	0.1004	0.0558	0.0457	0.048*
H26B	0.1761	0.0603	0.0597	0.048*
H26C	0.1245	0.0675	0.1122	0.048*
C23A	0.1806 (3)	−0.2011 (3)	0.2791 (3)	0.0362 (15)
H23A	0.1877	−0.2119	0.2388	0.043*
C14A	0.2988 (3)	0.3065 (3)	0.4392 (3)	0.0357 (14)
H14B	0.3198	0.3430	0.4486	0.043*
C3B	−0.4077 (3)	−0.1171 (2)	0.6048 (3)	0.0260 (11)

C15B	−0.5092 (3)	0.1662 (3)	0.3672 (3)	0.0361 (14)
H15B	−0.5410	0.1775	0.3390	0.043*
C20A	0.1611 (3)	−0.1704 (3)	0.3991 (3)	0.0350 (14)
H20A	0.1550	−0.1601	0.4396	0.042*
C29B	−0.0171 (3)	0.1440 (3)	0.5958 (3)	0.0423 (16)
H29A	−0.0028	0.1646	0.5613	0.051*
C24A	0.1787 (3)	−0.1395 (3)	0.2952 (3)	0.0293 (12)
H24A	0.1836	−0.1091	0.2661	0.035*
C28B	−0.0614 (3)	0.0964 (3)	0.5904 (3)	0.0345 (14)
H28B	−0.0765	0.0841	0.5525	0.041*
C24B	−0.0672 (3)	−0.0996 (3)	0.3792 (3)	0.0359 (14)
H24B	−0.0847	−0.0948	0.4179	0.043*
C20B	−0.0647 (3)	−0.0707 (3)	0.2736 (3)	0.0397 (16)
H20B	−0.0807	−0.0470	0.2418	0.048*
C31A	0.3280 (4)	−0.2347 (3)	0.1408 (4)	0.049 (2)
H31A	0.3238	−0.2665	0.1132	0.059*
C13A	0.3227 (3)	0.2704 (3)	0.3930 (3)	0.0364 (15)
H13B	0.3602	0.2824	0.3719	0.044*
C27B	−0.0828 (3)	0.0675 (3)	0.6423 (3)	0.0288 (12)
C7B	−0.4749 (3)	−0.1661 (3)	0.5300 (3)	0.0377 (15)
H7BA	−0.4827	−0.1767	0.4898	0.045*
C29A	0.3460 (4)	−0.1999 (3)	0.2423 (3)	0.0385 (15)
H29B	0.3547	−0.2079	0.2829	0.046*
C31B	−0.0147 (4)	0.1321 (3)	0.7028 (4)	0.0465 (19)
H31B	0.0012	0.1442	0.7405	0.056*
C23B	−0.0174 (3)	−0.1412 (3)	0.3685 (4)	0.0488 (19)
H23B	−0.0013	−0.1651	0.4001	0.059*
C6B	−0.5177 (3)	−0.1861 (3)	0.5756 (3)	0.0410 (16)
H6BA	−0.5546	−0.2094	0.5659	0.049*
C21B	−0.0157 (4)	−0.1112 (4)	0.2642 (4)	0.054 (2)
H21A	0.0022	−0.1150	0.2255	0.064*
C1B	−0.2946 (4)	0.1154 (3)	0.6781 (3)	0.0393 (16)
H1BA	−0.2964	0.1516	0.7025	0.059*
H1BB	−0.2590	0.1188	0.6496	0.059*
H1BC	−0.2875	0.0806	0.7036	0.059*
C17A	0.3338 (4)	−0.1480 (3)	0.4382 (3)	0.0423 (16)
H17A	0.3505	−0.1880	0.4295	0.063*
H17B	0.2894	−0.1511	0.4531	0.063*
H17C	0.3610	−0.1289	0.4684	0.063*
C21A	0.1621 (4)	−0.2304 (3)	0.3814 (3)	0.0409 (16)
H21B	0.1557	−0.2609	0.4102	0.049*
C30B	0.0062 (4)	0.1613 (3)	0.6519 (4)	0.0467 (18)
H30A	0.0364	0.1931	0.6549	0.056*
C32B	−0.0603 (3)	0.0837 (3)	0.6986 (3)	0.0359 (14)
H32A	−0.0747	0.0633	0.7331	0.043*
C30A	0.3386 (3)	−0.2479 (3)	0.2009 (3)	0.0406 (16)
H30B	0.3408	−0.2882	0.2139	0.049*
C32A	0.3235 (4)	−0.1758 (3)	0.1210 (3)	0.0436 (18)
H32B	0.3162	−0.1677	0.0802	0.052*

C7A	0.1799 (3)	0.2690 (3)	0.1201 (3)	0.0377 (15)
H7AA	0.1423	0.2812	0.1411	0.045*
C18B	0.0010 (4)	0.0596 (4)	0.4399 (4)	0.057 (2)
H18D	0.0426	0.0778	0.4501	0.085*
H18E	0.0053	0.0368	0.4030	0.085*
H18F	−0.0125	0.0328	0.4720	0.085*
C2A	0.4342 (4)	0.2487 (4)	0.1891 (4)	0.056 (2)
H2AA	0.4348	0.2896	0.2047	0.084*
H2AB	0.4164	0.2488	0.1488	0.084*
H2AC	0.4783	0.2328	0.1883	0.084*
C25A	0.1546 (4)	−0.1524 (3)	0.0805 (4)	0.054 (2)
H25A	0.1384	−0.1921	0.0911	0.081*
H25B	0.1969	−0.1563	0.0612	0.081*
H25C	0.1243	−0.1332	0.0531	0.081*
C22B	0.0087 (4)	−0.1475 (4)	0.3104 (4)	0.059 (3)
H22B	0.0421	−0.1755	0.3028	0.070*
C25B	0.0208 (4)	−0.0957 (5)	0.5471 (4)	0.074 (3)
H25D	0.0529	−0.0950	0.5151	0.112*
H25E	0.0252	−0.1329	0.5697	0.112*
H25F	0.0277	−0.0615	0.5735	0.112*
C17B	−0.1336 (6)	0.1828 (4)	0.3428 (4)	0.077 (3)
H17D	−0.1551	0.2218	0.3405	0.116*
H17E	−0.1489	0.1572	0.3105	0.116*
H17F	−0.0867	0.1883	0.3393	0.116*
C2B	−0.4780 (4)	0.0260 (4)	0.5525 (4)	0.056 (2)
H2BA	−0.5215	0.0420	0.5463	0.084*
H2BB	−0.4808	−0.0117	0.5746	0.084*
H2BC	−0.4574	0.0187	0.5140	0.084*
C9B	−0.4991 (3)	−0.0479 (4)	0.3695 (3)	0.059 (2)
H9BA	−0.5401	−0.0526	0.3907	0.088*
H9BB	−0.4958	−0.0785	0.3385	0.088*
H9BC	−0.4972	−0.0082	0.3513	0.088*
C9A	0.0787 (6)	0.2570 (4)	0.3137 (5)	0.081 (3)
H9AA	0.0798	0.2970	0.2959	0.122*
H9AB	0.1009	0.2578	0.3522	0.122*
H9AC	0.0337	0.2447	0.3195	0.122*
C26B	−0.1582 (6)	−0.1736 (4)	0.6266 (5)	0.082 (3)
H26D	−0.1546	−0.2160	0.6370	0.124*
H26E	−0.2017	−0.1655	0.6111	0.124*
H26F	−0.1506	−0.1491	0.6620	0.124*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1A	0.0243 (9)	0.0283 (12)	0.0158 (9)	−0.0001 (9)	−0.0007 (7)	−0.0010 (8)
Na1B	0.0395 (14)	0.0298 (11)	0.0232 (10)	0.0019 (11)	0.0037 (11)	0.0036 (8)
Nd1A	0.01981 (12)	0.01566 (10)	0.01529 (10)	0.00057 (13)	−0.00040 (10)	0.00040 (8)
Nd1B	0.01793 (11)	0.02086 (12)	0.01791 (11)	0.00030 (13)	−0.00023 (9)	0.00121 (8)

S1A	0.0194 (6)	0.0183 (6)	0.0194 (6)	−0.0004 (4)	0.0011 (4)	0.0012 (4)
P1A	0.0164 (6)	0.0216 (7)	0.0266 (7)	−0.0012 (5)	−0.0009 (5)	−0.0012 (5)
S4A	0.0295 (7)	0.0220 (7)	0.0127 (6)	0.0062 (5)	−0.0012 (5)	−0.0016 (5)
S2A	0.0222 (6)	0.0169 (6)	0.0212 (6)	−0.0008 (5)	0.0022 (5)	−0.0009 (4)
S3A	0.0184 (5)	0.0189 (6)	0.0162 (6)	−0.0003 (5)	0.0009 (4)	0.0017 (4)
P3A	0.0190 (6)	0.0192 (7)	0.0158 (6)	−0.0003 (5)	−0.0039 (4)	0.0019 (5)
S3B	0.0278 (7)	0.0296 (8)	0.0217 (6)	0.0046 (6)	0.0070 (5)	0.0010 (5)
S1B	0.0250 (7)	0.0231 (7)	0.0240 (6)	−0.0016 (5)	0.0005 (5)	0.0030 (5)
S4B	0.0313 (7)	0.0356 (9)	0.0237 (7)	−0.0061 (6)	−0.0101 (5)	0.0024 (6)
P2B	0.0193 (6)	0.0244 (7)	0.0201 (6)	0.0005 (5)	−0.0003 (5)	−0.0015 (5)
S2B	0.0232 (6)	0.0246 (7)	0.0211 (6)	0.0044 (5)	0.0011 (5)	0.0032 (5)
P2A	0.0208 (7)	0.0223 (7)	0.0271 (7)	0.0023 (5)	0.0009 (5)	0.0013 (5)
P4A	0.0296 (7)	0.0180 (7)	0.0204 (7)	−0.0020 (6)	−0.0095 (5)	−0.0009 (5)
P1B	0.0231 (6)	0.0227 (7)	0.0197 (6)	−0.0007 (5)	0.0014 (5)	−0.0008 (5)
P3B	0.0265 (7)	0.0220 (7)	0.0317 (8)	−0.0015 (6)	0.0071 (6)	0.0012 (6)
P4B	0.0303 (8)	0.0278 (8)	0.0345 (8)	0.0043 (6)	−0.0126 (6)	0.0018 (6)
O14A	0.0217 (17)	0.0210 (19)	0.0170 (17)	−0.0005 (14)	−0.0011 (13)	0.0002 (13)
O19A	0.032 (2)	0.020 (2)	0.0180 (18)	0.0054 (15)	−0.0031 (15)	−0.0028 (14)
O1A	0.0192 (16)	0.0197 (15)	0.0186 (14)	−0.0012 (15)	0.0003 (14)	0.0026 (11)
O4A	0.0204 (18)	0.024 (2)	0.0200 (19)	−0.0017 (15)	0.0007 (14)	−0.0025 (15)
O9A	0.0246 (18)	0.0167 (15)	0.0188 (15)	0.0005 (15)	0.0009 (15)	−0.0023 (11)
O13A	0.0244 (19)	0.031 (2)	0.0210 (18)	−0.0012 (16)	−0.0009 (14)	0.0009 (15)
O11B	0.0185 (18)	0.028 (2)	0.033 (2)	−0.0061 (15)	0.0044 (16)	−0.0012 (16)
O16A	0.0248 (19)	0.029 (2)	0.0149 (18)	−0.0106 (15)	−0.0038 (14)	0.0026 (14)
O6A	0.0214 (19)	0.029 (2)	0.022 (2)	0.0060 (16)	0.0022 (15)	−0.0015 (16)
O20A	0.035 (2)	0.029 (2)	0.023 (2)	0.0047 (18)	−0.0038 (16)	−0.0033 (17)
O1B	0.0202 (18)	0.022 (2)	0.0208 (17)	0.0022 (14)	0.0038 (13)	0.0037 (14)
O11A	0.0247 (19)	0.0212 (19)	0.0140 (17)	0.0044 (14)	−0.0011 (13)	−0.0022 (13)
O4B	0.0250 (19)	0.019 (2)	0.0265 (19)	−0.0013 (15)	0.0000 (15)	0.0005 (14)
O17A	0.047 (3)	0.025 (2)	0.039 (2)	−0.0103 (19)	−0.024 (2)	0.0026 (18)
O5A	0.035 (2)	0.0194 (19)	0.0201 (18)	0.0003 (16)	0.0030 (15)	0.0005 (14)
O2A	0.0197 (19)	0.033 (2)	0.028 (2)	0.0021 (16)	−0.0037 (15)	−0.0018 (16)
O15A	0.0197 (18)	0.032 (2)	0.0196 (18)	−0.0009 (16)	−0.0003 (14)	0.0020 (15)
O19B	0.027 (2)	0.033 (2)	0.024 (2)	−0.0045 (16)	−0.0024 (15)	−0.0064 (16)
O18A	0.031 (2)	0.030 (2)	0.032 (2)	−0.0028 (17)	−0.0101 (17)	−0.0022 (17)
O6B	0.0240 (19)	0.024 (2)	0.0203 (18)	−0.0038 (15)	−0.0058 (14)	0.0044 (14)
O9B	0.0230 (19)	0.027 (2)	0.0218 (18)	0.0053 (15)	−0.0007 (14)	0.0051 (14)
O10A	0.036 (2)	0.023 (2)	0.025 (2)	−0.0008 (16)	0.0050 (16)	0.0020 (15)
O10B	0.033 (2)	0.031 (2)	0.026 (2)	0.0048 (17)	0.0066 (17)	0.0028 (16)
O8A	0.023 (2)	0.030 (2)	0.033 (2)	0.0032 (16)	−0.0007 (16)	−0.0072 (17)
O3B	0.021 (2)	0.051 (3)	0.034 (2)	0.0014 (19)	−0.0024 (17)	0.001 (2)
O2B	0.035 (2)	0.021 (2)	0.028 (2)	0.0017 (16)	−0.0006 (17)	−0.0056 (15)
O14B	0.0210 (18)	0.027 (2)	0.0228 (18)	−0.0009 (15)	0.0044 (14)	0.0024 (14)
O16B	0.0220 (19)	0.036 (2)	0.0239 (19)	0.0060 (16)	−0.0058 (15)	−0.0004 (16)
O8B	0.029 (2)	0.030 (2)	0.026 (2)	−0.0052 (17)	0.0045 (16)	−0.0059 (16)
O3A	0.031 (2)	0.024 (2)	0.040 (2)	−0.0060 (17)	0.0005 (18)	−0.0051 (17)
O12A	0.030 (2)	0.019 (2)	0.026 (2)	0.0063 (15)	−0.0027 (16)	0.0041 (14)
O7A	0.049 (3)	0.025 (2)	0.045 (3)	0.014 (2)	0.001 (2)	0.0001 (19)
O15B	0.040 (2)	0.047 (3)	0.026 (2)	0.014 (2)	−0.0010 (17)	0.0037 (19)

O5B	0.041 (3)	0.033 (2)	0.024 (2)	−0.0029 (19)	−0.0086 (18)	0.0045 (16)
N3A	0.023 (2)	0.022 (2)	0.0128 (16)	−0.0041 (17)	−0.0023 (14)	0.0004 (13)
O20B	0.049 (3)	0.060 (3)	0.032 (2)	−0.023 (3)	−0.007 (2)	0.005 (2)
O7B	0.0184 (19)	0.065 (3)	0.028 (2)	0.001 (2)	0.0006 (16)	0.001 (2)
O13B	0.031 (2)	0.053 (3)	0.044 (3)	−0.009 (2)	0.003 (2)	0.003 (2)
N2A	0.017 (2)	0.029 (3)	0.036 (3)	0.0019 (18)	0.0028 (18)	−0.007 (2)
N1B	0.036 (3)	0.027 (3)	0.019 (2)	0.001 (2)	0.0051 (18)	−0.0023 (18)
N1A	0.022 (2)	0.023 (2)	0.026 (2)	0.0012 (17)	0.0002 (17)	0.0048 (17)
O12B	0.060 (3)	0.032 (3)	0.031 (2)	0.006 (2)	−0.001 (2)	0.0081 (18)
N4A	0.030 (2)	0.025 (2)	0.0164 (17)	0.005 (2)	−0.0042 (17)	−0.0014 (14)
N3B	0.031 (3)	0.027 (3)	0.038 (3)	−0.001 (2)	0.019 (2)	0.004 (2)
O18B	0.092 (4)	0.035 (3)	0.032 (3)	0.014 (3)	−0.015 (3)	0.001 (2)
C27A	0.023 (3)	0.018 (3)	0.025 (3)	0.0087 (19)	−0.0057 (19)	−0.0061 (19)
O17B	0.030 (3)	0.098 (5)	0.055 (3)	0.010 (3)	−0.010 (2)	0.007 (3)
C3A	0.026 (3)	0.013 (2)	0.027 (2)	0.0000 (18)	−0.005 (2)	−0.0001 (16)
N2B	0.040 (3)	0.030 (3)	0.016 (2)	0.001 (2)	−0.0113 (18)	0.0001 (18)
C11A	0.024 (3)	0.016 (2)	0.025 (2)	0.0031 (19)	−0.0043 (19)	0.0003 (17)
C1A	0.026 (3)	0.037 (4)	0.037 (3)	0.010 (2)	−0.010 (2)	0.003 (3)
C5A	0.061 (4)	0.019 (3)	0.030 (3)	0.002 (3)	0.005 (3)	0.010 (2)
C19A	0.017 (2)	0.019 (3)	0.028 (3)	−0.0076 (19)	−0.0051 (19)	0.0024 (19)
C11B	0.021 (3)	0.026 (3)	0.030 (3)	0.005 (2)	0.001 (2)	0.001 (2)
C10A	0.032 (3)	0.031 (3)	0.045 (4)	−0.005 (3)	0.001 (3)	0.001 (3)
C28A	0.042 (3)	0.017 (3)	0.027 (3)	0.005 (2)	0.014 (2)	0.001 (2)
C16B	0.034 (3)	0.023 (3)	0.029 (3)	0.003 (2)	−0.006 (2)	0.003 (2)
C4B	0.028 (3)	0.029 (3)	0.030 (3)	0.002 (2)	0.003 (2)	−0.001 (2)
C19B	0.015 (2)	0.032 (3)	0.040 (3)	0.000 (2)	−0.003 (2)	−0.009 (2)
C18A	0.040 (4)	0.035 (4)	0.038 (3)	−0.006 (3)	−0.013 (3)	0.001 (3)
C8A	0.025 (3)	0.025 (3)	0.032 (3)	0.003 (2)	0.002 (2)	0.005 (2)
C10B	0.029 (3)	0.041 (4)	0.024 (3)	0.005 (3)	0.009 (2)	−0.004 (2)
C12A	0.026 (3)	0.022 (3)	0.033 (3)	0.005 (2)	−0.002 (2)	−0.005 (2)
C15A	0.046 (4)	0.022 (3)	0.036 (3)	0.003 (3)	0.001 (3)	−0.011 (2)
C6A	0.058 (5)	0.022 (3)	0.043 (4)	0.005 (3)	−0.014 (3)	0.001 (3)
C22A	0.045 (4)	0.013 (3)	0.051 (4)	0.000 (2)	0.002 (3)	−0.005 (2)
N4B	0.042 (3)	0.028 (3)	0.054 (4)	0.003 (2)	−0.025 (3)	0.000 (2)
C14B	0.026 (3)	0.035 (4)	0.038 (3)	0.007 (2)	0.003 (2)	0.003 (3)
C4A	0.046 (4)	0.028 (3)	0.024 (3)	−0.006 (3)	0.007 (3)	0.004 (2)
C12B	0.034 (3)	0.037 (4)	0.026 (3)	0.016 (3)	−0.004 (2)	0.004 (2)
C5B	0.035 (3)	0.037 (4)	0.043 (4)	−0.005 (3)	0.011 (3)	0.007 (3)
C8B	0.030 (3)	0.029 (3)	0.030 (3)	−0.010 (2)	−0.003 (2)	0.008 (2)
C16A	0.041 (3)	0.025 (3)	0.027 (3)	−0.006 (2)	0.008 (2)	0.000 (2)
C13B	0.035 (3)	0.044 (4)	0.034 (3)	0.015 (3)	0.002 (3)	0.000 (3)
C26A	0.026 (3)	0.033 (3)	0.037 (3)	0.004 (2)	−0.006 (2)	0.003 (3)
C23A	0.047 (4)	0.022 (3)	0.039 (4)	−0.002 (3)	0.011 (3)	−0.009 (2)
C14A	0.044 (4)	0.023 (3)	0.040 (4)	−0.014 (3)	−0.002 (3)	−0.004 (2)
C3B	0.028 (3)	0.016 (3)	0.033 (3)	−0.001 (2)	0.000 (2)	0.002 (2)
C15B	0.030 (3)	0.036 (4)	0.042 (4)	0.008 (3)	−0.009 (3)	0.001 (3)
C20A	0.053 (4)	0.024 (3)	0.028 (3)	−0.006 (3)	−0.005 (3)	0.001 (2)
C29B	0.030 (3)	0.041 (4)	0.056 (4)	−0.004 (3)	−0.009 (3)	0.006 (3)
C24A	0.041 (3)	0.024 (3)	0.023 (3)	−0.009 (2)	0.010 (2)	−0.001 (2)

C28B	0.024 (3)	0.045 (4)	0.035 (3)	0.001 (3)	−0.011 (2)	0.008 (3)
C24B	0.019 (3)	0.033 (4)	0.056 (4)	−0.002 (2)	0.006 (3)	0.004 (3)
C20B	0.038 (4)	0.047 (4)	0.035 (3)	−0.005 (3)	0.005 (3)	−0.023 (3)
C31A	0.053 (4)	0.017 (3)	0.077 (6)	0.006 (3)	−0.023 (4)	−0.014 (3)
C13A	0.026 (3)	0.027 (3)	0.057 (4)	−0.008 (2)	0.009 (3)	−0.010 (3)
C27B	0.022 (3)	0.029 (3)	0.035 (3)	0.004 (2)	−0.003 (2)	−0.008 (2)
C7B	0.031 (3)	0.050 (4)	0.032 (3)	−0.009 (3)	0.001 (3)	0.003 (3)
C29A	0.052 (4)	0.030 (3)	0.034 (3)	0.007 (3)	0.007 (3)	0.012 (2)
C31B	0.044 (4)	0.042 (4)	0.053 (5)	0.006 (3)	−0.011 (3)	−0.023 (3)
C23B	0.027 (3)	0.035 (4)	0.084 (6)	−0.004 (3)	−0.015 (4)	0.008 (4)
C6B	0.029 (3)	0.040 (4)	0.053 (4)	−0.011 (3)	−0.002 (3)	0.001 (3)
C21B	0.032 (4)	0.066 (6)	0.063 (5)	−0.003 (3)	0.005 (3)	−0.034 (4)
C1B	0.057 (4)	0.022 (3)	0.039 (4)	−0.005 (3)	−0.009 (3)	−0.001 (2)
C17A	0.054 (4)	0.034 (4)	0.038 (4)	0.009 (3)	0.001 (3)	0.010 (3)
C21A	0.053 (4)	0.018 (3)	0.052 (4)	−0.007 (3)	−0.005 (3)	0.011 (3)
C30B	0.035 (4)	0.040 (4)	0.066 (5)	−0.003 (3)	−0.010 (3)	−0.005 (3)
C32B	0.026 (3)	0.043 (4)	0.038 (3)	0.006 (3)	−0.004 (2)	−0.021 (3)
C30A	0.040 (4)	0.018 (3)	0.064 (5)	−0.002 (3)	0.004 (3)	0.002 (3)
C32A	0.062 (5)	0.028 (3)	0.041 (4)	0.013 (3)	−0.019 (3)	−0.018 (3)
C7A	0.033 (3)	0.030 (4)	0.050 (4)	0.011 (3)	0.007 (3)	0.004 (3)
C18B	0.040 (4)	0.079 (6)	0.051 (5)	0.012 (4)	0.004 (3)	0.022 (4)
C2A	0.073 (6)	0.037 (4)	0.057 (5)	−0.021 (4)	0.007 (4)	0.000 (3)
C25A	0.076 (6)	0.033 (4)	0.053 (5)	−0.004 (4)	−0.027 (4)	−0.002 (3)
C22B	0.028 (4)	0.048 (5)	0.100 (7)	0.006 (3)	−0.004 (4)	−0.040 (5)
C25B	0.039 (5)	0.131 (10)	0.053 (5)	−0.008 (5)	−0.015 (4)	0.008 (6)
C17B	0.147 (10)	0.043 (5)	0.040 (5)	0.019 (6)	0.002 (5)	0.011 (4)
C2B	0.031 (4)	0.050 (5)	0.087 (6)	−0.004 (3)	−0.007 (4)	0.003 (4)
C9B	0.024 (3)	0.103 (7)	0.049 (5)	0.005 (4)	−0.004 (3)	−0.009 (5)
C9A	0.120 (10)	0.028 (5)	0.096 (8)	0.010 (5)	−0.012 (7)	−0.006 (4)
C26B	0.119 (9)	0.044 (6)	0.084 (8)	−0.013 (6)	0.017 (7)	0.006 (5)

Geometric parameters (Å, °)

Na1A—O10A^{i}	2.385 (4)	C19A—C24A	1.385 (8)
Na1A—O20A	2.411 (4)	C19A—C20A	1.390 (8)
Na1A—O5A	2.421 (4)	C11B—C12B	1.388 (8)
Na1A—O15A^{i}	2.433 (4)	C11B—C16B	1.388 (7)
Na1A—N3A^{i}	2.526 (4)	C10A—H10A	0.9600
Na1A—N4A	2.589 (5)	C10A—H10B	0.9600
Na1B—O15B	2.186 (5)	C10A—H10C	0.9600
Na1B—O20B^{ii}	2.211 (5)	C28A—C29A	1.379 (8)
Na1B—O5B^{ii}	2.242 (5)	C28A—H28A	0.9300
Na1B—O10B	2.261 (4)	C16B—C15B	1.389 (8)
Nd1A—O6A	2.362 (4)	C16B—H16A	0.9300
Nd1A—O4A	2.375 (4)	C4B—C5B	1.381 (9)
Nd1A—O16A	2.406 (4)	C4B—C3B	1.391 (8)
Nd1A—O11A	2.409 (4)	C4B—H4BA	0.9300
Nd1A—O9A	2.478 (3)	C19B—C24B	1.383 (9)

Nd1A—O1A	2.485 (3)	C19B—C20B	1.386 (8)
Nd1A—O19A	2.492 (4)	C18A—H18A	0.9600
Nd1A—O14A	2.515 (4)	C18A—H18B	0.9600
Nd1B—O1B	2.368 (4)	C18A—H18C	0.9600
Nd1B—O16B	2.372 (4)	C8A—C7A	1.379 (8)
Nd1B—O11B	2.380 (4)	C8A—H8AA	0.9300
Nd1B—O6B	2.382 (4)	C10B—H10D	0.9600
Nd1B—O19B	2.484 (4)	C10B—H10E	0.9600
Nd1B—O14B	2.493 (4)	C10B—H10F	0.9600
Nd1B—O4B	2.513 (4)	C12A—C13A	1.388 (8)
Nd1B—O9B	2.509 (4)	C12A—H12A	0.9300
S1A—O5A	1.442 (4)	C15A—C16A	1.378 (8)
S1A—O1A	1.465 (3)	C15A—C14A	1.391 (9)
S1A—N1A	1.547 (5)	C15A—H15A	0.9300
S1A—C3A	1.767 (5)	C6A—C7A	1.391 (9)
P1A—O4A	1.482 (4)	C6A—H6AA	0.9300
P1A—O2A	1.570 (4)	C22A—C21A	1.372 (10)
P1A—O3A	1.576 (4)	C22A—C23A	1.378 (9)
P1A—N1A	1.595 (5)	C22A—H22A	0.9300
S4A—O20A	1.452 (4)	C14B—C15B	1.369 (9)
S4A—O19A	1.461 (4)	C14B—C13B	1.372 (9)
S4A—N4A	1.561 (4)	C14B—H14A	0.9300
S4A—C27A	1.769 (5)	C4A—H4AA	0.9300
S2A—O10A	1.450 (4)	C12B—C13B	1.416 (8)
S2A—O9A	1.462 (4)	C12B—H12B	0.9300
S2A—N2A	1.561 (5)	C5B—C6B	1.376 (10)
S2A—C11A	1.783 (5)	C5B—H5BA	0.9300
S3A—O15A	1.452 (4)	C8B—C3B	1.382 (8)
S3A—O14A	1.453 (4)	C8B—C7B	1.384 (8)
S3A—N3A	1.566 (4)	C8B—H8BA	0.9300
S3A—C19A	1.766 (5)	C16A—H16B	0.9300
S3A—Na1A^{iii}	3.030 (2)	C13B—H13A	0.9300
P3A—O11A	1.495 (4)	C26A—H26A	0.9600
P3A—O12A	1.563 (4)	C26A—H26B	0.9600
P3A—O13A	1.570 (4)	C26A—H26C	0.9600
P3A—N3A	1.599 (4)	C23A—C24A	1.397 (8)
S3B—O15B	1.435 (4)	C23A—H23A	0.9300
S3B—O14B	1.467 (4)	C14A—C13A	1.378 (9)
S3B—N3B	1.530 (5)	C14A—H14B	0.9300
S3B—C19B	1.761 (6)	C15B—H15B	0.9300
S1B—O4B	1.462 (4)	C20A—C21A	1.373 (8)
S1B—O5B	1.467 (4)	C20A—H20A	0.9300
S1B—N1B	1.567 (5)	C29B—C30B	1.376 (10)
S1B—C3B	1.770 (6)	C29B—C28B	1.383 (9)
S1B—Na1B^{iv}	3.287 (2)	C29B—H29A	0.9300
S4B—O20B	1.431 (5)	C24A—H24A	0.9300
S4B—O19B	1.459 (4)	C28B—C27B	1.379 (9)
S4B—N4B	1.521 (6)	C28B—H28B	0.9300

S4B—C27B	1.769 (6)	C24B—C23B	1.382 (9)
P2B—O6B	1.488 (4)	C24B—H24B	0.9300
P2B—O8B	1.570 (4)	C20B—C21B	1.348 (10)
P2B—O7B	1.589 (4)	C20B—H20B	0.9300
P2B—N2B	1.591 (5)	C31A—C32A	1.367 (9)
S2B—O10B	1.442 (4)	C31A—C30A	1.372 (11)
S2B—O9B	1.456 (4)	C31A—H31A	0.9300
S2B—N2B	1.578 (5)	C13A—H13B	0.9300
S2B—C11B	1.767 (5)	C27B—C32B	1.369 (8)
P2A—O6A	1.486 (4)	C7B—C6B	1.399 (9)
P2A—O7A	1.565 (5)	C7B—H7BA	0.9300
P2A—O8A	1.567 (4)	C29A—C30A	1.400 (9)
P2A—N2A	1.584 (5)	C29A—H29B	0.9300
P4A—O16A	1.483 (4)	C31B—C30B	1.361 (11)
P4A—O17A	1.564 (4)	C31B—C32B	1.411 (10)
P4A—O18A	1.569 (4)	C31B—H31B	0.9300
P4A—N4A	1.601 (5)	C23B—C22B	1.394 (12)
P1B—O1B	1.485 (4)	C23B—H23B	0.9300
P1B—N1B	1.560 (5)	C6B—H6BA	0.9300
P1B—O2B	1.565 (4)	C21B—C22B	1.384 (12)
P1B—O3B	1.574 (4)	C21B—H21A	0.9300
P3B—O11B	1.493 (4)	C1B—H1BA	0.9600
P3B—O13B	1.555 (5)	C1B—H1BB	0.9600
P3B—O12B	1.562 (5)	C1B—H1BC	0.9600
P3B—N3B	1.600 (5)	C17A—H17A	0.9600
P4B—O16B	1.484 (4)	C17A—H17B	0.9600
P4B—O17B	1.559 (6)	C17A—H17C	0.9600
P4B—O18B	1.570 (5)	C21A—H21B	0.9300
P4B—N4B	1.589 (6)	C30B—H30A	0.9300
O13A—C18A	1.442 (8)	C32B—H32A	0.9300
O17A—C25A	1.438 (8)	C30A—H30B	0.9300
O2A—C1A	1.461 (7)	C32A—H32B	0.9300
O15A—Na1A^{iii}	2.433 (4)	C7A—H7AA	0.9300
O18A—C26A	1.469 (7)	C18B—H18D	0.9600
O10A—Na1A^{iii}	2.385 (4)	C18B—H18E	0.9600
O8A—C10A	1.458 (7)	C18B—H18F	0.9600
O3B—C2B	1.396 (8)	C2A—H2AA	0.9600
O2B—C1B	1.440 (8)	C2A—H2AB	0.9600
O8B—C10B	1.454 (6)	C2A—H2AC	0.9600
O3A—C2A	1.457 (8)	C25A—H25A	0.9600
O12A—C17A	1.445 (7)	C25A—H25B	0.9600
O7A—C9A	1.422 (10)	C25A—H25C	0.9600
O5B—Na1B^{iv}	2.242 (5)	C22B—H22B	0.9300
N3A—Na1A^{iii}	2.526 (4)	C25B—H25D	0.9600
O20B—Na1B^{iv}	2.211 (5)	C25B—H25E	0.9600
O7B—C9B	1.446 (8)	C25B—H25F	0.9600
O13B—C18B	1.429 (9)	C17B—H17D	0.9600
O12B—C17B	1.396 (9)	C17B—H17E	0.9600

O18B—C26B	1.375 (11)	C17B—H17F	0.9600
C27A—C32A	1.373 (7)	C2B—H2BA	0.9600
C27A—C28A	1.379 (8)	C2B—H2BB	0.9600
O17B—C25B	1.422 (9)	C2B—H2BC	0.9600
C3A—C8A	1.385 (7)	C9B—H9BA	0.9600
C3A—C4A	1.403 (7)	C9B—H9BB	0.9600
C11A—C12A	1.390 (8)	C9B—H9BC	0.9600
C11A—C16A	1.395 (7)	C9A—H9AA	0.9600
C1A—H1AA	0.9600	C9A—H9AB	0.9600
C1A—H1AB	0.9600	C9A—H9AC	0.9600
C1A—H1AC	0.9600	C26B—H26D	0.9600
C5A—C4A	1.367 (8)	C26B—H26E	0.9600
C5A—C6A	1.369 (10)	C26B—H26F	0.9600
C5A—H5AA	0.9300		
O10A^{i}—Na1A—O20A	97.60 (16)	C28A—C27A—S4A	120.7 (4)
O10A^{i}—Na1A—O5A	169.50 (17)	C25B—O17B—P4B	125.0 (5)
O20A—Na1A—O5A	90.13 (15)	C8A—C3A—C4A	120.4 (5)
O10A^{i}—Na1A—O15A^{i}	88.43 (15)	C8A—C3A—S1A	120.8 (4)
O20A—Na1A—O15A^{i}	119.79 (16)	C4A—C3A—S1A	118.8 (4)
O5A—Na1A—O15A^{i}	93.91 (15)	S2B—N2B—P2B	124.9 (3)
O10A^{i}—Na1A—N3A^{i}	84.84 (14)	C12A—C11A—C16A	122.0 (5)
O20A—Na1A—N3A^{i}	177.28 (17)	C12A—C11A—S2A	119.2 (4)
O5A—Na1A—N3A^{i}	87.60 (14)	C16A—C11A—S2A	118.8 (4)
O15A^{i}—Na1A—N3A^{i}	58.92 (13)	O2A—C1A—H1AA	109.5
O10A^{i}—Na1A—N4A	92.63 (15)	O2A—C1A—H1AB	109.5
O20A—Na1A—N4A	58.69 (15)	H1AA—C1A—H1AB	109.5
O5A—Na1A—N4A	85.30 (14)	O2A—C1A—H1AC	109.5
O15A^{i}—Na1A—N4A	178.26 (16)	H1AA—C1A—H1AC	109.5
N3A^{i}—Na1A—N4A	122.54 (16)	H1AB—C1A—H1AC	109.5
O15B—Na1B—O20B^{ii}	106.9 (2)	C4A—C5A—C6A	121.2 (6)
O15B—Na1B—O5B^{ii}	104.8 (2)	C4A—C5A—H5AA	119.4
O20B^{ii}—Na1B—O5B^{ii}	109.55 (17)	C6A—C5A—H5AA	119.4
O15B—Na1B—O10B	106.11 (17)	C24A—C19A—C20A	121.1 (5)
O20B^{ii}—Na1B—O10B	105.98 (19)	C24A—C19A—S3A	119.8 (4)
O5B^{ii}—Na1B—O10B	122.60 (19)	C20A—C19A—S3A	119.1 (4)
O6A—Nd1A—O4A	98.22 (12)	C12B—C11B—C16B	120.3 (5)
O6A—Nd1A—O16A	87.85 (14)	C12B—C11B—S2B	119.5 (4)
O4A—Nd1A—O16A	144.23 (13)	C16B—C11B—S2B	120.2 (4)
O6A—Nd1A—O11A	145.13 (13)	O8A—C10A—H10A	109.5
O4A—Nd1A—O11A	86.74 (13)	O8A—C10A—H10B	109.5
O16A—Nd1A—O11A	108.08 (14)	H10A—C10A—H10B	109.5
O6A—Nd1A—O9A	72.03 (13)	O8A—C10A—H10C	109.5
O4A—Nd1A—O9A	74.65 (12)	H10A—C10A—H10C	109.5
O16A—Nd1A—O9A	139.73 (12)	H10B—C10A—H10C	109.5
O11A—Nd1A—O9A	76.19 (11)	C27A—C28A—C29A	120.9 (6)

O6A—Nd1A—O1A	73.58 (13)	C27A—C28A—H28A	119.6
O4A—Nd1A—O1A	72.22 (12)	C29A—C28A—H28A	119.6
O16A—Nd1A—O1A	75.91 (12)	C11B—C16B—C15B	119.2 (6)
O11A—Nd1A—O1A	139.56 (12)	C11B—C16B—H16A	120.4
O9A—Nd1A—O1A	127.34 (11)	C15B—C16B—H16A	120.4
O6A—Nd1A—O19A	142.77 (13)	C5B—C4B—C3B	118.9 (6)
O4A—Nd1A—O19A	81.60 (13)	C5B—C4B—H4BA	120.6
O16A—Nd1A—O19A	72.94 (12)	C3B—C4B—H4BA	120.6
O11A—Nd1A—O19A	72.07 (12)	C24B—C19B—C20B	121.4 (6)
O9A—Nd1A—O19A	141.11 (12)	C24B—C19B—S3B	119.0 (5)
O1A—Nd1A—O19A	70.97 (12)	C20B—C19B—S3B	119.6 (5)
O6A—Nd1A—O14A	82.82 (13)	O13A—C18A—H18A	109.5
O4A—Nd1A—O14A	143.65 (12)	O13A—C18A—H18B	109.5
O16A—Nd1A—O14A	71.97 (12)	H18A—C18A—H18B	109.5
O11A—Nd1A—O14A	73.57 (11)	O13A—C18A—H18C	109.5
O9A—Nd1A—O14A	71.17 (11)	H18A—C18A—H18C	109.5
O1A—Nd1A—O14A	140.54 (12)	H18B—C18A—H18C	109.5
O19A—Nd1A—O14A	118.92 (13)	C7A—C8A—C3A	119.2 (6)
O1B—Nd1B—O16B	137.22 (12)	C7A—C8A—H8AA	120.4
O1B—Nd1B—O11B	105.85 (13)	C3A—C8A—H8AA	120.4
O16B—Nd1B—O11B	90.45 (15)	O8B—C10B—H10D	109.5
O1B—Nd1B—O6B	90.24 (14)	O8B—C10B—H10E	109.5
O16B—Nd1B—O6B	104.06 (13)	H10D—C10B—H10E	109.5
O11B—Nd1B—O6B	137.53 (13)	O8B—C10B—H10F	109.5
O1B—Nd1B—O19B	74.81 (13)	H10D—C10B—H10F	109.5
O16B—Nd1B—O19B	72.93 (13)	H10E—C10B—H10F	109.5
O11B—Nd1B—O19B	72.56 (13)	C13A—C12A—C11A	118.3 (5)
O6B—Nd1B—O19B	149.77 (13)	C13A—C12A—H12A	120.9
O1B—Nd1B—O14B	150.42 (12)	C11A—C12A—H12A	120.9
O16B—Nd1B—O14B	71.95 (13)	C16A—C15A—C14A	120.7 (5)
O11B—Nd1B—O14B	72.82 (13)	C16A—C15A—H15A	119.6
O6B—Nd1B—O14B	74.26 (13)	C14A—C15A—H15A	119.6
O19B—Nd1B—O14B	129.64 (13)	C5A—C6A—C7A	119.8 (6)
O1B—Nd1B—O4B	71.67 (12)	C5A—C6A—H6AA	120.1
O16B—Nd1B—O4B	74.48 (13)	C7A—C6A—H6AA	120.1
O11B—Nd1B—O4B	149.32 (13)	C21A—C22A—C23A	119.6 (6)
O6B—Nd1B—O4B	72.89 (12)	C21A—C22A—H22A	120.2
O19B—Nd1B—O4B	77.46 (13)	C23A—C22A—H22A	120.2
O14B—Nd1B—O4B	124.66 (12)	S4B—N4B—P4B	130.8 (3)
O1B—Nd1B—O9B	73.23 (12)	C15B—C14B—C13B	120.8 (6)
O16B—Nd1B—O9B	149.40 (13)	C15B—C14B—H14A	119.6
O11B—Nd1B—O9B	74.40 (13)	C13B—C14B—H14A	119.6
O6B—Nd1B—O9B	73.19 (13)	C5A—C4A—C3A	119.0 (6)
O19B—Nd1B—O9B	124.70 (13)	C5A—C4A—H4AA	120.5
O14B—Nd1B—O9B	78.15 (12)	C3A—C4A—H4AA	120.5
O4B—Nd1B—O9B	130.28 (13)	C11B—C12B—C13B	119.5 (5)
O5A—S1A—O1A	113.9 (2)	C11B—C12B—H12B	120.3
O5A—S1A—N1A	109.6 (2)	C13B—C12B—H12B	120.3
O1A—S1A—N1A	113.6 (2)	C6B—C5B—C4B	121.3 (6)

O5A—S1A—C3A	106.3 (2)	C6B—C5B—H5BA	119.3
O1A—S1A—C3A	104.3 (2)	C4B—C5B—H5BA	119.3
N1A—S1A—C3A	108.5 (2)	C3B—C8B—C7B	119.9 (6)
O4A—P1A—O2A	112.4 (2)	C3B—C8B—H8BA	120.1
O4A—P1A—O3A	107.7 (2)	C7B—C8B—H8BA	120.1
O2A—P1A—O3A	101.9 (2)	C15A—C16A—C11A	118.2 (5)
O4A—P1A—N1A	117.2 (2)	C15A—C16A—H16B	120.9
O2A—P1A—N1A	106.2 (2)	C11A—C16A—H16B	120.9
O3A—P1A—N1A	110.3 (2)	C14B—C13B—C12B	119.2 (6)
O20A—S4A—O19A	113.9 (2)	C14B—C13B—H13A	120.4
O20A—S4A—N4A	109.1 (2)	C12B—C13B—H13A	120.4
O19A—S4A—N4A	113.9 (2)	O18A—C26A—H26A	109.5
O20A—S4A—C27A	107.9 (3)	O18A—C26A—H26B	109.5
O19A—S4A—C27A	104.2 (2)	H26A—C26A—H26B	109.5
N4A—S4A—C27A	107.5 (2)	O18A—C26A—H26C	109.5
O20A—S4A—Na1A	51.33 (16)	H26A—C26A—H26C	109.5
O19A—S4A—Na1A	126.23 (17)	H26B—C26A—H26C	109.5
N4A—S4A—Na1A	58.53 (16)	C22A—C23A—C24A	121.0 (6)
C27A—S4A—Na1A	129.45 (18)	C22A—C23A—H23A	119.5
O10A—S2A—O9A	114.3 (2)	C24A—C23A—H23A	119.5
O10A—S2A—N2A	110.1 (3)	C13A—C14A—C15A	120.2 (5)
O9A—S2A—N2A	113.4 (2)	C13A—C14A—H14B	119.9
O10A—S2A—C11A	105.5 (2)	C15A—C14A—H14B	119.9
O9A—S2A—C11A	104.3 (2)	C8B—C3B—C4B	120.6 (5)
N2A—S2A—C11A	108.5 (2)	C8B—C3B—S1B	119.4 (4)
O15A—S3A—O14A	114.6 (2)	C4B—C3B—S1B	119.9 (5)
O15A—S3A—N3A	107.9 (2)	C14B—C15B—C16B	120.9 (6)
O14A—S3A—N3A	113.9 (2)	C14B—C15B—H15B	119.6
O15A—S3A—C19A	108.2 (2)	C16B—C15B—H15B	119.6
O14A—S3A—C19A	104.9 (2)	C21A—C20A—C19A	119.2 (6)
N3A—S3A—C19A	107.0 (2)	C21A—C20A—H20A	120.4
O15A—S3A—Na1A^{iii}	52.38 (15)	C19A—C20A—H20A	120.4
O14A—S3A—Na1A^{iii}	125.82 (16)	C30B—C29B—C28B	120.6 (7)
N3A—S3A—Na1A^{iii}	56.38 (15)	C30B—C29B—H29A	119.7
C19A—S3A—Na1A^{iii}	129.24 (19)	C28B—C29B—H29A	119.7
O11A—P3A—O12A	108.3 (2)	C19A—C24A—C23A	118.1 (5)
O11A—P3A—O13A	113.0 (2)	C19A—C24A—H24A	120.9
O12A—P3A—O13A	101.9 (2)	C23A—C24A—H24A	120.9
O11A—P3A—N3A	116.8 (2)	C27B—C28B—C29B	118.6 (6)
O12A—P3A—N3A	109.9 (2)	C27B—C28B—H28B	120.7
O13A—P3A—N3A	106.0 (2)	C29B—C28B—H28B	120.7
O15B—S3B—O14B	113.0 (3)	C23B—C24B—C19B	118.9 (7)
O15B—S3B—N3B	110.8 (3)	C23B—C24B—H24B	120.6
O14B—S3B—N3B	114.4 (2)	C19B—C24B—H24B	120.6
O15B—S3B—C19B	105.3 (3)	C21B—C20B—C19B	118.8 (8)
O14B—S3B—C19B	106.8 (3)	C21B—C20B—H20B	120.6
N3B—S3B—C19B	105.8 (3)	C19B—C20B—H20B	120.6
O14B—S3B—Na1B	109.83 (16)	C32A—C31A—C30A	121.2 (6)

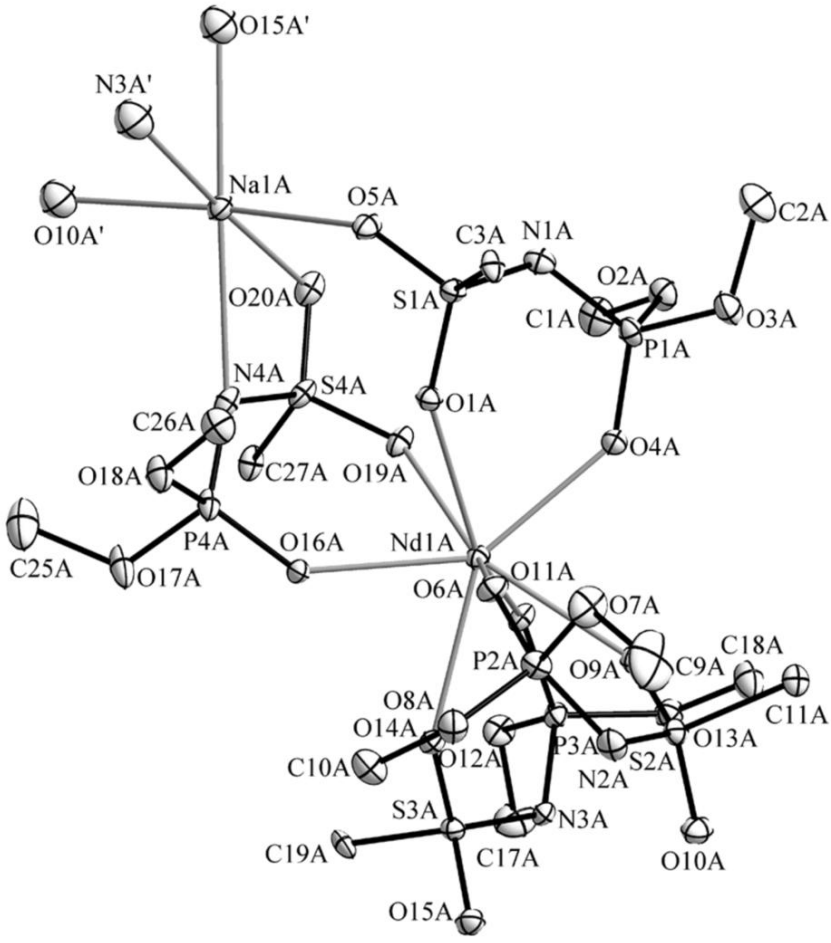
N3B—S3B—Na1B	90.8 (2)	C32A—C31A—H31A	119.4
C19B—S3B—Na1B	128.4 (2)	C30A—C31A—H31A	119.4
O4B—S1B—O5B	113.6 (3)	C14A—C13A—C12A	120.6 (6)
O4B—S1B—N1B	114.0 (2)	C14A—C13A—H13B	119.7
O5B—S1B—N1B	110.9 (3)	C12A—C13A—H13B	119.7
O4B—S1B—C3B	106.0 (3)	C32B—C27B—C28B	122.0 (6)
O5B—S1B—C3B	104.3 (3)	C32B—C27B—S4B	119.4 (5)
N1B—S1B—C3B	107.3 (3)	C28B—C27B—S4B	118.6 (5)
O4B—S1B—Na1B^{iv}	108.17 (17)	C8B—C7B—C6B	119.9 (6)
N1B—S1B—Na1B^{iv}	84.05 (19)	C8B—C7B—H7BA	120.1
C3B—S1B—Na1B^{iv}	135.3 (2)	C6B—C7B—H7BA	120.1
O20B—S4B—O19B	112.8 (3)	C28A—C29A—C30A	119.0 (6)
O20B—S4B—N4B	111.9 (3)	C28A—C29A—H29B	120.5
O19B—S4B—N4B	113.7 (3)	C30A—C29A—H29B	120.5
O20B—S4B—C27B	106.1 (3)	C30B—C31B—C32B	120.2 (7)
O19B—S4B—C27B	105.8 (3)	C30B—C31B—H31B	119.9
N4B—S4B—C27B	105.8 (3)	C32B—C31B—H31B	119.9
O6B—P2B—O8B	112.8 (2)	C24B—C23B—C22B	120.0 (7)
O6B—P2B—O7B	107.0 (2)	C24B—C23B—H23B	120.0
O8B—P2B—O7B	100.3 (2)	C22B—C23B—H23B	120.0
O6B—P2B—N2B	118.6 (2)	C5B—C6B—C7B	119.3 (6)
O8B—P2B—N2B	106.0 (2)	C5B—C6B—H6BA	120.3
O7B—P2B—N2B	110.8 (3)	C7B—C6B—H6BA	120.3
O10B—S2B—O9B	113.9 (2)	C20B—C21B—C22B	121.9 (8)
O10B—S2B—N2B	108.1 (3)	C20B—C21B—H21A	119.1
O9B—S2B—N2B	114.8 (2)	C22B—C21B—H21A	119.1
O10B—S2B—C11B	105.5 (3)	O2B—C1B—H1BA	109.5
O9B—S2B—C11B	106.7 (2)	O2B—C1B—H1BB	109.5
N2B—S2B—C11B	107.4 (3)	H1BA—C1B—H1BB	109.5
O9B—S2B—Na1B	110.68 (17)	O2B—C1B—H1BC	109.5
N2B—S2B—Na1B	77.58 (19)	H1BA—C1B—H1BC	109.5
C11B—S2B—Na1B	135.7 (2)	H1BB—C1B—H1BC	109.5
O6A—P2A—O7A	107.5 (2)	O12A—C17A—H17A	109.5
O6A—P2A—O8A	112.1 (2)	O12A—C17A—H17B	109.5
O7A—P2A—O8A	101.5 (3)	H17A—C17A—H17B	109.5
O6A—P2A—N2A	117.4 (2)	O12A—C17A—H17C	109.5
O7A—P2A—N2A	110.5 (3)	H17A—C17A—H17C	109.5
O8A—P2A—N2A	106.8 (2)	H17B—C17A—H17C	109.5
O16A—P4A—O17A	108.5 (2)	C20A—C21A—C22A	121.0 (6)
O16A—P4A—O18A	113.1 (2)	C20A—C21A—H21B	119.5
O17A—P4A—O18A	101.4 (2)	C22A—C21A—H21B	119.5
O16A—P4A—N4A	116.1 (2)	C31B—C30B—C29B	120.4 (7)
O17A—P4A—N4A	110.0 (3)	C31B—C30B—H30A	119.8
O18A—P4A—N4A	106.8 (2)	C29B—C30B—H30A	119.8
O1B—P1B—N1B	115.8 (2)	C27B—C32B—C31B	118.2 (7)
O1B—P1B—O2B	113.4 (2)	C27B—C32B—H32A	120.9
N1B—P1B—O2B	108.2 (2)	C31B—C32B—H32A	120.9
O1B—P1B—O3B	111.6 (2)	C31A—C30A—C29A	119.2 (6)

N1B—P1B—O3B	109.4 (3)	C31A—C30A—H30B	120.4
O2B—P1B—O3B	96.7 (2)	C29A—C30A—H30B	120.4
O11B—P3B—O13B	112.0 (3)	C31A—C32A—C27A	120.1 (7)
O11B—P3B—O12B	108.0 (3)	C31A—C32A—H32B	120.0
O13B—P3B—O12B	102.1 (3)	C27A—C32A—H32B	120.0
O11B—P3B—N3B	117.3 (2)	C8A—C7A—C6A	120.3 (6)
O13B—P3B—N3B	107.7 (3)	C8A—C7A—H7AA	119.8
O12B—P3B—N3B	108.7 (3)	C6A—C7A—H7AA	119.8
O16B—P4B—O17B	106.4 (3)	O13B—C18B—H18D	109.5
O16B—P4B—O18B	112.6 (3)	O13B—C18B—H18E	109.5
O17B—P4B—O18B	102.1 (3)	H18D—C18B—H18E	109.5
O16B—P4B—N4B	117.3 (3)	O13B—C18B—H18F	109.5
O17B—P4B—N4B	109.5 (3)	H18D—C18B—H18F	109.5
O18B—P4B—N4B	107.9 (3)	H18E—C18B—H18F	109.5
S3A—O14A—Nd1A	137.7 (2)	O3A—C2A—H2AA	109.5
S4A—O19A—Nd1A	138.4 (2)	O3A—C2A—H2AB	109.5
S1A—O1A—Nd1A	140.9 (2)	H2AA—C2A—H2AB	109.5
P1A—O4A—Nd1A	138.8 (2)	O3A—C2A—H2AC	109.5
S2A—O9A—Nd1A	140.9 (2)	H2AA—C2A—H2AC	109.5
C18A—O13A—P3A	121.5 (4)	H2AB—C2A—H2AC	109.5
P3B—O11B—Nd1B	139.6 (2)	O17A—C25A—H25A	109.5
P4A—O16A—Nd1A	137.1 (2)	O17A—C25A—H25B	109.5
P2A—O6A—Nd1A	139.2 (2)	H25A—C25A—H25B	109.5
S4A—O20A—Na1A	100.6 (2)	O17A—C25A—H25C	109.5
P1B—O1B—Nd1B	143.8 (2)	H25A—C25A—H25C	109.5
P3A—O11A—Nd1A	136.1 (2)	H25B—C25A—H25C	109.5
S1B—O4B—Nd1B	141.7 (2)	C21B—C22B—C23B	119.0 (7)
C25A—O17A—P4A	121.4 (5)	C21B—C22B—H22B	120.5
S1A—O5A—Na1A	142.3 (2)	C23B—C22B—H22B	120.5
C1A—O2A—P1A	118.5 (3)	O17B—C25B—H25D	109.5
S3A—O15A—Na1A^{iii}	99.42 (19)	O17B—C25B—H25E	109.5
S4B—O19B—Nd1B	143.1 (2)	H25D—C25B—H25E	109.5
C26A—O18A—P4A	121.9 (4)	O17B—C25B—H25F	109.5
P2B—O6B—Nd1B	140.1 (2)	H25D—C25B—H25F	109.5
S2B—O9B—Nd1B	141.2 (2)	H25E—C25B—H25F	109.5
S2A—O10A—Na1A^{iii}	145.9 (2)	O12B—C17B—H17D	109.5
S2B—O10B—Na1B	120.6 (2)	O12B—C17B—H17E	109.5
C10A—O8A—P2A	118.0 (4)	H17D—C17B—H17E	109.5
C2B—O3B—P1B	120.1 (5)	O12B—C17B—H17F	109.5
C1B—O2B—P1B	120.6 (4)	H17D—C17B—H17F	109.5
S3B—O14B—Nd1B	141.3 (2)	H17E—C17B—H17F	109.5
P4B—O16B—Nd1B	141.3 (2)	O3B—C2B—H2BA	109.5
C10B—O8B—P2B	119.5 (4)	O3B—C2B—H2BB	109.5
C2A—O3A—P1A	118.5 (4)	H2BA—C2B—H2BB	109.5
C17A—O12A—P3A	121.2 (4)	O3B—C2B—H2BC	109.5
C9A—O7A—P2A	119.0 (5)	H2BA—C2B—H2BC	109.5
S3B—O15B—Na1B	137.5 (3)	H2BB—C2B—H2BC	109.5
S1B—O5B—Na1B^{iv}	123.5 (3)	O7B—C9B—H9BA	109.5

S3A—N3A—P3A	122.8 (2)	O7B—C9B—H9BB	109.5
S3A—N3A—Na1A^{iii}	92.54 (19)	H9BA—C9B—H9BB	109.5
P3A—N3A—Na1A^{iii}	142.2 (2)	O7B—C9B—H9BC	109.5
S4B—O20B—Na1B^{iv}	141.3 (3)	H9BA—C9B—H9BC	109.5
C9B—O7B—P2B	119.7 (4)	H9BB—C9B—H9BC	109.5
C18B—O13B—P3B	121.9 (5)	O7A—C9A—H9AA	109.5
S2A—N2A—P2A	126.7 (3)	O7A—C9A—H9AB	109.5
P1B—N1B—S1B	129.5 (3)	H9AA—C9A—H9AB	109.5
S1A—N1A—P1A	126.5 (3)	O7A—C9A—H9AC	109.5
C17B—O12B—P3B	121.9 (5)	H9AA—C9A—H9AC	109.5
S4A—N4A—P4A	123.3 (2)	H9AB—C9A—H9AC	109.5
S4A—N4A—Na1A	90.5 (2)	O18B—C26B—H26D	109.5
P4A—N4A—Na1A	143.0 (2)	O18B—C26B—H26E	109.5
S3B—N3B—P3B	130.3 (3)	H26D—C26B—H26E	109.5
C26B—O18B—P4B	118.4 (6)	O18B—C26B—H26F	109.5
C32A—C27A—C28A	119.6 (6)	H26D—C26B—H26F	109.5
C32A—C27A—S4A	119.7 (5)	H26E—C26B—H26F	109.5

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

Fig. 1


O15A'
N3A'
Na1A
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P1A
N4A
S4A
O1A
C26A
O4A
O18A
C27A
O19A
P4A
O16A
Nd1A
C25A
O17A
O11A
O6A
O7A
C18A
P2A
O9A
C9A
O8A
C11A
O14A
O12A
P3A
O13A
C10A
S2A
N2A
S3A
N3A
C19A
C17A
O10A
O15A

Fig. 2

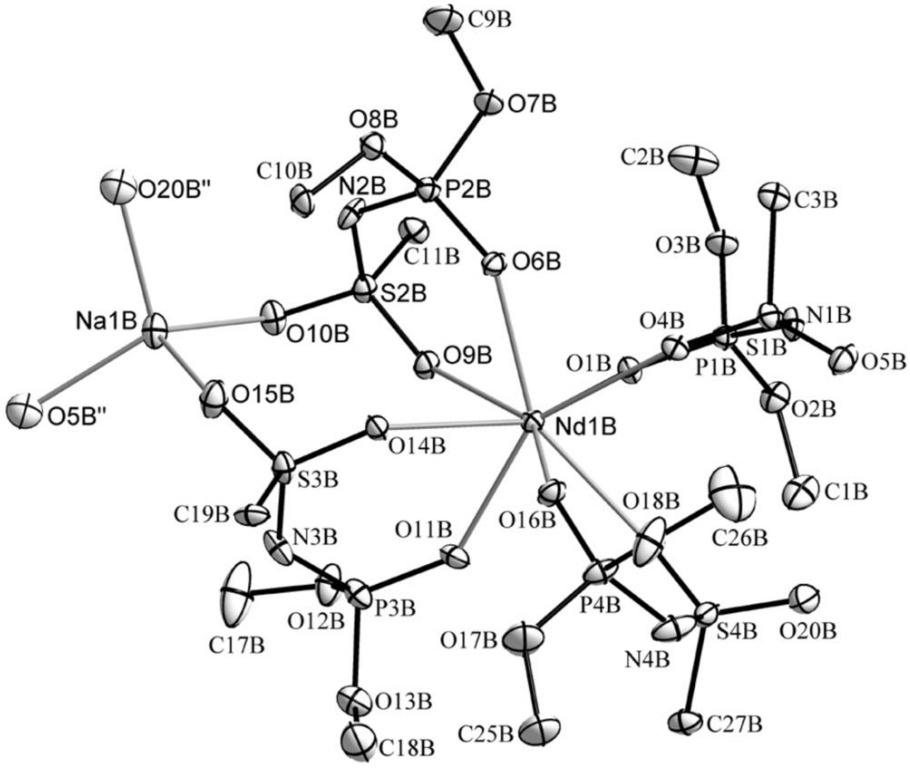
C9B
O7B
O8B
C10B
N2B
P2B
O20B"
C2B
C3B
O3B
C11B
O6B
S2B
Na1B
O10B
O4B
N1B
S1B
O1B
P1B
O5B
O9B
O15B
O5B"
O2B
Nd1B
O14B
S3B
C1B
C19B
O18B
O16B
O11B
N3B
C26B
P4B
P3B
O12B
S4B
O20B
C17B
O17B
N4B
O13B
C25B
C27B
C18B

Fig. 3