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Poly[[tetrakis(μ_2 -pyrazine N,N' -dioxide- $\kappa^2O:O'$)neodymium(III)] tris(perchlorate)]

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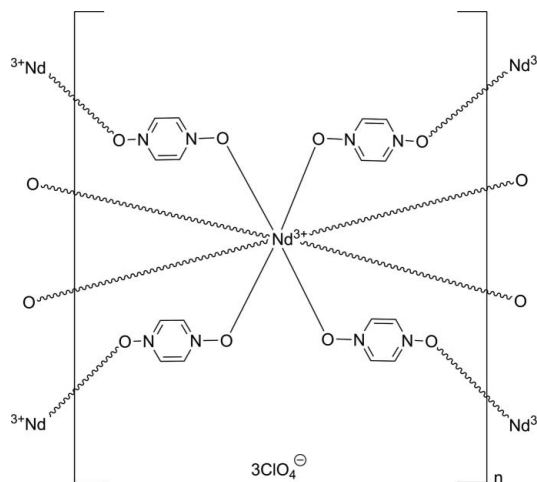
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.038; wR factor = 0.106; data-to-parameter ratio = 19.0.

The title three-dimensional coordination network, $\{[Nd(C_4H_4N_2O_2)_4](ClO_4)_3\}_n$, is isostructural to that of other lanthanides. The Nd^{3+} cation lies on a fourfold roto-inversion axis. It is coordinated in a distorted square-antiprismatic fashion by eight O atoms from bridging pyrazine N,N' -dioxide ligands. There are two unique pyrazine N,N' -dioxide ligands. One ring is located around an inversion center, and there is a twofold rotation axis at the center of the other ring. There are also two unique perchlorate anions. One is centered on a twofold rotation axis and the other on a fourfold roto-inversion axis. The perchlorate anions are located in channels that run perpendicular to (001) and (110) and interact with the coordination network through $C-H \cdots O$ hydrogen bonds.

Related literature

For the isostructural La, Ce, Pr, Sm, Eu, Gd, Tb and Y coordination networks, see: Sun *et al.* (2004). For the isostructural Dy, Ho, Er coordination networks, see: Quinn-Elmore *et al.* (2010); Buchner *et al.* (2010*a,b*), respectively. For a lanthanum 4,4'-bipyridine N,N' -dioxide coordination network of similar topology, see: Long *et al.* (2001). For additional discussions on Ln^{3+} ($Ln =$ lanthanide) coordination networks with aromatic N,N' -dioxide ligands, see: Cardoso *et al.* (2001); Hill *et al.* (2005). For background information on the applications of coordination networks, see: Roswell & Yaghi (2004); Rosi *et al.* (2003); Seo *et al.* (2000).



Experimental

Crystal data

$[Nd(C_4H_4N_2O_2)_4](ClO_4)_3$
 $M_r = 890.96$
 Tetragonal, $I4_1/acd$
 $a = 15.3804$ (4) Å
 $c = 22.9843$ (12) Å
 $V = 5437.1$ (3) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 2.32$ mm⁻¹
 $T = 100$ K
 $0.23 \times 0.23 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{min} = 0.593$, $T_{max} = 0.659$

30711 measured reflections
 2086 independent reflections
 1842 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.106$
 $S = 1.10$
 2086 reflections

110 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 2.27$ e Å⁻³
 $\Delta\rho_{min} = -1.95$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C2-H2 \cdots O2^i$	0.95	2.55	3.326 (3)	139
$C2-H2 \cdots O5$	0.95	2.43	3.194 (7)	137
$C3-H3 \cdots O1$	0.95	2.59	3.331 (3)	135
$C3-H3 \cdots O3$	0.95	2.51	3.260 (3)	136
$C4-H4 \cdots O3^{ii}$	0.95	2.41	3.289 (3)	154

Symmetry codes: (i) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-y + \frac{3}{4}, x - \frac{1}{4}, -z + \frac{1}{4}$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: X-SEED.

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Board of Regents (grant No. CAP-491) and by Youngstown State University. The authors would like to acknowledge Youngstown State University and the STaRBURSTT Cyber-Instrumentation Consortium for assistance with the crystallography.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2298).

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supporting information

Acta Cryst. (2010). E66, m1104–m1105 [https://doi.org/10.1107/S1600536810031818]

Poly[[tetrakis(μ_2 -pyrazine *N,N'*-dioxide- κ^2 O:O')neodymium(III)] tris-(perchlorate)]

Benjamin G. Quinn-Elmore, James D. Buchner, Keith B. Beach and Jacqueline M. Knaust

S1. Comment

The synthesis of lanthanide coordination networks has been of recent interest due to the potential of the flexible coordination sphere of the Ln^{+3} metal ions to produce coordination networks with new, unusual, or high connectivity topologies (Hill *et al.* 2005, Long *et al.* 2001, and Sun *et al.* 2004). Coordination networks with both a high connectivity topology and an open framework have potential for applications in areas such as absorption, ion exchange, or catalysis (Roswell *et al.* 2004, Rosi *et al.* 2003, and Seo *et al.* 2000). Aromatic *N,N'*-dioxide ligands have been attractive candidates for use with Ln^{+3} cations as the O-donor atoms of the ligand are complementary to the hard acid character of the lanthanide cations (Cardoso *et al.* 2001, Hill *et al.* 2005, Long *et al.* 2001, and Sun *et al.* 2004).

The description of the structure of the title compound is part of a series of consecutive papers on three-dimensional coordination networks of the type $\{[\text{Ln}(\text{C}_4\text{H}_4\text{N}_2\text{O}_2)_4](\text{ClO}_4)_3\}_n$, with Ln = Nd (this publication), Dy (Quinn-Elmore *et al.* 2010), Ho (Buchner *et al.* 2010*a*) and Er (Buchner *et al.* 2010*b*), respectively. All four compounds are also isostructural to the previously reported La, Ce, Pr, Sm, Eu, Gd, Tb and Y coordination networks (Sun *et al.* 2004).

The asymmetric unit of the title compound contains one quarter of a Nd^{+3} cation, half of two coordinated pyrazine *N,N'*-dioxide ligands, a quarter of one perchlorate anion, and a half of another perchlorate anion (Figure 1). The Nd^{+3} cation lies on a fourfold roto-inversion axis. One ligand (O1, N1, C1, C2) is located around an inversion center, and there is a twofold rotation axis at the center of the other (O2, N2, C3, C4). Both chlorine atoms of the perchlorate anions lie on special positions. Cl1 lies on a fourfold roto-inversion axis, and Cl2 is located on a twofold rotation axis. The high atomic displacement parameters for O4 and O5 bonded to Cl2, and the residual electron density around Cl2 indicate that this perchlorate anion is disordered; however, the disorder does not appear discreet. Only O4 and O5 are easily found in positions that agree with the site symmetry of the anion, therefore only one position was modeled.

The Nd^{+3} cation is coordinated in a distorted square anti-prismatic fashion by eight O atoms from bridging pyrazine *N,N'*-dioxide ligands forming a three-dimensional coordination network. The network topology is similar to that which is seen in $\{[\text{La}(4,4'\text{-bipyridine } N,N'\text{-dioxide})_4](\text{CF}_3\text{SO}_3)_3 \cdot 4.2\text{CH}_3\text{OH}\}_n$ in that it can be considered as being composed of two sets of intersecting (4,4) nets (Long *et al.* 2001). The nets are perpendicular to one another, but they are canted. One set of nets lies parallel to the (1 0 0) plane, and the other set lies parallel to the (0 1 0) plane (Figure 2).

The title compound forms five unique C—H \cdots O hydrogen bonds (Figure 3). There are two unique hydrogen bonds between pyrazine *N,N'*-dioxide ligands and another three hydrogen bonds between the perchlorate anions and pyrazine *N,N'*-dioxide ligands. The non-disordered perchlorate anion (Cl1 and O3) forms two unique hydrogen bonds with pyrazine *N,N'*-dioxide ligands resulting in a total of eight hydrogen bonds per ion with the network, but the disordered perchlorate (Cl2, O4, and O5) forms only one unique hydrogen bond with pyrazine *N,N'*-dioxide ligands resulting in a total of only two hydrogen bonds per ion with the network. As seen in the packing diagrams, the perchlorate anions are

located in two sets of channels (Figures 4 and 5). In channels that run perpendicular to the (0 0 1) plane only anions containing Cl2 are present. (Figure 4), but in the channels that run perpendicular to the (1 1 0) plane the anions containing Cl1 and Cl2 alternate (Figure 5).

S2. Experimental

Pyrazine *N,N'*-dioxide (0.025 g, 0.223 mmol) was dissolved in deionized water (1.5 ml) and methanol (1.5 ml). An aqueous solution of $\text{Nd}(\text{ClO}_4)_3$ (0.240 ml of a 0.1167 M solution, 0.028 mmol) was diluted with methanol (0.760 ml) and CH_2Cl_2 (2.5 ml). The pyrazine *N,N'*-dioxide solution was layered over the $\text{Nd}(\text{ClO}_4)_3$ solution, and the two solutions were allowed to slowly mix. Rose colored block-like crystals formed upon the slow evaporation of the resultant solution.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with $\text{C—H} = 0.95 \text{ \AA}$ and with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$.

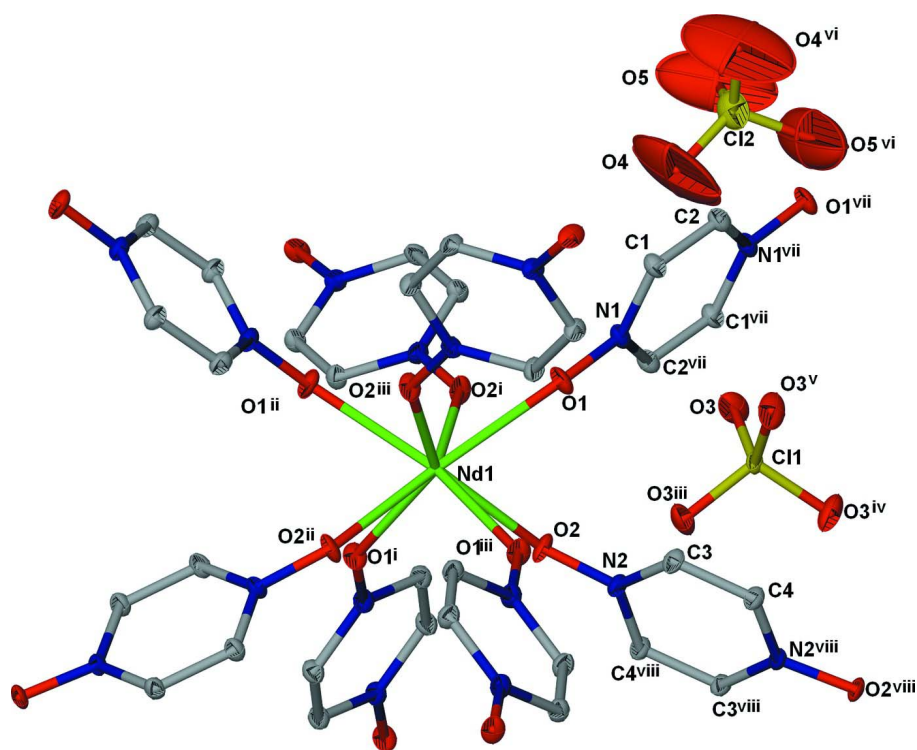


Figure 1

The coordination environment of the Nd^{3+} cation in title compound with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms have been omitted for clarity. Symmetry codes: (i) $y+1/4, x-1/4, -z+3/4$; (ii) $-y+3/4, -x+3/4, -z+3/4$; (iii) $-x+1, -y+1/2, z$; (iv) $-y+3/4, x-1/4, -z+1/4$; (v) $y+1/4, -x+3/4, -z+1/4$; (vi) $y+3/4, x-3/4, -z+1/4$; (vii) $-x+3/2, -y+1/2, -z+1/2$; (viii) $x, -y+1, -z+1/2$.

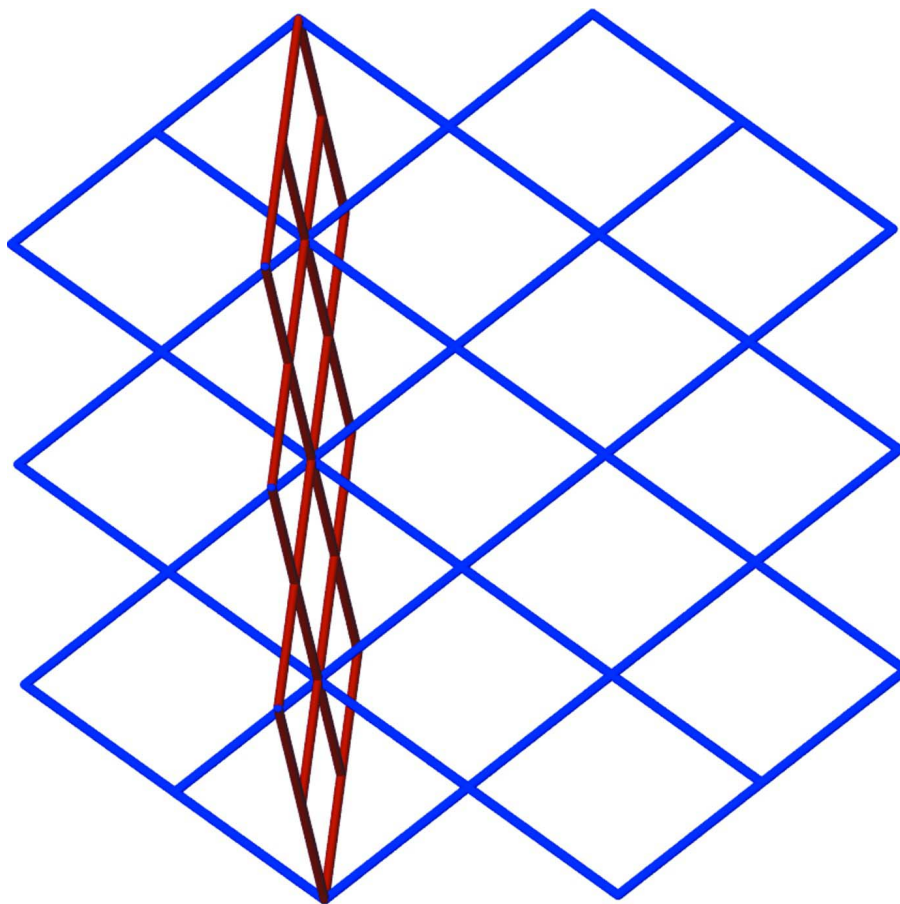


Figure 2

Schematic representation of the network topology seen in $\{[\text{Nd}(\text{C}_4\text{H}_4\text{N}_2\text{O}_2)_4](\text{ClO}_4)_3\}_n$. The net shown in red is parallel to the (1 0 0) plane, and the net shown in blue is parallel to the (0 1 0) plane.

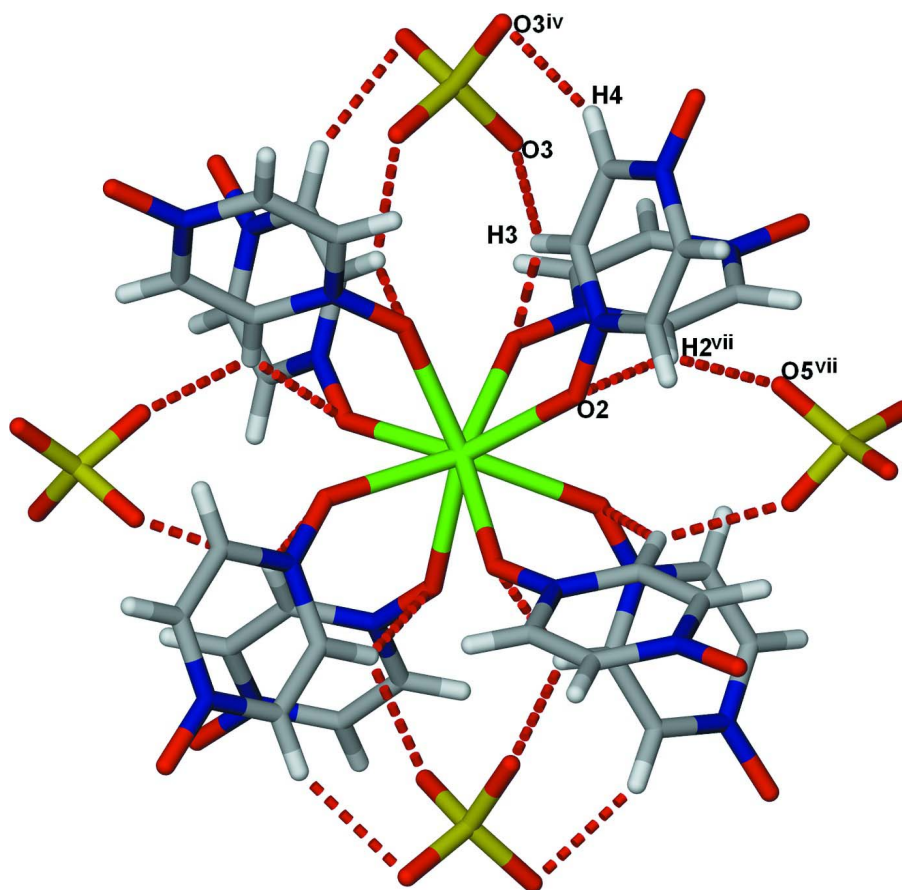


Figure 3

C—H...O hydrogen bonding interactions between pyrazine *N,N'*-dioxide ligands and between perchlorate anions and pyrazine *N,N'*-dioxide ligands. Hydrogen bonds are shown as dashed lines. Symmetry codes: (iv) $-y+3/4, x-1/4, -z+1/4$; (vi) $y+3/4, x-3/4, -z+1/4$; (vii) $-x+3/2, -y+1/2, -z+1/2$ Color scheme: Nd: green, C: grey, H: white, N: blue, O: red, Cl: yellow.

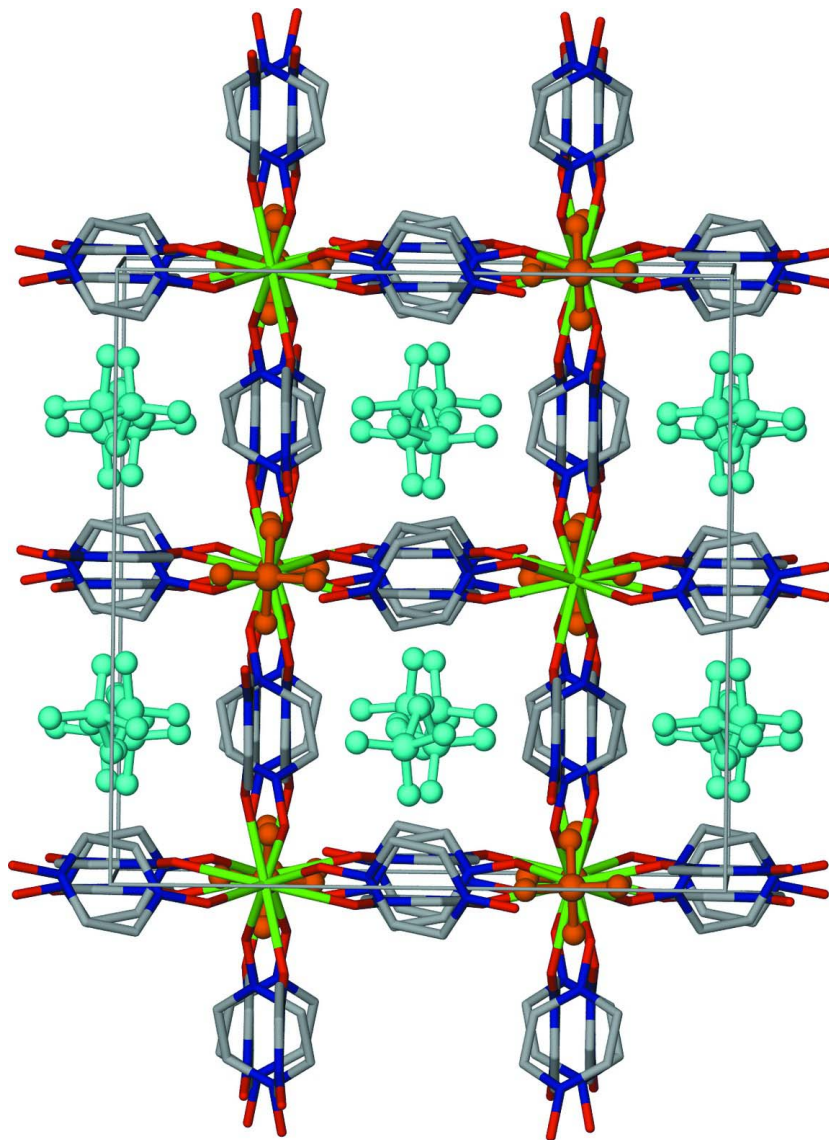


Figure 4

Packing of the title compound viewed perpendicular to the (0 0 1) with anions shown in ball and stick representation. In these channels there are only anions containing Cl2. Hydrogen atoms have been omitted for clarity. Color scheme: Nd: green, C: grey, H: white, N:blue, O: red, anions containing Cl1: orange, and anions containing Cl2: aqua.

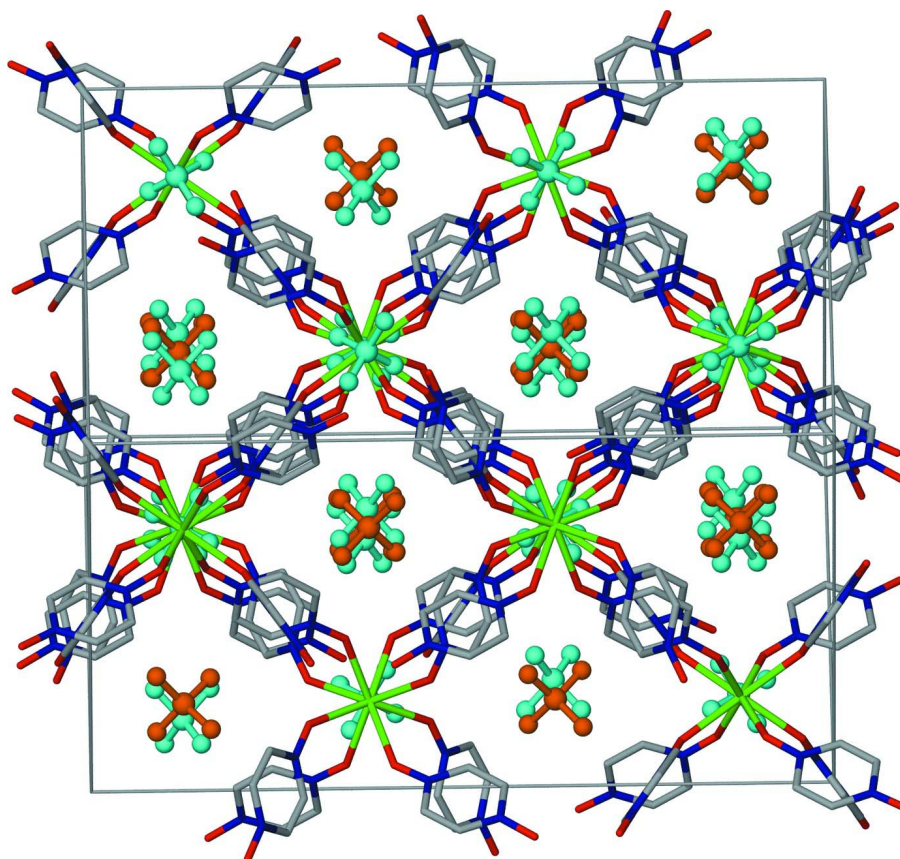


Figure 5

Packing of the title compound viewed perpendicular to the (1 1 0) plane with anions shown in ball and stick representation. The perchlorate anions in these channels alternate between those containing C11 and C12. Hydrogen atoms have been omitted for clarity. Color scheme: Nd: green, C: grey, H: white, N: blue, O: red, anions containing C11: orange, and anions containing C12: aqua.

Poly[[tetrakis(μ_2 -pyrazine *N,N'*-dioxide- κ^2 O:O')neodymium(III)] tris(perchlorate)]

Crystal data

[Nd(C₄H₄N₂O₂)₄](ClO₄)₃

$M_r = 890.96$

Tetragonal, $I4_1/acd$

Hall symbol: -I 4bd 2c

$a = 15.3804 (4) \text{ \AA}$

$c = 22.9843 (12) \text{ \AA}$

$V = 5437.1 (3) \text{ \AA}^3$

$Z = 8$

$F(000) = 3512$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

$D_x = 2.177 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 15053 reflections

$\theta = 2.6\text{--}30.5^\circ$

$\mu = 2.32 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, rose

$0.23 \times 0.23 \times 0.18 \text{ mm}$

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.593$, $T_{\max} = 0.659$

30711 measured reflections

2086 independent reflections

1842 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 2.6^\circ$

$h = -21 \rightarrow 21$
 $k = -21 \rightarrow 21$
 $l = -32 \rightarrow 32$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.106$
 $S = 1.10$
 2086 reflections
 110 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 38.356P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 2.27 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.95 \text{ e } \text{\AA}^{-3}$

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.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.5000	0.2500	0.3750	0.00589 (11)
Cl1	0.5000	0.2500	0.1250	0.0119 (3)
Cl2	0.72544 (6)	-0.02456 (6)	0.1250	0.0319 (3)
O1	0.59191 (12)	0.21965 (14)	0.29303 (8)	0.0171 (4)
O2	0.53338 (14)	0.39686 (12)	0.34324 (8)	0.0168 (4)
O3	0.57573 (16)	0.24613 (16)	0.16135 (10)	0.0277 (5)
O4	0.6477 (5)	-0.0172 (6)	0.1497 (5)	0.191 (4)
O5	0.7895 (5)	-0.0023 (6)	0.1623 (5)	0.180 (5)
N1	0.66963 (15)	0.23449 (15)	0.27293 (10)	0.0141 (4)
N2	0.52833 (15)	0.44642 (14)	0.29745 (9)	0.0129 (4)
C1	0.70832 (17)	0.17377 (17)	0.23897 (11)	0.0154 (5)
H1	0.6797	0.1202	0.2315	0.018*
C2	0.78886 (16)	0.18959 (17)	0.21540 (11)	0.0152 (5)
H2	0.8155	0.1475	0.1910	0.018*
C3	0.52715 (18)	0.41238 (16)	0.24314 (11)	0.0148 (5)
H3	0.5264	0.3511	0.2380	0.018*
C4	0.52702 (18)	0.46617 (16)	0.19547 (11)	0.0147 (5)
H4	0.5260	0.4420	0.1574	0.018*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00627 (13)	0.00627 (13)	0.00511 (16)	-0.00034 (7)	0.000	0.000
Cl1	0.0146 (4)	0.0146 (4)	0.0065 (6)	0.000	0.000	0.000
Cl2	0.0304 (4)	0.0304 (4)	0.0349 (6)	-0.0118 (5)	0.0035 (3)	-0.0035 (3)
O1	0.0112 (8)	0.0256 (10)	0.0146 (8)	-0.0032 (7)	0.0052 (7)	-0.0036 (7)
O2	0.0283 (10)	0.0114 (8)	0.0107 (8)	-0.0031 (7)	-0.0038 (7)	0.0049 (6)
O3	0.0195 (11)	0.0479 (15)	0.0156 (10)	0.0057 (9)	-0.0054 (8)	-0.0033 (8)
O4	0.085 (5)	0.154 (7)	0.335 (12)	-0.015 (4)	0.138 (7)	-0.028 (7)
O5	0.091 (5)	0.130 (6)	0.317 (15)	0.007 (4)	-0.066 (7)	-0.135 (8)
N1	0.0116 (10)	0.0198 (10)	0.0110 (9)	-0.0011 (8)	0.0022 (8)	-0.0013 (8)
N2	0.0160 (10)	0.0117 (9)	0.0111 (9)	0.0000 (8)	-0.0017 (7)	0.0028 (7)
C1	0.0149 (11)	0.0172 (11)	0.0140 (11)	-0.0008 (9)	0.0023 (8)	-0.0029 (9)
C2	0.0135 (11)	0.0188 (12)	0.0132 (10)	0.0000 (9)	0.0013 (8)	-0.0027 (9)
C3	0.0206 (12)	0.0104 (10)	0.0134 (11)	-0.0018 (9)	-0.0019 (9)	0.0006 (8)
C4	0.0209 (12)	0.0114 (10)	0.0118 (10)	-0.0002 (9)	-0.0002 (9)	0.0006 (8)

Geometric parameters (\AA , $^\circ$)

Nd1—O1 ⁱ	2.4012 (18)	Cl2—O5 ^{vi}	1.350 (7)
Nd1—O1 ⁱⁱ	2.4012 (18)	O1—N1	1.302 (3)
Nd1—O1	2.4012 (18)	O2—N2	1.302 (3)
Nd1—O1 ⁱⁱⁱ	2.4012 (18)	N1—C1	1.355 (3)
Nd1—O2 ⁱ	2.4286 (18)	N1—C2 ^{vii}	1.358 (3)
Nd1—O2 ⁱⁱ	2.4286 (18)	N2—C3	1.354 (3)
Nd1—O2	2.4286 (18)	N2—C4 ^{viii}	1.354 (3)
Nd1—O2 ⁱⁱⁱ	2.4287 (18)	C1—C2	1.374 (3)
Cl1—O3	1.435 (2)	C1—H1	0.9500
Cl1—O3 ^{iv}	1.435 (2)	C2—N1 ^{vii}	1.358 (3)
Cl1—O3 ⁱⁱⁱ	1.435 (2)	C2—H2	0.9500
Cl1—O3 ^v	1.435 (2)	C3—C4	1.373 (3)
Cl2—O4 ^{vi}	1.328 (5)	C3—H3	0.9500
Cl2—O4	1.328 (5)	C4—N2 ^{viii}	1.354 (3)
Cl2—O5	1.350 (7)	C4—H4	0.9500
O1 ⁱ —Nd1—O1 ⁱⁱ	76.62 (10)	O3 ^{iv} —Cl1—O3 ⁱⁱⁱ	109.83 (10)
O1 ⁱ —Nd1—O1	147.62 (10)	O3—Cl1—O3 ^v	109.83 (10)
O1 ⁱⁱ —Nd1—O1	112.75 (10)	O3 ^{iv} —Cl1—O3 ^v	108.76 (19)
O1 ⁱ —Nd1—O1 ⁱⁱⁱ	112.75 (10)	O3 ⁱⁱⁱ —Cl1—O3 ^v	109.83 (10)
O1 ⁱⁱ —Nd1—O1 ⁱⁱⁱ	147.62 (10)	O4 ^{vi} —Cl2—O4	109.6 (8)
O1—Nd1—O1 ⁱⁱⁱ	76.63 (10)	O4 ^{vi} —Cl2—O5	115.9 (6)
O1 ⁱ —Nd1—O2 ⁱ	79.66 (7)	O4—Cl2—O5	111.4 (7)
O1 ⁱⁱ —Nd1—O2 ⁱ	73.01 (7)	O4 ^{vi} —Cl2—O5 ^{vi}	111.4 (7)
O1—Nd1—O2 ⁱ	74.30 (6)	O4—Cl2—O5 ^{vi}	115.9 (6)
O1 ⁱⁱⁱ —Nd1—O2 ⁱ	137.92 (6)	O5—Cl2—O5 ^{vi}	91.8 (11)
O1 ⁱ —Nd1—O2 ⁱⁱ	73.01 (7)	N1—O1—Nd1	141.71 (16)
O1 ⁱⁱ —Nd1—O2 ⁱⁱ	79.66 (7)	N2—O2—Nd1	140.80 (15)

O1—Nd1—O2 ⁱⁱ	137.92 (6)	O1—N1—C1	119.1 (2)
O1 ⁱⁱⁱ —Nd1—O2 ⁱⁱ	74.30 (6)	O1—N1—C2 ^{vii}	120.8 (2)
O2 ⁱ —Nd1—O2 ⁱⁱ	145.02 (9)	C1—N1—C2 ^{vii}	120.0 (2)
O1 ⁱ —Nd1—O2	74.30 (6)	O2—N2—C3	121.3 (2)
O1 ⁱⁱ —Nd1—O2	137.92 (6)	O2—N2—C4 ^{viii}	119.0 (2)
O1—Nd1—O2	79.66 (7)	C3—N2—C4 ^{viii}	119.7 (2)
O1 ⁱⁱⁱ —Nd1—O2	73.01 (7)	N1—C1—C2	120.1 (2)
O2 ⁱ —Nd1—O2	72.37 (10)	N1—C1—H1	120.0
O2 ⁱⁱ —Nd1—O2	118.92 (10)	C2—C1—H1	120.0
O1 ⁱ —Nd1—O2 ⁱⁱⁱ	137.92 (6)	N1 ^{vii} —C2—C1	119.9 (2)
O1 ⁱⁱ —Nd1—O2 ⁱⁱⁱ	74.30 (6)	N1 ^{vii} —C2—H2	120.1
O1—Nd1—O2 ⁱⁱⁱ	73.01 (7)	C1—C2—H2	120.1
O1 ⁱⁱⁱ —Nd1—O2 ⁱⁱⁱ	79.66 (7)	N2—C3—C4	120.2 (2)
O2 ⁱ —Nd1—O2 ⁱⁱⁱ	118.92 (10)	N2—C3—H3	119.9
O2 ⁱⁱ —Nd1—O2 ⁱⁱⁱ	72.37 (10)	C4—C3—H3	119.9
O2—Nd1—O2 ⁱⁱⁱ	145.02 (9)	N2 ^{viii} —C4—C3	120.1 (2)
O3—C11—O3 ^{iv}	109.83 (10)	N2 ^{viii} —C4—H4	119.9
O3—C11—O3 ⁱⁱⁱ	108.76 (19)	C3—C4—H4	119.9

Symmetry codes: (i) $y+1/4, x-1/4, -z+3/4$; (ii) $-y+3/4, -x+3/4, -z+3/4$; (iii) $-x+1, -y+1/2, z$; (iv) $-y+3/4, x-1/4, -z+1/4$; (v) $y+1/4, -x+3/4, -z+1/4$; (vi) $y+3/4, x-3/4, -z+1/4$; (vii) $-x+3/2, -y+1/2, -z+1/2$; (viii) $x, -y+1, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O2 ^{vii}	0.95	2.55	3.326 (3)	139
C2—H2...O5	0.95	2.43	3.194 (7)	137
C3—H3...O1	0.95	2.59	3.331 (3)	135
C3—H3...O3	0.95	2.51	3.260 (3)	136
C4—H4...O3 ^{iv}	0.95	2.41	3.289 (3)	154

Symmetry codes: (iv) $-y+3/4, x-1/4, -z+1/4$; (vii) $-x+3/2, -y+1/2, -z+1/2$.