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Poly[μ_3-aqua-μ_2-2,4-dinitrophenolato-rubidium(I)]

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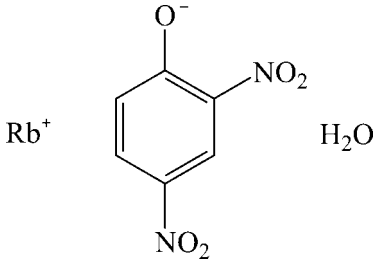
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 11.2.

The asymmetric unit of the title compound, $[Rb(C_6H_3N_2O_5)(H_2O)]_n$, comprises a rubidium cation, a 2,4-dinitrophenoxide anion and a water molecule. The Rb^+ cation is 11-coordinated by O atoms from 2,4-dinitrophenolate anions and water molecules. The metal centre is firstly coordinated by two μ_3-H_2O to form a one-dimensional ladder-shaped unit, $[Rb_2(\mu_3\text{-}H_2O)_2]$, which is further linked by 2,4-dinitrophenolate to give the three-dimensional framework of the title compound. The crystal structure involves O—H···O hydrogen bonds.

Related literature

For related literature, see: Abrahams *et al.* (1998); Brill *et al.* (2000); Cametti *et al.* (2005); Cole & Holt (1986); Devi & Vidyasagar (2000); Harrowfield *et al.* (1995); Hu *et al.* (2005); Klaui *et al.* (1987); Shannon (1976); von Prondzinski *et al.* (2007); Weinert *et al.* (2003).



Experimental

Crystal data

$[Rb(C_6H_3N_2O_5)(H_2O)]$
M_r = 286.59
Monoclinic, $P2_1/c$
a = 5.8519 (18) Å
b = 20.846 (7) Å
c = 7.412 (2) Å
β = 93.148 (5)°
V = 902.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.50 mm^{-1}
T = 293 (2) K
0.40 × 0.35 × 0.30 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.125, T_{max} = 0.202
4449 measured reflections
1599 independent reflections
1214 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.00
1599 reflections
143 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6B···O1^{i}	0.820 (10)	2.03 (2)	2.822 (5)	161 (6)
O6—H6A···O4^{ii}	0.818 (10)	2.27 (4)	2.919 (5)	137 (5)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*) and *DIAMOND* (Brandenburg & Brendt, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2074).

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supplementary materials

Acta Cryst. (2008). E**64**, m225 [**doi:10.1107/S1600536807066792**]

Poly[μ_3-aqua-μ_2-2,4-dinitrophenolato-rubidium(I)]

Z. Yang, M. Hu and X. Wang

Comment

Research on nitrogen-rich compounds is the focus of attention for their usage as energetic materials. Much work has concentrated on their alkaline or alkali-earth metal salts (Harrowfield *et al.*, 1995; Cole and Holt, 1986; von Prondzinski *et al.*, 2007), among which some polynitro-substituted phenoxide was found to be environment-friendly (Brill *et al.*, 2000). Our group has already demonstrated the structure of caesium 2,4-dinitrophenolate (Mancheng Hu *et al.*, 2005). Herein, we report its rubidium analogue [$Rb(OC_6H_3N_2O_4).H_2O$].

The asymmetric unit of the title compound comprises a rubidium cation, a 2,4-dinitrophenoxide anion and a water molecule. The central cation is coordinated to eleven O atoms (Fig. 1) with the Rb—O distances ranging from 2.914 (3) Å to 3.474 (4) Å, which are well within the range reported in the literature (Cametti *et al.*, 2005; Shannon, 1976; Devi and Vidyasagar, 2000).

The metal center is firstly coordinated by two μ_3-H_2O to form a one-dimensional ladder-shape unit, [$Rb_2(\mu_3$-$H_2O)_2$], which is further linked by 2,4-dinitrophenoxide to give the three-dimensional framework of the title compound. In the structure of [$Rb_2(\mu_3$-$H_2O)_2$] fragment (Fig.2), each rubidium ion is connected to three oxygen atoms of the water, and each water molecule is connected to three rubidium ions. The Rb—O—Rb angle along the sides of the ladder is 134.09 (13) °. It should be noted that the triply bridging water has been found in several lighter group I metal complexes (Klaui *et al.*, 1987; Abrahams *et al.*, 1998). A similar extended ladder-like structure motif was also found in the structure of [$Rb(OC_6H_3Ph_2$-2,6)]$_x$ (1) (Weinert *et al.*, 2003), however, each Rb atom in 1 is not connected to three water molecules but three O atoms from phenoxide. The corresponding Rb—O—Rb angle in 1 is about 155.5 (1) °, which is markedly larger than in the title compound.

The [$Rb_2(\mu_3$-$H_2O)_2$] fragments are connected to each other to form a two-dimensional netlike layer structure by the oxygen atoms from the nitro group and phenolate. Further, the two-dimensional layers are assembled *via* the 2,4-dinitrophenoxide into a three-dimensional framework in an ABAB fashion.

Experimental

To a solution of 10 mmol 2,4-dinitrophenol in 60 ml bidistilled water, a solution of an equimolar amount of rubidium hydroxide in 40 ml bidistilled water was added dropwise at room temperature. After vigorous stirring for 4 h, the resulting solution was then evaporated to a volume of about 20 ml in vacuum and filtered hot. The filtrate was then set aside for crystallization at room temperature. Three weeks later, yellow crystals of the title compound suitable for X-ray determination were isolated.

Refinement

The aromatic H atoms were placed at calculated positions (d(C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C)). Water H atoms were located and refined with distance restraints of d(O—H) = 0.82 (1) Å, their displacement parameters were set to 1.5 times U_{eq}(O).

Figures

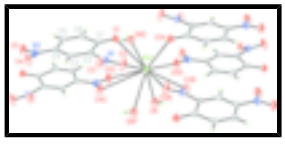

Fig. 1. Coordination sphere of Rb in [Rb($OC_6H_3N_2O_4$).H_2O]. Atoms marked with an A, B, C, D, E and F are at the symmetry positions (-*x*, 2 - *y*, 1 - *z*), (1 - *x*, 2 - *y*, 1 - *z*), (*x*, 3/2 - *y*, -1/2 + *z*), (-*x*, 1/2 + *y*, 1/2 - *z*), (-*x*,2 - *y*,-*z*), (1 - *x*, 2 - *y*, -*z*), respectively.

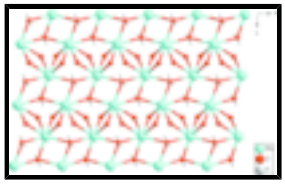

Fig. 2. The two-dimensional layer structure containing ladder-shape unit, [$Rb_2(\mu_3\text{-}H_2O)_2$]. All C atoms and N atoms were omitted for clarity.

Poly[μ_3-aqua-μ_2-2,4-dinitrophenolato-rubidium(I)]

Crystal data

[$Rb(C_6H_3N_2O_5)(H_2O)$]	F_{000} = 560
M_r = 286.59	D_x = 2.109 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1599 reflections
a = 5.8519 (18) Å	θ = 2.0–25.1°
b = 20.846 (7) Å	μ = 5.50 mm^{-1}
c = 7.412 (2) Å	T = 293 (2) K
β = 93.148 (5)°	Block, yellow
V = 902.8 (5) Å^3	0.40 × 0.35 × 0.30 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	1599 independent reflections
Radiation source: fine-focus sealed tube	1214 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.063
T = 293(2) K	θ_{max} = 25.1°
φ and ω scans	θ_{min} = 2.0°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→6
T_{min} = 0.125, T_{max} = 0.202	k = −20→24

4449 measured reflections

$l = -7 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.101$

$S = 1.00$

1599 reflections

143 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.12P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.50$ e Å^{-3}

$\Delta\rho_{min} = -0.71$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0120 (18)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ 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}
Rb1	0.18947 (8)	1.00955 (2)	0.24241 (6)	0.0381 (2)
O1	−0.0671 (5)	0.91314 (15)	0.4428 (4)	0.0404 (8)
O2	0.3775 (6)	0.93503 (16)	0.5483 (5)	0.0580 (11)
O3	0.5150 (5)	0.86504 (16)	0.7365 (4)	0.0456 (9)
O4	0.3512 (6)	0.64498 (16)	0.6287 (5)	0.0537 (10)
O5	0.0559 (6)	0.61696 (16)	0.4603 (5)	0.0562 (10)
O6	0.3268 (7)	1.03788 (18)	−0.1415 (5)	0.0526 (9)
H6A	0.382 (10)	1.0686 (17)	−0.086 (6)	0.079*
H6B	0.281 (10)	1.053 (2)	−0.239 (4)	0.079*
N1	0.3753 (6)	0.88137 (18)	0.6150 (5)	0.0331 (9)
N2	0.1790 (7)	0.65827 (18)	0.5345 (5)	0.0373 (9)
C1	−0.0063 (7)	0.8557 (2)	0.4619 (5)	0.0290 (10)
C2	0.2080 (7)	0.8349 (2)	0.5482 (5)	0.0261 (10)
C3	0.2641 (7)	0.7709 (2)	0.5735 (5)	0.0269 (10)

H3	0.4019	0.7594	0.6333	0.032*
C4	0.1145 (7)	0.7246 (2)	0.5096 (5)	0.0289 (10)
C5	−0.0968 (7)	0.7407 (2)	0.4243 (6)	0.0346 (11)
H5	−0.1973	0.7088	0.3830	0.042*
C6	−0.1537 (7)	0.8033 (2)	0.4023 (6)	0.0357 (11)
H6	−0.2952	0.8131	0.3458	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.0429 (3)	0.0320 (4)	0.0387 (3)	−0.0036 (2)	−0.0061 (2)	0.00384 (19)
O1	0.0411 (18)	0.029 (2)	0.050 (2)	0.0061 (15)	−0.0026 (16)	0.0050 (15)
O2	0.069 (2)	0.030 (2)	0.071 (3)	−0.0178 (18)	−0.032 (2)	0.0149 (18)
O3	0.0428 (19)	0.038 (2)	0.054 (2)	−0.0031 (15)	−0.0188 (17)	0.0056 (16)
O4	0.067 (2)	0.031 (2)	0.061 (3)	0.0131 (17)	−0.016 (2)	0.0011 (17)
O5	0.067 (2)	0.028 (2)	0.073 (3)	−0.0102 (18)	−0.003 (2)	−0.0112 (18)
O6	0.054 (2)	0.050 (2)	0.053 (2)	−0.005 (2)	−0.0014 (19)	0.0058 (19)
N1	0.032 (2)	0.031 (2)	0.036 (2)	−0.0009 (17)	−0.0042 (17)	0.0016 (17)
N2	0.049 (2)	0.026 (2)	0.038 (2)	−0.0007 (18)	0.0042 (19)	−0.0026 (17)
C1	0.029 (2)	0.030 (3)	0.028 (3)	0.0015 (19)	0.0013 (19)	0.0044 (19)
C2	0.026 (2)	0.023 (2)	0.029 (2)	−0.0053 (17)	−0.0047 (18)	−0.0001 (17)
C3	0.027 (2)	0.031 (3)	0.022 (2)	0.0001 (19)	−0.0010 (18)	0.0022 (18)
C4	0.036 (2)	0.023 (2)	0.027 (2)	0.000 (2)	0.0044 (18)	−0.0015 (18)
C5	0.035 (2)	0.035 (3)	0.034 (3)	−0.006 (2)	−0.001 (2)	−0.003 (2)
C6	0.027 (2)	0.045 (3)	0.035 (3)	0.001 (2)	−0.0053 (19)	−0.005 (2)

Geometric parameters (Å, °)

Rb1—O2	2.914 (3)	O4—Rb1^{vii}	3.474 (4)
Rb1—O1^{i}	2.956 (3)	O5—N2	1.232 (5)
Rb1—O1	2.957 (3)	O5—Rb1^{viii}	3.016 (3)
Rb1—O5^{ii}	3.016 (3)	O5—Rb1^{vii}	3.429 (4)
Rb1—O6	3.057 (4)	O6—Rb1^{iv}	3.127 (4)
Rb1—O2^{iii}	3.119 (3)	O6—Rb1^{v}	3.228 (4)
Rb1—O6^{iv}	3.127 (4)	O6—H6A	0.818 (10)
Rb1—O3^{iii}	3.134 (3)	O6—H6B	0.820 (10)
Rb1—O6^{v}	3.228 (4)	N1—C2	1.446 (5)
Rb1—O5^{vi}	3.429 (4)	N1—Rb1^{iii}	3.533 (4)
Rb1—O4^{vi}	3.474 (4)	N2—C4	1.443 (5)
Rb1—N1^{iii}	3.533 (4)	C1—C2	1.443 (5)
Rb1—H6A	3.00 (5)	C1—C6	1.446 (6)
O1—C1	1.255 (5)	C2—C3	1.384 (6)
O1—Rb1^{i}	2.956 (3)	C3—C4	1.369 (6)
O2—N1	1.223 (5)	C3—H3	0.9300
O2—Rb1^{iii}	3.119 (3)	C4—C5	1.398 (6)
O3—N1	1.231 (4)	C5—C6	1.353 (6)

O3—Rb1^{iii}	3.134 (3)	C5—H5	0.9300
O4—N2	1.226 (5)	C6—H6	0.9300
O2—Rb1—O1^{i}	76.94 (10)	O6^{v}—Rb1—N1^{iii}	156.48 (9)
O2—Rb1—O1	55.06 (9)	O5^{vi}—Rb1—N1^{iii}	144.49 (9)
O1^{i}—Rb1—O1	79.77 (10)	O4^{vi}—Rb1—N1^{iii}	117.89 (9)
O2—Rb1—O5^{ii}	158.84 (11)	O2—Rb1—H6A	135.0 (11)
O1^{i}—Rb1—O5^{ii}	81.90 (10)	O1^{i}—Rb1—H6A	122.3 (6)
O1—Rb1—O5^{ii}	120.93 (10)	O1—Rb1—H6A	155.4 (2)
O2—Rb1—O6	136.06 (12)	O5^{ii}—Rb1—H6A	58.7 (11)
O1^{i}—Rb1—O6	135.80 (9)	O6—Rb1—H6A	15.5 (2)
O1—Rb1—O6	139.96 (10)	O2^{iii}—Rb1—H6A	85.5 (6)
O5^{ii}—Rb1—O6	62.29 (11)	O6^{iv}—Rb1—H6A	63.4 (11)
O2—Rb1—O2^{iii}	63.18 (11)	O3^{iii}—Rb1—H6A	57.8 (2)
O1^{i}—Rb1—O2^{iii}	68.35 (10)	O6^{v}—Rb1—H6A	109.0 (8)
O1—Rb1—O2^{iii}	115.03 (9)	O5^{vi}—Rb1—H6A	84.5 (3)
O5^{ii}—Rb1—O2^{iii}	108.92 (10)	O4^{vi}—Rb1—H6A	93.7 (8)
O6—Rb1—O2^{iii}	98.24 (10)	N1^{iii}—Rb1—H6A	71.5 (4)
O2—Rb1—O6^{iv}	73.11 (11)	C1—O1—Rb1^{i}	120.7 (3)
O1^{i}—Rb1—O6^{iv}	128.52 (9)	C1—O1—Rb1	123.8 (3)
O1—Rb1—O6^{iv}	113.35 (9)	Rb1^{i}—O1—Rb1	100.23 (10)
O5^{ii}—Rb1—O6^{iv}	121.87 (11)	N1—O2—Rb1	142.2 (3)
O6—Rb1—O6^{iv}	63.31 (11)	N1—O2—Rb1^{iii}	99.5 (2)
O2^{iii}—Rb1—O6^{iv}	60.97 (10)	Rb1—O2—Rb1^{iii}	116.82 (11)
O2—Rb1—O3^{iii}	102.84 (9)	N1—O3—Rb1^{iii}	98.5 (2)
O1^{i}—Rb1—O3^{iii}	70.30 (9)	N2—O4—Rb1^{vii}	97.0 (3)
O1—Rb1—O3^{iii}	146.73 (9)	N2—O5—Rb1^{viii}	172.5 (3)
O5^{ii}—Rb1—O3^{iii}	69.62 (9)	N2—O5—Rb1^{vii}	99.1 (3)
O6—Rb1—O3^{iii}	73.29 (9)	Rb1^{viii}—O5—Rb1^{vii}	79.58 (8)
O2^{iii}—Rb1—O3^{iii}	40.11 (8)	Rb1—O6—Rb1^{iv}	116.69 (11)
O6^{iv}—Rb1—O3^{iii}	76.78 (9)	Rb1—O6—Rb1^{v}	82.29 (9)
O2—Rb1—O6^{v}	109.00 (9)	Rb1^{iv}—O6—Rb1^{v}	134.09 (13)
O1^{i}—Rb1—O6^{v}	94.91 (10)	Rb1—O6—H6A	78 (4)
O1—Rb1—O6^{v}	54.09 (9)	Rb1^{iv}—O6—H6A	92 (4)
O5^{ii}—Rb1—O6^{v}	72.43 (10)	Rb1^{v}—O6—H6A	134 (4)
O6—Rb1—O6^{v}	97.71 (9)	Rb1—O6—H6B	144 (4)
O2^{iii}—Rb1—O6^{v}	162.41 (11)	Rb1^{iv}—O6—H6B	100 (4)
O6^{iv}—Rb1—O6^{v}	134.09 (13)	Rb1^{v}—O6—H6B	70 (4)
O3^{iii}—Rb1—O6^{v}	140.73 (9)	H6A—O6—H6B	104.1 (17)
O2—Rb1—O5^{vi}	97.36 (9)	O2—N1—O3	121.8 (4)
O1^{i}—Rb1—O5^{vi}	147.52 (9)	O2—N1—C2	119.8 (3)
O1—Rb1—O5^{vi}	71.24 (9)	O3—N1—C2	118.4 (4)

O5^{ii}—Rb1—O5^{vi}	100.42 (8)	O2—N1—Rb1^{iii}	60.6 (2)
O6—Rb1—O5^{vi}	69.13 (9)	O3—N1—Rb1^{iii}	61.3 (2)
O2^{iii}—Rb1—O5^{vi}	137.72 (10)	C2—N1—Rb1^{iii}	176.1 (3)
O6^{iv}—Rb1—O5^{vi}	77.88 (10)	O4—N2—O5	122.6 (4)
O3^{iii}—Rb1—O5^{vi}	141.14 (9)	O4—N2—C4	119.4 (4)
O6^{v}—Rb1—O5^{vi}	56.22 (10)	O5—N2—C4	118.1 (4)
O2—Rb1—O4^{vi}	66.31 (9)	O1—C1—C2	124.8 (4)
O1^{i}—Rb1—O4^{vi}	141.08 (9)	O1—C1—C6	121.7 (4)
O1—Rb1—O4^{vi}	69.16 (9)	C2—C1—C6	113.4 (4)
O5^{ii}—Rb1—O4^{vi}	134.11 (9)	C3—C2—C1	123.0 (4)
O6—Rb1—O4^{vi}	82.20 (10)	C3—C2—N1	116.7 (3)
O2^{iii}—Rb1—O4^{vi}	103.85 (9)	C1—C2—N1	120.4 (4)
O6^{iv}—Rb1—O4^{vi}	52.17 (9)	C4—C3—C2	119.3 (4)
O3^{iii}—Rb1—O4^{vi}	128.95 (9)	C4—C3—H3	120.3
O6^{v}—Rb1—O4^{vi}	85.63 (9)	C2—C3—H3	120.3
O5^{vi}—Rb1—O4^{vi}	36.39 (8)	C3—C4—C5	121.3 (4)
O2—Rb1—N1^{iii}	82.82 (9)	C3—C4—N2	118.2 (4)
O1^{i}—Rb1—N1^{iii}	67.35 (9)	C5—C4—N2	120.5 (4)
O1—Rb1—N1^{iii}	131.67 (9)	C6—C5—C4	119.5 (4)
O5^{ii}—Rb1—N1^{iii}	89.25 (10)	C6—C5—H5	120.3
O6—Rb1—N1^{iii}	86.10 (9)	C4—C5—H5	120.3
O2^{iii}—Rb1—N1^{iii}	19.97 (8)	C5—C6—C1	123.5 (4)
O6^{iv}—Rb1—N1^{iii}	68.15 (9)	C5—C6—H6	118.2
O3^{iii}—Rb1—N1^{iii}	20.16 (8)	C1—C6—H6	118.2
O2—Rb1—O1—C1	−57.1 (3)	O6^{v}—Rb1—O6—Rb1^{iv}	−135.87 (16)
O1^{i}—Rb1—O1—C1	−138.2 (4)	O5^{vi}—Rb1—O6—Rb1^{iv}	−86.57 (13)
O5^{ii}—Rb1—O1—C1	147.8 (3)	O4^{vi}—Rb1—O6—Rb1^{iv}	−51.39 (12)
O6—Rb1—O1—C1	65.2 (4)	N1^{iii}—Rb1—O6—Rb1^{iv}	67.47 (12)
O2^{iii}—Rb1—O1—C1	−78.1 (3)	O2—Rb1—O6—Rb1^{v}	127.89 (11)
O6^{iv}—Rb1—O1—C1	−10.5 (3)	O1^{i}—Rb1—O6—Rb1^{v}	−105.25 (12)
O3^{iii}—Rb1—O1—C1	−112.3 (3)	O1—Rb1—O6—Rb1^{v}	40.64 (17)
O6^{v}—Rb1—O1—C1	118.0 (4)	O5^{ii}—Rb1—O6—Rb1^{v}	−65.46 (10)
O5^{vi}—Rb1—O1—C1	56.7 (3)	O2^{iii}—Rb1—O6—Rb1^{v}	−172.56 (9)
O4^{vi}—Rb1—O1—C1	18.0 (3)	O6^{iv}—Rb1—O6—Rb1^{v}	135.87 (16)
N1^{iii}—Rb1—O1—C1	−91.4 (3)	O3^{iii}—Rb1—O6—Rb1^{v}	−140.81 (10)
O2—Rb1—O1—Rb1^{i}	81.14 (12)	O6^{v}—Rb1—O6—Rb1^{v}	0.0
O1^{i}—Rb1—O1—Rb1^{i}	0.0	O5^{vi}—Rb1—O6—Rb1^{v}	49.30 (8)
O5^{ii}—Rb1—O1—Rb1^{i}	−74.03 (13)	O4^{vi}—Rb1—O6—Rb1^{v}	84.48 (8)
O6—Rb1—O1—Rb1^{i}	−156.60 (12)	N1^{iii}—Rb1—O6—Rb1^{v}	−156.66 (9)
O2^{iii}—Rb1—O1—Rb1^{i}	60.13 (12)	Rb1—O2—N1—O3	167.0 (4)

O6^{iv}—Rb1—O1—Rb1^{i}	127.69 (9)	Rb1^{iii}—O2—N1—O3	3.2 (5)
O3^{iii}—Rb1—O1—Rb1^{i}	25.93 (19)	Rb1—O2—N1—C2	−11.7 (7)
O6^{v}—Rb1—O1—Rb1^{i}	−103.77 (13)	Rb1^{iii}—O2—N1—C2	−175.5 (3)
O5^{vi}—Rb1—O1—Rb1^{i}	−165.14 (11)	Rb1—O2—N1—Rb1^{iii}	163.8 (6)
O4^{vi}—Rb1—O1—Rb1^{i}	156.16 (11)	Rb1^{iii}—O3—N1—O2	−3.2 (5)
N1^{iii}—Rb1—O1—Rb1^{i}	46.81 (14)	Rb1^{iii}—O3—N1—C2	175.5 (3)
O1^{i}—Rb1—O2—N1	125.8 (5)	Rb1^{vii}—O4—N2—O5	−23.8 (5)
O1—Rb1—O2—N1	39.3 (5)	Rb1^{vii}—O4—N2—C4	155.5 (3)
O5^{ii}—Rb1—O2—N1	125.4 (5)	Rb1^{vii}—O5—N2—O4	24.3 (5)
O6—Rb1—O2—N1	−89.1 (5)	Rb1^{vii}—O5—N2—C4	−155.1 (3)
O2^{iii}—Rb1—O2—N1	−162.0 (6)	Rb1^{i}—O1—C1—C2	−70.6 (5)
O6^{iv}—Rb1—O2—N1	−96.5 (5)	Rb1—O1—C1—C2	59.7 (5)
O3^{iii}—Rb1—O2—N1	−168.2 (5)	Rb1^{i}—O1—C1—C6	107.4 (4)
O6^{v}—Rb1—O2—N1	35.1 (5)	Rb1—O1—C1—C6	−122.3 (4)
O5^{vi}—Rb1—O2—N1	−21.6 (5)	O1—C1—C2—C3	177.1 (4)
O4^{vi}—Rb1—O2—N1	−41.1 (5)	C6—C1—C2—C3	−1.0 (6)
N1^{iii}—Rb1—O2—N1	−165.8 (5)	O1—C1—C2—N1	−2.2 (7)
O1^{i}—Rb1—O2—Rb1^{iii}	−72.12 (14)	C6—C1—C2—N1	179.7 (4)
O1—Rb1—O2—Rb1^{iii}	−158.66 (19)	O2—N1—C2—C3	155.4 (4)
O5^{ii}—Rb1—O2—Rb1^{iii}	−72.6 (3)	O3—N1—C2—C3	−23.3 (6)
O6—Rb1—O2—Rb1^{iii}	72.95 (19)	O2—N1—C2—C1	−25.2 (6)
O2^{iii}—Rb1—O2—Rb1^{iii}	0.0	O3—N1—C2—C1	156.0 (4)
O6^{iv}—Rb1—O2—Rb1^{iii}	65.50 (14)	C1—C2—C3—C4	2.1 (7)
O3^{iii}—Rb1—O2—Rb1^{iii}	−6.18 (17)	N1—C2—C3—C4	−178.6 (4)
O6^{v}—Rb1—O2—Rb1^{iii}	−162.86 (13)	C2—C3—C4—C5	−2.0 (6)
O5^{vi}—Rb1—O2—Rb1^{iii}	140.40 (14)	C2—C3—C4—N2	178.8 (4)
O4^{vi}—Rb1—O2—Rb1^{iii}	120.98 (17)	O4—N2—C4—C3	8.2 (6)
N1^{iii}—Rb1—O2—Rb1^{iii}	−3.78 (13)	O5—N2—C4—C3	−172.4 (4)
O2—Rb1—O6—Rb1^{iv}	−8.0 (2)	O4—N2—C4—C5	−171.0 (4)
O1^{i}—Rb1—O6—Rb1^{iv}	118.88 (14)	O5—N2—C4—C5	8.3 (7)
O1—Rb1—O6—Rb1^{iv}	−95.23 (16)	C3—C4—C5—C6	0.8 (7)
O5^{ii}—Rb1—O6—Rb1^{iv}	158.67 (17)	N2—C4—C5—C6	−180.0 (4)
O2^{iii}—Rb1—O6—Rb1^{iv}	51.57 (14)	C4—C5—C6—C1	0.3 (7)
O6^{iv}—Rb1—O6—Rb1^{iv}	0.0	O1—C1—C6—C5	−178.4 (4)
O3^{iii}—Rb1—O6—Rb1^{iv}	83.33 (12)	C2—C1—C6—C5	−0.2 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6B···O1^{v}	0.820 (10)	2.03 (2)	2.822 (5)	161 (6)

O6—H6A···O4^{ix}	0.818 (10)	2.27 (4)	2.919 (5)	137 (5)

Symmetry codes: (v) −*x*, −*y*+2, −*z*; (ix) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

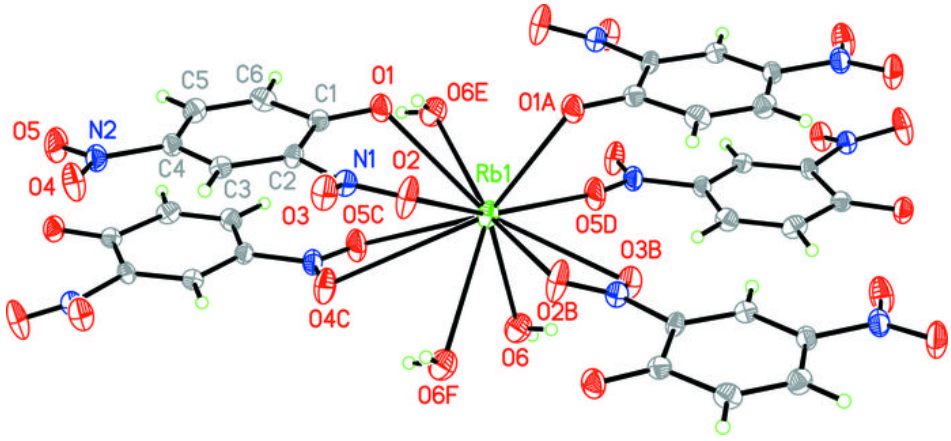

Fig. 2