

Crystal structure of poly[μ -acetato-bis[μ -2-oxo-2-(quinolin-8-yl)ethanoato]-trisodium]

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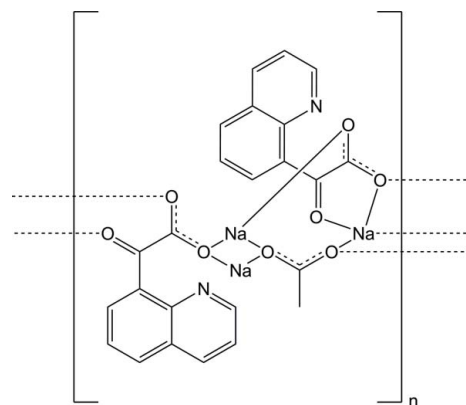
The title compound $[\text{Na}_3(\text{C}_{11}\text{H}_6\text{NO}_3)_2(\text{C}_2\text{H}_3\text{O}_2)]_n$, crystallized through diffusion of diethyl ether into methanol as needles. There are three crystallographically independent Na^+ cations present, each exhibiting a distorted octahedral coordination geometry, two through coordination by five O atoms and one N atom, and one through coordination by six O atoms. A series of intermolecular $\text{O}\cdots\text{Na}$ and $\text{N}\cdots\text{Na}$ contacts leads to the formation of chains along the a -axis direction.

Keywords: crystal structure; keto acid; sodium; acetate.

CCDC reference: 1030741

1. Related literature

The sodium salt of 2-oxo-2-(quinolin-8-yl)ethanoic acid was prepared as an authentic product during a catalytic process development within our group. Ethyl 2-oxo-2-(quinolin-8-yl)ethanoate was prepared by a literature procedure (Crespo-Peña *et al.*, 2012) and then hydrolysed under basic conditions to yield the title compound. For sodium salts of keto-acids, see; Lis & Matuszewski (1984); Jain *et al.* (1969); Tavale *et al.* (1961, 1964); Rach *et al.* (1988). A similar $\text{Na}\cdots\text{C}=\text{N}$ (quinoline) interaction is observed in a previously published samarium Schiff base complex (Li *et al.*, 2008).



2. Experimental

2.1. Crystal data

$[\text{Na}_3(\text{C}_{11}\text{H}_6\text{NO}_3)_2(\text{C}_2\text{H}_3\text{O}_2)]$
 $M_r = 528.35$
 Monoclinic, $P2_1/c$
 $a = 6.1101$ (5) Å
 $b = 22.7075$ (19) Å
 $c = 16.1587$ (12) Å
 $\beta = 94.626$ (7)°

$V = 2234.6$ (3) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 1.50$ mm⁻¹
 $T = 120$ K
 $0.19 \times 0.04 \times 0.03$ mm

2.2. Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
 Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2014), based on expressions derived by Clark & Reid (1995)]
 $T_{\min} = 0.887$, $T_{\max} = 0.971$

7799 measured reflections
 3943 independent reflections
 2557 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.130$
 $S = 0.99$
 3943 reflections

335 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.25$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: PJ2016).

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supporting information

Acta Cryst. (2014). E70, m385–m386 [doi:10.1107/S1600536814023423]

Crystal structure of poly[μ -acetato-bis[μ -2-oxo-2-(quinolin-8-yl)ethanoato]trisodium]

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S1. Comment

The sodium salt (1) of 2-oxo-2-(quinolin-8-yl)ethanoic acid was prepared as an authentic product during a catalytic process development within our group. Ethyl 2-oxo-2-(quinolin-8-yl)ethanoate was prepared by a literature procedure (Crespo-Peña *et al.*, 2012) and then hydrolysed under basic conditions to yield the title compound.

The asymmetric unit of 1 (Fig. 1) contains two crystallographically independent 2-oxo-2-(quinolin-8-yl)ethanoate anions, one acetate anion and three crystallographically independent sodium cations. Each sodium cation exhibits distorted octahedral geometry. One sodium cation (Na36) is coordinated by six oxygen atoms from the oxo-2'-quinolin-8'-yl-ethanoate and acetate ions. Na \cdots O bond distances are in the range 2.290 (3) to 2.610 (3) Å. The other two sodium cations (Na35, Na37) are coordinated by five oxygen atoms (2.272 (3)–2.727 (3) Å) and what appears to be an η_2 interaction with a C=N of the quinoline ring (Na \cdots N = 2.769 (3), 2.814 (3); Na \cdots C = 3.035 (4), 3.073 (4)). A similar Na \cdots C=N (quinoline) interaction is observed in a previously published samarium Schiff base complex (Li *et al.*, 2008), although this is somewhat shorter than that observed in 1. Na \cdots O bond lengths are comparable to previously published sodium salts of keto acids (Lis *et al.*, 1984, Jain *et al.*, 1969, Tavale *et al.*, 1961, 1964, Rach *et al.*, 1988).

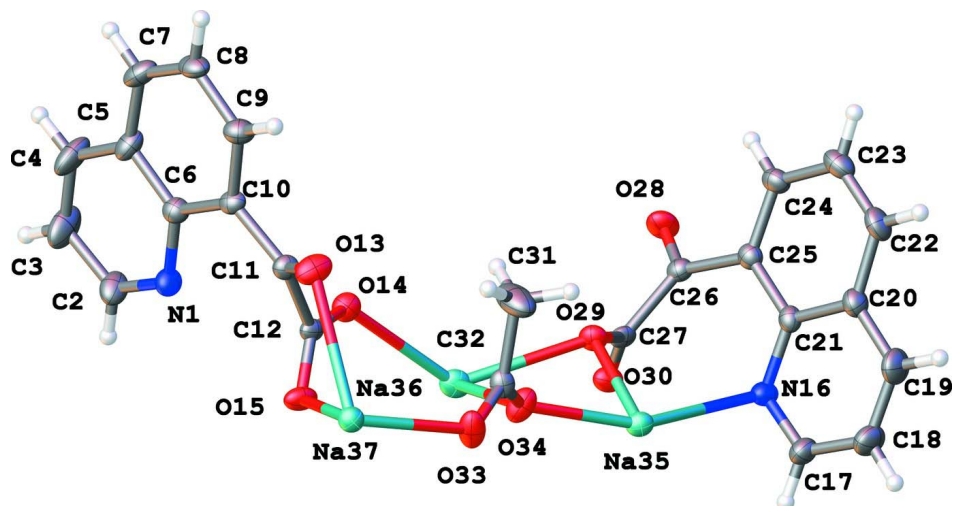
These Na \cdots O interactions lead to the formation of one-dimensional chains along the crystallographic *a*-axis (Fig. 2). The quinoline rings of the oxo(8-quinolyl)acetate groups and methyl groups of acetate ions appear to act as a hydrophobic sheath, encapsulating the Na \cdots O core of the chains, keeping them separated in the solid state. (Fig. 3).

S2. Experimental

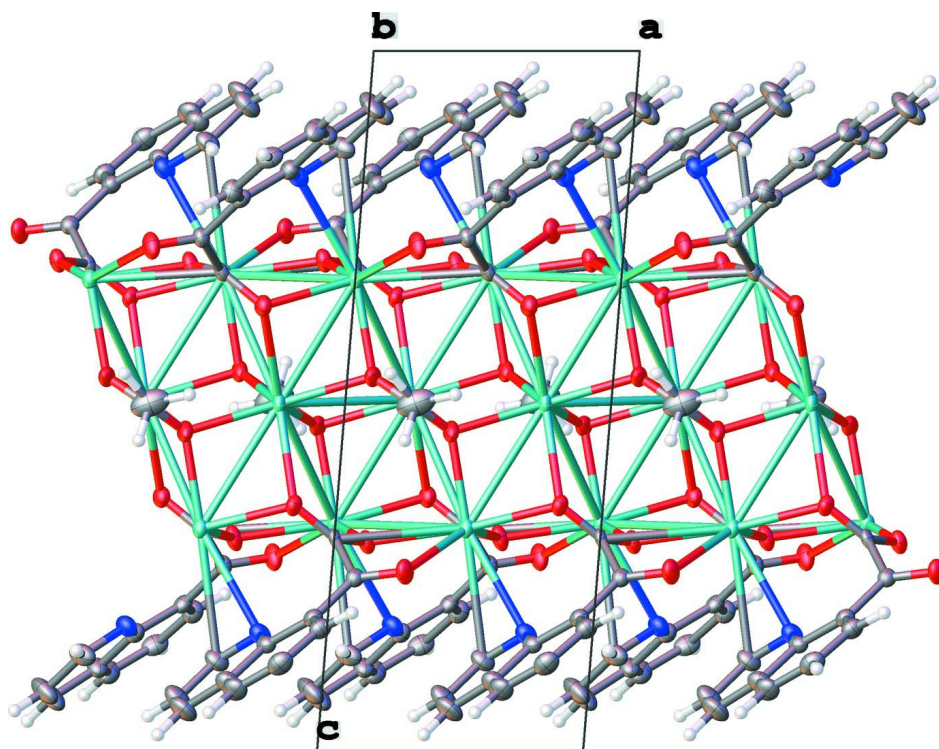
A solution of ethyl 2-oxo-2-(quinolin-8-yl)ethanoate (217 mg, 0.947 mmol) in methanol (3mL) was cooled to 0 °C and aqueous 2M NaOH (3 mL) added and stirred at room temperature for 90 min. The methanol was removed under vacuum and the remaining aqueous solution was washed at pH 9 with ethyl acetate (2 x 20 mL). The aqueous solution was acidified to pH 5 with 1M HCl and washed with ethyl acetate (2 x 20 mL). The remaining aqueous solution was reduced under vacuum to give a white solid (0.231 g) which was dissolved in methanol and filtered to remove NaCl. The product was recrystallised through diffusion of diethyl ether into a solution of the product in a minimum amount of methanol over three days to afford colourless needles.

S3. Refinement

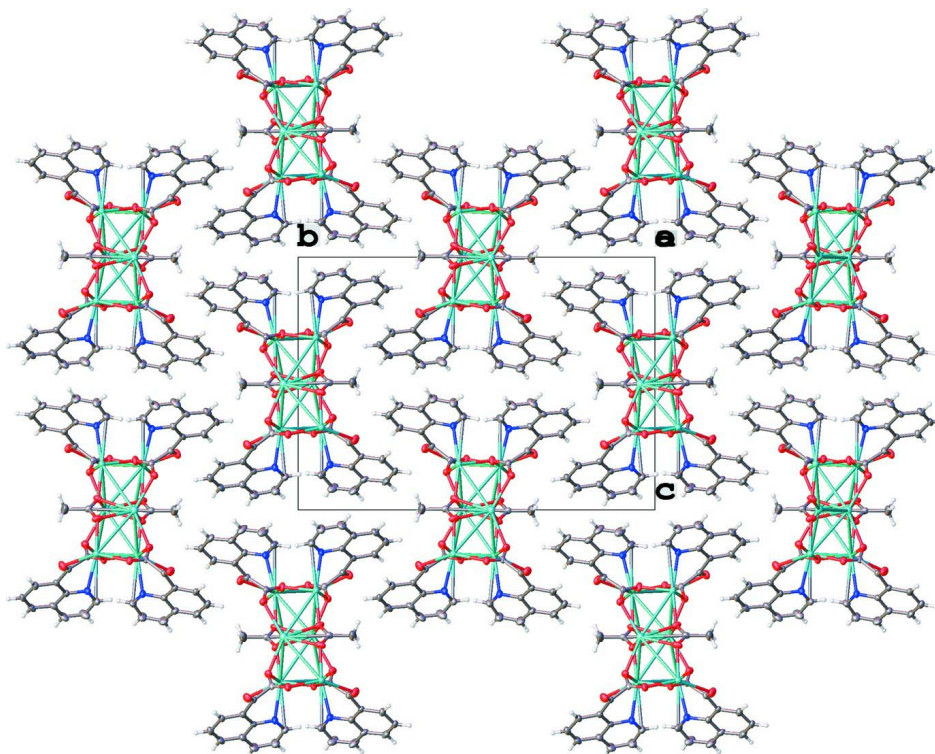
No special refinement procedures were applied to this crystal structure. All hydrogen atoms were placed in calculated positions and refined isotropically using a riding model.

**Figure 1**

The asymmetric unit of (1) showing the labelling scheme. Displacement ellipsoids are at the 50% probability level. Hydrogen atoms have been omitted for clarity.

**Figure 2**

Partial packing diagram of (1) showing the one-dimensional chain along the crystallographic *a*-axis. Displacement ellipsoids are at the 50% probability level.

**Figure 3**

Partial packing diagram of (1) viewed on the *bc* plane. Displacement ellipsoids are at the 50% probability level.

Poly[μ -acetato-bis[μ -2-oxo-2-(quinolin-8-yl)ethanoato]trisodium]

Crystal data

[Na₃(C₁₁H₆NO₃)₂(C₂H₃O₂)]

$M_r = 528.35$

Monoclinic, $P2_1/c$

$a = 6.1101 (5) \text{ \AA}$

$b = 22.7075 (19) \text{ \AA}$

$c = 16.1587 (12) \text{ \AA}$

$\beta = 94.626 (7)^\circ$

$V = 2234.6 (3) \text{ \AA}^3$

$Z = 4$

$F(000) = 1080$

$D_x = 1.570 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$

Cell parameters from 1524 reflections

$\theta = 5.5\text{--}72.4^\circ$

$\mu = 1.50 \text{ mm}^{-1}$

$T = 120 \text{ K}$

Needle, colourless

$0.19 \times 0.04 \times 0.03 \text{ mm}$

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer

Radiation source: sealed X-ray tube, SuperNova (Cu) X-ray Source

Mirror monochromator

Detector resolution: $10.6191 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: analytical

[*CrysAlis PRO* (Agilent, 2014), based on expressions derived by Clark & Reid (1995)]

$T_{\min} = 0.887$, $T_{\max} = 0.971$

7799 measured reflections

3943 independent reflections

2557 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

$\theta_{\max} = 66.6^\circ$, $\theta_{\min} = 3.4^\circ$

$h = -4 \rightarrow 7$

$k = -25 \rightarrow 26$

$l = -18 \rightarrow 19$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.050$ $wR(F^2) = 0.130$ $S = 0.99$

3943 reflections

335 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0475P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$ *Special details*

Experimental. Absorption correction: CrysAlisPro, Agilent Technologies, Version 1.171.37.33 (release 27-03-2014 CrysAlis171 .NET) (compiled Mar 27 2014,17:12:48) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.2460 (5)	0.59015 (12)	0.32073 (16)	0.0248 (6)
C2	0.0893 (6)	0.56634 (17)	0.3616 (2)	0.0324 (8)
H2	0.0647	0.5261	0.3557	0.039*
C3	-0.0423 (7)	0.59804 (19)	0.4134 (2)	0.0447 (11)
H3	-0.1491	0.5789	0.4413	0.054*
C4	-0.0117 (7)	0.65702 (19)	0.4222 (2)	0.0428 (10)
H4	-0.0980	0.6786	0.4561	0.051*
C5	0.1503 (5)	0.68536 (16)	0.3801 (2)	0.0267 (7)
C6	0.2792 (5)	0.65001 (14)	0.33027 (19)	0.0220 (7)
C7	0.1939 (6)	0.74641 (16)	0.3868 (2)	0.0303 (8)
H7	0.1080	0.7698	0.4186	0.036*
C8	0.3585 (6)	0.77153 (15)	0.3477 (2)	0.0281 (8)
H8	0.3841	0.8118	0.3524	0.034*
C9	0.4899 (6)	0.73642 (14)	0.3001 (2)	0.0259 (7)
H9	0.6058	0.7538	0.2752	0.031*
C10	0.4523 (5)	0.67691 (13)	0.28926 (18)	0.0197 (6)
C11	0.5912 (5)	0.64329 (14)	0.23363 (19)	0.0204 (7)
C12	0.5049 (5)	0.58940 (13)	0.18503 (18)	0.0180 (6)
O13	0.7770 (4)	0.66025 (11)	0.22217 (15)	0.0303 (6)
O14	0.3382 (4)	0.59685 (10)	0.13640 (13)	0.0237 (5)
O15	0.6225 (4)	0.54440 (10)	0.19491 (14)	0.0255 (5)

N16	0.2494 (4)	0.56492 (12)	-0.33221 (16)	0.0245 (6)
C17	0.4040 (6)	0.53700 (16)	-0.3695 (2)	0.0285 (8)
H17	0.4232	0.4970	-0.3590	0.034*
C18	0.5401 (7)	0.56398 (17)	-0.4235 (2)	0.0371 (9)
H18	0.6454	0.5422	-0.4487	0.045*
C19	0.5161 (7)	0.62277 (17)	-0.4390 (2)	0.0385 (9)
H19	0.6037	0.6413	-0.4755	0.046*
C20	0.3589 (6)	0.65517 (15)	-0.3995 (2)	0.0268 (7)
C21	0.2230 (5)	0.62401 (14)	-0.34723 (18)	0.0200 (6)
C22	0.3271 (6)	0.71665 (16)	-0.4110 (2)	0.0310 (8)
H22	0.4179	0.7375	-0.4440	0.037*
C23	0.1646 (6)	0.74553 (16)	-0.3741 (2)	0.0307 (8)
H23	0.1461	0.7859	-0.3816	0.037*
C24	0.0249 (5)	0.71412 (14)	-0.32455 (19)	0.0241 (7)
H24	-0.0893	0.7338	-0.3017	0.029*
C25	0.0544 (5)	0.65465 (14)	-0.30924 (18)	0.0208 (7)
C26	-0.0895 (5)	0.62462 (13)	-0.25169 (18)	0.0200 (6)
C27	-0.0049 (5)	0.57333 (13)	-0.19636 (19)	0.0182 (6)
O28	-0.2754 (4)	0.64243 (11)	-0.24306 (15)	0.0288 (5)
O29	0.1611 (3)	0.58346 (10)	-0.14860 (13)	0.0219 (5)
O30	-0.1234 (3)	0.52831 (10)	-0.20085 (13)	0.0232 (5)
C31	0.7331 (9)	0.65337 (18)	-0.0025 (3)	0.0526 (12)
H31A	0.5884	0.6654	0.0096	0.079*
H31B	0.7644	0.6685	-0.0557	0.079*
H31C	0.8387	0.6684	0.0395	0.079*
C32	0.7452 (5)	0.58759 (14)	-0.00364 (19)	0.0205 (7)
O33	0.9040 (4)	0.56211 (12)	0.03523 (14)	0.0312 (6)
O34	0.5933 (4)	0.55990 (11)	-0.04300 (14)	0.0278 (5)
Na35	0.50542 (19)	0.54983 (5)	-0.18100 (7)	0.0201 (3)
Na36	0.2478 (2)	0.54062 (6)	-0.00310 (8)	0.0247 (3)
Na37	0.99681 (19)	0.56515 (5)	0.17420 (7)	0.0198 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0263 (16)	0.0231 (15)	0.0257 (13)	-0.0049 (11)	0.0074 (11)	-0.0003 (12)
C2	0.041 (2)	0.0288 (19)	0.0285 (17)	-0.0146 (15)	0.0098 (15)	-0.0036 (15)
C3	0.044 (2)	0.053 (3)	0.041 (2)	-0.020 (2)	0.0246 (18)	-0.013 (2)
C4	0.041 (2)	0.049 (3)	0.041 (2)	-0.0106 (18)	0.0226 (18)	-0.0217 (19)
C5	0.0249 (19)	0.0326 (19)	0.0230 (16)	-0.0020 (14)	0.0042 (13)	-0.0095 (14)
C6	0.0215 (17)	0.0213 (17)	0.0228 (15)	-0.0020 (12)	0.0001 (12)	-0.0012 (13)
C7	0.0286 (19)	0.0312 (19)	0.0310 (18)	0.0072 (14)	0.0005 (14)	-0.0131 (15)
C8	0.040 (2)	0.0166 (16)	0.0269 (16)	0.0015 (14)	-0.0046 (15)	-0.0049 (14)
C9	0.0260 (18)	0.0201 (17)	0.0314 (17)	-0.0006 (13)	0.0007 (13)	-0.0020 (14)
C10	0.0200 (17)	0.0187 (16)	0.0199 (14)	-0.0002 (12)	-0.0030 (12)	-0.0037 (13)
C11	0.0175 (17)	0.0204 (16)	0.0237 (15)	-0.0006 (12)	0.0043 (12)	-0.0002 (13)
C12	0.0168 (16)	0.0168 (16)	0.0215 (14)	-0.0002 (12)	0.0080 (12)	0.0007 (12)
O13	0.0193 (13)	0.0291 (13)	0.0431 (13)	-0.0082 (9)	0.0065 (10)	-0.0104 (11)

O14	0.0174 (12)	0.0270 (12)	0.0267 (11)	-0.0040 (9)	0.0018 (9)	-0.0018 (10)
O15	0.0183 (12)	0.0200 (12)	0.0395 (13)	0.0009 (9)	0.0108 (10)	-0.0027 (10)
N16	0.0279 (16)	0.0189 (14)	0.0277 (14)	0.0010 (11)	0.0087 (11)	0.0011 (12)
C17	0.034 (2)	0.0255 (18)	0.0274 (16)	0.0027 (14)	0.0107 (14)	-0.0026 (14)
C18	0.041 (2)	0.034 (2)	0.0386 (19)	0.0038 (17)	0.0206 (17)	-0.0013 (17)
C19	0.045 (2)	0.040 (2)	0.0339 (19)	-0.0035 (17)	0.0211 (17)	0.0055 (18)
C20	0.0318 (19)	0.0251 (18)	0.0242 (15)	-0.0025 (14)	0.0059 (14)	0.0033 (14)
C21	0.0219 (17)	0.0211 (16)	0.0170 (14)	-0.0043 (12)	0.0012 (12)	0.0001 (12)
C22	0.035 (2)	0.030 (2)	0.0284 (17)	-0.0062 (15)	0.0047 (14)	0.0106 (15)
C23	0.036 (2)	0.0226 (18)	0.0320 (18)	-0.0030 (14)	-0.0043 (15)	0.0071 (15)
C24	0.0265 (18)	0.0204 (17)	0.0246 (16)	0.0025 (13)	-0.0027 (13)	0.0019 (13)
C25	0.0213 (17)	0.0215 (17)	0.0193 (14)	-0.0005 (12)	-0.0008 (12)	0.0008 (12)
C26	0.0201 (17)	0.0190 (16)	0.0206 (14)	0.0004 (12)	0.0007 (12)	-0.0029 (13)
C27	0.0133 (16)	0.0181 (16)	0.0245 (15)	0.0017 (11)	0.0085 (12)	-0.0015 (13)
O28	0.0186 (13)	0.0308 (13)	0.0375 (13)	0.0084 (10)	0.0045 (10)	0.0062 (11)
O29	0.0153 (12)	0.0242 (12)	0.0258 (11)	0.0035 (8)	-0.0010 (9)	0.0005 (9)
O30	0.0169 (12)	0.0212 (12)	0.0323 (12)	-0.0004 (9)	0.0070 (9)	0.0016 (10)
C31	0.084 (3)	0.025 (2)	0.046 (2)	-0.007 (2)	-0.013 (2)	0.0025 (18)
C32	0.0135 (15)	0.0274 (18)	0.0205 (14)	-0.0018 (12)	0.0004 (12)	0.0025 (13)
O33	0.0159 (12)	0.0532 (16)	0.0243 (11)	0.0085 (10)	0.0012 (9)	0.0068 (11)
O34	0.0150 (12)	0.0415 (15)	0.0269 (11)	-0.0051 (9)	0.0013 (9)	-0.0098 (11)
Na35	0.0146 (6)	0.0211 (6)	0.0245 (6)	0.0003 (4)	0.0016 (5)	-0.0015 (5)
Na36	0.0124 (6)	0.0279 (7)	0.0341 (7)	0.0005 (5)	0.0035 (5)	0.0016 (5)
Na37	0.0149 (6)	0.0221 (6)	0.0224 (6)	-0.0002 (4)	0.0019 (4)	0.0006 (5)

Geometric parameters (Å, °)

N1—C2	1.321 (4)	C24—H24	0.9300
N1—C6	1.381 (4)	C24—C25	1.382 (5)
N1—Na37 ⁱ	2.769 (3)	C25—C26	1.495 (4)
C2—H2	0.9300	C26—C27	1.532 (4)
C2—C3	1.406 (5)	C26—O28	1.224 (4)
C2—Na37 ⁱ	3.035 (4)	C27—O29	1.245 (4)
C3—H3	0.9300	C27—O30	1.252 (4)
C3—C4	1.358 (6)	C27—Na35 ⁱ	3.069 (3)
C4—H4	0.9300	O28—Na35 ⁱ	2.727 (3)
C4—C5	1.402 (5)	O29—Na35	2.337 (2)
C5—C6	1.419 (5)	O29—Na36	2.560 (2)
C5—C7	1.414 (5)	O30—Na35 ⁱ	2.367 (2)
C6—C10	1.430 (5)	O30—Na37 ⁱⁱ	2.288 (2)
C7—H7	0.9300	C31—H31A	0.9600
C7—C8	1.355 (5)	C31—H31B	0.9600
C8—H8	0.9300	C31—H31C	0.9600
C8—C9	1.404 (5)	C31—C32	1.496 (5)
C9—H9	0.9300	C32—O33	1.254 (4)
C9—C10	1.380 (5)	C32—O34	1.251 (4)
C10—C11	1.495 (4)	C32—Na36 ⁱⁱ	2.914 (4)
C11—C12	1.525 (4)	O33—Na36 ⁱⁱ	2.549 (3)

C11—O13	1.227 (4)	O33—Na36 ⁱⁱⁱ	2.290 (3)
C12—O14	1.247 (4)	O33—Na37	2.272 (2)
C12—O15	1.252 (4)	O34—Na35	2.263 (2)
C12—Na37	3.074 (3)	O34—Na36	2.299 (2)
O13—Na37	2.690 (3)	O34—Na36 ⁱⁱ	2.567 (3)
O14—Na36	2.610 (3)	Na35—O15 ⁱⁱ	2.283 (2)
O14—Na37 ⁱ	2.334 (2)	Na35—C27 ⁱⁱⁱ	3.069 (3)
O15—Na35 ⁱⁱ	2.283 (2)	Na35—O28 ⁱⁱⁱ	2.727 (3)
O15—Na37	2.385 (2)	Na35—O30 ⁱⁱⁱ	2.367 (2)
N16—C17	1.322 (4)	Na35—Na36 ⁱⁱ	3.8233 (18)
N16—C21	1.371 (4)	Na35—Na36	3.3934 (17)
N16—Na35	2.814 (3)	Na36—C32 ⁱⁱ	2.913 (4)
C17—H17	0.9300	Na36—O33 ⁱⁱ	2.549 (3)
C17—C18	1.395 (5)	Na36—O33 ⁱ	2.290 (3)
C17—Na35	3.073 (4)	Na36—O34 ⁱⁱ	2.567 (3)
C18—H18	0.9300	Na36—Na35 ⁱⁱ	3.8233 (18)
C18—C19	1.364 (6)	Na36—Na36 ^{iv}	3.554 (3)
C19—H19	0.9300	Na36—Na36 ⁱⁱ	3.586 (3)
C19—C20	1.403 (5)	Na36—Na37 ⁱ	3.4027 (16)
C20—C21	1.420 (4)	Na37—N1 ⁱⁱⁱ	2.769 (3)
C20—C22	1.420 (5)	Na37—C2 ⁱⁱⁱ	3.035 (4)
C21—C25	1.423 (4)	Na37—O14 ⁱⁱⁱ	2.334 (2)
C22—H22	0.9300	Na37—O30 ⁱⁱ	2.288 (2)
C22—C23	1.366 (5)	Na37—Na36 ⁱⁱⁱ	3.4026 (16)
C23—H23	0.9300	Na37—Na36 ⁱⁱ	3.8705 (18)
C23—C24	1.410 (5)		
C2—N1—C6	116.9 (3)	O29—Na35—Na36 ⁱⁱ	107.87 (7)
C2—N1—Na37 ⁱ	88.4 (2)	O29—Na35—Na37 ^v	154.51 (7)
C6—N1—Na37 ⁱ	111.3 (2)	O29—Na35—Na37 ⁱⁱ	60.34 (6)
N1—C2—H2	118.0	O30 ⁱⁱⁱ —Na35—N16	112.27 (9)
N1—C2—C3	124.1 (3)	O30 ⁱⁱⁱ —Na35—C17	87.99 (9)
N1—C2—Na37 ⁱ	65.77 (18)	O30 ⁱⁱⁱ —Na35—C27 ⁱⁱⁱ	22.17 (8)
C3—C2—H2	118.0	O30 ⁱⁱⁱ —Na35—O28 ⁱⁱⁱ	66.74 (8)
C3—C2—Na37 ⁱ	122.0 (3)	O30 ⁱⁱⁱ —Na35—Na36	128.10 (7)
Na37 ⁱ —C2—H2	82.7	O30 ⁱⁱⁱ —Na35—Na36 ⁱⁱ	70.88 (6)
C2—C3—H3	120.4	O30 ⁱⁱⁱ —Na35—Na37 ⁱⁱ	127.51 (7)
C4—C3—C2	119.1 (4)	O30 ⁱⁱⁱ —Na35—Na37 ^v	30.11 (6)
C4—C3—H3	120.4	O34—Na35—O15 ⁱⁱ	104.12 (10)
C3—C4—H4	120.0	O34—Na35—N16	156.15 (10)
C3—C4—C5	119.9 (3)	O34—Na35—C17	177.87 (10)
C5—C4—H4	120.0	O34—Na35—C27 ⁱⁱⁱ	84.64 (9)
C4—C5—C6	117.5 (3)	O34—Na35—O28 ⁱⁱⁱ	101.53 (9)
C4—C5—C7	123.3 (3)	O34—Na35—O29	83.84 (9)
C7—C5—C6	119.2 (3)	O34—Na35—O30 ⁱⁱⁱ	90.03 (9)
N1—C6—C5	122.5 (3)	O34—Na35—Na36 ⁱⁱ	40.55 (7)
N1—C6—C10	118.4 (3)	O34—Na35—Na36	42.34 (6)
C5—C6—C10	119.1 (3)	O34—Na35—Na37 ⁱⁱ	99.15 (7)

C5—C7—H7	119.4	O34—Na35—Na37 ^v	85.38 (7)
C8—C7—C5	121.3 (3)	Na36—Na35—Na36 ⁱⁱ	59.24 (4)
C8—C7—H7	119.4	Na36—Na35—Na37 ^v	109.87 (4)
C7—C8—H8	120.2	Na36 ⁱⁱ —Na35—Na37 ⁱⁱ	83.36 (3)
C7—C8—C9	119.6 (3)	Na36—Na35—Na37 ⁱⁱ	62.07 (3)
C9—C8—H8	120.2	Na36 ⁱⁱ —Na35—Na37 ^v	51.48 (3)
C8—C9—H9	119.0	Na37 ^v —Na35—Na37 ⁱⁱ	98.91 (4)
C10—C9—C8	122.0 (3)	O14—Na36—C32 ⁱⁱ	117.07 (9)
C10—C9—H9	119.0	O14—Na36—Na35	128.39 (7)
C6—C10—C11	122.5 (3)	O14—Na36—Na35 ⁱⁱ	63.15 (6)
C9—C10—C6	118.8 (3)	O14—Na36—Na36 ^{iv}	110.54 (7)
C9—C10—C11	118.7 (3)	O14—Na36—Na36 ⁱⁱ	96.09 (7)
C10—C11—C12	122.0 (3)	O14—Na36—Na37 ⁱ	43.22 (5)
O13—C11—C10	120.5 (3)	O29—Na36—O14	128.38 (9)
O13—C11—C12	117.4 (3)	O29—Na36—C32 ⁱⁱ	114.54 (9)
C11—C12—Na37	82.75 (17)	O29—Na36—O34 ⁱⁱ	130.52 (9)
O14—C12—C11	116.5 (3)	O29—Na36—Na35	43.48 (5)
O14—C12—O15	128.5 (3)	O29—Na36—Na35 ⁱⁱ	163.36 (7)
O14—C12—Na37	137.8 (2)	O29—Na36—Na36 ^{iv}	96.27 (7)
O15—C12—C11	114.7 (3)	O29—Na36—Na36 ⁱⁱ	109.56 (7)
O15—C12—Na37	46.18 (15)	O29—Na36—Na37 ⁱ	129.57 (7)
C11—O13—Na37	106.3 (2)	C32 ⁱⁱ —Na36—Na35	94.98 (7)
C12—O14—Na36	125.7 (2)	C32 ⁱⁱ —Na36—Na35 ⁱⁱ	55.28 (7)
C12—O14—Na37 ⁱ	119.68 (19)	C32 ⁱⁱ —Na36—Na36 ^{iv}	59.35 (7)
Na37 ⁱ —O14—Na36	86.79 (8)	C32 ⁱⁱ —Na36—Na36 ⁱⁱ	58.33 (7)
C12—O15—Na35 ⁱⁱ	124.3 (2)	C32 ⁱⁱ —Na36—Na37 ⁱ	97.95 (7)
C12—O15—Na37	111.58 (19)	O33 ⁱⁱ —Na36—O14	132.21 (9)
Na35 ⁱⁱ —O15—Na37	119.72 (10)	O33 ⁱ —Na36—O14	78.29 (9)
C17—N16—C21	117.8 (3)	O33 ⁱⁱ —Na36—O29	96.64 (8)
C17—N16—Na35	88.3 (2)	O33 ⁱ —Na36—O29	92.35 (8)
C21—N16—Na35	108.79 (19)	O33 ⁱⁱ —Na36—C32 ⁱⁱ	25.43 (8)
N16—C17—H17	118.0	O33 ⁱ —Na36—C32 ⁱⁱ	102.34 (10)
N16—C17—C18	123.9 (3)	O33 ⁱ —Na36—O33 ⁱⁱ	85.60 (10)
N16—C17—Na35	66.26 (18)	O33 ⁱ —Na36—O34	156.71 (11)
C18—C17—H17	118.0	O33 ⁱ —Na36—O34 ⁱⁱ	116.40 (10)
C18—C17—Na35	119.8 (3)	O33 ⁱⁱ —Na36—O34 ⁱⁱ	50.81 (7)
Na35—C17—H17	84.3	O33 ⁱⁱ —Na36—Na35 ⁱⁱ	77.35 (6)
C17—C18—H18	120.5	O33 ⁱ —Na36—Na35	135.58 (8)
C19—C18—C17	118.9 (3)	O33 ⁱ —Na36—Na35 ⁱⁱ	102.52 (7)
C19—C18—H18	120.5	O33 ⁱⁱ —Na36—Na35	94.01 (7)
C18—C19—H19	120.1	O33 ⁱⁱ —Na36—Na36 ⁱⁱ	80.37 (7)
C18—C19—C20	119.9 (3)	O33 ⁱ —Na36—Na36 ^{iv}	45.64 (8)
C20—C19—H19	120.1	O33 ⁱ —Na36—Na36 ⁱⁱ	155.10 (9)
C19—C20—C21	117.6 (3)	O33 ⁱⁱ —Na36—Na36 ^{iv}	39.97 (6)
C19—C20—C22	123.2 (3)	O33 ⁱⁱ —Na36—Na37 ⁱ	98.05 (7)
C22—C20—C21	119.2 (3)	O33 ⁱ —Na36—Na37 ⁱ	41.57 (6)
N16—C21—C20	121.8 (3)	O34 ⁱⁱ —Na36—O14	97.80 (8)
N16—C21—C25	118.8 (3)	O34—Na36—O14	90.80 (8)

C20—C21—C25	119.4 (3)	O34—Na36—O29	78.28 (8)
C20—C22—H22	119.6	O34 ⁱⁱ —Na36—C32 ⁱⁱ	25.40 (8)
C23—C22—C20	120.8 (3)	O34—Na36—C32 ⁱⁱ	100.94 (10)
C23—C22—H22	119.6	O34—Na36—O33 ⁱⁱ	116.40 (10)
C22—C23—H23	120.0	O34—Na36—O34 ⁱⁱ	85.21 (10)
C22—C23—C24	120.0 (3)	O34 ⁱⁱ —Na36—Na35 ⁱⁱ	34.96 (5)
C24—C23—H23	120.0	O34 ⁱⁱ —Na36—Na35	96.33 (6)
C23—C24—H24	119.3	O34—Na36—Na35 ⁱⁱ	90.41 (7)
C25—C24—C23	121.3 (3)	O34—Na36—Na35	41.53 (6)
C25—C24—H24	119.3	O34—Na36—Na36 ⁱⁱ	45.51 (7)
C21—C25—C26	121.9 (3)	O34 ⁱⁱ —Na36—Na36 ⁱⁱ	39.70 (6)
C24—C25—C21	119.3 (3)	O34 ⁱⁱ —Na36—Na36 ^{iv}	80.41 (7)
C24—C25—C26	118.8 (3)	O34—Na36—Na36 ^{iv}	155.59 (9)
C25—C26—C27	121.5 (3)	O34 ⁱⁱ —Na36—Na37 ⁱ	94.98 (6)
O28—C26—C25	121.2 (3)	O34—Na36—Na37 ⁱ	133.75 (8)
O28—C26—C27	117.2 (3)	Na35—Na36—Na35 ⁱⁱ	120.76 (4)
C26—C27—Na35 ⁱ	83.92 (17)	Na35—Na36—Na36 ⁱⁱ	66.36 (4)
O29—C27—C26	116.2 (3)	Na35—Na36—Na36 ^{iv}	120.68 (6)
O29—C27—O30	128.7 (3)	Na35—Na36—Na37 ⁱ	167.03 (5)
O29—C27—Na35 ⁱ	137.1 (2)	Na36 ⁱⁱ —Na36—Na35 ⁱⁱ	54.40 (4)
O30—C27—C26	114.9 (3)	Na36 ^{iv} —Na36—Na35 ⁱⁱ	89.01 (5)
O30—C27—Na35 ⁱ	45.52 (15)	Na36 ^{iv} —Na36—Na36 ⁱⁱ	117.67 (7)
C26—O28—Na35 ⁱ	105.9 (2)	Na37 ⁱ —Na36—Na35 ⁱⁱ	66.99 (4)
C27—O29—Na35	120.25 (19)	Na37 ⁱ —Na36—Na36 ⁱⁱ	120.36 (6)
C27—O29—Na36	126.7 (2)	Na37 ⁱ —Na36—Na36 ^{iv}	67.57 (4)
Na35—O29—Na36	87.60 (8)	N1 ⁱⁱⁱ —Na37—C2 ⁱⁱⁱ	25.79 (9)
C27—O30—Na35 ⁱ	112.32 (19)	N1 ⁱⁱⁱ —Na37—C12	112.78 (9)
C27—O30—Na37 ⁱⁱ	124.2 (2)	N1 ⁱⁱⁱ —Na37—Na35 ⁱⁱ	118.43 (7)
Na37 ⁱⁱ —O30—Na35 ⁱ	118.63 (10)	N1 ⁱⁱⁱ —Na37—Na35 ^v	75.29 (7)
H31A—C31—H31B	109.5	N1 ⁱⁱⁱ —Na37—Na36 ⁱⁱⁱ	119.97 (7)
H31A—C31—H31C	109.5	N1 ⁱⁱⁱ —Na37—Na36 ⁱⁱ	153.15 (7)
H31B—C31—H31C	109.5	C2 ⁱⁱⁱ —Na37—C12	92.63 (10)
C32—C31—H31A	109.5	C2 ⁱⁱⁱ —Na37—Na35 ⁱⁱ	93.41 (7)
C32—C31—H31B	109.5	C2 ⁱⁱⁱ —Na37—Na35 ^v	84.17 (8)
C32—C31—H31C	109.5	C2 ⁱⁱⁱ —Na37—Na36 ⁱⁱⁱ	141.35 (9)
C31—C32—Na36 ⁱⁱ	176.4 (3)	C2 ⁱⁱⁱ —Na37—Na36 ⁱⁱ	138.44 (8)
O33—C32—C31	119.4 (3)	C12—Na37—Na35 ⁱⁱ	50.62 (6)
O33—C32—Na36 ⁱⁱ	60.79 (18)	C12—Na37—Na35 ^v	149.24 (7)
O34—C32—C31	118.2 (3)	C12—Na37—Na36 ⁱⁱⁱ	125.90 (7)
O34—C32—O33	122.3 (3)	C12—Na37—Na36 ⁱⁱ	80.15 (6)
O34—C32—Na36 ⁱⁱ	61.64 (18)	O13—Na37—N1 ⁱⁱⁱ	80.90 (8)
C32—O33—Na36 ⁱⁱⁱ	130.7 (2)	O13—Na37—C2 ⁱⁱⁱ	76.26 (10)
C32—O33—Na36 ⁱⁱ	93.8 (2)	O13—Na37—C12	47.68 (8)
C32—O33—Na37	127.0 (2)	O13—Na37—Na35 ^v	155.72 (7)
Na36 ⁱⁱⁱ —O33—Na36 ⁱⁱ	94.40 (10)	O13—Na37—Na35 ⁱⁱ	96.49 (6)
Na37—O33—Na36 ⁱⁱ	106.67 (10)	O13—Na37—Na36 ⁱⁱ	122.07 (7)
Na37—O33—Na36 ⁱⁱⁱ	96.46 (10)	O13—Na37—Na36 ⁱⁱⁱ	130.05 (7)
C32—O34—Na35	131.2 (2)	O14 ⁱⁱⁱ —Na37—N1 ⁱⁱⁱ	73.69 (8)

C32—O34—Na36 ⁱⁱ	93.0 (2)	O14 ⁱⁱⁱ —Na37—C2 ⁱⁱⁱ	99.20 (9)
C32—O34—Na36	127.8 (2)	O14 ⁱⁱⁱ —Na37—C12	149.10 (9)
Na35—O34—Na36 ⁱⁱ	104.49 (10)	O14 ⁱⁱⁱ —Na37—O13	107.78 (9)
Na35—O34—Na36	96.13 (9)	O14 ⁱⁱⁱ —Na37—O15	170.06 (10)
Na36—O34—Na36 ⁱⁱ	94.80 (10)	O14 ⁱⁱⁱ —Na37—Na35 ^v	61.01 (6)
O15 ⁱⁱ —Na35—N16	82.34 (9)	O14 ⁱⁱⁱ —Na37—Na35 ⁱⁱ	154.67 (7)
O15 ⁱⁱ —Na35—C17	76.91 (9)	O14 ⁱⁱⁱ —Na37—Na36 ⁱⁱⁱ	49.99 (6)
O15 ⁱⁱ —Na35—C27 ⁱⁱⁱ	118.90 (9)	O14 ⁱⁱⁱ —Na37—Na36 ⁱⁱ	107.83 (7)
O15 ⁱⁱ —Na35—O28 ⁱⁱⁱ	149.41 (9)	O15—Na37—N1 ⁱⁱⁱ	112.82 (9)
O15 ⁱⁱ —Na35—O29	91.21 (9)	O15—Na37—C2 ⁱⁱⁱ	88.02 (10)
O15 ⁱⁱ —Na35—O30 ⁱⁱⁱ	96.73 (9)	O15—Na37—C12	22.25 (8)
O15 ⁱⁱ —Na35—Na36 ⁱⁱ	71.54 (7)	O15—Na37—O13	67.13 (8)
O15 ⁱⁱ —Na35—Na36	81.21 (7)	O15—Na37—Na35 ⁱⁱ	29.41 (6)
O15 ⁱⁱ —Na35—Na37 ⁱⁱ	30.87 (6)	O15—Na37—Na35 ^v	127.04 (7)
O15 ⁱⁱ —Na35—Na37 ^v	69.18 (6)	O15—Na37—Na36 ⁱⁱ	70.01 (6)
N16—Na35—C17	25.48 (9)	O15—Na37—Na36 ⁱⁱⁱ	126.03 (7)
N16—Na35—C27 ⁱⁱⁱ	112.70 (9)	O30 ⁱⁱ —Na37—N1 ⁱⁱⁱ	82.82 (9)
N16—Na35—Na36	118.67 (7)	O30 ⁱⁱ —Na37—C2 ⁱⁱⁱ	77.73 (10)
N16—Na35—Na36 ⁱⁱ	153.86 (7)	O30 ⁱⁱ —Na37—C12	118.21 (9)
N16—Na35—Na37 ^v	118.11 (7)	O30 ⁱⁱ —Na37—O13	149.27 (9)
N16—Na35—Na37 ⁱⁱ	74.45 (6)	O30 ⁱⁱ —Na37—O14 ⁱⁱⁱ	92.27 (9)
C17—Na35—Na36	139.79 (8)	O30 ⁱⁱ —Na37—O15	95.96 (9)
C17—Na35—Na36 ⁱⁱ	139.08 (8)	O30 ⁱⁱ —Na37—Na35 ^v	31.26 (6)
C17—Na35—Na37 ^v	93.29 (7)	O30 ⁱⁱ —Na37—Na35 ⁱⁱ	68.97 (6)
C17—Na35—Na37 ⁱⁱ	82.69 (7)	O30 ⁱⁱ —Na37—Na36 ⁱⁱ	70.37 (7)
C27 ⁱⁱⁱ —Na35—C17	93.22 (9)	O30 ⁱⁱ —Na37—Na36 ⁱⁱⁱ	80.69 (6)
C27 ⁱⁱⁱ —Na35—Na36	126.95 (7)	O33—Na37—N1 ⁱⁱⁱ	158.05 (10)
C27 ⁱⁱⁱ —Na35—Na36 ⁱⁱ	80.24 (7)	O33—Na37—C2 ⁱⁱⁱ	176.10 (11)
C27 ⁱⁱⁱ —Na35—Na37 ⁱⁱ	149.63 (7)	O33—Na37—C12	83.95 (9)
C27 ⁱⁱⁱ —Na35—Na37 ^v	51.11 (6)	O33—Na37—O13	102.63 (9)
O28 ⁱⁱⁱ —Na35—N16	80.90 (8)	O33—Na37—O14 ⁱⁱⁱ	84.70 (9)
O28 ⁱⁱⁱ —Na35—C17	76.96 (9)	O33—Na37—O15	88.11 (9)
O28 ⁱⁱⁱ —Na35—C27 ⁱⁱⁱ	47.57 (7)	O33—Na37—O30 ⁱⁱ	102.21 (10)
O28 ⁱⁱⁱ —Na35—Na36 ⁱⁱ	121.72 (6)	O33—Na37—Na35 ⁱⁱ	82.97 (7)
O28 ⁱⁱⁱ —Na35—Na36	129.36 (7)	O33—Na37—Na35 ^v	97.80 (7)
O28 ⁱⁱⁱ —Na35—Na37 ⁱⁱ	154.89 (7)	O33—Na37—Na36 ⁱⁱ	39.11 (7)
O28 ⁱⁱⁱ —Na35—Na37 ^v	96.80 (6)	O33—Na37—Na36 ⁱⁱⁱ	41.96 (6)
O29—Na35—N16	72.98 (8)	Na35 ^v —Na37—Na35 ⁱⁱ	98.91 (4)
O29—Na35—C17	98.04 (9)	Na36 ⁱⁱⁱ —Na37—Na35 ⁱⁱ	108.19 (4)
O29—Na35—C27 ⁱⁱⁱ	149.60 (9)	Na36 ⁱⁱ —Na37—Na35 ^v	82.16 (3)
O29—Na35—O28 ⁱⁱⁱ	107.95 (8)	Na36 ⁱⁱⁱ —Na37—Na35 ^v	61.53 (3)
O29—Na35—O30 ⁱⁱⁱ	170.97 (10)	Na36 ⁱⁱ —Na37—Na35 ⁱⁱ	50.77 (3)
O29—Na35—Na36	48.92 (6)	Na36 ⁱⁱⁱ —Na37—Na36 ⁱⁱ	58.08 (4)
N1—C2—C3—C4	0.9 (7)	C27 ⁱⁱⁱ —Na35—Na36—Na35 ⁱⁱ	-46.01 (9)
N1—C6—C10—C9	-178.4 (3)	C27 ⁱⁱⁱ —Na35—Na36—Na36 ⁱⁱ	-46.01 (9)
N1—C6—C10—C11	2.9 (5)	C27 ⁱⁱⁱ —Na35—Na36—Na36 ^{iv}	-155.26 (9)
C2—N1—C6—C5	-1.1 (5)	C27 ⁱⁱⁱ —Na35—Na36—Na37 ⁱ	77.9 (3)

C2—N1—C6—C10	177.9 (3)	O28—C26—C27—O29	-118.7 (3)
C2—C3—C4—C5	-0.3 (7)	O28—C26—C27—O30	55.8 (4)
C3—C4—C5—C6	-0.9 (6)	O28—C26—C27—Na35 ⁱ	21.5 (3)
C3—C4—C5—C7	-179.3 (4)	O28 ⁱⁱⁱ —Na35—Na36—O14	-29.13 (13)
C4—C5—C6—N1	1.7 (5)	O28 ⁱⁱⁱ —Na35—Na36—O29	79.27 (11)
C4—C5—C6—C10	-177.3 (3)	O28 ⁱⁱⁱ —Na35—Na36—C32 ⁱⁱ	-159.81 (10)
C4—C5—C7—C8	177.2 (4)	O28 ⁱⁱⁱ —Na35—Na36—O33 ⁱⁱ	174.69 (9)
C5—C6—C10—C9	0.6 (5)	O28 ⁱⁱⁱ —Na35—Na36—O33 ⁱ	86.89 (14)
C5—C6—C10—C11	-178.1 (3)	O28 ⁱⁱⁱ —Na35—Na36—O34	-58.92 (13)
C5—C7—C8—C9	-0.5 (5)	O28 ⁱⁱⁱ —Na35—Na36—O34 ⁱⁱ	-134.32 (9)
C6—N1—C2—C3	-0.2 (6)	O28 ⁱⁱⁱ —Na35—Na36—Na35 ⁱⁱ	-107.65 (9)
C6—N1—C2—Na37 ⁱ	113.2 (3)	O28 ⁱⁱⁱ —Na35—Na36—Na36 ⁱⁱ	-107.65 (9)
C6—C5—C7—C8	-1.1 (5)	O28 ⁱⁱⁱ —Na35—Na36—Na36 ^{iv}	143.10 (9)
C6—C10—C11—C12	28.7 (5)	O28 ⁱⁱⁱ —Na35—Na36—Na37 ⁱ	16.3 (3)
C6—C10—C11—O13	-155.2 (3)	O29—C27—O30—Na35 ⁱ	121.9 (3)
C7—C5—C6—N1	-179.9 (3)	O29—C27—O30—Na37 ⁱⁱ	-32.8 (4)
C7—C5—C6—C10	1.1 (5)	O29—Na35—Na36—O14	-108.40 (12)
C7—C8—C9—C10	2.3 (5)	O29—Na35—Na36—C32 ⁱⁱ	120.92 (11)
C8—C9—C10—C6	-2.4 (5)	O29—Na35—Na36—O33 ⁱ	7.62 (14)
C8—C9—C10—C11	176.4 (3)	O29—Na35—Na36—O33 ⁱⁱ	95.43 (10)
C9—C10—C11—C12	-150.0 (3)	O29—Na35—Na36—O34 ⁱⁱ	146.41 (10)
C9—C10—C11—O13	26.1 (4)	O29—Na35—Na36—O34	-138.19 (14)
C10—C11—C12—O14	58.0 (4)	O29—Na35—Na36—Na35 ⁱⁱ	173.08 (10)
C10—C11—C12—O15	-127.3 (3)	O29—Na35—Na36—Na36 ⁱⁱ	173.08 (10)
C10—C11—C12—Na37	-161.5 (3)	O29—Na35—Na36—Na36 ^{iv}	63.83 (10)
C10—C11—O13—Na37	157.1 (2)	O29—Na35—Na36—Na37 ⁱ	-63.0 (2)
C11—C12—O14—Na36	148.1 (2)	O30—C27—O29—Na35	84.3 (4)
C11—C12—O14—Na37 ⁱ	-102.7 (3)	O30—C27—O29—Na36	-27.7 (4)
C11—C12—O15—Na35 ⁱⁱ	153.0 (2)	O30 ⁱⁱⁱ —Na35—Na36—O14	60.53 (13)
C11—C12—O15—Na37	-50.6 (3)	O30 ⁱⁱⁱ —Na35—Na36—O29	168.92 (13)
C11—C12—Na37—N1 ⁱⁱⁱ	40.10 (18)	O30 ⁱⁱⁱ —Na35—Na36—C32 ⁱⁱ	-70.16 (11)
C11—C12—Na37—C2 ⁱⁱⁱ	56.71 (18)	O30 ⁱⁱⁱ —Na35—Na36—O33 ⁱ	176.54 (14)
C11—C12—Na37—O13	-11.98 (15)	O30 ⁱⁱⁱ —Na35—Na36—O33 ⁱⁱ	-95.65 (11)
C11—C12—Na37—O14 ⁱⁱⁱ	-56.1 (2)	O30 ⁱⁱⁱ —Na35—Na36—O34 ⁱⁱ	-44.66 (11)
C11—C12—Na37—O15	134.9 (3)	O30 ⁱⁱⁱ —Na35—Na36—O34	30.74 (13)
C11—C12—Na37—O30 ⁱⁱ	134.19 (17)	O30 ⁱⁱⁱ —Na35—Na36—Na35 ⁱⁱ	-17.99 (10)
C11—C12—Na37—O33	-125.17 (18)	O30 ⁱⁱⁱ —Na35—Na36—Na36 ^{iv}	-127.25 (10)
C11—C12—Na37—Na35 ⁱⁱ	148.96 (19)	O30 ⁱⁱⁱ —Na35—Na36—Na36 ⁱⁱ	-17.99 (10)
C11—C12—Na37—Na35 ^v	139.73 (16)	O30 ⁱⁱⁱ —Na35—Na36—Na37 ⁱ	105.9 (2)
C11—C12—Na37—Na36 ⁱⁱⁱ	-126.51 (16)	C31—C32—O33—Na36 ⁱⁱ	175.8 (3)
C11—C12—Na37—Na36 ⁱⁱ	-164.50 (17)	C31—C32—O33—Na36 ⁱⁱⁱ	-85.1 (4)
C11—O13—Na37—N1 ⁱⁱⁱ	-117.1 (2)	C31—C32—O33—Na37	61.6 (4)
C11—O13—Na37—C2 ⁱⁱⁱ	-91.2 (2)	C31—C32—O34—Na35	71.9 (4)
C11—O13—Na37—C12	15.48 (19)	C31—C32—O34—Na36	-77.5 (4)
C11—O13—Na37—O14 ⁱⁱⁱ	173.4 (2)	C31—C32—O34—Na36 ⁱⁱ	-175.9 (3)
C11—O13—Na37—O15	2.5 (2)	C32—O33—Na37—N1 ⁱⁱⁱ	-114.8 (3)
C11—O13—Na37—O30 ⁱⁱ	-58.2 (3)	C32—O33—Na37—C12	26.4 (3)
C11—O13—Na37—O33	85.0 (2)	C32—O33—Na37—O13	-17.8 (3)

C11—O13—Na37—Na35 ⁱⁱ	0.8 (2)	C32—O33—Na37—O14 ⁱⁱⁱ	-124.8 (3)
C11—O13—Na37—Na35 ^v	-128.4 (2)	C32—O33—Na37—O15	48.3 (3)
C11—O13—Na37—Na36 ⁱⁱ	47.9 (2)	C32—O33—Na37—O30 ⁱⁱ	144.0 (3)
C11—O13—Na37—Na36 ⁱⁱⁱ	121.2 (2)	C32—O33—Na37—Na35 ⁱⁱ	77.3 (3)
C12—C11—O13—Na37	-26.6 (3)	C32—O33—Na37—Na35 ^v	175.4 (3)
C12—O14—Na36—O29	-125.1 (2)	C32—O33—Na37—Na36 ⁱⁱ	108.2 (3)
C12—O14—Na36—C32 ⁱⁱ	53.2 (3)	C32—O33—Na37—Na36 ⁱⁱⁱ	-155.2 (3)
C12—O14—Na36—O33 ⁱ	151.2 (2)	C32—O34—Na35—O15 ⁱⁱ	144.5 (3)
C12—O14—Na36—O33 ⁱⁱ	78.3 (3)	C32—O34—Na35—N16	-112.2 (3)
C12—O14—Na36—O34 ⁱⁱ	35.8 (2)	C32—O34—Na35—C27 ⁱⁱⁱ	26.1 (3)
C12—O14—Na36—O34	-49.5 (2)	C32—O34—Na35—O28 ⁱⁱⁱ	-18.6 (3)
C12—O14—Na36—Na35 ⁱⁱ	40.6 (2)	C32—O34—Na35—O29	-125.8 (3)
C12—O14—Na36—Na35	-68.7 (3)	C32—O34—Na35—O30 ⁱⁱⁱ	47.6 (3)
C12—O14—Na36—Na36 ⁱⁱ	-4.2 (2)	C32—O34—Na35—Na36 ⁱⁱ	107.3 (3)
C12—O14—Na36—Na36 ^{iv}	118.4 (2)	C32—O34—Na35—Na36	-156.1 (3)
C12—O14—Na36—Na37 ⁱ	124.8 (3)	C32—O34—Na35—Na37 ⁱⁱ	175.7 (3)
C12—O15—Na37—N1 ⁱⁱⁱ	94.6 (2)	C32—O34—Na35—Na37 ^v	77.4 (3)
C12—O15—Na37—C2 ⁱⁱⁱ	101.9 (2)	C32—O34—Na36—O14	0.2 (3)
C12—O15—Na37—O13	26.0 (2)	C32—O34—Na36—O29	129.4 (3)
C12—O15—Na37—O30 ⁱⁱ	179.3 (2)	C32—O34—Na36—C32 ⁱⁱ	-117.5 (3)
C12—O15—Na37—O33	-78.6 (2)	C32—O34—Na36—O33 ⁱⁱ	-139.0 (3)
C12—O15—Na37—Na35 ⁱⁱ	-157.6 (3)	C32—O34—Na36—O33 ⁱ	61.5 (4)
C12—O15—Na37—Na35 ^v	-176.94 (18)	C32—O34—Na36—O34 ⁱⁱ	-97.5 (3)
C12—O15—Na37—Na36 ⁱⁱⁱ	-97.9 (2)	C32—O34—Na36—Na35	157.3 (3)
C12—O15—Na37—Na36 ⁱⁱ	-114.1 (2)	C32—O34—Na36—Na35 ⁱⁱ	-62.9 (3)
O13—C11—C12—O14	-118.2 (3)	C32—O34—Na36—Na36 ^{iv}	-151.4 (3)
O13—C11—C12—O15	56.5 (4)	C32—O34—Na36—Na36 ⁱⁱ	-97.5 (3)
O13—C11—C12—Na37	22.3 (3)	C32—O34—Na36—Na37 ⁱ	-5.2 (3)
O14—C12—O15—Na35 ⁱⁱ	-33.0 (4)	O33—C32—O34—Na35	-109.0 (3)
O14—C12—O15—Na37	123.3 (3)	O33—C32—O34—Na36 ⁱⁱ	3.2 (3)
O14—C12—Na37—N1 ⁱⁱⁱ	162.1 (3)	O33—C32—O34—Na36	101.6 (3)
O14—C12—Na37—C2 ⁱⁱⁱ	178.7 (3)	O34—C32—O33—Na36 ⁱⁱⁱ	95.9 (4)
O14—C12—Na37—O13	110.0 (3)	O34—C32—O33—Na36 ⁱⁱ	-3.3 (3)
O14—C12—Na37—O14 ⁱⁱⁱ	65.9 (4)	O34—C32—O33—Na37	-117.5 (3)
O14—C12—Na37—O15	-103.0 (4)	O34—Na35—Na36—O14	29.79 (12)
O14—C12—Na37—O30 ⁱⁱ	-103.8 (3)	O34—Na35—Na36—O29	138.19 (14)
O14—C12—Na37—O33	-3.1 (3)	O34—Na35—Na36—C32 ⁱⁱ	-100.89 (12)
O14—C12—Na37—Na35 ^v	-98.2 (3)	O34—Na35—Na36—O33 ⁱ	145.81 (17)
O14—C12—Na37—Na35 ⁱⁱ	-89.0 (3)	O34—Na35—Na36—O33 ⁱⁱ	-126.39 (12)
O14—C12—Na37—Na36 ⁱⁱⁱ	-4.5 (4)	O34—Na35—Na36—O34 ⁱⁱ	-75.40 (13)
O14—C12—Na37—Na36 ⁱⁱ	-42.5 (3)	O34—Na35—Na36—Na35 ⁱⁱ	-48.73 (10)
O15—C12—O14—Na36	-25.8 (4)	O34—Na35—Na36—Na36 ⁱⁱ	-48.73 (10)
O15—C12—O14—Na37 ⁱ	83.5 (4)	O34—Na35—Na36—Na36 ^{iv}	-157.98 (13)
O15—C12—Na37—N1 ⁱⁱⁱ	-94.8 (2)	O34—Na35—Na36—Na37 ⁱ	75.2 (2)
O15—C12—Na37—C2 ⁱⁱⁱ	-78.2 (2)	Na35 ⁱⁱ —O15—Na37—N1 ⁱⁱⁱ	-107.78 (12)
O15—C12—Na37—O13	-146.9 (2)	Na35 ⁱⁱ —O15—Na37—C2 ⁱⁱⁱ	-100.52 (13)
O15—C12—Na37—O14 ⁱⁱⁱ	168.9 (2)	Na35 ⁱⁱ —O15—Na37—C12	157.6 (3)
O15—C12—Na37—O30 ⁱⁱ	-0.8 (2)	Na35 ⁱⁱ —O15—Na37—O13	-176.45 (14)

O15—C12—Na37—O33	99.9 (2)	Na35 ⁱⁱ —O15—Na37—O30 ⁱⁱ	-23.08 (13)
O15—C12—Na37—Na35 ^v	4.8 (3)	Na35 ⁱⁱ —O15—Na37—O33	79.00 (13)
O15—C12—Na37—Na35 ⁱⁱ	14.02 (18)	Na35 ⁱⁱ —O15—Na37—Na35 ^v	-19.35 (15)
O15—C12—Na37—Na36 ⁱⁱⁱ	98.5 (2)	Na35 ⁱⁱ —O15—Na37—Na36 ⁱⁱⁱ	59.73 (14)
O15—C12—Na37—Na36 ⁱⁱ	60.6 (2)	Na35 ⁱⁱ —O15—Na37—Na36 ⁱⁱ	43.51 (10)
O15 ⁱⁱ —Na35—Na36—O14	152.22 (10)	Na35—N16—C17—C18	-110.9 (4)
O15 ⁱⁱ —Na35—Na36—O29	-99.39 (10)	Na35—N16—C21—C20	96.9 (3)
O15 ⁱⁱ —Na35—Na36—C32 ⁱⁱ	21.53 (9)	Na35—N16—C21—C25	-83.1 (3)
O15 ⁱⁱ —Na35—Na36—O33 ⁱⁱ	-3.96 (9)	Na35—C17—C18—C19	-79.3 (4)
O15 ⁱⁱ —Na35—Na36—O33 ⁱ	-91.77 (14)	Na35 ⁱ —C27—O29—Na35	147.06 (19)
O15 ⁱⁱ —Na35—Na36—O34	122.42 (13)	Na35 ⁱ —C27—O29—Na36	35.1 (4)
O15 ⁱⁱ —Na35—Na36—O34 ⁱⁱ	47.02 (9)	Na35 ⁱ —C27—O30—Na37 ⁱⁱ	-154.8 (3)
O15 ⁱⁱ —Na35—Na36—Na35 ⁱⁱ	73.70 (7)	Na35—O29—Na36—O14	108.43 (10)
O15 ⁱⁱ —Na35—Na36—Na36 ⁱⁱ	73.70 (7)	Na35—O29—Na36—C32 ⁱⁱ	-69.96 (10)
O15 ⁱⁱ —Na35—Na36—Na36 ^{iv}	-35.56 (9)	Na35—O29—Na36—O33 ⁱ	-174.67 (10)
O15 ⁱⁱ —Na35—Na36—Na37 ⁱ	-162.4 (2)	Na35—O29—Na36—O33 ⁱⁱ	-88.83 (9)
N16—C17—C18—C19	0.7 (6)	Na35—O29—Na36—O34	26.83 (9)
N16—C17—Na35—O15 ⁱⁱ	99.8 (2)	Na35—O29—Na36—O34 ⁱⁱ	-46.33 (13)
N16—C17—Na35—C27 ⁱⁱⁱ	-141.3 (2)	Na35—O29—Na36—Na35 ⁱⁱ	-21.2 (3)
N16—C17—Na35—O28 ⁱⁱⁱ	-96.2 (2)	Na35—O29—Na36—Na36 ⁱⁱ	-6.72 (9)
N16—C17—Na35—O29	10.4 (2)	Na35—O29—Na36—Na36 ^{iv}	-129.06 (7)
N16—C17—Na35—O30 ⁱⁱⁱ	-162.8 (2)	Na35—O29—Na36—Na37 ⁱ	164.97 (7)
N16—C17—Na35—Na36	41.0 (2)	Na35—O34—Na36—O14	-157.08 (9)
N16—C17—Na35—Na36 ⁱⁱ	139.93 (17)	Na35—O34—Na36—O29	-27.94 (9)
N16—C17—Na35—Na37 ^v	167.53 (19)	Na35—O34—Na36—C32 ⁱⁱ	85.13 (10)
N16—C17—Na35—Na37 ⁱⁱ	68.96 (19)	Na35—O34—Na36—O33 ⁱ	-95.8 (3)
N16—C21—C25—C24	-179.4 (3)	Na35—O34—Na36—O33 ⁱⁱ	63.71 (12)
N16—C21—C25—C26	1.9 (4)	Na35—O34—Na36—O34 ⁱⁱ	105.16 (11)
N16—Na35—Na36—O14	-131.57 (11)	Na35—O34—Na36—Na35 ⁱⁱ	139.77 (8)
N16—Na35—Na36—O29	-23.17 (10)	Na35—O34—Na36—Na36 ^{iv}	51.3 (3)
N16—Na35—Na36—C32 ⁱⁱ	97.75 (10)	Na35—O34—Na36—Na36 ⁱⁱ	105.16 (11)
N16—Na35—Na36—O33 ⁱ	-15.55 (15)	Na35—O34—Na36—Na37 ⁱ	-162.53 (7)
N16—Na35—Na36—O33 ⁱⁱ	72.25 (10)	Na36—O29—Na35—O15 ⁱⁱ	77.22 (9)
N16—Na35—Na36—O34 ⁱⁱ	123.24 (9)	Na36—O29—Na35—N16	158.84 (9)
N16—Na35—Na36—O34	-161.36 (13)	Na36—O29—Na35—C17	154.17 (9)
N16—Na35—Na36—Na35 ⁱⁱ	149.91 (8)	Na36—O29—Na35—C27 ⁱⁱⁱ	-95.16 (17)
N16—Na35—Na36—Na36 ⁱⁱ	149.91 (8)	Na36—O29—Na35—O28 ⁱⁱⁱ	-127.01 (8)
N16—Na35—Na36—Na36 ^{iv}	40.66 (10)	Na36—O29—Na35—O34	-26.85 (9)
N16—Na35—Na36—Na37 ⁱ	-86.2 (2)	Na36—O29—Na35—Na36 ⁱⁱ	6.24 (9)
C17—N16—C21—C20	-1.3 (5)	Na36—O29—Na35—Na37 ^v	38.65 (19)
C17—N16—C21—C25	178.6 (3)	Na36—O29—Na35—Na37 ⁱⁱ	77.37 (6)
C17—N16—Na35—O15 ⁱⁱ	-75.6 (2)	Na36 ⁱⁱ —C32—O33—Na36 ⁱⁱⁱ	99.1 (3)
C17—N16—Na35—C27 ⁱⁱⁱ	42.6 (2)	Na36 ⁱⁱ —C32—O33—Na37	-114.2 (2)
C17—N16—Na35—O28 ⁱⁱⁱ	78.7 (2)	Na36 ⁱⁱ —C32—O34—Na35	-112.2 (3)
C17—N16—Na35—O29	-169.2 (2)	Na36 ⁱⁱ —C32—O34—Na36	98.4 (2)
C17—N16—Na35—O30 ⁱⁱⁱ	18.6 (2)	Na36 ⁱⁱ —O33—Na37—N1 ⁱⁱⁱ	137.0 (2)
C17—N16—Na35—O34	176.7 (3)	Na36 ⁱⁱⁱ —O33—Na37—N1 ⁱⁱⁱ	40.5 (3)
C17—N16—Na35—Na36	-151.13 (18)	Na36 ⁱⁱⁱ —O33—Na37—C12	-178.38 (11)

C17—N16—Na35—Na36 ⁱⁱ	-73.2 (3)	Na36 ⁱⁱ —O33—Na37—C12	-81.81 (10)
C17—N16—Na35—Na37 ⁱⁱ	-106.1 (2)	Na36 ⁱⁱⁱ —O33—Na37—O13	137.47 (9)
C17—N16—Na35—Na37 ^v	-14.1 (2)	Na36 ⁱⁱ —O33—Na37—O13	-125.95 (9)
C17—C18—C19—C20	1.1 (6)	Na36 ⁱⁱ —O33—Na37—O14 ⁱⁱⁱ	126.98 (10)
C17—Na35—Na36—O14	-150.33 (13)	Na36 ⁱⁱⁱ —O33—Na37—O14 ⁱⁱⁱ	30.41 (10)
C17—Na35—Na36—O29	-41.94 (14)	Na36 ⁱⁱ —O33—Na37—O15	-59.89 (10)
C17—Na35—Na36—C32 ⁱⁱ	78.98 (14)	Na36 ⁱⁱⁱ —O33—Na37—O15	-156.47 (10)
C17—Na35—Na36—O33 ⁱ	-34.32 (18)	Na36 ⁱⁱ —O33—Na37—O30 ⁱⁱ	35.80 (11)
C17—Na35—Na36—O33 ⁱⁱ	53.49 (14)	Na36 ⁱⁱⁱ —O33—Na37—O30 ⁱⁱ	-60.78 (11)
C17—Na35—Na36—O34	179.87 (16)	Na36 ⁱⁱ —O33—Na37—Na35 ^v	67.25 (9)
C17—Na35—Na36—O34 ⁱⁱ	104.48 (13)	Na36 ⁱⁱⁱ —O33—Na37—Na35 ⁱⁱ	-127.41 (9)
C17—Na35—Na36—Na35 ⁱⁱ	131.15 (12)	Na36 ⁱⁱⁱ —O33—Na37—Na35 ^v	-29.33 (10)
C17—Na35—Na36—Na36 ^{iv}	21.89 (15)	Na36 ⁱⁱ —O33—Na37—Na35 ⁱⁱ	-30.84 (8)
C17—Na35—Na36—Na36 ⁱⁱ	131.15 (12)	Na36 ⁱⁱ —O33—Na37—Na36 ⁱⁱⁱ	96.57 (12)
C17—Na35—Na36—Na37 ⁱ	-104.9 (2)	Na36 ⁱⁱⁱ —O33—Na37—Na36 ⁱⁱ	-96.57 (12)
C18—C17—Na35—O15 ⁱⁱ	-143.4 (3)	Na36—O34—Na35—O15 ⁱⁱ	-59.34 (11)
C18—C17—Na35—N16	116.8 (4)	Na36 ⁱⁱ —O34—Na35—O15 ⁱⁱ	37.24 (11)
C18—C17—Na35—C27 ⁱⁱⁱ	-24.5 (3)	Na36 ⁱⁱ —O34—Na35—N16	140.5 (2)
C18—C17—Na35—O28 ⁱⁱⁱ	20.6 (3)	Na36—O34—Na35—N16	43.9 (3)
C18—C17—Na35—O29	127.2 (3)	Na36 ⁱⁱ —O34—Na35—C27 ⁱⁱⁱ	-81.24 (9)
C18—C17—Na35—O30 ⁱⁱⁱ	-46.0 (3)	Na36—O34—Na35—C27 ⁱⁱⁱ	-177.82 (10)
C18—C17—Na35—Na36 ⁱⁱ	-103.3 (3)	Na36—O34—Na35—O28 ⁱⁱⁱ	137.48 (9)
C18—C17—Na35—Na36	157.8 (2)	Na36 ⁱⁱ —O34—Na35—O28 ⁱⁱⁱ	-125.94 (9)
C18—C17—Na35—Na37 ⁱⁱ	-174.2 (3)	Na36 ⁱⁱ —O34—Na35—O29	126.94 (10)
C18—C17—Na35—Na37 ^v	-75.7 (3)	Na36—O34—Na35—O29	30.36 (10)
C18—C19—C20—C21	-2.8 (6)	Na36—O34—Na35—O30 ⁱⁱⁱ	-156.29 (10)
C18—C19—C20—C22	178.7 (4)	Na36 ⁱⁱ —O34—Na35—O30 ⁱⁱⁱ	-59.70 (10)
C19—C20—C21—N16	3.0 (5)	Na36—O34—Na35—Na36 ⁱⁱ	-96.58 (11)
C19—C20—C21—C25	-177.0 (3)	Na36 ⁱⁱ —O34—Na35—Na36	96.58 (11)
C19—C20—C22—C23	176.9 (4)	Na36 ⁱⁱ —O34—Na35—Na37 ^v	-29.93 (7)
C20—C21—C25—C24	0.5 (5)	Na36—O34—Na35—Na37 ^v	-126.51 (8)
C20—C21—C25—C26	-178.2 (3)	Na36—O34—Na35—Na37 ⁱⁱ	-28.20 (9)
C20—C22—C23—C24	-0.6 (5)	Na36 ⁱⁱ —O34—Na35—Na37 ⁱⁱ	68.38 (8)
C21—N16—C17—C18	-0.6 (5)	Na36 ⁱⁱ —O34—Na36—O14	97.76 (8)
C21—N16—C17—Na35	110.4 (3)	Na36 ⁱⁱ —O34—Na36—O29	-133.10 (9)
C21—N16—Na35—O15 ⁱⁱ	165.5 (2)	Na36 ⁱⁱ —O34—Na36—C32 ⁱⁱ	-20.03 (9)
C21—N16—Na35—C17	-118.9 (3)	Na36 ⁱⁱ —O34—Na36—O33 ⁱ	159.0 (2)
C21—N16—Na35—C27 ⁱⁱⁱ	-76.3 (2)	Na36 ⁱⁱ —O34—Na36—O33 ⁱⁱ	-41.45 (10)
C21—N16—Na35—O28 ⁱⁱⁱ	-40.1 (2)	Na36 ⁱⁱ —O34—Na36—O34 ⁱⁱ	0.0
C21—N16—Na35—O29	71.9 (2)	Na36 ⁱⁱ —O34—Na36—Na35 ⁱⁱ	34.61 (6)
C21—N16—Na35—O30 ⁱⁱⁱ	-100.3 (2)	Na36 ⁱⁱ —O34—Na36—Na35	-105.16 (11)
C21—N16—Na35—O34	57.8 (3)	Na36 ⁱⁱ —O34—Na36—Na36 ^{iv}	-53.9 (2)
C21—N16—Na35—Na36	90.0 (2)	Na36 ⁱⁱ —O34—Na36—Na37 ⁱ	92.31 (11)
C21—N16—Na35—Na36 ⁱⁱ	167.92 (17)	Na36 ⁱⁱ —Na35—Na36—O14	78.52 (9)
C21—N16—Na35—Na37 ^v	-133.04 (18)	Na36 ⁱⁱ —Na35—Na36—O29	-173.08 (10)
C21—N16—Na35—Na37 ⁱⁱ	135.0 (2)	Na36 ⁱⁱ —Na35—Na36—C32 ⁱⁱ	-52.16 (7)
C21—C20—C22—C23	-1.6 (5)	Na36 ⁱⁱ —Na35—Na36—O33 ⁱⁱ	-77.66 (7)
C21—C25—C26—C27	31.5 (4)	Na36 ⁱⁱ —Na35—Na36—O33 ⁱ	-165.47 (14)

C21—C25—C26—O28	-153.1 (3)	Na36 ⁱⁱ —Na35—Na36—O34 ⁱⁱ	-26.67 (5)
C22—C20—C21—N16	-178.4 (3)	Na36 ⁱⁱ —Na35—Na36—O34	48.73 (10)
C22—C20—C21—C25	1.6 (5)	Na36 ⁱⁱ —Na35—Na36—Na35 ⁱⁱ	0.0
C22—C23—C24—C25	2.9 (5)	Na36 ⁱⁱ —Na35—Na36—Na36 ^{iv}	-109.25 (8)
C23—C24—C25—C21	-2.8 (5)	Na36 ⁱⁱ —Na35—Na36—Na37 ⁱ	123.9 (2)
C23—C24—C25—C26	176.0 (3)	Na37 ⁱ —N1—C2—C3	-113.3 (4)
C24—C25—C26—C27	-147.2 (3)	Na37 ⁱ —N1—C6—C5	98.4 (3)
C24—C25—C26—O28	28.1 (4)	Na37 ⁱ —N1—C6—C10	-82.6 (3)
C25—C26—C27—O29	56.8 (4)	Na37 ⁱ —C2—C3—C4	-79.8 (5)
C25—C26—C27—O30	-128.7 (3)	Na37—C12—O14—Na36	38.1 (4)
C25—C26—C27—Na35 ⁱ	-163.0 (3)	Na37—C12—O14—Na37 ⁱ	147.35 (19)
C25—C26—O28—Na35 ⁱ	159.2 (2)	Na37—C12—O15—Na35 ⁱⁱ	-156.4 (3)
C26—C27—O29—Na35	-102.1 (3)	Na37 ⁱ —O14—Na36—O29	110.11 (10)
C26—C27—O29—Na36	145.9 (2)	Na37 ⁱ —O14—Na36—C32 ⁱⁱ	-71.52 (11)
C26—C27—O30—Na35 ⁱ	-51.8 (3)	Na37 ⁱ —O14—Na36—O33 ⁱ	26.48 (9)
C26—C27—O30—Na37 ⁱⁱ	153.47 (19)	Na37 ⁱ —O14—Na36—O33 ⁱⁱ	-46.44 (14)
C27—C26—O28—Na35 ⁱ	-25.2 (3)	Na37 ⁱ —O14—Na36—O34	-174.25 (9)
C27—O29—Na35—O15 ⁱⁱ	-54.6 (2)	Na37 ⁱ —O14—Na36—O34 ⁱⁱ	-88.98 (9)
C27—O29—Na35—N16	27.0 (2)	Na37 ⁱ —O14—Na36—Na35 ⁱⁱ	-84.20 (7)
C27—O29—Na35—C17	22.3 (2)	Na37 ⁱ —O14—Na36—Na35	166.51 (7)
C27—O29—Na35—C27 ⁱⁱⁱ	133.0 (3)	Na37 ⁱ —O14—Na36—Na36 ^{iv}	-6.35 (9)
C27—O29—Na35—O28 ⁱⁱⁱ	101.1 (2)	Na37 ⁱ —O14—Na36—Na36 ⁱⁱ	-128.95 (7)
C27—O29—Na35—O34	-158.7 (2)	Na37 ^v —Na35—Na36—O14	88.21 (9)
C27—O29—Na35—Na36 ⁱⁱ	-125.6 (2)	Na37 ⁱⁱ —Na35—Na36—O14	177.91 (9)
C27—O29—Na35—Na36	-131.9 (3)	Na37 ⁱⁱ —Na35—Na36—O29	-73.69 (8)
C27—O29—Na35—Na37 ^v	-93.2 (3)	Na37 ^v —Na35—Na36—O29	-163.40 (9)
C27—O29—Na35—Na37 ⁱⁱ	-54.5 (2)	Na37 ^v —Na35—Na36—C32 ⁱⁱ	-42.48 (8)
C27—O29—Na36—O14	-124.9 (2)	Na37 ⁱⁱ —Na35—Na36—C32 ⁱⁱ	47.23 (7)
C27—O29—Na36—C32 ⁱⁱ	56.7 (3)	Na37 ^v —Na35—Na36—O33 ⁱⁱ	-67.97 (7)
C27—O29—Na36—O33 ⁱ	-48.0 (2)	Na37 ⁱⁱ —Na35—Na36—O33 ⁱⁱ	21.73 (6)
C27—O29—Na36—O33 ⁱⁱ	37.8 (2)	Na37 ⁱⁱ —Na35—Na36—O33 ⁱ	-66.07 (12)
C27—O29—Na36—O34	153.5 (2)	Na37 ^v —Na35—Na36—O33 ⁱ	-155.78 (12)
C27—O29—Na36—O34 ⁱⁱ	80.3 (3)	Na37 ⁱⁱ —Na35—Na36—O34 ⁱⁱ	72.72 (6)
C27—O29—Na36—Na35	126.7 (3)	Na37 ^v —Na35—Na36—O34 ⁱⁱ	-16.98 (7)
C27—O29—Na36—Na35 ⁱⁱ	105.5 (3)	Na37 ⁱⁱ —Na35—Na36—O34	148.12 (11)
C27—O29—Na36—Na36 ^{iv}	-2.4 (2)	Na37 ^v —Na35—Na36—O34	58.42 (11)
C27—O29—Na36—Na36 ⁱⁱ	120.0 (2)	Na37 ^v —Na35—Na36—Na35 ⁱⁱ	9.69 (5)
C27—O29—Na36—Na37 ⁱ	-68.4 (3)	Na37 ⁱⁱ —Na35—Na36—Na35 ⁱⁱ	99.39 (5)
C27 ⁱⁱⁱ —Na35—Na36—O14	32.51 (13)	Na37 ⁱⁱ —Na35—Na36—Na36 ^{iv}	-9.86 (6)
C27 ⁱⁱⁱ —Na35—Na36—O29	140.91 (12)	Na37 ^v —Na35—Na36—Na36 ^{iv}	-99.57 (7)
C27 ⁱⁱⁱ —Na35—Na36—C32 ⁱⁱ	-98.17 (11)	Na37 ⁱⁱ —Na35—Na36—Na36 ⁱⁱ	99.39 (5)
C27 ⁱⁱⁱ —Na35—Na36—O33 ⁱ	148.52 (14)	Na37 ^v —Na35—Na36—Na36 ⁱⁱ	9.69 (5)
C27 ⁱⁱⁱ —Na35—Na36—O33 ⁱⁱ	-123.67 (10)	Na37 ^v —Na35—Na36—Na37 ⁱ	133.6 (2)
C27 ⁱⁱⁱ —Na35—Na36—O34 ⁱⁱ	-72.68 (10)	Na37 ⁱⁱ —Na35—Na36—Na37 ⁱ	-136.7 (2)
C27 ⁱⁱⁱ —Na35—Na36—O34	2.72 (13)		

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $x+1, y, z$; (iv) $-x, -y+1, -z$; (v) $-x+2, -y+1, -z$.