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catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')sodium(I)]-μ-aqua-[diaqua(1,10-phenanthroline-κ^2N,N')sodium(I)]-μ-aqua] dibromide 1,10-phenanthroline solvate]

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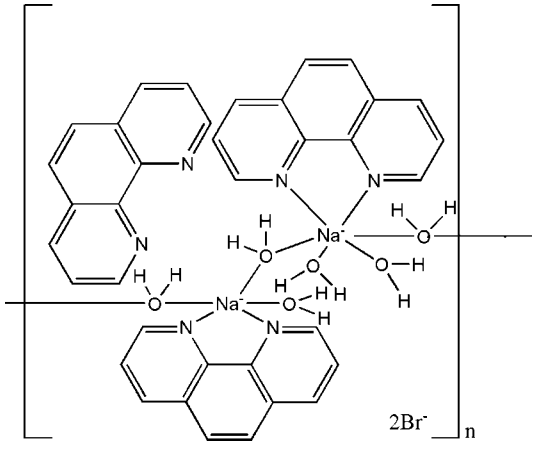
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.052; wR factor = 0.145; data-to-parameter ratio = 13.7.

In the title compound, $\{[Na_2(C_{12}H_8N_2)_2(H_2O)_5]Br_2\cdot C_{12}H_8N_2\}_n$, the Na^I ions in polymeric chains adopt two different types of coordination geometry. In one type, the Na^I ion is coordinated by two N atoms from 1,10-phenanthroline (L) and four water molecules in a distorted octahedral geometry, while in the other type, the Na^I ion is coordinated by two N atoms from L and three water molecules in a distorted trigonal–bipyramidal geometry. The coordinating bond lengths Na—N [2.425 (5)–2.517 (5) Å] and Na—O [2.353 (5)–2.574 (4) Å] are normal. The crystal packing exhibits an extensive hydrogen-bonding network (O—H···N, O—H···O and O—H···Br) and π–π interactions (centroid–centroid distances are 3.821 and 3.896 Å).

Related literature

For related sodium complexes with 1,10-phenanthroline, see: Qian *et al.* (1994).



Experimental

Crystal data

$[Na_2(C_{12}H_8N_2)_2(H_2O)_5]Br_2\cdot C_{12}H_8N_2$
M_r = 836.49
Monoclinic, $P2_1/c$
a = 12.833 (5) Å
b = 11.445 (5) Å
c = 24.888 (10) Å
β = 93.696 (6)°
V = 3648 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.30 mm^{-1}
T = 298 (2) K
0.66 × 0.32 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.313, T_{max} = 0.803
18042 measured reflections
6336 independent reflections
3007 reflections with $I > 2\sigma(I)$
R_{int} = 0.134

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.145
S = 0.85
6336 reflections
461 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H37···N5	0.85	2.10	2.925 (6)	164
O2—H39···Br2^{i}	0.85	2.60	3.388 (4)	156
O2—H40···N6^{i}	0.85	2.01	2.821 (5)	160
O3—H41···O2^{ii}	0.85	2.04	2.838 (5)	156
O3—H42···Br1	0.85	2.62	3.406 (4)	153
O4—H43···Br1	0.85	2.48	3.275 (4)	155
O4—H44···Br2^{i}	0.85	2.59	3.377 (4)	155
O5—H45···Br2	0.85	2.53	3.362 (4)	167
O5—H46···Br1^{i}	0.85	2.57	3.290 (4)	143

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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*); 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: CV2346).

References

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Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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supplementary materials

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catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')sodium(I)]-μ-aqua-[diaqua(1,10-phenanthroline-κ^2N,N')sodium(I)]-μ-aqua] dibromide 1,10-phenanthroline solvate]

J. Zhai, H. Yin and D. Wang

Comment

The structural chemistry of sodium complexes with 1,10-phenanthroline has been explored (Qian *et al.*, 1994). In continuation of our study of sodium complexes with 1,10-phenanthroline, we present here the synthesis and crystal structure of the title compound, (I).

In the title compound (Fig. 1), $[(Na_2L_2(H_2O)_5)^{2+}\cdot 2Br^{-}\cdot L]_n$, ($L$=1,10-phenanthroline), the Na^I ions in polymeric chains adopt two different coordinate fashions. The Na^I ions adopt different coordinate fashions. In one fashion, the Na^I ion is coordinated by two N atoms from L and four water molecules in a distorted octahedral geometry, while in another fashion, the Na^I ion is coordinated by two N atoms from L and three water molecules in a distorted trigonal-bipyramidal geometry. The coordinating bond lengths Na—N [2.425 (5)–2.517 (5) Å] and Na—O [2.353 (5)–2.574 (4) Å] are normal. The crystal packing exhibits an extensive hydrogen-bonding network formed by O—H···N, O—H···O and O—H···Br hydrogen bonds (Table 1) and π···π interactions, proved by short distances of 3.605 (4) and 3.821 (4) between the centroids of central and outer rings of L from neighbouring molecules.

Experimental

The title compound was prepared by the reaction of sodium(I) bromide (102.9 mg, 1 mmol) with 1,10-phenanthroline (198.2 mg, 1 mmol), in absolute ethanol. After stirring for 5 h at room temperature, the yellow paste was obtained and then filtered. Yellow crystals suitable for X-ray analysis were obtained by slow evaporation of ethanol/dichloromethane (1:1 *v*/*v*) solution over a period of two weeks (yield 82%. m.p. 452k).

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 Å for aromatic H atoms, O—H = 0.85 Å, and treated as riding on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C, O).

Figures

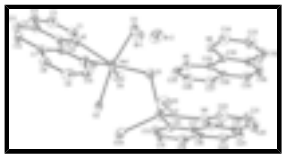


Fig. 1. View of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme [symmetry code: (A) −*x* + 1, *y* + 1/2, −*z* + 1/2]. H atoms have been omitted for clarity.

catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')sodium(I)]- μ-aqua-[diaqua(1,10-phenanthroline-κ^2N,N')sodium(I)]-μ-aqua] dibromide 1,10-phenanthroline solvate]

Crystal data

$[Na_2(C_{12}H_8N_2)_2(H_2O)_5]Br_2{\cdot}C_{12}H_8N_2$	F_{000} = 1696
M_r = 836.49	D_x = 1.523 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.833 (5) Å	Cell parameters from 2683 reflections
b = 11.445 (5) Å	θ = 2.4–20.9º
c = 24.888 (10) Å	μ = 2.30 mm^{-1}
β = 93.696 (6)º	T = 298 (2) K
V = 3648 (2) Å^3	Block, yellow
Z = 4	0.66 × 0.32 × 0.10 mm

Data collection

CCD area-detector diffractometer	6336 independent reflections
Radiation source: fine-focus sealed tube	3007 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.134
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→15
T_{min} = 0.313, T_{max} = 0.803	k = −13→13
18042 measured reflections	l = −29→27

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$w = 1/[\sigma^2(F_o^2)]$
$wR(F^2)$ = 0.145	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.85	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
6336 reflections	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
461 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0046 (4)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.39048 (15)	0.29514 (18)	0.25029 (8)	0.0471 (6)
Na2	0.69832 (15)	0.45126 (19)	0.26998 (9)	0.0512 (6)
Br1	0.27305 (5)	0.09245 (6)	0.39440 (3)	0.0635 (3)
Br2	0.72128 (5)	0.12723 (6)	0.14815 (3)	0.0717 (3)
N1	0.2206 (3)	0.2379 (4)	0.20115 (18)	0.0458 (12)
N2	0.3897 (3)	0.3228 (4)	0.15218 (17)	0.0405 (11)
N3	0.6562 (3)	0.4975 (4)	0.36179 (18)	0.0439 (12)
N4	0.8426 (3)	0.4056 (4)	0.33425 (19)	0.0440 (12)
N5	0.6283 (3)	0.1801 (4)	0.37083 (17)	0.0407 (11)
N6	0.7845 (3)	0.0744 (4)	0.31736 (18)	0.0394 (11)
O1	0.5907 (2)	0.2818 (3)	0.26352 (15)	0.0534 (11)
H37	0.6010	0.2396	0.2915	0.064*
H38	0.6015	0.2375	0.2370	0.064*
O2	0.3959 (2)	0.5093 (3)	0.24641 (14)	0.0487 (10)
H39	0.3860	0.5352	0.2777	0.058*
H40	0.3525	0.5385	0.2229	0.058*
O3	0.4043 (2)	0.0894 (3)	0.27973 (14)	0.0471 (10)
H41	0.4668	0.0645	0.2822	0.056*
H42	0.3934	0.0904	0.3131	0.056*
O4	0.3149 (3)	0.3385 (4)	0.33216 (17)	0.0831 (14)
H43	0.2852	0.2771	0.3428	0.100*
H44	0.2891	0.4022	0.3428	0.100*
O5	0.7918 (3)	0.3920 (4)	0.19641 (17)	0.0718 (13)
H45	0.7634	0.3287	0.1852	0.086*
H46	0.7714	0.4131	0.1647	0.086*
C1	0.1379 (5)	0.1980 (5)	0.2253 (3)	0.0556 (16)
H1	0.1443	0.1824	0.2621	0.067*
C2	0.0410 (4)	0.1790 (5)	0.1967 (3)	0.0614 (18)
H2A	−0.0154	0.1515	0.2147	0.074*
C3	0.0295 (4)	0.2006 (5)	0.1431 (3)	0.0560 (17)
H3	−0.0345	0.1881	0.1243	0.067*
C4	0.1144 (4)	0.2419 (5)	0.1165 (2)	0.0403 (14)
C5	0.2100 (4)	0.2599 (4)	0.1478 (2)	0.0353 (13)
C6	0.2977 (4)	0.3069 (4)	0.1214 (2)	0.0331 (13)
C7	0.2886 (4)	0.3349 (4)	0.0668 (2)	0.0378 (13)
C8	0.3746 (4)	0.3851 (5)	0.0433 (2)	0.0476 (15)
H8	0.3701	0.4057	0.0071	0.057*
C9	0.4642 (4)	0.4031 (5)	0.0740 (3)	0.0540 (17)
H9	0.5219	0.4371	0.0595	0.065*
C10	0.4678 (4)	0.3695 (5)	0.1279 (3)	0.0496 (16)
H10	0.5302	0.3809	0.1483	0.060*
C11	0.1097 (4)	0.2689 (5)	0.0603 (2)	0.0522 (17)
H11	0.0482	0.2545	0.0396	0.063*
C12	0.1908 (4)	0.3140 (5)	0.0370 (2)	0.0459 (15)
H12	0.1841	0.3324	0.0006	0.055*

C13	0.5678 (4)	0.5410 (5)	0.3758 (3)	0.0530 (17)
H13	0.5160	0.5541	0.3486	0.064*
C14	0.5449 (5)	0.5694 (5)	0.4282 (3)	0.0562 (17)
H14	0.4809	0.6017	0.4355	0.067*
C15	0.6198 (5)	0.5479 (5)	0.4681 (3)	0.0557 (17)
H15	0.6072	0.5649	0.5036	0.067*
C16	0.7162 (4)	0.5002 (5)	0.4557 (2)	0.0443 (15)
C17	0.7323 (4)	0.4761 (4)	0.4011 (2)	0.0390 (14)
C18	0.8299 (4)	0.4284 (4)	0.3866 (2)	0.0383 (14)
C19	0.9086 (4)	0.4064 (5)	0.4284 (2)	0.0441 (15)
C20	1.0038 (5)	0.3614 (5)	0.4122 (3)	0.0618 (19)
H20	1.0580	0.3460	0.4378	0.074*
C21	1.0167 (4)	0.3404 (5)	0.3599 (3)	0.0645 (19)
H21	1.0796	0.3110	0.3491	0.077*
C22	0.9332 (5)	0.3640 (5)	0.3217 (3)	0.0550 (17)
H22	0.9430	0.3493	0.2856	0.066*
C23	0.7965 (5)	0.4725 (5)	0.4960 (2)	0.0561 (17)
H23	0.7852	0.4851	0.5321	0.067*
C24	0.8876 (5)	0.4289 (5)	0.4826 (3)	0.0571 (18)
H24	0.9389	0.4127	0.5097	0.069*
C25	0.5517 (4)	0.2223 (5)	0.3984 (3)	0.0533 (16)
H25	0.4899	0.2447	0.3796	0.064*
C26	0.5591 (5)	0.2346 (5)	0.4542 (3)	0.0595 (18)
H26	0.5020	0.2608	0.4720	0.071*
C27	0.6503 (5)	0.2081 (5)	0.4823 (2)	0.0581 (17)
H27	0.6571	0.2193	0.5193	0.070*
C28	0.7335 (4)	0.1641 (5)	0.4552 (2)	0.0440 (14)
C29	0.7192 (4)	0.1479 (4)	0.3996 (2)	0.0375 (14)
C30	0.8015 (4)	0.0986 (4)	0.3698 (2)	0.0360 (13)
C31	0.8991 (4)	0.0763 (5)	0.3987 (3)	0.0435 (15)
C32	0.9783 (4)	0.0304 (5)	0.3684 (3)	0.0536 (17)
H32	1.0435	0.0147	0.3853	0.064*
C33	0.9615 (4)	0.0087 (5)	0.3154 (3)	0.0587 (18)
H33	1.0147	−0.0198	0.2954	0.070*
C34	0.8624 (4)	0.0300 (5)	0.2914 (2)	0.0523 (16)
H34	0.8501	0.0121	0.2550	0.063*
C35	0.8314 (5)	0.1364 (5)	0.4821 (2)	0.0576 (18)
H35	0.8407	0.1462	0.5191	0.069*
C36	0.9105 (5)	0.0961 (5)	0.4546 (3)	0.0605 (18)
H36	0.9746	0.0809	0.4729	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0494 (12)	0.0529 (15)	0.0386 (14)	0.0009 (10)	−0.0001 (10)	0.0058 (11)
Na2	0.0506 (13)	0.0624 (16)	0.0397 (15)	−0.0020 (11)	−0.0049 (11)	0.0047 (11)
Br1	0.0607 (4)	0.0888 (6)	0.0419 (4)	−0.0109 (4)	0.0097 (3)	−0.0017 (3)
Br2	0.0713 (5)	0.0805 (6)	0.0630 (5)	−0.0209 (4)	0.0012 (4)	0.0103 (4)

N1	0.046 (3)	0.054 (3)	0.038 (3)	0.005 (2)	0.002 (2)	0.007 (2)
N2	0.039 (3)	0.051 (3)	0.032 (3)	−0.006 (2)	0.001 (2)	−0.006 (2)
N3	0.038 (3)	0.051 (3)	0.043 (3)	0.003 (2)	−0.003 (2)	0.002 (2)
N4	0.043 (3)	0.050 (3)	0.039 (3)	0.002 (2)	0.004 (2)	0.001 (2)
N5	0.036 (2)	0.049 (3)	0.038 (3)	−0.002 (2)	0.010 (2)	0.002 (2)
N6	0.038 (3)	0.049 (3)	0.031 (3)	−0.003 (2)	0.006 (2)	−0.003 (2)
O1	0.057 (2)	0.052 (3)	0.050 (3)	−0.0047 (19)	−0.002 (2)	0.005 (2)
O2	0.050 (2)	0.063 (3)	0.032 (2)	0.0016 (19)	−0.0075 (18)	0.0049 (19)
O3	0.044 (2)	0.063 (3)	0.034 (2)	0.0036 (18)	0.0029 (17)	0.0087 (19)
O4	0.118 (4)	0.067 (3)	0.069 (3)	0.015 (3)	0.046 (3)	0.004 (2)
O5	0.081 (3)	0.083 (4)	0.052 (3)	−0.002 (2)	0.010 (2)	−0.001 (2)
C1	0.063 (4)	0.056 (4)	0.049 (4)	0.002 (3)	0.014 (3)	0.005 (3)
C2	0.045 (4)	0.062 (5)	0.080 (6)	−0.004 (3)	0.026 (4)	0.010 (4)
C3	0.041 (3)	0.054 (4)	0.072 (5)	−0.005 (3)	0.002 (3)	−0.001 (4)
C4	0.034 (3)	0.043 (4)	0.043 (4)	0.001 (3)	−0.002 (3)	−0.001 (3)
C5	0.039 (3)	0.029 (3)	0.039 (4)	0.007 (2)	0.009 (3)	0.004 (3)
C6	0.040 (3)	0.032 (3)	0.028 (3)	0.005 (2)	0.006 (3)	−0.005 (2)
C7	0.053 (3)	0.032 (3)	0.028 (3)	0.007 (3)	0.001 (3)	−0.005 (3)
C8	0.059 (4)	0.049 (4)	0.036 (4)	0.000 (3)	0.014 (3)	0.007 (3)
C9	0.052 (4)	0.058 (4)	0.054 (5)	−0.013 (3)	0.022 (3)	−0.004 (3)
C10	0.045 (3)	0.049 (4)	0.055 (5)	−0.010 (3)	0.003 (3)	−0.013 (3)
C11	0.050 (4)	0.052 (4)	0.052 (5)	−0.001 (3)	−0.020 (3)	−0.003 (3)
C12	0.052 (4)	0.060 (4)	0.025 (3)	0.002 (3)	−0.004 (3)	0.000 (3)
C13	0.036 (3)	0.050 (4)	0.073 (5)	0.006 (3)	−0.002 (3)	0.004 (3)
C14	0.051 (4)	0.060 (5)	0.058 (5)	0.006 (3)	0.013 (4)	−0.004 (4)
C15	0.067 (4)	0.054 (4)	0.048 (4)	0.000 (3)	0.012 (4)	−0.009 (3)
C16	0.048 (3)	0.042 (4)	0.043 (4)	−0.005 (3)	0.002 (3)	−0.006 (3)
C17	0.044 (3)	0.033 (3)	0.040 (4)	−0.009 (3)	0.005 (3)	0.003 (3)
C18	0.036 (3)	0.034 (3)	0.043 (4)	0.001 (2)	−0.005 (3)	0.001 (3)
C19	0.042 (3)	0.044 (4)	0.044 (4)	−0.004 (3)	−0.009 (3)	0.003 (3)
C20	0.044 (4)	0.074 (5)	0.066 (5)	0.005 (3)	−0.004 (4)	−0.001 (4)
C21	0.043 (4)	0.069 (5)	0.084 (6)	0.010 (3)	0.013 (4)	0.007 (4)
C22	0.057 (4)	0.061 (4)	0.049 (4)	0.006 (3)	0.014 (3)	0.005 (3)
C23	0.074 (4)	0.059 (4)	0.034 (4)	−0.006 (4)	−0.005 (3)	0.002 (3)
C24	0.062 (4)	0.058 (4)	0.047 (5)	0.003 (3)	−0.025 (4)	0.005 (3)
C25	0.046 (4)	0.059 (4)	0.055 (5)	−0.007 (3)	0.005 (3)	0.001 (3)
C26	0.054 (4)	0.065 (5)	0.063 (5)	−0.005 (3)	0.030 (4)	−0.004 (4)
C27	0.076 (4)	0.062 (5)	0.039 (4)	−0.013 (4)	0.019 (4)	−0.005 (3)
C28	0.055 (4)	0.042 (4)	0.036 (4)	−0.008 (3)	0.004 (3)	0.002 (3)
C29	0.033 (3)	0.039 (3)	0.041 (4)	−0.006 (2)	0.002 (3)	0.010 (3)
C30	0.032 (3)	0.036 (3)	0.039 (4)	−0.007 (2)	0.002 (3)	−0.002 (3)
C31	0.039 (3)	0.040 (4)	0.050 (4)	−0.003 (3)	−0.007 (3)	0.009 (3)
C32	0.032 (3)	0.054 (4)	0.075 (5)	0.004 (3)	−0.005 (3)	0.010 (4)
C33	0.039 (4)	0.066 (5)	0.072 (5)	−0.001 (3)	0.016 (4)	0.003 (4)
C34	0.051 (4)	0.060 (4)	0.047 (4)	−0.009 (3)	0.013 (3)	−0.008 (3)
C35	0.075 (5)	0.064 (5)	0.031 (4)	−0.014 (4)	−0.015 (4)	0.004 (3)
C36	0.054 (4)	0.064 (5)	0.061 (5)	0.008 (3)	−0.017 (4)	0.015 (4)

Geometric parameters (Å, °)

Na1—O4	2.365 (5)	C8—C9	1.356 (7)
Na1—O2	2.454 (4)	C8—H8	0.9300
Na1—N2	2.462 (5)	C9—C10	1.392 (8)
Na1—O3	2.469 (4)	C9—H9	0.9300
Na1—N1	2.517 (5)	C10—H10	0.9300
Na1—O1	2.574 (4)	C11—C12	1.328 (7)
Na1—Na2^{i}	4.119 (3)	C11—H11	0.9300
Na2—O5	2.353 (5)	C12—H12	0.9300
Na2—O3^{ii}	2.357 (4)	C13—C14	1.393 (8)
Na2—O1	2.380 (4)	C13—H13	0.9300
Na2—N4	2.425 (5)	C14—C15	1.359 (7)
Na2—N3	2.440 (5)	C14—H14	0.9300
Na2—Na1^{ii}	4.119 (3)	C15—C16	1.405 (7)
N1—C1	1.334 (7)	C15—H15	0.9300
N1—C5	1.350 (6)	C16—C17	1.413 (7)
N2—C10	1.317 (7)	C16—C23	1.427 (7)
N2—C6	1.376 (6)	C17—C18	1.433 (7)
N3—C13	1.306 (6)	C18—C19	1.424 (7)
N3—C17	1.360 (6)	C19—C20	1.408 (8)
N4—C22	1.312 (6)	C19—C24	1.417 (8)
N4—C18	1.350 (7)	C20—C21	1.343 (9)
N5—C25	1.326 (7)	C20—H20	0.9300
N5—C29	1.380 (6)	C21—C22	1.412 (8)
N6—C34	1.327 (7)	C21—H21	0.9300
N6—C30	1.338 (6)	C22—H22	0.9300
O1—H37	0.8500	C23—C24	1.333 (8)
O1—H38	0.8500	C23—H23	0.9300
O2—H39	0.8500	C24—H24	0.9300
O2—H40	0.8500	C25—C26	1.391 (8)
O3—Na2^{i}	2.357 (4)	C25—H25	0.9300
O3—H41	0.8500	C26—C27	1.359 (7)
O3—H42	0.8499	C26—H26	0.9300
O4—H43	0.8499	C27—C28	1.393 (7)
O4—H44	0.8500	C27—H27	0.9300
O5—H45	0.8501	C28—C29	1.395 (7)
O5—H46	0.8500	C28—C35	1.421 (7)
C1—C2	1.410 (8)	C29—C30	1.444 (7)
C1—H1	0.9300	C30—C31	1.427 (7)
C2—C3	1.354 (8)	C31—C32	1.406 (8)
C2—H2A	0.9300	C31—C36	1.408 (8)
C3—C4	1.394 (7)	C32—C33	1.345 (8)
C3—H3	0.9300	C32—H32	0.9300
C4—C5	1.425 (6)	C33—C34	1.392 (7)
C4—C11	1.428 (7)	C33—H33	0.9300
C5—C6	1.444 (7)	C34—H34	0.9300

C6—C7	1.394 (7)	C35—C36	1.342 (8)
C7—C8	1.404 (7)	C35—H35	0.9300
C7—C12	1.436 (7)	C36—H36	0.9300
O4—Na1—O2	80.71 (15)	C6—C7—C12	118.7 (5)
O4—Na1—N2	148.42 (17)	C8—C7—C12	122.5 (5)
O2—Na1—N2	80.27 (14)	C9—C8—C7	119.3 (5)
O4—Na1—O3	88.29 (15)	C9—C8—H8	120.4
O2—Na1—O3	164.26 (14)	C7—C8—H8	120.4
N2—Na1—O3	114.36 (15)	C8—C9—C10	118.3 (5)
O4—Na1—N1	94.76 (17)	C8—C9—H9	120.8
O2—Na1—N1	105.47 (14)	C10—C9—H9	120.8
N2—Na1—N1	66.62 (15)	N2—C10—C9	125.1 (5)
O3—Na1—N1	86.52 (14)	N2—C10—H10	117.4
O4—Na1—O1	111.33 (16)	C9—C10—H10	117.4
O2—Na1—O1	91.93 (12)	C12—C11—C4	121.8 (5)
N2—Na1—O1	94.29 (14)	C12—C11—H11	119.1
O3—Na1—O1	81.57 (12)	C4—C11—H11	119.1
N1—Na1—O1	150.81 (16)	C11—C12—C7	121.5 (5)
O4—Na1—Na2^{i}	100.40 (13)	C11—C12—H12	119.2
O2—Na1—Na2^{i}	163.28 (10)	C7—C12—H12	119.2
N2—Na1—Na2^{i}	91.01 (12)	N3—C13—C14	125.3 (6)
O3—Na1—Na2^{i}	30.59 (8)	N3—C13—H13	117.4
N1—Na1—Na2^{i}	57.83 (11)	C14—C13—H13	117.4
O1—Na1—Na2^{i}	103.00 (10)	C15—C14—C13	117.4 (6)
O5—Na2—O3^{ii}	94.63 (15)	C15—C14—H14	121.3
O5—Na2—O1	92.00 (16)	C13—C14—H14	121.3
O3^{ii}—Na2—O1	102.07 (14)	C14—C15—C16	120.0 (6)
O5—Na2—N4	92.58 (17)	C14—C15—H15	120.0
O3^{ii}—Na2—N4	150.24 (17)	C16—C15—H15	120.0
O1—Na2—N4	106.50 (16)	C15—C16—C17	118.2 (5)
O5—Na2—N3	161.14 (16)	C15—C16—C23	122.5 (6)
O3^{ii}—Na2—N3	101.31 (16)	C17—C16—C23	119.2 (5)
O1—Na2—N3	94.43 (15)	N3—C17—C16	120.9 (5)
N4—Na2—N3	68.60 (16)	N3—C17—C18	119.1 (5)
O5—Na2—Na1^{ii}	109.34 (13)	C16—C17—C18	120.0 (5)
O3^{ii}—Na2—Na1^{ii}	32.22 (9)	N4—C18—C19	123.0 (5)
O1—Na2—Na1^{ii}	127.99 (11)	N4—C18—C17	118.7 (5)
N4—Na2—Na1^{ii}	118.71 (13)	C19—C18—C17	118.3 (5)
N3—Na2—Na1^{ii}	80.29 (12)	C20—C19—C24	124.2 (5)
C1—N1—C5	118.4 (4)	C20—C19—C18	116.3 (6)
C1—N1—Na1	124.0 (4)	C24—C19—C18	119.5 (5)
C5—N1—Na1	117.3 (3)	C21—C20—C19	120.4 (6)
C10—N2—C6	116.7 (5)	C21—C20—H20	119.8
C10—N2—Na1	123.6 (4)	C19—C20—H20	119.8
C6—N2—Na1	118.9 (3)	C20—C21—C22	118.8 (6)
C13—N3—C17	118.2 (5)	C20—C21—H21	120.6

C13—N3—Na2	125.5 (4)	C22—C21—H21	120.6
C17—N3—Na2	116.3 (4)	N4—C22—C21	123.7 (6)
C22—N4—C18	117.7 (5)	N4—C22—H22	118.2
C22—N4—Na2	124.9 (4)	C21—C22—H22	118.2
C18—N4—Na2	117.4 (3)	C24—C23—C16	120.8 (6)
C25—N5—C29	117.3 (5)	C24—C23—H23	119.6
C34—N6—C30	118.3 (4)	C16—C23—H23	119.6
Na2—O1—Na1	122.02 (16)	C23—C24—C19	122.0 (5)
Na2—O1—H37	110.4	C23—C24—H24	119.0
Na1—O1—H37	103.9	C19—C24—H24	119.0
Na2—O1—H38	114.6	N5—C25—C26	123.3 (5)
Na1—O1—H38	98.4	N5—C25—H25	118.4
H37—O1—H38	105.8	C26—C25—H25	118.4
Na1—O2—H39	107.8	C27—C26—C25	119.5 (6)
Na1—O2—H40	113.6	C27—C26—H26	120.3
H39—O2—H40	111.3	C25—C26—H26	120.3
$Na2^{i}$—O3—Na1	117.19 (15)	C26—C27—C28	119.5 (6)
$Na2^{i}$—O3—H41	107.9	C26—C27—H27	120.2
Na1—O3—H41	113.0	C28—C27—H27	120.2
$Na2^{i}$—O3—H42	113.6	C27—C28—C29	118.2 (5)
Na1—O3—H42	105.3	C27—C28—C35	122.3 (6)
H41—O3—H42	98.4	C29—C28—C35	119.5 (6)
Na1—O4—H43	108.2	N5—C29—C28	122.1 (5)
Na1—O4—H44	129.6	N5—C29—C30	117.3 (5)
H43—O4—H44	114.9	C28—C29—C30	120.5 (5)
Na2—O5—H45	105.8	N6—C30—C31	122.4 (5)
Na2—O5—H46	119.8	N6—C30—C29	120.3 (4)
H45—O5—H46	80.6	C31—C30—C29	117.3 (5)
N1—C1—C2	121.7 (6)	C32—C31—C36	123.9 (5)
N1—C1—H1	119.1	C32—C31—C30	116.0 (6)
C2—C1—H1	119.1	C36—C31—C30	120.1 (5)
C3—C2—C1	120.4 (6)	C33—C32—C31	121.3 (5)
C3—C2—H2A	119.8	C33—C32—H32	119.3
C1—C2—H2A	119.8	C31—C32—H32	119.3
C2—C3—C4	119.4 (5)	C32—C33—C34	118.2 (6)
C2—C3—H3	120.3	C32—C33—H33	120.9
C4—C3—H3	120.3	C34—C33—H33	120.9
C3—C4—C5	117.4 (5)	N6—C34—C33	123.6 (6)
C3—C4—C11	123.6 (5)	N6—C34—H34	118.2
C5—C4—C11	119.0 (5)	C33—C34—H34	118.2
N1—C5—C4	122.7 (5)	C36—C35—C28	120.8 (6)
N1—C5—C6	119.0 (4)	C36—C35—H35	119.6
C4—C5—C6	118.3 (5)	C28—C35—H35	119.6
N2—C6—C7	121.8 (5)	C35—C36—C31	121.7 (5)
N2—C6—C5	117.5 (5)	C35—C36—H36	119.2
C7—C6—C5	120.7 (4)	C31—C36—H36	119.2
C6—C7—C8	118.7 (5)		

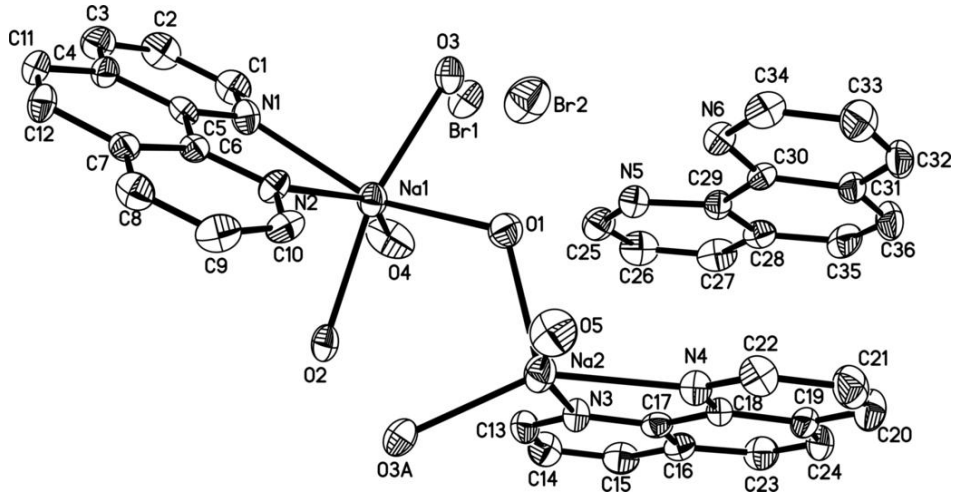
Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H37···N5	0.85	2.10	2.925 (6)	164
O2—H39···Br2^{ii}	0.85	2.60	3.388 (4)	156
O2—H40···N6^{ii}	0.85	2.01	2.821 (5)	160
O3—H41···O2^{i}	0.85	2.04	2.838 (5)	156
O3—H42···Br1	0.85	2.62	3.406 (4)	153
O4—H43···Br1	0.85	2.48	3.275 (4)	155
O4—H44···Br2^{ii}	0.85	2.59	3.377 (4)	155
O5—H45···Br2	0.85	2.53	3.362 (4)	167
O5—H46···Br1^{ii}	0.85	2.57	3.290 (4)	143

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

Fig. 1


C3
C2
C11
C4
C1
N1
C12
C5
C6
C7
N2
C8
C9
C10
Na1
O3
Br1
Br2
O4
O2
O1
O5
Na2
N3
C13
O3A
C14
C15
C16
C17
N4
C22
C21
C18
C19
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C23
C24
N5
C29
C30
C34
C33
N6
C32
C31
C25
C26
C27
C28
C35
C36