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(Isopropyl xanthato-κ^2S,S')bis(1,10-phenanthroline-κ^2N,N')sodium(I)

Feng Li

Department of Chemistry, Luliang Higher College, Shanxi 033000, People's Republic of China
Correspondence e-mail: lifeng1982@163.com

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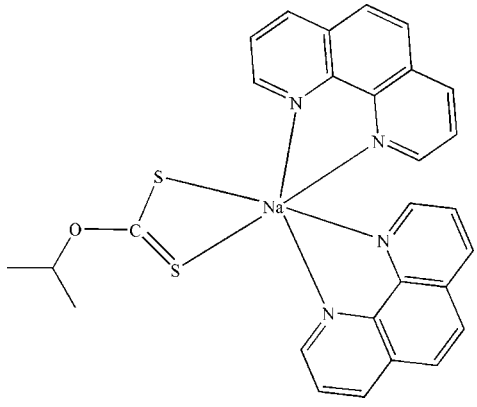
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.127; data-to-parameter ratio = 13.7.

The title compound, $[Na(C_4H_7OS_2)(C_{12}H_8N_2)_2]$, is monomeric, with the Na atom chelated by the S atoms of an *i*-propylxanthate ligand and the N atoms of two 1,10-phenanthroline (phen) ligands. The Na atom is six-coordinate in a distorted trigonal antiprism. A number of π–π stacking interactions involving the phen rings help to consolidate the crystal packing (centroid–centroid distances lie in the range 3.338–3.443 Å).

Related literature

For the structures of related complexes, see: Arnold (1995). For a comparison of π–π stacking interactions, see: Janiak (2000).



Experimental

Crystal data

$[Na(C_4H_7OS_2)(C_{12}H_8N_2)_2]$
M_r = 518.61
Monoclinic, $P2_1/c$
a = 16.529 (4) Å
b = 12.153 (3) Å
c = 13.002 (3) Å
β = 102.557 (4)°
V = 2549.5 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 298 (2) K
0.23 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.944, T_{max} = 0.960
13248 measured reflections
4495 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 1.00
4495 reflections
327 parameters
102 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Na1—N3	2.470 (3)	Na1—N1	2.523 (3)
Na1—N4	2.492 (3)	Na1—S1	2.9188 (15)
Na1—N2	2.501 (3)	Na1—S2	3.1265 (16)
N3—Na1—N4	66.79 (9)	N2—Na1—S1	145.46 (8)
N3—Na1—N2	94.11 (10)	N1—Na1—S1	85.78 (7)
N4—Na1—N2	88.26 (9)	N3—Na1—S2	134.91 (8)
N3—Na1—N1	92.54 (9)	N4—Na1—S2	85.99 (7)
N4—Na1—N1	146.48 (10)	N2—Na1—S2	121.38 (8)
N2—Na1—N1	66.31 (9)	N1—Na1—S2	125.37 (7)
N3—Na1—S1	107.62 (7)	S1—Na1—S2	58.81 (4)
N4—Na1—S1	124.66 (7)		

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SQ2005).

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(Isopropyl xanthato-κ^2S,S')bis(1,10-phenanthroline-κ^2N,N')sodium(I)

Feng Li

S1. Comment

So far only a handful of sodium chalcogenolates have been investigated in the solid state (Arnold *et al.*, 1995). As a continuation of our interest in sulfur-containing ligands, in this paper we report the synthesis and structural characterization of the title compound, (I).

The title compound, (I), is monomeric, with the Na atom chelated by the S atoms of an i-propylxanthate ligand and the nitrogen atoms of two 1,10-phenanthroline ligands (Fig. 1). The metal is six-coordinate in a coordination polyhedron that can be described as a distorted trigonal antiprism. The plane defined by S1, N1 and N3 is essentially parallel to that defined by S2, N2 and N4 (the two planes are inclined by 7.1°) and Na is displaced by 1.35 and 1.24 Å away from these planes, respectively.

A number of π-π stacking interactions involving the phen rings help to consolidate the crystal packing (Fig. 2). The *Cg*···*Cg* (*Cg* = ring centroid) distances lie in the range 3.338–3.443 Å, which is normal for such interactions (Janiak, 2000) and lead to the formation of an infinite one-dimensional chain network structure along the *a* axis.

S2. Experimental

To an acetonitrile solution of NaI (1.0 mmol) was added another acetonitrile solution of sodium i-propylxanthate (1.0 mmol) and phenanthroline (2.0 mmol). The resulting solution was stirred for 3.0 h at room temperature and a yellow-red solid was obtained by filtration. The product was recrystallized in acetone to give yellow-red crystals. Yield 82%. m.p.:436 K. Anal. Calcd. (%) for $C_{28}H_{23}NaON_4S_2$ (Mr = 518.61): C, 64.84; H, 4.47; N, 10.80. Found (%): C, 64.52; H, 4.23; N, 10.67.

S3. Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms [C—H = 0.93Å and U_{iso} = 1.2*U_{eq}(C) for CH (aromatic), C—H = 0.96Å and U_{iso} = 1.5*U_{eq}(C) for CH_3, C—H = 0.98Å and U_{iso} = 1.2*U_{eq}(C) for CH (aliphatic)].

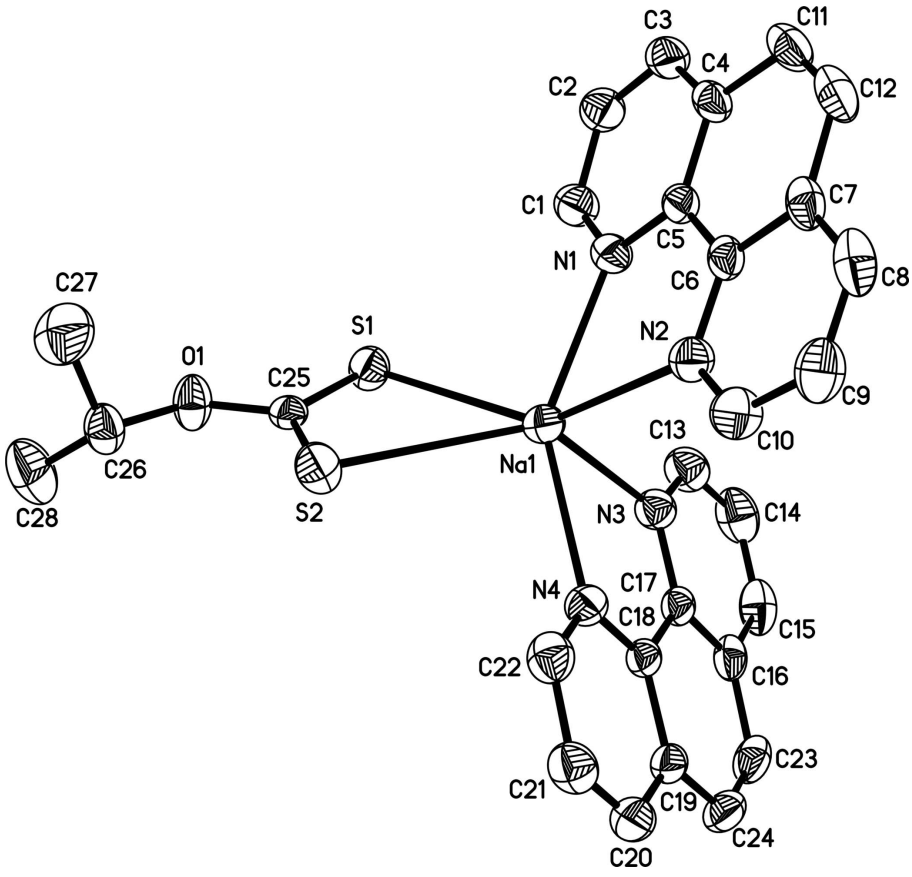

Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

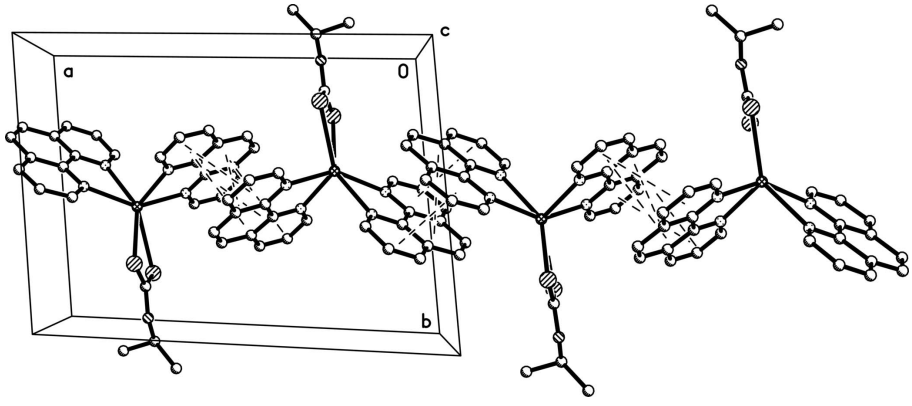

Figure 2

Crystal packing of (I) showing π-π stacking interactions (dashed lines) along the *a* axis.

(Isopropyl xanthato-κ^2S,S')bis(1,10-phenanthroline-κ^2N,N')sodium(I)

Crystal data

$[Na(C_4H_7OS_2)(C_{12}H_8N_2)_2]$
$M_r = 518.61$
Monoclinic, $P2_1/c$
$a = 16.529\ (4)$ Å
$b = 12.153\ (3)$ Å
$c = 13.002\ (3)$ Å

β = 102.557 (4)°
V = 2549.5 (11) Å^3
Z = 4
F(000) = 1080
D_x = 1.351 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2319 reflections
θ = 2.3–21.4°
μ = 0.26 mm^{-1}
T = 298 K
Block, yellow
0.23 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.944, T_{max} = 0.960

13248 measured reflections
4495 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −16→19
k = −13→14
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 1.00
4495 reflections
327 parameters
102 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
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.6823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Na1	0.24442 (7)	0.42828 (10)	0.49678 (9)	0.0561 (4)
S1	0.23574 (6)	0.23226 (7)	0.36513 (6)	0.0594 (3)
S2	0.26704 (6)	0.19302 (7)	0.59616 (6)	0.0652 (3)
N1	0.11912 (15)	0.4938 (2)	0.3635 (2)	0.0542 (7)
N2	0.16281 (16)	0.5731 (2)	0.5659 (2)	0.0571 (7)
N3	0.33660 (16)	0.5616 (2)	0.4359 (2)	0.0543 (7)
N4	0.36660 (15)	0.4814 (2)	0.6368 (2)	0.0522 (7)
O1	0.25533 (14)	0.04248 (16)	0.44589 (16)	0.0656 (7)
C1	0.0964 (2)	0.4556 (3)	0.2670 (3)	0.0641 (10)
H1	0.1330	0.4096	0.2423	0.077*

C2	0.0208 (2)	0.4798 (3)	0.1992 (3)	0.0664 (10)
H2	0.0079	0.4511	0.1313	0.080*
C3	−0.0334 (2)	0.5456 (3)	0.2341 (3)	0.0631 (10)
H3	−0.0845	0.5617	0.1905	0.076*
C4	−0.01268 (19)	0.5897 (2)	0.3358 (3)	0.0534 (8)
C5	0.06533 (18)	0.5611 (2)	0.3984 (2)	0.0481 (8)
C6	0.08858 (19)	0.6039 (2)	0.5051 (2)	0.0483 (8)
C7	0.0332 (2)	0.6737 (2)	0.5417 (3)	0.0569 (9)
C8	0.0581 (3)	0.7141 (3)	0.6447 (3)	0.0719 (11)
H8	0.0236	0.7611	0.6720	0.086*
C9	0.1327 (3)	0.6846 (3)	0.7041 (3)	0.0757 (11)
H9	0.1504	0.7116	0.7722	0.091*
C10	0.1822 (2)	0.6135 (3)	0.6620 (3)	0.0680 (10)
H10	0.2327	0.5928	0.7045	0.082*
C11	−0.0666 (2)	0.6609 (3)	0.3771 (3)	0.0670 (10)
H11	−0.1178	0.6797	0.3352	0.080*
C12	−0.0449 (2)	0.7008 (3)	0.4744 (3)	0.0708 (11)
H12	−0.0811	0.7472	0.4992	0.085*
C13	0.3242 (2)	0.6017 (3)	0.3396 (3)	0.0688 (10)
H13	0.2752	0.5827	0.2930	0.083*
C14	0.3786 (3)	0.6699 (3)	0.3027 (3)	0.0802 (12)
H14	0.3661	0.6958	0.2338	0.096*
C15	0.4505 (3)	0.6979 (3)	0.3695 (3)	0.0717 (11)
H15	0.4884	0.7428	0.3464	0.086*
C16	0.4675 (2)	0.6591 (2)	0.4731 (3)	0.0541 (8)
C17	0.40810 (18)	0.5912 (2)	0.5034 (2)	0.0455 (8)
C18	0.42288 (18)	0.5493 (2)	0.6098 (2)	0.0440 (7)
C19	0.49649 (19)	0.5806 (2)	0.6811 (3)	0.0514 (8)
C20	0.5093 (2)	0.5388 (3)	0.7836 (3)	0.0644 (10)
H20	0.5570	0.5575	0.8330	0.077*
C21	0.4525 (2)	0.4713 (3)	0.8106 (3)	0.0667 (10)
H21	0.4601	0.4436	0.8787	0.080*
C22	0.3821 (2)	0.4440 (3)	0.7342 (3)	0.0647 (9)
H22	0.3438	0.3965	0.7532	0.078*
C23	0.5415 (2)	0.6870 (3)	0.5485 (3)	0.0651 (10)
H23	0.5808	0.7320	0.5282	0.078*
C24	0.5552 (2)	0.6498 (3)	0.6469 (3)	0.0641 (10)
H24	0.6038	0.6693	0.6942	0.077*
C25	0.25295 (16)	0.1505 (2)	0.4714 (2)	0.0446 (7)
C26	0.2626 (2)	−0.0430 (3)	0.5236 (2)	0.0622 (10)
H26	0.2900	−0.0141	0.5928	0.075*
C27	0.1785 (3)	−0.0821 (4)	0.5268 (3)	0.1047 (14)
H27A	0.1458	−0.0214	0.5420	0.157*
H27B	0.1822	−0.1370	0.5808	0.157*
H27C	0.1529	−0.1134	0.4599	0.157*
C28	0.3157 (3)	−0.1305 (3)	0.4899 (3)	0.1062 (15)
H28A	0.2909	−0.1542	0.4196	0.159*
H28B	0.3202	−0.1920	0.5371	0.159*

H28C	0.3699	−0.1012	0.4913	0.159*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0451 (7)	0.0543 (7)	0.0660 (8)	−0.0008 (6)	0.0060 (6)	−0.0073 (6)
S1	0.0697 (6)	0.0538 (5)	0.0522 (5)	−0.0038 (4)	0.0078 (4)	0.0015 (4)
S2	0.0852 (7)	0.0600 (5)	0.0466 (5)	0.0113 (5)	0.0062 (4)	−0.0070 (4)
N1	0.0462 (17)	0.0547 (16)	0.0613 (18)	0.0053 (14)	0.0110 (14)	−0.0046 (14)
N2	0.0554 (18)	0.0576 (16)	0.0582 (18)	0.0005 (14)	0.0122 (14)	−0.0064 (14)
N3	0.0547 (18)	0.0561 (16)	0.0509 (17)	0.0019 (13)	0.0088 (14)	0.0003 (14)
N4	0.0458 (16)	0.0530 (15)	0.0581 (17)	−0.0046 (13)	0.0123 (13)	0.0032 (14)
O1	0.1042 (19)	0.0457 (13)	0.0483 (13)	0.0012 (12)	0.0195 (12)	−0.0033 (11)
C1	0.058 (2)	0.067 (2)	0.066 (2)	0.0055 (18)	0.0102 (19)	−0.0034 (19)
C2	0.067 (3)	0.067 (2)	0.061 (2)	−0.002 (2)	0.005 (2)	0.0041 (19)
C3	0.057 (2)	0.060 (2)	0.068 (2)	0.0004 (19)	0.0049 (19)	0.0182 (19)
C4	0.047 (2)	0.0450 (18)	0.069 (2)	0.0067 (16)	0.0158 (17)	0.0201 (17)
C5	0.0429 (19)	0.0396 (17)	0.063 (2)	−0.0008 (15)	0.0148 (16)	0.0059 (16)
C6	0.050 (2)	0.0354 (16)	0.062 (2)	−0.0004 (15)	0.0191 (17)	0.0068 (15)
C7	0.068 (2)	0.0387 (18)	0.071 (2)	0.0048 (17)	0.030 (2)	0.0101 (17)
C8	0.101 (3)	0.047 (2)	0.081 (3)	0.012 (2)	0.048 (2)	0.005 (2)
C9	0.102 (3)	0.064 (2)	0.067 (2)	−0.001 (2)	0.031 (2)	−0.009 (2)
C10	0.069 (3)	0.073 (2)	0.063 (2)	0.003 (2)	0.017 (2)	−0.007 (2)
C11	0.057 (2)	0.058 (2)	0.088 (3)	0.0176 (18)	0.021 (2)	0.027 (2)
C12	0.075 (3)	0.052 (2)	0.094 (3)	0.0234 (19)	0.037 (2)	0.018 (2)
C13	0.073 (3)	0.072 (2)	0.058 (2)	0.009 (2)	0.009 (2)	−0.001 (2)
C14	0.115 (4)	0.069 (3)	0.059 (2)	0.019 (3)	0.027 (3)	0.014 (2)
C15	0.096 (3)	0.048 (2)	0.084 (3)	0.004 (2)	0.049 (2)	0.005 (2)
C16	0.059 (2)	0.0376 (17)	0.072 (2)	0.0038 (16)	0.0283 (19)	−0.0034 (17)
C17	0.0429 (19)	0.0378 (16)	0.058 (2)	0.0023 (14)	0.0158 (16)	−0.0065 (15)
C18	0.0393 (18)	0.0377 (16)	0.056 (2)	0.0007 (14)	0.0126 (15)	−0.0033 (15)
C19	0.045 (2)	0.0425 (17)	0.065 (2)	0.0022 (15)	0.0076 (17)	−0.0132 (16)
C20	0.063 (2)	0.060 (2)	0.064 (2)	0.0070 (19)	0.0011 (19)	−0.0125 (19)
C21	0.080 (3)	0.068 (2)	0.050 (2)	0.008 (2)	0.011 (2)	0.0039 (18)
C22	0.069 (3)	0.060 (2)	0.068 (2)	−0.0030 (19)	0.020 (2)	0.0069 (19)
C23	0.058 (2)	0.0467 (19)	0.097 (3)	−0.0148 (17)	0.031 (2)	−0.011 (2)
C24	0.047 (2)	0.058 (2)	0.087 (3)	−0.0102 (18)	0.0121 (19)	−0.019 (2)
C25	0.0343 (17)	0.0451 (17)	0.0536 (18)	0.0008 (13)	0.0076 (14)	−0.0052 (15)
C26	0.083 (3)	0.050 (2)	0.051 (2)	0.0037 (18)	0.0111 (19)	0.0061 (16)
C27	0.110 (4)	0.111 (3)	0.095 (3)	−0.022 (3)	0.027 (3)	0.028 (3)
C28	0.138 (4)	0.079 (3)	0.101 (3)	0.039 (3)	0.023 (3)	0.001 (2)

Geometric parameters (Å, º)

Na1—N3	2.470 (3)	C10—H10	0.9300
Na1—N4	2.492 (3)	C11—C12	1.329 (5)
Na1—N2	2.501 (3)	C11—H11	0.9300
Na1—N1	2.523 (3)	C12—H12	0.9300

Na1—S1	2.9188 (15)	C13—C14	1.383 (5)
Na1—S2	3.1265 (16)	C13—H13	0.9300
S1—C25	1.675 (3)	C14—C15	1.354 (5)
S2—C25	1.670 (3)	C14—H14	0.9300
N1—C1	1.314 (4)	C15—C16	1.397 (5)
N1—C5	1.357 (4)	C15—H15	0.9300
N2—C10	1.315 (4)	C16—C17	1.403 (4)
N2—C6	1.360 (4)	C16—C23	1.432 (4)
N3—C13	1.317 (4)	C17—C18	1.444 (4)
N3—C17	1.359 (3)	C18—C19	1.412 (4)
N4—C22	1.316 (4)	C19—C20	1.399 (4)
N4—C18	1.346 (4)	C19—C24	1.425 (4)
O1—C25	1.357 (3)	C20—C21	1.349 (4)
O1—C26	1.435 (3)	C20—H20	0.9300
C1—C2	1.395 (4)	C21—C22	1.396 (4)
C1—H1	0.9300	C21—H21	0.9300
C2—C3	1.351 (4)	C22—H22	0.9300
C2—H2	0.9300	C23—C24	1.329 (4)
C3—C4	1.398 (4)	C23—H23	0.9300
C3—H3	0.9300	C24—H24	0.9300
C4—C5	1.411 (4)	C26—C27	1.478 (5)
C4—C11	1.429 (4)	C26—C28	1.504 (5)
C5—C6	1.452 (4)	C26—H26	0.9800
C6—C7	1.405 (4)	C27—H27A	0.9600
C7—C8	1.402 (5)	C27—H27B	0.9600
C7—C12	1.431 (4)	C27—H27C	0.9600
C8—C9	1.354 (5)	C28—H28A	0.9600
C8—H8	0.9300	C28—H28B	0.9600
C9—C10	1.382 (5)	C28—H28C	0.9600
C9—H9	0.9300		

N3—Na1—N4	66.79 (9)	C4—C11—H11	119.4
N3—Na1—N2	94.11 (10)	C11—C12—C7	121.3 (3)
N4—Na1—N2	88.26 (9)	C11—C12—H12	119.3
N3—Na1—N1	92.54 (9)	C7—C12—H12	119.3
N4—Na1—N1	146.48 (10)	N3—C13—C14	125.0 (4)
N2—Na1—N1	66.31 (9)	N3—C13—H13	117.5
N3—Na1—S1	107.62 (7)	C14—C13—H13	117.5
N4—Na1—S1	124.66 (7)	C15—C14—C13	118.3 (4)
N2—Na1—S1	145.46 (8)	C15—C14—H14	120.9
N1—Na1—S1	85.78 (7)	C13—C14—H14	120.9
N3—Na1—S2	134.91 (8)	C14—C15—C16	119.9 (4)
N4—Na1—S2	85.99 (7)	C14—C15—H15	120.0
N2—Na1—S2	121.38 (8)	C16—C15—H15	120.0
N1—Na1—S2	125.37 (7)	C15—C16—C17	117.5 (3)
S1—Na1—S2	58.81 (4)	C15—C16—C23	123.0 (3)
C25—S1—Na1	91.28 (11)	C17—C16—C23	119.5 (3)
C25—S2—Na1	84.41 (11)	N3—C17—C16	122.5 (3)

C1—N1—C5	117.4 (3)	N3—C17—C18	117.9 (3)
C1—N1—Na1	124.5 (2)	C16—C17—C18	119.6 (3)
C5—N1—Na1	117.4 (2)	N4—C18—C19	122.7 (3)
C10—N2—C6	116.9 (3)	N4—C18—C17	118.9 (3)
C10—N2—Na1	124.4 (2)	C19—C18—C17	118.4 (3)
C6—N2—Na1	118.3 (2)	C20—C19—C18	117.2 (3)
C13—N3—C17	116.8 (3)	C20—C19—C24	122.6 (3)
C13—N3—Na1	124.6 (2)	C18—C19—C24	120.1 (3)
C17—N3—Na1	118.5 (2)	C21—C20—C19	120.0 (3)
C22—N4—C18	117.5 (3)	C21—C20—H20	120.0
C22—N4—Na1	124.8 (2)	C19—C20—H20	120.0
C18—N4—Na1	117.7 (2)	C20—C21—C22	118.5 (3)
C25—O1—C26	122.0 (2)	C20—C21—H21	120.7
N1—C1—C2	124.0 (3)	C22—C21—H21	120.7
N1—C1—H1	118.0	N4—C22—C21	124.1 (3)
C2—C1—H1	118.0	N4—C22—H22	117.9
C3—C2—C1	118.7 (3)	C21—C22—H22	117.9
C3—C2—H2	120.6	C24—C23—C16	121.3 (3)
C1—C2—H2	120.6	C24—C23—H23	119.3
C2—C3—C4	120.1 (3)	C16—C23—H23	119.3
C2—C3—H3	120.0	C23—C24—C19	121.1 (3)
C4—C3—H3	120.0	C23—C24—H24	119.5
C3—C4—C5	117.2 (3)	C19—C24—H24	119.5
C3—C4—C11	122.9 (3)	O1—C25—S2	122.1 (2)
C5—C4—C11	119.9 (3)	O1—C25—S1	112.4 (2)
N1—C5—C4	122.6 (3)	S2—C25—S1	125.50 (18)
N1—C5—C6	118.6 (3)	O1—C26—C27	108.5 (3)
C4—C5—C6	118.8 (3)	O1—C26—C28	105.7 (3)
N2—C6—C7	122.8 (3)	C27—C26—C28	113.1 (3)
N2—C6—C5	118.4 (3)	O1—C26—H26	109.8
C7—C6—C5	118.9 (3)	C27—C26—H26	109.8
C8—C7—C6	117.2 (3)	C28—C26—H26	109.8
C8—C7—C12	122.9 (3)	C26—C27—H27A	109.5
C6—C7—C12	119.9 (3)	C26—C27—H27B	109.5
C9—C8—C7	119.6 (4)	H27A—C27—H27B	109.5
C9—C8—H8	120.2	C26—C27—H27C	109.5
C7—C8—H8	120.2	H27A—C27—H27C	109.5
C8—C9—C10	118.9 (4)	H27B—C27—H27C	109.5
C8—C9—H9	120.5	C26—C28—H28A	109.5
C10—C9—H9	120.5	C26—C28—H28B	109.5
N2—C10—C9	124.5 (4)	H28A—C28—H28B	109.5
N2—C10—H10	117.7	C26—C28—H28C	109.5
C9—C10—H10	117.7	H28A—C28—H28C	109.5
C12—C11—C4	121.1 (3)	H28B—C28—H28C	109.5
C12—C11—H11	119.4		