Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis(acetone)bis[μ-4-[(5-chloro-2-oxidophenyl)diazenyl]-3-oxido-*N*-phenylnaphthalene-2-carboxamidato]-sodium(I)ferrate(III)]

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Received 1 April 2007; accepted 8 April 2007

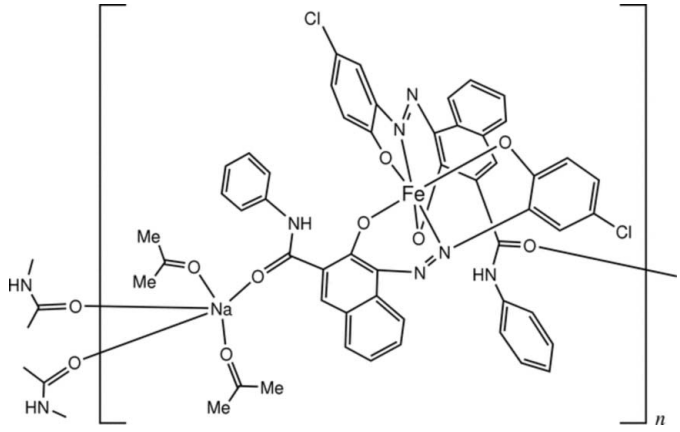
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.163; data-to-parameter ratio = 21.9.

The title compound, $[FeNa(C_{23}H_{14}ClN_3O_3)_2(C_3H_6O)_2]_n$, has a skeleton of an azo–Fe^{III} anion complex with a sodium cation, used widely as a charge-control agent (CCA) of the negative type in electrophotography. In the Fe^{III} anion-complex, the Fe^{III} atom is coordinated by four carbonyl O atoms and two N atoms of the diazo groups from two azo ligands lying *cis* to each other. There are two N—H···O intramolecular hydrogen bonds between the NH group and the carbonyl O atom. In the crystal structure, there exists a sodium-cation dimer bridged by the carbonyl O atoms at the periphery of the anion complex. An interesting aspect of this structure is that each sodium cation unites three different Fe-anion complexes through the carbonyl O atom, generating a quasi-two-dimensional network parallel to the (001) plane. At the same time, the sodium cation accommodates two acetone molecules, linked through the carbonyl O atom.

Related literature

Two related structural studies of azo–Fe anion complexes with a different cation (*viz.* ammonium cation) have been reported: a methanol-solvated complex (Mizuguchi, Sato & Uta, 2007) and an acetone-solvated one (Mizuguchi, Uta & Sato, 2007).

For related literature, see: Mizuguchi, Sato, Uta & Sato (2007); Tanaka (1995); Yasumatsu *et al.* (2006).



Experimental

Crystal data

$[FeNa(C_{23}H_{14}ClN_3O_3)_2(C_3H_6O)_2]$
M_r = 1026.64
Triclinic, $P\overline{1}$
a = 13.8165 (4) Å
b = 13.8623 (4) Å
c = 14.1524 (5) Å
α = 98.8719 (10)°
β = 105.3882 (10)°
γ = 109.0641 (8)°
V = 2382.21 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 93.1 K
0.18 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.918, T_{max} = 0.951
29200 measured reflections
13791 independent reflections
9943 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.163
S = 1.05
13791 reflections
631 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.9837 (13)	Na1—O5	2.3346 (16)
Fe1—O2	1.966 (2)	Na1—O5^{i}	2.320 (2)
Fe1—O3	1.950 (2)	Na1—O6^{ii}	2.342 (2)
Fe1—O4	1.9695 (16)	Na1—O7	2.2894 (19)
Fe1—N5	2.1411 (19)	Na1—O8	2.272 (2)
Fe1—N7	2.1236 (19)		
Na1···Na1^{i}	3.5581 (13)		
O1—Fe1—O2	86.60 (7)	O3—Fe1—O4	98.69 (7)
O1—Fe1—O3	92.44 (7)	O3—Fe1—N5	79.47 (7)
O1—Fe1—O4	157.75 (7)	O3—Fe1—N7	93.57 (8)
O1—Fe1—N5	101.35 (6)	O4—Fe1—N5	99.60 (6)
O1—Fe1—N7	80.70 (6)	O4—Fe1—N7	79.44 (6)
O2—Fe1—O3	160.13 (7)	N5—Fe1—N7	172.78 (8)
O2—Fe1—O4	89.25 (7)	O5—Na1—O5^{i}	80.28 (6)
O2—Fe1—N5	81.27 (7)	O5—Na1—O6^{ii}	83.32 (7)
O2—Fe1—N7	105.83 (8)	O5^{i}—Na1—O6^{ii}	162.26 (7)

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

 doi:10.1107/S1600536807017369

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3N···O2	0.88	1.99	2.660 (3)	132
N4—H4N···O1	0.88	1.96	2.658 (2)	135

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2155).

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supplementary materials

Acta Cryst. (2007). E**63**, m1377-m1378 [**doi:10.1107/S1600536807017369**]

Poly[bis(acetone)bis[μ-4-[(5-chloro-2-oxidophenyl)diazenyl]-3-oxido-*N*-phenylnaphthalene-2-carboxamidato]sodium(I)ferrate(III)]

J. Mizuguchi, Y. Sato and K. Uta

Comment

Charge-control agents play an important role in the electrophotographic process and are usually added to toners to create a desired charge level and polarity. The purpose of the present investigation has been set out in our previous investigation (Mizuguchi, Sato, Uta & Sato, 2007). We have been so far involved in the structure of a methanol-solvated azo-iron complex with the ammonium cation (Mizuguchi, Sato & Uta, 2007) and also of an acetone-solvated one (Mizuguchi, Uta & Sato, 2007). In the present investigation, the same azo-Fe^{III} complex but with a different cation (*i.e.* sodium cation) is used in place of the ammonium one. The ammonium salt is more widely used in practice as compared with the sodium one, because of its stable operation against temperature and humidity. To clarify this, the present structure analysis has been undertaken.

In the title compound, (I), there found two intramolecular hydrogen bonds, N3—H3N···O2 and N4—H4N···O1, between the NH group and the carbonyl O atom (Fig. 1 and Table 2). The sodium cation is found to form a dimer with another sodium one (Fig. 2), where each sodium cation is coordinated by five ligands: O5, O7, O8, $O5^{i}$ and $O6^{ii}$ [symmetry code: (i) $-x$, $1-y$, $1-z$; (ii) $1-x$, $1-y$, $1-z$]. Atoms Na1, O5, O7 and O8 are on the plane as characterized by the mean deviation of 0.0243 Å from the plane. It is interesting to note that each sodium cation unites three different anion complexes through the carbonyl O atoms: O5, $O5^{i}$ and $O6^{ii}$. This indicates that compound (I) forms a quasi two-dimensional network parallel to the (001) plane. This kind of the sheet-like network has not been observed in our methanol and acetone-solvated azo-Fe complexes with the ammonium cation (Mizuguchi, Sato & Uta, 2007;

Mizuguchi, Uta & Sato, 2007). Then, it is highly expected that the charge-control characteristics can greatly be affected by the species of cations. Correlation between structure and charge-control ability is now under investigation and will be shortly reported elsewhere.

Experimental

The title compound was prepared according to the methods previously reported (Yasumatsu *et al.*, 2006). Single crystals of (I) were obtained from an acetone solution.

Refinement

All H atoms were placed in geometrically idealized positions (C—H = 0.95 and 0.98 Å, and N—H = 0.88 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

Figures

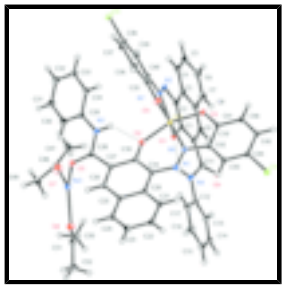


Fig. 1. The asymmetric unit of (I), showing 30% displacement ellipsoids. Dotted lines indicate intramolecular hydrogen bonds.

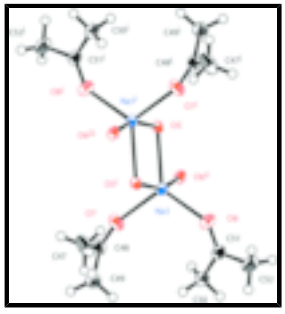


Fig. 2. The sodium cation dimer with four acetone molecules. Each sodium cation is coordinated by five ligands. The atom Na1 unites three different azo-Fe anion-complexes through the carbonyl O atoms: O5, O5^{i} and O6^{ii}. [Symmetry codes: (i) −*x*, 1 − *y*, 1 − *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) −1 + *x*, *y*, *z*].

Poly[bis(acetone)bis[μ-4-[(5-chloro-2-oxidophenyl)diazenyl]-3-oxido-N– phenylnaphthalene-2-carboxamidato]sodium(I)ferrate(III)]

Crystal data

$[FeNa(C_{23}H_{14}ClN_3O_3)_2(C_3H_6O)_2]$	$Z = 2$
$M_r = 1026.64$	$F_{000} = 1058.00$
Triclinic, $P\overline{1}$	$D_x = 1.431$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71075 Å
$a = 13.8165$ (4) Å	Cell parameters from 21230 reflections
$b = 13.8623$ (4) Å	θ = 3.1–30.0º
$c = 14.1524$ (5) Å	μ = 0.50 mm^{-1}
α = 98.8719 (10)º	$T = 93.1$ K
β = 105.3882 (10)º	Block, black
γ = 109.0641 (8)º	0.18 × 0.10 × 0.10 mm
$V = 2382.21$ (13) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	9943 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	$R_{int} = 0.043$
ω scans	$\theta_{max} = 30.0$º
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -19\rightarrow19$
$T_{min} = 0.918$, $T_{max} = 0.951$	$k = -18\rightarrow19$

29200 measured reflections
13791 independent reflections

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.056$

$wR(F^2) = 0.163$

$S = 1.05$

13791 reflections

631 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.6174P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.67$ e Å^{-3}

$\Delta\rho_{min} = -0.66$ e Å^{-3}

Extinction correction: none

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}
Fe1	0.31606 (2)	0.16230 (2)	0.47513 (2)	0.01612 (8)
Cl1	0.38547 (5)	−0.07025 (5)	0.04068 (4)	0.03048 (14)
Cl2	0.19145 (5)	0.04986 (5)	0.89961 (5)	0.02991 (14)
Na1	0.13517 (8)	0.58239 (7)	0.51452 (7)	0.0225 (2)
O1	0.44066 (13)	0.30060 (12)	0.51878 (12)	0.0196 (3)
O2	0.22198 (13)	0.24151 (13)	0.44431 (12)	0.0202 (3)
O3	0.40711 (13)	0.08387 (13)	0.45764 (12)	0.0210 (3)
O4	0.19287 (13)	0.04703 (13)	0.48461 (12)	0.0227 (3)
O5	0.02589 (13)	0.40350 (12)	0.47922 (12)	0.0201 (3)
O6	0.72706 (13)	0.48182 (13)	0.48145 (13)	0.0243 (3)
O7	0.23557 (17)	0.68164 (16)	0.67806 (15)	0.0382 (4)
O8	0.14432 (15)	0.67557 (15)	0.39620 (16)	0.0333 (4)
N1	0.20889 (15)	0.14164 (15)	0.24167 (14)	0.0179 (3)
N2	0.45392 (15)	0.23816 (15)	0.70695 (14)	0.0187 (3)
N3	0.10993 (16)	0.30301 (15)	0.55036 (15)	0.0200 (3)
N4	0.54202 (16)	0.42610 (16)	0.42128 (15)	0.0230 (4)
N5	0.27647 (15)	0.12597 (14)	0.31353 (14)	0.0170 (3)
N7	0.36381 (15)	0.18355 (14)	0.63488 (14)	0.0176 (3)
C1	0.53196 (18)	0.33593 (17)	0.59485 (17)	0.0176 (4)
C2	0.53897 (18)	0.30636 (17)	0.68714 (17)	0.0185 (4)

C3	0.63941 (18)	0.35065 (18)	0.77251 (17)	0.0206 (4)
C4	0.64824 (19)	0.32463 (19)	0.86600 (18)	0.0227 (4)
C5	0.7462 (2)	0.3664 (2)	0.94388 (19)	0.0276 (5)
C6	0.8399 (2)	0.4360 (2)	0.93258 (19)	0.0291 (5)
C7	0.8337 (2)	0.4644 (2)	0.8437 (2)	0.0277 (5)
C8	0.73351 (19)	0.42249 (19)	0.76142 (18)	0.0229 (4)
C9	0.72539 (19)	0.44944 (19)	0.66820 (18)	0.0215 (4)
C10	0.63053 (18)	0.40934 (18)	0.58666 (18)	0.0200 (4)
C11	0.63754 (19)	0.44278 (18)	0.49172 (18)	0.0202 (4)
C12	0.5242 (2)	0.44629 (19)	0.32462 (18)	0.0224 (4)
C13	0.6035 (2)	0.5190 (2)	0.2988 (2)	0.0259 (4)
C14	0.5776 (2)	0.5339 (2)	0.2018 (2)	0.0315 (5)
C15	0.4748 (2)	0.4791 (2)	0.1311 (2)	0.0345 (6)
C16	0.3955 (2)	0.4077 (2)	0.1567 (2)	0.0339 (5)
C17	0.4192 (2)	0.3912 (2)	0.2527 (2)	0.0280 (5)
C18	0.15271 (18)	0.24337 (17)	0.36269 (17)	0.0182 (4)
C19	0.14686 (18)	0.19647 (17)	0.26329 (16)	0.0177 (4)
C20	0.06999 (17)	0.20183 (17)	0.17447 (17)	0.0185 (4)
C21	0.0596 (2)	0.1544 (2)	0.07434 (17)	0.0238 (4)
C22	−0.0169 (2)	0.1596 (2)	−0.00840 (18)	0.0263 (5)
C23	−0.0858 (2)	0.2119 (2)	0.00479 (19)	0.0280 (5)
C24	−0.07693 (19)	0.2589 (2)	0.10065 (18)	0.0238 (4)
C25	0.00035 (19)	0.25475 (18)	0.18712 (17)	0.0201 (4)
C26	0.00764 (18)	0.30062 (17)	0.28715 (17)	0.0191 (4)
C27	0.07859 (18)	0.29493 (17)	0.37230 (16)	0.0172 (4)
C28	0.07078 (17)	0.33964 (17)	0.47220 (17)	0.0177 (4)
C29	0.11155 (19)	0.32857 (19)	0.65212 (17)	0.0212 (4)
C30	0.1169 (2)	0.4258 (2)	0.70109 (19)	0.0285 (5)
C31	0.1244 (2)	0.4459 (2)	0.80263 (19)	0.0327 (5)
C32	0.1279 (2)	0.3701 (2)	0.8558 (2)	0.0325 (5)
C33	0.1233 (2)	0.2736 (2)	0.8072 (2)	0.0340 (6)
C34	0.1134 (2)	0.2520 (2)	0.70495 (19)	0.0281 (5)
C35	0.19117 (19)	0.04498 (18)	0.57723 (17)	0.0208 (4)
C36	0.1017 (2)	−0.02391 (19)	0.59606 (19)	0.0235 (4)
C37	0.1024 (2)	−0.02095 (19)	0.69418 (19)	0.0254 (4)
C38	0.1935 (2)	0.04924 (19)	0.77662 (18)	0.0221 (4)
C39	0.28331 (19)	0.11807 (18)	0.76252 (17)	0.0206 (4)
C40	0.28146 (18)	0.11585 (17)	0.66251 (17)	0.0191 (4)
C41	0.40286 (18)	0.04753 (18)	0.36382 (16)	0.0185 (4)
C42	0.33457 (18)	0.06816 (17)	0.28179 (16)	0.0177 (4)
C43	0.32719 (19)	0.03125 (18)	0.18136 (17)	0.0210 (4)
C44	0.38792 (19)	−0.02652 (19)	0.16375 (17)	0.0218 (4)
C45	0.45506 (19)	−0.04928 (18)	0.24313 (18)	0.0210 (4)
C46	0.46185 (18)	−0.01315 (18)	0.34240 (17)	0.0205 (4)
C47	0.3919 (3)	0.7379 (2)	0.8251 (2)	0.0517 (9)
C48	0.3028 (2)	0.7536 (2)	0.75075 (19)	0.0278 (5)
C49	0.2974 (2)	0.8606 (2)	0.7686 (2)	0.0349 (6)
C50	0.3021 (2)	0.8333 (2)	0.4768 (2)	0.0341 (6)
C51	0.2019 (2)	0.7614 (2)	0.3904 (2)	0.0274 (5)

C52	0.1753 (2)	0.7969 (2)	0.2955 (2)	0.0398 (6)
H3N	0.1386	0.2567	0.5366	0.024*
H4	0.5858	0.2778	0.8752	0.027*
H4N	0.4835	0.3993	0.4376	0.028*
H5	0.7508	0.3479	1.0064	0.033*
H6	0.9074	0.4634	0.9868	0.035*
H7	0.8969	0.5126	0.8368	0.033*
H9	0.7887	0.4977	0.6616	0.026*
H13	0.6743	0.5577	0.3470	0.031*
H14	0.6317	0.5827	0.1839	0.038*
H15	0.4584	0.4902	0.0651	0.041*
H16	0.3247	0.3699	0.1081	0.041*
H17	0.3644	0.3427	0.2700	0.034*
H20	−0.0229	0.1273	−0.0751	0.032*
H21	0.1056	0.1187	0.0639	0.029*
H23	−0.1384	0.2146	−0.0526	0.034*
H24	−0.1231	0.2949	0.1095	0.029*
H26	−0.0387	0.3367	0.2952	0.023*
H30	0.1154	0.4783	0.6655	0.034*
H31	0.1272	0.5122	0.8360	0.039*
H32	0.1335	0.3847	0.9253	0.039*
H33	0.1268	0.2220	0.8436	0.041*
H34	0.1079	0.1847	0.6711	0.034*
H36	0.0404	−0.0729	0.5406	0.028*
H37	0.0410	−0.0666	0.7058	0.030*
H39	0.3446	0.1656	0.8189	0.025*
H43	0.2816	0.0456	0.1269	0.025*
H45	0.4959	−0.0895	0.2287	0.025*
H46	0.5065	−0.0295	0.3960	0.025*
H47a	0.3674	0.7153	0.8800	0.062*
H47b	0.4559	0.8045	0.8536	0.062*
H47c	0.4109	0.6834	0.7906	0.062*
H49a	0.3399	0.9037	0.7337	0.042*
H49b	0.3273	0.8952	0.8416	0.042*
H49c	0.2215	0.8532	0.7421	0.042*
H50a	0.3556	0.8755	0.4503	0.041*
H50b	0.3330	0.7910	0.5153	0.041*
H50c	0.2836	0.8805	0.5215	0.041*
H52a	0.2109	0.7733	0.2505	0.048*
H52b	0.2012	0.8742	0.3130	0.048*
H53c	0.0963	0.7662	0.2607	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01826 (16)	0.02073 (16)	0.01130 (14)	0.00860 (13)	0.00639 (11)	0.00470 (11)
Cl1	0.0409 (3)	0.0459 (3)	0.0157 (2)	0.0273 (3)	0.0143 (2)	0.0073 (2)
Cl2	0.0375 (3)	0.0376 (3)	0.0227 (2)	0.0147 (2)	0.0183 (2)	0.0152 (2)

Na1	0.0227 (4)	0.0219 (4)	0.0250 (4)	0.0087 (4)	0.0112 (3)	0.0062 (3)
O1	0.0194 (7)	0.0231 (7)	0.0176 (7)	0.0082 (6)	0.0065 (6)	0.0080 (6)
O2	0.0217 (7)	0.0271 (8)	0.0128 (7)	0.0122 (6)	0.0050 (5)	0.0036 (6)
O3	0.0267 (8)	0.0287 (8)	0.0120 (6)	0.0155 (7)	0.0075 (6)	0.0051 (6)
O4	0.0227 (8)	0.0248 (8)	0.0162 (7)	0.0045 (7)	0.0060 (6)	0.0041 (6)
O5	0.0208 (7)	0.0213 (7)	0.0206 (7)	0.0101 (6)	0.0087 (6)	0.0044 (6)
O6	0.0218 (7)	0.0284 (8)	0.0273 (8)	0.0098 (7)	0.0140 (6)	0.0099 (7)
O7	0.0369 (10)	0.0368 (10)	0.0290 (10)	0.0089 (9)	0.0065 (8)	−0.0041 (8)
O8	0.0308 (9)	0.0347 (10)	0.0406 (11)	0.0123 (8)	0.0173 (8)	0.0186 (8)
N1	0.0190 (8)	0.0232 (9)	0.0143 (8)	0.0096 (7)	0.0067 (6)	0.0068 (7)
N2	0.0182 (8)	0.0221 (9)	0.0169 (8)	0.0086 (7)	0.0071 (7)	0.0049 (7)
N3	0.0246 (9)	0.0213 (8)	0.0182 (8)	0.0112 (8)	0.0105 (7)	0.0055 (7)
N4	0.0229 (9)	0.0293 (10)	0.0219 (9)	0.0100 (8)	0.0124 (7)	0.0118 (8)
N5	0.0191 (8)	0.0194 (8)	0.0155 (8)	0.0093 (7)	0.0075 (6)	0.0066 (6)
N7	0.0201 (8)	0.0195 (8)	0.0167 (8)	0.0090 (7)	0.0092 (7)	0.0056 (7)
C1	0.0194 (9)	0.0192 (9)	0.0171 (9)	0.0090 (8)	0.0093 (8)	0.0037 (7)
C2	0.0183 (9)	0.0201 (10)	0.0170 (9)	0.0074 (8)	0.0063 (8)	0.0043 (8)
C3	0.0205 (10)	0.0235 (10)	0.0187 (10)	0.0099 (9)	0.0077 (8)	0.0037 (8)
C4	0.0218 (10)	0.0246 (11)	0.0206 (10)	0.0084 (9)	0.0065 (8)	0.0054 (8)
C5	0.0276 (12)	0.0354 (13)	0.0172 (10)	0.0122 (11)	0.0043 (9)	0.0055 (9)
C6	0.0210 (11)	0.0396 (14)	0.0200 (11)	0.0103 (11)	0.0016 (9)	0.0023 (10)
C7	0.0216 (11)	0.0305 (12)	0.0258 (12)	0.0065 (10)	0.0063 (9)	0.0034 (9)
C8	0.0212 (10)	0.0269 (11)	0.0198 (10)	0.0087 (9)	0.0080 (8)	0.0037 (8)
C9	0.0185 (10)	0.0239 (10)	0.0226 (10)	0.0069 (9)	0.0090 (8)	0.0067 (8)
C10	0.0192 (10)	0.0220 (10)	0.0207 (10)	0.0087 (9)	0.0086 (8)	0.0057 (8)
C11	0.0217 (10)	0.0205 (10)	0.0207 (10)	0.0077 (9)	0.0108 (8)	0.0059 (8)
C12	0.0282 (11)	0.0260 (11)	0.0229 (11)	0.0155 (10)	0.0148 (9)	0.0116 (9)
C13	0.0292 (12)	0.0289 (11)	0.0264 (11)	0.0129 (10)	0.0151 (9)	0.0124 (9)
C14	0.0387 (14)	0.0378 (14)	0.0341 (14)	0.0209 (12)	0.0240 (11)	0.0200 (11)
C15	0.0493 (16)	0.0487 (16)	0.0247 (12)	0.0308 (14)	0.0219 (11)	0.0198 (11)
C16	0.0372 (14)	0.0440 (15)	0.0238 (12)	0.0188 (13)	0.0101 (10)	0.0116 (11)
C17	0.0295 (12)	0.0321 (12)	0.0276 (12)	0.0131 (11)	0.0130 (10)	0.0138 (10)
C18	0.0187 (9)	0.0182 (9)	0.0167 (9)	0.0047 (8)	0.0073 (8)	0.0054 (7)
C19	0.0203 (10)	0.0209 (10)	0.0147 (9)	0.0097 (9)	0.0073 (7)	0.0056 (7)
C20	0.0169 (9)	0.0219 (10)	0.0164 (9)	0.0055 (9)	0.0067 (7)	0.0068 (8)
C21	0.0257 (11)	0.0352 (12)	0.0163 (10)	0.0162 (10)	0.0095 (8)	0.0082 (9)
C22	0.0292 (12)	0.0372 (13)	0.0142 (10)	0.0149 (11)	0.0074 (9)	0.0065 (9)
C23	0.0296 (12)	0.0377 (13)	0.0181 (10)	0.0159 (11)	0.0052 (9)	0.0095 (10)
C24	0.0238 (11)	0.0311 (12)	0.0209 (10)	0.0156 (10)	0.0065 (8)	0.0092 (9)
C25	0.0225 (10)	0.0237 (10)	0.0162 (9)	0.0095 (9)	0.0081 (8)	0.0066 (8)
C26	0.0203 (10)	0.0208 (10)	0.0186 (10)	0.0092 (9)	0.0081 (8)	0.0059 (8)
C27	0.0186 (9)	0.0179 (9)	0.0157 (9)	0.0064 (8)	0.0077 (7)	0.0043 (7)
C28	0.0171 (9)	0.0164 (9)	0.0171 (9)	0.0035 (8)	0.0068 (7)	0.0027 (7)
C29	0.0217 (10)	0.0267 (11)	0.0175 (10)	0.0102 (9)	0.0097 (8)	0.0053 (8)
C30	0.0406 (14)	0.0240 (11)	0.0199 (11)	0.0116 (11)	0.0103 (10)	0.0044 (9)
C31	0.0461 (15)	0.0334 (13)	0.0186 (11)	0.0168 (12)	0.0114 (10)	0.0028 (10)
C32	0.0454 (15)	0.0415 (14)	0.0183 (11)	0.0216 (13)	0.0157 (10)	0.0099 (10)
C33	0.0538 (17)	0.0433 (15)	0.0251 (12)	0.0317 (14)	0.0232 (12)	0.0187 (11)
C34	0.0426 (14)	0.0325 (12)	0.0223 (11)	0.0241 (12)	0.0169 (10)	0.0113 (9)

C35	0.0229 (10)	0.0231 (10)	0.0194 (10)	0.0112 (9)	0.0075 (8)	0.0081 (8)
C36	0.0227 (11)	0.0235 (11)	0.0222 (11)	0.0065 (9)	0.0069 (8)	0.0065 (9)
C37	0.0252 (11)	0.0250 (11)	0.0275 (12)	0.0073 (10)	0.0123 (9)	0.0101 (9)
C38	0.0283 (11)	0.0266 (11)	0.0186 (10)	0.0134 (10)	0.0124 (9)	0.0110 (8)
C39	0.0212 (10)	0.0234 (10)	0.0171 (10)	0.0074 (9)	0.0079 (8)	0.0056 (8)
C40	0.0217 (10)	0.0211 (10)	0.0186 (10)	0.0096 (9)	0.0097 (8)	0.0084 (8)
C41	0.0224 (10)	0.0230 (10)	0.0124 (9)	0.0104 (9)	0.0069 (7)	0.0054 (8)
C42	0.0209 (10)	0.0210 (10)	0.0139 (9)	0.0097 (9)	0.0075 (7)	0.0055 (7)
C43	0.0239 (10)	0.0276 (11)	0.0146 (9)	0.0124 (9)	0.0077 (8)	0.0065 (8)
C44	0.0268 (11)	0.0285 (11)	0.0127 (9)	0.0122 (10)	0.0093 (8)	0.0043 (8)
C45	0.0244 (10)	0.0239 (10)	0.0188 (10)	0.0123 (9)	0.0099 (8)	0.0056 (8)
C46	0.0221 (10)	0.0250 (10)	0.0164 (10)	0.0114 (9)	0.0066 (8)	0.0055 (8)
C47	0.062 (2)	0.059 (2)	0.0353 (16)	0.0415 (18)	0.0037 (15)	−0.0011 (14)
C48	0.0294 (12)	0.0326 (12)	0.0238 (11)	0.0119 (11)	0.0139 (9)	0.0057 (10)
C49	0.0408 (15)	0.0336 (13)	0.0343 (14)	0.0170 (12)	0.0150 (12)	0.0101 (11)
C50	0.0413 (15)	0.0314 (13)	0.0290 (13)	0.0100 (12)	0.0135 (11)	0.0119 (10)
C51	0.0278 (12)	0.0294 (12)	0.0328 (13)	0.0141 (11)	0.0164 (10)	0.0115 (10)
C52	0.0360 (15)	0.0411 (15)	0.0366 (15)	0.0070 (13)	0.0073 (12)	0.0204 (13)

Geometric parameters (Å, °)

Fe1—O1	1.9837 (13)	C18—C27	1.449 (3)
Fe1—O2	1.966 (2)	C19—C20	1.444 (3)
Fe1—O3	1.950 (2)	C20—C21	1.416 (3)
Fe1—O4	1.9695 (16)	C20—C25	1.417 (4)
Fe1—N5	2.1411 (19)	C21—C22	1.383 (3)
Fe1—N7	2.1236 (19)	C21—H21	0.950
Cl1—C44	1.741 (2)	C22—C23	1.404 (4)
Cl2—C38	1.747 (2)	C22—H20	0.950
Na1—O5	2.3346 (16)	C23—C24	1.366 (3)
Na1—O5^{i}	2.320 (2)	C23—H23	0.950
Na1—O6^{ii}	2.342 (2)	C24—C25	1.418 (3)
Na1—O7	2.2894 (19)	C24—H24	0.950
Na1—O8	2.272 (2)	C25—C26	1.422 (3)
O1—C1	1.305 (2)	C26—C27	1.368 (3)
O2—C18	1.300 (2)	C26—H26	0.950
O3—C41	1.324 (2)	C27—C28	1.500 (3)
O4—C35	1.322 (3)	C29—C30	1.386 (3)
O5—C28	1.242 (3)	C29—C34	1.392 (4)
O6—C11	1.235 (3)	C30—C31	1.390 (3)
O7—C48	1.220 (2)	C30—H30	0.950
O8—C51	1.226 (3)	C31—C32	1.389 (4)
N1—N5	1.285 (2)	C31—H31	0.950
N1—C19	1.378 (3)	C32—C33	1.380 (4)
N2—N7	1.279 (2)	C32—H32	0.950
N2—C2	1.373 (3)	C33—C34	1.392 (4)
N3—C28	1.345 (3)	C33—H33	0.950
N3—C29	1.421 (3)	C34—H34	0.950
N3—H3N	0.880	C35—C36	1.412 (3)

N4—C11	1.349 (3)	C35—C40	1.419 (2)
N4—C12	1.412 (3)	C36—C37	1.380 (3)
N4—H4N	0.880	C36—H36	0.950
N5—C42	1.410 (3)	C37—C38	1.401 (2)
N7—C40	1.407 (3)	C37—H37	0.950
C1—C2	1.417 (3)	C38—C39	1.381 (3)
C1—C10	1.456 (3)	C39—C40	1.404 (3)
C2—C3	1.445 (2)	C39—H39	0.950
C3—C4	1.409 (3)	C41—C42	1.420 (3)
C3—C8	1.420 (3)	C41—C46	1.401 (4)
C4—C5	1.372 (3)	C42—C43	1.399 (3)
C4—H4	0.950	C43—C44	1.377 (4)
C5—C6	1.405 (3)	C43—H43	0.950
C5—H5	0.950	C44—C45	1.403 (3)
C6—C7	1.364 (4)	C45—C46	1.384 (3)
C6—H6	0.950	C45—H45	0.950
C7—C8	1.421 (3)	C46—H46	0.950
C7—H7	0.950	C47—C48	1.493 (4)
C8—C9	1.412 (3)	C47—H47a	0.980
C9—C10	1.372 (2)	C47—H47b	0.980
C9—H9	0.950	C47—H47c	0.980
C10—C11	1.504 (3)	C48—C49	1.496 (4)
C12—C13	1.398 (3)	C49—H49a	0.980
C12—C17	1.406 (3)	C49—H49b	0.980
C13—C14	1.389 (4)	C49—H49c	0.980
C13—H13	0.950	C50—C51	1.493 (3)
C14—C15	1.379 (3)	C50—H50a	0.980
C14—H14	0.950	C50—H50b	0.980
C15—C16	1.388 (4)	C50—H50c	0.980
C15—H15	0.950	C51—C52	1.497 (4)
C16—C17	1.383 (4)	C52—H52a	0.980
C16—H16	0.950	C52—H52b	0.980
C17—H17	0.950	C52—H53c	0.980
C18—C19	1.425 (3)		
Na1···Na1^{i}	3.5581 (13)	N2···H45^{iv}	2.595
Cl1···H49b^{iii}	2.635	C6···H32^{vi}	2.797
O3···H46^{iv}	2.458	C18···H37^{vii}	2.778
O3···H50a^{v}	2.718	C46···H50a^{v}	2.703
O1—Fe1—O2	86.60 (7)	C20—C21—C22	120.5 (2)
O1—Fe1—O3	92.44 (7)	C20—C21—H21	119.7
O1—Fe1—O4	157.75 (7)	C22—C21—H21	119.8
O1—Fe1—N5	101.35 (6)	C21—C22—C23	121.0 (2)
O1—Fe1—N7	80.70 (6)	C21—C22—H20	119.5
O2—Fe1—O3	160.13 (7)	C23—C22—H20	119.5
O2—Fe1—O4	89.25 (7)	C22—C23—C24	119.6 (2)
O2—Fe1—N5	81.27 (7)	C22—C23—H23	120.2
O2—Fe1—N7	105.83 (8)	C24—C23—H23	120.2
O3—Fe1—O4	98.69 (7)	C23—C24—C25	120.9 (2)

O3—Fe1—N5	79.47 (7)	C23—C24—H24	119.6
O3—Fe1—N7	93.57 (8)	C25—C24—H24	119.6
O4—Fe1—N5	99.60 (6)	C20—C25—C24	119.8 (2)
O4—Fe1—N7	79.44 (6)	C20—C25—C26	119.0 (2)
N5—Fe1—N7	172.78 (8)	C24—C25—C26	121.1 (2)
O5—Na1—O5^{i}	80.28 (6)	C25—C26—C27	122.7 (2)
O5—Na1—O6^{ii}	83.32 (7)	C25—C26—H26	118.6
O5—Na1—O7	121.07 (8)	C27—C26—H26	118.6
O5—Na1—O8	124.62 (6)	C18—C27—C26	120.0 (2)
O5^{i}—Na1—O6^{ii}	162.26 (7)	C18—C27—C28	123.4 (2)
O5^{i}—Na1—O7	94.92 (8)	C26—C27—C28	116.5 (2)
O5^{i}—Na1—O8	92.23 (8)	O5—C28—N3	123.0 (2)
O6^{ii}—Na1—O7	87.74 (8)	O5—C28—C27	120.5 (2)
O6^{ii}—Na1—O8	102.69 (8)	N3—C28—C27	116.4 (2)
O7—Na1—O8	114.20 (7)	N3—C29—C30	123.6 (2)
Fe1—O1—C1	129.50 (16)	N3—C29—C34	116.6 (2)
Fe1—O2—C18	135.37 (16)	C30—C29—C34	119.7 (2)
Fe1—O3—C41	117.35 (16)	C29—C30—C31	119.6 (2)
Fe1—O4—C35	116.21 (11)	C29—C30—H30	120.2
Na1—O5—Na1^{i}	99.72 (8)	C31—C30—H30	120.2
Na1—O5—C28	116.87 (13)	C30—C31—C32	120.7 (2)
Na1^{i}—O5—C28	143.08 (14)	C30—C31—H31	119.6
Na1^{ii}—O6—C11	131.51 (18)	C32—C31—H31	119.6
Na1—O7—C48	161.6 (2)	C31—C32—C33	119.7 (2)
Na1—O8—C51	138.02 (17)	C31—C32—H32	120.2
N5—N1—C19	120.6 (2)	C33—C32—H32	120.2
N7—N2—C2	119.9 (2)	C32—C33—C34	120.0 (3)
C28—N3—C29	129.1 (2)	C32—C33—H33	120.0
C28—N3—H3N	115.5	C34—C33—H33	120.0
C29—N3—H3N	115.5	C29—C34—C33	120.3 (2)
C11—N4—C12	128.1 (2)	C29—C34—H34	119.9
C11—N4—H4N	115.9	C33—C34—H34	119.9
C12—N4—H4N	115.9	O4—C35—C36	122.86 (17)
Fe1—N5—N1	133.58 (18)	O4—C35—C40	119.5 (2)
Fe1—N5—C42	111.06 (14)	C36—C35—C40	117.6 (2)
N1—N5—C42	115.27 (19)	C35—C36—C37	120.76 (18)
Fe1—N7—N2	132.41 (17)	C35—C36—H36	119.6
Fe1—N7—C40	111.44 (11)	C37—C36—H36	119.6
N2—N7—C40	115.84 (19)	C36—C37—C38	120.1 (2)
O1—C1—C2	122.2 (2)	C36—C37—H37	120.0
O1—C1—C10	119.8 (2)	C38—C37—H37	120.0
C2—C1—C10	117.99 (18)	Cl2—C38—C37	118.6 (2)
N2—C2—C1	125.19 (18)	Cl2—C38—C39	119.82 (15)
N2—C2—C3	113.3 (2)	C37—C38—C39	121.5 (2)
C1—C2—C3	121.4 (2)	C38—C39—C40	118.12 (17)
C2—C3—C4	122.7 (2)	C38—C39—H39	120.9
C2—C3—C8	118.7 (2)	C40—C39—H39	120.9

C4—C3—C8	118.60 (18)	N7—C40—C35	112.7 (2)
C3—C4—C5	120.6 (2)	N7—C40—C39	125.32 (16)
C3—C4—H4	119.7	C35—C40—C39	121.9 (2)
C5—C4—H4	119.7	O3—C41—C42	119.3 (2)
C4—C5—C6	121.0 (2)	O3—C41—C46	122.0 (2)
C4—C5—H5	119.5	C42—C41—C46	118.7 (2)
C6—C5—H5	119.5	N5—C42—C41	112.8 (2)
C5—C6—C7	119.9 (2)	N5—C42—C43	125.8 (2)
C5—C6—H6	120.0	C41—C42—C43	121.4 (2)
C7—C6—H6	120.0	C42—C43—C44	118.1 (2)
C6—C7—C8	120.5 (2)	C42—C43—H43	121.0
C6—C7—H7	119.7	C44—C43—H43	121.0
C8—C7—H7	119.7	Cl1—C44—C43	119.91 (19)
C3—C8—C7	119.4 (2)	Cl1—C44—C45	118.3 (2)
C3—C8—C9	119.03 (19)	C43—C44—C45	121.8 (2)
C7—C8—C9	121.6 (2)	C44—C45—C46	120.1 (2)
C8—C9—C10	123.2 (2)	C44—C45—H45	120.0
C8—C9—H9	118.4	C46—C45—H45	120.0
C10—C9—H9	118.4	C41—C46—C45	120.0 (2)
C1—C10—C9	119.6 (2)	C41—C46—H46	120.0
C1—C10—C11	124.15 (18)	C45—C46—H46	120.0
C9—C10—C11	116.2 (2)	C48—C47—H47a	109.5
O6—C11—N4	124.0 (2)	C48—C47—H47b	109.5
O6—C11—C10	120.0 (2)	C48—C47—H47c	109.5
N4—C11—C10	116.0 (2)	H47a—C47—H47b	109.5
N4—C12—C13	123.72 (19)	H47a—C47—H47c	109.5
N4—C12—C17	116.9 (2)	H47b—C47—H47c	109.5
C13—C12—C17	119.4 (2)	O7—C48—C47	121.5 (2)
C12—C13—C14	119.4 (2)	O7—C48—C49	120.6 (2)
C12—C13—H13	120.3	C47—C48—C49	117.9 (2)
C14—C13—H13	120.3	C48—C49—H49a	109.5
C13—C14—C15	121.1 (2)	C48—C49—H49b	109.5
C13—C14—H14	119.5	C48—C49—H49c	109.5
C15—C14—H14	119.5	H49a—C49—H49b	109.5
C14—C15—C16	119.8 (2)	H49a—C49—H49c	109.5
C14—C15—H15	120.1	H49b—C49—H49c	109.5
C16—C15—H15	120.1	C51—C50—H50a	109.5
C15—C16—C17	120.3 (2)	C51—C50—H50b	109.5
C15—C16—H16	119.9	C51—C50—H50c	109.5
C17—C16—H16	119.9	H50a—C50—H50b	109.5
C12—C17—C16	120.1 (2)	H50a—C50—H50c	109.5
C12—C17—H17	120.0	H50b—C50—H50c	109.5
C16—C17—H17	120.0	O8—C51—C50	121.3 (2)
O2—C18—C19	122.3 (2)	O8—C51—C52	121.0 (2)
O2—C18—C27	119.3 (2)	C50—C51—C52	117.7 (2)
C19—C18—C27	118.4 (2)	C51—C52—H52a	109.5
N1—C19—C18	125.3 (2)	C51—C52—H52b	109.5
N1—C19—C20	114.0 (2)	C51—C52—H53c	109.5
C18—C19—C20	120.6 (2)	H52a—C52—H52b	109.5

C19—C20—C21	122.6 (2)	H52a—C52—H53c	109.5
C19—C20—C25	119.2 (2)	H52b—C52—H53c	109.5
C21—C20—C25	118.2 (2)		
O1—Fe1—O2—C18	116.7 (2)	O1—C1—C2—N2	0.9 (4)
O2—Fe1—O1—C1	141.4 (2)	O1—C1—C2—C3	−176.6 (2)
O1—Fe1—O3—C41	−101.36 (15)	O1—C1—C10—C9	177.5 (2)
O3—Fe1—O1—C1	−58.5 (2)	O1—C1—C10—C11	−4.7 (4)
O1—Fe1—O4—C35	−19.9 (3)	C2—C1—C10—C9	−1.7 (3)
O4—Fe1—O1—C1	61.8 (3)	C2—C1—C10—C11	176.1 (2)
O1—Fe1—N5—N1	−93.59 (19)	C10—C1—C2—N2	−179.95 (19)
O1—Fe1—N5—C42	90.08 (14)	C10—C1—C2—C3	2.6 (3)
N5—Fe1—O1—C1	−138.2 (2)	N2—C2—C3—C4	0.7 (3)
O1—Fe1—N7—N2	−23.2 (2)	N2—C2—C3—C8	180.0 (2)
O1—Fe1—N7—C40	163.59 (18)	C1—C2—C3—C4	178.5 (2)
N7—Fe1—O1—C1	34.8 (2)	C1—C2—C3—C8	−2.2 (4)
O2—Fe1—O3—C41	−14.6 (2)	C2—C3—C4—C5	178.1 (2)
O3—Fe1—O2—C18	28.9 (3)	C2—C3—C8—C7	−178.2 (2)
O2—Fe1—O4—C35	−99.02 (19)	C2—C3—C8—C9	1.0 (4)
O4—Fe1—O2—C18	−85.2 (2)	C4—C3—C8—C7	1.1 (4)
O2—Fe1—N5—N1	−8.87 (18)	C4—C3—C8—C9	−179.7 (2)
O2—Fe1—N5—C42	174.80 (14)	C8—C3—C4—C5	−1.2 (4)
N5—Fe1—O2—C18	14.6 (2)	C3—C4—C5—C6	0.1 (3)
O2—Fe1—N7—N2	−106.9 (2)	C4—C5—C6—C7	1.1 (4)
O2—Fe1—N7—C40	79.84 (17)	C5—C6—C7—C8	−1.2 (4)
N7—Fe1—O2—C18	−164.0 (2)	C6—C7—C8—C3	0.1 (3)
O3—Fe1—O4—C35	99.27 (19)	C6—C7—C8—C9	−179.1 (2)
O4—Fe1—O3—C41	97.97 (15)	C3—C8—C9—C10	−0.2 (4)
O3—Fe1—N5—N1	176.02 (19)	C7—C8—C9—C10	179.0 (2)
O3—Fe1—N5—C42	−0.31 (13)	C8—C9—C10—C1	0.5 (4)
N5—Fe1—O3—C41	−0.26 (14)	C8—C9—C10—C11	−177.4 (2)
O3—Fe1—N7—N2	68.7 (2)	C1—C10—C11—O6	−161.0 (2)
O3—Fe1—N7—C40	−104.53 (17)	C1—C10—C11—N4	18.2 (3)
N7—Fe1—O3—C41	177.82 (14)	C9—C10—C11—O6	16.8 (3)
O4—Fe1—N5—N1	78.87 (19)	C9—C10—C11—N4	−163.9 (2)
O4—Fe1—N5—C42	−97.46 (14)	N4—C12—C13—C14	−179.4 (2)
N5—Fe1—O4—C35	179.97 (14)	N4—C12—C17—C16	179.5 (2)
O4—Fe1—N7—N2	166.9 (2)	C13—C12—C17—C16	1.2 (4)
O4—Fe1—N7—C40	−6.34 (17)	C17—C12—C13—C14	−1.3 (4)
N7—Fe1—O4—C35	7.23 (19)	C12—C13—C14—C15	0.7 (5)
O5—Na1—O5^{i}—C28^{i}	−172.4 (2)	C13—C14—C15—C16	−0.1 (4)
O5^{i}—Na1—O5—C28	−174.88 (17)	C14—C15—C16—C17	−0.0 (4)
O5—Na1—O6^{ii}—C11^{ii}	158.7 (2)	C15—C16—C17—C12	−0.5 (5)
O6^{ii}—Na1—O5—Na1^{i}	173.20 (7)	O2—C18—C19—N1	2.5 (3)
O6^{ii}—Na1—O5—C28	−1.68 (17)	O2—C18—C19—C20	−178.92 (19)
O5—Na1—O7—C48	165.7 (7)	O2—C18—C27—C26	177.85 (19)
O7—Na1—O5—Na1^{i}	89.91 (11)	O2—C18—C27—C28	−5.0 (3)
O7—Na1—O5—C28	−84.96 (19)	C19—C18—C27—C26	−2.0 (3)

O5—Na1—O8—C51	−167.7 (3)	C19—C18—C27—C28	175.07 (19)
O8—Na1—O5—Na1^{i}	−85.97 (11)	C27—C18—C19—N1	−177.63 (19)
O8—Na1—O5—C28	99.15 (18)	C27—C18—C19—C20	1.0 (3)
O5^{i}—Na1—O6^{ii}—C11^{ii}	−178.8 (2)	N1—C19—C20—C21	0.2 (3)
O6^{ii}—Na1—O5^{i}—Na1^{i}	−22.7 (2)	N1—C19—C20—C25	178.98 (19)
O6^{ii}—Na1—O5^{i}—C28^{i}	164.9 (2)	C18—C19—C20—C21	−178.5 (2)
O5^{i}—Na1—O7—C48	−112.7 (7)	C18—C19—C20—C25	0.2 (3)
O7—Na1—O5^{i}—Na1^{i}	−120.71 (8)	C19—C20—C21—C22	178.5 (2)
O7—Na1—O5^{i}—C28^{i}	66.9 (2)	C19—C20—C25—C24	−178.8 (2)
O5^{i}—Na1—O8—C51	112.6 (3)	C19—C20—C25—C26	−0.4 (3)
O8—Na1—O5^{i}—Na1^{i}	124.76 (7)	C21—C20—C25—C24	0.0 (2)
O8—Na1—O5^{i}—C28^{i}	−47.6 (2)	C21—C20—C25—C26	178.4 (2)
O6^{ii}—Na1—O7—C48	84.9 (7)	C25—C20—C21—C22	−0.2 (3)
O7—Na1—O6^{ii}—C11^{ii}	−79.6 (2)	C20—C21—C22—C23	0.0 (2)
O6^{ii}—Na1—O8—C51	−77.1 (3)	C21—C22—C23—C24	0.4 (3)
O8—Na1—O6^{ii}—C11^{ii}	34.7 (2)	C22—C23—C24—C25	−0.6 (3)
O7—Na1—O8—C51	16.2 (3)	C23—C24—C25—C20	0.4 (3)
O8—Na1—O7—C48	−18.0 (8)	C23—C24—C25—C26	−178.0 (2)
Fe1—O1—C1—C2	−32.1 (3)	C20—C25—C26—C27	−0.7 (3)
Fe1—O1—C1—C10	148.77 (19)	C24—C25—C26—C27	177.7 (2)
Fe1—O2—C18—C19	−14.7 (3)	C25—C26—C27—C18	2.0 (3)
Fe1—O2—C18—C27	165.40 (15)	C25—C26—C27—C28	−175.36 (19)
Fe1—O3—C41—C42	0.8 (2)	C18—C27—C28—O5	163.18 (19)
Fe1—O3—C41—C46	−177.58 (15)	C18—C27—C28—N3	−19.8 (2)
Fe1—O4—C35—C36	171.6 (2)	C26—C27—C28—O5	−19.6 (2)
Fe1—O4—C35—C40	−7.1 (3)	C26—C27—C28—N3	157.38 (19)
Na1—O5—C28—N3	95.0 (2)	N3—C29—C30—C31	−176.3 (2)
Na1—O5—C28—C27	−88.25 (17)	N3—C29—C34—C33	175.2 (2)
Na1^{i}—O5—C28—N3	−76.6 (2)	C30—C29—C34—C33	−1.6 (4)
Na1^{i}—O5—C28—C27	100.2 (2)	C34—C29—C30—C31	0.2 (3)
Na1^{ii}—O6—C11—N4	−122.2 (2)	C29—C30—C31—C32	0.7 (4)
Na1^{ii}—O6—C11—C10	57.0 (2)	C30—C31—C32—C33	−0.4 (4)
Na1—O7—C48—C47	−116.2 (7)	C31—C32—C33—C34	−1.0 (4)
Na1—O7—C48—C49	64.5 (8)	C32—C33—C34—C29	2.0 (4)
Na1—O8—C51—C50	4.8 (5)	O4—C35—C36—C37	−178.0 (2)
Na1—O8—C51—C52	−176.5 (2)	O4—C35—C40—N7	1.2 (3)
N5—N1—C19—C18	2.4 (3)	O4—C35—C40—C39	179.1 (2)
N5—N1—C19—C20	−176.30 (18)	C36—C35—C40—N7	−177.6 (2)
C19—N1—N5—Fe1	3.3 (2)	C36—C35—C40—C39	0.3 (4)
C19—N1—N5—C42	179.52 (18)	C40—C35—C36—C37	0.7 (4)
N7—N2—C2—C1	10.7 (4)	C35—C36—C37—C38	−1.5 (4)
N7—N2—C2—C3	−171.6 (2)	C36—C37—C38—Cl2	−179.6 (2)
C2—N2—N7—Fe1	7.0 (3)	C36—C37—C38—C39	1.3 (4)
C2—N2—N7—C40	179.96 (17)	Cl2—C38—C39—C40	−179.4 (2)
C28—N3—C29—C30	−29.4 (3)	C37—C38—C39—C40	−0.3 (4)

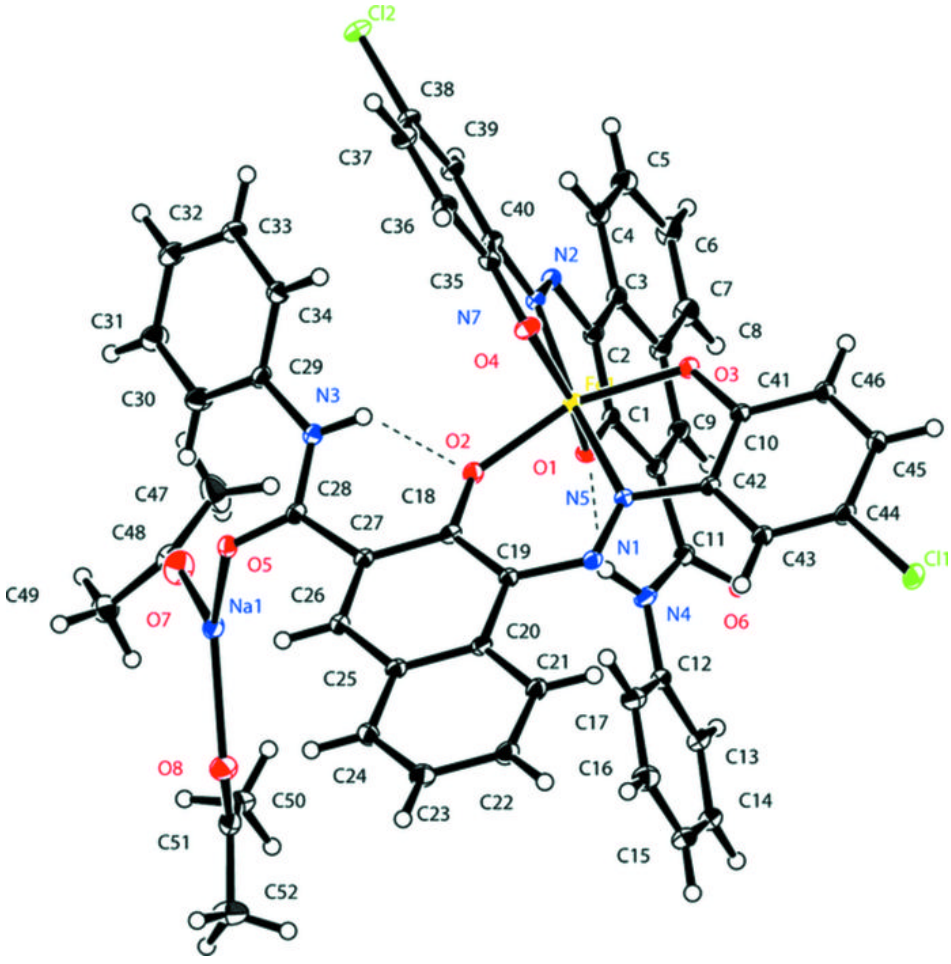
C28—N3—C29—C34	153.9 (2)	C38—C39—C40—N7	177.1 (2)
C29—N3—C28—O5	−1.6 (3)	C38—C39—C40—C35	−0.5 (4)
C29—N3—C28—C27	−178.50 (18)	O3—C41—C42—N5	−1.1 (2)
C11—N4—C12—C13	−22.6 (4)	O3—C41—C42—C43	−179.87 (19)
C11—N4—C12—C17	159.2 (2)	O3—C41—C46—C45	−179.87 (19)
C12—N4—C11—O6	1.5 (4)	C42—C41—C46—C45	1.7 (3)
C12—N4—C11—C10	−177.7 (2)	C46—C41—C42—N5	177.39 (18)
Fe1—N5—C42—C41	0.8 (2)	C46—C41—C42—C43	−1.4 (3)
Fe1—N5—C42—C43	179.51 (17)	N5—C42—C43—C44	−178.3 (2)
N1—N5—C42—C41	−176.27 (17)	C41—C42—C43—C44	0.3 (3)
N1—N5—C42—C43	2.4 (3)	C42—C43—C44—Cl1	−177.69 (16)
Fe1—N7—C40—C35	4.6 (2)	C42—C43—C44—C45	0.5 (3)
Fe1—N7—C40—C39	−173.2 (2)	Cl1—C44—C45—C46	178.04 (17)
N2—N7—C40—C35	−169.8 (2)	C43—C44—C45—C46	−0.2 (3)
N2—N7—C40—C39	12.4 (3)	C44—C45—C46—C41	−0.9 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O2	0.88	1.99	2.660 (3)	132
N4—H4N···O1	0.88	1.96	2.658 (2)	135

Fig. 1


Cl2
C38
C39
C37
C5
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C36
C40
C4
C6
N2
C35
C3
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C34
N7
C8
O4
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O3
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N4
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C20
C21
C12
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C13
O8
C24
C16
C14
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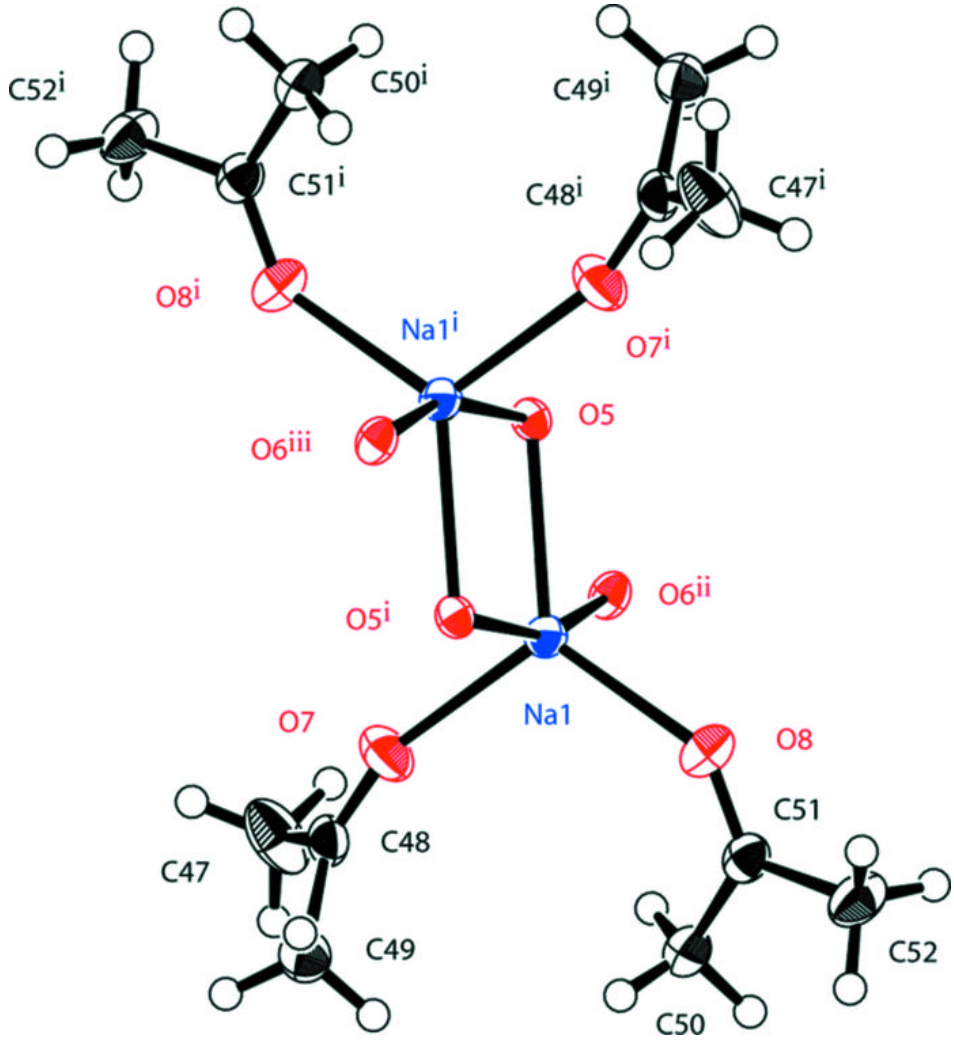
C22
C51
C15
C52

Fig. 2


C52i
C50i
C49i
C51i
C48i
C47i
O8i
Na1i
O7i
O5
O6iii
O5i
O6ii
Na1
O7
O8
C51
C48
C47
C49
C52
C50