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Diacetonitriletetrakis{μ_2-3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholato}tetraaquadiiron(III)disodium(I) dihydrate

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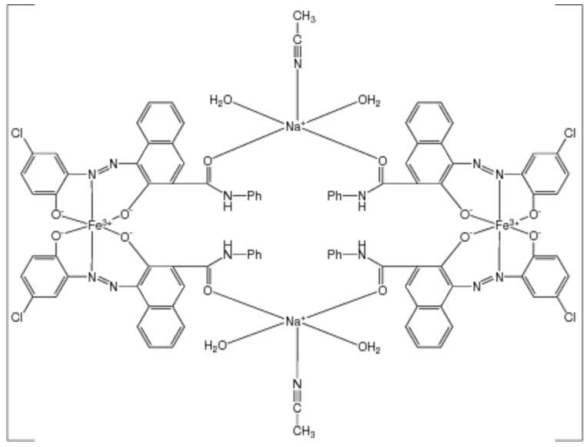
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.009 Å; H-atom completeness 84%; R factor = 0.086; wR factor = 0.264; data-to-parameter ratio = 13.4.

The title compound, $[Fe_2Na_2(C_{23}H_{14}ClN_3O_3)_4(C_2H_3N)_2(H_2O)_4]\cdot 2H_2O$, is a hydrated Fe–azo complex dimer that is used as a charge-control agent in electrophotography. The molecule is a centrosymmetric dimer with two octahedral Fe^{III} units linked by two bridging five-coordinate Na^{I} cations. Each Fe^{III} atom is chelated by the N and two O atoms from two 3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholate ligands. The Na^+ cation is coordinated by a carbonyl O atom from the two ligands of each octahedral Fe^{III} unit, two water molecules and the N atom of an acetonitrile molecule. Two solvent water molecules complete the structure. In the crystal structure, the dimeric molecules are bridged by a pair of discrete intermolecular O—H···O hydrogen bonds, one of which involves a sodium-bound water molecule and a hydrate water, and the other a 5-chlorophenolate O atom and a water molecule to form an extended chain along b.

Related literature

For general background to charge-control agents, see Tanaka (1995); and for the preparation of the title compound, see Yasumatsu *et al.* (2006). For related structures, see: Mizuguchi, Sato, Uta & Sato (2007); Mizuguchi *et al.* (2007*a*,*b*); Mizuguchi, Uta & Sato (2007).



Experimental

Crystal data

$[Fe_2Na_2(C_{23}H_{14}ClN_3O_3)_4(C_2H_3N)_2(H_2O)_4]\cdot 2H_2O$
M_r = 2011.21
Triclinic, $P\overline{1}$
a = 11.4416 (5) Å
b = 14.1161 (7) Å
c = 15.0105 (7) Å
α = 72.396 (1)°
β = 76.2850 (9)°
γ = 83.015 (1)°
V = 2241.67 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 93.1 K
0.30 × 0.09 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.793, T_{max} = 0.976
40907 measured reflections
8133 independent reflections
4163 reflections with $I > 2\sigma(I)$
R_{int} = 0.125

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.264
S = 0.97
8133 reflections
607 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.970 (4)	Na1—O5^{i}	2.222 (4)
Fe1—O2	1.944 (3)	Na1—O6	2.238 (5)
Fe1—O3	1.986 (3)	Na1—O7	2.508 (7)
Fe1—O4	1.976 (4)	Na1—O8	2.329 (6)
Fe1—N1	2.127 (4)	Na1—N7	2.381 (9)
Fe1—N4	2.161 (4)		
O1—Fe1—O2	90.26 (17)	O4—Fe1—N4	87.69 (18)
O1—Fe1—O3	85.60 (17)	N1—Fe1—N4	166.3 (2)
O1—Fe1—O4	160.14 (15)	O5^{i}—Na1—O6	97.7 (2)
O1—Fe1—N1	81.72 (18)	O5^{i}—Na1—O7	88.35 (19)
O1—Fe1—N4	111.90 (19)	O5^{i}—Na1—O8	108.0 (2)
O2—Fe1—O3	155.71 (17)	O5^{i}—Na1—N7	149.5 (3)
O2—Fe1—O4	96.86 (18)	O6—Na1—O7	92.9 (2)
O2—Fe1—N1	100.35 (16)	O6—Na1—O8	101.3 (2)
O2—Fe1—N4	79.14 (16)	O6—Na1—N7	107.6 (2)
O3—Fe1—O4	95.02 (17)	O7—Na1—O8	156.4 (2)
O3—Fe1—N1	102.70 (16)	O7—Na1—N7	73.9 (2)
O3—Fe1—N4	80.26 (17)	O8—Na1—N7	83.8 (2)
O4—Fe1—N1	78.78 (18)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3N···O1	0.86	1.94	2.644 (7)	138
N6—H6N···O3	0.86	1.97	2.664 (6)	138
O8—H···O9	–	–	2.730 (7)	–
O9—H···O4^{iii}	–	–	2.710 (6)	–

Symmetry code: (iii) $x, y-1, z$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); 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: SJ2453).

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supplementary materials

Acta Cryst. (2008). E**64**, m240-m241 [**doi:10.1107/S1600536807066895**]

Diacetonitriletetrakis{$_2$-3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholato}tetraaquadiiron(III)disodium(I) dihydrate

S. Yohei, U. Kazuya and J. Mizuguchi

Comment

The title compound, I, is a hydrated Fe-azo complex dimer that is used as a charge-control agent (CCA) of the negative type in electrophotography (Tanaka, 1995). The purpose of the investigation has been set out in our previous paper (Mizuguchi, Sato, Uta & Sato, 2007). We have previously reported the structure of a methanol-solvated Fe-azo complex with an ammonium cation (Mizuguchi *et al.*, 2007*a*) and its acetone solvate (Mizuguchi, Uta & Sato, 2007). together with the structure of an acetone-solvated Fe-azo complex with a sodium cation, in place of the ammonium (Mizuguchi *et al.*, 2007*b*). In this molecule, the sodium cation is found to bridge three different Fe-azo complexes through the Na—O bonds between the sodium cation and the carbonyl O atoms of the Fe-azo complex. The present paper reports a related hydrated Fe-azo complex dimer bridged by two sodium cations.

Fig. 1 shows the asymmetric unit of the complex with the complete centrosymmetric dimer molecule shown in Fig. 2. The dimer comprises two octahedral Fe^{III} units linked by two bridging five-coordinate Na^{I} cations. Each Fe^{III} atom is chelated by the N and two O atoms from two 3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholate ligands with the naphtholate and chloro-2-oxidophenyl O atoms mutually *cis*. In each octahedral Fe^{III} unit, there are two intramolecular N3—H3N···O1 and N6—H6N···O3 hydrogen bonds that effect the conformation of the molecule (Table 2). The five-coordinate Na cation binds to N7 of the acetonitrile molecule, the O7 and O8 atoms of the two coordinated water molecules, and to the O6 and $O5^{i}$ carbonyl O atoms from of each octahedral Fe^{III} unit [symmetry code (i): $1-x, -y, 1-z$]. There are also two hydrated water molecules O9 and $O9^{ii}$ [symmetry code (ii): $x, y-1, z$].

In the crystal structure the dimeric molecules are bridged by a pair of discrete intermolecular O—H···O hydrogen bonds as shown in Fig. 3. One of these involves a sodium bound water molecule and a hydrate water, and the other a 5-chlorphenolate O atom and a hydrate water to form an extended chain along *b*. The atoms involved are: O8—(H)···O9 and O9—(H)···$O4^{ii}$ [symmetry code: (ii) $x, -1+y, z$] with the H atoms in parenthesis not located. The H atoms on the O7, O8 and O9 atoms of the water molecules could not be found in difference density maps. However the bond distances O8—O9, 2.730 (7) and O9—$O4^{ii}$, 2.710 (6) Å [symmetry code: (ii) $x, -1+y, z$] strongly suggest the presence of classical hydrogen bonds.

Experimental

Compound I was prepared according to the previously reported method (Yasumatsu *et al.*, 2006). Single crystals of (I) were recrystallized from an acetonitrile solution as blocks over a 48 h period.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 except for C—H in methyl groups (0.96) and N—H = 0.86 A, and U_{iso} (H) = 1.2 U_{eq} (parent atom). Six H atoms on the three water molecules (O7, O8 and O9) were not located in difference electron density maps.

R-merge for the reflection data was 12.5%. This indicates poor crystal quality resulting in a rather high value of the *R* factor.

Figures

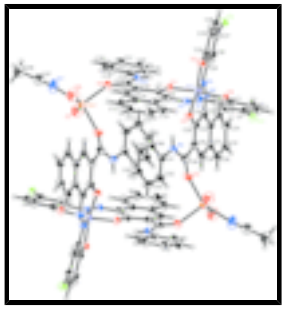


Fig. 1. A view of the molecular structure of (I), showing 30% displacement ellipsoids.

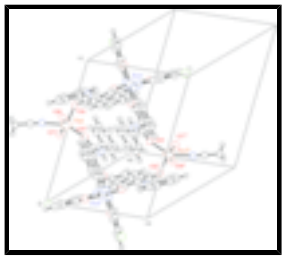


Fig. 2. The centrosymmetric complex dimer. The two Fe-azo complexes are bridged by Na1 and Na1^{i} cations through Na1—O5^{i} and Na1—O6, and Na1^{i}—O5 and Na1^{i}—O6^{i} bonds, respectively [symmetry code(i): 1 − *x*, −*y*, 1 − *z*].

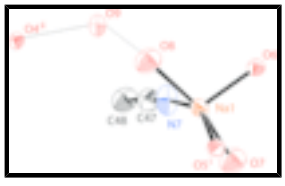


Fig. 3. shows two distinct intermolecular O···O interactions, dashed lines, that link two azo-Fe complex dimers: O8···O9 and O9···O4^{ii} Hydrogen atoms on O8 and O9 could not be located in difference electron density maps [symmetry codes (i): −*x* + 1, −*y*, −*z* + 1 and (ii): *x*, −1 + *y*, *z*].

Diacetonitriletetrakis{μ$_2$-3-anilinocarbonyl-1-[(5-chloro-2- oxidophenyl)diazenyl]-2-naphtholato}tetraaquadiiron(III)disodium(I) dihydrate

Crystal data

$[Fe_2Na_2(C_{23}H_{14}ClN_3O_3)_4(C_2H_3N)_2(H_2O)_4]\cdot 2H_2O$	$Z = 1$
$M_r = 2011.21$	$F_{000} = 1022.0$
Triclinic, $P\bar{1}$	$D_x = 1.481$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71075 Å
$a = 11.4416$ (5) Å	Cell parameters from 18467 reflections
$b = 14.1161$ (7) Å	θ = 3.0–25.3°

c = 15.0105 (7) Å
α = 72.396 (1)º
β = 76.2850 (9)º
γ = 83.015 (1)º
V = 2241.67 (18) Å^3

μ = 0.53 mm^{-1}
T = 93.1 K
Block, black
0.30 × 0.09 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.793, T_{max} = 0.976
40907 measured reflections
8133 independent reflections

4163 reflections with $I > 2\sigma(I)$
R_{int} = 0.125
θ_{max} = 25.4º
h = −13→13
k = −16→16
l = −18→18

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.264
S = 0.97
8133 reflections
607 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1531P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 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 $F^2 > 2$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	0.35889 (7)	0.15898 (6)	0.81868 (6)	0.0419 (3)
Cl1	0.89755 (14)	0.08974 (12)	0.97345 (11)	0.0493 (4)
Cl2	−0.13236 (15)	0.46998 (12)	0.94460 (12)	0.0570 (4)
Na1	0.1669 (2)	−0.2788 (2)	0.66698 (19)	0.0631 (7)

O1	0.3035 (3)	0.0314 (2)	0.8208 (2)	0.0431 (9)
O2	0.2505 (3)	0.1532 (2)	0.9412 (2)	0.0455 (10)
O3	0.4037 (3)	0.1844 (2)	0.6776 (2)	0.0441 (10)
O4	0.4653 (3)	0.2573 (2)	0.8224 (2)	0.0435 (10)
O5	0.6633 (4)	0.2145 (3)	0.4266 (3)	0.0565 (11)
O6	0.1263 (3)	−0.1752 (3)	0.7588 (2)	0.0506 (11)
O7	0.0555 (5)	−0.1671 (4)	0.5459 (4)	0.1103 (15)
O8	0.2170 (5)	−0.4270 (4)	0.7749 (4)	0.1103 (15)
O9	0.3764 (4)	−0.5671 (3)	0.8564 (3)	0.0660 (13)
N1	0.5057 (4)	0.0648 (3)	0.8650 (3)	0.0397 (11)
N2	0.5346 (4)	−0.0289 (3)	0.8773 (3)	0.0398 (11)
N3	0.1124 (4)	−0.0205 (3)	0.7800 (3)	0.0454 (12)
N4	0.2318 (4)	0.2816 (3)	0.7769 (3)	0.0413 (11)
N5	0.2329 (4)	0.3526 (3)	0.6989 (3)	0.0430 (12)
N6	0.5554 (4)	0.1015 (3)	0.5544 (3)	0.0449 (12)
N7	−0.0136 (6)	−0.3582 (5)	0.6870 (6)	0.101 (2)
C1	0.5628 (5)	0.2210 (4)	0.8598 (4)	0.0422 (14)
C2	0.6393 (5)	0.2825 (4)	0.8750 (4)	0.0448 (15)
C3	0.7400 (5)	0.2409 (4)	0.9114 (4)	0.0473 (15)
C4	0.7679 (5)	0.1382 (4)	0.9319 (4)	0.0451 (14)
C5	0.6932 (5)	0.0759 (4)	0.9196 (4)	0.0428 (14)
C6	0.5913 (5)	0.1184 (4)	0.8821 (4)	0.0436 (14)
C7	0.3479 (5)	−0.0602 (4)	0.8343 (4)	0.0392 (13)
C8	0.4605 (5)	−0.0899 (4)	0.8615 (4)	0.0386 (13)
C9	0.5082 (5)	−0.1914 (4)	0.8752 (4)	0.0402 (14)
C10	0.6220 (5)	−0.2231 (4)	0.8991 (4)	0.0486 (15)
C11	0.6632 (6)	−0.3209 (4)	0.9089 (5)	0.0593 (18)
C12	0.5984 (6)	−0.3902 (4)	0.8959 (5)	0.0592 (18)
C13	0.4881 (6)	−0.3611 (4)	0.8720 (5)	0.0544 (17)
C14	0.4414 (5)	−0.2609 (4)	0.8604 (4)	0.0454 (15)
C15	0.3295 (5)	−0.2294 (4)	0.8330 (4)	0.0450 (14)
C16	0.2828 (5)	−0.1335 (4)	0.8186 (4)	0.0398 (13)
C17	0.1688 (5)	−0.1119 (4)	0.7845 (4)	0.0424 (14)
C18	0.0062 (5)	0.0210 (4)	0.7457 (4)	0.0452 (15)
C19	−0.0736 (6)	−0.0332 (5)	0.7267 (4)	0.0573 (17)
C20	−0.1751 (6)	0.0128 (5)	0.6939 (4)	0.0605 (18)
C21	−0.1973 (6)	0.1163 (5)	0.6778 (4)	0.0573 (18)
C22	−0.1186 (5)	0.1703 (5)	0.6963 (4)	0.0530 (17)
C23	−0.0168 (5)	0.1234 (5)	0.7317 (4)	0.0502 (16)
C24	0.1631 (5)	0.2232 (4)	0.9440 (4)	0.0415 (14)
C25	0.0855 (5)	0.2317 (4)	1.0296 (4)	0.0434 (14)
C26	−0.0026 (5)	0.3072 (4)	1.0291 (4)	0.0471 (15)
C27	−0.0182 (5)	0.3765 (4)	0.9418 (4)	0.0444 (14)
C28	0.0548 (5)	0.3704 (4)	0.8564 (4)	0.0468 (15)
C29	0.1455 (5)	0.2944 (4)	0.8573 (4)	0.0421 (14)
C30	0.4013 (5)	0.2678 (4)	0.6089 (4)	0.0452 (15)
C31	0.3192 (5)	0.3486 (4)	0.6182 (4)	0.0456 (15)
C32	0.3197 (5)	0.4395 (4)	0.5399 (4)	0.0437 (14)
C33	0.2371 (5)	0.5215 (4)	0.5450 (4)	0.0484 (15)

C34	0.2456 (6)	0.6069 (4)	0.4700 (4)	0.0541 (17)
C35	0.3359 (6)	0.6164 (4)	0.3864 (4)	0.0548 (17)
C36	0.4139 (6)	0.5365 (4)	0.3802 (4)	0.0510 (16)
C37	0.4090 (5)	0.4471 (4)	0.4548 (4)	0.0442 (14)
C38	0.4904 (5)	0.3653 (4)	0.4471 (4)	0.0476 (15)
C39	0.4874 (5)	0.2775 (4)	0.5180 (4)	0.0452 (15)
C40	0.5767 (6)	0.1949 (5)	0.4971 (4)	0.0505 (16)
C41	0.6173 (5)	0.0108 (4)	0.5470 (4)	0.0435 (14)
C42	0.7141 (5)	0.0022 (5)	0.4734 (4)	0.0564 (17)
C43	0.7690 (6)	−0.0910 (5)	0.4735 (5)	0.068 (2)
C44	0.7300 (6)	−0.1763 (5)	0.5459 (4)	0.0577 (17)
C45	0.6337 (5)	−0.1664 (5)	0.6187 (4)	0.0523 (16)
C46	0.5787 (5)	−0.0738 (4)	0.6184 (4)	0.0462 (15)
C47	−0.0920 (8)	−0.4004 (6)	0.6882 (6)	0.081 (2)
C48	−0.1940 (8)	−0.4558 (7)	0.6902 (6)	0.103 (3)
H2	0.6224	0.3509	0.8605	0.054*
H3	0.7899	0.2816	0.9224	0.057*
H3N	0.1456	0.0176	0.8008	0.054*
H5	0.7097	0.0074	0.9356	0.051*
H6N	0.4958	0.0970	0.6024	0.054*
H10	0.6683	−0.1784	0.9082	0.058*
H11	0.7379	−0.3410	0.9248	0.071*
H12	0.6288	−0.4557	0.9033	0.071*
H13	0.4439	−0.4072	0.8634	0.066*
H15	0.2858	−0.2758	0.8242	0.053*
H19	−0.0590	−0.1018	0.7363	0.068*
H20	−0.2287	−0.0245	0.6825	0.073*
H21	−0.2649	0.1478	0.6548	0.069*
H22	−0.1329	0.2388	0.6852	0.064*
H23	0.0350	0.1602	0.7457	0.060*
H25	0.0940	0.1857	1.0872	0.052*
H26	−0.0521	0.3128	1.0863	0.057*
H28	0.0441	0.4159	0.7991	0.056*
H33	0.1765	0.5177	0.5995	0.058*
H34	0.1901	0.6600	0.4747	0.065*
H35	0.3421	0.6754	0.3369	0.066*
H36	0.4726	0.5412	0.3246	0.061*
H38	0.5489	0.3713	0.3911	0.057*
H42	0.7418	0.0583	0.4246	0.068*
H43	0.8335	−0.0967	0.4239	0.082*
H44	0.7678	−0.2384	0.5453	0.069*
H45	0.6060	−0.2222	0.6679	0.063*
H46	0.5138	−0.0684	0.6677	0.055*
H48A	−0.1883	−0.4635	0.6279	0.123*
H48B	−0.2682	−0.4198	0.7081	0.123*
H48C	−0.1919	−0.5202	0.7358	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0437 (5)	0.0388 (5)	0.0420 (5)	0.0055 (3)	−0.0130 (4)	−0.0097 (3)
Cl1	0.0459 (8)	0.0517 (9)	0.0505 (9)	0.0036 (7)	−0.0165 (7)	−0.0122 (7)
Cl2	0.0557 (10)	0.0513 (10)	0.0614 (11)	0.0143 (7)	−0.0124 (8)	−0.0188 (8)
Na1	0.0676 (17)	0.0632 (18)	0.0588 (17)	−0.0126 (14)	0.0001 (13)	−0.0248 (13)
O1	0.044 (2)	0.040 (2)	0.046 (2)	0.0014 (18)	−0.0145 (19)	−0.0111 (18)
O2	0.049 (2)	0.041 (2)	0.047 (2)	0.0134 (19)	−0.0170 (19)	−0.0129 (19)
O3	0.049 (2)	0.040 (2)	0.041 (2)	0.0019 (18)	−0.0088 (19)	−0.0106 (18)
O4	0.044 (2)	0.040 (2)	0.049 (2)	0.0070 (18)	−0.0202 (19)	−0.0115 (18)
O5	0.057 (2)	0.054 (2)	0.052 (2)	0.006 (2)	−0.002 (2)	−0.016 (2)
O6	0.049 (2)	0.053 (2)	0.051 (2)	−0.001 (2)	−0.013 (2)	−0.014 (2)
O7	0.114 (3)	0.112 (3)	0.107 (3)	−0.011 (2)	−0.047 (3)	−0.014 (2)
O8	0.114 (3)	0.112 (3)	0.107 (3)	−0.011 (2)	−0.047 (3)	−0.014 (2)
O9	0.067 (3)	0.050 (2)	0.084 (3)	−0.001 (2)	−0.019 (2)	−0.022 (2)
N1	0.038 (2)	0.040 (2)	0.039 (2)	0.001 (2)	−0.007 (2)	−0.011 (2)
N2	0.050 (3)	0.033 (2)	0.034 (2)	0.005 (2)	−0.011 (2)	−0.009 (2)
N3	0.046 (2)	0.046 (3)	0.047 (3)	0.003 (2)	−0.015 (2)	−0.016 (2)
N4	0.042 (2)	0.040 (2)	0.041 (2)	0.001 (2)	−0.009 (2)	−0.012 (2)
N5	0.049 (3)	0.040 (2)	0.033 (2)	0.003 (2)	−0.010 (2)	−0.002 (2)
N6	0.050 (3)	0.039 (3)	0.041 (2)	0.003 (2)	−0.008 (2)	−0.009 (2)
N7	0.073 (4)	0.088 (5)	0.164 (8)	0.003 (4)	−0.057 (5)	−0.047 (5)
C1	0.042 (3)	0.047 (3)	0.037 (3)	0.003 (2)	−0.010 (2)	−0.012 (2)
C2	0.048 (3)	0.037 (3)	0.051 (3)	0.010 (2)	−0.022 (3)	−0.010 (2)
C3	0.046 (3)	0.044 (3)	0.052 (4)	−0.002 (2)	−0.005 (3)	−0.017 (2)
C4	0.045 (3)	0.046 (3)	0.047 (3)	−0.001 (2)	−0.014 (2)	−0.014 (2)
C5	0.048 (3)	0.041 (3)	0.042 (3)	0.007 (2)	−0.018 (2)	−0.013 (2)
C6	0.050 (3)	0.038 (3)	0.042 (3)	0.001 (2)	−0.016 (2)	−0.008 (2)
C7	0.046 (3)	0.034 (3)	0.041 (3)	0.005 (2)	−0.011 (2)	−0.018 (2)
C8	0.038 (3)	0.038 (3)	0.039 (3)	0.010 (2)	−0.016 (2)	−0.009 (2)
C9	0.044 (3)	0.038 (3)	0.039 (3)	0.007 (2)	−0.010 (2)	−0.013 (2)
C10	0.057 (3)	0.040 (3)	0.052 (3)	0.003 (3)	−0.020 (3)	−0.012 (2)
C11	0.052 (4)	0.050 (4)	0.080 (5)	0.016 (3)	−0.029 (3)	−0.021 (3)
C12	0.060 (4)	0.038 (3)	0.089 (5)	0.017 (3)	−0.034 (3)	−0.024 (3)
C13	0.059 (4)	0.039 (3)	0.072 (4)	−0.001 (3)	−0.019 (3)	−0.022 (3)
C14	0.050 (3)	0.038 (3)	0.048 (3)	0.003 (2)	−0.010 (2)	−0.015 (2)
C15	0.043 (3)	0.044 (3)	0.049 (3)	−0.001 (2)	−0.010 (2)	−0.015 (2)
C16	0.040 (3)	0.043 (3)	0.039 (3)	0.003 (2)	−0.017 (2)	−0.010 (2)
C17	0.047 (3)	0.037 (3)	0.041 (3)	0.005 (2)	−0.011 (2)	−0.010 (2)
C18	0.042 (3)	0.054 (4)	0.040 (3)	0.005 (3)	−0.013 (2)	−0.014 (2)
C19	0.055 (4)	0.060 (4)	0.059 (4)	0.014 (3)	−0.024 (3)	−0.018 (3)
C20	0.058 (4)	0.070 (5)	0.055 (4)	0.003 (3)	−0.019 (3)	−0.017 (3)
C21	0.055 (4)	0.061 (4)	0.060 (4)	0.015 (3)	−0.026 (3)	−0.019 (3)
C22	0.049 (3)	0.059 (4)	0.048 (4)	0.019 (3)	−0.019 (3)	−0.013 (3)
C23	0.049 (3)	0.057 (4)	0.043 (3)	0.005 (3)	−0.007 (2)	−0.016 (3)
C24	0.047 (3)	0.037 (3)	0.040 (3)	−0.001 (2)	−0.011 (2)	−0.009 (2)

C25	0.048 (3)	0.039 (3)	0.042 (3)	0.002 (2)	−0.015 (2)	−0.006 (2)
C26	0.046 (3)	0.049 (3)	0.048 (3)	0.003 (3)	−0.012 (2)	−0.017 (3)
C27	0.046 (3)	0.038 (3)	0.051 (3)	0.015 (2)	−0.016 (2)	−0.016 (2)
C28	0.053 (3)	0.039 (3)	0.047 (3)	0.005 (2)	−0.013 (3)	−0.012 (2)
C29	0.037 (3)	0.041 (3)	0.048 (3)	0.004 (2)	−0.014 (2)	−0.011 (2)
C30	0.053 (3)	0.041 (3)	0.037 (3)	−0.003 (2)	−0.012 (2)	−0.003 (2)
C31	0.058 (4)	0.034 (3)	0.046 (3)	0.008 (2)	−0.018 (3)	−0.013 (2)
C32	0.050 (3)	0.042 (3)	0.037 (3)	0.002 (2)	−0.012 (2)	−0.007 (2)
C33	0.055 (3)	0.045 (3)	0.046 (3)	0.006 (3)	−0.013 (3)	−0.014 (2)
C34	0.061 (4)	0.040 (3)	0.058 (4)	0.011 (3)	−0.019 (3)	−0.009 (3)
C35	0.073 (4)	0.045 (4)	0.041 (3)	−0.003 (3)	−0.009 (3)	−0.006 (2)
C36	0.062 (4)	0.047 (4)	0.043 (3)	−0.003 (3)	−0.011 (3)	−0.011 (2)
C37	0.051 (3)	0.043 (3)	0.037 (3)	0.006 (2)	−0.013 (2)	−0.010 (2)
C38	0.057 (4)	0.045 (3)	0.039 (3)	−0.004 (3)	−0.008 (3)	−0.010 (2)
C39	0.043 (3)	0.047 (3)	0.047 (3)	0.006 (2)	−0.014 (2)	−0.015 (2)
C40	0.056 (4)	0.054 (4)	0.044 (3)	0.004 (3)	−0.015 (3)	−0.015 (3)
C41	0.050 (3)	0.041 (3)	0.043 (3)	0.002 (2)	−0.015 (2)	−0.014 (2)
C42	0.060 (4)	0.046 (4)	0.051 (4)	0.000 (3)	0.000 (3)	−0.006 (3)
C43	0.070 (4)	0.052 (4)	0.064 (4)	−0.001 (3)	0.010 (3)	−0.008 (3)
C44	0.064 (4)	0.050 (4)	0.052 (4)	0.013 (3)	−0.006 (3)	−0.015 (3)
C45	0.054 (4)	0.048 (4)	0.051 (4)	−0.004 (3)	−0.011 (3)	−0.010 (3)
C46	0.047 (3)	0.047 (3)	0.041 (3)	0.003 (2)	−0.010 (2)	−0.009 (2)
C47	0.069 (5)	0.086 (6)	0.089 (6)	0.012 (4)	−0.027 (4)	−0.024 (4)
C48	0.097 (7)	0.106 (7)	0.105 (7)	−0.010 (5)	−0.039 (6)	−0.015 (5)

Geometric parameters (Å, °)

Fe1—O1	1.970 (4)	C15—C16	1.366 (8)
Fe1—O2	1.944 (3)	C15—H15	0.930
Fe1—O3	1.986 (3)	C16—C17	1.477 (8)
Fe1—O4	1.976 (4)	C18—C19	1.387 (11)
Fe1—N1	2.127 (4)	C18—C23	1.397 (9)
Fe1—N4	2.161 (4)	C19—C20	1.381 (10)
Cl1—C4	1.729 (6)	C19—H19	0.930
Cl2—C27	1.743 (6)	C20—C21	1.408 (10)
Na1—O5^{i}	2.222 (4)	C20—H20	0.930
Na1—O6	2.238 (5)	C21—C22	1.373 (11)
Na1—O7	2.508 (7)	C21—H21	0.930
Na1—O8	2.329 (6)	C22—C23	1.404 (9)
Na1—N7	2.381 (9)	C22—H22	0.930
O1—C7	1.304 (6)	C23—H23	0.930
O2—C24	1.320 (6)	C24—C25	1.407 (8)
O3—C30	1.312 (6)	C24—C29	1.424 (7)
O4—C1	1.344 (7)	C25—C26	1.375 (8)
O5—C40	1.253 (7)	C25—H25	0.930
O6—C17	1.258 (8)	C26—C27	1.413 (8)
N1—N2	1.290 (6)	C26—H26	0.930
N1—C6	1.420 (9)	C27—C28	1.375 (8)
N2—C8	1.384 (8)	C28—C29	1.398 (8)

N3—C17	1.361 (7)	C28—H28	0.930
N3—C18	1.424 (8)	C30—C31	1.406 (8)
N3—H3N	0.860	C30—C39	1.460 (8)
N4—N5	1.289 (5)	C31—C32	1.455 (7)
N4—C29	1.409 (7)	C32—C33	1.412 (8)
N5—C31	1.380 (7)	C32—C37	1.418 (7)
N6—C40	1.353 (7)	C33—C34	1.373 (7)
N6—C41	1.407 (7)	C33—H33	0.930
N6—H6N	0.860	C34—C35	1.406 (8)
N7—C47	1.130 (13)	C34—H34	0.930
C1—C2	1.404 (10)	C35—C36	1.363 (9)
C1—C6	1.400 (8)	C35—H35	0.930
C2—C3	1.382 (8)	C36—C37	1.408 (7)
C2—H2	0.930	C36—H36	0.930
C3—C4	1.401 (8)	C37—C38	1.408 (8)
C3—H3	0.930	C38—C39	1.366 (7)
C4—C5	1.376 (10)	C38—H38	0.930
C5—C6	1.404 (8)	C39—C40	1.511 (9)
C5—H5	0.930	C41—C42	1.390 (8)
C7—C8	1.420 (8)	C41—C46	1.379 (7)
C7—C16	1.449 (9)	C42—C43	1.387 (9)
C8—C9	1.441 (7)	C42—H42	0.930
C9—C10	1.417 (8)	C43—C44	1.393 (8)
C9—C14	1.410 (10)	C43—H43	0.930
C10—C11	1.379 (9)	C44—C45	1.382 (8)
C10—H10	0.930	C44—H44	0.930
C11—C12	1.380 (11)	C45—C46	1.379 (9)
C11—H11	0.930	C45—H45	0.930
C12—C13	1.374 (10)	C46—H46	0.930
C12—H12	0.930	C47—C48	1.472 (14)
C13—C14	1.424 (8)	C48—H48A	0.960
C13—H13	0.930	C48—H48B	0.960
C14—C15	1.417 (9)	C48—H48C	0.960
O4···O9^{ii}	2.710 (6)	O9···O4^{iii}	2.710 (6)
O8···O9	2.730 (7)	O9···O8	2.730 (7)
O1—Fe1—O2	90.26 (17)	N3—C17—C16	117.7 (6)
O1—Fe1—O3	85.60 (17)	N3—C18—C19	124.4 (5)
O1—Fe1—O4	160.14 (15)	N3—C18—C23	116.0 (6)
O1—Fe1—N1	81.72 (18)	C19—C18—C23	119.5 (5)
O1—Fe1—N4	111.90 (19)	C18—C19—C20	120.8 (6)
O2—Fe1—O3	155.71 (17)	C18—C19—H19	119.9
O2—Fe1—O4	96.86 (18)	C20—C19—H19	119.3
O2—Fe1—N1	100.35 (16)	C19—C20—C21	119.9 (7)
O2—Fe1—N4	79.14 (16)	C19—C20—H20	120.1
O3—Fe1—O4	95.02 (17)	C21—C20—H20	120.1
O3—Fe1—N1	102.70 (16)	C20—C21—C22	119.5 (6)
O3—Fe1—N4	80.26 (17)	C20—C21—H21	120.2
O4—Fe1—N1	78.78 (18)	C22—C21—H21	120.2

O4—Fe1—N4	87.69 (18)	C21—C22—C23	120.7 (6)
N1—Fe1—N4	166.3 (2)	C21—C22—H22	119.6
$O5^{i}$—Na1—O6	97.7 (2)	C23—C22—H22	119.6
$O5^{i}$—Na1—O7	88.35 (19)	C18—C23—C22	119.5 (7)
$O5^{i}$—Na1—O8	108.0 (2)	C18—C23—H23	120.3
$O5^{i}$—Na1—N7	149.5 (3)	C22—C23—H23	120.3
O6—Na1—O7	92.9 (2)	O2—C24—C25	123.0 (4)
O6—Na1—O8	101.3 (2)	O2—C24—C29	119.4 (4)
O6—Na1—N7	107.6 (2)	C25—C24—C29	117.6 (5)
O7—Na1—O8	156.4 (2)	C24—C25—C26	120.8 (5)
O7—Na1—N7	73.9 (2)	C24—C25—H25	119.6
O8—Na1—N7	83.8 (2)	C26—C25—H25	119.6
Fe1—O1—C7	136.1 (4)	C25—C26—C27	120.2 (5)
Fe1—O2—C24	117.8 (3)	C25—C26—H26	119.9
Fe1—O3—C30	130.3 (4)	C27—C26—H26	119.9
Fe1—O4—C1	116.7 (3)	Cl2—C27—C26	118.6 (4)
$Na1^{i}$—O5—C40	159.8 (5)	Cl2—C27—C28	120.6 (4)
Na1—O6—C17	145.0 (3)	C26—C27—C28	120.8 (5)
Fe1—N1—N2	133.6 (4)	C27—C28—C29	118.8 (5)
Fe1—N1—C6	112.0 (3)	C27—C28—H28	120.6
N2—N1—C6	114.3 (4)	C29—C28—H28	120.6
N1—N2—C8	120.5 (4)	N4—C29—C24	112.6 (4)
C17—N3—C18	129.2 (6)	N4—C29—C28	125.6 (5)
C17—N3—H3N	115.4	C24—C29—C28	121.7 (5)
C18—N3—H3N	115.4	O3—C30—C31	123.1 (5)
Fe1—N4—N5	132.3 (3)	O3—C30—C39	118.8 (5)
Fe1—N4—C29	110.8 (3)	C31—C30—C39	118.1 (4)
N5—N4—C29	115.6 (4)	N5—C31—C30	125.8 (4)
N4—N5—C31	119.2 (4)	N5—C31—C32	113.0 (5)
C40—N6—C41	129.3 (4)	C30—C31—C32	121.1 (5)
C40—N6—H6N	115.3	C31—C32—C33	123.2 (5)
C41—N6—H6N	115.4	C31—C32—C37	118.6 (5)
Na1—N7—C47	171.9 (8)	C33—C32—C37	118.2 (4)
O4—C1—C2	122.4 (5)	C32—C33—C34	120.4 (5)
O4—C1—C6	119.0 (6)	C32—C33—H33	119.8
C2—C1—C6	118.5 (5)	C34—C33—H33	119.8
C1—C2—C3	119.7 (5)	C33—C34—C35	121.9 (5)
C1—C2—H2	120.1	C33—C34—H34	119.0
C3—C2—H2	120.1	C35—C34—H34	119.0
C2—C3—C4	120.8 (6)	C34—C35—C36	117.9 (5)
C2—C3—H3	119.6	C34—C35—H35	121.1
C4—C3—H3	119.6	C36—C35—H35	121.1
Cl1—C4—C3	119.3 (5)	C35—C36—C37	122.6 (5)
Cl1—C4—C5	120.0 (4)	C35—C36—H36	118.7
C3—C4—C5	120.7 (5)	C37—C36—H36	118.7
C4—C5—C6	118.3 (5)	C32—C37—C36	119.0 (5)
C4—C5—H5	120.8	C32—C37—C38	119.2 (4)
C6—C5—H5	120.8	C36—C37—C38	121.8 (5)

N1—C6—C1	112.8 (5)	C37—C38—C39	123.0 (5)
N1—C6—C5	125.3 (5)	C37—C38—H38	118.5
C1—C6—C5	121.9 (6)	C39—C38—H38	118.5
O1—C7—C8	121.8 (6)	C30—C39—C38	119.8 (5)
O1—C7—C16	119.5 (5)	C30—C39—C40	123.5 (4)
C8—C7—C16	118.7 (5)	C38—C39—C40	116.7 (5)
N2—C8—C7	125.9 (5)	O5—C40—N6	123.1 (5)
N2—C8—C9	113.4 (5)	O5—C40—C39	119.5 (5)
C7—C8—C9	120.8 (6)	N6—C40—C39	117.3 (4)
C8—C9—C10	122.4 (6)	N6—C41—C42	124.1 (4)
C8—C9—C14	118.9 (5)	N6—C41—C46	117.0 (4)
C10—C9—C14	118.7 (5)	C42—C41—C46	118.9 (5)
C9—C10—C11	119.3 (6)	C41—C42—C43	119.3 (5)
C9—C10—H10	120.4	C41—C42—H42	120.3
C11—C10—H10	120.4	C43—C42—H42	120.3
C10—C11—C12	122.8 (6)	C42—C43—C44	121.6 (6)
C10—C11—H11	118.6	C42—C43—H43	119.2
C12—C11—H11	118.6	C44—C43—H43	119.2
C11—C12—C13	119.0 (6)	C43—C44—C45	118.3 (6)
C11—C12—H12	120.5	C43—C44—H44	120.8
C13—C12—H12	120.5	C45—C44—H44	120.8
C12—C13—C14	120.7 (7)	C44—C45—C46	120.1 (5)
C12—C13—H13	119.5	C44—C45—H45	119.9
C14—C13—H13	119.8	C46—C45—H45	120.0
C9—C14—C13	119.6 (5)	C41—C46—C45	121.8 (5)
C9—C14—C15	119.3 (5)	C41—C46—H46	119.1
C13—C14—C15	121.1 (6)	C45—C46—H46	119.1
C14—C15—C16	123.0 (6)	N7—C47—C48	179.8 (9)
C14—C15—H15	118.7	C47—C48—H48A	109.5
C16—C15—H15	118.3	C47—C48—H48B	109.5
C7—C16—C15	119.3 (5)	C47—C48—H48C	109.5
C7—C16—C17	124.6 (5)	H48A—C48—H48B	109.5
C15—C16—C17	116.1 (6)	H48A—C48—H48C	109.5
O6—C17—N3	121.1 (5)	H48B—C48—H48C	109.5
O6—C17—C16	121.2 (5)		
O1—Fe1—O2—C24	−116.4 (4)	C3—C4—C5—C6	2.7 (8)
O2—Fe1—O1—C7	−107.1 (5)	C4—C5—C6—N1	179.9 (4)
O1—Fe1—O3—C30	145.6 (5)	C4—C5—C6—C1	−1.8 (8)
O3—Fe1—O1—C7	96.8 (5)	O1—C7—C8—N2	0.3 (6)
O1—Fe1—O4—C1	−18.3 (7)	O1—C7—C8—C9	−179.5 (4)
O4—Fe1—O1—C7	4.2 (8)	O1—C7—C16—C15	−179.8 (3)
O1—Fe1—N1—N2	4.6 (4)	O1—C7—C16—C17	2.3 (8)
O1—Fe1—N1—C6	−178.2 (3)	C8—C7—C16—C15	1.8 (7)
N1—Fe1—O1—C7	−6.7 (5)	C8—C7—C16—C17	−176.1 (5)
O1—Fe1—N4—N5	−105.7 (6)	C16—C7—C8—N2	178.7 (4)
O1—Fe1—N4—C29	88.5 (4)	C16—C7—C8—C9	−1.2 (7)
N4—Fe1—O1—C7	174.5 (4)	N2—C8—C9—C10	−2.1 (7)
O2—Fe1—O3—C30	64.8 (7)	N2—C8—C9—C14	−179.5 (4)
O3—Fe1—O2—C24	−36.6 (7)	C7—C8—C9—C10	177.8 (5)

O2—Fe1—O4—C1	91.9 (3)	C7—C8—C9—C14	0.4 (6)
O4—Fe1—O2—C24	82.2 (4)	C8—C9—C10—C11	−178.4 (5)
O2—Fe1—N1—N2	93.4 (4)	C8—C9—C14—C13	178.9 (5)
O2—Fe1—N1—C6	−89.4 (3)	C8—C9—C14—C15	−0.2 (6)
N1—Fe1—O2—C24	162.0 (4)	C10—C9—C14—C13	1.4 (8)
O2—Fe1—N4—N5	168.5 (6)	C10—C9—C14—C15	−177.7 (5)
O2—Fe1—N4—C29	2.6 (4)	C14—C9—C10—C11	−1.0 (8)
N4—Fe1—O2—C24	−4.1 (4)	C9—C10—C11—C12	0.2 (7)
O3—Fe1—O4—C1	−109.3 (3)	C10—C11—C12—C13	0.2 (7)
O4—Fe1—O3—C30	−54.3 (5)	C11—C12—C13—C14	0.2 (7)
O3—Fe1—N1—N2	−78.9 (4)	C12—C13—C14—C9	−1.0 (9)
O3—Fe1—N1—C6	98.3 (3)	C12—C13—C14—C15	178.1 (6)
N1—Fe1—O3—C30	−133.9 (5)	C9—C14—C15—C16	0.9 (8)
O3—Fe1—N4—N5	−24.5 (6)	C13—C14—C15—C16	−178.2 (5)
O3—Fe1—N4—C29	169.7 (4)	C14—C15—C16—C7	−1.7 (8)
N4—Fe1—O3—C30	32.5 (5)	C14—C15—C16—C17	176.4 (5)
O4—Fe1—N1—N2	−171.6 (4)	C7—C16—C17—O6	169.3 (5)
O4—Fe1—N1—C6	5.6 (3)	C7—C16—C17—N3	−9.5 (7)
N1—Fe1—O4—C1	−7.3 (3)	C15—C16—C17—O6	−8.7 (7)
O4—Fe1—N4—N5	71.0 (6)	C15—C16—C17—N3	172.5 (4)
O4—Fe1—N4—C29	−94.8 (4)	N3—C18—C19—C20	179.7 (5)
N4—Fe1—O4—C1	170.7 (3)	N3—C18—C23—C22	178.8 (5)
N1—Fe1—N4—N5	79.3 (10)	C19—C18—C23—C22	−1.7 (8)
N1—Fe1—N4—C29	−86.5 (7)	C23—C18—C19—C20	0.2 (7)
N4—Fe1—N1—N2	179.9 (5)	C18—C19—C20—C21	1.1 (9)
N4—Fe1—N1—C6	−2.9 (9)	C19—C20—C21—C22	−1.0 (9)
$O5^{i}$—Na1—O6—C17	−15.9 (6)	C20—C21—C22—C23	−0.4 (8)
O6—Na1—$O5^{i}$—$C40^{i}$	−161.4 (11)	C21—C22—C23—C18	1.8 (8)
O7—Na1—$O5^{i}$—$C40^{i}$	−68.7 (12)	O2—C24—C25—C26	178.6 (6)
O8—Na1—$O5^{i}$—$C40^{i}$	94.0 (12)	O2—C24—C29—N4	−2.4 (9)
N7—Na1—$O5^{i}$—$C40^{i}$	−15.1 (14)	O2—C24—C29—C28	−179.6 (6)
O7—Na1—O6—C17	−104.7 (6)	C25—C24—C29—N4	177.1 (6)
O8—Na1—O6—C17	94.3 (6)	C25—C24—C29—C28	−0.0 (9)
N7—Na1—O6—C17	−178.7 (6)	C29—C24—C25—C26	−1.0 (10)
Fe1—O1—C7—C8	5.8 (8)	C24—C25—C26—C27	1.3 (10)
Fe1—O1—C7—C16	−172.5 (3)	C25—C26—C27—Cl2	179.2 (5)
Fe1—O2—C24—C25	−174.4 (5)	C25—C26—C27—C28	−0.7 (10)
Fe1—O2—C24—C29	5.1 (8)	Cl2—C27—C28—C29	179.9 (4)
Fe1—O3—C30—C31	−29.3 (10)	C26—C27—C28—C29	−0.3 (8)
Fe1—O3—C30—C39	151.0 (5)	C27—C28—C29—N4	−176.1 (6)
Fe1—O4—C1—C2	−173.9 (4)	C27—C28—C29—C24	0.6 (10)
Fe1—O4—C1—C6	8.1 (6)	O3—C30—C31—N5	0.9 (12)
$Na1^{i}$—O5—C40—N6	−117.5 (11)	O3—C30—C31—C32	−179.8 (6)
$Na1^{i}$—O5—C40—C39	65.3 (14)	O3—C30—C39—C38	−176.9 (6)
Na1—O6—C17—N3	128.1 (5)	O3—C30—C39—C40	2.4 (10)
Na1—O6—C17—C16	−50.6 (8)	C31—C30—C39—C38	3.4 (10)
Fe1—N1—N2—C8	−1.7 (7)	C31—C30—C39—C40	−177.3 (7)

Fe1—N1—C6—C1	−3.2 (5)	C39—C30—C31—N5	−179.4 (6)
Fe1—N1—C6—C5	175.3 (4)	C39—C30—C31—C32	−0.0 (9)
N2—N1—C6—C1	174.6 (4)	N5—C31—C32—C33	−2.4 (10)
N2—N1—C6—C5	−7.0 (7)	N5—C31—C32—C37	176.3 (6)
C6—N1—N2—C8	−178.9 (4)	C30—C31—C32—C33	178.2 (7)
N1—N2—C8—C7	−2.0 (7)	C30—C31—C32—C37	−3.1 (10)
N1—N2—C8—C9	177.9 (4)	C31—C32—C33—C34	177.1 (7)
C17—N3—C18—C19	13.2 (8)	C31—C32—C37—C36	−177.0 (6)
C17—N3—C18—C23	−167.3 (5)	C31—C32—C37—C38	2.9 (10)
C18—N3—C17—O6	−2.3 (8)	C33—C32—C37—C36	1.7 (10)
C18—N3—C17—C16	176.5 (4)	C33—C32—C37—C38	−178.3 (7)
Fe1—N4—N5—C31	10.9 (9)	C37—C32—C33—C34	−1.6 (11)
Fe1—N4—C29—C24	−0.9 (7)	C32—C33—C34—C35	−0.3 (9)
Fe1—N4—C29—C28	176.0 (5)	C33—C34—C35—C36	1.9 (12)
N5—N4—C29—C24	−169.4 (5)	C34—C35—C36—C37	−1.7 (12)
N5—N4—C29—C28	7.6 (10)	C35—C36—C37—C32	−0.0 (10)
C29—N4—N5—C31	176.2 (6)	C35—C36—C37—C38	180.0 (7)
N4—N5—C31—C30	7.2 (11)	C32—C37—C38—C39	0.4 (11)
N4—N5—C31—C32	−172.2 (6)	C36—C37—C38—C39	−179.6 (7)
C40—N6—C41—C42	−2.0 (12)	C37—C38—C39—C30	−3.7 (11)
C40—N6—C41—C46	177.4 (7)	C37—C38—C39—C40	177.0 (7)
C41—N6—C40—O5	−2.7 (12)	C30—C39—C40—O5	−165.1 (7)
C41—N6—C40—C39	174.5 (6)	C30—C39—C40—N6	17.5 (11)
O4—C1—C2—C3	−178.3 (5)	C38—C39—C40—O5	14.1 (11)
O4—C1—C6—N1	−2.8 (7)	C38—C39—C40—N6	−163.2 (7)
O4—C1—C6—C5	178.7 (5)	N6—C41—C42—C43	179.6 (7)
C2—C1—C6—N1	179.0 (4)	N6—C41—C46—C45	−179.3 (6)
C2—C1—C6—C5	0.5 (8)	C42—C41—C46—C45	0.1 (8)
C6—C1—C2—C3	−0.2 (6)	C46—C41—C42—C43	0.2 (8)
C1—C2—C3—C4	1.1 (8)	C41—C42—C43—C44	−0.4 (10)
C2—C3—C4—Cl1	177.8 (4)	C42—C43—C44—C45	0.3 (9)
C2—C3—C4—C5	−2.4 (8)	C43—C44—C45—C46	0.1 (10)
Cl1—C4—C5—C6	−177.5 (4)	C44—C45—C46—C41	−0.3 (9)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O1	0.86	1.94	2.644 (7)	138
N6—H6N···O3	0.86	1.97	2.664 (6)	138
O8—H···O9	.	.	2.730 (7)	.
O9—H···O4^{iii}	.	.	2.710 (6)	.

Symmetry codes: (iii) *x*, *y*−1, *z*.

Fig. 1

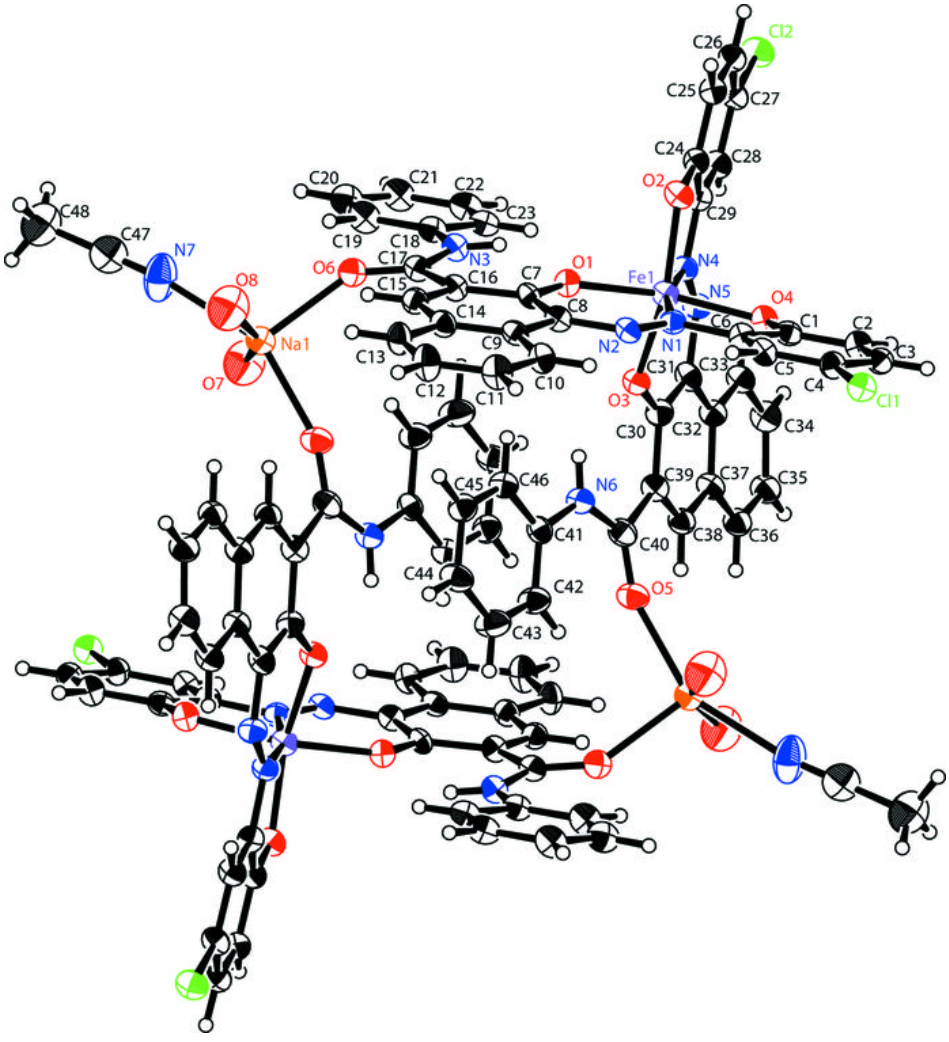

Cl2
C26
C25
C27
C24
C28
O2
C29
C20
C21
C22
C23
C48
C47
N7
C19
C18
N3
O8
O6
C17
C16
C7
O1
Fe1
N4
C15
C14
C8
N5
O4
Na1
C9
N2
N1
C6
C1
C2
C3
C13
C31
C33
C5
C4
Cl1
O7
C12
C11
C10
O3
C30
C32
C34
C45
C46
N6
C39
C37
C35
C41
C40
C38
C36
C44
C42
O5
C43

Fig. 2

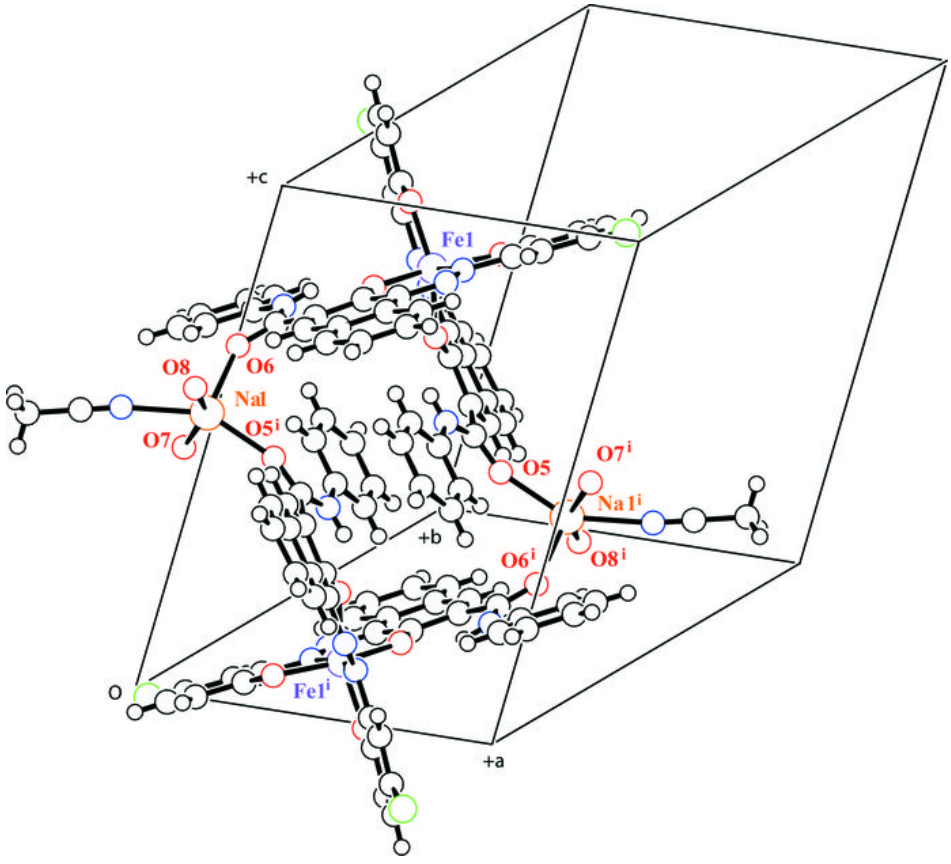
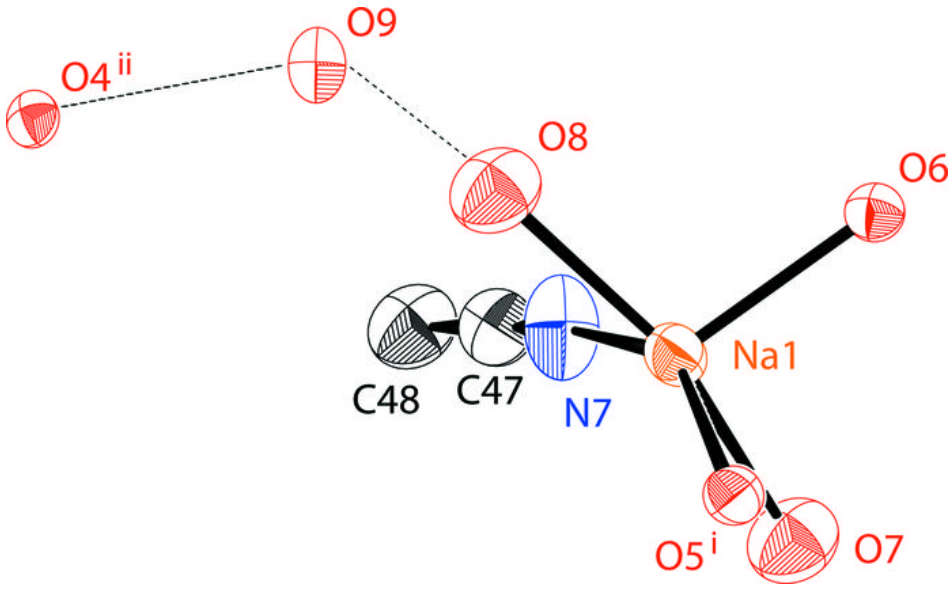


Fig. 3



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Diacetonitriletetrakis{μ_2-3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholato}tetraaquadiiron(III)disodium(I) dihydrate. Corrigendum

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Corrections are made to the names of the first two authors in Yohei, Kazuya & Mizuguchi [*Acta Cryst.* (2008), E**64**, m240–m241].

In the paper by Yohei, Kazuya & Mizuguchi [*Acta Cryst.* (2008), E**64**, m240–m241], the names of the first two authors are given incorrectly. The correct names should be Yohei Sato and Kazuya Uta, as given above.