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Diethanolaminium *cyclo*-octa-μ_2-fluoro-hexadeca-μ_2-trimethylacetato-$\kappa^{32}O{:}O'$-heptachromium(III)nickel(II) ethyl acetate 0.5-solvate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.007 Å
Some non-H atoms missing
Disorder in main residue
R factor = 0.089
wR factor = 0.255
Data-to-parameter ratio = 35.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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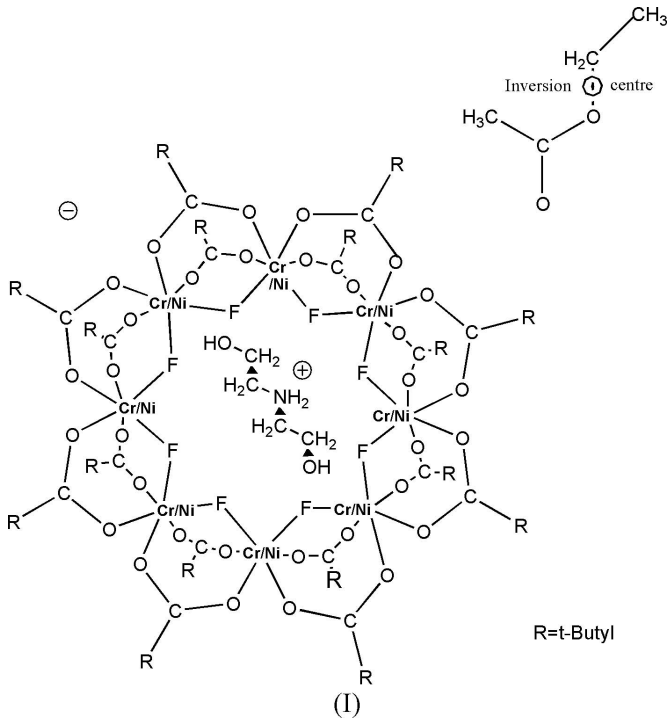
The title compound, $[N(C_2H_4OH)_2H_2][Cr_7NiF_8(C_5H_9O_2)_{16}]\cdot 0.5C_4H_8O_2$, is a heterometallic wheel templated by a protonated amino alcohol. It consists of an octagon of metal centres, with each edge of the octagon bridged by a single F^- anion and two carboxylate groups. Each metal atom is octahedrally coordinated. The protonated amine molecule protrudes through the cavity of the ring, while a solvent ethyl acetate molecule fills up the vacant space between the ring anions. It appears that the one equivalent of Ni atoms is unevenly distributed among the eight metal sites.

Comment

Our recent report (Larsen, McInnes *et al.*, 2003) of a series of octanuclear $\{Cr_7M\}$ heterometallic wheel-type complexes with the general formula $[NR_2H_2][Cr_7MF_8(O_2CCMe_3)_{16}]$ was the first report of anti-ferromagnetically coupled cyclic molecules that have a non-diamagnetic ground state. There has been considerable interest in such molecules for applications as diverse as olefin polymerization catalysis (Lassahn *et al.*, 2004), magnetic cooling (Affronte *et al.*, 2004) and quantum computing (Meier *et al.*, 2003). They were synthesized using a secondary ammonium cation, $[NR_2H_2]^+$, which is a protonated alkyl-chain secondary amine with $R = CH_3(CH_2)_n$ (*e.g.* n = 0–7). It acts as a template in the reaction of $CrF_3\cdot 4H_2O$ with pivalic acid in the presence of a second divalent metal cation (M^{2+} = Ni, Co, Mn, Fe, Zn or Cd). This procedure gives $\{Cr_7M\}$ ring compounds in good yield (Larsen, Overgaard *et al.*, 2003; Larsen, McInnes *et al.*, 2003). In each case, the amines are found to be hydrogen-bonded at the centre of the metal ring. The protonated N atoms are not involved in the packing of the molecules in the crystal structure, because they are accommodated completely in the cavity (void) of the wheels. However, it was found that the choice of R can influence the packing of the rings in the crystal structure, regardless of the solvent used for crystallization. For example, both short and very long alkyl chains lead to packing where the octanuclear wheels are coplanar (generally tetragonal or orthorhombic crystals), but for intermediate chain lengths (Et or ^{n}Pr), monoclinic crystals are found, where the rings pack with an angle of *ca* 50° between the mean planes of neighbouring rings (Larsen, Overgaard *et al.*, 2003).

The purpose of this paper is to extend further our studies of heterometallic wheels, by the preparation and structural characterization of the new title complex, $[N(CH_2CH_2OH)_2H_2][Cr_7NiF_8(O_2CCMe_3)_{16}][C_4H_8O_2]_{0.5}$, (I). Using a protonated secondary amino alcohol as a template, we wished to investigate the influence of the alcohol group on the accommodation of the amine group in the void of the wheel, and also how the –OH group might influence the packing of

the anionic rings in the crystal structure. A further goal was to obtain a complex for the synthesis of further polymetallic cage complexes, using the two OH groups of the diethanolamine to bind to further metal centres.



(I)

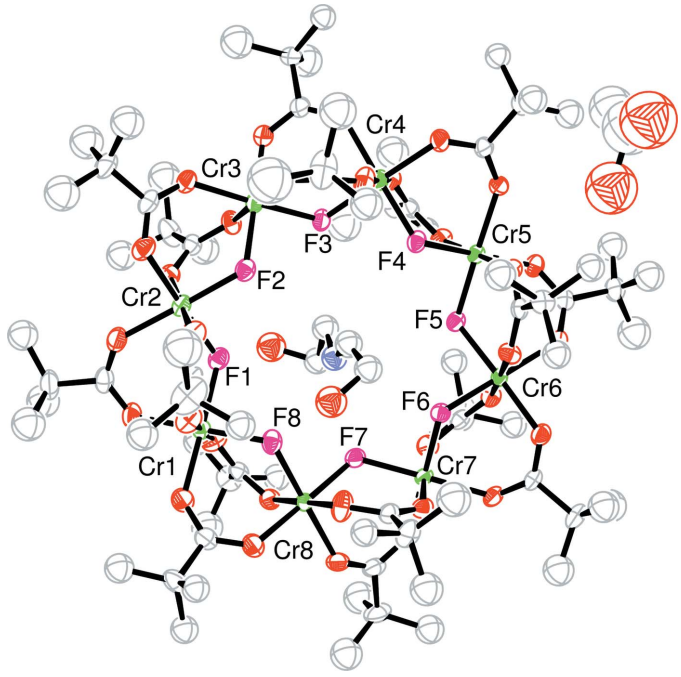


Figure 1
A view of (I), showing 50% displacement ellipsoids, with selected atoms labelled. Only one orientation is shown for the disorder components. Colour key: Cr/Ni green, F pink, O red, C grey, N blue. H atoms have been omitted.

For five of the 16 bridging pivalate groups in (I), two possible positions were located and refined for the *tert*-butyl methyl groups. The occupation factors for the major component of these five disordered pivalate groups, of which two are on either face, while one is on the edge of the circular ring molecule, are in the range 0.521 (10)–0.592 (9). For all pivalate groups, a restraint was imposed in order to maintain tetrahedral coordination of the CMe_3 groups, and a common C—C bond length was restrained to 1.521 (1) Å.

Compound (I) was crystallized from an ethyl acetate solution and a molecule of ethyl acetate is incorporated in the crystal structure. It is situated near a centre of symmetry and is disordered over two positions, with two of the atom positions coinciding. The protonated ethanolamine molecule appears to be disordered over three orientations in the void of the octagonal ring, with one major [0.444 (5)] and two minor [0.251 (5) and 0.302 (5)] orientations. The amine N atom of the main component sits significantly closer to one side of the ring than the other. The N···F distances vary systematically around the ring: N1···F1 = 3.104 (3), N1···F2 = 3.408 (3), N1···F3 = 3.730 (3), N1···F4 = 3.829 (3), N1···F5 = 3.557 (3), N1···F6 = 3.215 (3), N1···F7 = 2.878 (3) and N1···F8 = 2.855 (3) Å.

In the final cycles of refinement, all Cr/Ni atoms were refined using Cr scattering factors. The metal atoms on the side of the ring with the shorter N···F separations tend to have smaller values for their equivalent isotropic displacement parameters: U_{eq}(Cr1) = 0.0238 (1), U_{eq}(Cr2) = 0.0281 (1), U_{eq}(Cr3) = 0.0286 (1), U_{eq}(Cr4) = 0.0308 (1), U_{eq}(Cr5) = 0.0234 (1), U_{eq}(Cr6) = 0.0222 (1), U_{eq}(Cr7) = 0.0238 (1) and U_{eq}(Cr8) = 0.0257 (1) Å^2. Since Ni has four more electrons than Cr, it is conceivable that the Cr atoms with lower U_{eq} values may have greater Ni occupancy, so there is an indication of an uneven distribution of Ni around the ring.

The O atoms of the ethanolamine molecule are found to have short distances to the same F atoms which are involved in the shortest N···F separation [O2*A*···F1 = 2.952 (3) and O2*B*···F8 = 2.933 (3) Å]. The minor disorder components of the ethanolammonium cation show short N···F distances to other F atoms than found for the major component and of similar lengths: N1*C*···F1 = 2.721 (3), N1*C*···F2 = 2.922 (3) and N1*C*···F8 = 2.939 (3) Å, and N1*E*···F6 = 2.837 (3), N1*E*···F7 = 2.940 (3) and N1*E*···F5 = 3.084 (3) Å.

Experimental

Compound (I) was synthesized in approximately 65% yield in a similar way to the analogues reported earlier (Larsen, Overgaard *et al.*, 2003), except that the amine used was diethanolamine and the product was crystallized from ethyl acetate. Elemental analysis (dried sample), calculated for $C_{84}H_{156}Cr_7F_8N_1Ni_1O_{34}$: Cr 15.83, Ni 2.55, C 43.89, H 6.84, N 0.61%; found: Cr 15.28, Ni 2.72, C 43.89, H 7.00, N 0.62%. ES–MS (2 THF/MeOH *m*/*z*): −2191 [$Cr_7NiF_8(O_2CCMe_3)_{16}$], 2298 [$M^-$], 2321 [$M$+Na]$^+$.

Crystal data

$(C_4H_{12}NO_2)[Cr_7NiF_8(C_5H_9O_2)_{16}]\cdot 0.5C_4H_8O_2$	$D_x = 1.294$ Mg m^{-3}
$M_r = 2342.85$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 9946 reflections
$a = 24.9892$ (15) Å	$\theta = 2.2$–31.0°
$b = 16.6220$ (9) Å	$\mu = 0.78$ mm^{-1}
$c = 30.8299$ (19) Å	$T = 100$ (2) K
$\beta = 110.506$ (3)°	Block, green
$V = 11994.4$ (12) Å^3	0.38 × 0.3 × 0.25 mm
$Z = 4$	

Data collection

Bruker X8 APEX-II diffractometer	28754 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 31.1^\circ$
$T_{min} = 0.723$, $T_{max} = 0.823$	$h = -36 \rightarrow 35$
209153 measured reflections	$k = -23 \rightarrow 24$
38517 independent reflections	$l = -44 \rightarrow 44$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1134P)^2 + 52.1149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.091$	$(\Delta/\sigma)_{max} = 0.006$
$wR(F^2) = 0.258$	$\Delta\rho_{max} = 2.10$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -1.17$ e Å^{-3}
38517 reflections	
1066 parameters	
H-atom parameters constrained	

Methyl H atoms were located in idealized positions, with C—H = 0.98 Å, and refined as riding, with the constraint $U_{iso}(H) = 1.5U_{iso}(C)$. N-bound H atoms were located in idealized positions, with N—H = 0.92 Å, and refined as riding, with the constraint $U_{iso}(H) = 1.2U_{iso}(N)$. The highest difference peak is 0.39 Å from H20*C* and the deepest difference hole is 0.51 Å from C28.

Data collection: *APEX-II* (Bruker–Nonius, 2004); cell refinement: *SAINT-Plus* (Bruker–Nonius, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *enCIFer* (Version 1.1; Allen *et al.*, 2004) and *WinGX* (Version 1.70.00; Farrugia, 1999).

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supporting information

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$V = 11994.4\ (12)$ Å^3
$Z = 4$
$F(000) = 4908$
$D_x = 1.294$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9946 reflections
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Block, green
0.38 × 0.3 × 0.25 mm

Data collection

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Radiation source: fine-focus sealed tube
Graphite monochromator
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Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.723$, $T_{max} = 0.823$
209153 measured reflections
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$\theta_{max} = 31.1°$, $\theta_{min} = 2.5°$
$h = -36\rightarrow35$
$k = -23\rightarrow24$
$l = -44\rightarrow44$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.091$
$wR(F^2) = 0.258$
$S = 1.04$
38517 reflections
1066 parameters
141 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
$w = 1/[\sigma^2(F_o^2) + (0.1134P)^2 + 52.1149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 2.10$ e Å^{-3}
$\Delta\rho_{min} = -1.17$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cr1	0.24845 (2)	0.30732 (3)	0.53149 (2)	0.02378 (12)	
Cr2	0.17266 (3)	0.23451 (4)	0.59513 (2)	0.02810 (13)	
Cr3	0.12131 (3)	0.31986 (4)	0.67277 (2)	0.02856 (13)	
Cr4	0.15764 (3)	0.48148 (4)	0.74459 (2)	0.03080 (14)	
Cr5	0.22740 (2)	0.65434 (3)	0.740880 (19)	0.02338 (12)	
Cr6	0.32644 (2)	0.70831 (3)	0.694543 (19)	0.02222 (11)	
Cr7	0.35228 (2)	0.64380 (4)	0.599364 (19)	0.02382 (12)	
Cr8	0.33790 (2)	0.46585 (4)	0.543084 (19)	0.02571 (12)	
F1	0.19865 (10)	0.32329 (14)	0.56776 (9)	0.0325 (5)	
F2	0.18121 (10)	0.30385 (14)	0.64808 (8)	0.0319 (5)	
F3	0.14510 (10)	0.43013 (13)	0.68579 (8)	0.0302 (5)	
F4	0.21990 (10)	0.53930 (14)	0.73597 (8)	0.0303 (5)	
F5	0.25624 (9)	0.65394 (13)	0.69092 (7)	0.0270 (4)	
F6	0.33767 (10)	0.62235 (13)	0.65650 (7)	0.0283 (4)	
F7	0.30798 (10)	0.54933 (16)	0.57288 (8)	0.0333 (5)	
F8	0.29877 (11)	0.38951 (15)	0.56946 (8)	0.0346 (5)	
O11	0.19584 (14)	0.2266 (2)	0.49306 (11)	0.0409 (7)	
O12	0.16241 (13)	0.16393 (19)	0.54221 (12)	0.0398 (7)	
O13	0.29402 (13)	0.22558 (19)	0.57568 (12)	0.0398 (7)	
O14	0.25123 (14)	0.1987 (2)	0.62736 (12)	0.0426 (7)	
O21	0.14561 (14)	0.14517 (18)	0.62421 (12)	0.0391 (7)	
O22	0.09468 (14)	0.20917 (18)	0.66065 (11)	0.0374 (6)	
O23	0.09225 (12)	0.26815 (18)	0.56420 (10)	0.0323 (6)	
O24	0.06884 (12)	0.35197 (18)	0.61191 (10)	0.0338 (6)	
O31	0.05925 (14)	0.3370 (2)	0.69615 (11)	0.0390 (7)	
O32	0.09342 (15)	0.4260 (2)	0.75357 (11)	0.0423 (8)	
O33	0.17371 (15)	0.28622 (19)	0.73370 (10)	0.0411 (7)	
O34	0.21066 (16)	0.3958 (2)	0.77585 (11)	0.0438 (8)	
O41	0.17130 (15)	0.5347 (2)	0.80388 (10)	0.0419 (7)	
O42	0.19833 (12)	0.65794 (17)	0.79206 (9)	0.0291 (5)	
O43	0.10292 (12)	0.56438 (18)	0.71131 (10)	0.0338 (6)	
O44	0.15052 (12)	0.66674 (19)	0.69496 (10)	0.0329 (6)	
O51	0.23345 (12)	0.77042 (16)	0.74569 (10)	0.0304 (5)	
O52	0.31486 (12)	0.79640 (16)	0.73316 (10)	0.0303 (5)	
O53	0.30420 (11)	0.64100 (16)	0.78710 (9)	0.0261 (5)	

O54	0.36780 (12)	0.64591 (18)	0.75064 (9)	0.0303 (5)	
O61	0.39856 (12)	0.75736 (18)	0.69798 (10)	0.0329 (6)	
O62	0.39842 (12)	0.73888 (18)	0.62611 (10)	0.0315 (6)	
O63	0.28298 (12)	0.77293 (16)	0.64041 (9)	0.0294 (5)	
O64	0.28194 (12)	0.70839 (19)	0.57637 (10)	0.0343 (6)	
O71	0.36455 (14)	0.6663 (2)	0.54189 (10)	0.0378 (7)	
O72	0.37709 (13)	0.5440 (2)	0.51640 (10)	0.0391 (7)	
O73	0.42339 (11)	0.58215 (19)	0.62410 (10)	0.0320 (6)	
O74	0.40570 (14)	0.4546 (2)	0.60022 (12)	0.0456 (8)	
O81	0.36965 (12)	0.3782 (2)	0.51689 (12)	0.0408 (7)	
O82	0.29876 (13)	0.2873 (2)	0.49591 (12)	0.0403 (7)	
O83	0.27102 (12)	0.47890 (19)	0.48589 (9)	0.0333 (6)	
O84	0.20475 (12)	0.3890 (2)	0.48759 (11)	0.0394 (7)	
C11	0.16754 (17)	0.1735 (3)	0.50323 (16)	0.0357 (9)	
C12	0.1376 (2)	0.1122 (3)	0.46613 (18)	0.0533 (13)	
C13	0.1004 (4)	0.0577 (6)	0.4835 (4)	0.066 (3)*	0.521 (10)
H13A	0.0655	0.0864	0.4819	0.098*	0.521 (10)
H13B	0.1215	0.0421	0.5156	0.098*	0.521 (10)
H13C	0.0902	0.0093	0.4641	0.098*	0.521 (10)
C14	0.1866 (4)	0.0632 (7)	0.4613 (4)	0.081 (4)*	0.521 (10)
H14A	0.1712	0.0178	0.4403	0.121*	0.521 (10)
H14B	0.2106	0.0429	0.4918	0.121*	0.521 (10)
H14C	0.2096	0.0973	0.4487	0.121*	0.521 (10)
C15	0.1026 (4)	0.1490 (7)	0.4203 (3)	0.082 (4)*	0.521 (10)
H15A	0.0847	0.1062	0.3981	0.123*	0.521 (10)
H15B	0.1275	0.1812	0.4086	0.123*	0.521 (10)
H15C	0.0730	0.1835	0.4244	0.123*	0.521 (10)
C13B	0.0739 (3)	0.1290 (9)	0.4534 (6)	0.123 (8)*	0.479 (10)
H13D	0.0662	0.1857	0.4446	0.185*	0.479 (10)
H13E	0.0624	0.1174	0.4800	0.185*	0.479 (10)
H13F	0.0522	0.0948	0.4272	0.185*	0.479 (10)
C14B	0.1492 (6)	0.0242 (4)	0.4788 (5)	0.072 (4)*	0.479 (10)
H14D	0.1236	0.0056	0.4946	0.107*	0.479 (10)
H14E	0.1889	0.0176	0.4995	0.107*	0.479 (10)
H14F	0.1426	−0.0076	0.4507	0.107*	0.479 (10)
C15B	0.1543 (7)	0.1304 (9)	0.4240 (4)	0.102 (7)*	0.479 (10)
H15D	0.1312	0.0975	0.3977	0.153*	0.479 (10)
H15E	0.1948	0.1180	0.4312	0.153*	0.479 (10)
H15F	0.1476	0.1875	0.4160	0.153*	0.479 (10)
C16	0.29254 (17)	0.1951 (2)	0.61281 (18)	0.0394 (10)	
C17	0.3461 (2)	0.1472 (3)	0.6404 (2)	0.0670 (19)	
C18	0.3603 (5)	0.0895 (5)	0.6071 (3)	0.063 (3)*	0.551 (11)
H18A	0.3966	0.0623	0.6235	0.095*	0.551 (11)
H18B	0.3637	0.1200	0.5810	0.095*	0.551 (11)
H18C	0.3298	0.0495	0.5956	0.095*	0.551 (11)
C19	0.3948 (4)	0.2080 (5)	0.6578 (3)	0.054 (3)*	0.551 (11)
H19A	0.3881	0.2431	0.6810	0.081*	0.551 (11)
H19B	0.3964	0.2405	0.6318	0.081*	0.551 (11)

H19C	0.4310	0.1793	0.6719	0.081*	0.551 (11)
C20	0.3410 (6)	0.1000 (6)	0.6806 (3)	0.096 (5)*	0.551 (11)
H20A	0.3711	0.0589	0.6902	0.144*	0.551 (11)
H20B	0.3035	0.0739	0.6712	0.144*	0.551 (11)
H20C	0.3452	0.1364	0.7066	0.144*	0.551 (11)
C18A	0.3264 (8)	0.0605 (5)	0.6293 (6)	0.103 (7)*	0.449 (11)
H18D	0.3052	0.0553	0.5960	0.154*	0.449 (11)
H18E	0.3016	0.0456	0.6465	0.154*	0.449 (11)
H18F	0.3598	0.0249	0.6382	0.154*	0.449 (11)
C19A	0.4044 (5)	0.1580 (13)	0.6362 (7)	0.167 (14)*	0.449 (11)
H19D	0.4198	0.2108	0.6484	0.250*	0.449 (11)
H19E	0.4007	0.1544	0.6035	0.250*	0.449 (11)
H19F	0.4302	0.1157	0.6538	0.250*	0.449 (11)
C20A	0.3507 (8)	0.1652 (11)	0.6903 (3)	0.093 (6)*	0.449 (11)
H20D	0.3575	0.2228	0.6965	0.139*	0.449 (11)
H20E	0.3824	0.1344	0.7117	0.139*	0.449 (11)
H20F	0.3149	0.1499	0.6945	0.139*	0.449 (11)
C21	0.11039 (19)	0.1471 (2)	0.64461 (16)	0.0366 (9)	
C22	0.08358 (19)	0.0693 (2)	0.65217 (16)	0.0528 (13)	
C23	0.0950 (3)	0.0584 (4)	0.70373 (15)	0.0746 (19)*	
H23A	0.0792	0.1041	0.7152	0.112*	
H23B	0.1363	0.0554	0.7205	0.112*	
H23C	0.0770	0.0085	0.7086	0.112*	
C24	0.1076 (3)	−0.0021 (4)	0.6344 (2)	0.085 (2)*	
H24A	0.0963	−0.0520	0.6457	0.128*	
H24B	0.1494	0.0016	0.6454	0.128*	
H24C	0.0926	−0.0020	0.6004	0.128*	
C25	0.0197 (2)	0.0756 (5)	0.6265 (2)	0.080 (2)*	
H25A	0.0051	0.1244	0.6364	0.121*	
H25B	0.0007	0.0284	0.6334	0.121*	
H25C	0.0121	0.0783	0.5931	0.121*	
C26	0.05805 (16)	0.3135 (2)	0.57419 (13)	0.0296 (7)	
C27	−0.00216 (17)	0.3226 (3)	0.53950 (13)	0.0487 (12)	
C28	−0.0131 (3)	0.2666 (3)	0.49829 (19)	0.0694 (17)*	
H28A	−0.0519	0.2751	0.4763	0.104*	
H28B	−0.0088	0.2107	0.5090	0.104*	
H28C	0.0145	0.2780	0.4830	0.104*	
C29	−0.0442 (3)	0.3027 (4)	0.5638 (2)	0.084 (2)*	
H29A	−0.0414	0.3435	0.5874	0.125*	
H29B	−0.0350	0.2498	0.5785	0.125*	
H29C	−0.0831	0.3020	0.5411	0.125*	
C30	−0.0104 (3)	0.4092 (3)	0.5231 (2)	0.0745 (19)*	
H30A	−0.0066	0.4447	0.5494	0.112*	
H30B	−0.0485	0.4157	0.4996	0.112*	
H30C	0.0187	0.4233	0.5098	0.112*	
C31	0.0558 (2)	0.3782 (3)	0.72922 (15)	0.0388 (9)	
C32	0.00116 (18)	0.3710 (2)	0.73978 (12)	0.0472 (12)	
C33	−0.0287 (3)	0.2920 (3)	0.7217 (2)	0.081 (2)*	

H33A	−0.0427	0.2923	0.6878	0.122*
H33B	−0.0611	0.2853	0.7324	0.122*
H33C	−0.0018	0.2474	0.7333	0.122*
C34	0.0144 (2)	0.3773 (3)	0.79158 (12)	0.0459 (10)*
H34A	0.0385	0.3320	0.8072	0.069*
H34B	−0.0214	0.3762	0.7980	0.069*
H34C	0.0345	0.4279	0.8030	0.069*
C35	−0.0368 (3)	0.4407 (3)	0.71530 (19)	0.080 (2)*
H35A	−0.0202	0.4913	0.7303	0.120*
H35B	−0.0749	0.4338	0.7171	0.120*
H35C	−0.0397	0.4418	0.6828	0.120*
C36	0.2088 (2)	0.3221 (3)	0.76840 (15)	0.0424 (10)
C37	0.2507 (2)	0.2700 (3)	0.80539 (16)	0.0646 (18)
C38	0.2276 (3)	0.2657 (5)	0.8450 (3)	0.088 (2)*
H38A	0.2547	0.2362	0.8710	0.132*
H38B	0.1908	0.2377	0.8345	0.132*
H38C	0.2226	0.3202	0.8549	0.132*
C39	0.2554 (4)	0.1856 (4)	0.7884 (4)	0.135 (4)*
H39A	0.2670	0.1884	0.7612	0.202*
H39B	0.2183	0.1586	0.7800	0.202*
H39C	0.2840	0.1552	0.8130	0.202*
C40	0.3091 (2)	0.3099 (4)	0.8224 (2)	0.0664 (16)*
H40A	0.3214	0.3200	0.7960	0.100*
H40B	0.3366	0.2743	0.8445	0.100*
H40C	0.3068	0.3609	0.8375	0.100*
C41	0.18395 (18)	0.6070 (3)	0.81547 (13)	0.0323 (8)
C42	0.18162 (15)	0.6330 (2)	0.86237 (12)	0.0397 (9)
C43	0.12469 (15)	0.6078 (3)	0.86543 (17)	0.0459 (11)*
H43A	0.0938	0.6379	0.8426	0.069*
H43B	0.1245	0.6192	0.8966	0.069*
H43C	0.1189	0.5501	0.8591	0.069*
C44	0.1890 (2)	0.7234 (2)	0.8690 (2)	0.0592 (14)*
H44A	0.2236	0.7403	0.8635	0.089*
H44B	0.1924	0.7373	0.9008	0.089*
H44C	0.1558	0.7508	0.8471	0.089*
C45	0.23001 (17)	0.5899 (3)	0.89922 (18)	0.0558 (13)*
H45A	0.2284	0.5323	0.8921	0.084*
H45B	0.2263	0.5978	0.9295	0.084*
H45C	0.2667	0.6118	0.8998	0.084*
C46	0.10582 (16)	0.6268 (2)	0.68924 (13)	0.0291 (7)
C47	0.05108 (16)	0.6549 (2)	0.65207 (14)	0.0436 (11)
C48	0.0570 (3)	0.7396 (3)	0.6360 (2)	0.0589 (14)*
H48A	0.0650	0.7769	0.6621	0.088*
H48B	0.0214	0.7554	0.6115	0.088*
H48C	0.0885	0.7413	0.6239	0.088*
C49	0.0383 (4)	0.5965 (3)	0.6120 (2)	0.092 (3)*
H49A	0.0696	0.5975	0.5998	0.138*
H49B	0.0026	0.6122	0.5875	0.138*

H49C	0.0343	0.5421	0.6227	0.138*	
C50	0.0030 (3)	0.6527 (4)	0.6716 (3)	0.084 (2)*	
H50A	−0.0043	0.5969	0.6781	0.126*	
H50B	−0.0317	0.6757	0.6489	0.126*	
H50C	0.0140	0.6841	0.7003	0.126*	
C51	0.27450 (16)	0.8159 (2)	0.74661 (12)	0.0271 (7)	
C52	0.27662 (17)	0.8975 (2)	0.76893 (14)	0.0427 (10)	
C53	0.3191 (2)	0.8888 (4)	0.81820 (16)	0.0676 (17)*	
H53A	0.3553	0.8676	0.8173	0.101*	
H53B	0.3037	0.8517	0.8356	0.101*	
H53C	0.3257	0.9415	0.8334	0.101*	
C54	0.21884 (17)	0.9206 (4)	0.7710 (2)	0.0650 (16)*	
H54A	0.2211	0.9745	0.7844	0.097*	
H54B	0.2078	0.8817	0.7903	0.097*	
H54C	0.1903	0.9204	0.7396	0.097*	
C55	0.2975 (3)	0.9608 (4)	0.7434 (2)	0.085 (2)*	
H55A	0.2701	0.9662	0.7118	0.127*	
H55B	0.3347	0.9447	0.7423	0.127*	
H55C	0.3012	1.0124	0.7596	0.127*	
C56	0.35379 (15)	0.6328 (2)	0.78561 (12)	0.0253 (6)	
C57	0.40057 (15)	0.6057 (2)	0.82961 (12)	0.0334 (8)	
C58	0.4001 (3)	0.6561 (4)	0.8703 (2)	0.052 (2)*	0.592 (9)
H58A	0.4278	0.6343	0.8989	0.078*	0.592 (9)
H58B	0.3618	0.6550	0.8723	0.078*	0.592 (9)
H58C	0.4104	0.7117	0.8661	0.078*	0.592 (9)
C59	0.4593 (2)	0.6095 (5)	0.8252 (3)	0.052 (2)*	0.592 (9)
H59A	0.4876	0.5849	0.8525	0.078*	0.592 (9)
H59B	0.4696	0.6657	0.8228	0.078*	0.592 (9)
H59C	0.4585	0.5802	0.7974	0.078*	0.592 (9)
C60	0.3871 (4)	0.5184 (3)	0.8372 (3)	0.063 (3)*	0.592 (9)
H60A	0.3873	0.4858	0.8107	0.094*	0.592 (9)
H60B	0.3493	0.5154	0.8400	0.094*	0.592 (9)
H60C	0.4160	0.4979	0.8656	0.094*	0.592 (9)
C58B	0.4311 (6)	0.6858 (5)	0.8455 (5)	0.072 (5)*	0.408 (9)
H58D	0.4591	0.6799	0.8769	0.108*	0.408 (9)
H58E	0.4030	0.7270	0.8455	0.108*	0.408 (9)
H58F	0.4507	0.7019	0.8244	0.108*	0.408 (9)
C59B	0.4424 (5)	0.5456 (6)	0.8226 (5)	0.074 (5)*	0.408 (9)
H59D	0.4733	0.5359	0.8521	0.111*	0.408 (9)
H59E	0.4584	0.5671	0.8001	0.111*	0.408 (9)
H59F	0.4226	0.4949	0.8109	0.111*	0.408 (9)
C60B	0.3781 (6)	0.5752 (7)	0.8665 (4)	0.066 (4)*	0.408 (9)
H60D	0.3580	0.5242	0.8564	0.099*	0.408 (9)
H60E	0.3517	0.6149	0.8713	0.099*	0.408 (9)
H60F	0.4102	0.5670	0.8956	0.099*	0.408 (9)
C61	0.41897 (16)	0.7671 (2)	0.66619 (14)	0.0285 (7)	
C62	0.47217 (16)	0.8189 (2)	0.67716 (14)	0.0426 (10)	
C63	0.5139 (3)	0.7983 (4)	0.72488 (15)	0.0676 (17)*	

H63A	0.5464	0.8354	0.7330	0.101*	
H63B	0.5276	0.7430	0.7249	0.101*	
H63C	0.4948	0.8031	0.7476	0.101*	
C64	0.5009 (3)	0.8091 (4)	0.64143 (18)	0.0706 (18)*	
H64A	0.4745	0.8262	0.6110	0.106*	
H64B	0.5111	0.7524	0.6400	0.106*	
H64C	0.5355	0.8422	0.6502	0.106*	
C65	0.4514 (3)	0.9049 (3)	0.6766 (2)	0.080 (2)*	
H65A	0.4251	0.9182	0.6454	0.121*	
H65B	0.4842	0.9416	0.6850	0.121*	
H65C	0.4317	0.9104	0.6988	0.121*	
C66	0.26545 (16)	0.7626 (2)	0.59714 (13)	0.0289 (7)	
C67	0.2201 (2)	0.8229 (3)	0.56924 (14)	0.0560 (15)	
C68	0.2415 (4)	0.9083 (4)	0.5823 (3)	0.059 (3)*	0.580 (13)
H68A	0.2117	0.9465	0.5651	0.088*	0.580 (13)
H68B	0.2758	0.9173	0.5745	0.088*	0.580 (13)
H68C	0.2506	0.9162	0.6156	0.088*	0.580 (13)
C69	0.2028 (3)	0.8110 (5)	0.51746 (17)	0.042 (2)*	0.580 (13)
H69A	0.1682	0.8421	0.5016	0.063*	0.580 (13)
H69B	0.1954	0.7538	0.5100	0.063*	0.580 (13)
H69C	0.2337	0.8294	0.5072	0.063*	0.580 (13)
C70	0.1679 (3)	0.8096 (5)	0.5835 (3)	0.055 (3)*	0.580 (13)
H70A	0.1771	0.8256	0.6159	0.082*	0.580 (13)
H70B	0.1573	0.7526	0.5800	0.082*	0.580 (13)
H70C	0.1359	0.8421	0.5638	0.082*	0.580 (13)
C68B	0.2670 (8)	0.8720 (14)	0.5607 (7)	0.143 (12)*	0.420 (13)
H68D	0.2541	0.8892	0.5283	0.215*	0.420 (13)
H68E	0.3015	0.8389	0.5675	0.215*	0.420 (13)
H68F	0.2757	0.9194	0.5809	0.215*	0.420 (13)
C69B	0.1840 (7)	0.8778 (14)	0.5872 (8)	0.179 (17)*	0.420 (13)
H69D	0.2059	0.9262	0.6007	0.269*	0.420 (13)
H69E	0.1734	0.8495	0.6108	0.269*	0.420 (13)
H69F	0.1494	0.8932	0.5615	0.269*	0.420 (13)
C70B	0.1829 (6)	0.7846 (10)	0.5239 (4)	0.075 (5)*	0.420 (13)
H70D	0.1632	0.7377	0.5304	0.112*	0.420 (13)
H70E	0.2070	0.7677	0.5063	0.112*	0.420 (13)
H70F	0.1547	0.8239	0.5057	0.112*	0.420 (13)
C71	0.37694 (18)	0.6202 (3)	0.51482 (14)	0.0374 (9)	
C72	0.38918 (17)	0.6637 (3)	0.47535 (14)	0.0534 (14)	
C73	0.4240 (2)	0.7391 (3)	0.4936 (2)	0.0634 (15)*	
H73A	0.4579	0.7254	0.5204	0.095*	
H73B	0.4007	0.7782	0.5029	0.095*	
H73C	0.4360	0.7625	0.4692	0.095*	
C74	0.4206 (3)	0.6089 (4)	0.4532 (2)	0.078 (2)*	
H74A	0.4316	0.6393	0.4304	0.117*	
H74B	0.3957	0.5642	0.4378	0.117*	
H74C	0.4550	0.5878	0.4771	0.117*	
C75	0.33163 (19)	0.6872 (4)	0.4398 (2)	0.082 (2)*	

H75A	0.3106	0.7202	0.4547	0.123*	
H75B	0.3096	0.6385	0.4270	0.123*	
H75C	0.3377	0.7179	0.4148	0.123*	
C76	0.43675 (16)	0.5094 (3)	0.62478 (13)	0.0305 (7)	
C77	0.49638 (15)	0.4863 (2)	0.65641 (14)	0.0440 (11)	
C78	0.5379 (3)	0.5254 (3)	0.6368 (2)	0.0737 (18)*	
H78A	0.5354	0.4987	0.6079	0.111*	
H78B	0.5769	0.5204	0.6592	0.111*	
H78C	0.5282	0.5825	0.6308	0.111*	
C79	0.5057 (3)	0.5193 (3)	0.70440 (18)	0.077 (2)*	
H79A	0.5044	0.5782	0.7032	0.116*	
H79B	0.5430	0.5017	0.7258	0.116*	
H79C	0.4756	0.4992	0.7152	0.116*	
C80	0.5051 (2)	0.3958 (2)	0.65897 (18)	0.0494 (11)*	
H80A	0.4737	0.3700	0.6658	0.074*	
H80B	0.5414	0.3829	0.6835	0.074*	
H80C	0.5058	0.3760	0.6292	0.074*	
C81	0.34801 (17)	0.3118 (3)	0.49980 (14)	0.0352 (8)	
C82	0.38529 (15)	0.2574 (2)	0.48293 (12)	0.0435 (10)	
C83	0.43838 (18)	0.2379 (3)	0.52423 (13)	0.0500 (12)*	
H83A	0.4280	0.2036	0.5459	0.075*	
H83B	0.4555	0.2879	0.5398	0.075*	
H83C	0.4659	0.2095	0.5137	0.075*	
C84	0.3536 (2)	0.1807 (3)	0.46268 (18)	0.0604 (14)*	
H84A	0.3745	0.1517	0.4459	0.091*	
H84B	0.3152	0.1940	0.4413	0.091*	
H84C	0.3507	0.1467	0.4877	0.091*	
C85	0.4017 (2)	0.3020 (3)	0.44652 (15)	0.0542 (13)*	
H85A	0.4259	0.3481	0.4608	0.081*	
H85B	0.3671	0.3210	0.4220	0.081*	
H85C	0.4228	0.2657	0.4332	0.081*	
C86	0.22150 (16)	0.4486 (2)	0.47059 (13)	0.0289 (7)	
C87	0.17905 (17)	0.4863 (3)	0.42719 (14)	0.0443 (10)	
C88	0.1795 (4)	0.5767 (3)	0.4357 (3)	0.056 (3)*	0.565 (12)
H88A	0.1744	0.5868	0.4653	0.085*	0.565 (12)
H88B	0.1483	0.6021	0.4106	0.085*	0.565 (12)
H88C	0.2161	0.5993	0.4365	0.085*	0.565 (12)
C89	0.1189 (3)	0.4543 (5)	0.4144 (4)	0.062 (3)*	0.565 (12)
H89A	0.1045	0.4656	0.4395	0.094*	0.565 (12)
H89B	0.1190	0.3960	0.4095	0.094*	0.565 (12)
H89C	0.0943	0.4803	0.3859	0.094*	0.565 (12)
C90	0.2020 (5)	0.4703 (6)	0.3884 (3)	0.080 (4)*	0.565 (12)
H90A	0.2395	0.4956	0.3959	0.120*	0.565 (12)
H90B	0.1756	0.4928	0.3594	0.120*	0.565 (12)
H90C	0.2055	0.4121	0.3849	0.120*	0.565 (12)
C88B	0.1932 (7)	0.5660 (5)	0.4096 (6)	0.098 (7)*	0.435 (12)
H88D	0.2199	0.5568	0.3932	0.147*	0.435 (12)
H88E	0.2107	0.6022	0.4358	0.147*	0.435 (12)

H88F	0.1581	0.5903	0.3883	0.147*	0.435 (12)
C89B	0.1226 (4)	0.4946 (8)	0.4356 (5)	0.067 (4)*	0.435 (12)
H89D	0.0936	0.5174	0.4080	0.100*	0.435 (12)
H89E	0.1279	0.5303	0.4621	0.100*	0.435 (12)
H89F	0.1101	0.4416	0.4421	0.100*	0.435 (12)
C90B	0.1717 (6)	0.4219 (7)	0.3903 (4)	0.078 (5)*	0.435 (12)
H90D	0.1496	0.3769	0.3958	0.118*	0.435 (12)
H90E	0.2094	0.4026	0.3917	0.118*	0.435 (12)
H90F	0.1515	0.4449	0.3596	0.118*	0.435 (12)
O2A	0.1362 (4)	0.4768 (6)	0.5417 (3)	0.0651 (13)*	0.444 (5)
C2A	0.1719 (8)	0.5362 (8)	0.5625 (5)	0.0533 (15)*	0.444 (5)
H2A1	0.1520	0.5878	0.5623	0.064*	0.444 (5)
H2A2	0.2030	0.5437	0.5500	0.064*	0.444 (5)
C1A	0.1938 (6)	0.4922 (9)	0.6139 (4)	0.0521 (18)*	0.444 (5)
H1A1	0.1872	0.5288	0.6369	0.063*	0.444 (5)
H1A2	0.1712	0.4427	0.6125	0.063*	0.444 (5)
N1	0.2508 (5)	0.4727 (8)	0.6282 (4)	0.0456 (17)*	0.444 (5)
H1A	0.2686	0.5186	0.6236	0.055*	0.444 (5)
H1B	0.2536	0.4360	0.6068	0.055*	0.444 (5)
C1B	0.2863 (6)	0.4428 (12)	0.6711 (6)	0.0521 (18)*	0.444 (5)
H1B1	0.2708	0.3881	0.6719	0.063*	0.444 (5)
H1B2	0.2746	0.4745	0.6935	0.063*	0.444 (5)
C2B	0.3455 (6)	0.4325 (7)	0.6943 (4)	0.0533 (15)*	0.444 (5)
H2B1	0.3658	0.4843	0.6963	0.064*	0.444 (5)
H2B2	0.3533	0.4118	0.7260	0.064*	0.444 (5)
O2B	0.3624 (4)	0.3796 (6)	0.6693 (4)	0.0651 (13)*	0.444 (5)
O2C	0.3036 (8)	0.3207 (10)	0.7024 (6)	0.0651 (13)*	0.251 (4)
C2C	0.3205 (10)	0.3816 (12)	0.6822 (8)	0.0533 (15)*	0.251 (4)
H2C1	0.3223	0.3656	0.6517	0.064*	0.251 (4)
H2C2	0.3583	0.4025	0.7020	0.064*	0.251 (4)
C1C	0.2744 (12)	0.4412 (13)	0.6770 (15)	0.0521 (18)*	0.251 (4)
H1C1	0.2916	0.4945	0.6879	0.063*	0.251 (4)
H1C2	0.2520	0.4248	0.6964	0.063*	0.251 (4)
N1C	0.2365 (8)	0.4472 (12)	0.6285 (6)	0.0456 (17)*	0.251 (4)
H1C3	0.2589	0.4387	0.6108	0.055*	0.251 (4)
H1C4	0.2118	0.4042	0.6232	0.055*	0.251 (4)
C1D	0.2050 (13)	0.5106 (14)	0.6111 (10)	0.0521 (18)*	0.251 (4)
H1D1	0.2204	0.5254	0.5866	0.063*	0.251 (4)
H1D2	0.2226	0.5500	0.6362	0.063*	0.251 (4)
C2D	0.1492 (10)	0.5433 (9)	0.5920 (8)	0.0533 (15)*	0.251 (4)
H2D1	0.1324	0.5321	0.5584	0.064*	0.251 (4)
H2D2	0.1238	0.5210	0.6075	0.064*	0.251 (4)
O2D	0.1574 (8)	0.6220 (9)	0.6000 (7)	0.0651 (13)*	0.251 (4)
O2E	0.3730 (6)	0.4797 (9)	0.7166 (5)	0.0651 (13)*	0.302 (5)
C2E	0.3278 (7)	0.4363 (11)	0.7159 (7)	0.0533 (15)*	0.302 (5)
H2E1	0.3203	0.4453	0.7450	0.064*	0.302 (5)
H2E2	0.3363	0.3784	0.7141	0.064*	0.302 (5)
C1E	0.2824 (8)	0.4551 (15)	0.6808 (12)	0.0521 (18)*	0.302 (5)

H1E1	0.2674	0.4004	0.6708	0.063*	0.302 (5)
H1E2	0.2580	0.4754	0.6977	0.063*	0.302 (5)
N1E	0.2587 (7)	0.4936 (10)	0.6413 (6)	0.0456 (17)*	0.302 (5)
H1E3	0.2662	0.4616	0.6198	0.055*	0.302 (5)
H1E4	0.2810	0.5387	0.6441	0.055*	0.302 (5)
C1F	0.1998 (12)	0.5223 (13)	0.6177 (7)	0.0521 (18)*	0.302 (5)
H1F1	0.1752	0.4896	0.6300	0.063*	0.302 (5)
H1F2	0.1985	0.5780	0.6288	0.063*	0.302 (5)
C2F	0.1720 (13)	0.5244 (10)	0.5688 (8)	0.0533 (15)*	0.302 (5)
H2F1	0.1876	0.4829	0.5534	0.064*	0.302 (5)
H2F2	0.1303	0.5163	0.5600	0.064*	0.302 (5)
O2F	0.1839 (7)	0.5984 (8)	0.5579 (5)	0.0651 (13)*	0.302 (5)
O99	0.4693 (4)	0.5143 (7)	0.9913 (4)	0.164 (4)*	
C99	0.4441 (9)	0.5166 (7)	1.0299 (7)	0.181 (7)*	
O98	0.4767 (11)	0.4978 (13)	1.0601 (10)	0.192 (10)*	0.50
C98	0.3844 (10)	0.5449 (15)	1.0045 (9)	0.129 (8)*	0.50
H98A	0.3660	0.5091	0.9782	0.194*	0.50
H98B	0.3854	0.5998	0.9932	0.194*	0.50
H98C	0.3627	0.5443	1.0255	0.194*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0180 (2)	0.0254 (3)	0.0247 (3)	0.00061 (19)	0.00350 (19)	−0.0014 (2)
Cr2	0.0238 (3)	0.0240 (3)	0.0340 (3)	−0.0023 (2)	0.0072 (2)	0.0009 (2)
Cr3	0.0337 (3)	0.0261 (3)	0.0229 (3)	−0.0072 (2)	0.0061 (2)	−0.0003 (2)
Cr4	0.0382 (3)	0.0297 (3)	0.0224 (3)	−0.0123 (2)	0.0080 (2)	−0.0024 (2)
Cr5	0.0227 (2)	0.0247 (3)	0.0194 (2)	−0.00281 (19)	0.00320 (19)	0.00213 (19)
Cr6	0.0235 (2)	0.0214 (2)	0.0192 (2)	−0.00308 (19)	0.00432 (19)	0.00107 (18)
Cr7	0.0211 (2)	0.0301 (3)	0.0197 (2)	−0.0060 (2)	0.00641 (19)	0.0007 (2)
Cr8	0.0200 (2)	0.0357 (3)	0.0199 (2)	−0.0056 (2)	0.00509 (19)	−0.0050 (2)
F1	0.0266 (10)	0.0292 (11)	0.0396 (13)	−0.0005 (9)	0.0090 (9)	0.0003 (9)
F2	0.0301 (11)	0.0327 (11)	0.0278 (11)	−0.0046 (9)	0.0039 (9)	0.0011 (9)
F3	0.0387 (12)	0.0251 (10)	0.0237 (10)	−0.0068 (9)	0.0072 (9)	−0.0003 (8)
F4	0.0339 (11)	0.0281 (11)	0.0251 (10)	−0.0056 (9)	0.0055 (9)	0.0013 (8)
F5	0.0266 (10)	0.0293 (10)	0.0215 (9)	−0.0049 (8)	0.0039 (8)	0.0025 (8)
F6	0.0332 (11)	0.0287 (10)	0.0232 (10)	−0.0046 (9)	0.0099 (8)	0.0026 (8)
F7	0.0298 (11)	0.0448 (13)	0.0250 (10)	−0.0113 (10)	0.0093 (9)	−0.0041 (9)
F8	0.0388 (13)	0.0334 (12)	0.0257 (11)	−0.0041 (10)	0.0037 (9)	−0.0006 (9)
O11	0.0400 (16)	0.0384 (16)	0.0396 (16)	−0.0095 (13)	0.0080 (13)	−0.0114 (13)
O12	0.0341 (15)	0.0307 (14)	0.0542 (19)	−0.0060 (12)	0.0149 (14)	−0.0086 (13)
O13	0.0276 (14)	0.0365 (15)	0.0490 (18)	0.0057 (11)	0.0056 (13)	0.0100 (13)
O14	0.0369 (16)	0.0389 (17)	0.0452 (18)	0.0025 (13)	0.0059 (14)	0.0119 (14)
O21	0.0398 (16)	0.0281 (14)	0.0512 (19)	−0.0024 (12)	0.0184 (14)	0.0049 (13)
O22	0.0458 (17)	0.0290 (14)	0.0391 (16)	−0.0100 (12)	0.0170 (13)	−0.0015 (12)
O23	0.0269 (13)	0.0353 (14)	0.0330 (14)	−0.0033 (11)	0.0084 (11)	−0.0051 (11)
O24	0.0310 (14)	0.0352 (14)	0.0298 (14)	0.0022 (11)	0.0040 (11)	−0.0052 (11)
O31	0.0446 (17)	0.0399 (16)	0.0356 (15)	−0.0147 (13)	0.0178 (13)	−0.0095 (12)

O32	0.0535 (19)	0.0455 (18)	0.0318 (15)	−0.0232 (15)	0.0199 (14)	−0.0101 (13)
O33	0.0556 (19)	0.0310 (14)	0.0274 (14)	−0.0081 (13)	0.0031 (13)	0.0060 (11)
O34	0.057 (2)	0.0355 (16)	0.0273 (14)	−0.0120 (14)	0.0002 (13)	0.0053 (12)
O41	0.058 (2)	0.0424 (17)	0.0265 (14)	−0.0203 (15)	0.0162 (14)	−0.0070 (12)
O42	0.0320 (13)	0.0316 (13)	0.0240 (12)	−0.0042 (10)	0.0099 (10)	−0.0009 (10)
O43	0.0296 (13)	0.0365 (15)	0.0343 (14)	−0.0055 (11)	0.0096 (11)	−0.0053 (12)
O44	0.0260 (13)	0.0401 (15)	0.0268 (13)	−0.0020 (11)	0.0018 (10)	0.0059 (11)
O51	0.0307 (13)	0.0234 (12)	0.0339 (14)	−0.0001 (10)	0.0073 (11)	0.0024 (10)
O52	0.0312 (13)	0.0257 (12)	0.0318 (13)	−0.0043 (10)	0.0083 (11)	−0.0027 (10)
O53	0.0237 (11)	0.0307 (13)	0.0204 (11)	−0.0023 (9)	0.0032 (9)	0.0018 (9)
O54	0.0298 (13)	0.0378 (14)	0.0208 (11)	0.0038 (11)	0.0058 (10)	0.0034 (10)
O61	0.0297 (13)	0.0359 (14)	0.0299 (13)	−0.0078 (11)	0.0065 (11)	−0.0013 (11)
O62	0.0281 (13)	0.0339 (14)	0.0308 (13)	−0.0096 (11)	0.0083 (11)	0.0022 (11)
O63	0.0301 (13)	0.0271 (12)	0.0272 (12)	−0.0004 (10)	0.0056 (10)	0.0061 (10)
O64	0.0304 (14)	0.0440 (16)	0.0237 (12)	−0.0013 (12)	0.0036 (11)	0.0030 (11)
O71	0.0395 (16)	0.0469 (17)	0.0304 (14)	−0.0072 (13)	0.0164 (12)	0.0059 (12)
O72	0.0303 (14)	0.060 (2)	0.0301 (14)	−0.0110 (13)	0.0147 (12)	−0.0077 (13)
O73	0.0218 (12)	0.0435 (16)	0.0286 (13)	−0.0050 (11)	0.0060 (10)	−0.0013 (11)
O74	0.0350 (16)	0.0436 (18)	0.0416 (17)	−0.0045 (13)	−0.0073 (13)	−0.0041 (14)
O81	0.0248 (13)	0.0529 (19)	0.0423 (17)	−0.0023 (12)	0.0090 (12)	−0.0165 (14)
O82	0.0274 (14)	0.0489 (18)	0.0422 (17)	−0.0003 (12)	0.0091 (12)	−0.0115 (14)
O83	0.0321 (14)	0.0429 (16)	0.0231 (12)	−0.0047 (12)	0.0076 (11)	−0.0022 (11)
O84	0.0227 (13)	0.0508 (18)	0.0375 (16)	−0.0020 (12)	0.0016 (11)	0.0089 (13)
C11	0.0240 (17)	0.0305 (18)	0.044 (2)	0.0014 (14)	0.0014 (16)	−0.0079 (16)
C12	0.046 (3)	0.041 (3)	0.069 (4)	−0.008 (2)	0.016 (2)	−0.026 (2)
C16	0.0255 (17)	0.0224 (17)	0.061 (3)	0.0016 (13)	0.0029 (18)	0.0101 (17)
C17	0.045 (3)	0.049 (3)	0.090 (5)	0.017 (2)	0.002 (3)	0.036 (3)
C21	0.039 (2)	0.0261 (17)	0.042 (2)	−0.0062 (15)	0.0112 (18)	0.0054 (15)
C22	0.065 (3)	0.028 (2)	0.076 (4)	−0.012 (2)	0.037 (3)	−0.002 (2)
C26	0.0280 (17)	0.0311 (18)	0.0261 (16)	−0.0017 (14)	0.0049 (14)	0.0001 (13)
C27	0.036 (2)	0.062 (3)	0.035 (2)	0.012 (2)	−0.0039 (18)	−0.014 (2)
C31	0.048 (2)	0.040 (2)	0.0307 (19)	−0.0153 (19)	0.0169 (18)	−0.0042 (16)
C32	0.057 (3)	0.056 (3)	0.038 (2)	−0.023 (2)	0.029 (2)	−0.012 (2)
C36	0.057 (3)	0.036 (2)	0.0241 (18)	−0.0062 (19)	0.0021 (18)	0.0082 (15)
C37	0.079 (4)	0.045 (3)	0.043 (3)	−0.003 (3)	−0.012 (3)	0.014 (2)
C41	0.0334 (19)	0.039 (2)	0.0219 (16)	−0.0104 (15)	0.0061 (14)	−0.0023 (14)
C42	0.054 (3)	0.039 (2)	0.0268 (18)	−0.0122 (19)	0.0151 (18)	−0.0052 (16)
C46	0.0245 (16)	0.0366 (19)	0.0244 (16)	−0.0004 (14)	0.0063 (13)	−0.0091 (14)
C47	0.0261 (19)	0.048 (3)	0.046 (2)	0.0070 (17)	−0.0007 (17)	−0.011 (2)
C51	0.0306 (17)	0.0242 (15)	0.0230 (15)	−0.0002 (13)	0.0049 (13)	0.0017 (12)
C52	0.049 (3)	0.030 (2)	0.051 (3)	−0.0029 (18)	0.021 (2)	−0.0084 (18)
C56	0.0275 (16)	0.0227 (15)	0.0204 (14)	−0.0010 (12)	0.0017 (12)	−0.0005 (11)
C57	0.0284 (17)	0.041 (2)	0.0244 (17)	0.0059 (15)	0.0017 (14)	0.0084 (15)
C61	0.0260 (16)	0.0231 (15)	0.0336 (18)	−0.0057 (12)	0.0069 (14)	0.0023 (13)
C62	0.035 (2)	0.038 (2)	0.051 (3)	−0.0161 (18)	0.0104 (19)	−0.0024 (19)
C66	0.0251 (16)	0.0284 (17)	0.0301 (17)	−0.0042 (13)	0.0056 (13)	0.0072 (13)
C67	0.063 (3)	0.039 (2)	0.042 (3)	0.003 (2)	−0.012 (2)	0.012 (2)
C71	0.0283 (18)	0.058 (3)	0.0250 (17)	−0.0134 (18)	0.0087 (14)	0.0006 (17)

C72	0.050 (3)	0.083 (4)	0.033 (2)	−0.025 (3)	0.021 (2)	0.002 (2)
C76	0.0231 (16)	0.041 (2)	0.0253 (16)	−0.0029 (14)	0.0056 (13)	0.0001 (14)
C77	0.0220 (17)	0.049 (3)	0.050 (3)	−0.0013 (17)	−0.0003 (17)	−0.001 (2)
C81	0.0274 (18)	0.045 (2)	0.0302 (18)	0.0038 (16)	0.0069 (15)	−0.0043 (16)
C82	0.034 (2)	0.056 (3)	0.041 (2)	0.0109 (19)	0.0133 (18)	−0.009 (2)
C86	0.0248 (16)	0.0371 (19)	0.0230 (15)	0.0017 (14)	0.0063 (13)	−0.0026 (14)
C87	0.039 (2)	0.051 (3)	0.035 (2)	0.0108 (19)	0.0019 (18)	0.0066 (19)

Geometric parameters (Å, º)

Cr1—F8	1.946 (2)	C49—H49A	0.9800
Cr1—O84	1.957 (3)	C49—H49B	0.9800
Cr1—O11	1.960 (3)	C49—H49C	0.9800
Cr1—F1	1.961 (3)	C50—H50A	0.9800
Cr1—O82	1.965 (3)	C50—H50B	0.9800
Cr1—O13	1.978 (3)	C50—H50C	0.9800
Cr2—F1	1.922 (2)	C51—C52	1.515 (5)
Cr2—F2	1.948 (2)	C52—C55	1.511 (3)
Cr2—O12	1.952 (3)	C52—C54	1.516 (3)
Cr2—O14	1.957 (3)	C52—C53	1.525 (3)
Cr2—O21	1.972 (3)	C53—H53A	0.9800
Cr2—O23	1.979 (3)	C53—H53B	0.9800
Cr3—F2	1.921 (3)	C53—H53C	0.9800
Cr3—F3	1.925 (2)	C54—H54A	0.9800
Cr3—O31	1.946 (3)	C54—H54B	0.9800
Cr3—O22	1.948 (3)	C54—H54C	0.9800
Cr3—O24	1.950 (3)	C55—H55A	0.9800
Cr3—O33	1.958 (3)	C55—H55B	0.9800
Cr4—F4	1.925 (2)	C55—H55C	0.9800
Cr4—F3	1.927 (2)	C56—C57	1.517 (5)
Cr4—O41	1.950 (3)	C57—C58	1.513 (3)
Cr4—O32	1.953 (3)	C57—C59B	1.515 (3)
Cr4—O34	1.954 (4)	C57—C60B	1.519 (3)
Cr4—O43	1.959 (3)	C57—C59	1.521 (3)
Cr5—F5	1.916 (2)	C57—C60	1.526 (3)
Cr5—F4	1.922 (2)	C57—C58B	1.528 (3)
Cr5—O51	1.937 (3)	C58—H58A	0.9800
Cr5—O42	1.956 (3)	C58—H58B	0.9800
Cr5—O44	1.958 (3)	C58—H58C	0.9800
Cr5—O53	1.961 (3)	C59—H59A	0.9800
Cr6—F6	1.931 (2)	C59—H59B	0.9800
Cr6—F5	1.941 (2)	C59—H59C	0.9800
Cr6—O61	1.947 (3)	C60—H60A	0.9800
Cr6—O63	1.962 (3)	C60—H60B	0.9800
Cr6—O54	1.971 (3)	C60—H60C	0.9800
Cr6—O52	1.971 (3)	C58B—H58D	0.9800
Cr7—F7	1.930 (2)	C58B—H58E	0.9800
Cr7—O71	1.938 (3)	C58B—H58F	0.9800

Cr7—F6	1.953 (2)	C59B—H59D	0.9800
Cr7—O73	1.959 (3)	C59B—H59E	0.9800
Cr7—O62	1.960 (3)	C59B—H59F	0.9800
Cr7—O64	1.968 (3)	C60B—H60D	0.9800
Cr8—F8	1.945 (3)	C60B—H60E	0.9800
Cr8—F7	1.952 (3)	C60B—H60F	0.9800
Cr8—O81	1.962 (3)	C61—C62	1.520 (5)
Cr8—O83	1.971 (3)	C62—C63	1.515 (3)
Cr8—O72	1.972 (3)	C62—C65	1.518 (3)
Cr8—O74	1.979 (3)	C62—C64	1.519 (3)
O11—C11	1.238 (6)	C63—H63A	0.9800
O12—C11	1.262 (6)	C63—H63B	0.9800
O13—C16	1.264 (6)	C63—H63C	0.9800
O14—C16	1.263 (6)	C64—H64A	0.9800
O21—C21	1.249 (6)	C64—H64B	0.9800
O22—C21	1.264 (6)	C64—H64C	0.9800
O23—C26	1.257 (5)	C65—H65A	0.9800
O24—C26	1.270 (5)	C65—H65B	0.9800
O31—C31	1.256 (5)	C65—H65C	0.9800
O32—C31	1.258 (5)	C66—C67	1.532 (5)
O33—C36	1.269 (5)	C67—C69	1.514 (3)
O34—C36	1.244 (6)	C67—C69B	1.517 (3)
O41—C41	1.262 (5)	C67—C68	1.521 (3)
O42—C41	1.245 (5)	C67—C70B	1.521 (3)
O43—C46	1.257 (5)	C67—C68B	1.525 (3)
O44—C46	1.258 (5)	C67—C70	1.532 (3)
O51—C51	1.266 (5)	C68—H68A	0.9800
O52—C51	1.260 (5)	C68—H68B	0.9800
O53—C56	1.263 (5)	C68—H68C	0.9800
O54—C56	1.263 (5)	C69—H69A	0.9800
O61—C61	1.264 (5)	C69—H69B	0.9800
O62—C61	1.251 (5)	C69—H69C	0.9800
O63—C66	1.262 (5)	C70—H70A	0.9800
O64—C66	1.255 (5)	C70—H70B	0.9800
O71—C71	1.250 (6)	C70—H70C	0.9800
O72—C71	1.267 (6)	C68B—H68D	0.9800
O73—C76	1.252 (5)	C68B—H68E	0.9800
O74—C76	1.263 (5)	C68B—H68F	0.9800
O81—C81	1.261 (6)	C69B—H69D	0.9800
O82—C81	1.261 (5)	C69B—H69E	0.9800
O83—C86	1.264 (5)	C69B—H69F	0.9800
O84—C86	1.259 (5)	C70B—H70D	0.9800
C11—C12	1.519 (6)	C70B—H70E	0.9800
C12—C15	1.507 (3)	C70B—H70F	0.9800
C12—C14B	1.516 (3)	C71—C72	1.536 (6)
C12—C14	1.521 (3)	C72—C74	1.512 (3)
C12—C13	1.522 (3)	C72—C73	1.518 (3)
C12—C13B	1.526 (3)	C72—C75	1.522 (3)

C12—C15B	1.529 (3)	C73—H73A	0.9800
C13—H13A	0.9800	C73—H73B	0.9800
C13—H13B	0.9800	C73—H73C	0.9800
C13—H13C	0.9800	C74—H74A	0.9800
C14—H14A	0.9800	C74—H74B	0.9800
C14—H14B	0.9800	C74—H74C	0.9800
C14—H14C	0.9800	C75—H75A	0.9800
C15—H15A	0.9800	C75—H75B	0.9800
C15—H15B	0.9800	C75—H75C	0.9800
C15—H15C	0.9800	C76—C77	1.517 (5)
C13B—H13D	0.9800	C77—C78	1.518 (3)
C13B—H13E	0.9800	C77—C79	1.518 (3)
C13B—H13F	0.9800	C77—C80	1.518 (3)
C14B—H14D	0.9800	C78—H78A	0.9800
C14B—H14E	0.9800	C78—H78B	0.9800
C14B—H14F	0.9800	C78—H78C	0.9800
C15B—H15D	0.9800	C79—H79A	0.9800
C15B—H15E	0.9800	C79—H79B	0.9800
C15B—H15F	0.9800	C79—H79C	0.9800
C16—C17	1.534 (6)	C80—H80A	0.9800
C17—C20	1.511 (3)	C80—H80B	0.9800
C17—C19A	1.517 (3)	C80—H80C	0.9800
C17—C18A	1.522 (3)	C81—C82	1.515 (6)
C17—C19	1.526 (3)	C82—C84	1.515 (3)
C17—C20A	1.530 (3)	C82—C83	1.518 (3)
C17—C18	1.534 (3)	C82—C85	1.517 (3)
C18—H18A	0.9800	C83—H83A	0.9800
C18—H18B	0.9800	C83—H83B	0.9800
C18—H18C	0.9800	C83—H83C	0.9800
C19—H19A	0.9800	C84—H84A	0.9800
C19—H19B	0.9800	C84—H84B	0.9800
C19—H19C	0.9800	C84—H84C	0.9800
C20—H20A	0.9800	C85—H85A	0.9800
C20—H20B	0.9800	C85—H85B	0.9800
C20—H20C	0.9800	C85—H85C	0.9800
C18A—H18D	0.9800	C86—C87	1.521 (5)
C18A—H18E	0.9800	C87—C89	1.510 (3)
C18A—H18F	0.9800	C87—C88B	1.519 (3)
C19A—H19D	0.9800	C87—C90	1.520 (3)
C19A—H19E	0.9800	C87—C88	1.524 (3)
C19A—H19F	0.9800	C87—C90B	1.527 (3)
C20A—H20D	0.9800	C87—C89B	1.528 (3)
C20A—H20E	0.9800	C88—H88A	0.9800
C20A—H20F	0.9800	C88—H88B	0.9800
C21—C22	1.512 (6)	C88—H88C	0.9800
C22—C25	1.517 (3)	C89—H89A	0.9800
C22—C24	1.517 (3)	C89—H89B	0.9800
C22—C23	1.524 (3)	C89—H89C	0.9800

C23—H23A	0.9800	C90—H90A	0.9800
C23—H23B	0.9800	C90—H90B	0.9800
C23—H23C	0.9800	C90—H90C	0.9800
C24—H24A	0.9800	C88B—H88D	0.9800
C24—H24B	0.9800	C88B—H88E	0.9800
C24—H24C	0.9800	C88B—H88F	0.9800
C25—H25A	0.9800	C89B—H89D	0.9800
C25—H25B	0.9800	C89B—H89E	0.9800
C25—H25C	0.9800	C89B—H89F	0.9800
C26—C27	1.517 (5)	C90B—H90D	0.9800
C27—C30	1.516 (3)	C90B—H90E	0.9800
C27—C28	1.520 (3)	C90B—H90F	0.9800
C27—C29	1.525 (3)	O2A—C2A	1.334 (6)
C28—H28A	0.9800	C2A—C1A	1.65 (2)
C28—H28B	0.9800	C2A—H2A1	0.9900
C28—H28C	0.9800	C2A—H2A2	0.9900
C29—H29A	0.9800	C1A—N1	1.372 (18)
C29—H29B	0.9800	C1A—H1A1	0.9900
C29—H29C	0.9800	C1A—H1A2	0.9900
C30—H30A	0.9800	N1—C1B	1.401 (19)
C30—H30B	0.9800	N1—H1A	0.9200
C30—H30C	0.9800	N1—H1B	0.9200
C31—C32	1.516 (6)	C1B—C2B	1.410 (19)
C32—C33	1.517 (3)	C1B—H1B1	0.9900
C32—C34	1.517 (3)	C1B—H1B2	0.9900
C32—C35	1.520 (3)	C2B—O2B	1.333 (6)
C33—H33A	0.9800	C2B—H2B1	0.9900
C33—H33B	0.9800	C2B—H2B2	0.9900
C33—H33C	0.9800	O2C—C2C	1.334 (6)
C34—H34A	0.9800	C2C—C1C	1.49 (3)
C34—H34B	0.9800	C2C—H2C1	0.9900
C34—H34C	0.9800	C2C—H2C2	0.9900
C35—H35A	0.9800	C1C—N1C	1.47 (4)
C35—H35B	0.9800	C1C—H1C1	0.9900
C35—H35C	0.9800	C1C—H1C2	0.9900
C36—C37	1.520 (6)	N1C—C1D	1.31 (3)
C37—C39	1.518 (3)	N1C—H1C3	0.9200
C37—C40	1.519 (3)	N1C—H1C4	0.9200
C37—C38	1.523 (3)	C1D—C2D	1.42 (3)
C38—H38A	0.9800	C1D—H1D1	0.9900
C38—H38B	0.9800	C1D—H1D2	0.9900
C38—H38C	0.9800	C2D—O2D	1.335 (6)
C39—H39A	0.9800	C2D—H2D1	0.9900
C39—H39B	0.9800	C2D—H2D2	0.9900
C39—H39C	0.9800	O2E—C2E	1.334 (6)
C40—H40A	0.9800	C2E—C1E	1.30 (3)
C40—H40B	0.9800	C2E—H2E1	0.9900
C40—H40C	0.9800	C2E—H2E2	0.9900

C41—C42	1.529 (5)	C1E—N1E	1.32 (4)
C42—C43	1.517 (3)	C1E—H1E1	0.9900
C42—C45	1.517 (3)	C1E—H1E2	0.9900
C42—C44	1.519 (3)	N1E—C1F	1.48 (3)
C43—H43A	0.9800	N1E—H1E3	0.9200
C43—H43B	0.9800	N1E—H1E4	0.9200
C43—H43C	0.9800	C1F—C2F	1.42 (3)
C44—H44A	0.9800	C1F—H1F1	0.9900
C44—H44B	0.9800	C1F—H1F2	0.9900
C44—H44C	0.9800	C2F—O2F	1.335 (6)
C45—H45A	0.9800	C2F—H2F1	0.9900
C45—H45B	0.9800	C2F—H2F2	0.9900
C45—H45C	0.9800	O99—O99^{i}	1.515 (19)
C46—C47	1.518 (5)	O99—C99	1.53 (2)
C47—C49	1.515 (3)	C99—O98	1.05 (3)
C47—C48	1.517 (3)	C99—C98	1.497 (16)
C47—C50	1.521 (3)	C98—H98A	0.9800
C48—H48A	0.9800	C98—H98B	0.9800
C48—H48B	0.9800	C98—H98C	0.9800
C48—H48C	0.9800		

F8—Cr1—O84	90.89 (12)	H48B—C48—H48C	109.5
F8—Cr1—O11	178.32 (13)	C47—C49—H49A	109.5
O84—Cr1—O11	87.90 (14)	C47—C49—H49B	109.5
F8—Cr1—F1	88.13 (11)	H49A—C49—H49B	109.5
O84—Cr1—F1	89.34 (12)	C47—C49—H49C	109.5
O11—Cr1—F1	90.69 (13)	H49A—C49—H49C	109.5
F8—Cr1—O82	92.85 (12)	H49B—C49—H49C	109.5
O84—Cr1—O82	92.44 (15)	C47—C50—H50A	109.5
O11—Cr1—O82	88.37 (14)	C47—C50—H50B	109.5
F1—Cr1—O82	177.95 (13)	H50A—C50—H50B	109.5
F8—Cr1—O13	88.46 (12)	C47—C50—H50C	109.5
O84—Cr1—O13	178.86 (14)	H50A—C50—H50C	109.5
O11—Cr1—O13	92.77 (14)	H50B—C50—H50C	109.5
F1—Cr1—O13	91.57 (13)	O52—C51—O51	125.1 (3)
O82—Cr1—O13	86.67 (15)	O52—C51—C52	118.4 (3)
F1—Cr2—F2	87.65 (11)	O51—C51—C52	116.4 (3)
F1—Cr2—O12	93.44 (13)	C55—C52—C51	110.5 (4)
F2—Cr2—O12	178.61 (12)	C55—C52—C54	110.7 (3)
F1—Cr2—O14	91.33 (12)	C51—C52—C54	111.3 (4)
F2—Cr2—O14	87.62 (13)	C55—C52—C53	109.7 (3)
O12—Cr2—O14	93.21 (15)	C51—C52—C53	105.6 (4)
F1—Cr2—O21	178.68 (13)	C54—C52—C53	108.9 (2)
F2—Cr2—O21	91.09 (12)	C52—C53—H53A	109.5
O12—Cr2—O21	87.81 (14)	C52—C53—H53B	109.5
O14—Cr2—O21	89.02 (14)	H53A—C53—H53B	109.5
F1—Cr2—O23	90.78 (11)	C52—C53—H53C	109.5
F2—Cr2—O23	91.81 (11)	H53A—C53—H53C	109.5

O12—Cr2—O23	87.31 (13)	H53B—C53—H53C	109.5
O14—Cr2—O23	177.78 (14)	C52—C54—H54A	109.5
O21—Cr2—O23	88.85 (13)	C52—C54—H54B	109.5
F2—Cr3—F3	89.30 (10)	H54A—C54—H54B	109.5
F2—Cr3—O31	178.45 (13)	C52—C54—H54C	109.5
F3—Cr3—O31	90.64 (12)	H54A—C54—H54C	109.5
F2—Cr3—O22	93.12 (12)	H54B—C54—H54C	109.5
F3—Cr3—O22	177.58 (13)	C52—C55—H55A	109.5
O31—Cr3—O22	86.94 (14)	C52—C55—H55B	109.5
F2—Cr3—O24	90.64 (12)	H55A—C55—H55B	109.5
F3—Cr3—O24	89.68 (11)	C52—C55—H55C	109.5
O31—Cr3—O24	87.81 (14)	H55A—C55—H55C	109.5
O22—Cr3—O24	90.26 (13)	H55B—C55—H55C	109.5
F2—Cr3—O33	89.34 (13)	O54—C56—O53	125.5 (3)
F3—Cr3—O33	91.03 (11)	O54—C56—C57	117.2 (3)
O31—Cr3—O33	92.21 (15)	O53—C56—C57	117.3 (3)
O22—Cr3—O33	89.03 (13)	C58—C57—C59B	133.7 (7)
O24—Cr3—O33	179.29 (14)	C58—C57—C56	110.4 (4)
F4—Cr4—F3	87.95 (10)	C59B—C57—C56	115.0 (6)
F4—Cr4—O41	91.05 (12)	C58—C57—C60B	56.7 (5)
F3—Cr4—O41	178.99 (13)	C59B—C57—C60B	110.0 (3)
F4—Cr4—O32	178.23 (14)	C56—C57—C60B	113.4 (6)
F3—Cr4—O32	93.05 (12)	C58—C57—C59	109.9 (3)
O41—Cr4—O32	87.95 (13)	C59B—C57—C59	43.9 (5)
F4—Cr4—O34	89.47 (13)	C56—C57—C59	111.9 (4)
F3—Cr4—O34	90.00 (12)	C60B—C57—C59	134.5 (7)
O41—Cr4—O34	90.15 (15)	C58—C57—C60	109.5 (3)
O32—Cr4—O34	91.99 (16)	C59B—C57—C60	66.1 (5)
F4—Cr4—O43	91.49 (11)	C56—C57—C60	106.1 (5)
F3—Cr4—O43	88.01 (11)	C60B—C57—C60	53.9 (5)
O41—Cr4—O43	91.86 (14)	C59—C57—C60	108.9 (3)
O32—Cr4—O43	87.08 (15)	C58—C57—C58B	53.0 (5)
O34—Cr4—O43	177.75 (13)	C59B—C57—C58B	109.2 (3)
F5—Cr5—F4	89.26 (10)	C56—C57—C58B	99.7 (6)
F5—Cr5—O51	91.36 (11)	C60B—C57—C58B	108.9 (3)
F4—Cr5—O51	178.91 (12)	C59—C57—C58B	66.7 (5)
F5—Cr5—O42	178.42 (11)	C60—C57—C58B	153.2 (7)
F4—Cr5—O42	92.32 (11)	C57—C58—H58A	109.5
O51—Cr5—O42	87.07 (12)	C57—C58—H58B	109.5
F5—Cr5—O44	88.23 (11)	H58A—C58—H58B	109.5
F4—Cr5—O44	90.22 (12)	C57—C58—H58C	109.5
O51—Cr5—O44	88.91 (12)	H58A—C58—H58C	109.5
O42—Cr5—O44	91.86 (12)	H58B—C58—H58C	109.5
F5—Cr5—O53	92.05 (10)	C57—C59—H59A	109.5
F4—Cr5—O53	89.34 (11)	C57—C59—H59B	109.5
O51—Cr5—O53	91.53 (12)	H59A—C59—H59B	109.5
O42—Cr5—O53	87.87 (11)	C57—C59—H59C	109.5
O44—Cr5—O53	179.47 (13)	H59A—C59—H59C	109.5

F6—Cr6—F5	86.63 (10)	H59B—C59—H59C	109.5
F6—Cr6—O61	90.81 (11)	C57—C60—H60A	109.5
F5—Cr6—O61	177.00 (12)	C57—C60—H60B	109.5
F6—Cr6—O63	92.48 (11)	H60A—C60—H60B	109.5
F5—Cr6—O63	89.21 (10)	C57—C60—H60C	109.5
O61—Cr6—O63	92.47 (12)	H60A—C60—H60C	109.5
F6—Cr6—O54	90.03 (11)	H60B—C60—H60C	109.5
F5—Cr6—O54	89.48 (11)	C57—C58B—H58D	109.5
O61—Cr6—O54	88.95 (12)	C57—C58B—H58E	109.5
O63—Cr6—O54	177.09 (13)	H58D—C58B—H58E	109.5
F6—Cr6—O52	179.75 (13)	C57—C58B—H58F	109.5
F5—Cr6—O52	93.41 (11)	H58D—C58B—H58F	109.5
O61—Cr6—O52	89.15 (12)	H58E—C58B—H58F	109.5
O63—Cr6—O52	87.28 (12)	C57—C59B—H59D	109.5
O54—Cr6—O52	90.21 (12)	C57—C59B—H59E	109.5
F7—Cr7—O71	91.22 (12)	H59D—C59B—H59E	109.5
F7—Cr7—F6	88.42 (10)	C57—C59B—H59F	109.5
O71—Cr7—F6	178.33 (12)	H59D—C59B—H59F	109.5
F7—Cr7—O73	92.68 (12)	H59E—C59B—H59F	109.5
O71—Cr7—O73	92.56 (13)	C57—C60B—H60D	109.5
F6—Cr7—O73	89.08 (11)	C57—C60B—H60E	109.5
F7—Cr7—O62	179.01 (12)	H60D—C60B—H60E	109.5
O71—Cr7—O62	88.31 (13)	C57—C60B—H60F	109.5
F6—Cr7—O62	92.07 (11)	H60D—C60B—H60F	109.5
O73—Cr7—O62	86.46 (12)	H60E—C60B—H60F	109.5
F7—Cr7—O64	89.08 (12)	O62—C61—O61	125.5 (3)
O71—Cr7—O64	88.42 (13)	O62—C61—C62	117.2 (3)
F6—Cr7—O64	89.94 (11)	O61—C61—C62	117.3 (3)
O73—Cr7—O64	177.96 (13)	C63—C62—C65	109.9 (3)
O62—Cr7—O64	91.79 (13)	C63—C62—C64	109.9 (2)
F8—Cr8—F7	86.30 (10)	C65—C62—C64	109.8 (3)
F8—Cr8—O81	91.31 (13)	C63—C62—C61	109.8 (4)
F7—Cr8—O81	176.36 (13)	C65—C62—C61	105.3 (4)
F8—Cr8—O83	93.02 (11)	C64—C62—C61	112.1 (4)
F7—Cr8—O83	89.89 (11)	C62—C63—H63A	109.5
O81—Cr8—O83	92.97 (13)	C62—C63—H63B	109.5
F8—Cr8—O72	179.48 (13)	H63A—C63—H63B	109.5
F7—Cr8—O72	93.22 (12)	C62—C63—H63C	109.5
O81—Cr8—O72	89.18 (15)	H63A—C63—H63C	109.5
O83—Cr8—O72	86.77 (13)	H63B—C63—H63C	109.5
F8—Cr8—O74	88.01 (13)	C62—C64—H64A	109.5
F7—Cr8—O74	89.88 (13)	C62—C64—H64B	109.5
O81—Cr8—O74	87.29 (14)	H64A—C64—H64B	109.5
O83—Cr8—O74	178.93 (15)	C62—C64—H64C	109.5
O72—Cr8—O74	92.20 (14)	H64A—C64—H64C	109.5
Cr2—F1—Cr1	121.73 (12)	H64B—C64—H64C	109.5
Cr3—F2—Cr2	122.83 (12)	C62—C65—H65A	109.5
Cr3—F3—Cr4	123.65 (12)	C62—C65—H65B	109.5

Cr5—F4—Cr4	123.17 (13)	H65A—C65—H65B	109.5
Cr5—F5—Cr6	122.62 (11)	C62—C65—H65C	109.5
Cr6—F6—Cr7	121.72 (11)	H65A—C65—H65C	109.5
Cr7—F7—Cr8	121.34 (12)	H65B—C65—H65C	109.5
Cr1—F8—Cr8	121.33 (12)	O64—C66—O63	125.6 (4)
C11—O11—Cr1	131.0 (3)	O64—C66—C67	119.6 (4)
C11—O12—Cr2	133.8 (3)	O63—C66—C67	114.8 (4)
C16—O13—Cr1	135.0 (3)	C69—C67—C69B	118.4 (9)
C16—O14—Cr2	129.3 (3)	C69—C67—C68	110.1 (3)
C21—O21—Cr2	128.6 (3)	C69B—C67—C68	62.6 (9)
C21—O22—Cr3	135.5 (3)	C69—C67—C70B	28.2 (7)
C26—O23—Cr2	135.6 (3)	C69B—C67—C70B	109.7 (3)
C26—O24—Cr3	126.8 (3)	C68—C67—C70B	132.7 (8)
C31—O31—Cr3	132.1 (3)	C69—C67—C68B	80.8 (7)
C31—O32—Cr4	133.8 (3)	C69B—C67—C68B	109.4 (3)
C36—O33—Cr3	135.0 (3)	C68—C67—C68B	47.6 (9)
C36—O34—Cr4	130.6 (3)	C70B—C67—C68B	108.9 (3)
C41—O41—Cr4	129.9 (3)	C69—C67—C70	109.1 (3)
C41—O42—Cr5	135.4 (3)	C69B—C67—C70	46.2 (10)
C46—O43—Cr4	134.6 (3)	C68—C67—C70	108.3 (3)
C46—O44—Cr5	130.1 (3)	C70B—C67—C70	84.1 (7)
C51—O51—Cr5	129.6 (3)	C68B—C67—C70	155.5 (10)
C51—O52—Cr6	133.9 (3)	C69—C67—C66	112.8 (5)
C56—O53—Cr5	135.1 (2)	C69B—C67—C66	127.4 (10)
C56—O54—Cr6	128.5 (2)	C68—C67—C66	109.9 (5)
C61—O61—Cr6	129.0 (3)	C70B—C67—C66	109.6 (7)
C61—O62—Cr7	134.0 (3)	C68B—C67—C66	89.1 (11)
C66—O63—Cr6	135.1 (3)	C70—C67—C66	106.3 (5)
C66—O64—Cr7	128.3 (3)	C67—C68—H68A	109.5
C71—O71—Cr7	130.3 (3)	C67—C68—H68B	109.5
C71—O72—Cr8	132.8 (3)	H68A—C68—H68B	109.5
C76—O73—Cr7	135.3 (3)	C67—C68—H68C	109.5
C76—O74—Cr8	128.3 (3)	H68A—C68—H68C	109.5
C81—O81—Cr8	130.2 (3)	H68B—C68—H68C	109.5
C81—O82—Cr1	133.3 (3)	C67—C69—H69A	109.5
C86—O83—Cr8	134.6 (3)	C67—C69—H69B	109.5
C86—O84—Cr1	130.3 (3)	H69A—C69—H69B	109.5
O11—C11—O12	126.0 (4)	C67—C69—H69C	109.5
O11—C11—C12	117.5 (4)	H69A—C69—H69C	109.5
O12—C11—C12	116.4 (4)	H69B—C69—H69C	109.5
C15—C12—C14B	129.1 (8)	C67—C70—H70A	109.5
C15—C12—C11	113.9 (6)	C67—C70—H70B	109.5
C14B—C12—C11	117.0 (7)	H70A—C70—H70B	109.5
C15—C12—C14	110.4 (3)	C67—C70—H70C	109.5
C14B—C12—C14	54.6 (6)	H70A—C70—H70C	109.5
C11—C12—C14	103.4 (6)	H70B—C70—H70C	109.5
C15—C12—C13	110.3 (3)	C67—C68B—H68D	109.5
C14B—C12—C13	54.6 (6)	C67—C68B—H68E	109.5

C11—C12—C13	109.6 (6)	H68D—C68B—H68E	109.5
C14—C12—C13	109.1 (3)	C67—C68B—H68F	109.5
C15—C12—C13B	58.3 (7)	H68D—C68B—H68F	109.5
C14B—C12—C13B	109.4 (3)	H68E—C68B—H68F	109.5
C11—C12—C13B	105.4 (8)	C67—C69B—H69D	109.5
C14—C12—C13B	151.2 (8)	C67—C69B—H69E	109.5
C13—C12—C13B	59.3 (6)	H69D—C69B—H69E	109.5
C15—C12—C15B	50.4 (7)	C67—C69B—H69F	109.5
C14B—C12—C15B	109.1 (3)	H69D—C69B—H69F	109.5
C11—C12—C15B	107.3 (8)	H69E—C69B—H69F	109.5
C14—C12—C15B	63.5 (6)	C67—C70B—H70D	109.5
C13—C12—C15B	143.0 (8)	C67—C70B—H70E	109.5
C13B—C12—C15B	108.4 (3)	H70D—C70B—H70E	109.5
C12—C13—H13A	109.5	C67—C70B—H70F	109.5
C12—C13—H13B	109.5	H70D—C70B—H70F	109.5
H13A—C13—H13B	109.5	H70E—C70B—H70F	109.5
C12—C13—H13C	109.5	O71—C71—O72	125.9 (4)
H13A—C13—H13C	109.5	O71—C71—C72	113.9 (4)
H13B—C13—H13C	109.5	O72—C71—C72	120.2 (4)
C12—C14—H14A	109.5	C74—C72—C73	110.1 (3)
C12—C14—H14B	109.5	C74—C72—C75	109.8 (3)
H14A—C14—H14B	109.5	C73—C72—C75	109.2 (3)
C12—C14—H14C	109.5	C74—C72—C71	110.7 (5)
H14A—C14—H14C	109.5	C73—C72—C71	110.1 (4)
H14B—C14—H14C	109.5	C75—C72—C71	106.9 (4)
C12—C15—H15A	109.5	C72—C73—H73A	109.5
C12—C15—H15B	109.5	C72—C73—H73B	109.5
H15A—C15—H15B	109.5	H73A—C73—H73B	109.5
C12—C15—H15C	109.5	C72—C73—H73C	109.5
H15A—C15—H15C	109.5	H73A—C73—H73C	109.5
H15B—C15—H15C	109.5	H73B—C73—H73C	109.5
C12—C13B—H13D	109.5	C72—C74—H74A	109.5
C12—C13B—H13E	109.5	C72—C74—H74B	109.5
H13D—C13B—H13E	109.5	H74A—C74—H74B	109.5
C12—C13B—H13F	109.5	C72—C74—H74C	109.5
H13D—C13B—H13F	109.5	H74A—C74—H74C	109.5
H13E—C13B—H13F	109.5	H74B—C74—H74C	109.5
C12—C14B—H14D	109.5	C72—C75—H75A	109.5
C12—C14B—H14E	109.5	C72—C75—H75B	109.5
H14D—C14B—H14E	109.5	H75A—C75—H75B	109.5
C12—C14B—H14F	109.5	C72—C75—H75C	109.5
H14D—C14B—H14F	109.5	H75A—C75—H75C	109.5
H14E—C14B—H14F	109.5	H75B—C75—H75C	109.5
C12—C15B—H15D	109.5	O73—C76—O74	125.6 (4)
C12—C15B—H15E	109.5	O73—C76—C77	116.9 (3)
H15D—C15B—H15E	109.5	O74—C76—C77	117.4 (4)
C12—C15B—H15F	109.5	C78—C77—C79	109.9 (2)
H15D—C15B—H15F	109.5	C78—C77—C80	109.9 (2)

H15E—C15B—H15F	109.5	C79—C77—C80	109.7 (2)
O14—C16—O13	126.1 (4)	C78—C77—C76	106.8 (4)
O14—C16—C17	119.4 (4)	C79—C77—C76	108.4 (4)
O13—C16—C17	114.4 (4)	C80—C77—C76	112.1 (3)
C20—C17—C19A	119.4 (11)	C77—C78—H78A	109.5
C20—C17—C18A	65.1 (7)	C77—C78—H78B	109.5
C19A—C17—C18A	109.6 (3)	H78A—C78—H78B	109.5
C20—C17—C19	109.9 (3)	C77—C78—H78C	109.5
C19A—C17—C19	44.1 (7)	H78A—C78—H78C	109.5
C18A—C17—C19	149.4 (9)	H78B—C78—H78C	109.5
C20—C17—C20A	43.5 (7)	C77—C79—H79A	109.5
C19A—C17—C20A	109.1 (3)	C77—C79—H79B	109.5
C18A—C17—C20A	108.4 (3)	H79A—C79—H79B	109.5
C19—C17—C20A	75.4 (7)	C77—C79—H79C	109.5
C20—C17—C18	109.3 (3)	H79A—C79—H79C	109.5
C19A—C17—C18	64.0 (7)	H79B—C79—H79C	109.5
C18A—C17—C18	52.4 (7)	C77—C80—H80A	109.5
C19—C17—C18	107.8 (3)	C77—C80—H80B	109.5
C20A—C17—C18	147.2 (8)	H80A—C80—H80B	109.5
C20—C17—C16	114.7 (7)	C77—C80—H80C	109.5
C19A—C17—C16	124.6 (10)	H80A—C80—H80C	109.5
C18A—C17—C16	102.5 (8)	H80B—C80—H80C	109.5
C19—C17—C16	106.5 (5)	O81—C81—O82	125.7 (4)
C20A—C17—C16	101.5 (8)	O81—C81—C82	116.2 (4)
C18—C17—C16	108.4 (6)	O82—C81—C82	118.1 (4)
C17—C18—H18A	109.5	C84—C82—C81	110.4 (4)
C17—C18—H18B	109.5	C84—C82—C83	110.0 (2)
H18A—C18—H18B	109.5	C81—C82—C83	107.6 (3)
C17—C18—H18C	109.5	C84—C82—C85	110.1 (2)
H18A—C18—H18C	109.5	C81—C82—C85	108.7 (4)
H18B—C18—H18C	109.5	C83—C82—C85	110.0 (2)
C17—C19—H19A	109.5	C82—C83—H83A	109.5
C17—C19—H19B	109.5	C82—C83—H83B	109.5
H19A—C19—H19B	109.5	H83A—C83—H83B	109.5
C17—C19—H19C	109.5	C82—C83—H83C	109.5
H19A—C19—H19C	109.5	H83A—C83—H83C	109.5
H19B—C19—H19C	109.5	H83B—C83—H83C	109.5
C17—C20—H20A	109.5	C82—C84—H84A	109.5
C17—C20—H20B	109.5	C82—C84—H84B	109.5
H20A—C20—H20B	109.5	H84A—C84—H84B	109.5
C17—C20—H20C	109.5	C82—C84—H84C	109.5
H20A—C20—H20C	109.5	H84A—C84—H84C	109.5
H20B—C20—H20C	109.5	H84B—C84—H84C	109.5
C17—C18A—H18D	109.5	C82—C85—H85A	109.5
C17—C18A—H18E	109.5	C82—C85—H85B	109.5
H18D—C18A—H18E	109.5	H85A—C85—H85B	109.5
C17—C18A—H18F	109.5	C82—C85—H85C	109.5
H18D—C18A—H18F	109.5	H85A—C85—H85C	109.5

H18E—C18A—H18F	109.5	H85B—C85—H85C	109.5
C17—C19A—H19D	109.5	O84—C86—O83	125.7 (4)
C17—C19A—H19E	109.5	O84—C86—C87	117.3 (3)
H19D—C19A—H19E	109.5	O83—C86—C87	117.0 (4)
C17—C19A—H19F	109.5	C89—C87—C88B	123.3 (8)
H19D—C19A—H19F	109.5	C89—C87—C90	110.3 (3)
H19E—C19A—H19F	109.5	C88B—C87—C90	70.9 (6)
C17—C20A—H20D	109.5	C89—C87—C86	114.1 (5)
C17—C20A—H20E	109.5	C88B—C87—C86	119.7 (7)
H20D—C20A—H20E	109.5	C90—C87—C86	106.3 (5)
C17—C20A—H20F	109.5	C89—C87—C88	109.9 (3)
H20D—C20A—H20F	109.5	C88B—C87—C88	38.1 (6)
H20E—C20A—H20F	109.5	C90—C87—C88	109.0 (3)
O21—C21—O22	126.0 (4)	C86—C87—C88	107.1 (5)
O21—C21—C22	119.0 (4)	C89—C87—C90B	73.1 (5)
O22—C21—C22	115.0 (4)	C88B—C87—C90B	109.1 (3)
C21—C22—C25	107.6 (4)	C90—C87—C90B	43.1 (5)
C21—C22—C24	111.1 (4)	C86—C87—C90B	103.4 (7)
C25—C22—C24	110.0 (3)	C88—C87—C90B	144.2 (7)
C21—C22—C23	109.4 (4)	C89—C87—C89B	35.2 (5)
C25—C22—C23	109.4 (3)	C88B—C87—C89B	109.0 (3)
C24—C22—C23	109.3 (3)	C90—C87—C89B	140.8 (7)
C22—C23—H23A	109.5	C86—C87—C89B	106.8 (6)
C22—C23—H23B	109.5	C88—C87—C89B	80.4 (6)
H23A—C23—H23B	109.5	C90B—C87—C89B	108.3 (3)
C22—C23—H23C	109.5	C87—C88—H88A	109.5
H23A—C23—H23C	109.5	C87—C88—H88B	109.5
H23B—C23—H23C	109.5	H88A—C88—H88B	109.5
C22—C24—H24A	109.5	C87—C88—H88C	109.5
C22—C24—H24B	109.5	H88A—C88—H88C	109.5
H24A—C24—H24B	109.5	H88B—C88—H88C	109.5
C22—C24—H24C	109.5	C87—C89—H89A	109.5
H24A—C24—H24C	109.5	C87—C89—H89B	109.5
H24B—C24—H24C	109.5	H89A—C89—H89B	109.5
C22—C25—H25A	109.5	C87—C89—H89C	109.5
C22—C25—H25B	109.5	H89A—C89—H89C	109.5
H25A—C25—H25B	109.5	H89B—C89—H89C	109.5
C22—C25—H25C	109.5	C87—C90—H90A	109.5
H25A—C25—H25C	109.5	C87—C90—H90B	109.5
H25B—C25—H25C	109.5	H90A—C90—H90B	109.5
O23—C26—O24	125.6 (4)	C87—C90—H90C	109.5
O23—C26—C27	118.6 (3)	H90A—C90—H90C	109.5
O24—C26—C27	115.8 (3)	H90B—C90—H90C	109.5
C30—C27—C26	108.3 (4)	C87—C88B—H88D	109.5
C30—C27—C28	109.8 (3)	C87—C88B—H88E	109.5
C26—C27—C28	111.8 (4)	H88D—C88B—H88E	109.5
C30—C27—C29	109.5 (3)	C87—C88B—H88F	109.5
C26—C27—C29	108.4 (4)	H88D—C88B—H88F	109.5

C28—C27—C29	109.0 (3)	H88E—C88B—H88F	109.5
C27—C28—H28A	109.5	C87—C89B—H89D	109.5
C27—C28—H28B	109.5	C87—C89B—H89E	109.5
H28A—C28—H28B	109.5	H89D—C89B—H89E	109.5
C27—C28—H28C	109.5	C87—C89B—H89F	109.5
H28A—C28—H28C	109.5	H89D—C89B—H89F	109.5
H28B—C28—H28C	109.5	H89E—C89B—H89F	109.5
C27—C29—H29A	109.5	C87—C90B—H90D	109.5
C27—C29—H29B	109.5	C87—C90B—H90E	109.5
H29A—C29—H29B	109.5	H90D—C90B—H90E	109.5
C27—C29—H29C	109.5	C87—C90B—H90F	109.5
H29A—C29—H29C	109.5	H90D—C90B—H90F	109.5
H29B—C29—H29C	109.5	H90E—C90B—H90F	109.5
C27—C30—H30A	109.5	O2A—C2A—C1A	94.3 (9)
C27—C30—H30B	109.5	O2A—C2A—H2A1	112.9
H30A—C30—H30B	109.5	C1A—C2A—H2A1	112.9
C27—C30—H30C	109.5	O2A—C2A—H2A2	112.9
H30A—C30—H30C	109.5	C1A—C2A—H2A2	112.9
H30B—C30—H30C	109.5	H2A1—C2A—H2A2	110.3
O31—C31—O32	125.4 (4)	N1—C1A—C2A	111.8 (13)
O31—C31—C32	117.0 (4)	N1—C1A—H1A1	109.3
O32—C31—C32	117.6 (4)	C2A—C1A—H1A1	109.3
C31—C32—C33	110.8 (4)	N1—C1A—H1A2	109.3
C31—C32—C34	109.9 (4)	C2A—C1A—H1A2	109.3
C33—C32—C34	110.2 (2)	H1A1—C1A—H1A2	107.9
C31—C32—C35	106.5 (4)	C1A—N1—C1B	129.0 (12)
C33—C32—C35	109.6 (3)	C1A—N1—H1A	105.0
C34—C32—C35	109.7 (3)	C1B—N1—H1A	105.0
C32—C33—H33A	109.5	C1A—N1—H1B	105.0
C32—C33—H33B	109.5	C1B—N1—H1B	105.0
H33A—C33—H33B	109.5	H1A—N1—H1B	105.9
C32—C33—H33C	109.5	N1—C1B—C2B	136.6 (14)
H33A—C33—H33C	109.5	N1—C1B—H1B1	103.0
H33B—C33—H33C	109.5	C2B—C1B—H1B1	103.0
C32—C34—H34A	109.5	N1—C1B—H1B2	103.0
C32—C34—H34B	109.5	C2B—C1B—H1B2	103.0
H34A—C34—H34B	109.5	H1B1—C1B—H1B2	105.1
C32—C34—H34C	109.5	O2B—C2B—C1B	106.1 (11)
H34A—C34—H34C	109.5	O2B—C2B—H2B1	110.5
H34B—C34—H34C	109.5	C1B—C2B—H2B1	110.5
C32—C35—H35A	109.5	O2B—C2B—H2B2	110.5
C32—C35—H35B	109.5	C1B—C2B—H2B2	110.5
H35A—C35—H35B	109.5	H2B1—C2B—H2B2	108.7
C32—C35—H35C	109.5	O2C—C2C—C1C	101.2 (18)
H35A—C35—H35C	109.5	O2C—C2C—H2C1	111.5
H35B—C35—H35C	109.5	C1C—C2C—H2C1	111.5
O34—C36—O33	126.1 (4)	O2C—C2C—H2C2	111.5
O34—C36—C37	116.8 (4)	C1C—C2C—H2C2	111.5

O33—C36—C37	117.1 (4)	H2C1—C2C—H2C2	109.3
C39—C37—C40	109.9 (3)	C2C—C1C—N1C	111 (3)
C39—C37—C36	112.6 (6)	C2C—C1C—H1C1	109.5
C40—C37—C36	109.7 (4)	N1C—C1C—H1C1	109.5
C39—C37—C38	109.3 (3)	C2C—C1C—H1C2	109.5
C40—C37—C38	109.4 (3)	N1C—C1C—H1C2	109.5
C36—C37—C38	105.9 (5)	H1C1—C1C—H1C2	108.1
C37—C38—H38A	109.5	C1D—N1C—C1C	124 (2)
C37—C38—H38B	109.5	C1D—N1C—H1C3	106.4
H38A—C38—H38B	109.5	C1C—N1C—H1C3	106.4
C37—C38—H38C	109.5	C1D—N1C—H1C4	106.4
H38A—C38—H38C	109.5	C1C—N1C—H1C4	106.4
H38B—C38—H38C	109.5	H1C3—N1C—H1C4	106.5
C37—C39—H39A	109.5	N1C—C1D—C2D	147 (3)
C37—C39—H39B	109.5	N1C—C1D—H1D1	100.1
H39A—C39—H39B	109.5	C2D—C1D—H1D1	100.1
C37—C39—H39C	109.5	N1C—C1D—H1D2	100.1
H39A—C39—H39C	109.5	C2D—C1D—H1D2	100.1
H39B—C39—H39C	109.5	H1D1—C1D—H1D2	104.2
C37—C40—H40A	109.5	O2D—C2D—C1D	103.5 (18)
C37—C40—H40B	109.5	O2D—C2D—H2D1	111.1
H40A—C40—H40B	109.5	C1D—C2D—H2D1	111.1
C37—C40—H40C	109.5	O2D—C2D—H2D2	111.1
H40A—C40—H40C	109.5	C1D—C2D—H2D2	111.1
H40B—C40—H40C	109.5	H2D1—C2D—H2D2	109.0
O42—C41—O41	125.3 (4)	O2E—C2E—C1E	111.8 (18)
O42—C41—C42	118.1 (3)	O2E—C2E—H2E1	109.3
O41—C41—C42	116.6 (3)	C1E—C2E—H2E1	109.3
C43—C42—C45	110.0 (2)	O2E—C2E—H2E2	109.3
C43—C42—C44	109.6 (2)	C1E—C2E—H2E2	109.3
C45—C42—C44	109.7 (2)	H2E1—C2E—H2E2	107.9
C43—C42—C41	109.2 (3)	N1E—C1E—C2E	150 (3)
C45—C42—C41	106.9 (4)	N1E—C1E—H1E1	99.3
C44—C42—C41	111.4 (4)	C2E—C1E—H1E1	99.3
C42—C43—H43A	109.5	N1E—C1E—H1E2	99.3
C42—C43—H43B	109.5	C2E—C1E—H1E2	99.3
H43A—C43—H43B	109.5	H1E1—C1E—H1E2	104.0
C42—C43—H43C	109.5	C1E—N1E—C1F	131.4 (19)
H43A—C43—H43C	109.5	C1E—N1E—H1E3	104.4
H43B—C43—H43C	109.5	C1F—N1E—H1E3	104.4
C42—C44—H44A	109.5	C1E—N1E—H1E4	104.4
C42—C44—H44B	109.5	C1F—N1E—H1E4	104.4
H44A—C44—H44B	109.5	H1E3—N1E—H1E4	105.6
C42—C44—H44C	109.5	C2F—C1F—N1E	124 (2)
H44A—C44—H44C	109.5	C2F—C1F—H1F1	106.2
H44B—C44—H44C	109.5	N1E—C1F—H1F1	106.2
C42—C45—H45A	109.5	C2F—C1F—H1F2	106.2
C42—C45—H45B	109.5	N1E—C1F—H1F2	106.2

H45A—C45—H45B	109.5	H1F1—C1F—H1F2	106.4
C42—C45—H45C	109.5	O2F—C2F—C1F	102.7 (16)
H45A—C45—H45C	109.5	O2F—C2F—H2F1	111.2
H45B—C45—H45C	109.5	C1F—C2F—H2F1	111.2
O43—C46—O44	125.2 (4)	O2F—C2F—H2F2	111.2
O43—C46—C47	117.1 (3)	C1F—C2F—H2F2	111.2
O44—C46—C47	117.7 (4)	H2F1—C2F—H2F2	109.1
C49—C47—C48	110.2 (3)	O99^{i}—O99—C99	112.0 (14)
C49—C47—C46	107.2 (4)	O98—C99—C98	152 (3)
C48—C47—C46	111.5 (4)	O98—C99—O99	106 (2)
C49—C47—C50	109.7 (3)	C98—C99—O99	102.0 (17)
C48—C47—C50	109.4 (2)	C99—C98—H98A	109.5
C46—C47—C50	108.8 (4)	C99—C98—H98B	109.5
C47—C48—H48A	109.5	H98A—C98—H98B	109.5
C47—C48—H48B	109.5	C99—C98—H98C	109.5
H48A—C48—H48B	109.5	H98A—C98—H98C	109.5
C47—C48—H48C	109.5	H98B—C98—H98C	109.5
H48A—C48—H48C	109.5		

F2—Cr2—F1—Cr1	142.52 (15)	O83—Cr8—O81—C81	−56.9 (4)
O12—Cr2—F1—Cr1	−38.35 (16)	O72—Cr8—O81—C81	−143.7 (4)
O14—Cr2—F1—Cr1	54.95 (17)	O74—Cr8—O81—C81	124.1 (4)
O21—Cr2—F1—Cr1	160 (6)	F8—Cr1—O82—C81	7.1 (4)
O23—Cr2—F1—Cr1	−125.70 (15)	O84—Cr1—O82—C81	98.1 (4)
F8—Cr1—F1—Cr2	−129.30 (15)	O11—Cr1—O82—C81	−174.1 (4)
O84—Cr1—F1—Cr2	139.79 (16)	F1—Cr1—O82—C81	−111 (3)
O11—Cr1—F1—Cr2	51.89 (17)	O13—Cr1—O82—C81	−81.2 (4)
O82—Cr1—F1—Cr2	−11 (3)	F8—Cr8—O83—C86	−1.6 (4)
O13—Cr1—F1—Cr2	−40.90 (16)	F7—Cr8—O83—C86	−87.9 (4)
F3—Cr3—F2—Cr2	−144.00 (15)	O81—Cr8—O83—C86	89.8 (4)
O31—Cr3—F2—Cr2	−56 (5)	O72—Cr8—O83—C86	178.9 (4)
O22—Cr3—F2—Cr2	35.97 (17)	O74—Cr8—O83—C86	−166 (8)
O24—Cr3—F2—Cr2	−54.32 (16)	F8—Cr1—O84—C86	43.7 (4)
O33—Cr3—F2—Cr2	124.96 (16)	O11—Cr1—O84—C86	−137.5 (4)
F1—Cr2—F2—Cr3	128.26 (15)	F1—Cr1—O84—C86	131.8 (4)
O12—Cr2—F2—Cr3	−13 (6)	O82—Cr1—O84—C86	−49.2 (4)
O14—Cr2—F2—Cr3	−140.31 (16)	O13—Cr1—O84—C86	−11 (8)
O21—Cr2—F2—Cr3	−51.34 (16)	Cr1—O11—C11—O12	7.0 (7)
O23—Cr2—F2—Cr3	37.55 (16)	Cr1—O11—C11—C12	−170.9 (3)
F2—Cr3—F3—Cr4	−131.21 (15)	Cr2—O12—C11—O11	21.3 (7)
O31—Cr3—F3—Cr4	50.34 (17)	Cr2—O12—C11—C12	−160.8 (3)
O22—Cr3—F3—Cr4	50 (3)	O11—C11—C12—C15	−50.2 (6)
O24—Cr3—F3—Cr4	138.15 (17)	O12—C11—C12—C15	131.7 (5)
O33—Cr3—F3—Cr4	−41.88 (18)	O11—C11—C12—C14B	126.4 (7)
F4—Cr4—F3—Cr3	143.88 (16)	O12—C11—C12—C14B	−51.6 (7)
O41—Cr4—F3—Cr3	153 (9)	O11—C11—C12—C14	69.5 (6)
O32—Cr4—F3—Cr3	−37.58 (18)	O12—C11—C12—C14	−108.5 (5)
O34—Cr4—F3—Cr3	54.41 (17)	O11—C11—C12—C13	−174.2 (5)

O43—Cr4—F3—Cr3	−124.55 (16)	O12—C11—C12—C13	7.7 (6)
F5—Cr5—F4—Cr4	−142.77 (14)	O11—C11—C12—C13B	−111.9 (7)
O51—Cr5—F4—Cr4	−18 (6)	O12—C11—C12—C13B	70.1 (7)
O42—Cr5—F4—Cr4	37.33 (15)	O11—C11—C12—C15B	3.5 (7)
O44—Cr5—F4—Cr4	−54.54 (15)	O12—C11—C12—C15B	−174.6 (6)
O53—Cr5—F4—Cr4	125.16 (15)	Cr2—O14—C16—O13	11.2 (7)
F3—Cr4—F4—Cr5	127.87 (14)	Cr2—O14—C16—C17	−166.0 (3)
O41—Cr4—F4—Cr5	−51.98 (17)	Cr1—O13—C16—O14	16.1 (7)
O32—Cr4—F4—Cr5	4 (4)	Cr1—O13—C16—C17	−166.5 (3)
O34—Cr4—F4—Cr5	−142.11 (16)	O14—C16—C17—C20	6.8 (7)
O43—Cr4—F4—Cr5	39.92 (15)	O13—C16—C17—C20	−170.8 (5)
F4—Cr5—F5—Cr6	−129.51 (14)	O14—C16—C17—C19A	−160.2 (9)
O51—Cr5—F5—Cr6	51.38 (15)	O13—C16—C17—C19A	22.2 (10)
O42—Cr5—F5—Cr6	47 (4)	O14—C16—C17—C18A	74.9 (8)
O44—Cr5—F5—Cr6	140.25 (15)	O13—C16—C17—C18A	−102.7 (8)
O53—Cr5—F5—Cr6	−40.20 (15)	O14—C16—C17—C19	−115.1 (5)
F6—Cr6—F5—Cr5	146.17 (14)	O13—C16—C17—C19	67.3 (6)
O61—Cr6—F5—Cr5	115 (2)	O14—C16—C17—C20A	−37.1 (8)
O63—Cr6—F5—Cr5	−121.30 (15)	O13—C16—C17—C20A	145.3 (7)
O54—Cr6—F5—Cr5	56.11 (15)	O14—C16—C17—C18	129.1 (5)
O52—Cr6—F5—Cr5	−34.07 (15)	O13—C16—C17—C18	−48.5 (6)
F5—Cr6—F6—Cr7	127.31 (14)	Cr2—O21—C21—O22	−18.2 (7)
O61—Cr6—F6—Cr7	−54.26 (15)	Cr2—O21—C21—C22	162.8 (3)
O63—Cr6—F6—Cr7	38.25 (15)	Cr3—O22—C21—O21	−12.7 (8)
O54—Cr6—F6—Cr7	−143.21 (15)	Cr3—O22—C21—C22	166.4 (3)
O52—Cr6—F6—Cr7	26 (25)	O21—C21—C22—C25	−118.0 (4)
F7—Cr7—F6—Cr6	−144.23 (14)	O22—C21—C22—C25	62.8 (5)
O71—Cr7—F6—Cr6	−67 (4)	O21—C21—C22—C24	2.6 (6)
O73—Cr7—F6—Cr6	123.06 (15)	O22—C21—C22—C24	−176.6 (4)
O62—Cr7—F6—Cr6	36.63 (15)	O21—C21—C22—C23	123.3 (4)
O64—Cr7—F6—Cr6	−55.15 (15)	O22—C21—C22—C23	−55.8 (5)
O71—Cr7—F7—Cr8	53.04 (17)	Cr2—O23—C26—O24	−1.5 (7)
F6—Cr7—F7—Cr8	−128.59 (15)	Cr2—O23—C26—C27	−179.6 (3)
O73—Cr7—F7—Cr8	−39.58 (16)	Cr3—O24—C26—O23	−30.2 (6)
O62—Cr7—F7—Cr8	−9 (7)	Cr3—O24—C26—C27	148.0 (3)
O64—Cr7—F7—Cr8	141.44 (15)	O23—C26—C27—C30	−115.8 (4)
F8—Cr8—F7—Cr7	143.50 (15)	O24—C26—C27—C30	65.9 (4)
O81—Cr8—F7—Cr7	94.5 (18)	O23—C26—C27—C28	5.3 (5)
O83—Cr8—F7—Cr7	−123.46 (16)	O24—C26—C27—C28	−172.9 (4)
O72—Cr8—F7—Cr7	−36.70 (16)	O23—C26—C27—C29	125.5 (4)
O74—Cr8—F7—Cr7	55.50 (17)	O24—C26—C27—C29	−52.8 (5)
O84—Cr1—F8—Cr8	−53.43 (17)	Cr3—O31—C31—O32	6.8 (8)
O11—Cr1—F8—Cr8	−97 (5)	Cr3—O31—C31—C32	−174.6 (3)
F1—Cr1—F8—Cr8	−142.74 (16)	Cr4—O32—C31—O31	20.2 (8)
O82—Cr1—F8—Cr8	39.06 (18)	Cr4—O32—C31—C32	−158.4 (3)
O13—Cr1—F8—Cr8	125.64 (17)	O31—C31—C32—C33	23.0 (5)
F7—Cr8—F8—Cr1	129.53 (16)	O32—C31—C32—C33	−158.3 (4)
O81—Cr8—F8—Cr1	−53.22 (17)	O31—C31—C32—C34	145.0 (4)

O83—Cr8—F8—Cr1	39.83 (17)	O32—C31—C32—C34	−36.3 (5)
O72—Cr8—F8—Cr1	107 (15)	O31—C31—C32—C35	−96.2 (5)
O74—Cr8—F8—Cr1	−140.46 (18)	O32—C31—C32—C35	82.5 (5)
F8—Cr1—O11—C11	−84 (5)	Cr4—O34—C36—O33	9.5 (8)
O84—Cr1—O11—C11	−128.0 (4)	Cr4—O34—C36—C37	−167.6 (3)
F1—Cr1—O11—C11	−38.6 (4)	Cr3—O33—C36—O34	15.7 (9)
O82—Cr1—O11—C11	139.5 (4)	Cr3—O33—C36—C37	−167.2 (4)
O13—Cr1—O11—C11	53.0 (4)	O34—C36—C37—C39	−165.8 (5)
F1—Cr2—O12—C11	−3.6 (4)	O33—C36—C37—C39	16.9 (6)
F2—Cr2—O12—C11	138 (5)	O34—C36—C37—C40	−43.0 (6)
O14—Cr2—O12—C11	−95.1 (4)	O33—C36—C37—C40	139.6 (5)
O21—Cr2—O12—C11	176.0 (4)	O34—C36—C37—C38	74.9 (6)
O23—Cr2—O12—C11	87.0 (4)	O33—C36—C37—C38	−102.5 (5)
F8—Cr1—O13—C16	87.8 (4)	Cr5—O42—C41—O41	−19.0 (7)
O84—Cr1—O13—C16	143 (8)	Cr5—O42—C41—C42	160.5 (3)
O11—Cr1—O13—C16	−91.0 (4)	Cr4—O41—C41—O42	−10.8 (7)
F1—Cr1—O13—C16	−0.3 (4)	Cr4—O41—C41—C42	169.7 (3)
O82—Cr1—O13—C16	−179.2 (4)	O42—C41—C42—C43	130.1 (4)
F1—Cr2—O14—C16	−41.6 (4)	O41—C41—C42—C43	−50.3 (5)
F2—Cr2—O14—C16	−129.2 (4)	O42—C41—C42—C45	−111.0 (4)
O12—Cr2—O14—C16	51.9 (4)	O41—C41—C42—C45	68.6 (4)
O21—Cr2—O14—C16	139.7 (4)	O42—C41—C42—C44	8.9 (5)
O23—Cr2—O14—C16	156 (4)	O41—C41—C42—C44	−171.5 (4)
F1—Cr2—O21—C21	27 (6)	Cr4—O43—C46—O44	−24.4 (6)
F2—Cr2—O21—C21	44.3 (4)	Cr4—O43—C46—C47	154.3 (3)
O12—Cr2—O21—C21	−134.9 (4)	Cr5—O44—C46—O43	−5.4 (6)
O14—Cr2—O21—C21	131.9 (4)	Cr5—O44—C46—C47	176.0 (3)
O23—Cr2—O21—C21	−47.5 (4)	O43—C46—C47—C49	−72.4 (4)
F2—Cr3—O22—C21	2.6 (4)	O44—C46—C47—C49	106.4 (4)
F3—Cr3—O22—C21	−178 (100)	O43—C46—C47—C48	166.9 (3)
O31—Cr3—O22—C21	−178.9 (4)	O44—C46—C47—C48	−14.3 (5)
O24—Cr3—O22—C21	93.3 (4)	O43—C46—C47—C50	46.1 (4)
O33—Cr3—O22—C21	−86.7 (4)	O44—C46—C47—C50	−135.1 (4)
F1—Cr2—O23—C26	−90.0 (4)	Cr6—O52—C51—O51	16.1 (6)
F2—Cr2—O23—C26	−2.3 (4)	Cr6—O52—C51—C52	−168.6 (3)
O12—Cr2—O23—C26	176.6 (4)	Cr5—O51—C51—O52	18.7 (6)
O14—Cr2—O23—C26	73 (4)	Cr5—O51—C51—C52	−156.6 (3)
O21—Cr2—O23—C26	88.7 (4)	O52—C51—C52—C55	41.0 (5)
F2—Cr3—O24—C26	51.9 (3)	O51—C51—C52—C55	−143.3 (4)
F3—Cr3—O24—C26	141.2 (3)	O52—C51—C52—C54	164.5 (3)
O31—Cr3—O24—C26	−128.2 (4)	O51—C51—C52—C54	−19.8 (5)
O22—Cr3—O24—C26	−41.2 (4)	O52—C51—C52—C53	−77.5 (4)
O33—Cr3—O24—C26	−37 (12)	O51—C51—C52—C53	98.2 (4)
F2—Cr3—O31—C31	−125 (4)	Cr6—O54—C56—O53	18.0 (5)
F3—Cr3—O31—C31	−37.1 (4)	Cr6—O54—C56—C57	−161.5 (3)
O22—Cr3—O31—C31	142.9 (4)	Cr5—O53—C56—O54	13.8 (6)
O24—Cr3—O31—C31	−126.7 (4)	Cr5—O53—C56—C57	−166.7 (3)
O33—Cr3—O31—C31	54.0 (4)	O54—C56—C57—C58	130.2 (4)

F4—Cr4—O32—C31	121 (4)	O53—C56—C57—C58	−49.4 (5)
F3—Cr4—O32—C31	−3.6 (5)	O54—C56—C57—C59B	−40.4 (6)
O41—Cr4—O32—C31	176.2 (5)	O53—C56—C57—C59B	140.0 (6)
O34—Cr4—O32—C31	−93.7 (5)	O54—C56—C57—C60B	−168.2 (6)
O43—Cr4—O32—C31	84.3 (5)	O53—C56—C57—C60B	12.2 (6)
F2—Cr3—O33—C36	90.3 (5)	O54—C56—C57—C59	7.5 (5)
F3—Cr3—O33—C36	1.0 (5)	O53—C56—C57—C59	−172.1 (4)
O31—Cr3—O33—C36	−89.7 (5)	O54—C56—C57—C60	−111.2 (4)
O22—Cr3—O33—C36	−176.6 (5)	O53—C56—C57—C60	69.3 (4)
O24—Cr3—O33—C36	179 (100)	O54—C56—C57—C58B	76.2 (6)
F4—Cr4—O34—C36	−126.6 (5)	O53—C56—C57—C58B	−103.4 (6)
F3—Cr4—O34—C36	−38.6 (5)	Cr7—O62—C61—O61	−27.8 (6)
O41—Cr4—O34—C36	142.4 (5)	Cr7—O62—C61—C62	153.7 (3)
O32—Cr4—O34—C36	54.4 (5)	Cr6—O61—C61—O62	−7.7 (6)
O43—Cr4—O34—C36	−11 (4)	Cr6—O61—C61—C62	170.8 (3)
F4—Cr4—O41—C41	40.5 (4)	O62—C61—C62—C63	−138.2 (4)
F3—Cr4—O41—C41	32 (9)	O61—C61—C62—C63	43.2 (5)
O32—Cr4—O41—C41	−138.0 (4)	O62—C61—C62—C65	103.5 (4)
O34—Cr4—O41—C41	130.0 (4)	O61—C61—C62—C65	−75.1 (4)
O43—Cr4—O41—C41	−51.0 (4)	O62—C61—C62—C64	−15.8 (5)
F5—Cr5—O42—C41	−172 (34)	O61—C61—C62—C64	165.6 (4)
F4—Cr5—O42—C41	4.5 (4)	Cr7—O64—C66—O63	−19.2 (6)
O51—Cr5—O42—C41	−176.4 (4)	Cr7—O64—C66—C67	161.0 (3)
O44—Cr5—O42—C41	94.8 (4)	Cr6—O63—C66—O64	−14.7 (6)
O53—Cr5—O42—C41	−84.8 (4)	Cr6—O63—C66—C67	165.2 (3)
F4—Cr4—O43—C46	5.8 (4)	O64—C66—C67—C69	−3.3 (5)
F3—Cr4—O43—C46	−82.1 (4)	O63—C66—C67—C69	176.8 (4)
O41—Cr4—O43—C46	96.9 (4)	O64—C66—C67—C69B	163.0 (12)
O32—Cr4—O43—C46	−175.2 (4)	O63—C66—C67—C69B	−16.8 (12)
O34—Cr4—O43—C46	−110 (4)	O64—C66—C67—C68	−126.7 (4)
F5—Cr5—O44—C46	128.1 (4)	O63—C66—C67—C68	53.4 (5)
F4—Cr5—O44—C46	38.8 (4)	O64—C66—C67—C70B	26.8 (8)
O51—Cr5—O44—C46	−140.6 (4)	O63—C66—C67—C70B	−153.1 (8)
O42—Cr5—O44—C46	−53.5 (4)	O64—C66—C67—C68B	−83.0 (9)
O53—Cr5—O44—C46	6 (17)	O63—C66—C67—C68B	97.1 (8)
F5—Cr5—O51—C51	−47.1 (3)	O64—C66—C67—C70	116.2 (4)
F4—Cr5—O51—C51	−172 (100)	O63—C66—C67—C70	−63.7 (5)
O42—Cr5—O51—C51	132.8 (3)	Cr7—O71—C71—O72	9.9 (7)
O44—Cr5—O51—C51	−135.3 (3)	Cr7—O71—C71—C72	−173.9 (3)
O53—Cr5—O51—C51	45.0 (3)	Cr8—O72—C71—O71	23.0 (7)
F6—Cr6—O52—C51	95 (25)	Cr8—O72—C71—C72	−153.0 (3)
F5—Cr6—O52—C51	−6.7 (4)	O71—C71—C72—C74	162.8 (4)
O61—Cr6—O52—C51	174.8 (4)	O72—C71—C72—C74	−20.7 (5)
O63—Cr6—O52—C51	82.3 (4)	O71—C71—C72—C73	40.9 (5)
O54—Cr6—O52—C51	−96.2 (4)	O72—C71—C72—C73	−142.6 (4)
F5—Cr5—O53—C56	−1.8 (3)	O71—C71—C72—C75	−77.6 (4)
F4—Cr5—O53—C56	87.4 (3)	O72—C71—C72—C75	98.8 (5)
O51—Cr5—O53—C56	−93.2 (4)	Cr7—O73—C76—O74	14.4 (7)

O42—Cr5—O53—C56	179.8 (4)	Cr7—O73—C76—C77	−168.4 (3)
O44—Cr5—O53—C56	121 (16)	Cr8—O74—C76—O73	17.8 (7)
F6—Cr6—O54—C56	−133.0 (3)	Cr8—O74—C76—C77	−159.5 (3)
F5—Cr6—O54—C56	−46.4 (3)	O73—C76—C77—C78	−66.8 (4)
O61—Cr6—O54—C56	136.2 (3)	O74—C76—C77—C78	110.7 (4)
O63—Cr6—O54—C56	17 (3)	O73—C76—C77—C79	51.6 (4)
O52—Cr6—O54—C56	47.1 (3)	O74—C76—C77—C79	−131.0 (4)
F6—Cr6—O61—C61	42.9 (3)	O73—C76—C77—C80	172.8 (3)
F5—Cr6—O61—C61	74 (2)	O74—C76—C77—C80	−9.7 (5)
O63—Cr6—O61—C61	−49.6 (4)	Cr8—O81—C81—O82	0.2 (7)
O54—Cr6—O61—C61	132.9 (3)	Cr8—O81—C81—C82	−179.5 (3)
O52—Cr6—O61—C61	−136.9 (3)	Cr1—O82—C81—O81	−28.9 (7)
F7—Cr7—O62—C61	−108 (7)	Cr1—O82—C81—C82	150.7 (3)
O71—Cr7—O62—C61	−170.7 (4)	O81—C81—C82—C84	−179.1 (4)
F6—Cr7—O62—C61	10.9 (4)	O82—C81—C82—C84	1.2 (5)
O73—Cr7—O62—C61	−78.1 (4)	O81—C81—C82—C83	60.8 (5)
O64—Cr7—O62—C61	100.9 (4)	O82—C81—C82—C83	−118.8 (4)
F6—Cr6—O63—C66	3.6 (4)	O81—C81—C82—C85	−58.2 (5)
F5—Cr6—O63—C66	−83.0 (4)	O82—C81—C82—C85	122.1 (4)
O61—Cr6—O63—C66	94.5 (4)	Cr1—O84—C86—O83	−16.2 (6)
O54—Cr6—O63—C66	−146 (2)	Cr1—O84—C86—C87	162.2 (3)
O52—Cr6—O63—C66	−176.4 (4)	Cr8—O83—C86—O84	−11.4 (7)
F7—Cr7—O64—C66	136.3 (3)	Cr8—O83—C86—C87	170.2 (3)
O71—Cr7—O64—C66	−132.5 (3)	O84—C86—C87—C89	8.8 (6)
F6—Cr7—O64—C66	47.9 (3)	O83—C86—C87—C89	−172.6 (5)
O73—Cr7—O64—C66	−14 (4)	O84—C86—C87—C88B	170.1 (7)
O62—Cr7—O64—C66	−44.2 (3)	O83—C86—C87—C88B	−11.4 (8)
F7—Cr7—O71—C71	−43.1 (4)	O84—C86—C87—C90	−113.0 (5)
F6—Cr7—O71—C71	−121 (4)	O83—C86—C87—C90	65.6 (5)
O73—Cr7—O71—C71	49.6 (4)	O84—C86—C87—C88	130.6 (5)
O62—Cr7—O71—C71	136.0 (4)	O83—C86—C87—C88	−50.8 (5)
O64—Cr7—O71—C71	−132.2 (4)	O84—C86—C87—C90B	−68.4 (7)
F8—Cr8—O72—C71	16 (15)	O83—C86—C87—C90B	110.1 (6)
F7—Cr8—O72—C71	−7.3 (4)	O84—C86—C87—C89B	45.7 (7)
O81—Cr8—O72—C71	175.5 (4)	O83—C86—C87—C89B	−135.7 (6)
O83—Cr8—O72—C71	82.5 (4)	O2A—C2A—C1A—N1	115.2 (15)
O74—Cr8—O72—C71	−97.3 (4)	C2A—C1A—N1—C1B	172.7 (15)
F7—Cr7—O73—C76	−2.2 (4)	C1A—N1—C1B—C2B	−166.7 (17)
O71—Cr7—O73—C76	−93.5 (4)	N1—C1B—C2B—O2B	−64 (3)
F6—Cr7—O73—C76	86.2 (4)	O2C—C2C—C1C—N1C	−107 (2)
O62—Cr7—O73—C76	178.3 (4)	C2C—C1C—N1C—C1D	−157 (2)
O64—Cr7—O73—C76	148 (4)	C1C—N1C—C1D—C2D	−113 (5)
F8—Cr8—O74—C76	−133.0 (4)	N1C—C1D—C2D—O2D	156 (4)
F7—Cr8—O74—C76	−46.7 (4)	O2E—C2E—C1E—N1E	10 (6)
O81—Cr8—O74—C76	135.6 (4)	C2E—C1E—N1E—C1F	−156 (4)
O83—Cr8—O74—C76	31 (9)	C1E—N1E—C1F—C2F	−146 (2)
O72—Cr8—O74—C76	46.5 (4)	N1E—C1F—C2F—O2F	−92 (3)

F8—Cr8—O81—C81	36.2 (4)	O99^{i}—O99—C99—O98	0.7 (14)
F7—Cr8—O81—C81	85.0 (18)	O99^{i}—O99—C99—C98	−179.2 (14)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.