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catena-Poly[[[pentaaquadysprosium(III)]-μ-5-azaniumylisophthalato] dichloride monohydrate]

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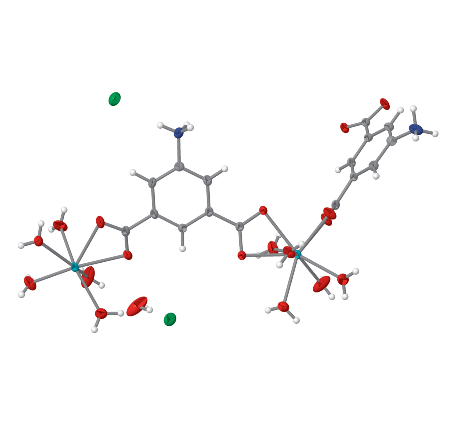
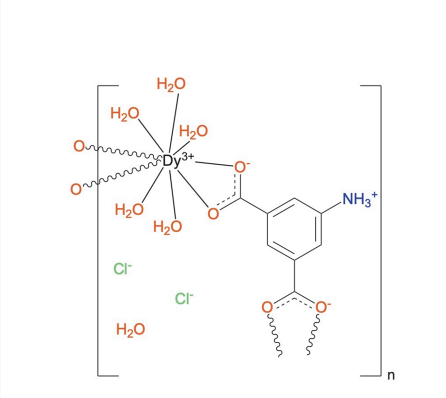
In the title compound, $\{[Dy(C_8H_6NO_4)(H_2O)_5]Cl_2{\cdot}H_2O\}_n$ the central Dy^{III} atom is nine-coordinated by four oxygen atoms from two symmetry-related chelating carboxylate groups and five water molecules, resulting in a distorted polyhedral geometry best described as 'muffin'-type by continuous shape measure analysis. The bridging ligands generate infinite [10$\bar{1}$] chains and the structure is consolidated by an extensive hydrogen-bonding network and weak π–π stacking interactions.

3D view



Chemical scheme



Structure description

Single-crystal X-ray diffraction analysis reveals that the title compound, (**I**), crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit consists of one Dy^{3+} ion, one 5-azaniumylisophthalate ligand ($C_8H_6NO_4^-$ or AIP^-), five coordinating water molecules, two chloride anions and one water molecule of crystallization (O6*W*). Both carboxylate groups of the AIP ligand are deprotonated and the amino group is protonated.

The metal ion in (**I**) exhibits a DyO_9 coordination environment (Fig. 1): four oxygen atoms (O1 + O2 and O3 + O4) originate from symmetry-related chelating carboxylate groups of two AIP^- ligands and the remaining atoms (O1*W*–O5*W*) arise from coordinating water molecules. The Dy—O bond lengths range from 2.362 (3) to 2.4770 (19) Å (Table 1) and the O—Dy—O bond angles span the range 52.67 (6)° to 147.25 (9)°. An analysis of the DyO_9 coordination polyhedron using the continuous shape measure (CShM) approach, as implemented in the *SHAPE* program (Casanova *et al.*, 2004), indicates that the DyO_9 environment in (**I**) is intermediate between several ideal polyhedra, with the lowest deviation corresponding to a muffin-type geometry with C_s local symmetry (Table 2 and Fig. 2).

Each AIP^- ligand chelates two symmetry-equivalent Dy^{3+} ions *via* its carboxylate groups, which leads to the formation of an infinite [10$\bar{1}$] zigzag polymeric chain (Fig. 3).

Table 1
Selected geometric parameters (Å, °).

Dy1—O1	2.446 (2)	Dy1—O4W	2.449 (4)
Dy1—O1W	2.362 (3)	Dy1—O5W	2.367 (3)
Dy1—O2	2.407 (2)	Dy1—O3^{i}	2.468 (2)
Dy1—O2W	2.396 (3)	Dy1—O4^{i}	2.4770 (19)
Dy1—O3W	2.423 (2)		
O1—Dy1—O2	53.71 (8)	O3^{i}—Dy1—O4^{i}	52.67 (6)

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

Table 2
Analysis of the shapes of the coordination polyhedron of the Dy^{3+} ion performed by the *SHAPE* program.

Shape	Deviation
Spherical-relaxed capped cube	9.13
Capped square antiprism	2.47
Spherical capped square antiprism	1.65
Tricapped trigonal prism	2.82
Spherical tricapped trigonal prism	1.62
Tridiminished icosahedron	11.27
Hula-hoop	10.29
Muffin	1.55

The shortest Dy···Dy separation within the chain is 9.8546 (5) Å while the shortest distance between chains is 6.2048 (4) Å. Otherwise, the geometrical parameters for (**I**) are consistent with reported values for similar compounds (Queirós *et al.*, 2021; Kariem *et al.*, 2017; Zhao *et al.*, 2012; Yan *et al.*, 2009; Ye *et al.*, 2008).

In the extended structure of (**I**), adjacent chains are cross-linked by an extensive hydrogen-bonding network featuring O—H···O, O—H···Cl, N—H···O and N—H···Cl interactions, some of which are bifurcated (Table 3) and slightly offset π–π stacking interactions between centrosymmetrically related phenyl rings [$Cg1\cdots Cg1$ = 3.4693 (18) Å, slippage = 1.237 Å] also occur. Collectively, these interactions generate a

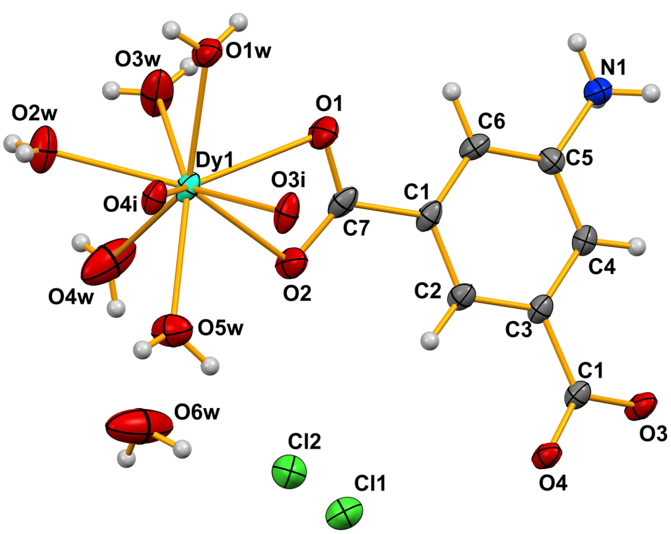


Figure 1
The asymmetric unit of (**I**) expanded to show the complete metal-ion coordination polyhedron with displacement ellipsoids for non-H atoms drawn at the 50% probability level. Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

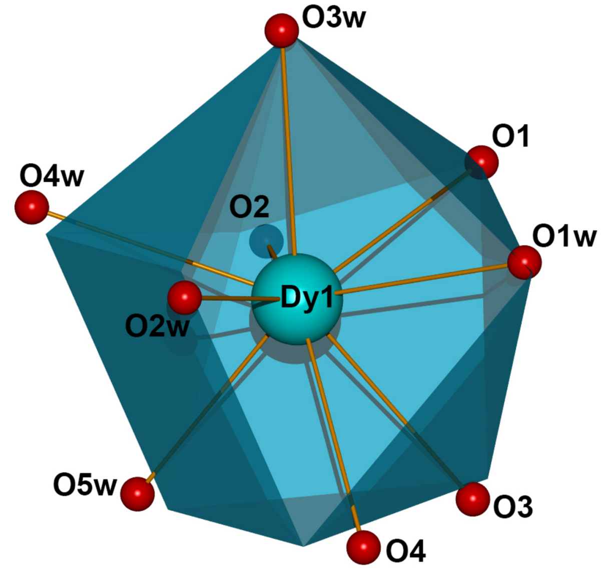


Figure 2
Distorted muffin-type coordination polyhedron of the nine-coordinate Dy1 atom in (**I**).

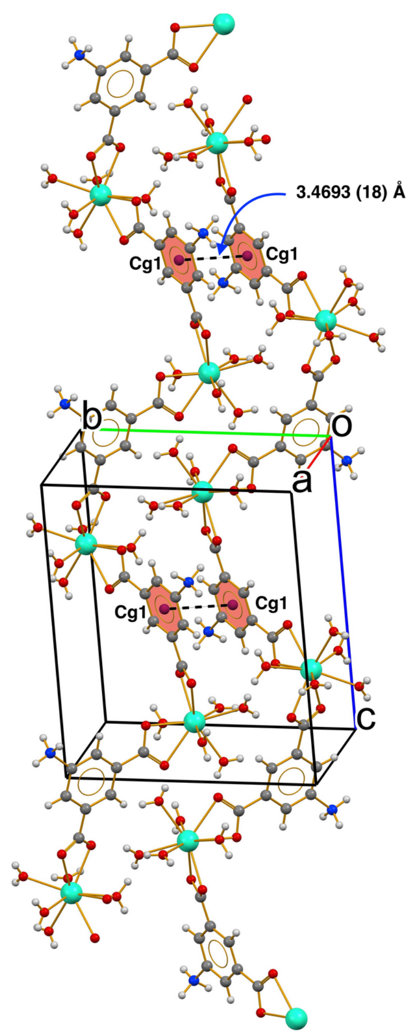


Figure 3
View of a fragment of an infinite [10$\overline{1}$] chain in (**I**) constructed by bridging AIP ligands and π–π stacking interactions represented as black dashed lines.

Table 3
Hydrogen-bond geometry (Å, °).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N1—H1*A*···Cl2^{ii}	0.90 (5)	2.24 (5)	3.127 (4)	166 (4)
N1—H1*B*···Cl1	0.86 (3)	2.29 (4)	3.141 (4)	171 (3)
N1—H1*C*···O2^{iii}	0.94 (5)	1.97 (4)	2.870 (4)	158 (4)
O1*W*—H1*WA*···O4^{iv}	0.77 (5)	1.95 (5)	2.718 (3)	175 (5)
O1*W*—H1*WB*···Cl2^{iv}	0.77 (5)	2.36 (5)	3.097 (3)	162 (4)
O2*W*—H2*WA*···Cl1^{v}	0.85 (6)	2.38 (6)	3.209 (3)	163 (4)
O2*W*—H2*WB*···O6*W*^{vi}	0.69 (6)	2.57 (6)	3.128 (5)	141 (7)
O3*W*—H3*WA*···Cl1^{v}	0.77 (5)	2.44 (5)	3.186 (3)	163 (4)
O3*W*—H3*WB*···O3^{iii}	0.75 (5)	2.12 (5)	2.780 (3)	148 (4)
O4*W*—H4*WA*···O6*W*	0.77 (5)	1.95 (5)	2.721 (5)	178 (5)
O4*W*—H4*WB*···Cl2^{vii}	0.75 (6)	2.81 (5)	3.261 (4)	122 (4)
O4*W*—H4*WB*···Cl1^{v}	0.75 (6)	2.64 (6)	3.273 (4)	144 (5)
O5*W*—H5*WA*···Cl1^{viii}	0.77 (5)	2.32 (5)	3.085 (3)	170 (4)
O5*W*—H5*WB*···Cl2	0.87 (6)	2.21 (6)	3.075 (3)	171 (5)
O6*W*—H6*WA*···O1*W*^{ix}	0.85	2.52	3.039 (4)	120
O6*W*—H6*WA*···O3^{x}	0.85	2.49	3.161 (4)	137
O6*W*—H6*WB*···Cl2	0.85	2.32	3.126 (4)	158

Symmetry codes: (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (vi) $-x+1, -y+1, -z$; (vii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (viii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ix) $x+1, y, z$; (x) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

three-dimensional supramolecular network. For packing views, see Figs. S1–S3 in the supporting information.

Synthesis and crystallization

A methanolic solution of 5-aminoisophthalic acid (0.181 g, 1.00 mmol in 10 ml methanol) was added dropwise, under stirring, to a separate methanolic solution of $DyCl_3·6H_2O$ (0.094 g, 0.25 mmol). Upon stirring for several minutes, the reaction mixture yielded a white precipitate, which was collected by filtration and discarded. The colourless filtrate was allowed to evaporate slowly at room temperature over the course of one week, resulting in the formation of colorless blocks of (**I**), suitable for X-ray diffraction analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4.

Acknowledgements

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Table 4
Experimental details.

Crystal data	
Chemical formula	$[Dy(C_8H_6NO_4)(H_2O)_5]Cl_2·H_2O$
M_r	521.63
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	8.7274 (2), 11.9281 (3), 15.4697 (4)
β (°)	100.480 (1)
V (Å^3)	1583.55 (7)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	5.10
Crystal size (mm)	0.13 × 0.12 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.675, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16994, 4086, 3470
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.022, 0.052, 1.01
No. of reflections	4086
No. of parameters	266
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.63

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2019/3* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2020).

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full crystallographic data

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catena-Poly[[[pentaaquadysprosium(III)]-μ-5-azaniumylisophthalato] dichloride monohydrate]

Ahlem Linda Boulkedid, Mehdi Boutebdja and Rochdi Ghallab

catena-Poly[[[pentaaquadysprosium(III)]-μ-5-azaniumylisophthalato] dichloride monohydrate]

Crystal data

$[Dy(C_8H_6NO_4)(H_2O)_5]Cl_2 \cdot H_2O$
M_r = 521.63
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.7274 (2) Å
b = 11.9281 (3) Å
c = 15.4697 (4) Å
β = 100.480 (1)°
V = 1583.55 (7) Å^3
Z = 4
$F(000)$ = 1012
D_x = 2.188 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8978 reflections
θ = 2.7–34.0°
μ = 5.10 mm^{-1}
T = 296 K
Block, colourless
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.675, T_{max} = 0.747
16994 measured reflections
4086 independent reflections
3470 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 28.7°, θ_{min} = 2.2°
h = −11→11
k = −13→16
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.052
S = 1.01
4086 reflections
266 parameters
0 restraints
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
W = $1/[\Sigma^2(FO^2) + (0.0152P)^2 + 1.8767P]$ WHERE $P = (FO^2 + 2FC^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Dy1	0.29223 (2)	0.48158 (2)	0.14719 (2)	0.0189 (1)
Cl1	0.02552 (10)	0.70815 (8)	0.56158 (6)	0.0377 (3)
Cl2	0.64436 (11)	0.17687 (9)	0.24575 (6)	0.0430 (3)
O1	0.2208 (3)	0.4945 (2)	0.29260 (14)	0.0313 (7)
O1W	0.0349 (3)	0.5510 (2)	0.12853 (16)	0.0277 (7)
O2	0.4427 (3)	0.4136 (2)	0.28306 (12)	0.0295 (7)
O2W	0.2900 (3)	0.5851 (3)	0.01427 (17)	0.0365 (9)
O3	0.6343 (3)	0.18700 (19)	0.66052 (12)	0.0262 (6)
O3W	0.3298 (4)	0.6758 (2)	0.19189 (18)	0.0424 (9)
O4	0.6313 (2)	0.12560 (18)	0.52657 (12)	0.0216 (6)
O4W	0.5608 (4)	0.5387 (3)	0.1444 (3)	0.0608 (13)
O5W	0.4398 (3)	0.3280 (2)	0.11052 (18)	0.0356 (8)
N1	0.2551 (4)	0.5119 (3)	0.63105 (19)	0.0283 (9)
C1	0.3633 (3)	0.4088 (2)	0.42259 (16)	0.0197 (8)
C2	0.4623 (3)	0.3207 (3)	0.45410 (17)	0.0202 (8)
C3	0.4866 (3)	0.2926 (2)	0.54279 (17)	0.0188 (8)
C4	0.4162 (3)	0.3562 (3)	0.59983 (18)	0.0206 (8)
C5	0.3188 (3)	0.4431 (3)	0.56745 (18)	0.0205 (8)
C6	0.2882 (3)	0.4697 (3)	0.47899 (18)	0.0205 (8)
C7	0.3396 (4)	0.4414 (3)	0.32713 (17)	0.0225 (8)
C8	0.5899 (3)	0.1970 (2)	0.57829 (17)	0.0193 (8)
O6W	0.8027 (3)	0.3937 (3)	0.1901 (3)	0.0748 (16)
H1A	0.208 (5)	0.465 (4)	0.664 (3)	0.045 (12)*
H1B	0.188 (4)	0.561 (3)	0.607 (2)	0.026 (9)*
H1C	0.339 (5)	0.550 (4)	0.666 (3)	0.042 (11)*
H2	0.508 (4)	0.281 (3)	0.414 (2)	0.024 (8)*
H1WA	−0.007 (5)	0.574 (4)	0.084 (3)	0.045 (12)*
H4	0.431 (3)	0.340 (3)	0.659 (2)	0.021 (8)*
H1WB	0.007 (5)	0.578 (4)	0.168 (3)	0.048 (13)*
H4WA	0.631 (5)	0.499 (4)	0.157 (3)	0.034 (12)*
H6	0.223 (5)	0.532 (3)	0.458 (3)	0.040 (11)*
H3WA	0.368 (5)	0.716 (4)	0.163 (3)	0.057 (15)*
H3WB	0.309 (5)	0.700 (4)	0.233 (3)	0.058 (15)*
H4WB	0.590 (6)	0.597 (5)	0.141 (3)	0.070 (18)*
H5WA	0.437 (5)	0.301 (4)	0.065 (3)	0.058 (15)*
H5WB	0.490 (6)	0.287 (5)	0.153 (4)	0.09 (2)*
H2WA	0.351 (6)	0.641 (5)	0.015 (3)	0.09 (2)*
H2WB	0.255 (7)	0.562 (6)	−0.025 (4)	0.09 (2)*
H6WA	0.90093	0.40173	0.20341	0.1120*
H6WB	0.78481	0.33146	0.21305	0.1120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.0253 (1)	0.0155 (1)	0.0139 (1)	−0.0019 (1)	−0.0019 (1)	0.0003 (1)

Cl1	0.0421 (5)	0.0308 (5)	0.0412 (4)	0.0098 (4)	0.0102 (4)	0.0073 (4)
Cl2	0.0492 (5)	0.0431 (6)	0.0411 (5)	0.0161 (4)	0.0199 (4)	0.0112 (4)
O1	0.0359 (12)	0.0381 (15)	0.0179 (10)	0.0113 (10)	−0.0005 (9)	0.0068 (9)
O1W	0.0351 (12)	0.0284 (14)	0.0184 (11)	0.0103 (10)	0.0017 (9)	0.0028 (9)
O2	0.0401 (12)	0.0321 (14)	0.0146 (9)	0.0116 (10)	0.0005 (8)	−0.0006 (8)
O2W	0.0479 (15)	0.0388 (17)	0.0216 (12)	−0.0139 (13)	0.0031 (11)	0.0039 (11)
O3	0.0396 (12)	0.0226 (12)	0.0135 (9)	0.0113 (10)	−0.0025 (8)	−0.0010 (8)
O3W	0.080 (2)	0.0229 (15)	0.0264 (13)	−0.0117 (14)	0.0156 (13)	−0.0065 (11)
O4	0.0292 (10)	0.0184 (11)	0.0153 (9)	0.0058 (9)	−0.0009 (8)	−0.0009 (8)
O4W	0.0394 (17)	0.034 (2)	0.099 (3)	−0.0118 (15)	−0.0143 (16)	0.0201 (18)
O5W	0.0393 (14)	0.0370 (16)	0.0275 (13)	0.0097 (11)	−0.0022 (11)	−0.0086 (11)
N1	0.0331 (14)	0.0288 (17)	0.0247 (13)	0.0124 (13)	0.0099 (11)	0.0066 (11)
C1	0.0273 (14)	0.0151 (15)	0.0143 (12)	−0.0024 (11)	−0.0027 (10)	0.0011 (10)
C2	0.0289 (15)	0.0149 (15)	0.0154 (13)	0.0018 (12)	0.0006 (11)	−0.0013 (10)
C3	0.0233 (13)	0.0150 (15)	0.0170 (12)	−0.0010 (11)	0.0009 (10)	0.0019 (10)
C4	0.0238 (14)	0.0203 (16)	0.0174 (13)	−0.0007 (11)	0.0031 (10)	0.0040 (11)
C5	0.0199 (13)	0.0220 (16)	0.0201 (13)	0.0013 (11)	0.0053 (10)	0.0003 (11)
C6	0.0213 (13)	0.0164 (16)	0.0216 (13)	0.0026 (11)	−0.0019 (10)	0.0025 (11)
C7	0.0330 (15)	0.0125 (15)	0.0188 (13)	−0.0014 (12)	−0.0035 (11)	0.0001 (11)
C8	0.0239 (14)	0.0150 (15)	0.0176 (12)	0.0000 (11)	0.0004 (10)	0.0015 (10)
O6W	0.0356 (15)	0.035 (2)	0.156 (4)	0.0001 (14)	0.023 (2)	−0.004 (2)

Geometric parameters (Å, º)

Dy1—O1	2.446 (2)	O4W—H4WB	0.75 (6)
Dy1—O1W	2.362 (3)	O4W—H4WA	0.77 (5)
Dy1—O2	2.407 (2)	O5W—H5WA	0.77 (5)
Dy1—O2W	2.396 (3)	O5W—H5WB	0.87 (6)
Dy1—O3W	2.423 (2)	N1—H1A	0.90 (5)
Dy1—O4W	2.449 (4)	N1—H1B	0.86 (3)
Dy1—O5W	2.367 (3)	N1—H1C	0.94 (5)
Dy1—O3^{i}	2.468 (2)	C1—C6	1.388 (4)
Dy1—O4^{i}	2.4770 (19)	C1—C7	1.505 (4)
O1—C7	1.249 (4)	C1—C2	1.391 (4)
O2—C7	1.268 (4)	C2—C3	1.391 (4)
O3—C8	1.266 (3)	C3—C8	1.495 (4)
O4—C8	1.265 (3)	C3—C4	1.389 (4)
N1—C5	1.466 (4)	C4—C5	1.376 (5)
O1W—H1WA	0.77 (5)	C5—C6	1.383 (4)
O1W—H1WB	0.77 (5)	C2—H2	0.93 (3)
O2W—H2WA	0.85 (6)	C4—H4	0.92 (3)
O2W—H2WB	0.69 (6)	C6—H6	0.96 (4)
O3W—H3WB	0.75 (5)	O6W—H6WA	0.8500
O3W—H3WA	0.77 (5)	O6W—H6WB	0.8500
O1—Dy1—O1W	72.21 (8)	Dy1—O2W—H2WB	119 (6)
O1—Dy1—O2	53.71 (8)	H2WA—O2W—H2WB	120 (7)
O1—Dy1—O2W	142.49 (10)	Dy1—O2W—H2WA	119 (3)

O1—Dy1—O3W	73.81 (9)	Dy1—O3W—H3WA	119 (3)
O1—Dy1—O4W	113.80 (12)	Dy1—O3W—H3WB	125 (4)
O1—Dy1—O5W	120.66 (9)	H3WA—O3W—H3WB	117 (5)
O1—Dy1—O3^{i}	74.62 (7)	Dy1—O4W—H4WA	123 (3)
O1—Dy1—O4^{i}	121.39 (7)	H4WA—O4W—H4WB	109 (5)
O1W—Dy1—O2	125.48 (8)	Dy1—O4W—H4WB	127 (4)
O1W—Dy1—O2W	81.68 (9)	H5WA—O5W—H5WB	113 (5)
O1W—Dy1—O3W	77.05 (10)	Dy1—O5W—H5WA	128 (3)
O1W—Dy1—O4W	142.40 (10)	Dy1—O5W—H5WB	118 (4)
O1W—Dy1—O5W	142.09 (9)	C6—C1—C7	119.0 (2)
O1W—Dy1—O3^{i}	76.27 (8)	C2—C1—C6	120.6 (2)
O1W—Dy1—O4^{i}	72.10 (7)	C2—C1—C7	120.3 (2)
O2—Dy1—O2W	147.25 (9)	C5—N1—H1B	114 (2)
O2—Dy1—O3W	92.80 (9)	C5—N1—H1C	108 (3)
O2—Dy1—O4W	74.77 (12)	H1A—N1—H1B	109 (4)
O2—Dy1—O5W	73.40 (9)	H1A—N1—H1C	111 (4)
O2—Dy1—O3^{i}	82.93 (8)	H1B—N1—H1C	108 (4)
O2—Dy1—O4^{i}	128.93 (7)	C5—N1—H1A	107 (3)
O2W—Dy1—O3W	74.44 (10)	C1—C2—C3	120.1 (3)
O2W—Dy1—O4W	72.53 (12)	C2—C3—C4	119.3 (3)
O2W—Dy1—O5W	96.49 (10)	C4—C3—C8	119.4 (2)
O2W—Dy1—O3^{i}	125.05 (9)	C2—C3—C8	121.3 (2)
O2W—Dy1—O4^{i}	72.81 (9)	C3—C4—C5	119.7 (3)
O3W—Dy1—O4W	70.05 (12)	C4—C5—C6	121.9 (3)
O3W—Dy1—O5W	139.22 (10)	N1—C5—C6	120.5 (3)
O3^{i}—Dy1—O3W	143.51 (10)	N1—C5—C4	117.5 (3)
O3W—Dy1—O4^{i}	137.50 (9)	C1—C6—C5	118.3 (3)
O4W—Dy1—O5W	69.32 (11)	O1—C7—C1	120.4 (3)
O3^{i}—Dy1—O4W	141.18 (10)	O1—C7—O2	121.2 (3)
O4^{i}—Dy1—O4W	122.94 (11)	O2—C7—C1	118.4 (3)
O3^{i}—Dy1—O5W	74.09 (8)	O4—C8—C3	120.2 (2)
O4^{i}—Dy1—O5W	71.26 (8)	O3—C8—O4	120.1 (2)
O3^{i}—Dy1—O4^{i}	52.67 (6)	O3—C8—C3	119.7 (2)
Dy1—O1—C7	91.76 (18)	C1—C2—H2	118 (2)
Dy1—O2—C7	93.07 (18)	C3—C2—H2	122 (2)
Dy1^{ii}—O3—C8	93.80 (16)	C3—C4—H4	121 (2)
Dy1^{ii}—O4—C8	93.39 (15)	C5—C4—H4	119 (2)
Dy1—O1W—H1WA	121 (3)	C1—C6—H6	121 (3)
Dy1—O1W—H1WB	119 (3)	C5—C6—H6	121 (3)
H1WA—O1W—H1WB	113 (5)	H6WA—O6W—H6WB	105.00

O1W—Dy1—O1—C7	169.7 (2)	O5W—Dy1—O4^{i}—C8^{i}	82.71 (16)
O2—Dy1—O1—C7	−2.97 (19)	Dy1—O1—C7—O2	5.3 (3)
O2W—Dy1—O1—C7	−142.2 (2)	Dy1—O1—C7—C1	−174.6 (3)
O3W—Dy1—O1—C7	−109.0 (2)	Dy1—O2—C7—O1	−5.4 (3)
O4W—Dy1—O1—C7	−50.1 (2)	Dy1—O2—C7—C1	174.5 (3)
O5W—Dy1—O1—C7	29.1 (2)	Dy1^{ii}—O3—C8—O4	2.3 (3)
O3^{i}—Dy1—O1—C7	89.5 (2)	Dy1^{ii}—O3—C8—C3	−178.6 (2)

O4^{i}—Dy1—O1—C7	114.8 (2)	Dy1^{ii}—O4—C8—O3	−2.2 (3)
O1—Dy1—O2—C7	2.93 (19)	Dy1^{ii}—O4—C8—C3	178.6 (2)
O1W—Dy1—O2—C7	−5.6 (2)	C6—C1—C2—C3	0.2 (4)
O2W—Dy1—O2—C7	135.6 (2)	C7—C1—C2—C3	178.5 (3)
O3W—Dy1—O2—C7	70.5 (2)	C2—C1—C6—C5	2.3 (4)
O4W—Dy1—O2—C7	138.9 (2)	C7—C1—C6—C5	−176.1 (3)
O5W—Dy1—O2—C7	−148.6 (2)	C2—C1—C7—O1	158.3 (3)
O3^{i}—Dy1—O2—C7	−73.2 (2)	C2—C1—C7—O2	−21.6 (4)
O4^{i}—Dy1—O2—C7	−100.8 (2)	C6—C1—C7—O1	−23.3 (4)
O1—Dy1—O3^{i}—C8^{i}	154.02 (19)	C6—C1—C7—O2	156.7 (3)
O1W—Dy1—O3^{i}—C8^{i}	79.03 (18)	C1—C2—C3—C4	−2.6 (4)
O2—Dy1—O3^{i}—C8^{i}	−151.75 (18)	C1—C2—C3—C8	178.8 (2)
O2W—Dy1—O3^{i}—C8^{i}	9.7 (2)	C2—C3—C4—C5	2.6 (4)
O3W—Dy1—O3^{i}—C8^{i}	123.13 (19)	C8—C3—C4—C5	−178.9 (3)
O4W—Dy1—O3^{i}—C8^{i}	−97.0 (2)	C2—C3—C8—O3	166.1 (3)
O5W—Dy1—O3^{i}—C8^{i}	−77.05 (18)	C2—C3—C8—O4	−14.8 (4)
O1—Dy1—O4^{i}—C8^{i}	−32.37 (18)	C4—C3—C8—O3	−12.5 (4)
O1W—Dy1—O4^{i}—C8^{i}	−87.40 (16)	C4—C3—C8—O4	166.7 (3)
O2—Dy1—O4^{i}—C8^{i}	34.15 (18)	C3—C4—C5—N1	−176.3 (3)
O2W—Dy1—O4^{i}—C8^{i}	−174.00 (17)	C3—C4—C5—C6	0.0 (5)
O3W—Dy1—O4^{i}—C8^{i}	−132.88 (18)	N1—C5—C6—C1	173.8 (3)
O4W—Dy1—O4^{i}—C8^{i}	131.09 (17)	C4—C5—C6—C1	−2.4 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl2^{iii}	0.90 (5)	2.24 (5)	3.127 (4)	166 (4)
N1—H1*B*···Cl1	0.86 (3)	2.29 (4)	3.141 (4)	171 (3)
N1—H1*C*···O2^{iv}	0.94 (5)	1.97 (4)	2.870 (4)	158 (4)
O1*W*—H1*WA*···O4^{v}	0.77 (5)	1.95 (5)	2.718 (3)	175 (5)
O1*W*—H1*WB*···Cl2^{v}	0.77 (5)	2.36 (5)	3.097 (3)	162 (4)
O2*W*—H2*WA*···Cl1^{vi}	0.85 (6)	2.38 (6)	3.209 (3)	163 (4)
O2*W*—H2*WB*···O6*W*^{vii}	0.69 (6)	2.57 (6)	3.128 (5)	141 (7)
O3*W*—H3*WA*···Cl1^{vi}	0.77 (5)	2.44 (5)	3.186 (3)	163 (4)
O3*W*—H3*WB*···O3^{iv}	0.75 (5)	2.12 (5)	2.780 (3)	148 (4)
O4*W*—H4*WA*···O6*W*	0.77 (5)	1.95 (5)	2.721 (5)	178 (5)
O4*W*—H4*WB*···Cl2^{viii}	0.75 (6)	2.81 (5)	3.261 (4)	122 (4)
O4*W*—H4*WB*···Cl1^{vi}	0.75 (6)	2.64 (6)	3.273 (4)	144 (5)
O5*W*—H5*WA*···Cl1^{ix}	0.77 (5)	2.32 (5)	3.085 (3)	170 (4)
O5*W*—H5*WB*···Cl2	0.87 (6)	2.21 (6)	3.075 (3)	171 (5)
O6*W*—H6*WA*···O1*W*^{x}	0.85	2.52	3.039 (4)	120
O6*W*—H6*WA*···O3^{xi}	0.85	2.49	3.161 (4)	137
O6*W*—H6*WB*···Cl2	0.85	2.32	3.126 (4)	158

Symmetry codes: (iii) *x*−1/2, −*y*+1/2, *z*+1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1/2, *y*+1/2, −*z*+1/2; (vi) *x*+1/2, −*y*+3/2, *z*−1/2; (vii) −*x*+1, −*y*+1, −*z*; (viii) −*x*+3/2, *y*+1/2, −*z*+1/2; (ix) −*x*+1/2, *y*−1/2, −*z*+1/2; (x) *x*+1, *y*, *z*; (xi) *x*+1/2, −*y*+1/2, *z*−1/2.