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Octadecabromidobis(dicarbido)decadysprosium, [$Dy_{10}Br_{18}(C_2)_2$]

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.016 Å; R factor = 0.033; wR factor = 0.079; data-to-parameter ratio = 28.9.

Single crystals of [$Dy_{10}Br_{18}(C_2)_2$] were obtained during the reaction of $DyBr_3$ with dysprosium metal and graphite in a sealed tantalum container. In the crystal structure, the Dy atoms form dimers of edge-sharing octahedra, each encapsulating a C_2 unit. The metal atoms are surrounded by Br atoms above the cluster edges and vertices, respectively. The dimers are connected to each other by Br atoms, leading to a three-dimensional network. [$Dy_{10}Br_{18}(C_2)_2$] is isotypic with its iodido analogue [$Dy_{10}I_{18}(C_2)_2$].

Related literature

Details of ternary and quaternary halides of the rare earth elements have been compiled by Meyer & Wickleder (2000). Bromides with the formula [$RE_{10}Br_{18}(C_2)_2$], where RE is Gd, Tb or Er, have been studied by Liess (1996), Mattausch *et al.* (2002) and Uhrlandt *et al.* (1994). Recently, the first dysprosium compound belonging to this structural family, [$Dy_{10}I_{18}(C_2)_2$], was reported by Mattausch *et al.* (2007). [$Dy_{10}Br_{18}(C_2)_2$] is obtained by reduction of $DyBr_3$ with dysprosium and graphite. For the synthesis of the starting material $DyBr_3$, see Meyer *et al.* (1987).

Experimental

Crystal data

[$Dy_{10}Br_{18}(C_2)_2$]	Monoclinic, $P2_1/c$
M_r = 3111.42	a = 9.7399 (12) Å
b = 16.3398 (15) Å	Mo $K\alpha$ radiation
c = 13.2469 (19) Å	μ = 40.24 mm^{-1}
β = 120.869 (9)°	T = 293 (2) K
V = 1809.6 (4) Å^3	0.20 × 0.20 × 0.20 mm
Z = 2	

Data collection

Stoe IPDSII diffractometer	23768 measured reflections
Absorption correction: numerical [*X-RED* (Stoe & Cie, 2001) and *X-SHAPE* (Stoe & Cie, 1999)]	3935 independent reflections
T_{min} = 0.015, T_{max} = 0.063	2989 reflections with $I > 2\sigma(I)$
	R_{int} = 0.096

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033	136 parameters
$wR(F^2)$ = 0.079	$\Delta\rho_{max}$ = 2.44 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −1.75 e Å^{-3}
3935 reflections	

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2169).

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supplementary materials

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Octadecabromidobis(dicarbido)decadysprosium, [$Dy_{10}Br_{18}(C_2)_2$]

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Comment

A number of ternary and quaternary halides of the general formulae [$\{RE_{10}(C_2)_2\}X_n$] with RE = Gd, Tb, Er, Y; X = Cl, Br, I; n = 17–19 and $A_x[\{RE_{10}(C_2)_2\}X_n]$ with A = K, Rb, Cs; x = 1–3; n = 18–21 have been observed and were compiled by Meyer and Wickleder (2000). Among these halides, three bromides with the formula [$\{RE_{10}(C_2)_2\}Br_{18}$], where RE is Gd, Tb, and Er, are known and were structurally studied by Ließ (1996), Mattausch *et al.* (2002) and Uhrlandt *et al.* (1994).

The crystal structure of the title compound is isotypic with the iodide analogue [$\{Dy_{10}(C_2)_2\}I_{18}$] studied recently by Mattausch *et al.* (2007). As many reduced rare earth halides, the cluster compound [$\{Dy_{10}(C_2)_2\}Br_{18}$] consists of an octahedral arrangement of dysprosium atoms stabilized by an interstitial C_2 dumbbell. The dysprosium octahedra are connected *via* common edges leading to the formation of dimers. The cluster cores are surrounded by bromine atoms above the cluster edges and vertices, respectively (Fig. 1). Some of the bromine atoms belong to a single dimeric unit while others connect neighbouring dimers, thus leading to a three-dimensional network (Fig. 2). Due to the slight elongation of the dysprosium octahedra established roughly parallel to the axis of the C_2 units, the Dy—Dy distances range from 3.1832 (11) to 4.0369 (9) Å. The Dy—Br distances in [$\{Dy_{10}(C_2)_2\}Br_{18}$] vary between 2.7157 (15) and 3.3231 (12) Å with the distances to the edge-bridging bromine atoms that are placed between two condensed octahedra significantly larger than those to the other ligands. The C—C bond length is 1.437 (13) Å.

Experimental

Black parallelepipedic crystals of [$\{Dy_{10}(C_2)_2\}Br_{18}$] were obtained by the reaction of $DyBr_3$ (150 mg) with dysprosium powder (85 mg, Chempur, 99,9%) and graphite (8 mg, Merck, p.a.) in a tantalum container at 1273 K. $DyBr_3$ had been synthesized previously according to the ammonium bromide route (Meyer *et al.*, 1987), followed by sublimation in high vacuum for purification. Due to air and moisture sensitivity of both reagents and products, all handlings were carried out in an argon-filled glove box (*M*. Braun, Garching, Germany).

Refinement

The highest peak in the final difference Fourier map is 0.99 Å from atom Dy4 and the deepest hole is 0.88 Å from the same atom.

Figures

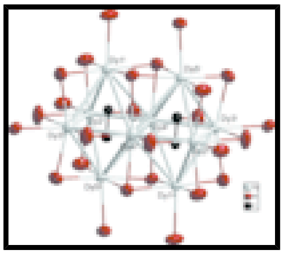

Fig. 1. : The dimeric unit in [$\{Dy_{10}(C_2)_2\}Br_{18}$] with displacement ellipsoids drawn at the 90% probability level [Symmetry codes: (i) $1 - x$, $1/2 + y$, $1.5 - z$; (ii) x, $0.5 - y$, $1/2 + z$].

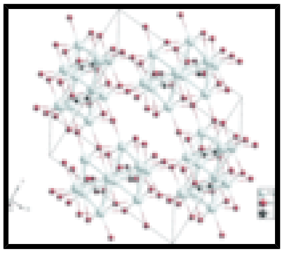

Fig. 2. : View of the crystal structure of [$\{Dy_{10}(C_2)_2\}Br_{18}$] emphasizing the connection between the dimers *via* bromine atoms.

Octadecabromidobis(dicarbido)decadysprosium

Crystal data

[$Dy_{10}Br_{18}(C_2)_2$]

$M_r = 3111.42$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.7399$ (12) Å

$b = 16.3398$ (15) Å

$c = 13.2469$ (19) Å

$\beta = 120.869$ (9)°

$V = 1809.6$ (4) Å^3

$Z = 2$

$F_{000} = 2628$

$D_x = 5.710$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 14525 reflections

$\theta = 2.1$–27.1°

$\mu = 40.24$ mm^{-1}

$T = 293$ (2) K

Parallelepiped, black

0.20 × 0.20 × 0.20 mm

Data collection

Stoe IPDSII
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

φ scans

Absorption correction: numerical
[X-RED (Stoe & Cie, 2001) and X-SHAPE (Stoe & Cie, 1999)]

$T_{min} = 0.015$, $T_{max} = 0.063$

23768 measured reflections

3935 independent reflections

2989 reflections with $I > 2\sigma(I)$

$R_{int} = 0.096$

$\theta_{max} = 27.3$°

$\theta_{min} = 2.2$°

$h = -12 \rightarrow 12$

$k = -20 \rightarrow 20$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.079$

$S = 1.01$

3935 reflections

136 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 2.44$ e Å^{-3}

$\Delta\rho_{min} = -1.75$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00038 (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 $F^2 > 2\text{sigma}(F^2)$ 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}
Dy1	0.72140 (7)	−0.18631 (3)	0.55464 (5)	0.01642 (12)
Dy2	0.86572 (6)	−0.05763 (3)	0.81405 (4)	0.01581 (12)
Dy3	0.49120 (6)	0.16312 (3)	0.27712 (5)	0.01646 (13)
Dy4	0.66436 (6)	0.04537 (3)	0.53869 (5)	0.01672 (12)
Dy5	0.49942 (6)	−0.05623 (3)	0.23673 (5)	0.01640 (12)
Br1	0.79002 (15)	0.17718 (7)	0.46836 (11)	0.0267 (3)
Br2	0.18295 (15)	−0.05866 (7)	0.03920 (11)	0.0261 (3)
Br3	0.81121 (14)	−0.06564 (6)	0.44345 (10)	0.0199 (2)
Br4	0.19236 (15)	0.18349 (7)	0.05984 (11)	0.0270 (3)
Br5	0.60176 (17)	−0.19122 (6)	0.14246 (12)	0.0282 (3)
Br6	0.59583 (16)	0.06929 (7)	0.14910 (12)	0.0273 (3)
Br7	1.01722 (16)	−0.18152 (7)	0.75532 (12)	0.0274 (3)
Br8	0.97720 (15)	0.06689 (7)	0.73923 (11)	0.0265 (3)
Br9	0.58632 (14)	0.19733 (6)	0.66855 (10)	0.0198 (2)
C1	0.6314 (13)	−0.0891 (5)	0.6212 (9)	0.0118 (18)*
C2	0.4262 (13)	0.0309 (6)	0.3277 (9)	0.0144 (19)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.0185 (3)	0.0131 (2)	0.0193 (3)	0.00139 (17)	0.0109 (2)	−0.00086 (17)
Dy2	0.0133 (3)	0.0157 (2)	0.0161 (3)	−0.00058 (17)	0.0058 (2)	0.00070 (17)
Dy3	0.0170 (3)	0.0136 (2)	0.0190 (3)	−0.00068 (17)	0.0094 (2)	0.00148 (17)
Dy4	0.0136 (3)	0.0162 (2)	0.0177 (3)	−0.00185 (17)	0.0061 (2)	0.00218 (17)
Dy5	0.0162 (3)	0.0138 (2)	0.0191 (3)	0.00202 (17)	0.0089 (2)	−0.00146 (17)
Br1	0.0196 (6)	0.0273 (5)	0.0261 (6)	−0.0087 (4)	0.0066 (5)	0.0045 (4)
Br2	0.0170 (6)	0.0321 (6)	0.0209 (6)	0.0031 (4)	0.0037 (5)	−0.0070 (5)
Br3	0.0161 (6)	0.0213 (5)	0.0235 (6)	0.0005 (4)	0.0110 (5)	0.0020 (4)
Br4	0.0214 (7)	0.0287 (5)	0.0247 (6)	−0.0059 (4)	0.0073 (5)	0.0103 (4)
Br5	0.0435 (8)	0.0148 (5)	0.0400 (7)	0.0018 (4)	0.0313 (7)	−0.0017 (4)
Br6	0.0361 (7)	0.0225 (5)	0.0354 (7)	−0.0012 (5)	0.0271 (6)	0.0002 (5)
Br7	0.0191 (6)	0.0298 (5)	0.0281 (7)	0.0066 (4)	0.0083 (5)	−0.0031 (4)
Br8	0.0182 (6)	0.0291 (5)	0.0248 (6)	−0.0074 (4)	0.0057 (5)	0.0056 (4)
Br9	0.0189 (6)	0.0163 (4)	0.0235 (6)	−0.0005 (4)	0.0104 (5)	−0.0009 (4)

Geometric parameters (Å, °)

Dy1—C1	2.205 (9)	Dy4—C2	2.568 (11)
Dy1—Br7	2.7413 (15)	Dy4—C1^{ii}	2.652 (10)
Dy1—Br5^{i}	2.8473 (12)	Dy4—C2^{ii}	2.659 (10)
Dy1—Br3	2.8539 (12)	Dy4—Br8	2.8564 (14)
Dy1—Br9^{ii}	2.9434 (14)	Dy4—Br1	2.8591 (12)
Dy1—Br4^{iii}	2.9730 (12)	Dy4—Br3	2.9630 (12)
Dy1—Dy2	3.6399 (8)	Dy4—Dy4^{ii}	3.1832 (11)
Dy1—Dy3^{ii}	3.7595 (9)	Dy4—Br9	3.3231 (12)
Dy1—Dy4	3.8163 (7)	Dy5—C2	2.207 (10)
Dy2—C1	2.453 (10)	Dy5—Br6	2.7485 (12)
Dy2—C2^{ii}	2.515 (11)	Dy5—Br2	2.8413 (14)
Dy2—Br8	2.7213 (12)	Dy5—Br3	2.8655 (14)
Dy2—Br7	2.8388 (13)	Dy5—Br9^{ii}	2.9432 (12)
Dy2—Br4^{ii}	2.8827 (12)	Dy5—Br5	2.9488 (12)
Dy2—Br2^{ii}	2.9258 (13)	Dy5—Dy2^{ii}	3.7560 (8)
Dy2—Br2^{iv}	2.9978 (14)	Br2—Dy2^{ii}	2.9258 (13)
Dy2—Dy3^{ii}	3.4938 (8)	Br2—Dy2^{vii}	2.9978 (14)
Dy2—Dy4	3.5558 (9)	Br4—Dy2^{ii}	2.8827 (12)
Dy2—Dy5^{ii}	3.7560 (8)	Br4—Dy1^{v}	2.9730 (12)
Dy3—C2	2.439 (9)	Br5—Dy1^{viii}	2.8473 (12)
Dy3—C1^{ii}	2.520 (10)	Br5—Dy3^{iii}	2.9340 (12)
Dy3—Br1	2.7157 (15)	Br9—Dy5^{ii}	2.9432 (12)
Dy3—Br6	2.8354 (13)	Br9—Dy1^{ii}	2.9434 (14)
Dy3—Br4	2.8759 (14)	Br9—Dy3^{ix}	3.0812 (12)

Dy3—Br5^{v}	2.9340 (12)	C1—C2^{ii}	1.437 (13)
Dy3—Br9^{vi}	3.0812 (12)	C1—Dy3^{ii}	2.520 (10)
Dy3—Dy2^{ii}	3.4938 (8)	C1—Dy4^{ii}	2.652 (10)
Dy3—Dy4	3.5434 (8)	C2—C1^{ii}	1.437 (13)
Dy3—Dy5	3.6309 (7)	C2—Dy2^{ii}	2.515 (11)
Dy3—Dy1^{ii}	3.7595 (8)	C2—Dy4^{ii}	2.659 (10)
Dy4—C1	2.547 (9)		
C1—Dy1—Br7	91.6 (3)	C2—Dy4—C2^{ii}	105.0 (3)
C1—Dy1—Br5^{i}	90.7 (2)	C1^{ii}—Dy4—C2^{ii}	93.6 (3)
Br7—Dy1—Br5^{i}	94.05 (4)	C1—Dy4—Br8	90.9 (2)
C1—Dy1—Br3	89.9 (2)	C2—Dy4—Br8	163.8 (2)
Br7—Dy1—Br3	91.88 (4)	C1^{ii}—Dy4—Br8	155.9 (2)
Br5^{i}—Dy1—Br3	174.01 (4)	C2^{ii}—Dy4—Br8	89.9 (2)
C1—Dy1—Br9^{ii}	92.1 (3)	C1—Dy4—Br1	163.6 (2)
Br7—Dy1—Br9^{ii}	176.15 (4)	C2—Dy4—Br1	90.8 (2)
Br5^{i}—Dy1—Br9^{ii}	87.03 (4)	C1^{ii}—Dy4—Br1	90.5 (2)
Br3—Dy1—Br9^{ii}	87.00 (4)	C2^{ii}—Dy4—Br1	156.1 (2)
C1—Dy1—Br4^{iii}	173.6 (3)	Br8—Dy4—Br1	77.27 (4)
Br7—Dy1—Br4^{iii}	94.80 (4)	C1—Dy4—Br3	81.3 (2)
Br5^{i}—Dy1—Br4^{iii}	89.28 (4)	C2—Dy4—Br3	81.0 (2)
Br3—Dy1—Br4^{iii}	89.40 (4)	C1^{ii}—Dy4—Br3	112.9 (2)
Br9^{ii}—Dy1—Br4^{iii}	81.51 (4)	C2^{ii}—Dy4—Br3	113.2 (2)
C1—Dy1—Dy2	41.1 (3)	Br8—Dy4—Br3	87.35 (4)
Br7—Dy1—Dy2	50.46 (3)	Br1—Dy4—Br3	86.65 (4)
Br5^{i}—Dy1—Dy2	93.50 (3)	C1—Dy4—Dy4^{ii}	53.8 (2)
Br3—Dy1—Dy2	90.92 (3)	C2—Dy4—Dy4^{ii}	53.8 (2)
Br9^{ii}—Dy1—Dy2	133.21 (3)	C1^{ii}—Dy4—Dy4^{ii}	50.8 (2)
Br4^{iii}—Dy1—Dy2	145.25 (3)	C2^{ii}—Dy4—Dy4^{ii}	51.2 (2)
C1—Dy1—Dy3^{ii}	40.3 (2)	Br8—Dy4—Dy4^{ii}	140.68 (4)
Br7—Dy1—Dy3^{ii}	92.68 (3)	Br1—Dy4—Dy4^{ii}	140.71 (4)
Br5^{i}—Dy1—Dy3^{ii}	50.45 (2)	Br3—Dy4—Dy4^{ii}	101.73 (3)
Br3—Dy1—Dy3^{ii}	130.11 (3)	C1—Dy4—Br9	108.0 (2)
Br9^{ii}—Dy1—Dy3^{ii}	90.85 (3)	C2—Dy4—Br9	108.3 (2)
Br4^{iii}—Dy1—Dy3^{ii}	139.48 (3)	C1^{ii}—Dy4—Br9	76.7 (2)
Dy2—Dy1—Dy3^{ii}	56.324 (16)	C2^{ii}—Dy4—Br9	76.3 (2)
C1—Dy1—Dy4	39.8 (2)	Br8—Dy4—Br9	81.07 (4)
Br7—Dy1—Dy4	94.36 (3)	Br1—Dy4—Br9	81.70 (4)
Br5^{i}—Dy1—Dy4	129.89 (3)	Br3—Dy4—Br9	165.10 (3)
Br3—Dy1—Dy4	50.25 (2)	Dy4^{ii}—Dy4—Br9	93.17 (3)
Br9^{ii}—Dy1—Dy4	87.75 (2)	C1—Dy4—Dy3	141.9 (2)
Br4^{iii}—Dy1—Dy4	138.84 (3)	C2—Dy4—Dy3	43.5 (2)

Dy2—Dy1—Dy4	56.906 (14)
Dy3^{ii}—Dy1—Dy4	79.866 (14)
C1—Dy2—C2^{ii}	33.6 (3)
C1—Dy2—Br8	96.3 (2)
C2^{ii}—Dy2—Br8	96.2 (2)
C1—Dy2—Br7	84.4 (2)
C2^{ii}—Dy2—Br7	117.8 (2)
Br8—Dy2—Br7	94.17 (4)
C1—Dy2—Br4^{ii}	95.7 (2)
C2^{ii}—Dy2—Br4^{ii}	94.2 (2)
Br8—Dy2—Br4^{ii}	167.98 (4)
Br7—Dy2—Br4^{ii}	86.23 (4)
C1—Dy2—Br2^{ii}	116.5 (2)
C2^{ii}—Dy2—Br2^{ii}	82.9 (2)
Br8—Dy2—Br2^{ii}	89.27 (4)
Br7—Dy2—Br2^{ii}	158.35 (4)
Br4^{ii}—Dy2—Br2^{ii}	86.07 (4)
C1—Dy2—Br2^{iv}	165.5 (2)
C2^{ii}—Dy2—Br2^{iv}	159.6 (2)
Br8—Dy2—Br2^{iv}	88.07 (4)
Br7—Dy2—Br2^{iv}	81.56 (4)
Br4^{ii}—Dy2—Br2^{iv}	80.09 (4)
Br2^{ii}—Dy2—Br2^{iv}	77.19 (4)
C1—Dy2—Dy3^{ii}	46.2 (2)
C2^{ii}—Dy2—Dy3^{ii}	44.3 (2)
Br8—Dy2—Dy3^{ii}	139.04 (3)
Br7—Dy2—Dy3^{ii}	96.80 (3)
Br4^{ii}—Dy2—Dy3^{ii}	52.56 (3)
Br2^{ii}—Dy2—Dy3^{ii}	94.50 (3)
Br2^{iv}—Dy2—Dy3^{ii}	132.53 (3)
C1—Dy2—Dy4	45.7 (2)
C2^{ii}—Dy2—Dy4	48.3 (2)
Br8—Dy2—Dy4	52.09 (3)
Br7—Dy2—Dy4	98.46 (3)
Br4^{ii}—Dy2—Dy4	139.75 (3)
Br2^{ii}—Dy2—Dy4	100.49 (3)
Br2^{iv}—Dy2—Dy4	140.15 (3)
Dy3^{ii}—Dy2—Dy4	87.228 (19)
C1—Dy2—Dy1	36.2 (2)
C2^{ii}—Dy2—Dy1	69.8 (2)
Br8—Dy2—Dy1	96.95 (3)
Br7—Dy2—Dy1	48.13 (3)
C1^{ii}—Dy4—Dy3	45.2 (2)
C2^{ii}—Dy4—Dy3	138.7 (2)
Br8—Dy4—Dy3	126.02 (3)
Br1—Dy4—Dy3	48.77 (3)
Br3—Dy4—Dy3	90.43 (3)
Dy4^{ii}—Dy4—Dy3	92.44 (2)
Br9—Dy4—Dy3	88.85 (3)
C1—Dy4—Dy2	43.6 (2)
C2—Dy4—Dy2	142.0 (2)
C1^{ii}—Dy4—Dy2	138.4 (2)
C2^{ii}—Dy4—Dy2	44.9 (2)
Br8—Dy4—Dy2	48.74 (3)
Br1—Dy4—Dy2	126.00 (3)
Br3—Dy4—Dy2	90.82 (3)
Dy4^{ii}—Dy4—Dy2	92.53 (2)
Br9—Dy4—Dy2	88.56 (3)
Dy3—Dy4—Dy2	174.519 (19)
C1—Dy4—Dy1	33.6 (2)
C2—Dy4—Dy1	89.6 (2)
C1^{ii}—Dy4—Dy1	112.27 (19)
C2^{ii}—Dy4—Dy1	65.6 (2)
Br8—Dy4—Dy1	90.87 (3)
Br1—Dy4—Dy1	133.69 (3)
Br3—Dy4—Dy1	47.77 (2)
Dy4^{ii}—Dy4—Dy1	69.484 (18)
Br9—Dy4—Dy1	141.07 (3)
Dy3—Dy4—Dy1	125.134 (19)
Dy2—Dy4—Dy1	59.047 (14)
C2—Dy5—Br6	91.4 (3)
C2—Dy5—Br2	90.6 (3)
Br6—Dy5—Br2	93.77 (4)
C2—Dy5—Br3	89.6 (3)
Br6—Dy5—Br3	91.11 (4)
Br2—Dy5—Br3	175.10 (4)
C2—Dy5—Br9^{ii}	91.8 (3)
Br6—Dy5—Br9^{ii}	176.15 (4)
Br2—Dy5—Br9^{ii}	88.32 (4)
Br3—Dy5—Br9^{ii}	86.79 (3)
C2—Dy5—Br5	171.1 (3)
Br6—Dy5—Br5	96.68 (4)
Br2—Dy5—Br5	92.42 (4)
Br3—Dy5—Br5	86.67 (4)

Br4^{ii}—Dy2—Dy1	92.26 (3)	Br9^{ii}—Dy5—Br5	79.99 (3)
Br2^{ii}—Dy2—Dy1	152.46 (3)	C2—Dy5—Dy3	41.0 (3)
Br2^{iv}—Dy2—Dy1	129.62 (3)	Br6—Dy5—Dy3	50.49 (3)
Dy3^{ii}—Dy2—Dy1	63.568 (16)	Br2—Dy5—Dy3	93.10 (3)
Dy4—Dy2—Dy1	64.047 (17)	Br3—Dy5—Dy3	90.27 (2)
C1—Dy2—Dy5^{ii}	68.1 (2)	Br9^{ii}—Dy5—Dy3	132.68 (3)
C2^{ii}—Dy2—Dy5^{ii}	34.5 (2)	Br5—Dy5—Dy3	146.99 (3)
Br8—Dy2—Dy5^{ii}	94.73 (3)	C2—Dy5—Dy2^{ii}	40.2 (3)
Br7—Dy2—Dy5^{ii}	151.85 (3)	Br6—Dy5—Dy2^{ii}	92.98 (3)
Br4^{ii}—Dy2—Dy5^{ii}	90.45 (3)	Br2—Dy5—Dy2^{ii}	50.35 (3)
Br2^{ii}—Dy2—Dy5^{ii}	48.39 (3)	Br3—Dy5—Dy2^{ii}	129.76 (3)
Br2^{iv}—Dy2—Dy5^{ii}	125.37 (3)	Br9^{ii}—Dy5—Dy2^{ii}	90.84 (3)
Dy3^{ii}—Dy2—Dy5^{ii}	59.980 (16)	Br5—Dy5—Dy2^{ii}	142.13 (3)
Dy4—Dy2—Dy5^{ii}	66.960 (16)	Dy3—Dy5—Dy2^{ii}	56.425 (13)
Dy1—Dy2—Dy5^{ii}	104.213 (19)	C2—Dy5—Dy4	39.8 (3)
C2—Dy3—C1^{ii}	33.6 (3)	Br6—Dy5—Dy4	93.80 (3)
C2—Dy3—Br1	97.1 (3)	Br2—Dy5—Dy4	129.92 (3)
C1^{ii}—Dy3—Br1	96.7 (2)	Br3—Dy5—Dy4	49.90 (3)
C2—Dy3—Br6	84.8 (2)	Br9^{ii}—Dy5—Dy4	87.31 (3)
C1^{ii}—Dy3—Br6	118.3 (2)	Br5—Dy5—Dy4	135.47 (3)
Br1—Dy3—Br6	93.53 (4)	Dy3—Dy5—Dy4	56.545 (13)
C2—Dy3—Br4	96.1 (3)	Dy2^{ii}—Dy5—Dy4	79.862 (17)
C1^{ii}—Dy3—Br4	94.4 (2)	Dy3—Br1—Dy4	78.88 (3)
Br1—Dy3—Br4	166.85 (4)	Dy5—Br2—Dy2^{ii}	81.26 (3)
Br6—Dy3—Br4	87.35 (4)	Dy5—Br2—Dy2^{vii}	173.49 (5)
C2—Dy3—Br5^{v}	116.5 (2)	Dy2^{ii}—Br2—Dy2^{vii}	102.81 (4)
C1^{ii}—Dy3—Br5^{v}	82.9 (2)	Dy1—Br3—Dy5	94.31 (4)
Br1—Dy3—Br5^{v}	88.59 (4)	Dy1—Br3—Dy4	81.98 (3)
Br6—Dy3—Br5^{v}	158.19 (4)	Dy5—Br3—Dy4	82.40 (3)
Br4—Dy3—Br5^{v}	85.82 (4)	Dy3—Br4—Dy2^{ii}	74.70 (3)
C2—Dy3—Br9^{vi}	165.0 (2)	Dy3—Br4—Dy1^{v}	100.81 (4)
C1^{ii}—Dy3—Br9^{vi}	160.6 (2)	Dy2^{ii}—Br4—Dy1^{v}	175.51 (5)
Br1—Dy3—Br9^{vi}	86.44 (4)	Dy1^{viii}—Br5—Dy3^{iii}	81.11 (3)
Br6—Dy3—Br9^{vi}	80.48 (3)	Dy1^{viii}—Br5—Dy5	175.47 (5)
Br4—Dy3—Br9^{vi}	80.76 (3)	Dy3^{iii}—Br5—Dy5	102.63 (4)
Br5^{v}—Dy3—Br9^{vi}	77.99 (3)	Dy5—Br6—Dy3	81.10 (3)
C2—Dy3—Dy2^{ii}	46.0 (3)	Dy1—Br7—Dy2	81.41 (4)
C1^{ii}—Dy3—Dy2^{ii}	44.6 (2)	Dy2—Br8—Dy4	79.17 (3)
Br1—Dy3—Dy2^{ii}	139.84 (3)	Dy5^{ii}—Br9—Dy1^{ii}	90.85 (3)
Br6—Dy3—Dy2^{ii}	97.22 (3)	Dy5^{ii}—Br9—Dy3^{ix}	99.30 (4)
Br4—Dy3—Dy2^{ii}	52.74 (3)	Dy1^{ii}—Br9—Dy3^{ix}	96.84 (4)

Br5^{v}—Dy3—Dy2^{ii}	95.05 (3)	Dy5^{ii}—Br9—Dy4	79.96 (3)
Br9^{vi}—Dy3—Dy2^{ii}	133.46 (3)	Dy1^{ii}—Br9—Dy4	79.62 (3)
C2—Dy3—Dy4	46.4 (3)	Dy3^{ix}—Br9—Dy4	176.35 (4)
C1^{ii}—Dy3—Dy4	48.3 (2)	C2^{ii}—C1—Dy1	174.9 (7)
Br1—Dy3—Dy4	52.35 (3)	C2^{ii}—C1—Dy2	75.6 (6)
Br6—Dy3—Dy4	98.89 (3)	Dy1—C1—Dy2	102.7 (4)
Br4—Dy3—Dy4	140.45 (3)	C2^{ii}—C1—Dy3^{ii}	70.1 (5)
Br5^{v}—Dy3—Dy4	99.56 (3)	Dy1—C1—Dy3^{ii}	105.2 (3)
Br9^{vi}—Dy3—Dy4	138.77 (3)	Dy2—C1—Dy3^{ii}	89.3 (3)
Dy2^{ii}—Dy3—Dy4	87.713 (18)	C2^{ii}—C1—Dy4	78.3 (5)
C2—Dy3—Dy5	36.4 (2)	Dy1—C1—Dy4	106.6 (4)
C1^{ii}—Dy3—Dy5	70.0 (2)	Dy2—C1—Dy4	90.7 (3)
Br1—Dy3—Dy5	97.29 (3)	Dy3^{ii}—C1—Dy4	147.4 (4)
Br6—Dy3—Dy5	48.41 (2)	C2^{ii}—C1—Dy4^{ii}	70.8 (6)
Br4—Dy3—Dy5	93.11 (3)	Dy1—C1—Dy4^{ii}	111.5 (4)
Br5^{v}—Dy3—Dy5	152.68 (3)	Dy2—C1—Dy4^{ii}	145.5 (4)
Br9^{vi}—Dy3—Dy5	128.83 (3)	Dy3^{ii}—C1—Dy4^{ii}	86.4 (3)
Dy2^{ii}—Dy3—Dy5	63.595 (14)	Dy4—C1—Dy4^{ii}	75.5 (3)
Dy4—Dy3—Dy5	64.703 (15)	C1^{ii}—C2—Dy5	175.8 (8)
C2—Dy3—Dy1^{ii}	68.1 (2)	C1^{ii}—C2—Dy3	76.3 (5)
C1^{ii}—Dy3—Dy1^{ii}	34.5 (2)	Dy5—C2—Dy3	102.7 (4)
Br1—Dy3—Dy1^{ii}	95.23 (4)	C1^{ii}—C2—Dy2^{ii}	70.8 (6)
Br6—Dy3—Dy1^{ii}	152.30 (3)	Dy5—C2—Dy2^{ii}	105.2 (4)
Br4—Dy3—Dy1^{ii}	89.95 (3)	Dy3—C2—Dy2^{ii}	89.7 (3)
Br5^{v}—Dy3—Dy1^{ii}	48.44 (2)	C1^{ii}—C2—Dy4	77.3 (6)
Br9^{vi}—Dy3—Dy1^{ii}	126.24 (3)	Dy5—C2—Dy4	106.8 (4)
Dy2^{ii}—Dy3—Dy1^{ii}	60.109 (16)	Dy3—C2—Dy4	90.0 (3)
Dy4—Dy3—Dy1^{ii}	66.772 (17)	Dy2^{ii}—C2—Dy4	147.2 (4)
Dy5—Dy3—Dy1^{ii}	104.320 (16)	C1^{ii}—C2—Dy4^{ii}	69.7 (5)
C1—Dy4—C2	98.4 (3)	Dy5—C2—Dy4^{ii}	111.8 (4)
C1—Dy4—C1^{ii}	104.5 (3)	Dy3—C2—Dy4^{ii}	145.0 (4)
C2—Dy4—C1^{ii}	31.9 (3)	Dy2^{ii}—C2—Dy4^{ii}	86.8 (3)
C1—Dy4—C2^{ii}	32.0 (3)	Dy4—C2—Dy4^{ii}	75.0 (3)

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

Fig. 1

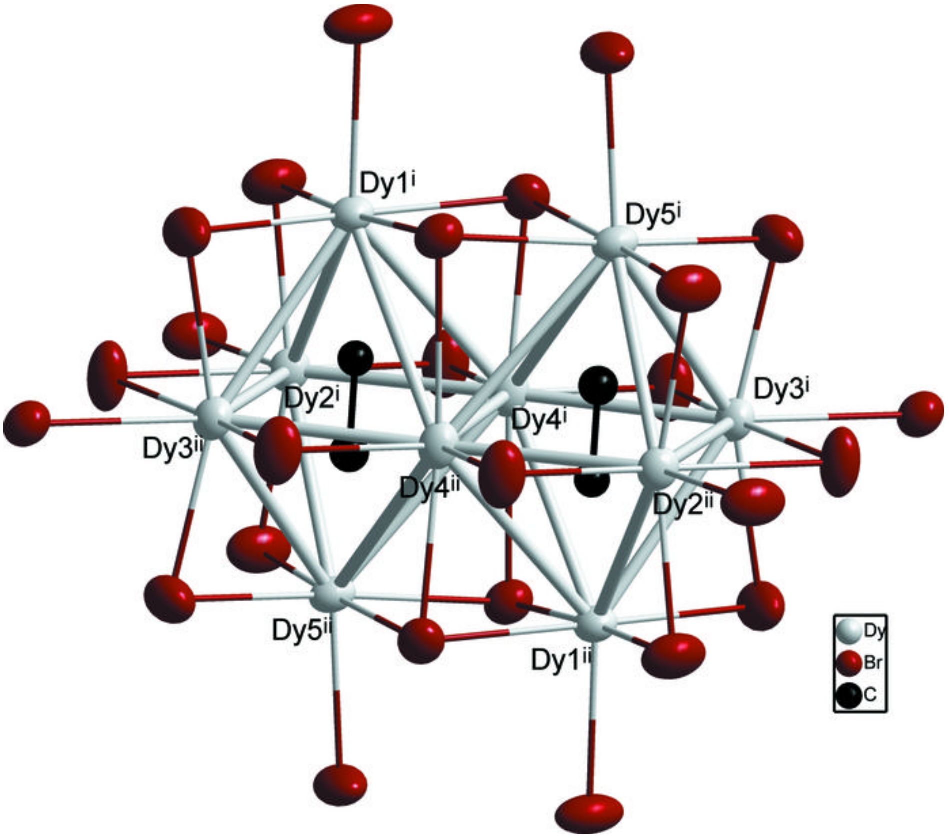
Dy1ⁱ
Dy5ⁱ
Dy2ⁱ
Dy4ⁱ
Dy3ⁱ
Dy3ⁱⁱ
Dy4ⁱⁱ
Dy2ⁱⁱ
Dy5ⁱⁱ
Dy1ⁱⁱ
Dy
Br
C

Fig. 2