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$Dy_8SnS_{13.61}O_{0.39}$ from single-crystal data

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Sn–S) = 0.004 Å; disorder in main residue; R factor = 0.026; wR factor = 0.038; data-to-parameter ratio = 16.2.

Crystals of the title dysprosium tin sulfide oxide, $Dy_8SnS_{13}S_{1-x}O_x$ [x = 0.39 (4)], were obtained unintentionally from the Dy–Sn–S system. A statistical mixture of sulfur and oxygen was assumed for one position in the structure. S and O atoms surround each of the eight symmetrically non-equivalent dysprosium atoms. The Sn atoms are located in tetrahedral surroundings of sulfur atoms. Trigonal prisms and tetrahedra are connected to each other by their edges. All atoms are situated in mirror planes.

Related literature

For previous structures with a statistical mixture of sulfur and oxygen, see: Besançon *et al.* (1973); Schleid (1991).

Experimental

Crystal data

$Dy_8SnS_{13.61}O_{0.39}$
M_r = 1861.27
Orthorhombic, $Cmc2_1$
a = 3.7822 (8) Å
b = 23.620 (5) Å
c = 21.271 (4) Å
V = 1900.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 33.80 mm^{-1}
T = 293 (2) K
0.14 × 0.01 × 0.01 mm

Data collection

KUMA KM-4 CCD area-detector diffractometer
Absorption correction: numerical (CrysAlis; Oxford Diffraction, 2007)
T_{min} = 0.104, T_{max} = 0.716
11655 measured reflections
2287 independent reflections
1910 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.038
S = 0.89
2287 reflections
141 parameters
1 restraint
$\Delta\rho_{max}$ = 3.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.56 e Å^{-3}
Absolute structure: Flack (1983), 1089 Friedel pairs
Flack parameter: 0.0 (2)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *publCIF* (Westrip, 2007) and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2066).

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supplementary materials

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$Dy_8SnS_{13.61}O_{0.39}$ from single-crystal data

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Comment

An attempt to synthesize Dy_2SnS_5, a compound with the La_2SnS_5 type structure was unsuccessful, resulting in a multiphase product. However, the formation of the new compound, $Dy_8SnS_{13}S_{1-x}O_x$ (x = 0.39 (4)) was achieved. The structure of this compound was investigated by means of single-crystal X-ray diffraction. In the initial stage of refinement, the composition Dy_8SnS_{14} was assumed. However, unusually short Dy2—S14 (2.399 (5) Å) and Dy3—S14 (2.508 (7) Å) distances and a large value for the displacement parameter of S14 were observed. To complete the refinement, a statistical mixture (S and O) was assumed at the site of S14. Refinement of this model reduced the unusual displacement parameter to a physically reasonable value. The final composition was $Dy_8SnS_{13}S_{1-x}O_x$ (x = 0.39 (4)). The values of the Dy2—S14 (2.399 (5) Å) and Dy3—S14 (2.508 (7) Å) distances are intermediate between the Dy—O (2.220–2.264 Å) and Dy–S (2.704–2.742 Å) distances in Dy_2OS_2 (Schleid, 1991). A similar substitution of S by O in one position has also been observed in the structure of the $La_{10}S_{14}S_{1-x}O_x$ ($x \simeq 1/2$) compound (Besançon *et al.*, 1973).

The unit cell and coordination polyhedra of the Dy and Sn atoms in the structure of the $Dy_8SnS_{14-x}O_x$ (x = 0.39 (4)) compound are shown in Fig. 1. Sulfur and oxygen atoms surround each of eight symmetrically non-equivalent dysprosium atoms. However, only one mono-capped trigonal prism is evident (Dy1) along with seven bi-capped trigonal prisms around the remaining Dy atoms. The Sn atoms are located in tetrahedral surroundings of sulfur atoms. Trigonal prisms and tetrahedra are connected to each other by edges.

Experimental

Single crystals of the title compound were grown by fusion of the elemental constituents (Alfa Aesar; purity > 99.9%$_{wt}$) in evacuated silica ampoules. The ampoule was heated in a tube furnace with a heating rate of 30 K/h to 1420 K and kept at this temperature for 4 h. It was then cooled down slowly (10 K/h) to 870 K and annealed at this temperature for further 240 h and finally quenched in cold water. The product was a brown-coloured compact alloy containing red crystals with a prismatic habit and maximal lengths of 0.2 mm. An EDAX PV9800 microanalyser was used for the confirmation of the composition of the Dy, Sn and S in the crystal. The content of oxygen (<2%) was out of the limit of the microanalyser.

Refinement

A statistical mixture of the sulfur and oxygen was assumed in the refinement with the same anisotropic displacement parameters for the S14 and O14 atoms. The space group $Cmc2_1$ was confirmed with *PLATON* (Spek, 2003).

Figures

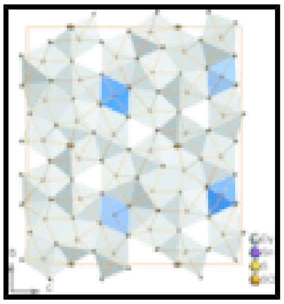

Fig. 1. The structure of $Dy_8SnS_{13.61}O_{0.39}$ viewed down the *a* axis. Displacement ellipsoids are shown at the 50% probability level.

Dysprosium tin sulfide oxide

Crystal data

$Dy_8Sn_1S_{13.61}O_{0.39}$	F_{000} = 3196
M_r = 1861.27	D_x = 6.506 Mg m^{-3}
Orthorhombic, *Cmc*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2c -2	Cell parameters from 1910 reflections
a = 3.7822 (8) Å	θ = 2.6–26.7º
b = 23.620 (5) Å	μ = 33.80 mm^{-1}
c = 21.271 (4) Å	*T* = 293 (2) K
V = 1900.3 (7) Å^3	Needle, red
Z = 4	0.14 × 0.01 × 0.01 mm

Data collection

KUMA KM-4 with CCD area-detector diffractometer	2287 independent reflections
Radiation source: fine-focus sealed tube	1910 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
Detector resolution: 1024x1024 with blocks 2x2, 33.133pixel/mm pixels mm^{-1}	θ_{max} = 26.7º
T = 293(2) K	θ_{min} = 2.6º
ω–scan	*h* = −4→4
Absorption correction: numerical (CrysAlis; Oxford Diffraction, 2007)	*k* = −29→29
T_{min} = 0.104, T_{max} = 0.716	*l* = −26→26
11655 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0128P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.026$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.038$	$\Delta\rho_{max} = 3.05$ e Å^{-3}
$S = 0.89$	$\Delta\rho_{min} = -1.56$ e Å^{-3}
2287 reflections	Extinction correction: none
141 parameters	Absolute structure: Flack (1983), 1089 Friedel pairs
1 restraint	Flack parameter: 0.0 (2)
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Dy1	0.0000	0.69122 (4)	0.08524 (3)	0.0086 (2)	
Dy2	0.0000	0.44849 (4)	0.24158 (5)	0.0242 (3)	
Dy3	0.0000	0.10373 (4)	0.23391 (4)	0.0132 (2)	
Dy4	0.0000	0.04543 (4)	0.40541 (5)	0.0125 (2)	
Dy5	0.0000	0.85422 (4)	0.07459 (5)	0.0106 (2)	
Dy6	0.0000	0.27636 (4)	0.24724 (4)	0.0100 (2)	
Dy7	0.0000	0.37415 (4)	0.41648 (5)	0.0109 (2)	
Dy8	0.5000	0.52208 (3)	0.07589 (4)	0.01244 (19)	
Sn1	0.0000	0.70904 (6)	0.40908 (8)	0.0076 (2)	
S1	0.0000	0.85740 (18)	0.2105 (2)	0.0088 (11)	
S2	0.5000	0.43628 (19)	0.3487 (2)	0.0100 (10)	
S3	0.5000	0.7734 (2)	0.1121 (2)	0.0089 (10)	
S4	0.0000	0.48205 (18)	0.4751 (2)	0.0086 (9)	
S5	0.0000	0.55462 (18)	0.3115 (2)	0.0100 (10)	
S6	0.5000	0.63430 (18)	0.0139 (2)	0.0084 (10)	
S7	0.0000	0.4362 (2)	0.1072 (2)	0.0121 (11)	
S8	0.0000	0.58602 (18)	0.13619 (19)	0.0105 (9)	
S9	0.5000	0.7460 (2)	0.4772 (2)	0.0141 (10)	
S10	0.0000	0.1733 (2)	0.3409 (2)	0.0169 (10)	
S11	0.0000	0.69522 (18)	0.21604 (19)	0.0079 (9)	
S12	0.0000	0.6207 (2)	0.4722 (2)	0.0112 (10)	
S13	0.0000	0.80025 (18)	0.3496 (2)	0.0096 (9)	
O14	0.0000	0.0010 (3)	0.2040 (4)	0.034 (3)	0.39 (4)
S14	0.0000	0.0010 (3)	0.2040 (4)	0.034 (3)	0.61 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.0068 (4)	0.0089 (5)	0.0101 (5)	0.000	0.000	−0.0003 (4)
Dy2	0.0243 (5)	0.0308 (6)	0.0174 (7)	0.000	0.000	−0.0128 (5)
Dy3	0.0077 (4)	0.0231 (5)	0.0089 (5)	0.000	0.000	0.0020 (4)
Dy4	0.0095 (5)	0.0173 (5)	0.0106 (5)	0.000	0.000	0.0007 (4)
Dy5	0.0062 (4)	0.0107 (4)	0.0149 (5)	0.000	0.000	0.0034 (4)
Dy6	0.0069 (4)	0.0122 (4)	0.0110 (5)	0.000	0.000	0.0010 (4)
Dy7	0.0083 (4)	0.0162 (5)	0.0083 (5)	0.000	0.000	−0.0014 (4)
Dy8	0.0062 (4)	0.0104 (4)	0.0207 (5)	0.000	0.000	−0.0021 (4)
Sn1	0.0069 (4)	0.0080 (5)	0.0079 (5)	0.000	0.000	0.0016 (4)
S1	0.012 (3)	0.010 (2)	0.005 (3)	0.000	0.000	−0.0009 (18)
S2	0.007 (2)	0.013 (2)	0.010 (2)	0.000	0.000	−0.004 (2)
S3	0.006 (2)	0.010 (2)	0.010 (3)	0.000	0.000	−0.002 (2)
S4	0.008 (2)	0.008 (2)	0.010 (2)	0.000	0.000	0.0019 (18)
S5	0.009 (2)	0.014 (2)	0.006 (2)	0.000	0.000	0.0020 (17)
S6	0.008 (2)	0.009 (2)	0.008 (2)	0.000	0.000	0.0006 (16)
S7	0.008 (2)	0.014 (2)	0.014 (3)	0.000	0.000	−0.006 (2)
S8	0.011 (2)	0.012 (2)	0.009 (2)	0.000	0.000	−0.0014 (16)
S9	0.009 (2)	0.021 (3)	0.013 (2)	0.000	0.000	−0.0090 (18)
S10	0.009 (2)	0.029 (3)	0.012 (2)	0.000	0.000	−0.011 (2)
S11	0.010 (2)	0.007 (2)	0.007 (2)	0.000	0.000	0.0045 (17)
S12	0.013 (2)	0.012 (2)	0.009 (2)	0.000	0.000	0.001 (2)
S13	0.013 (2)	0.008 (2)	0.008 (2)	0.000	0.000	0.0007 (18)
O14	0.023 (4)	0.022 (5)	0.056 (6)	0.000	0.000	−0.004 (4)
S14	0.023 (4)	0.022 (5)	0.056 (6)	0.000	0.000	−0.004 (4)

Geometric parameters (Å, °)

Dy1—S8	2.711 (4)	Dy7—S13^{vii}	2.940 (3)
Dy1—S9^{i}	2.735 (5)	Dy7—S13^{viii}	2.940 (3)
Dy1—S3	2.769 (3)	Dy7—Dy7^{ii}	3.7822 (8)
Dy1—S3^{ii}	2.769 (3)	Dy7—Dy7^{iii}	3.7822 (8)
Dy1—S6^{ii}	2.772 (3)	Dy7—Dy1^{xii}	3.9078 (15)
Dy1—S6	2.772 (3)	Dy8—S8^{iii}	2.739 (3)
Dy1—S11	2.784 (4)	Dy8—S8	2.739 (3)
Dy1—Dy1^{ii}	3.7822 (8)	Dy8—S14^{v}	2.770 (8)
Dy1—Dy1^{iii}	3.7822 (8)	Dy8—O14^{v}	2.770 (8)
Dy1—Dy5	3.8567 (14)	Dy8—S7	2.852 (4)
Dy1—Dy7^{iv}	3.9078 (15)	Dy8—S7^{iii}	2.852 (4)
Dy2—S14^{v}	2.399 (5)	Dy8—S4^{iv}	2.861 (3)
Dy2—O14^{v}	2.399 (5)	Dy8—S4^{xiii}	2.861 (3)
Dy2—S14^{vi}	2.399 (5)	Dy8—S6	2.960 (4)
Dy2—O14^{vi}	2.399 (5)	Dy8—Dy8^{ii}	3.7822 (8)

Dy2—S7	2.873 (5)	Dy8—Dy8^{iii}	3.7822 (8)
Dy2—S5	2.914 (5)	Dy8—Dy3^{v}	3.8753 (14)
Dy2—S1^{vii}	2.940 (3)	Sn1—S12	2.481 (5)
Dy2—S1^{viii}	2.940 (3)	Sn1—S13	2.498 (5)
Dy2—S2	2.976 (4)	Sn1—S10^{vi}	2.529 (3)
Dy2—S2^{ii}	2.976 (4)	Sn1—S10^{v}	2.529 (3)
Dy2—Dy2^{ii}	3.7822 (8)	Sn1—S9	2.537 (3)
Dy2—Dy2^{iii}	3.7822 (8)	Sn1—S9^{ii}	2.537 (3)
Dy3—O14	2.508 (7)	S1—Dy6^{vi}	2.802 (3)
Dy3—S5^{viii}	2.765 (3)	S1—Dy6^{v}	2.802 (3)
Dy3—S5^{vii}	2.765 (3)	S1—Dy2^{v}	2.940 (3)
Dy3—S10	2.807 (5)	S1—Dy2^{vi}	2.940 (3)
Dy3—S8^{vii}	2.841 (3)	S2—Dy7^{iii}	2.794 (4)
Dy3—S8^{viii}	2.841 (3)	S2—Dy4^{v}	2.846 (5)
Dy3—S11^{viii}	2.897 (3)	S2—Dy2^{iii}	2.976 (4)
Dy3—S11^{vii}	2.897 (3)	S3—Dy1^{iii}	2.769 (3)
Dy3—Dy3^{ii}	3.7822 (8)	S3—Dy5^{iii}	2.803 (4)
Dy3—Dy3^{iii}	3.7822 (8)	S3—Dy6^{v}	2.876 (5)
Dy3—Dy8^{vii}	3.8753 (14)	S4—Dy4^{v}	2.831 (3)
Dy4—S5^{vii}	2.760 (3)	S4—Dy4^{vi}	2.831 (3)
Dy4—S5^{viii}	2.760 (3)	S4—Dy8^{xi}	2.861 (3)
Dy4—S4^{viii}	2.831 (3)	S4—Dy8^{xii}	2.861 (3)
Dy4—S4^{vii}	2.831 (3)	S5—Dy4^{v}	2.760 (3)
Dy4—S2^{vii}	2.846 (5)	S5—Dy4^{vi}	2.760 (3)
Dy4—S12^{viii}	2.960 (4)	S5—Dy3^{vi}	2.765 (3)
Dy4—S12^{vii}	2.960 (4)	S5—Dy3^{v}	2.765 (3)
Dy4—Dy4^{iii}	3.7822 (8)	S6—Dy1^{iii}	2.772 (3)
Dy4—Dy4^{ii}	3.7822 (8)	S6—Dy7^{iv}	2.813 (3)
Dy4—Dy8^{ix}	3.9612 (17)	S6—Dy7^{xiii}	2.813 (3)
Dy5—S7^{v}	2.794 (4)	S7—Dy5^{vii}	2.794 (4)
Dy5—S7^{vi}	2.794 (4)	S7—Dy5^{viii}	2.794 (4)
Dy5—S3	2.803 (4)	S7—Dy8^{ii}	2.852 (4)
Dy5—S3^{ii}	2.803 (4)	S8—Dy8^{ii}	2.739 (3)
Dy5—S1	2.892 (5)	S8—Dy3^{v}	2.841 (3)
Dy5—S12^{x}	2.944 (4)	S8—Dy3^{vi}	2.841 (3)
Dy5—S12^{i}	2.944 (4)	S9—Sn1^{iii}	2.537 (3)
Dy5—S9^{i}	3.145 (5)	S9—Dy1^{xiv}	2.735 (5)
Dy5—Dy5^{ii}	3.7822 (8)	S9—Dy5^{xiv}	3.145 (5)
Dy5—Dy5^{iii}	3.7822 (8)	S10—Sn1^{viii}	2.529 (3)
Dy5—Dy8^{vi}	3.9649 (15)	S10—Sn1^{vii}	2.529 (3)
Dy6—S11^{vii}	2.773 (3)	S11—Dy6^{v}	2.773 (3)

Dy6—S11^{viii}	2.773 (3)	S11—Dy6^{vi}	2.773 (3)
Dy6—S1^{viii}	2.802 (3)	S11—Dy3^{vi}	2.897 (3)
Dy6—S1^{vii}	2.802 (3)	S11—Dy3^{v}	2.897 (3)
Dy6—S3^{vii}	2.876 (5)	S12—Dy5^{xiv}	2.944 (4)
Dy6—S13^{viii}	2.939 (3)	S12—Dy5^{xv}	2.944 (4)
Dy6—S13^{vii}	2.939 (3)	S12—Dy4^{vi}	2.960 (4)
Dy6—S10	3.145 (5)	S12—Dy4^{v}	2.960 (4)
Dy6—Dy6^{iii}	3.7822 (8)	S13—Dy6^{vi}	2.939 (3)
Dy6—Dy6^{ii}	3.7822 (8)	S13—Dy6^{v}	2.939 (3)
Dy7—S2	2.794 (4)	S13—Dy7^{v}	2.940 (3)
Dy7—S2^{ii}	2.794 (4)	S13—Dy7^{vi}	2.940 (3)
Dy7—S6^{xi}	2.813 (3)	O14—Dy2^{vii}	2.399 (5)
Dy7—S6^{xii}	2.813 (3)	O14—Dy2^{viii}	2.399 (5)
Dy7—S4	2.837 (5)	O14—Dy8^{vii}	2.770 (8)

S8—Dy1—S9^{i}	146.41 (14)	S11^{vii}—Dy6—S1^{viii}	149.95 (14)
S8—Dy1—S3	124.06 (10)	S11^{viii}—Dy6—S1^{viii}	86.85 (10)
S9^{i}—Dy1—S3	78.05 (13)	S11^{vii}—Dy6—S1^{vii}	86.85 (9)
S8—Dy1—S3^{ii}	124.06 (10)	S11^{viii}—Dy6—S1^{vii}	149.95 (14)
S9^{i}—Dy1—S3^{ii}	78.05 (13)	S1^{viii}—Dy6—S1^{vii}	84.89 (12)
S3—Dy1—S3^{ii}	86.14 (13)	S11^{vii}—Dy6—S3^{vii}	75.16 (11)
S8—Dy1—S6^{ii}	76.95 (11)	S11^{viii}—Dy6—S3^{vii}	75.16 (11)
S9^{i}—Dy1—S6^{ii}	78.66 (12)	S1^{viii}—Dy6—S3^{vii}	74.79 (12)
S3—Dy1—S6^{ii}	156.70 (14)	S1^{vii}—Dy6—S3^{vii}	74.79 (12)
S3^{ii}—Dy1—S6^{ii}	89.24 (10)	S11^{vii}—Dy6—S13^{viii}	138.49 (12)
S8—Dy1—S6	76.95 (11)	S11^{viii}—Dy6—S13^{viii}	82.60 (10)
S9^{i}—Dy1—S6	78.66 (12)	S1^{viii}—Dy6—S13^{viii}	68.99 (11)
S3—Dy1—S6	89.24 (10)	S1^{vii}—Dy6—S13^{viii}	120.66 (12)
S3^{ii}—Dy1—S6	156.70 (14)	S3^{vii}—Dy6—S13^{viii}	138.20 (6)
S6^{ii}—Dy1—S6	86.02 (13)	S11^{vii}—Dy6—S13^{vii}	82.60 (10)
S8—Dy1—S11	68.38 (12)	S11^{viii}—Dy6—S13^{vii}	138.49 (12)
S9^{i}—Dy1—S11	145.21 (13)	S1^{viii}—Dy6—S13^{vii}	120.66 (12)
S3—Dy1—S11	76.72 (12)	S1^{vii}—Dy6—S13^{vii}	68.99 (11)
S3^{ii}—Dy1—S11	76.72 (12)	S3^{vii}—Dy6—S13^{vii}	138.20 (6)
S6^{ii}—Dy1—S11	124.29 (10)	S13^{viii}—Dy6—S13^{vii}	80.09 (11)
S6—Dy1—S11	124.29 (10)	S11^{vii}—Dy6—S10	67.46 (10)
S8—Dy1—Dy1^{ii}	90.0	S11^{viii}—Dy6—S10	67.46 (10)
S9^{i}—Dy1—Dy1^{ii}	90.0	S1^{viii}—Dy6—S10	134.86 (8)
S3—Dy1—Dy1^{ii}	133.07 (7)	S1^{vii}—Dy6—S10	134.86 (8)
S3^{ii}—Dy1—Dy1^{ii}	46.93 (7)	S3^{vii}—Dy6—S10	127.89 (13)
S6^{ii}—Dy1—Dy1^{ii}	46.99 (6)	S13^{viii}—Dy6—S10	71.30 (10)

S6—Dy1—Dy1^{ii}	133.01 (6)	S13^{vii}—Dy6—S10	71.30 (10)
S11—Dy1—Dy1^{ii}	90.0	S11^{vii}—Dy6—Dy6^{iii}	133.00 (6)
S8—Dy1—Dy1^{iii}	90.0	S11^{viii}—Dy6—Dy6^{iii}	47.00 (6)
S9^{i}—Dy1—Dy1^{iii}	90.0	S1^{viii}—Dy6—Dy6^{iii}	47.55 (6)
S3—Dy1—Dy1^{iii}	46.93 (7)	S1^{vii}—Dy6—Dy6^{iii}	132.45 (6)
S3^{ii}—Dy1—Dy1^{iii}	133.07 (7)	S3^{vii}—Dy6—Dy6^{iii}	90.0
S6^{ii}—Dy1—Dy1^{iii}	133.01 (6)	S13^{viii}—Dy6—Dy6^{iii}	49.95 (5)
S6—Dy1—Dy1^{iii}	46.99 (6)	S13^{vii}—Dy6—Dy6^{iii}	130.05 (5)
S11—Dy1—Dy1^{iii}	90.0	S10—Dy6—Dy6^{iii}	90.0
Dy1^{ii}—Dy1—Dy1^{iii}	180.00 (5)	S11^{vii}—Dy6—Dy6^{ii}	47.00 (6)
S8—Dy1—Dy5	159.81 (9)	S11^{viii}—Dy6—Dy6^{ii}	133.00 (6)
S9^{i}—Dy1—Dy5	53.78 (10)	S1^{viii}—Dy6—Dy6^{ii}	132.45 (6)
S3—Dy1—Dy5	46.56 (8)	S1^{vii}—Dy6—Dy6^{ii}	47.55 (6)
S3^{ii}—Dy1—Dy5	46.56 (8)	S3^{vii}—Dy6—Dy6^{ii}	90.0
S6^{ii}—Dy1—Dy5	116.87 (9)	S13^{viii}—Dy6—Dy6^{ii}	130.05 (5)
S6—Dy1—Dy5	116.87 (9)	S13^{vii}—Dy6—Dy6^{ii}	49.95 (5)
S11—Dy1—Dy5	91.43 (9)	S10—Dy6—Dy6^{ii}	90.0
Dy1^{ii}—Dy1—Dy5	90.0	Dy6^{iii}—Dy6—Dy6^{ii}	180.00 (5)
Dy1^{iii}—Dy1—Dy5	90.0	S2—Dy7—S2^{ii}	85.20 (14)
S8—Dy1—Dy7^{iv}	90.29 (9)	S2—Dy7—S6^{xi}	87.83 (11)
S9^{i}—Dy1—Dy7^{iv}	56.12 (10)	S2^{ii}—Dy7—S6^{xi}	150.73 (13)
S3—Dy1—Dy7^{iv}	117.79 (10)	S2—Dy7—S6^{xii}	150.73 (13)
S3^{ii}—Dy1—Dy7^{iv}	117.79 (10)	S2^{ii}—Dy7—S6^{xii}	87.83 (11)
S6^{ii}—Dy1—Dy7^{iv}	46.02 (7)	S6^{xi}—Dy7—S6^{xii}	84.49 (13)
S6—Dy1—Dy7^{iv}	46.02 (7)	S2—Dy7—S4	75.80 (11)
S11—Dy1—Dy7^{iv}	158.67 (9)	S2^{ii}—Dy7—S4	75.80 (11)
Dy1^{ii}—Dy1—Dy7^{iv}	90.0	S6^{xi}—Dy7—S4	74.93 (11)
Dy1^{iii}—Dy1—Dy7^{iv}	90.0	S6^{xii}—Dy7—S4	74.93 (11)
Dy5—Dy1—Dy7^{iv}	109.91 (3)	S2—Dy7—S13^{vii}	119.86 (13)
S14^{v}—Dy2—O14^{v}	0.0 (5)	S2^{ii}—Dy7—S13^{vii}	68.11 (12)
S14^{v}—Dy2—S14^{vi}	104.1 (3)	S6^{xi}—Dy7—S13^{vii}	138.30 (12)
O14^{v}—Dy2—S14^{vi}	104.1 (3)	S6^{xii}—Dy7—S13^{vii}	83.21 (10)
S14^{v}—Dy2—O14^{vi}	104.1 (3)	S4—Dy7—S13^{vii}	138.23 (6)
O14^{v}—Dy2—O14^{vi}	104.1 (3)	S2—Dy7—S13^{viii}	68.11 (12)
S14^{vi}—Dy2—O14^{vi}	0.0 (4)	S2^{ii}—Dy7—S13^{viii}	119.86 (13)
S14^{v}—Dy2—S7	73.79 (19)	S6^{xi}—Dy7—S13^{viii}	83.21 (10)
O14^{v}—Dy2—S7	73.79 (19)	S6^{xii}—Dy7—S13^{viii}	138.30 (12)
S14^{vi}—Dy2—S7	73.79 (19)	S4—Dy7—S13^{viii}	138.23 (6)
O14^{vi}—Dy2—S7	73.79 (19)	S13^{vii}—Dy7—S13^{viii}	80.06 (11)
S14^{v}—Dy2—S5	74.03 (17)	S2—Dy7—Dy7^{ii}	132.60 (7)
O14^{v}—Dy2—S5	74.03 (17)	S2^{ii}—Dy7—Dy7^{ii}	47.40 (7)

S14^{vi}—Dy2—S5	74.03 (17)	S6^{xi}—Dy7—Dy7^{ii}	132.25 (6)
O14^{vi}—Dy2—S5	74.03 (17)	S6^{xii}—Dy7—Dy7^{ii}	47.75 (6)
S7—Dy2—S5	126.46 (14)	S4—Dy7—Dy7^{ii}	90.0
S14^{v}—Dy2—S1^{vii}	144.2 (2)	S13^{vii}—Dy7—Dy7^{ii}	49.97 (6)
O14^{v}—Dy2—S1^{vii}	144.2 (2)	S13^{viii}—Dy7—Dy7^{ii}	130.03 (6)
S14^{vi}—Dy2—S1^{vii}	78.26 (16)	S2—Dy7—Dy7^{iii}	47.40 (7)
O14^{vi}—Dy2—S1^{vii}	78.26 (16)	S2^{ii}—Dy7—Dy7^{iii}	132.60 (7)
S7—Dy2—S1^{vii}	72.68 (12)	S6^{xi}—Dy7—Dy7^{iii}	47.75 (6)
S5—Dy2—S1^{vii}	138.10 (7)	S6^{xii}—Dy7—Dy7^{iii}	132.25 (6)
S14^{v}—Dy2—S1^{viii}	78.26 (16)	S4—Dy7—Dy7^{iii}	90.0
O14^{v}—Dy2—S1^{viii}	78.26 (16)	S13^{vii}—Dy7—Dy7^{iii}	130.03 (6)
S14^{vi}—Dy2—S1^{viii}	144.2 (2)	S13^{viii}—Dy7—Dy7^{iii}	49.97 (6)
O14^{vi}—Dy2—S1^{viii}	144.2 (2)	Dy7^{ii}—Dy7—Dy7^{iii}	180.00 (8)
S7—Dy2—S1^{viii}	72.68 (12)	S2—Dy7—Dy1^{xii}	132.94 (8)
S5—Dy2—S1^{viii}	138.10 (7)	S2^{ii}—Dy7—Dy1^{xii}	132.94 (8)
S1^{vii}—Dy2—S1^{viii}	80.07 (11)	S6^{xi}—Dy7—Dy1^{xii}	45.18 (7)
S14^{v}—Dy2—S2	78.71 (18)	S6^{xii}—Dy7—Dy1^{xii}	45.18 (7)
O14^{v}—Dy2—S2	78.71 (18)	S4—Dy7—Dy1^{xii}	87.21 (9)
S14^{vi}—Dy2—S2	143.7 (2)	S13^{vii}—Dy7—Dy1^{xii}	102.10 (8)
O14^{vi}—Dy2—S2	143.7 (2)	S13^{viii}—Dy7—Dy1^{xii}	102.10 (8)
S7—Dy2—S2	138.79 (7)	Dy7^{ii}—Dy7—Dy1^{xii}	90.0
S5—Dy2—S2	72.10 (11)	Dy7^{iii}—Dy7—Dy1^{xii}	90.0
S1^{vii}—Dy2—S2	120.68 (12)	S8^{iii}—Dy8—S8	87.33 (13)
S1^{viii}—Dy2—S2	72.10 (11)	S8^{iii}—Dy8—S14^{v}	68.79 (14)
S14^{v}—Dy2—S2^{ii}	143.7 (2)	S8—Dy8—S14^{v}	68.79 (14)
O14^{v}—Dy2—S2^{ii}	143.7 (2)	S8^{iii}—Dy8—O14^{v}	68.79 (14)
S14^{vi}—Dy2—S2^{ii}	78.71 (18)	S8—Dy8—O14^{v}	68.79 (14)
O14^{vi}—Dy2—S2^{ii}	78.71 (18)	S14^{v}—Dy8—O14^{v}	0.0 (3)
S7—Dy2—S2^{ii}	138.79 (7)	S8^{iii}—Dy8—S7	137.78 (12)
S5—Dy2—S2^{ii}	72.10 (11)	S8—Dy8—S7	79.92 (11)
S1^{vii}—Dy2—S2^{ii}	72.10 (11)	S14^{v}—Dy8—S7	69.06 (15)
S1^{viii}—Dy2—S2^{ii}	120.68 (12)	O14^{v}—Dy8—S7	69.06 (15)
S2—Dy2—S2^{ii}	78.91 (12)	S8^{iii}—Dy8—S7^{iii}	79.92 (11)
S14^{v}—Dy2—Dy2^{ii}	142.03 (14)	S8—Dy8—S7^{iii}	137.78 (12)
O14^{v}—Dy2—Dy2^{ii}	142.03 (14)	S14^{v}—Dy8—S7^{iii}	69.06 (15)
S14^{vi}—Dy2—Dy2^{ii}	37.97 (14)	O14^{v}—Dy8—S7^{iii}	69.06 (15)
O14^{vi}—Dy2—Dy2^{ii}	37.97 (14)	S7—Dy8—S7^{iii}	83.07 (13)
S7—Dy2—Dy2^{ii}	90.0	S8^{iii}—Dy8—S4^{iv}	145.71 (13)
S5—Dy2—Dy2^{ii}	90.0	S8—Dy8—S4^{iv}	85.03 (10)
S1^{vii}—Dy2—Dy2^{ii}	49.97 (6)	S14^{v}—Dy8—S4^{iv}	136.99 (8)
S1^{viii}—Dy2—Dy2^{ii}	130.03 (6)	O14^{v}—Dy8—S4^{iv}	136.99 (8)

$S2—Dy2—Dy2^{ii}$	129.46 (6)	$S7—Dy8—S4^{iv}$	73.29 (12)
$S2^{ii}—Dy2—Dy2^{ii}$	50.54 (6)	$S7^{iii}—Dy8—S4^{iv}$	126.09 (13)
$S14^{v}—Dy2—Dy2^{iii}$	37.97 (14)	$S8^{iii}—Dy8—S4^{xiii}$	85.03 (10)
$O14^{v}—Dy2—Dy2^{iii}$	37.97 (14)	$S8—Dy8—S4^{xiii}$	145.71 (13)
$S14^{vi}—Dy2—Dy2^{iii}$	142.03 (14)	$S14^{v}—Dy8—S4^{xiii}$	136.99 (8)
$O14^{vi}—Dy2—Dy2^{iii}$	142.03 (14)	$O14^{v}—Dy8—S4^{xiii}$	136.99 (8)
$S7—Dy2—Dy2^{iii}$	90.0	$S7—Dy8—S4^{xiii}$	126.09 (13)
$S5—Dy2—Dy2^{iii}$	90.0	$S7^{iii}—Dy8—S4^{xiii}$	73.29 (12)
$S1^{vii}—Dy2—Dy2^{iii}$	130.03 (6)	$S4^{iv}—Dy8—S4^{xiii}$	82.77 (12)
$S1^{viii}—Dy2—Dy2^{iii}$	49.97 (6)	$S8^{iii}—Dy8—S6$	73.43 (10)
$S2—Dy2—Dy2^{iii}$	50.54 (6)	$S8—Dy8—S6$	73.43 (10)
$S2^{ii}—Dy2—Dy2^{iii}$	129.46 (6)	$S14^{v}—Dy8—S6$	126.78 (17)
$Dy2^{ii}—Dy2—Dy2^{iii}$	180.00 (6)	$O14^{v}—Dy8—S6$	126.78 (17)
$O14—Dy3—S5^{viii}$	75.25 (16)	$S7—Dy8—S6$	137.80 (7)
$O14—Dy3—S5^{vii}$	75.25 (16)	$S7^{iii}—Dy8—S6$	137.80 (7)
$S5^{viii}—Dy3—S5^{vii}$	86.32 (13)	$S4^{iv}—Dy8—S6$	72.35 (11)
$O14—Dy3—S10$	140.5 (2)	$S4^{xiii}—Dy8—S6$	72.35 (11)
$S5^{viii}—Dy3—S10$	76.23 (12)	$S8^{iii}—Dy8—Dy8^{ii}$	133.66 (6)
$S5^{vii}—Dy3—S10$	76.23 (12)	$S8—Dy8—Dy8^{ii}$	46.34 (6)
$O14—Dy3—S8^{vii}$	70.86 (16)	$S14^{v}—Dy8—Dy8^{ii}$	90.0
$S5^{viii}—Dy3—S8^{vii}$	146.11 (13)	$O14^{v}—Dy8—Dy8^{ii}$	90.0
$S5^{vii}—Dy3—S8^{vii}$	85.38 (10)	$S7—Dy8—Dy8^{ii}$	48.47 (7)
$S10—Dy3—S8^{vii}$	132.79 (8)	$S7^{iii}—Dy8—Dy8^{ii}$	131.53 (7)
$O14—Dy3—S8^{viii}$	70.86 (16)	$S4^{iv}—Dy8—Dy8^{ii}$	48.62 (6)
$S5^{viii}—Dy3—S8^{viii}$	85.38 (10)	$S4^{xiii}—Dy8—Dy8^{ii}$	131.38 (6)
$S5^{vii}—Dy3—S8^{viii}$	146.11 (13)	$S6—Dy8—Dy8^{ii}$	90.0
$S10—Dy3—S8^{viii}$	132.79 (8)	$S8^{iii}—Dy8—Dy8^{iii}$	46.34 (6)
$S8^{vii}—Dy3—S8^{viii}$	83.46 (11)	$S8—Dy8—Dy8^{iii}$	133.66 (6)
$O14—Dy3—S11^{viii}$	133.50 (11)	$S14^{v}—Dy8—Dy8^{iii}$	90.0
$S5^{viii}—Dy3—S11^{viii}$	86.83 (9)	$O14^{v}—Dy8—Dy8^{iii}$	90.0
$S5^{vii}—Dy3—S11^{viii}$	146.92 (13)	$S7—Dy8—Dy8^{iii}$	131.53 (7)
$S10—Dy3—S11^{viii}$	70.70 (11)	$S7^{iii}—Dy8—Dy8^{iii}$	48.47 (7)
$S8^{vii}—Dy3—S11^{viii}$	116.65 (11)	$S4^{iv}—Dy8—Dy8^{iii}$	131.38 (6)
$S8^{viii}—Dy3—S11^{viii}$	65.12 (11)	$S4^{xiii}—Dy8—Dy8^{iii}$	48.62 (6)
$O14—Dy3—S11^{vii}$	133.50 (11)	$S6—Dy8—Dy8^{iii}$	90.0
$S5^{viii}—Dy3—S11^{vii}$	146.92 (13)	$Dy8^{ii}—Dy8—Dy8^{iii}$	180.0
$S5^{vii}—Dy3—S11^{vii}$	86.83 (9)	$S8^{iii}—Dy8—Dy3^{v}$	47.11 (7)
$S10—Dy3—S11^{vii}$	70.70 (11)	$S8—Dy8—Dy3^{v}$	47.11 (7)
$S8^{vii}—Dy3—S11^{vii}$	65.12 (11)	$S14^{v}—Dy8—Dy3^{v}$	40.19 (15)
$S8^{viii}—Dy3—S11^{vii}$	116.65 (11)	$O14^{v}—Dy8—Dy3^{v}$	40.19 (15)
$S11^{viii}—Dy3—S11^{vii}$	81.52 (11)	$S7—Dy8—Dy3^{v}$	98.71 (10)

O14—Dy3—Dy3^{ii}	90.0	S7^{iii}—Dy8—Dy3^{v}	98.71 (10)
S5^{viii}—Dy3—Dy3^{ii}	133.16 (6)	S4^{iv}—Dy8—Dy3^{v}	131.84 (7)
S5^{vii}—Dy3—Dy3^{ii}	46.84 (6)	S4^{xiii}—Dy8—Dy3^{v}	131.84 (7)
S10—Dy3—Dy3^{ii}	90.0	S6—Dy8—Dy3^{v}	86.59 (9)
S8^{vii}—Dy3—Dy3^{ii}	48.27 (6)	Dy8^{ii}—Dy8—Dy3^{v}	90.0
S8^{viii}—Dy3—Dy3^{ii}	131.73 (6)	Dy8^{iii}—Dy8—Dy3^{v}	90.0
S11^{viii}—Dy3—Dy3^{ii}	130.76 (5)	S12—Sn1—S13	177.64 (19)
S11^{vii}—Dy3—Dy3^{ii}	49.24 (5)	S12—Sn1—S10^{vi}	91.72 (15)
O14—Dy3—Dy3^{iii}	90.0	S13—Sn1—S10^{vi}	89.85 (14)
S5^{viii}—Dy3—Dy3^{iii}	46.84 (6)	S12—Sn1—S10^{v}	91.72 (15)
S5^{vii}—Dy3—Dy3^{iii}	133.16 (6)	S13—Sn1—S10^{v}	89.85 (14)
S10—Dy3—Dy3^{iii}	90.0	S10^{vi}—Sn1—S10^{v}	96.82 (16)
S8^{vii}—Dy3—Dy3^{iii}	131.73 (6)	S12—Sn1—S9	88.85 (14)
S8^{viii}—Dy3—Dy3^{iii}	48.27 (6)	S13—Sn1—S9	89.58 (14)
S11^{viii}—Dy3—Dy3^{iii}	49.24 (5)	S10^{vi}—Sn1—S9	179.39 (19)
S11^{vii}—Dy3—Dy3^{iii}	130.76 (5)	S10^{v}—Sn1—S9	83.40 (8)
Dy3^{ii}—Dy3—Dy3^{iii}	180.00 (3)	S12—Sn1—S9^{ii}	88.85 (14)
O14—Dy3—Dy8^{vii}	45.47 (18)	S13—Sn1—S9^{ii}	89.58 (13)
S5^{viii}—Dy3—Dy8^{vii}	107.98 (9)	S10^{vi}—Sn1—S9^{ii}	83.40 (8)
S5^{vii}—Dy3—Dy8^{vii}	107.98 (9)	S10^{v}—Sn1—S9^{ii}	179.39 (19)
S10—Dy3—Dy8^{vii}	174.01 (11)	S9—Sn1—S9^{ii}	96.38 (16)
S8^{vii}—Dy3—Dy8^{vii}	44.94 (7)	Dy6^{vi}—S1—Dy6^{v}	84.89 (12)
S8^{viii}—Dy3—Dy8^{vii}	44.94 (7)	Dy6^{vi}—S1—Dy5	105.14 (12)
S11^{viii}—Dy3—Dy8^{vii}	104.92 (9)	Dy6^{v}—S1—Dy5	105.14 (12)
S11^{vii}—Dy3—Dy8^{vii}	104.92 (8)	Dy6^{vi}—S1—Dy2^{v}	150.61 (19)
Dy3^{ii}—Dy3—Dy8^{vii}	90.0	Dy6^{v}—S1—Dy2^{v}	90.17 (6)
Dy3^{iii}—Dy3—Dy8^{vii}	90.0	Dy5—S1—Dy2^{v}	104.12 (12)
S5^{vii}—Dy4—S5^{viii}	86.51 (13)	Dy6^{vi}—S1—Dy2^{vi}	90.17 (6)
S5^{vii}—Dy4—S4^{viii}	151.45 (13)	Dy6^{v}—S1—Dy2^{vi}	150.61 (19)
S5^{viii}—Dy4—S4^{viii}	87.87 (10)	Dy5—S1—Dy2^{vi}	104.12 (12)
S5^{vii}—Dy4—S4^{vii}	87.87 (10)	Dy2^{v}—S1—Dy2^{vi}	80.07 (11)
S5^{viii}—Dy4—S4^{vii}	151.45 (13)	Dy7—S2—Dy7^{iii}	85.20 (14)
S4^{viii}—Dy4—S4^{vii}	83.83 (12)	Dy7—S2—Dy4^{v}	104.92 (13)
S5^{vii}—Dy4—S2^{vii}	76.38 (11)	Dy7^{iii}—S2—Dy4^{v}	104.92 (13)
S5^{viii}—Dy4—S2^{vii}	76.38 (11)	Dy7—S2—Dy2	90.90 (5)
S4^{viii}—Dy4—S2^{vii}	75.09 (11)	Dy7^{iii}—S2—Dy2	151.17 (18)
S4^{vii}—Dy4—S2^{vii}	75.09 (11)	Dy4^{v}—S2—Dy2	103.69 (13)
S5^{vii}—Dy4—S12^{viii}	137.58 (12)	Dy7—S2—Dy2^{iii}	151.17 (18)
S5^{viii}—Dy4—S12^{viii}	82.10 (11)	Dy7^{iii}—S2—Dy2^{iii}	90.90 (5)
S4^{viii}—Dy4—S12^{viii}	68.88 (12)	Dy4^{v}—S2—Dy2^{iii}	103.69 (13)
S4^{vii}—Dy4—S12^{viii}	119.56 (13)	Dy2—S2—Dy2^{iii}	78.91 (12)

$S2^{vii}$—Dy4—$S12^{viii}$	138.40 (7)	Dy1—S3—$Dy1^{iii}$	86.14 (13)
$S5^{vii}$—Dy4—$S12^{vii}$	82.10 (11)	Dy1—S3—$Dy5^{iii}$	151.58 (19)
$S5^{viii}$—Dy4—$S12^{vii}$	137.58 (12)	$Dy1^{iii}$—S3—$Dy5^{iii}$	87.60 (5)
$S4^{viii}$—Dy4—$S12^{vii}$	119.56 (13)	Dy1—S3—Dy5	87.60 (5)
$S4^{vii}$—Dy4—$S12^{vii}$	68.88 (12)	$Dy1^{iii}$—S3—Dy5	151.58 (19)
$S2^{vii}$—Dy4—$S12^{vii}$	138.40 (7)	$Dy5^{iii}$—S3—Dy5	84.86 (13)
$S12^{viii}$—Dy4—$S12^{vii}$	79.43 (12)	Dy1—S3—$Dy6^{v}$	102.89 (13)
$S5^{vii}$—Dy4—$Dy4^{iii}$	133.25 (7)	$Dy1^{iii}$—S3—$Dy6^{v}$	102.89 (13)
$S5^{viii}$—Dy4—$Dy4^{iii}$	46.75 (7)	$Dy5^{iii}$—S3—$Dy6^{v}$	105.53 (13)
$S4^{viii}$—Dy4—$Dy4^{iii}$	48.09 (6)	Dy5—S3—$Dy6^{v}$	105.53 (13)
$S4^{vii}$—Dy4—$Dy4^{iii}$	131.91 (6)	$Dy4^{v}$—S4—$Dy4^{vi}$	83.83 (12)
$S2^{vii}$—Dy4—$Dy4^{iii}$	90.0	$Dy4^{v}$—S4—Dy7	104.18 (12)
$S12^{viii}$—Dy4—$Dy4^{iii}$	50.28 (6)	$Dy4^{vi}$—S4—Dy7	104.18 (12)
$S12^{vii}$—Dy4—$Dy4^{iii}$	129.72 (6)	$Dy4^{v}$—S4—$Dy8^{xi}$	88.21 (5)
$S5^{vii}$—Dy4—$Dy4^{ii}$	46.75 (7)	$Dy4^{vi}$—S4—$Dy8^{xi}$	148.43 (17)
$S5^{viii}$—Dy4—$Dy4^{ii}$	133.25 (7)	Dy7—S4—$Dy8^{xi}$	107.38 (12)
$S4^{viii}$—Dy4—$Dy4^{ii}$	131.91 (6)	$Dy4^{v}$—S4—$Dy8^{xii}$	148.43 (17)
$S4^{vii}$—Dy4—$Dy4^{ii}$	48.09 (6)	$Dy4^{vi}$—S4—$Dy8^{xii}$	88.21 (5)
$S2^{vii}$—Dy4—$Dy4^{ii}$	90.0	Dy7—S4—$Dy8^{xii}$	107.38 (12)
$S12^{viii}$—Dy4—$Dy4^{ii}$	129.72 (6)	$Dy8^{xi}$—S4—$Dy8^{xii}$	82.77 (12)
$S12^{vii}$—Dy4—$Dy4^{ii}$	50.28 (6)	$Dy4^{v}$—S5—$Dy4^{vi}$	86.51 (13)
$Dy4^{iii}$—Dy4—$Dy4^{ii}$	180.00 (5)	$Dy4^{v}$—S5—$Dy3^{vi}$	159.03 (18)
$S5^{vii}$—Dy4—Dy3	45.15 (7)	$Dy4^{vi}$—S5—$Dy3^{vi}$	89.79 (4)
$S5^{viii}$—Dy4—Dy3	45.15 (7)	$Dy4^{v}$—S5—$Dy3^{v}$	89.79 (4)
$S4^{viii}$—Dy4—Dy3	132.57 (7)	$Dy4^{vi}$—S5—$Dy3^{v}$	159.03 (18)
$S4^{vii}$—Dy4—Dy3	132.57 (7)	$Dy3^{vi}$—S5—$Dy3^{v}$	86.32 (13)
$S2^{vii}$—Dy4—Dy3	85.62 (10)	$Dy4^{v}$—S5—Dy2	107.56 (12)
$S12^{viii}$—Dy4—Dy3	103.71 (10)	$Dy4^{vi}$—S5—Dy2	107.56 (12)
$S12^{vii}$—Dy4—Dy3	103.71 (10)	$Dy3^{vi}$—S5—Dy2	93.24 (12)
$Dy4^{iii}$—Dy4—Dy3	90.0	$Dy3^{v}$—S5—Dy2	93.24 (12)
$Dy4^{ii}$—Dy4—Dy3	90.0	$Dy1^{iii}$—S6—Dy1	86.02 (13)
$S5^{vii}$—Dy4—$Dy8^{ix}$	133.99 (7)	$Dy1^{iii}$—S6—$Dy7^{iv}$	153.67 (17)
$S5^{viii}$—Dy4—$Dy8^{ix}$	133.99 (7)	Dy1—S6—$Dy7^{iv}$	88.80 (5)
$S4^{viii}$—Dy4—$Dy8^{ix}$	46.20 (7)	$Dy1^{iii}$—S6—$Dy7^{xiii}$	88.80 (5)
$S4^{vii}$—Dy4—$Dy8^{ix}$	46.20 (7)	Dy1—S6—$Dy7^{xiii}$	153.67 (17)
$S2^{vii}$—Dy4—$Dy8^{ix}$	91.32 (10)	$Dy7^{iv}$—S6—$Dy7^{xiii}$	84.49 (13)
$S12^{viii}$—Dy4—$Dy8^{ix}$	78.60 (10)	$Dy1^{iii}$—S6—Dy8	100.99 (12)
$S12^{vii}$—Dy4—$Dy8^{ix}$	78.60 (10)	Dy1—S6—Dy8	100.99 (12)
$Dy4^{iii}$—Dy4—$Dy8^{ix}$	90.0	$Dy7^{iv}$—S6—Dy8	105.34 (11)
$Dy4^{ii}$—Dy4—$Dy8^{ix}$	90.0	$Dy7^{xiii}$—S6—Dy8	105.34 (11)
Dy3—Dy4—$Dy8^{ix}$	176.94 (3)	$Dy5^{vii}$—S7—$Dy5^{viii}$	85.19 (13)

$S7^{v}$—Dy5—$S7^{vi}$	85.19 (13)	$Dy5^{vii}$—S7—$Dy8^{ii}$	89.21 (5)
$S7^{v}$—Dy5—S3	86.84 (11)	$Dy5^{viii}$—S7—$Dy8^{ii}$	152.1 (2)
$S7^{vi}$—Dy5—S3	149.10 (16)	$Dy5^{vii}$—S7—Dy8	152.1 (2)
$S7^{v}$—Dy5—$S3^{ii}$	149.10 (16)	$Dy5^{viii}$—S7—Dy8	89.21 (5)
$S7^{vi}$—Dy5—$S3^{ii}$	86.84 (11)	$Dy8^{ii}$—S7—Dy8	83.07 (13)
S3—Dy5—$S3^{ii}$	84.86 (13)	$Dy5^{vii}$—S7—Dy2	108.48 (14)
$S7^{v}$—Dy5—S1	74.57 (12)	$Dy5^{viii}$—S7—Dy2	108.48 (14)
$S7^{vi}$—Dy5—S1	74.57 (12)	$Dy8^{ii}$—S7—Dy2	99.23 (13)
S3—Dy5—S1	74.54 (12)	Dy8—S7—Dy2	99.23 (13)
$S3^{ii}$—Dy5—S1	74.54 (12)	Dy1—S8—$Dy8^{ii}$	108.55 (12)
$S7^{v}$—Dy5—$S12^{x}$	118.62 (13)	Dy1—S8—Dy8	108.55 (12)
$S7^{vi}$—Dy5—$S12^{x}$	67.02 (12)	$Dy8^{ii}$—S8—Dy8	87.33 (13)
S3—Dy5—$S12^{x}$	141.31 (14)	Dy1—S8—$Dy3^{v}$	99.06 (12)
$S3^{ii}$—Dy5—$S12^{x}$	85.06 (11)	$Dy8^{ii}$—S8—$Dy3^{v}$	152.05 (17)
S1—Dy5—$S12^{x}$	137.24 (8)	Dy8—S8—$Dy3^{v}$	87.95 (5)
$S7^{v}$—Dy5—$S12^{i}$	67.02 (12)	Dy1—S8—$Dy3^{vi}$	99.06 (12)
$S7^{vi}$—Dy5—$S12^{i}$	118.62 (13)	$Dy8^{ii}$—S8—$Dy3^{vi}$	87.95 (5)
S3—Dy5—$S12^{i}$	85.06 (11)	Dy8—S8—$Dy3^{vi}$	152.05 (17)
$S3^{ii}$—Dy5—$S12^{i}$	141.31 (14)	$Dy3^{v}$—S8—$Dy3^{vi}$	83.46 (11)
S1—Dy5—$S12^{i}$	137.24 (8)	Sn1—S9—$Sn1^{iii}$	96.38 (16)
$S12^{x}$—Dy5—$S12^{i}$	79.93 (13)	Sn1—S9—$Dy1^{xiv}$	131.79 (8)
$S7^{v}$—Dy5—$S9^{i}$	133.23 (9)	$Sn1^{iii}$—S9—$Dy1^{xiv}$	131.79 (8)
$S7^{vi}$—Dy5—$S9^{i}$	133.23 (9)	Sn1—S9—$Dy5^{xiv}$	96.74 (13)
S3—Dy5—$S9^{i}$	71.02 (11)	$Sn1^{iii}$—S9—$Dy5^{xiv}$	96.74 (13)
$S3^{ii}$—Dy5—$S9^{i}$	71.02 (11)	$Dy1^{xiv}$—S9—$Dy5^{xiv}$	81.66 (13)
S1—Dy5—$S9^{i}$	132.68 (13)	$Sn1^{viii}$—S10—$Sn1^{vii}$	96.82 (16)
$S12^{x}$—Dy5—$S9^{i}$	70.38 (11)	$Sn1^{viii}$—S10—Dy3	131.34 (8)
$S12^{i}$—Dy5—$S9^{i}$	70.38 (11)	$Sn1^{vii}$—S10—Dy3	131.34 (8)
$S7^{v}$—Dy5—$Dy5^{ii}$	132.60 (7)	$Sn1^{viii}$—S10—Dy6	96.03 (14)
$S7^{vi}$—Dy5—$Dy5^{ii}$	47.40 (7)	$Sn1^{vii}$—S10—Dy6	96.03 (14)
S3—Dy5—$Dy5^{ii}$	132.43 (7)	Dy3—S10—Dy6	86.55 (13)
$S3^{ii}$—Dy5—$Dy5^{ii}$	47.57 (7)	$Dy6^{v}$—S11—$Dy6^{vi}$	85.99 (12)
S1—Dy5—$Dy5^{ii}$	90.0	$Dy6^{v}$—S11—Dy1	105.23 (11)
$S12^{x}$—Dy5—$Dy5^{ii}$	50.03 (6)	$Dy6^{vi}$—S11—Dy1	105.23 (11)
$S12^{i}$—Dy5—$Dy5^{ii}$	129.97 (6)	$Dy6^{v}$—S11—$Dy3^{vi}$	158.35 (16)
$S9^{i}$—Dy5—$Dy5^{ii}$	90.0	$Dy6^{vi}$—S11—$Dy3^{vi}$	92.23 (4)
$S7^{v}$—Dy5—$Dy5^{iii}$	47.40 (7)	Dy1—S11—$Dy3^{vi}$	96.07 (11)
$S7^{vi}$—Dy5—$Dy5^{iii}$	132.60 (7)	$Dy6^{v}$—S11—$Dy3^{v}$	92.23 (4)
S3—Dy5—$Dy5^{iii}$	47.57 (7)	$Dy6^{vi}$—S11—$Dy3^{v}$	158.35 (16)
$S3^{ii}$—Dy5—$Dy5^{iii}$	132.43 (7)	Dy1—S11—$Dy3^{v}$	96.07 (11)
S1—Dy5—$Dy5^{iii}$	90.0	$Dy3^{vi}$—S11—$Dy3^{v}$	81.52 (11)

S12^{x}—Dy5—Dy5^{iii}	129.97 (6)	Sn1—S12—Dy5^{xiv}	103.38 (14)
S12^{i}—Dy5—Dy5^{iii}	50.03 (6)	Sn1—S12—Dy5^{xv}	103.38 (14)
S9^{i}—Dy5—Dy5^{iii}	90.0	Dy5^{xiv}—S12—Dy5^{xv}	79.93 (13)
Dy5^{ii}—Dy5—Dy5^{iii}	180.0	Sn1—S12—Dy4^{vi}	104.21 (14)
S7^{v}—Dy5—Dy1	132.63 (8)	Dy5^{xiv}—S12—Dy4^{vi}	152.42 (18)
S7^{vi}—Dy5—Dy1	132.63 (8)	Dy5^{xv}—S12—Dy4^{vi}	93.75 (5)
S3—Dy5—Dy1	45.84 (7)	Sn1—S12—Dy4^{v}	104.21 (14)
S3^{ii}—Dy5—Dy1	45.84 (7)	Dy5^{xiv}—S12—Dy4^{v}	93.75 (5)
S1—Dy5—Dy1	88.12 (9)	Dy5^{xv}—S12—Dy4^{v}	152.42 (18)
S12^{x}—Dy5—Dy1	104.13 (10)	Dy4^{vi}—S12—Dy4^{v}	79.43 (12)
S12^{i}—Dy5—Dy1	104.13 (10)	Sn1—S13—Dy6^{vi}	102.09 (12)
S9^{i}—Dy5—Dy1	44.56 (9)	Sn1—S13—Dy6^{v}	102.09 (12)
Dy5^{ii}—Dy5—Dy1	90.0	Dy6^{vi}—S13—Dy6^{v}	80.09 (11)
Dy5^{iii}—Dy5—Dy1	90.0	Sn1—S13—Dy7^{v}	105.50 (12)
S7^{v}—Dy5—Dy8^{vi}	45.99 (8)	Dy6^{vi}—S13—Dy7^{v}	152.39 (16)
S7^{vi}—Dy5—Dy8^{vi}	45.99 (8)	Dy6^{v}—S13—Dy7^{v}	93.35 (5)
S3—Dy5—Dy8^{vi}	132.78 (8)	Sn1—S13—Dy7^{vi}	105.50 (12)
S3^{ii}—Dy5—Dy8^{vi}	132.78 (8)	Dy6^{vi}—S13—Dy7i	93.35 (5)
S1—Dy5—Dy8^{vi}	88.11 (9)	Dy6i—S13—Dy7i	152.39 (16)
S12^{x}—Dy5—Dy8^{vi}	78.71 (9)	Dy7i—S13—Dy7i	80.06 (11)
S12^{i}—Dy5—Dy8^{vi}	78.71 (9)	Dy2i—O14—Dy2i	104.1 (3)
S9^{i}—Dy5—Dy8^{vi}	139.21 (9)	Dy2i—O14—Dy3	114.6 (2)
Dy5^{ii}—Dy5—Dy8^{vi}	90.0	Dy2i—O14—Dy3	114.6 (2)
Dy5^{iii}—Dy5—Dy8^{vi}	90.0	Dy2i—O14—Dy8i	114.9 (2)
Dy1—Dy5—Dy8^{vi}	176.23 (4)	Dy2i—O14—Dy8i	114.9 (2)
S11^{vii}—Dy6—S11^{viii}	85.99 (12)	Dy3—O14—Dy8i	94.3 (2)

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

Fig. 1