Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(18-Crown-6)bis(tetrahydrofuran-κO)-potassium(I) [1,2-bis(fluoren-9-yl-carbonyl)benzene(2−)]bis(η^5-cyclopentadienyl)dysprosate(III)

Ahmad Zaeni,[a] Falk Olbrich,[b] Steffen Blaurock[a] and Frank T. Edelmann[a]*

[a]Chemisches Institut der Otto-von-Guericke-Universität, Universitätsplatz 2, 39116 Magdeburg, Germany, and [b]Institut für Anorganische und Angewandte Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany
Correspondence e-mail: frank.edelmann@ovgu.de

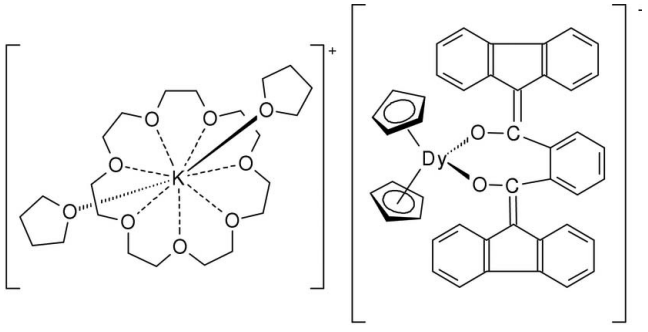
Received 6 July 2007; accepted 22 July 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.067; data-to-parameter ratio = 19.7.

The title compound, $[K(C_{20}H_{40}O_8)(C_4H_8O)_2][Dy(C_5H_5)_2(C_{34}H_{20}O_2)]$, was isolated serendipitously from a reaction of anhydrous $DyCl_3$ and KCp (Cp = cyclopentadienyl) in tetrahydrofuran (THF), followed by addition of KFl(18-crown-6) (Fl = fluorenide). In the cation, K^+ is coordinated by 18-crown-6 and two THF ligands, while the anion is an 'ate' complex of Dy^{III}, containing two η^5-Cp ligands and the novel chelating ligand *o*-phenylenebis(fluorenylideneacylate).

Related literature

For related literature, see: Edelmann *et al.* (2007); Goldschmidt & Nagel (1930); Greenhow *et al.* (1953); Harcourt & O'Ferrall (1995); Meyer & Gottlieb-Billroth (1921).



Experimental

Crystal data

$[K(C_{20}H_{40}O_8)(C_4H_8O)_2]$-$[Dy(C_5H_5)_2(C_{34}H_{20}O_2)]$
M_r = 1200.80
Triclinic, $P\overline{1}$
a = 12.0798 (2) Å
b = 13.0513 (2) Å
c = 19.3154 (3) Å
α = 85.1700 (8)°
β = 73.1480 (7)°
γ = 74.5617 (8)°
V = 2809.20 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 173 (2) K
0.60 × 0.40 × 0.30 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.455, T_{max} = 0.641
19240 measured reflections
13639 independent reflections
12598 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.02
13639 reflections
691 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.31 e Å^{-3}
$\Delta\rho_{min}$ = −1.40 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The authors thank the Otto-von-Guericke-Universität, Magdeburg, for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2211).

References

Bruker (1997). *SMART* and *SAINT*. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.
Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Edelmann, F. T., Zaeni, A., Blaurock, S. & Olbrich, F. (2007). Unpublished results.
Goldschmidt, S. & Nagel, F. (1930). *Ber. Dtsch. Chem. Ges.* **63**, 1212–1217.
Greenhow, E. J., White, E. N. & McNeill, D. (1953). *J. Chem. Soc.* pp. 3099–3105.
Harcourt, M. P. & O'Ferrall, R. A. M. (1995). *J. Chem. Soc. Perkin Trans. 2*, pp. 1415–1425.
Meyer, K. H. & Gottlieb-Billroth, H. (1921). *Ber. Dtsch. Chem. Ges.* **54**, 575–578.
Sheldrick, G. M. (1997). *SADABS*. University of Göttingen, Germany.

  doi:10.1107/S1600536807035738

supplementary materials

Acta Cryst. (2007). E**63**, m2218 [**doi:10.1107/S1600536807035738**]

(18-Crown-6)bis(tetrahydrofuran-κO)potassium(I) [1,2-bis(fluoren-9-ylcarbonyl)benzene(2-)]bis(η^5-cyclopentadienyl)dysprosate(III)

A. Zaeni, F. Olbrich, S. Blaurock and F. T. Edelmann

Comment

As part of a research project on the synthesis and structural characterization of new lanthanide fluorenyl complexes we investigated the possibility of preparing an anionic "ate" complex of dysprosium containing two cyclopentadienyl and two fluorenyl ligands. The title compound was isolated serendipitously and in small amounts from a reaction of anhydrous $DyCl_3$ and KCp in THF, followed by addition of KFl(18-crown-6) (Fl = fluorenide). The structure comprises discrete $[K(18\text{-crown-}6)(THF)_2]^+$ cations and unprecedented $[DyCp_2(C_6H_4(OC{=}C_{13}H_8)_2)]^-$ anions (Figure 1).

In the cation, K^+ is coordinated by 18-crown-6 and two THF ligands. This cation is not unusual and has been observed in the potassium fluorenide derivative $[K(18\text{-crown-}6)(THF)_2]^+Fl^-$ (Edelmann *et al.*, 2007). The surprising result of this reaction is the formation of the unprecedented $C_6H_4(OC{=}C_{13}H_8)_2^{2-}$ ligand in the $[DyCp_2(C_6H_4(OC{=}C_{13}H_8)_2)]^-$ anion. In this ligand, a central phenyl ring is substituted in *ortho* positions by two fluorenylideneacylate groups. While the origin of the fluorenyl group is certain, the formation of the entire ligand system remains speculative. The new ligand is coordinated as a dianion *via* its two acyl O atoms·The bonds C37—C69 (1.373 (2) Å) and C38—C49 (1.380 (3) Å) are clearly double bonds. Thus, the new ligand can be regarded as a chelating phenylene-1,2-bis(fluorenylideneacylate)dianion. It is well established that 9-acylfluorenes exhibit keto-enol tautomerism (Meyer & Gottlieb-Billroth (1921); Goldschmidt & Nagel (1930); Greenhow *et al.* (1953); Harcourt & O'Ferrall (1995)). In the title compound, the dianion of the bis-enol form is coordinated to Dy. We were unable to prepare the new ligand independently by treatment of phthalic dichloride with two equivalents of sodium fluorenide.

Experimental

0.27 g (1.0 mmol) of anhydrous $DyCl_3$ and 0.312 g (3.0 mmol) of KCp were dissolved in 20 ml of THF under nitrogen and stirred at reflux temperature for 1 h. The yellow reaction mixture was filtered and 0.15 g (1 mmol) of KFl(18-crown-6) were added with stirring. After filtering again, the solution was carefully layered with *n*-hexane (10 ml). After several days a small amount of well formed dark green crystals were obtained at room temperature. *M*.p. 663 K.

Refinement

H atoms were placed geometrically and refined using a riding model with C—H = 0.95–0.99 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

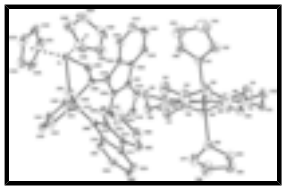


Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at the 50% probability level. H atoms are omitted.

(I)

Crystal data

$[K(C_{20}H_{40}O_8)(C_4H_8O)_2][Dy(C_5H_5)_2(C_{34}H_{20}O_2)]$	$Z = 2$
$M_r = 1200.80$	$F_{000} = 1238$
Triclinic, $P\overline{1}$	$D_x = 1.420$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 663 K
$a = 12.0798$ (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.0513$ (2) Å	Cell parameters from 100 reflections
$c = 19.3154$ (3) Å	$\theta = 1.6$–29.2^o
$\alpha = 85.1700$ (8)º	$\mu = 1.46$ mm^{-1}
$\beta = 73.1480$ (7)º	$T = 173$ (2) K
$\gamma = 74.5617$ (8)º	Plate, dark green
$V = 2809.20$ (8) Å^3	0.60 × 0.40 × 0.30 mm

Data collection

Siemens SMART CCD diffractometer	13639 independent reflections
Radiation source: fine-focus sealed tube	12598 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 173$(2) K	$\theta_{max} = 29.2^o$
ω scans	$\theta_{min} = 1.6^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	$h = -13 \rightarrow 16$
$T_{min} = 0.455$, $T_{max} = 0.641$	$k = -17 \rightarrow 17$
19240 measured reflections	$l = -26 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.3278P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$

13639 reflections	$\Delta\rho_{max} = 1.31$ e Å^{-3}
691 parameters	$\Delta\rho_{min} = -1.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ 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}
K	0.48016 (4)	0.52461 (3)	0.25229 (2)	0.02541 (8)
O1	0.59368 (13)	0.67575 (13)	0.17793 (8)	0.0329 (3)
O2	0.46758 (14)	0.58350 (13)	0.10802 (9)	0.0376 (4)
O3	0.32065 (15)	0.46039 (13)	0.19874 (10)	0.0392 (4)
O4	0.36303 (13)	0.37716 (12)	0.32869 (9)	0.0337 (3)
O5	0.49545 (14)	0.46832 (12)	0.39557 (8)	0.0321 (3)
O6	0.65250 (14)	0.58081 (12)	0.30114 (8)	0.0325 (3)
O7	0.64954 (16)	0.33991 (13)	0.20525 (11)	0.0477 (4)
O8	0.30420 (16)	0.71086 (13)	0.29797 (10)	0.0444 (4)
C1	0.5992 (2)	0.6930 (2)	0.10353 (12)	0.0400 (5)
H1A	0.6649	0.6377	0.0739	0.0452 (16)*
H1B	0.6147	0.7633	0.0878	0.0452 (16)*
C2	0.4818 (2)	0.6886 (2)	0.09360 (14)	0.0428 (6)
H2A	0.4155	0.7389	0.1270	0.0452 (16)*
H2B	0.4797	0.7094	0.0434	0.0452 (16)*
C3	0.3584 (2)	0.5744 (2)	0.09790 (16)	0.0480 (6)
H3A	0.3612	0.5844	0.0461	0.0452 (16)*
H3B	0.2909	0.6302	0.1257	0.0452 (16)*
C4	0.3399 (3)	0.4670 (2)	0.12292 (15)	0.0458 (6)
H4A	0.2699	0.4566	0.1103	0.0452 (16)*
H4B	0.4112	0.4110	0.0990	0.0452 (16)*
C5	0.2871 (2)	0.36662 (18)	0.23024 (15)	0.0405 (5)
H5A	0.3537	0.3032	0.2129	0.0452 (16)*
H5B	0.2168	0.3596	0.2163	0.0452 (16)*
C6	0.2575 (2)	0.37470 (18)	0.31050 (15)	0.0396 (5)
H6A	0.1939	0.4402	0.3275	0.0452 (16)*
H6B	0.2283	0.3129	0.3341	0.0452 (16)*
C7	0.3468 (2)	0.37626 (19)	0.40446 (13)	0.0395 (5)

H7A	0.3170	0.3142	0.4270	0.0452 (16)*
H7B	0.2876	0.4417	0.4263	0.0452 (16)*
C8	0.4653 (2)	0.37009 (18)	0.41659 (13)	0.0393 (5)
H8A	0.4610	0.3555	0.4683	0.0452 (16)*
H8B	0.5273	0.3116	0.3877	0.0452 (16)*
C9	0.6100 (2)	0.46734 (19)	0.40246 (13)	0.0368 (5)
H9A	0.6718	0.4091	0.3732	0.0452 (16)*
H9B	0.6106	0.4552	0.4536	0.0452 (16)*
C10	0.6367 (2)	0.57188 (18)	0.37680 (12)	0.0343 (4)
H10A	0.5699	0.6307	0.4018	0.0452 (16)*
H10B	0.7103	0.5765	0.3879	0.0452 (16)*
C11	0.6827 (2)	0.67701 (17)	0.27198 (13)	0.0341 (4)
H11A	0.7559	0.6820	0.2833	0.0452 (16)*
H11B	0.6169	0.7389	0.2936	0.0452 (16)*
C12	0.70304 (18)	0.67746 (18)	0.19195 (13)	0.0333 (4)
H12A	0.7281	0.7420	0.1703	0.0452 (16)*
H12B	0.7670	0.6144	0.1704	0.0452 (16)*
C13	0.7340 (2)	0.3667 (2)	0.14170 (18)	0.0533 (7)
H13A	0.8074	0.3700	0.1536	0.083 (3)*
H13B	0.6993	0.4372	0.1229	0.083 (3)*
C14	0.7642 (3)	0.2830 (3)	0.08531 (18)	0.0694 (9)
H14A	0.8448	0.2353	0.0805	0.083 (3)*
H14B	0.7602	0.3155	0.0376	0.083 (3)*
C15	0.6671 (3)	0.2232 (3)	0.11543 (18)	0.0608 (8)
H15A	0.5958	0.2553	0.0981	0.083 (3)*
H15B	0.6971	0.1473	0.1017	0.083 (3)*
C16	0.6390 (2)	0.23608 (19)	0.19600 (15)	0.0442 (6)
H16A	0.5571	0.2295	0.2207	0.083 (3)*
H16B	0.6964	0.1816	0.2159	0.083 (3)*
C17	0.2078 (3)	0.7031 (3)	0.35854 (19)	0.0627 (9)
H17A	0.2008	0.6288	0.3657	0.083 (3)*
H17B	0.1318	0.7490	0.3519	0.083 (3)*
C18	0.2349 (4)	0.7394 (3)	0.42263 (18)	0.0727 (10)
H18A	0.2747	0.6781	0.4481	0.083 (3)*
H18B	0.1608	0.7792	0.4572	0.083 (3)*
C19	0.3177 (3)	0.8110 (2)	0.38960 (15)	0.0459 (6)
H19A	0.3954	0.7842	0.4008	0.083 (3)*
H19B	0.2813	0.8846	0.4077	0.083 (3)*
C20	0.3334 (2)	0.80660 (17)	0.30879 (14)	0.0383 (5)
H20A	0.2793	0.8693	0.2930	0.083 (3)*
H20B	0.4169	0.8049	0.2811	0.083 (3)*
Dy	0.136270 (7)	0.070125 (6)	0.128562 (4)	0.02123 (3)
O31	0.00368 (12)	0.22074 (10)	0.16913 (7)	0.0233 (3)
O36	0.20241 (12)	0.08247 (11)	0.22062 (7)	0.0266 (3)
C21	0.1169 (3)	−0.12320 (19)	0.18210 (15)	0.0455 (6)
H21	0.1679	−0.1568	0.2112	0.061 (3)*
C22	0.1438 (2)	−0.13181 (17)	0.10779 (14)	0.0396 (5)
H22	0.2167	−0.1719	0.0772	0.061 (3)*
C23	0.0467 (2)	−0.07224 (18)	0.08566 (14)	0.0392 (5)

H23	0.0414	−0.0648	0.0373	0.061 (3)*
C24	−0.0422 (2)	−0.02476 (19)	0.14642 (18)	0.0473 (6)
H24	−0.1183	0.0206	0.1469	0.061 (3)*
C25	0.0021 (3)	−0.0567 (2)	0.20691 (15)	0.0505 (7)
H25	−0.0387	−0.0367	0.2557	0.061 (3)*
C26	0.3442 (2)	0.1093 (3)	0.05106 (13)	0.0459 (6)
H26	0.4046	0.0992	0.0751	0.061 (3)*
C27	0.3277 (2)	0.0325 (2)	0.01099 (14)	0.0502 (6)
H27	0.3743	−0.0388	0.0034	0.061 (3)*
C28	0.2296 (2)	0.0806 (2)	−0.01572 (12)	0.0449 (6)
H28	0.1981	0.0473	−0.0449	0.061 (3)*
C29	0.1866 (2)	0.1847 (2)	0.00774 (12)	0.0407 (5)
H29	0.1206	0.2352	−0.0028	0.061 (3)*
C30	0.2561 (2)	0.2034 (2)	0.04943 (12)	0.0397 (5)
H30	0.2456	0.2681	0.0725	0.061 (3)*
C31	−0.04811 (16)	0.18802 (13)	0.29644 (10)	0.0201 (3)
C32	−0.16929 (17)	0.19355 (15)	0.32745 (11)	0.0257 (4)
H32	−0.2269	0.2398	0.3069	0.038 (3)*
C33	−0.20713 (19)	0.13260 (17)	0.38785 (12)	0.0315 (4)
H33	−0.2900	0.1380	0.4088	0.038 (3)*
C34	−0.1237 (2)	0.06409 (17)	0.41735 (12)	0.0321 (4)
H34	−0.1490	0.0229	0.4590	0.038 (3)*
C35	−0.00246 (19)	0.05567 (15)	0.38580 (11)	0.0270 (4)
H35	0.0545	0.0068	0.4056	0.038 (3)*
C36	0.03767 (17)	0.11766 (14)	0.32550 (10)	0.0210 (3)
C37	−0.01876 (15)	0.26107 (14)	0.23298 (9)	0.0196 (3)
C38	0.16958 (17)	0.09984 (14)	0.29021 (10)	0.0211 (3)
C41	0.13554 (19)	0.16799 (15)	0.45819 (11)	0.0271 (4)
H41	0.0588	0.1889	0.4499	0.037 (2)*
C42	0.1486 (2)	0.18555 (16)	0.52531 (11)	0.0316 (4)
H42	0.0800	0.2176	0.5627	0.037 (2)*
C43	0.2601 (2)	0.15705 (16)	0.53864 (12)	0.0353 (5)
H43	0.2670	0.1690	0.5849	0.037 (2)*
C44	0.3608 (2)	0.11125 (16)	0.48450 (12)	0.0325 (4)
H44	0.4373	0.0925	0.4931	0.037 (2)*
C45	0.56362 (19)	0.01110 (17)	0.33670 (13)	0.0329 (4)
H45	0.6014	0.0093	0.3738	0.037 (2)*
C46	0.6306 (2)	−0.02579 (18)	0.26798 (13)	0.0365 (5)
H46	0.7147	−0.0533	0.2579	0.037 (2)*
C47	0.57487 (19)	−0.02271 (17)	0.21366 (12)	0.0337 (4)
H47	0.6218	−0.0482	0.1669	0.037 (2)*
C48	0.45198 (18)	0.01696 (16)	0.22662 (11)	0.0277 (4)
H48	0.4152	0.0191	0.1890	0.037 (2)*
C49	0.25310 (17)	0.09335 (14)	0.32737 (10)	0.0219 (3)
C50	0.23571 (18)	0.11955 (14)	0.40321 (10)	0.0233 (4)
C51	0.34947 (19)	0.09260 (14)	0.41686 (11)	0.0258 (4)
C52	0.44031 (18)	0.05074 (15)	0.35057 (11)	0.0259 (4)
C53	0.38291 (17)	0.05385 (14)	0.29597 (10)	0.0233 (4)
C61	−0.07294 (17)	0.38101 (14)	0.38571 (10)	0.0225 (3)

H61	−0.0829	0.3112	0.3970	0.032 (2)*
C62	−0.08552 (18)	0.44884 (16)	0.44059 (11)	0.0265 (4)
H62	−0.1029	0.4242	0.4893	0.032 (2)*
C63	−0.07322 (19)	0.55228 (16)	0.42597 (11)	0.0275 (4)
H63	−0.0824	0.5974	0.4645	0.032 (2)*
C64	−0.04756 (18)	0.58916 (15)	0.35525 (11)	0.0254 (4)
H64	−0.0397	0.6598	0.3449	0.032 (2)*
C65	0.01487 (18)	0.63022 (15)	0.18095 (11)	0.0271 (4)
H65	0.0115	0.6928	0.2041	0.032 (2)*
C66	0.0401 (2)	0.62683 (17)	0.10631 (12)	0.0307 (4)
H66	0.0539	0.6877	0.0780	0.032 (2)*
C67	0.0454 (2)	0.53472 (17)	0.07253 (11)	0.0309 (4)
H67	0.0632	0.5336	0.0213	0.032 (2)*
C68	0.02505 (18)	0.44395 (15)	0.11257 (10)	0.0255 (4)
H68	0.0284	0.3818	0.0889	0.032 (2)*
C69	−0.02338 (16)	0.36481 (14)	0.24407 (10)	0.0202 (3)
C70	−0.04538 (16)	0.41586 (14)	0.31351 (10)	0.0198 (3)
C71	−0.03333 (16)	0.52160 (14)	0.29937 (10)	0.0213 (3)
C72	−0.00544 (16)	0.54005 (14)	0.22144 (10)	0.0216 (3)
C73	−0.00025 (16)	0.44578 (14)	0.18781 (10)	0.0203 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K	0.02496 (19)	0.02416 (18)	0.02657 (19)	−0.00700 (15)	−0.00607 (15)	0.00129 (15)
O1	0.0241 (7)	0.0446 (9)	0.0315 (8)	−0.0146 (6)	−0.0076 (6)	0.0109 (6)
O2	0.0318 (8)	0.0444 (9)	0.0414 (9)	−0.0120 (7)	−0.0183 (7)	0.0114 (7)
O3	0.0391 (9)	0.0347 (8)	0.0537 (10)	−0.0167 (7)	−0.0237 (8)	0.0076 (7)
O4	0.0248 (7)	0.0359 (8)	0.0381 (8)	−0.0092 (6)	−0.0057 (6)	0.0068 (6)
O5	0.0334 (8)	0.0288 (7)	0.0322 (8)	−0.0058 (6)	−0.0097 (6)	0.0057 (6)
O6	0.0355 (8)	0.0318 (7)	0.0331 (8)	−0.0102 (6)	−0.0128 (6)	0.0015 (6)
O7	0.0413 (10)	0.0317 (8)	0.0615 (12)	−0.0077 (7)	0.0001 (9)	−0.0098 (8)
O8	0.0408 (9)	0.0282 (8)	0.0580 (11)	−0.0088 (7)	−0.0015 (8)	−0.0093 (7)
C1	0.0375 (12)	0.0509 (14)	0.0314 (11)	−0.0190 (11)	−0.0066 (9)	0.0153 (10)
C2	0.0456 (14)	0.0489 (14)	0.0377 (12)	−0.0160 (11)	−0.0189 (11)	0.0172 (11)
C3	0.0440 (14)	0.0561 (15)	0.0557 (16)	−0.0163 (12)	−0.0331 (13)	0.0155 (13)
C4	0.0445 (14)	0.0477 (14)	0.0567 (16)	−0.0143 (12)	−0.0303 (12)	0.0038 (12)
C5	0.0322 (11)	0.0290 (10)	0.0687 (17)	−0.0121 (9)	−0.0246 (11)	0.0055 (11)
C6	0.0247 (10)	0.0305 (11)	0.0638 (16)	−0.0115 (9)	−0.0106 (10)	0.0072 (10)
C7	0.0413 (12)	0.0315 (11)	0.0367 (12)	−0.0121 (9)	0.0041 (10)	0.0046 (9)
C8	0.0566 (15)	0.0299 (11)	0.0305 (11)	−0.0107 (10)	−0.0132 (10)	0.0081 (9)
C9	0.0360 (11)	0.0384 (11)	0.0348 (11)	−0.0018 (9)	−0.0156 (9)	0.0023 (9)
C10	0.0318 (11)	0.0396 (11)	0.0331 (11)	−0.0045 (9)	−0.0149 (9)	−0.0024 (9)
C11	0.0279 (10)	0.0320 (10)	0.0450 (12)	−0.0092 (8)	−0.0133 (9)	0.0010 (9)
C12	0.0213 (9)	0.0352 (11)	0.0434 (12)	−0.0110 (8)	−0.0069 (8)	0.0041 (9)
C13	0.0325 (12)	0.0431 (14)	0.075 (2)	−0.0077 (11)	−0.0033 (13)	0.0038 (13)
C14	0.069 (2)	0.082 (2)	0.0484 (17)	−0.0144 (19)	−0.0091 (16)	0.0017 (16)
C15	0.066 (2)	0.0591 (18)	0.064 (2)	−0.0085 (16)	−0.0333 (17)	−0.0094 (15)

C16	0.0425 (13)	0.0336 (12)	0.0571 (16)	−0.0090 (10)	−0.0146 (12)	−0.0032 (11)
C17	0.0485 (16)	0.0518 (16)	0.082 (2)	−0.0283 (14)	0.0079 (15)	−0.0103 (15)
C18	0.096 (3)	0.072 (2)	0.0519 (18)	−0.049 (2)	−0.0002 (18)	0.0077 (16)
C19	0.0481 (14)	0.0371 (12)	0.0525 (15)	−0.0109 (11)	−0.0144 (12)	0.0016 (11)
C20	0.0338 (11)	0.0263 (10)	0.0512 (14)	−0.0077 (9)	−0.0061 (10)	−0.0011 (9)
Dy	0.02097 (5)	0.02315 (5)	0.01945 (5)	−0.00487 (3)	−0.00488 (3)	−0.00452 (3)
O31	0.0272 (7)	0.0204 (6)	0.0210 (6)	−0.0025 (5)	−0.0074 (5)	−0.0026 (5)
O36	0.0258 (7)	0.0332 (7)	0.0206 (6)	−0.0055 (6)	−0.0072 (5)	−0.0038 (5)
C21	0.0659 (17)	0.0322 (11)	0.0546 (15)	−0.0230 (12)	−0.0359 (14)	0.0131 (11)
C22	0.0425 (13)	0.0227 (10)	0.0536 (14)	−0.0033 (9)	−0.0155 (11)	−0.0085 (9)
C23	0.0509 (14)	0.0334 (11)	0.0451 (13)	−0.0156 (10)	−0.0268 (11)	−0.0014 (10)
C24	0.0300 (11)	0.0313 (11)	0.085 (2)	−0.0097 (9)	−0.0183 (12)	−0.0086 (12)
C25	0.0702 (19)	0.0479 (14)	0.0388 (13)	−0.0419 (14)	0.0038 (12)	−0.0096 (11)
C26	0.0253 (10)	0.0837 (19)	0.0298 (11)	−0.0217 (12)	−0.0061 (9)	0.0130 (12)
C27	0.0368 (13)	0.0538 (15)	0.0413 (13)	−0.0002 (11)	0.0092 (11)	−0.0059 (11)
C28	0.0406 (13)	0.0729 (18)	0.0215 (10)	−0.0209 (12)	0.0002 (9)	−0.0119 (10)
C29	0.0305 (11)	0.0603 (15)	0.0253 (10)	−0.0116 (11)	−0.0015 (8)	0.0103 (10)
C30	0.0410 (13)	0.0514 (14)	0.0272 (10)	−0.0244 (11)	0.0006 (9)	0.0032 (9)
C31	0.0235 (8)	0.0165 (7)	0.0207 (8)	−0.0049 (6)	−0.0064 (7)	−0.0019 (6)
C32	0.0228 (9)	0.0262 (9)	0.0284 (9)	−0.0067 (7)	−0.0067 (7)	−0.0024 (7)
C33	0.0277 (10)	0.0324 (10)	0.0345 (11)	−0.0135 (8)	−0.0026 (8)	−0.0029 (8)
C34	0.0390 (11)	0.0276 (10)	0.0303 (10)	−0.0157 (9)	−0.0054 (9)	0.0048 (8)
C35	0.0342 (10)	0.0205 (8)	0.0270 (9)	−0.0076 (8)	−0.0097 (8)	0.0030 (7)
C36	0.0261 (9)	0.0178 (8)	0.0203 (8)	−0.0058 (7)	−0.0076 (7)	−0.0012 (6)
C37	0.0168 (7)	0.0208 (8)	0.0212 (8)	−0.0037 (6)	−0.0062 (6)	0.0002 (6)
C38	0.0250 (9)	0.0171 (7)	0.0215 (8)	−0.0039 (6)	−0.0080 (7)	0.0001 (6)
C41	0.0359 (11)	0.0188 (8)	0.0264 (9)	−0.0021 (7)	−0.0127 (8)	−0.0008 (7)
C42	0.0470 (12)	0.0217 (9)	0.0251 (9)	−0.0051 (8)	−0.0111 (9)	−0.0025 (7)
C43	0.0578 (15)	0.0251 (9)	0.0283 (10)	−0.0077 (9)	−0.0226 (10)	−0.0003 (8)
C44	0.0421 (12)	0.0280 (10)	0.0348 (11)	−0.0077 (9)	−0.0235 (9)	0.0018 (8)
C45	0.0290 (10)	0.0306 (10)	0.0438 (12)	−0.0081 (8)	−0.0185 (9)	0.0064 (9)
C46	0.0240 (10)	0.0347 (11)	0.0486 (13)	−0.0058 (8)	−0.0100 (9)	0.0062 (10)
C47	0.0274 (10)	0.0317 (10)	0.0365 (11)	−0.0057 (8)	−0.0031 (8)	0.0021 (9)
C48	0.0277 (10)	0.0265 (9)	0.0277 (9)	−0.0056 (8)	−0.0075 (8)	0.0008 (7)
C49	0.0254 (9)	0.0177 (8)	0.0223 (8)	−0.0027 (7)	−0.0087 (7)	0.0001 (6)
C50	0.0304 (9)	0.0160 (8)	0.0251 (9)	−0.0041 (7)	−0.0124 (7)	0.0015 (7)
C51	0.0333 (10)	0.0176 (8)	0.0295 (9)	−0.0046 (7)	−0.0154 (8)	0.0015 (7)
C52	0.0294 (10)	0.0195 (8)	0.0321 (10)	−0.0060 (7)	−0.0147 (8)	0.0033 (7)
C53	0.0244 (9)	0.0186 (8)	0.0275 (9)	−0.0043 (7)	−0.0098 (7)	0.0013 (7)
C61	0.0237 (9)	0.0208 (8)	0.0241 (9)	−0.0044 (7)	−0.0095 (7)	0.0005 (7)
C62	0.0294 (10)	0.0274 (9)	0.0236 (9)	−0.0038 (8)	−0.0111 (7)	−0.0024 (7)
C63	0.0319 (10)	0.0270 (9)	0.0265 (9)	−0.0060 (8)	−0.0118 (8)	−0.0072 (7)
C64	0.0268 (9)	0.0209 (8)	0.0309 (10)	−0.0063 (7)	−0.0105 (8)	−0.0033 (7)
C65	0.0271 (9)	0.0232 (9)	0.0342 (10)	−0.0098 (7)	−0.0112 (8)	0.0026 (8)
C66	0.0330 (10)	0.0289 (10)	0.0349 (11)	−0.0144 (8)	−0.0140 (9)	0.0113 (8)
C67	0.0354 (11)	0.0366 (11)	0.0259 (10)	−0.0147 (9)	−0.0138 (8)	0.0084 (8)
C68	0.0285 (9)	0.0261 (9)	0.0252 (9)	−0.0090 (7)	−0.0108 (7)	0.0013 (7)
C69	0.0200 (8)	0.0203 (8)	0.0210 (8)	−0.0045 (6)	−0.0073 (6)	−0.0001 (6)
C70	0.0176 (8)	0.0190 (8)	0.0232 (8)	−0.0027 (6)	−0.0075 (6)	−0.0020 (6)

C71	0.0197 (8)	0.0200 (8)	0.0254 (9)	−0.0043 (6)	−0.0084 (7)	−0.0011 (7)
C72	0.0194 (8)	0.0215 (8)	0.0255 (9)	−0.0060 (7)	−0.0085 (7)	0.0012 (7)
C73	0.0197 (8)	0.0192 (8)	0.0235 (8)	−0.0050 (6)	−0.0083 (7)	0.0008 (6)

Geometric parameters (Å, °)

K—O7	2.7364 (18)	Dy—C25	2.691 (2)
K—O3	2.7652 (16)	Dy—C28	2.693 (2)
K—O4	2.7649 (15)	Dy—C27	2.699 (2)
K—O1	2.7669 (15)	O31—C37	1.308 (2)
K—O8	2.7800 (18)	O36—C38	1.308 (2)
K—O6	2.7983 (15)	C21—C22	1.384 (4)
K—O5	2.8488 (15)	C21—C25	1.397 (4)
K—O2	2.8638 (16)	C21—H21	0.950
K—C13	3.434 (3)	C22—C23	1.383 (3)
O1—C1	1.421 (3)	C22—H22	0.950
O1—C12	1.429 (2)	C23—C24	1.397 (4)
O2—C2	1.422 (3)	C23—H23	0.950
O2—C3	1.424 (3)	C24—C25	1.410 (4)
O3—C4	1.414 (3)	C24—H24	0.950
O3—C5	1.424 (3)	C25—H25	0.950
O4—C7	1.419 (3)	C26—C30	1.399 (4)
O4—C6	1.426 (3)	C26—C27	1.403 (4)
O5—C8	1.420 (3)	C26—H26	0.950
O5—C9	1.424 (3)	C27—C28	1.403 (4)
O6—C10	1.417 (3)	C27—H27	0.950
O6—C11	1.425 (3)	C28—C29	1.384 (4)
O7—C16	1.425 (3)	C28—H28	0.950
O7—C13	1.436 (3)	C29—C30	1.395 (3)
O8—C17	1.410 (3)	C29—H29	0.950
O8—C20	1.432 (3)	C30—H30	0.950
C1—C2	1.501 (3)	C31—C32	1.396 (3)
C1—H1A	0.990	C31—C36	1.406 (2)
C1—H1B	0.990	C31—C37	1.506 (2)
C2—H2A	0.990	C32—C33	1.390 (3)
C2—H2B	0.990	C32—H32	0.950
C3—C4	1.496 (4)	C33—C34	1.381 (3)
C3—H3A	0.990	C33—H33	0.950
C3—H3B	0.990	C34—C35	1.392 (3)
C4—H4A	0.990	C34—H34	0.950
C4—H4B	0.990	C35—C36	1.403 (2)
C5—C6	1.493 (4)	C35—H35	0.950
C5—H5A	0.990	C36—C38	1.502 (3)
C5—H5B	0.990	C37—C69	1.373 (2)
C6—H6A	0.990	C38—C49	1.380 (2)
C6—H6B	0.990	C41—C42	1.395 (3)
C7—C8	1.497 (4)	C41—C50	1.397 (3)
C7—H7A	0.990	C41—H41	0.950
C7—H7B	0.990	C42—C43	1.392 (3)

C8—H8A	0.990	C42—H42	0.950
C8—H8B	0.990	C43—C44	1.382 (3)
C9—C10	1.497 (3)	C43—H43	0.950
C9—H9A	0.990	C44—C51	1.400 (3)
C9—H9B	0.990	C44—H44	0.950
C10—H10A	0.990	C45—C46	1.388 (3)
C10—H10B	0.990	C45—C52	1.393 (3)
C11—C12	1.493 (3)	C45—H45	0.950
C11—H11A	0.990	C46—C47	1.394 (3)
C11—H11B	0.990	C46—H46	0.950
C12—H12A	0.990	C47—C48	1.390 (3)
C12—H12B	0.990	C47—H47	0.950
C13—C14	1.507 (5)	C48—C53	1.403 (3)
C13—H13A	0.990	C48—H48	0.950
C13—H13B	0.990	C49—C53	1.471 (3)
C14—C15	1.529 (5)	C49—C50	1.475 (3)
C14—H14A	0.990	C50—C51	1.421 (3)
C14—H14B	0.990	C51—C52	1.458 (3)
C15—C16	1.508 (4)	C52—C53	1.413 (3)
C15—H15A	0.990	C61—C62	1.387 (3)
C15—H15B	0.990	C61—C70	1.402 (2)
C16—H16A	0.990	C61—H61	0.950
C16—H16B	0.990	C62—C63	1.394 (3)
C17—C18	1.510 (5)	C62—H62	0.950
C17—H17A	0.990	C63—C64	1.385 (3)
C17—H17B	0.990	C63—H63	0.950
C18—C19	1.520 (4)	C64—C71	1.394 (3)
C18—H18A	0.990	C64—H64	0.950
C18—H18B	0.990	C65—C66	1.387 (3)
C19—C20	1.521 (4)	C65—C72	1.394 (3)
C19—H19A	0.990	C65—H65	0.950
C19—H19B	0.990	C66—C67	1.394 (3)
C20—H20A	0.990	C66—H66	0.950
C20—H20B	0.990	C67—C68	1.397 (3)
Dy—O36	2.1832 (13)	C67—H67	0.950
Dy—O31	2.2134 (13)	C68—C73	1.397 (3)
Dy—C30	2.658 (2)	C68—H68	0.950
Dy—C29	2.670 (2)	C69—C73	1.471 (2)
Dy—C22	2.673 (2)	C69—C70	1.471 (2)
Dy—C23	2.675 (2)	C70—C71	1.422 (2)
Dy—C26	2.680 (2)	C71—C72	1.458 (3)
Dy—C24	2.687 (2)	C72—C73	1.418 (2)
Dy—C21	2.688 (2)		
O7—K—O3	90.26 (6)	C30—Dy—C24	146.66 (9)
O7—K—O4	79.66 (5)	C29—Dy—C24	116.67 (9)
O3—K—O4	60.37 (5)	C22—Dy—C24	49.80 (8)
O7—K—O1	101.60 (5)	C23—Dy—C24	30.21 (8)
O3—K—O1	119.84 (5)	C26—Dy—C24	151.47 (9)
O4—K—O1	178.69 (5)	O36—Dy—C21	85.56 (6)

O7—K—O8	178.42 (6)	O31—Dy—C21	124.28 (8)
O3—K—O8	88.18 (5)	C30—Dy—C21	153.13 (9)
O4—K—O8	99.79 (5)	C29—Dy—C21	144.81 (9)
O1—K—O8	78.96 (5)	C22—Dy—C21	29.92 (8)
O7—K—O6	86.54 (5)	C23—Dy—C21	49.48 (7)
O3—K—O6	176.62 (5)	C26—Dy—C21	123.02 (9)
O4—K—O6	119.97 (5)	C24—Dy—C21	49.83 (8)
O1—K—O6	59.89 (4)	O36—Dy—C25	90.05 (7)
O8—K—O6	95.01 (5)	O31—Dy—C25	95.24 (8)
O7—K—O5	88.51 (5)	C30—Dy—C25	176.30 (9)
O3—K—O5	120.51 (5)	C29—Dy—C25	147.02 (8)
O4—K—O5	60.96 (5)	C22—Dy—C25	49.69 (8)
O1—K—O5	118.58 (5)	C23—Dy—C25	49.81 (8)
O8—K—O5	92.51 (5)	C26—Dy—C25	153.07 (10)
O6—K—O5	60.55 (4)	C24—Dy—C25	30.39 (9)
O7—K—O2	91.62 (6)	C21—Dy—C25	30.10 (9)
O3—K—O2	60.48 (5)	O36—Dy—C28	133.37 (7)
O4—K—O2	120.04 (5)	O31—Dy—C28	110.54 (7)
O1—K—O2	60.43 (5)	C30—Dy—C28	49.93 (8)
O8—K—O2	87.38 (5)	C29—Dy—C28	29.91 (8)
O6—K—O2	118.47 (5)	C22—Dy—C28	86.15 (8)
O5—K—O2	179.00 (5)	C23—Dy—C28	79.85 (8)
O7—K—C13	23.63 (6)	C26—Dy—C28	49.77 (7)
O3—K—C13	96.02 (7)	C24—Dy—C28	104.90 (9)
O4—K—C13	102.42 (6)	C21—Dy—C28	115.57 (9)
O1—K—C13	78.87 (6)	C25—Dy—C28	129.56 (8)
O8—K—C13	156.45 (6)	O36—Dy—C27	106.91 (8)
O6—K—C13	80.61 (6)	O31—Dy—C27	130.21 (7)
O5—K—C13	105.02 (6)	C30—Dy—C27	50.12 (9)
O2—K—C13	74.82 (6)	C29—Dy—C27	49.72 (8)
C1—O1—C12	111.96 (16)	C22—Dy—C27	82.24 (9)
C1—O1—K	118.11 (13)	C23—Dy—C27	91.29 (9)
C12—O1—K	116.56 (11)	C26—Dy—C27	30.24 (9)
C2—O2—C3	111.57 (18)	C24—Dy—C27	121.31 (9)
C2—O2—K	108.88 (13)	C21—Dy—C27	105.07 (9)
C3—O2—K	111.25 (14)	C25—Dy—C27	131.83 (9)
C4—O3—C5	113.67 (19)	C28—Dy—C27	30.16 (8)
C4—O3—K	116.46 (14)	C37—O31—Dy	125.31 (11)
C5—O3—K	116.24 (13)	C38—O36—Dy	143.67 (12)
C7—O4—C6	112.76 (18)	C22—C21—C25	108.3 (2)
C7—O4—K	114.76 (13)	C22—C21—Dy	74.44 (13)
C6—O4—K	114.96 (12)	C25—C21—Dy	75.08 (13)
C8—O5—C9	112.41 (17)	C22—C21—H21	125.9
C8—O5—K	110.42 (12)	C25—C21—H21	125.9
C9—O5—K	111.21 (12)	Dy—C21—H21	116.7
C10—O6—C11	112.36 (17)	C23—C22—C21	108.4 (2)
C10—O6—K	115.49 (12)	C23—C22—Dy	75.12 (13)
C11—O6—K	115.85 (12)	C21—C22—Dy	75.64 (13)
C16—O7—C13	108.1 (2)	C23—C22—H22	125.8

C16—O7—K	131.44 (15)	C21—C22—H22	125.8
C13—O7—K	106.58 (14)	Dy—C22—H22	115.6
C17—O8—C20	104.91 (19)	C22—C23—C24	108.5 (2)
C17—O8—K	116.98 (16)	C22—C23—Dy	74.91 (13)
C20—O8—K	121.67 (14)	C24—C23—Dy	75.35 (13)
O1—C1—C2	108.38 (18)	C22—C23—H23	125.7
O1—C1—H1A	110.0	C24—C23—H23	125.7
C2—C1—H1A	110.0	Dy—C23—H23	116.1
O1—C1—H1B	110.0	C23—C24—C25	107.2 (2)
C2—C1—H1B	110.0	C23—C24—Dy	74.44 (13)
H1A—C1—H1B	108.4	C25—C24—Dy	74.97 (13)
O2—C2—C1	109.29 (19)	C23—C24—H24	126.4
O2—C2—H2A	109.8	C25—C24—H24	126.4
C1—C2—H2A	109.8	Dy—C24—H24	116.4
O2—C2—H2B	109.8	C21—C25—C24	107.5 (2)
C1—C2—H2B	109.8	C21—C25—Dy	74.82 (14)
H2A—C2—H2B	108.3	C24—C25—Dy	74.64 (14)
O2—C3—C4	109.51 (19)	C21—C25—H25	126.2
O2—C3—H3A	109.8	C24—C25—H25	126.2
C4—C3—H3A	109.8	Dy—C25—H25	116.5
O2—C3—H3B	109.8	C30—C26—C27	108.2 (2)
C4—C3—H3B	109.8	C30—C26—Dy	73.93 (13)
H3A—C3—H3B	108.2	C27—C26—Dy	75.61 (14)
O3—C4—C3	108.5 (2)	C30—C26—H26	125.9
O3—C4—H4A	110.0	C27—C26—H26	125.9
C3—C4—H4A	110.0	Dy—C26—H26	116.6
O3—C4—H4B	110.0	C28—C27—C26	107.4 (2)
C3—C4—H4B	110.0	C28—C27—Dy	74.70 (14)
H4A—C4—H4B	108.4	C26—C27—Dy	74.15 (14)
O3—C5—C6	108.22 (19)	C28—C27—H27	126.3
O3—C5—H5A	110.1	C26—C27—H27	126.3
C6—C5—H5A	110.1	Dy—C27—H27	117.0
O3—C5—H5B	110.1	C29—C28—C27	108.2 (2)
C6—C5—H5B	110.1	C29—C28—Dy	74.11 (13)
H5A—C5—H5B	108.4	C27—C28—Dy	75.14 (14)
O4—C6—C5	108.32 (19)	C29—C28—H28	125.9
O4—C6—H6A	110.0	C27—C28—H28	125.9
C5—C6—H6A	110.0	Dy—C28—H28	116.9
O4—C6—H6B	110.0	C28—C29—C30	108.7 (2)
C5—C6—H6B	110.0	C28—C29—Dy	75.98 (14)
H6A—C6—H6B	108.4	C30—C29—Dy	74.35 (12)
O4—C7—C8	107.72 (18)	C28—C29—H29	125.6
O4—C7—H7A	110.2	C30—C29—H29	125.6
C8—C7—H7A	110.2	Dy—C29—H29	116.1
O4—C7—H7B	110.2	C29—C30—C26	107.5 (2)
C8—C7—H7B	110.2	C29—C30—Dy	75.29 (13)
H7A—C7—H7B	108.5	C26—C30—Dy	75.69 (13)
O5—C8—C7	108.91 (18)	C29—C30—H30	126.2
O5—C8—H8A	109.9	C26—C30—H30	126.2

C7—C8—H8A	109.9	Dy—C30—H30	115.1
O5—C8—H8B	109.9	C32—C31—C36	119.63 (17)
C7—C8—H8B	109.9	C32—C31—C37	116.15 (16)
H8A—C8—H8B	108.3	C36—C31—C37	124.22 (16)
O5—C9—C10	109.02 (17)	C33—C32—C31	121.17 (18)
O5—C9—H9A	109.9	C33—C32—H32	119.4
C10—C9—H9A	109.9	C31—C32—H32	119.4
O5—C9—H9B	109.9	C34—C33—C32	119.69 (19)
C10—C9—H9B	109.9	C34—C33—H33	120.2
H9A—C9—H9B	108.3	C32—C33—H33	120.2
O6—C10—C9	108.91 (18)	C33—C34—C35	119.73 (19)
O6—C10—H10A	109.9	C33—C34—H34	120.1
C9—C10—H10A	109.9	C35—C34—H34	120.1
O6—C10—H10B	109.9	C34—C35—C36	121.53 (18)
C9—C10—H10B	109.9	C34—C35—H35	119.2
H10A—C10—H10B	108.3	C36—C35—H35	119.2
O6—C11—C12	108.73 (18)	C35—C36—C31	118.21 (17)
O6—C11—H11A	109.9	C35—C36—C38	119.36 (16)
C12—C11—H11A	109.9	C31—C36—C38	122.18 (16)
O6—C11—H11B	109.9	O31—C37—C69	123.84 (16)
C12—C11—H11B	109.9	O31—C37—C31	115.80 (15)
H11A—C11—H11B	108.3	C69—C37—C31	120.25 (15)
O1—C12—C11	108.16 (17)	O36—C38—C49	121.02 (17)
O1—C12—H12A	110.1	O36—C38—C36	114.67 (15)
C11—C12—H12A	110.1	C49—C38—C36	124.12 (16)
O1—C12—H12B	110.1	C42—C41—C50	119.7 (2)
C11—C12—H12B	110.1	C42—C41—H41	120.1
H12A—C12—H12B	108.4	C50—C41—H41	120.1
O7—C13—C14	108.6 (2)	C43—C42—C41	121.4 (2)
O7—C13—K	49.80 (11)	C43—C42—H42	119.3
C14—C13—K	137.2 (2)	C41—C42—H42	119.3
O7—C13—H13A	110.0	C44—C43—C42	119.90 (19)
C14—C13—H13A	110.0	C44—C43—H43	120.0
K—C13—H13A	112.4	C42—C43—H43	120.0
O7—C13—H13B	110.0	C43—C44—C51	119.6 (2)
C14—C13—H13B	110.0	C43—C44—H44	120.2
K—C13—H13B	62.1	C51—C44—H44	120.2
H13A—C13—H13B	108.3	C46—C45—C52	119.1 (2)
C13—C14—C15	102.7 (3)	C46—C45—H45	120.5
C13—C14—H14A	111.2	C52—C45—H45	120.5
C15—C14—H14A	111.2	C45—C46—C47	120.3 (2)
C13—C14—H14B	111.2	C45—C46—H46	119.9
C15—C14—H14B	111.2	C47—C46—H46	119.9
H14A—C14—H14B	109.1	C48—C47—C46	121.3 (2)
C16—C15—C14	102.8 (2)	C48—C47—H47	119.4
C16—C15—H15A	111.2	C46—C47—H47	119.4
C14—C15—H15A	111.2	C47—C48—C53	119.14 (19)
C16—C15—H15B	111.2	C47—C48—H48	120.4
C14—C15—H15B	111.2	C53—C48—H48	120.4

H15A—C15—H15B	109.1	C38—C49—C53	124.13 (17)
O7—C16—C15	105.3 (2)	C38—C49—C50	129.77 (18)
O7—C16—H16A	110.7	C53—C49—C50	106.08 (15)
C15—C16—H16A	110.7	C41—C50—C51	118.51 (17)
O7—C16—H16B	110.7	C41—C50—C49	133.20 (17)
C15—C16—H16B	110.7	C51—C50—C49	108.18 (17)
H16A—C16—H16B	108.8	C44—C51—C50	120.9 (2)
O8—C17—C18	106.2 (2)	C44—C51—C52	130.50 (19)
O8—C17—H17A	110.5	C50—C51—C52	108.56 (16)
C18—C17—H17A	110.5	C45—C52—C53	121.1 (2)
O8—C17—H17B	110.5	C45—C52—C51	130.64 (19)
C18—C17—H17B	110.5	C53—C52—C51	108.27 (17)
H17A—C17—H17B	108.7	C48—C53—C52	119.12 (18)
C17—C18—C19	104.1 (2)	C48—C53—C49	131.99 (17)
C17—C18—H18A	110.9	C52—C53—C49	108.81 (17)
C19—C18—H18A	110.9	C62—C61—C70	119.77 (17)
C17—C18—H18B	110.9	C62—C61—H61	120.1
C19—C18—H18B	110.9	C70—C61—H61	120.1
H18A—C18—H18B	109.0	C61—C62—C63	121.54 (18)
C18—C19—C20	103.9 (2)	C61—C62—H62	119.2
C18—C19—H19A	111.0	C63—C62—H62	119.2
C20—C19—H19A	111.0	C64—C63—C62	119.87 (18)
C18—C19—H19B	111.0	C64—C63—H63	120.1
C20—C19—H19B	111.0	C62—C63—H63	120.1
H19A—C19—H19B	109.0	C63—C64—C71	119.31 (17)
O8—C20—C19	105.66 (19)	C63—C64—H64	120.3
O8—C20—H20A	110.6	C71—C64—H64	120.3
C19—C20—H20A	110.6	C66—C65—C72	118.80 (18)
O8—C20—H20B	110.6	C66—C65—H65	120.6
C19—C20—H20B	110.6	C72—C65—H65	120.6
H20A—C20—H20B	108.7	C65—C66—C67	120.44 (18)
O36—Dy—O31	84.77 (5)	C65—C66—H66	119.8
O36—Dy—C30	92.15 (7)	C67—C66—H66	119.8
O31—Dy—C30	82.00 (7)	C66—C67—C68	121.24 (19)
O36—Dy—C29	122.30 (7)	C66—C67—H67	119.4
O31—Dy—C29	82.68 (7)	C68—C67—H67	119.4
C30—Dy—C29	30.36 (7)	C73—C68—C67	119.14 (18)
O36—Dy—C22	110.75 (7)	C73—C68—H68	120.4
O31—Dy—C22	139.57 (7)	C67—C68—H68	120.4
C30—Dy—C22	131.84 (8)	C37—C69—C73	126.39 (16)
C29—Dy—C22	114.91 (8)	C37—C69—C70	127.37 (16)
O36—Dy—C23	134.82 (6)	C73—C69—C70	106.16 (15)
O31—Dy—C23	114.59 (7)	C61—C70—C71	118.11 (16)
C30—Dy—C23	129.23 (8)	C61—C70—C69	133.47 (16)
C29—Dy—C23	101.20 (8)	C71—C70—C69	108.42 (15)
C22—Dy—C23	29.97 (7)	C64—C71—C70	121.39 (17)
O36—Dy—C26	83.65 (6)	C64—C71—C72	130.18 (17)
O31—Dy—C26	110.14 (8)	C70—C71—C72	108.43 (15)
C30—Dy—C26	30.38 (8)	C65—C72—C73	121.37 (17)

C29—Dy—C26	49.84 (7)	C65—C72—C71	130.35 (18)
C22—Dy—C26	108.58 (9)	C73—C72—C71	108.28 (15)
C23—Dy—C26	121.53 (9)	C68—C73—C72	119.00 (16)
O36—Dy—C24	119.37 (8)	C68—C73—C69	132.30 (17)
O31—Dy—C24	89.86 (7)	C72—C73—C69	108.70 (15)
O7—K—O1—C1	77.07 (16)	C22—C23—C24—C25	−0.2 (3)
O3—K—O1—C1	−20.00 (17)	Dy—C23—C24—C25	−68.40 (16)
O8—K—O1—C1	−101.42 (16)	C22—C23—C24—Dy	68.21 (16)
O6—K—O1—C1	156.11 (17)	O36—Dy—C24—C23	−129.87 (15)
O5—K—O1—C1	171.75 (15)	O31—Dy—C24—C23	146.21 (15)
O2—K—O1—C1	−8.15 (15)	C30—Dy—C24—C23	71.1 (2)
C13—K—O1—C1	70.59 (16)	C29—Dy—C24—C23	64.49 (17)
O7—K—O1—C12	−60.74 (15)	C22—Dy—C24—C23	−36.62 (14)
O3—K—O1—C12	−157.81 (14)	C26—Dy—C24—C23	10.4 (3)
O8—K—O1—C12	120.77 (15)	C21—Dy—C24—C23	−76.13 (16)
O6—K—O1—C12	18.30 (14)	C25—Dy—C24—C23	−113.1 (2)
O5—K—O1—C12	33.94 (16)	C28—Dy—C24—C23	34.96 (17)
O2—K—O1—C12	−145.96 (16)	C27—Dy—C24—C23	7.26 (19)
C13—K—O1—C12	−67.22 (15)	O36—Dy—C24—C25	−16.72 (19)
O7—K—O2—C2	−128.46 (15)	O31—Dy—C24—C25	−100.64 (16)
O3—K—O2—C2	142.16 (16)	C30—Dy—C24—C25	−175.76 (16)
O4—K—O2—C2	152.56 (14)	C29—Dy—C24—C25	177.63 (16)
O1—K—O2—C2	−26.03 (14)	C22—Dy—C24—C25	76.52 (17)
O8—K—O2—C2	52.77 (15)	C23—Dy—C24—C25	113.1 (2)
O6—K—O2—C2	−41.51 (16)	C26—Dy—C24—C25	123.6 (2)
C13—K—O2—C2	−111.67 (15)	C21—Dy—C24—C25	37.02 (16)
O7—K—O2—C3	108.18 (17)	C28—Dy—C24—C25	148.10 (17)
O3—K—O2—C3	18.80 (16)	C27—Dy—C24—C25	120.40 (18)
O4—K—O2—C3	29.20 (18)	C22—C21—C25—C24	0.4 (3)
O1—K—O2—C3	−149.39 (18)	Dy—C21—C25—C24	68.06 (16)
O8—K—O2—C3	−70.59 (16)	C22—C21—C25—Dy	−67.63 (17)
O6—K—O2—C3	−164.87 (16)	C23—C24—C25—C21	−0.1 (3)
C13—K—O2—C3	124.97 (17)	Dy—C24—C25—C21	−68.18 (16)
O7—K—O3—C4	−75.56 (16)	C23—C24—C25—Dy	68.03 (16)
O4—K—O3—C4	−153.48 (17)	O36—Dy—C25—C21	−81.04 (15)
O1—K—O3—C4	28.00 (18)	O31—Dy—C25—C21	−165.79 (15)
O8—K—O3—C4	104.18 (16)	C29—Dy—C25—C21	109.6 (2)
O5—K—O3—C4	−163.98 (15)	C22—Dy—C25—C21	36.60 (14)
O2—K—O3—C4	16.16 (15)	C23—Dy—C25—C21	76.20 (16)
C13—K—O3—C4	−52.60 (17)	C26—Dy—C25—C21	−5.1 (3)
O7—K—O3—C5	62.62 (17)	C24—Dy—C25—C21	113.5 (2)
O4—K—O3—C5	−15.30 (16)	C28—Dy—C25—C21	72.0 (2)
O1—K—O3—C5	166.18 (16)	C27—Dy—C25—C21	32.0 (2)
O8—K—O3—C5	−117.64 (17)	O36—Dy—C25—C24	165.48 (16)
O5—K—O3—C5	−25.80 (18)	O31—Dy—C25—C24	80.72 (16)
O2—K—O3—C5	154.34 (18)	C29—Dy—C25—C24	−3.9 (3)
C13—K—O3—C5	85.58 (17)	C22—Dy—C25—C24	−76.89 (16)
O7—K—O4—C7	111.16 (15)	C23—Dy—C25—C24	−37.28 (15)
O3—K—O4—C7	−152.57 (16)	C26—Dy—C25—C24	−118.6 (2)

O8—K—O4—C7	−70.34 (15)	C21—Dy—C25—C24	−113.5 (2)
O6—K—O4—C7	31.30 (16)	C28—Dy—C25—C24	−41.5 (2)
O5—K—O4—C7	17.09 (14)	C27—Dy—C25—C24	−81.5 (2)
O2—K—O4—C7	−162.98 (14)	O36—Dy—C26—C30	−105.33 (15)
C13—K—O4—C7	117.53 (15)	O31—Dy—C26—C30	−23.29 (16)
O7—K—O4—C6	−115.64 (16)	C29—Dy—C26—C30	37.55 (14)
O3—K—O4—C6	−19.38 (15)	C22—Dy—C26—C30	144.87 (15)
O8—K—O4—C6	62.86 (16)	C23—Dy—C26—C30	114.86 (16)
O6—K—O4—C6	164.50 (14)	C24—Dy—C26—C30	108.7 (2)
O5—K—O4—C6	150.28 (16)	C21—Dy—C26—C30	174.18 (14)
O2—K—O4—C6	−29.79 (17)	C25—Dy—C26—C30	177.21 (16)
C13—K—O4—C6	−109.28 (16)	C28—Dy—C26—C30	77.04 (16)
O7—K—O5—C8	−59.85 (15)	C27—Dy—C26—C30	114.1 (2)
O3—K—O5—C8	29.57 (16)	O36—Dy—C26—C27	140.54 (17)
O4—K—O5—C8	19.14 (14)	O31—Dy—C26—C27	−137.42 (16)
O1—K—O5—C8	−162.26 (14)	C30—Dy—C26—C27	−114.1 (2)
O8—K—O5—C8	118.94 (15)	C29—Dy—C26—C27	−76.58 (17)
O6—K—O5—C8	−146.72 (16)	C22—Dy—C26—C27	30.74 (18)
C13—K—O5—C8	−76.93 (15)	C23—Dy—C26—C27	0.73 (19)
O7—K—O5—C9	65.65 (14)	C24—Dy—C26—C27	−5.4 (3)
O3—K—O5—C9	155.07 (13)	C21—Dy—C26—C27	60.05 (18)
O4—K—O5—C9	144.64 (14)	C25—Dy—C26—C27	63.1 (2)
O1—K—O5—C9	−36.76 (15)	C28—Dy—C26—C27	−37.09 (16)
O8—K—O5—C9	−115.56 (14)	C30—C26—C27—C28	0.5 (3)
O6—K—O5—C9	−21.22 (13)	Dy—C26—C27—C28	67.89 (17)
C13—K—O5—C9	48.57 (14)	C30—C26—C27—Dy	−67.36 (16)
O7—K—O6—C10	−104.07 (14)	O36—Dy—C27—C28	−154.88 (16)
O4—K—O6—C10	−28.10 (15)	O31—Dy—C27—C28	−57.3 (2)
O1—K—O6—C10	150.39 (15)	C30—Dy—C27—C28	−76.59 (18)
O8—K—O6—C10	76.23 (14)	C29—Dy—C27—C28	−36.57 (16)
O5—K—O6—C10	−13.83 (13)	C22—Dy—C27—C28	95.71 (18)
O2—K—O6—C10	165.96 (13)	C23—Dy—C27—C28	67.06 (17)
C13—K—O6—C10	−127.10 (14)	C26—Dy—C27—C28	−113.6 (2)
O7—K—O6—C11	121.56 (15)	C24—Dy—C27—C28	63.41 (19)
O4—K—O6—C11	−162.47 (14)	C21—Dy—C27—C28	115.23 (17)
O1—K—O6—C11	16.02 (14)	C25—Dy—C27—C28	99.26 (19)
O8—K—O6—C11	−58.14 (15)	O36—Dy—C27—C26	−41.32 (17)
O5—K—O6—C11	−148.20 (16)	O31—Dy—C27—C26	56.29 (19)
O2—K—O6—C11	31.59 (16)	C30—Dy—C27—C26	36.98 (15)
C13—K—O6—C11	98.53 (15)	C29—Dy—C27—C26	77.00 (17)
O3—K—O7—C16	−29.6 (2)	C22—Dy—C27—C26	−150.73 (17)
O4—K—O7—C16	30.2 (2)	C23—Dy—C27—C26	−179.37 (16)
O1—K—O7—C16	−150.2 (2)	C24—Dy—C27—C26	176.98 (15)
O6—K—O7—C16	151.5 (2)	C21—Dy—C27—C26	−131.21 (16)
O5—K—O7—C16	90.9 (2)	C25—Dy—C27—C26	−147.18 (16)
O2—K—O7—C16	−90.1 (2)	C28—Dy—C27—C26	113.6 (2)
C13—K—O7—C16	−134.1 (3)	C26—C27—C28—C29	−0.2 (3)
O3—K—O7—C13	104.55 (17)	Dy—C27—C28—C29	67.34 (16)
O4—K—O7—C13	164.33 (17)	C26—C27—C28—Dy	−67.52 (17)

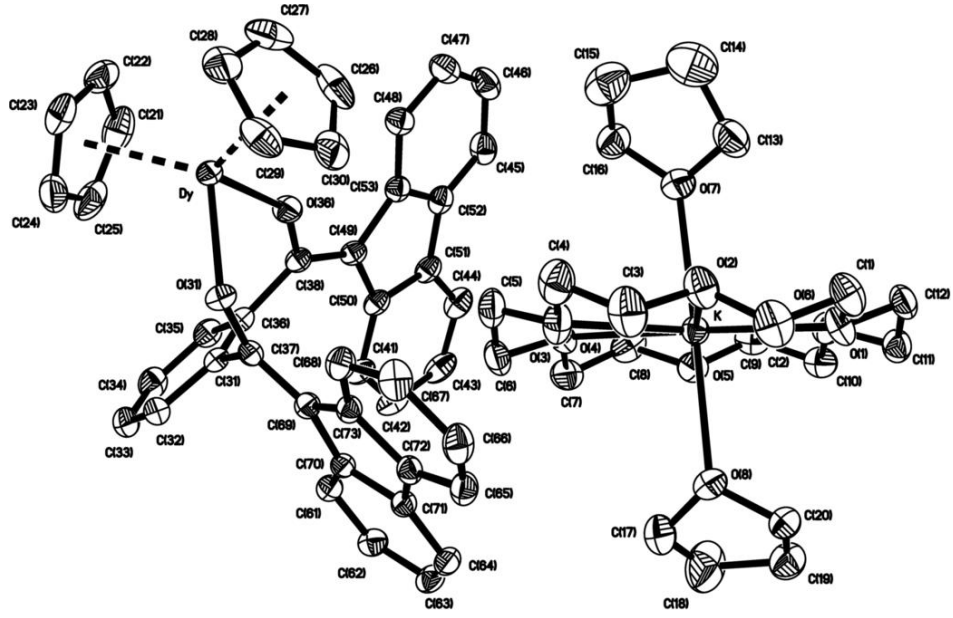
O1—K—O7—C13	−16.04 (17)	O36—Dy—C28—C29	−80.32 (17)
O6—K—O7—C13	−74.35 (17)	O31—Dy—C28—C29	22.40 (16)
O5—K—O7—C13	−134.93 (17)	C30—Dy—C28—C29	−36.98 (14)
O2—K—O7—C13	44.08 (17)	C22—Dy—C28—C29	164.54 (15)
O3—K—O8—C17	73.3 (2)	C23—Dy—C28—C29	135.00 (16)
O4—K—O8—C17	13.8 (2)	C26—Dy—C28—C29	−77.08 (17)
O1—K—O8—C17	−165.8 (2)	C24—Dy—C28—C29	117.97 (15)
O6—K—O8—C17	−107.8 (2)	C21—Dy—C28—C29	170.18 (14)
O5—K—O8—C17	−47.1 (2)	C25—Dy—C28—C29	138.25 (16)
O2—K—O8—C17	133.8 (2)	C27—Dy—C28—C29	−114.3 (2)
C13—K—O8—C17	174.3 (2)	O36—Dy—C28—C27	34.0 (2)
O3—K—O8—C20	−155.90 (17)	O31—Dy—C28—C27	136.68 (16)
O4—K—O8—C20	144.59 (17)	C30—Dy—C28—C27	77.30 (18)
O1—K—O8—C20	−35.00 (17)	C29—Dy—C28—C27	114.3 (2)
O6—K—O8—C20	22.98 (17)	C22—Dy—C28—C27	−81.18 (18)
O5—K—O8—C20	83.63 (17)	C23—Dy—C28—C27	−110.72 (18)
O2—K—O8—C20	−95.37 (17)	C26—Dy—C28—C27	37.20 (17)
C13—K—O8—C20	−55.0 (3)	C24—Dy—C28—C27	−127.76 (17)
C12—O1—C1—C2	179.31 (19)	C21—Dy—C28—C27	−75.54 (18)
K—O1—C1—C2	39.7 (2)	C25—Dy—C28—C27	−107.47 (19)
C3—O2—C2—C1	−178.8 (2)	C27—C28—C29—C30	−0.3 (3)
K—O2—C2—C1	58.0 (2)	Dy—C28—C29—C30	67.78 (15)
O1—C1—C2—O2	−66.6 (3)	C27—C28—C29—Dy	−68.03 (17)
C2—O2—C3—C4	−172.6 (2)	O36—Dy—C29—C28	122.03 (14)
K—O2—C3—C4	−50.8 (3)	O31—Dy—C29—C28	−158.92 (15)
C5—O3—C4—C3	172.6 (2)	C30—Dy—C29—C28	114.4 (2)
K—O3—C4—C3	−48.2 (2)	C22—Dy—C29—C28	−17.05 (17)
O2—C3—C4—O3	67.0 (3)	C23—Dy—C29—C28	−45.20 (16)
C4—O3—C5—C6	−174.27 (19)	C26—Dy—C29—C28	76.84 (17)
K—O3—C5—C6	46.4 (2)	C24—Dy—C29—C28	−72.78 (16)
C7—O4—C6—C5	−175.28 (17)	C21—Dy—C29—C28	−15.5 (2)
K—O4—C6—C5	50.6 (2)	C25—Dy—C29—C28	−70.6 (2)
O3—C5—C6—O4	−63.7 (2)	C27—Dy—C29—C28	36.89 (15)
C6—O4—C7—C8	175.49 (18)	O36—Dy—C29—C30	7.62 (18)
K—O4—C7—C8	−50.3 (2)	O31—Dy—C29—C30	86.67 (16)
C9—O5—C8—C7	−177.39 (19)	C22—Dy—C29—C30	−131.47 (16)
K—O5—C8—C7	−52.6 (2)	C23—Dy—C29—C30	−159.62 (16)
O4—C7—C8—O5	70.3 (2)	C26—Dy—C29—C30	−37.58 (16)
C8—O5—C9—C10	177.95 (19)	C24—Dy—C29—C30	172.81 (15)
K—O5—C9—C10	53.6 (2)	C21—Dy—C29—C30	−129.90 (18)
C11—O6—C10—C9	−177.89 (18)	C25—Dy—C29—C30	175.01 (16)
K—O6—C10—C9	46.2 (2)	C28—Dy—C29—C30	−114.4 (2)
O5—C9—C10—O6	−67.9 (2)	C27—Dy—C29—C30	−77.53 (17)
C10—O6—C11—C12	177.42 (17)	C28—C29—C30—C26	0.6 (3)
K—O6—C11—C12	−46.8 (2)	Dy—C29—C30—C26	69.45 (15)
C1—O1—C12—C11	170.67 (19)	C28—C29—C30—Dy	−68.87 (16)
K—O1—C12—C11	−49.0 (2)	C27—C26—C30—C29	−0.7 (3)
O6—C11—C12—O1	62.6 (2)	Dy—C26—C30—C29	−69.18 (15)
C16—O7—C13—C14	8.8 (3)	C27—C26—C30—Dy	68.48 (17)

K—O7—C13—C14	−136.7 (2)	O36—Dy—C30—C29	−173.56 (15)
C16—O7—C13—K	145.5 (2)	O31—Dy—C30—C29	−89.15 (15)
O3—K—C13—O7	−76.72 (17)	C22—Dy—C30—C29	65.81 (19)
O4—K—C13—O7	−15.79 (18)	C23—Dy—C30—C29	26.2 (2)
O1—K—C13—O7	163.98 (17)	C26—Dy—C30—C29	112.9 (2)
O8—K—C13—O7	−176.05 (15)	C24—Dy—C30—C29	−11.7 (2)
O6—K—C13—O7	103.04 (17)	C21—Dy—C30—C29	102.0 (2)
O5—K—C13—O7	47.12 (17)	C28—Dy—C30—C29	36.39 (15)
O2—K—C13—O7	−133.90 (17)	C27—Dy—C30—C29	76.08 (17)
O7—K—C13—C14	72.8 (3)	O36—Dy—C30—C26	73.57 (15)
O3—K—C13—C14	−3.9 (3)	O31—Dy—C30—C26	157.98 (15)
O4—K—C13—C14	57.0 (3)	C29—Dy—C30—C26	−112.9 (2)
O1—K—C13—C14	−123.2 (3)	C22—Dy—C30—C26	−47.06 (19)
O8—K—C13—C14	−103.3 (3)	C23—Dy—C30—C26	−86.70 (17)
O6—K—C13—C14	175.8 (3)	C24—Dy—C30—C26	−124.62 (18)
O5—K—C13—C14	119.9 (3)	C21—Dy—C30—C26	−10.8 (3)
O2—K—C13—C14	−61.1 (3)	C28—Dy—C30—C26	−76.48 (17)
O7—C13—C14—C15	13.6 (3)	C27—Dy—C30—C26	−36.79 (15)
K—C13—C14—C15	−36.8 (4)	C36—C31—C32—C33	1.7 (3)
C13—C14—C15—C16	−29.3 (3)	C37—C31—C32—C33	−177.68 (17)
C13—O7—C16—C15	−28.1 (3)	C31—C32—C33—C34	−0.9 (3)
K—O7—C16—C15	105.6 (2)	C32—C33—C34—C35	−0.8 (3)
C14—C15—C16—O7	35.8 (3)	C33—C34—C35—C36	1.8 (3)
C20—O8—C17—C18	−39.0 (3)	C34—C35—C36—C31	−1.1 (3)
K—O8—C17—C18	99.2 (2)	C34—C35—C36—C38	−175.57 (18)
O8—C17—C18—C19	24.5 (4)	C32—C31—C36—C35	−0.6 (3)
C17—C18—C19—C20	−1.6 (3)	C37—C31—C36—C35	178.66 (16)
C17—O8—C20—C19	37.8 (3)	C32—C31—C36—C38	173.66 (17)
K—O8—C20—C19	−98.0 (2)	C37—C31—C36—C38	−7.0 (3)
C18—C19—C20—O8	−21.4 (3)	Dy—O31—C37—C69	130.86 (15)
O36—Dy—O31—C37	−13.93 (14)	Dy—O31—C37—C31	−53.02 (19)
C30—Dy—O31—C37	−106.84 (15)	C32—C31—C37—O31	−93.0 (2)
C29—Dy—O31—C37	−137.48 (15)	C36—C31—C37—O31	87.7 (2)
C22—Dy—O31—C37	102.26 (16)	C32—C31—C37—C69	83.3 (2)
C23—Dy—O31—C37	123.52 (14)	C36—C31—C37—C69	−96.0 (2)
C26—Dy—O31—C37	−95.19 (14)	Dy—O36—C38—C49	176.34 (14)
C24—Dy—O31—C37	105.59 (15)	Dy—O36—C38—C36	1.1 (3)
C21—Dy—O31—C37	67.07 (15)	C35—C36—C38—O36	126.44 (18)
C25—Dy—O31—C37	75.64 (15)	C31—C36—C38—O36	−47.8 (2)
C28—Dy—O31—C37	−148.52 (14)	C35—C36—C38—C49	−48.6 (3)
C27—Dy—O31—C37	−121.69 (15)	C31—C36—C38—C49	137.18 (18)
O31—Dy—O36—C38	48.1 (2)	C50—C41—C42—C43	0.9 (3)
C30—Dy—O36—C38	129.9 (2)	C41—C42—C43—C44	0.6 (3)
C29—Dy—O36—C38	126.0 (2)	C42—C43—C44—C51	−0.9 (3)
C22—Dy—O36—C38	−93.4 (2)	C52—C45—C46—C47	0.2 (3)
C23—Dy—O36—C38	−71.8 (2)	C45—C46—C47—C48	0.0 (3)
C26—Dy—O36—C38	159.1 (2)	C46—C47—C48—C53	−0.4 (3)
C24—Dy—O36—C38	−38.8 (2)	O36—C38—C49—C53	−8.3 (3)
C21—Dy—O36—C38	−77.0 (2)	C36—C38—C49—C53	166.44 (16)

C25—Dy—O36—C38	−47.2 (2)	O36—C38—C49—C50	173.43 (17)
C28—Dy—O36—C38	161.6 (2)	C36—C38—C49—C50	−11.8 (3)
C27—Dy—O36—C38	178.6 (2)	C42—C41—C50—C51	−2.0 (3)
O36—Dy—C21—C22	−147.92 (16)	C42—C41—C50—C49	−177.68 (19)
O31—Dy—C21—C22	131.50 (15)	C38—C49—C50—C41	−7.8 (3)
C30—Dy—C21—C22	−61.9 (2)	C53—C49—C50—C41	173.65 (19)
C29—Dy—C21—C22	−2.8 (2)	C38—C49—C50—C51	176.21 (18)
C23—Dy—C21—C22	36.91 (15)	C53—C49—C50—C51	−2.32 (19)
C26—Dy—C21—C22	−68.45 (17)	C43—C44—C51—C50	−0.4 (3)
C24—Dy—C21—C22	76.90 (17)	C43—C44—C51—C52	176.7 (2)
C25—Dy—C21—C22	114.3 (2)	C41—C50—C51—C44	1.8 (3)
C28—Dy—C21—C22	−11.33 (18)	C49—C50—C51—C44	178.47 (17)
C27—Dy—C21—C22	−41.58 (17)	C41—C50—C51—C52	−175.86 (16)
O36—Dy—C21—C25	97.79 (16)	C49—C50—C51—C52	0.8 (2)
O31—Dy—C21—C25	17.20 (18)	C46—C45—C52—C53	0.0 (3)
C30—Dy—C21—C25	−176.22 (16)	C46—C45—C52—C51	179.1 (2)
C29—Dy—C21—C25	−117.14 (19)	C44—C51—C52—C45	4.6 (3)
C22—Dy—C21—C25	−114.3 (2)	C50—C51—C52—C45	−178.0 (2)
C23—Dy—C21—C25	−77.38 (17)	C44—C51—C52—C53	−176.26 (19)
C26—Dy—C21—C25	177.26 (15)	C50—C51—C52—C53	1.1 (2)
C24—Dy—C21—C25	−37.39 (16)	C47—C48—C53—C52	0.7 (3)
C28—Dy—C21—C25	−125.63 (16)	C47—C48—C53—C49	−175.67 (19)
C27—Dy—C21—C25	−155.88 (16)	C45—C52—C53—C48	−0.5 (3)
C25—C21—C22—C23	−0.5 (3)	C51—C52—C53—C48	−179.71 (17)
Dy—C21—C22—C23	−68.61 (16)	C45—C52—C53—C49	176.67 (17)
C25—C21—C22—Dy	68.06 (16)	C51—C52—C53—C49	−2.6 (2)
O36—Dy—C22—C23	148.43 (15)	C38—C49—C53—C48	1.0 (3)
O31—Dy—C22—C23	41.3 (2)	C50—C49—C53—C48	179.65 (19)
C30—Dy—C22—C23	−98.43 (18)	C38—C49—C53—C52	−175.60 (17)
C29—Dy—C22—C23	−67.87 (17)	C50—C49—C53—C52	3.03 (19)
C26—Dy—C22—C23	−121.42 (16)	C70—C61—C62—C63	1.0 (3)
C24—Dy—C22—C23	36.93 (16)	C61—C62—C63—C64	−0.2 (3)
C21—Dy—C22—C23	113.9 (2)	C62—C63—C64—C71	−0.5 (3)
C25—Dy—C22—C23	77.11 (18)	C72—C65—C66—C67	−0.2 (3)
C28—Dy—C22—C23	−76.30 (17)	C65—C66—C67—C68	0.3 (3)
C27—Dy—C22—C23	−106.36 (17)	C66—C67—C68—C73	−0.4 (3)
O36—Dy—C22—C21	34.49 (17)	O31—C37—C69—C73	−2.4 (3)
O31—Dy—C22—C21	−72.63 (18)	C31—C37—C69—C73	−178.34 (16)
C30—Dy—C22—C21	147.64 (16)	O31—C37—C69—C70	−178.60 (17)
C29—Dy—C22—C21	178.19 (15)	C31—C37—C69—C70	5.4 (3)
C23—Dy—C22—C21	−113.9 (2)	C62—C61—C70—C71	−1.1 (3)
C26—Dy—C22—C21	124.64 (16)	C62—C61—C70—C69	178.18 (19)
C24—Dy—C22—C21	−77.01 (18)	C37—C69—C70—C61	−3.7 (3)
C25—Dy—C22—C21	−36.83 (16)	C73—C69—C70—C61	179.44 (19)
C28—Dy—C22—C21	169.76 (17)	C37—C69—C70—C71	175.59 (17)
C27—Dy—C22—C21	139.70 (17)	C73—C69—C70—C71	−1.23 (19)
C21—C22—C23—C24	0.5 (3)	C63—C64—C71—C70	0.4 (3)
Dy—C22—C23—C24	−68.50 (16)	C63—C64—C71—C72	−179.41 (19)
C21—C22—C23—Dy	68.96 (16)	C61—C70—C71—C64	0.4 (3)

O36—Dy—C23—C22	−43.6 (2)	C69—C70—C71—C64	−179.04 (17)
O31—Dy—C23—C22	−151.92 (15)	C61—C70—C71—C72	−179.74 (16)
C30—Dy—C23—C22	107.94 (17)	C69—C70—C71—C72	0.8 (2)
C29—Dy—C23—C22	121.08 (16)	C66—C65—C72—C73	0.2 (3)
C26—Dy—C23—C22	71.61 (17)	C66—C65—C72—C71	179.97 (19)
C24—Dy—C23—C22	−114.2 (2)	C64—C71—C72—C65	0.0 (3)
C21—Dy—C23—C22	−36.85 (16)	C70—C71—C72—C65	−179.81 (19)
C25—Dy—C23—C22	−76.70 (18)	C64—C71—C72—C73	179.78 (19)
C28—Dy—C23—C22	100.01 (17)	C70—C71—C72—C73	−0.1 (2)
C27—Dy—C23—C22	71.98 (17)	C67—C68—C73—C72	0.5 (3)
O36—Dy—C23—C24	70.57 (18)	C67—C68—C73—C69	−178.81 (19)
O31—Dy—C23—C24	−37.70 (17)	C65—C72—C73—C68	−0.4 (3)
C30—Dy—C23—C24	−137.84 (16)	C71—C72—C73—C68	179.83 (16)
C29—Dy—C23—C24	−124.70 (16)	C65—C72—C73—C69	179.05 (17)
C22—Dy—C23—C24	114.2 (2)	C71—C72—C73—C69	−0.7 (2)
C26—Dy—C23—C24	−174.17 (15)	C37—C69—C73—C68	3.7 (3)
C21—Dy—C23—C24	77.37 (18)	C70—C69—C73—C68	−179.46 (19)
C25—Dy—C23—C24	37.52 (16)	C37—C69—C73—C72	−175.67 (17)
C28—Dy—C23—C24	−145.77 (17)	C70—C69—C73—C72	1.20 (19)
C27—Dy—C23—C24	−173.80 (16)		

Fig. 1


C(27)
C(28)
C(22)
C(47)
C(46)
C(26)
C(48)
C(23)
C(21)
C(45)
C(29)
C(30)
C(53)
Dy
C(52)
O(36)
C(24)
C(25)
C(49)
C(51)
C(4)
C(44)
O(31)
C(38)
C(50)
C(5)
C(3)
O(2)
C(1)
C(12)
O(6)
C(35)
C(36)
K
C(37)
C(41)
O(3)
O(4)
C(9)
C(2)
O(1)
C(11)
C(34)
C(31)
C(68)
C(43)
C(6)
C(8)
O(5)
C(10)
C(67)
C(7)
C(33)
C(32)
C(69)
C(73)
C(42)
C(66)
C(72)
C(70)
O(8)
C(65)
C(71)
C(61)
C(20)
C(17)
C(64)
C(62)
C(19)
C(63)
C(18)