Supplementary Information for

Organolanthanoid-Halide Synthons – A New General Route to Monofunctionalized Lanthanoid(II) Compounds?

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General Considerations

All manipulations were carried out under N_2 atmosphere using standard Schlenk, vacuum line, and drybox techniques. Solvents were stored over Na/K alloy and distilled prior to use. 3,5-Diphenylpyrazole[i] (HPh_2pz) was prepared according to a literature procedure. All other reagents were purchased from commercial sources. Elemental Analyses (C, H, N) were performed by the Campbell Microanalytical Laboratories, University of Otago, New Zealand, on samples sealed under argon. Metal analyses were performed by EDTA titrations with Xylenol orange indicator, following acid digestion and buffering with hexamine.[ii] IR spectra are for Nujol mulls on NaCl plates using a *Perkin-Elmer 1600 FTIR* instrument. NMR spectra were obtained using a *Bruker DPX* 300 MHz spectrometer. ^{171}Yb-NMR spectra are referenced to 0.15 M $[Yb(C_5Me_5)_2(THF)]$ in thf/10 % C_6D_6. GC/MS experiments were performed on samples hydrolyzed with H_2O/EtOH (1:2) with a *Hewlett Packard 6890 Plus GC* with an *Agilent 5973N* detector.

X-ray Crystallography

Crystals of **1** and **2** were obtained from thf. Crystals of **3** from dme/*n*-hexane. A suitable crystal was covered in viscous mineral oil and mounted onto a glass fiber. The crystal was transferred directly to a cold (123 K) N_2 stream of a Bruker X8 Apex II CCD diffractometer. The structures were solved using conventional methods and refined with anisotropic thermal parameter forms for the non-hydrogen atoms by full-matrix least square on all F^2.data using SHELX97.[iii] Hydrogen atoms were included in calculated positions. The coordinating thf molecules in **1** and **2** were modelled as disordered (with C10A/B and C13A/B disordered over two positions, C16

disordered with half occupancy over a symmetry site). In the structure of **3** two of the total 16 phenyl ligands in the asymmetric unit were modelled as disordered over two positions and were refined using an idealized hexagonal geometry (groups consisting of C55, C56A/B to C60A/B and C121 to 126, C158 to 163 respectively). Two dme molecules around Yb4 show high thermal parameters indicating disorder (C82 and C87) which could not be resolved. In addition two dme molecules in the lattice of **3** were found. One of the molecules was treated as isotropic and refined as disordered over two positions with half occupancy (C145 to C150, O25 to O27). The second (C151 to 154, O29 and O30) was refined giving approximate atomic positions although residual electron density indicates additional disorder (we avoided use of the program SQUEEZE). All efforts to obtain improved structural data for **3** failed, partly due to quick decomposition of the compound upon selection and mounting of the crystals.

Table 1. Crystallographic details of **1**-**3**.

	1	**2**	2 (**3**·dme)
formula	C_{31} H_{43} Eu I N_2 O_4	C_{31} H_{43} Yb I N_2 O_4	C_{152} H_{220} O_{28} Yb_6
formula weight	786.53 mol	807.61	1766.76
space group	*Pmn*21	*Pmn*21	*P*-1
a [Å]	17.7513(3)	17.6761(8)	20.1461(7)
b [Å]	8.7645(2)	8.7327(4)	20.3068(6)
c [Å]	10.3139(2)	10.1877(5)	22.5761(12)
α [°]	90	90	110.121(2)
β [°]	90	90	103.298(2)
γ [°]	90	90	106.657(2)
V [Å^3]	1604.65(6)	1572.57(13)	7734.1(5)
Z	2	2	2
$\rho_{calc.}$ [g/cm^3]	1.628	1.316	1.517

radiation	MoKα (λ = 0.71073 Å)	MoKα (λ = 0.71073 Å)	MoKα (λ = 0.71073 Å)
μ [mm^{-1}]	2.952	3.991	3.656
T [K]	123(1)	123(1)	123(1)
abs. correction	Multi-scan	Multi-scan	Multi-scan
reflections; collected	13764	13478	54801
reflections; unique	3616 (R_{int} = 0.0204)	3722 (R_{int} = 0.0492)	27110 (R_{int} = 0.0578)
reflections; observed	3573	3515	27110
data, parameters	3616, 212	3722, 213	17319, 1756
*R*1	0.0136	0.0246	0.0485
*wR*2	0.0319	0.0489	0.0972
GOF	1.060	1.002	0.992

Experimental Supplement

Crystallization attempts on "PhYbI(thf)$_n$":

Yb metal filings (433 mg, 2.5 mmol) were suspended in thf (15 mL) and at -78 °C PhI (408 mg, 2 mmol) was added. The mixture was sonicated for 10 sec. developing a red colour. The mixture was stirred for 3 h at -50 °C and subsequently filtered through a glass frit. The resulting dark red solution was topped with ~ 7 mL of *n*-hexane and cooled to -25 °C. Overnight crystals of $[YbI_2(thf)_4]^{iv}$ and $[YbPh_3(thf)_3]^{v}$ had formed and were identified by determination of the unit cell by single crystal X-ray diffraction studies.

Hydrolysis of "PhYbI(thf)$_n$":

To a solution of "PhYbI(thf)$_n$" (obtained from Yb and PhI in thf; 3 h at -50° C as described above) a 1:2 mixture of water/EtOH was added at -50° C and slowly warmed to room

temperature. Following a GC/MS analysis the following compounds were identified: Biphenyl: *m/z* = 154 (M^+), 153 (M^+ - H), 77 (M^+ - C_6H_5), 76 (M^+ - C_6H_6); Phenyltetrahydrofuran: *m/z* = 148 (M^+), 147 (M^+ - H), 106 (M^+ - $(CH_2)_3$), 105 (M^+ - $(CH_2)_3$ –H).

Hydrolysis of "$PhYbI(dme)_n$":
To a solution of "$PhYbI(dme)_n$" (obtained from Yb and PhI in dme; 3 h at -78° C as described for the synthesis of **3**) a 1:2 mixture of water/EtOH was added at -50° C and slowly warmed to room temperature. Following a GC/MS analysis the following compounds were identified: Biphenyl: *m/z* = 154 (M^+), 153 (M^+ - H), 77 (M^+ - C_6H_5), 76 (M^+ - C_6H_6); Terphenyl: *m/z* = 230 (M^+); Triphenylbenzene: *m/z* = 306 (M^+).

Hydrolysis of crude $[Yb(Ph_2pz)I(thf)_4]$ (**2**):
To the mother liquor obtained after isolation of **2** a 1:2 mixture of water/EtOH was added at r.t.. Following a GC/MS analysis biphenyl was identified: Biphenyl: *m/z* = 154 (M^+), 153 (M^+ - H), 77 (M^+ - C_6H_5), 76 (M^+ - C_6H_6).

Structural Tables

Table 2: Bond lengths [Å] and angles [°] for **1**.

Eu(1)-N(1)	2.5353(17)	C(14)-C(13A)	1.475(6)
Eu(1)-N(1)#1	2.5353(17)	C(14)-C(14)#1	1.508(5)
Eu(1)-O(3)	2.558(2)	C(14)-C(13B)	1.515(7)
Eu(1)-O(1)#1	2.5770(14)	C(15)-C(16)	1.560(6)
Eu(1)-O(1)	2.5770(14)	C(15)-C(16)#1	1.560(6)
Eu(1)-O(2)	2.616(2)	C(16)-C(17)	1.470(6)
Eu(1)-I(1)	3.1983(2)	C(17)-C(16)#1	1.470(6)
O(1)-C(9)	1.438(3)	C(17)-C(18)	1.506(5)
O(1)-C(12)	1.438(3)		
N(1)-C(1)	1.348(3)	N(1)-Eu(1)-N(1)#1	31.58(8)
N(1)-N(1)#1	1.380(3)	N(1)-Eu(1)-O(3)	82.52(6)
C(1)-C(2)	1.393(3)	N(1)#1-Eu(1)-O(3)	82.52(6)
C(1)-C(3)	1.470(3)	N(1)-Eu(1)-O(1)#1	116.76(5)
O(2)-C(13B)#1	1.429(6)	N(1)#1-Eu(1)-O(1)#1	85.30(5)
O(2)-C(13B)	1.429(6)	O(3)-Eu(1)-O(1)#1	86.64(4)
O(2)-C(13A)#1	1.440(6)	N(1)-Eu(1)-O(1)	85.30(5)
O(2)-C(13A)	1.440(6)	N(1)#1-Eu(1)-O(1)	116.76(5)
C(2)-C(1)#1	1.393(3)	O(3)-Eu(1)-O(1)	86.64(4)
O(3)-C(15)	1.447(4)	O(1)#1-Eu(1)-O(1)	155.81(7)
O(3)-C(18)	1.450(4)	N(1)-Eu(1)-O(2)	156.27(6)
C(3)-C(8)	1.390(4)	N(1)#1-Eu(1)-O(2)	156.27(6)
C(3)-C(4)	1.398(3)	O(3)-Eu(1)-O(2)	79.83(7)
C(4)-C(5)	1.389(3)	O(1)#1-Eu(1)-O(2)	77.97(3)
C(5)-C(6)	1.385(4)	O(1)-Eu(1)-O(2)	77.97(3)
C(6)-C(7)	1.373(3)	N(1)-Eu(1)-I(1)	108.60(4)
C(7)-C(8)	1.393(3)	N(1)#1-Eu(1)-I(1)	108.60(4)
C(9)-C(10B)	1.446(7)	O(3)-Eu(1)-I(1)	168.42(5)
C(9)-C(10A)	1.504(8)	O(1)#1-Eu(1)-I(1)	90.98(3)
C(11)-C(10A)	1.419(8)	O(1)-Eu(1)-I(1)	90.98(3)
C(11)-C(12)	1.503(4)	O(2)-Eu(1)-I(1)	88.58(5)
C(11)-C(10B)	1.573(8)	C(9)-O(1)-C(12)	109.31(18)

C(9)-O(1)-Eu(1)	131.06(14)
C(12)-O(1)-Eu(1)	119.58(14)
C(1)-N(1)-N(1)#1	107.75(12)
C(1)-N(1)-Eu(1)	175.44(15)
N(1)#1-N(1)-Eu(1)	74.21(4)
N(1)-C(1)-C(2)	110.00(19)
N(1)-C(1)-C(3)	121.44(19)
C(2)-C(1)-C(3)	128.6(2)
C(13B)#1-O(2)-C(13B)	95.7(5)
C(13B)#1-O(2)-C(13A)#1	33.8(3)
C(13B)-O(2)-C(13A)#1	109.0(3)
C(13B)#1-O(2)-C(13A)	109.0(3)
C(13B)-O(2)-C(13A)	33.8(3)
C(13A)#1-O(2)-C(13A)	102.5(5)
C(13B)#1-O(2)-Eu(1)	130.2(2)
C(13B)-O(2)-Eu(1)	130.2(2)
C(13A)#1-O(2)-Eu(1)	119.8(2)
C(13A)-O(2)-Eu(1)	119.8(2)
C(1)#1-C(2)-C(1)	104.5(3)
C(15)-O(3)-C(18)	109.1(3)
C(15)-O(3)-Eu(1)	126.82(19)
C(18)-O(3)-Eu(1)	124.0(2)
C(8)-C(3)-C(4)	118.04(19)
C(8)-C(3)-C(1)	120.9(2)
C(4)-C(3)-C(1)	121.08(19)
C(5)-C(4)-C(3)	120.8(2)
C(6)-C(5)-C(4)	120.1(2)
C(7)-C(6)-C(5)	119.9(2)
C(6)-C(7)-C(8)	120.1(2)
C(3)-C(8)-C(7)	121.1(2)
O(1)-C(9)-C(10B)	109.3(3)
O(1)-C(9)-C(10A)	102.9(4)
C(10B)-C(9)-C(10A)	33.7(3)
C(10A)-C(11)-C(12)	102.0(4)
C(10A)-C(11)-C(10B)	32.8(3)
C(12)-C(11)-C(10B)	105.5(3)
O(1)-C(12)-C(11)	106.9(2)
C(13A)-C(14)-C(14)#1	104.5(2)
C(13A)-C(14)-C(13B)	32.4(3)
C(14)#1-C(14)-C(13B)	101.6(3)
O(3)-C(15)-C(16)	102.6(3)
O(3)-C(15)-C(16)#1	102.6(3)
C(16)-C(15)-C(16)#1	47.9(5)
C(17)-C(16)-C(15)	100.5(3)
C(16)#1-C(17)-C(16)	51.1(5)
C(16)#1-C(17)-C(18)	104.3(3)
C(16)-C(17)-C(18)	104.3(3)
O(3)-C(18)-C(17)	105.6(3)
C(9)-C(10B)-C(11)	102.7(4)
C(11)-C(10A)-C(9)	107.5(4)
O(2)-C(13B)-C(14)	105.6(4)
O(2)-C(13A)-C(14)	107.2(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,z

Table 3: Bond lengths [Å] and angles [°] for **2**.

Yb(1)-N(1)	2.433(3)	C(14)-C(14)#1	1.520(11)
Yb(1)-N(1)#1	2.433(3)	C(15)-C(16)#1	1.551(11)
Yb(1)-O(3)	2.441(4)	C(15)-C(16)	1.551(11)
Yb(1)-O(1)	2.473(3)	C(16)-C(17)	1.443(11)
Yb(1)-O(1)#1	2.473(3)	C(17)-C(16)#1	1.443(11)
Yb(1)-O(2)	2.518(4)	C(17)-C(18)	1.501(9)
Yb(1)-I(1)	3.0966(4)		
O(1)-C(12)	1.440(5)	N(1)#1-Yb(1)-N(1)	33.02(15)
O(1)-C(9)	1.448(5)	N(1)#1-Yb(1)-O(3)	84.61(11)
N(1)-C(1)	1.361(5)	N(1)-Yb(1)-O(3)	84.61(11)
N(1)-N(1)#1	1.383(6)	N(1)#1-Yb(1)-O(1)	117.63(10)
C(1)-C(2)	1.392(5)	N(1)-Yb(1)-O(1)	84.71(10)
C(1)-C(3)	1.458(6)	O(3)-Yb(1)-O(1)	86.91(7)
O(2)-C(13B)	1.439(11)	N(1)#1-Yb(1)-O(1)#1	84.71(10)
O(2)-C(13B)#1	1.439(11)	N(1)-Yb(1)-O(1)#1	117.63(10)
O(2)-C(13A)	1.468(10)	O(3)-Yb(1)-O(1)#1	86.91(7)
O(2)-C(13A)#1	1.468(10)	O(1)-Yb(1)-O(1)#1	156.09(13)
C(2)-C(1)#1	1.392(5)	N(1)#1-Yb(1)-O(2)	157.47(10)
O(3)-C(15)	1.457(7)	N(1)-Yb(1)-O(2)	157.47(10)
O(3)-C(18)	1.464(7)	O(3)-Yb(1)-O(2)	80.07(13)
C(3)-C(4)	1.398(6)	O(1)-Yb(1)-O(2)	78.09(6)
C(3)-C(8)	1.404(7)	O(1)#1-Yb(1)-O(2)	78.09(6)
C(4)-C(5)	1.392(7)	N(1)#1-Yb(1)-I(1)	106.42(7)
C(5)-C(6)	1.392(7)	N(1)-Yb(1)-I(1)	106.42(7)
C(6)-C(7)	1.378(6)	O(3)-Yb(1)-I(1)	168.48(9)
C(7)-C(8)	1.381(6)	O(1)-Yb(1)-I(1)	90.74(6)
C(9)-C(10B)	1.427(16)	O(1)#1-Yb(1)-I(1)	90.74(6)
C(9)-C(10A)	1.521(13)	O(2)-Yb(1)-I(1)	88.40(9)
C(10A)-C(11)	1.396(14)	C(12)-O(1)-C(9)	109.0(4)
C(11)-C(12)	1.504(7)	C(12)-O(1)-Yb(1)	120.0(3)
C(11)-C(10B)	1.581(15)	C(9)-O(1)-Yb(1)	130.6(3)
C(14)-C(13A)	1.467(11)	C(1)-N(1)-N(1)#1	107.7(2)
C(14)-C(13B)	1.518(12)	C(1)-N(1)-Yb(1)	174.5(3)

N(1)#1-N(1)-Yb(1)	73.49(8)
N(1)-C(1)-C(2)	109.8(4)
N(1)-C(1)-C(3)	121.5(4)
C(2)-C(1)-C(3)	128.8(4)
C(13B)-O(2)-C(13B)#1	96.3(9)
C(13B)-O(2)-C(13A)	33.8(5)
C(13B)#1-O(2)-C(13A)	109.1(5)
C(13B)-O(2)-C(13A)#1	109.1(5)
C(13B)#1-O(2)-C(13A)#1	33.8(5)
C(13A)-O(2)-C(13A)#1	102.0(9)
C(13B)-O(2)-Yb(1)	130.0(5)
C(13B)#1-O(2)-Yb(1)	130.0(5)
C(13A)-O(2)-Yb(1)	119.9(4)
C(13A)#1-O(2)-Yb(1)	119.9(4)
C(1)-C(2)-C(1)#1	105.1(5)
C(15)-O(3)-C(18)	108.5(4)
C(15)-O(3)-Yb(1)	127.6(3)
C(18)-O(3)-Yb(1)	123.9(4)
C(4)-C(3)-C(8)	117.5(4)
C(4)-C(3)-C(1)	121.9(4)
C(8)-C(3)-C(1)	120.6(4)
C(5)-C(4)-C(3)	121.3(4)
C(4)-C(5)-C(6)	119.8(4)
C(7)-C(6)-C(5)	119.6(4)
C(6)-C(7)-C(8)	120.7(4)
C(7)-C(8)-C(3)	121.1(5)
C(10B)-C(9)-O(1)	110.9(6)
C(10B)-C(9)-C(10A)	33.0(7)
O(1)-C(9)-C(10A)	101.8(6)
C(11)-C(10A)-C(9)	107.5(7)
C(10A)-C(11)-C(12)	103.0(6)
C(10A)-C(11)-C(10B)	32.1(6)
C(12)-C(11)-C(10B)	105.7(6)
C(12)-C(11)-H(11B)	110.6
O(1)-C(12)-C(11)	107.0(4)
C(13A)-C(14)-C(13B)	32.9(5)
C(13A)-C(14)-C(14)#1	105.1(4)
C(13B)-C(14)-C(14)#1	101.9(5)
O(2)-C(13A)-C(14)	106.6(7)
O(3)-C(15)-C(16)#1	102.9(5)
O(3)-C(15)-C(16)	102.9(5)
C(16)#1-C(15)-C(16)	44.6(9)
C(17)-C(16)-C(15)	101.9(6)
C(16)-C(17)-C(16)#1	48.1(9)
C(16)-C(17)-C(18)	105.4(5)
C(16)#1-C(17)-C(18)	105.4(5)
O(3)-C(18)-C(17)	105.4(5)
C(9)-C(10B)-C(11)	102.8(10)
O(2)-C(13B)-C(14)	105.4(8)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,z

Table 2: Bond lengths [Å] and angles [°] for **3**.

Yb(1)-O(1)	2.547(6)	Yb(5)-C(105)	2.481(9)
Yb(1)-O(2)	2.462(5)	Yb(5)-C(111)	2.442(8)
Yb(1)-O(3)	2.511(5)	Yb(6)-O(23)	2.469(5)
Yb(1)-O(4)	2.524(6)	Yb(6)-O(24)	2.469(6)
Yb(1)-O(5)	2.550(6)	Yb(6)-C(121)	2.486(10)
Yb(1)-O(6)	2.509(5)	Yb(6)-C(127)	2.462(9)
Yb(1)-O(7)	2.500(5)	Yb(6)-C(133)	2.419(10)
Yb(1)-O(8)	2.506(6)	Yb(6)-C(139)	2.466(10)
Yb(2)-O(9)	2.441(5)	Yb(6)-C(158)	2.534(11)
Yb(2)-O(10)	2.481(6)	O(1)-C(2)	1.413(10)
Yb(2)-C(21)	2.458(9)	O(1)-C(1)	1.427(10)
Yb(2)-C(27)	2.427(9)	O(2)-C(4)	1.394(10)
Yb(2)-C(33)	2.432(8)	O(2)-C(3)	1.397(10)
Yb(2)-C(39)	2.475(9)	O(3)-C(6)	1.412(9)
Yb(3)-O(11)	2.461(5)	O(3)-C(5)	1.438(10)
Yb(3)-O(12)	2.423(6)	O(4)-C(7)	1.428(10)
Yb(3)-C(49)	2.456(9)	O(4)-C(8)	1.430(10)
Yb(3)-C(55)	2.430(6)	O(5)-C(10)	1.438(9)
Yb(3)-C(61)	2.424(8)	O(5)-C(9)	1.446(10)
Yb(3)-C(67)	2.466(8)	O(6)-C(11)	1.434(10)
Yb(4)-O(13)	2.477(7)	O(6)-C(12)	1.437(10)
Yb(4)-O(14)	2.483(6)	O(7)-C(13)	1.417(10)
Yb(4)-O(15)	2.515(7)	O(7)-C(14)	1.452(10)
Yb(4)-O(16)	2.424(6)	O(8)-C(16)	1.402(10)
Yb(4)-O(17)	2.462(7)	O(8)-C(15)	1.441(10)
Yb(4)-O(18)	2.526(8)	O(9)-C(17)	1.430(10)
Yb(4)-O(19)	2.496(7)	O(9)-C(18)	1.436(10)
Yb(4)-O(20)	2.483(7)	O(10)-C(20)	1.423(10)
Yb(5)-O(21)	2.453(6)	O(10)-C(19)	1.440(9)
Yb(5)-O(22)	2.439(5)	O(11)-C(45)	1.415(10)
Yb(5)-C(93)	2.459(9)	O(11)-C(46)	1.449(11)
Yb(5)-C(99)	2.409(10)	O(12)-C(48)	1.423(10)

O(12)-C(47)	1.426(9)	C(2)-C(3)	1.447(13)
O(13)-C(73)	1.437(11)	C(6)-C(7)	1.468(12)
O(13)-C(74)	1.509(12)	C(10)-C(11)	1.478(13)
O(14)-C(75)	1.408(13)	C(14)-C(15)	1.474(12)
O(14)-C(76)	1.430(11)	C(18)-C(19)	1.477(12)
O(15)-C(77)	1.370(15)	C(21)-C(22)	1.390(11)
O(15)-C(78)	1.445(12)	C(21)-C(26)	1.419(12)
O(16)-C(80)	1.362(12)	C(22)-C(23)	1.409(13)
O(16)-C(79)	1.417(13)	C(23)-C(24)	1.376(13)
O(17)-C(81)	1.384(15)	C(24)-C(25)	1.390(13)
O(17)-C(82)	1.469(17)	C(25)-C(26)	1.397(13)
O(18)-C(84)	1.386(16)	C(27)-C(32)	1.405(12)
O(18)-C(83)	1.413(15)	C(27)-C(28)	1.422(12)
O(19)-C(85)	1.397(11)	C(28)-C(29)	1.395(12)
O(19)-C(86)	1.406(13)	C(29)-C(30)	1.368(12)
O(20)-C(87)	1.402(15)	C(30)-C(31)	1.373(12)
O(20)-C(88)	1.418(11)	C(31)-C(32)	1.394(12)
O(21)-C(90)	1.439(10)	C(33)-C(34)	1.392(11)
O(21)-C(89)	1.449(10)	C(33)-C(38)	1.421(13)
O(22)-C(91)	1.392(11)	C(34)-C(35)	1.371(11)
O(22)-C(92)	1.438(10)	C(35)-C(36)	1.398(12)
O(23)-C(118)	1.418(11)	C(36)-C(37)	1.375(11)
O(23)-C(117)	1.462(10)	C(37)-C(38)	1.364(11)
O(24)-C(119)	1.439(10)	C(39)-C(44)	1.388(12)
O(24)-C(120)	1.445(10)	C(39)-C(40)	1.401(12)
O(25)-C(146)	1.292(15)	C(40)-C(41)	1.401(12)
O(25)-C(145)	1.34(3)	C(41)-C(42)	1.348(14)
O(26)-C(147)	1.39(3)	C(42)-C(43)	1.363(13)
O(26)-C(148)	1.394(17)	C(43)-C(44)	1.400(12)
O(27)-C(149)	1.45(3)	C(46)-C(47)	1.473(12)
O(28)-C(150)	1.38(2)	C(49)-C(54)	1.400(12)
O(29)-C(152)	1.27(3)	C(49)-C(50)	1.416(12)
O(29)-C(151)	1.28(3)	C(50)-C(51)	1.395(12)
O(30)-C(153)	1.35(3)	C(51)-C(52)	1.333(13)
O(30)-C(154)	1.51(4)	C(52)-C(53)	1.378(14)

C(53)-C(54)	1.375(12)	C(97)-C(98)	1.393(13)
C(55)-C(60A)	1.377(8)	C(99)-C(104)	1.381(13)
C(55)-C(56B)	1.399(8)	C(99)-C(100)	1.394(13)
C(55)-C(56A)	1.403(8)	C(100)-C(101)	1.385(13)
C(55)-C(60B)	1.407(8)	C(101)-C(102)	1.358(15)
C(56A)-C(57A)	1.395(8)	C(102)-C(103)	1.365(15)
C(56B)-C(57B)	1.389(8)	C(103)-C(104)	1.409(14)
C(57A)-C(58A)	1.390(8)	C(105)-C(106)	1.385(12)
C(57B)-C(58B)	1.387(8)	C(105)-C(110)	1.391(12)
C(58A)-C(59A)	1.392(8)	C(106)-C(107)	1.353(13)
C(58B)-C(59B)	1.393(8)	C(107)-C(108)	1.387(14)
C(59A)-C(60A)	1.393(8)	C(108)-C(109)	1.362(13)
C(59B)-C(60B)	1.389(8)	C(109)-C(110)	1.372(12)
C(61)-C(66)	1.379(12)	C(111)-C(116)	1.365(12)
C(61)-C(62)	1.397(11)	C(111)-C(112)	1.407(12)
C(62)-C(63)	1.401(13)	C(112)-C(113)	1.386(11)
C(63)-C(64)	1.364(14)	C(113)-C(114)	1.378(14)
C(64)-C(65)	1.354(13)	C(114)-C(115)	1.351(15)
C(65)-C(66)	1.387(12)	C(115)-C(116)	1.384(12)
C(67)-C(68)	1.379(11)	C(118)-C(119)	1.483(13)
C(67)-C(72)	1.417(12)	C(121)-C(122)	1.394(8)
C(68)-C(69)	1.381(12)	C(121)-C(126)	1.400(8)
C(69)-C(70)	1.387(12)	C(122)-C(123)	1.384(8)
C(70)-C(71)	1.379(12)	C(123)-C(124)	1.395(8)
C(71)-C(72)	1.394(13)	C(124)-C(125)	1.385(8)
C(74)-C(75)	1.409(16)	C(125)-C(126)	1.392(8)
C(78)-C(79)	1.515(16)	C(127)-C(132)	1.392(13)
C(82)-C(83)	1.40(2)	C(127)-C(128)	1.396(14)
C(86)-C(87)	1.450(16)	C(128)-C(129)	1.380(14)
C(90)-C(91)	1.468(13)	C(129)-C(130)	1.324(19)
C(93)-C(98)	1.403(12)	C(130)-C(131)	1.390(19)
C(93)-C(94)	1.425(11)	C(131)-C(132)	1.401(13)
C(94)-C(95)	1.374(12)	C(133)-C(134)	1.391(13)
C(95)-C(96)	1.371(12)	C(133)-C(138)	1.412(12)
C(96)-C(97)	1.383(12)	C(134)-C(135)	1.395(13)

C(135)-C(136)	1.360(13)	O(8)-Yb(1)-O(1)	109.00(19)
C(136)-C(137)	1.357(13)	O(6)-Yb(1)-O(1)	135.7(2)
C(137)-C(138)	1.405(13)	O(3)-Yb(1)-O(1)	89.39(19)
C(139)-C(144)	1.395(14)	O(4)-Yb(1)-O(1)	71.6(2)
C(139)-C(140)	1.397(14)	O(2)-Yb(1)-O(5)	133.4(2)
C(140)-C(141)	1.405(17)	O(7)-Yb(1)-O(5)	87.76(18)
C(141)-C(142)	1.39(2)	O(8)-Yb(1)-O(5)	72.13(19)
C(142)-C(143)	1.34(2)	O(6)-Yb(1)-O(5)	64.78(18)
C(143)-C(144)	1.367(16)	O(3)-Yb(1)-O(5)	76.85(19)
C(146)-C(147)	1.50(3)	O(4)-Yb(1)-O(5)	115.87(18)
C(158)-C(163)	1.398(8)	O(1)-Yb(1)-O(5)	158.5(2)
C(158)-C(159)	1.399(8)	C(27)-Yb(2)-C(33)	106.8(3)
C(159)-C(160)	1.388(8)	C(27)-Yb(2)-O(9)	95.4(2)
C(160)-C(161)	1.391(8)	C(33)-Yb(2)-O(9)	157.2(3)
C(161)-C(162)	1.386(8)	C(27)-Yb(2)-C(21)	90.9(3)
C(162)-C(163)	1.390(8)	C(33)-Yb(2)-C(21)	99.7(3)
C(152)-C(153)	1.48(3)	O(9)-Yb(2)-C(21)	85.2(2)
		C(27)-Yb(2)-C(39)	95.6(3)
O(2)-Yb(1)-O(7)	105.50(18)	C(33)-Yb(2)-C(39)	90.8(3)
O(2)-Yb(1)-O(8)	73.9(2)	O(9)-Yb(2)-C(39)	81.3(2)
O(7)-Yb(1)-O(8)	64.84(18)	C(21)-Yb(2)-C(39)	165.5(3)
O(2)-Yb(1)-O(6)	84.69(19)	C(27)-Yb(2)-O(10)	161.3(2)
O(7)-Yb(1)-O(6)	148.18(19)	C(33)-Yb(2)-O(10)	91.5(2)
O(8)-Yb(1)-O(6)	90.37(18)	O(9)-Yb(2)-O(10)	66.94(18)
O(2)-Yb(1)-O(3)	147.7(2)	C(21)-Yb(2)-O(10)	82.1(3)
O(7)-Yb(1)-O(3)	83.38(17)	C(39)-Yb(2)-O(10)	87.8(2)
O(8)-Yb(1)-O(3)	135.73(19)	O(12)-Yb(3)-C(61)	93.7(2)
O(6)-Yb(1)-O(3)	104.18(17)	O(12)-Yb(3)-C(55)	162.8(2)
O(2)-Yb(1)-O(4)	87.02(19)	C(61)-Yb(3)-C(55)	103.5(3)
O(7)-Yb(1)-O(4)	133.55(19)	O(12)-Yb(3)-C(49)	82.5(2)
O(8)-Yb(1)-O(4)	157.57(19)	C(61)-Yb(3)-C(49)	96.6(3)
O(6)-Yb(1)-O(4)	75.94(19)	C(55)-Yb(3)-C(49)	96.6(3)
O(3)-Yb(1)-O(4)	65.93(18)	O(12)-Yb(3)-O(11)	68.12(19)
O(2)-Yb(1)-O(1)	64.5(2)	C(61)-Yb(3)-O(11)	161.7(2)
O(7)-Yb(1)-O(1)	74.19(19)	C(55)-Yb(3)-O(11)	94.8(2)

C(49)-Yb(3)-O(11)	80.4(2)	C(99)-Yb(5)-C(111)	108.3(3)
O(12)-Yb(3)-C(67)	79.6(2)	O(22)-Yb(5)-C(111)	156.5(3)
C(61)-Yb(3)-C(67)	94.7(3)	C(99)-Yb(5)-O(21)	160.5(2)
C(55)-Yb(3)-C(67)	97.5(3)	O(22)-Yb(5)-O(21)	66.78(19)
C(49)-Yb(3)-C(67)	159.4(3)	C(111)-Yb(5)-O(21)	90.3(2)
O(11)-Yb(3)-C(67)	83.5(2)	C(99)-Yb(5)-C(93)	89.9(3)
O(16)-Yb(4)-O(17)	78.6(3)	O(22)-Yb(5)-C(93)	85.1(2)
O(16)-Yb(4)-O(13)	120.2(3)	C(111)-Yb(5)-C(93)	96.9(3)
O(17)-Yb(4)-O(13)	127.6(3)	O(21)-Yb(5)-C(93)	81.6(3)
O(16)-Yb(4)-O(14)	76.0(2)	C(99)-Yb(5)-C(105)	95.0(3)
O(17)-Yb(4)-O(14)	154.5(3)	O(22)-Yb(5)-C(105)	79.5(2)
O(13)-Yb(4)-O(14)	65.4(2)	C(111)-Yb(5)-C(105)	95.7(3)
O(16)-Yb(4)-O(20)	155.1(2)	O(21)-Yb(5)-C(105)	89.0(2)
O(17)-Yb(4)-O(20)	76.6(3)	C(93)-Yb(5)-C(105)	164.2(3)
O(13)-Yb(4)-O(20)	77.8(3)	C(133)-Yb(6)-C(127)	110.6(3)
O(14)-Yb(4)-O(20)	128.9(2)	C(133)-Yb(6)-C(139)	92.8(3)
O(16)-Yb(4)-O(19)	128.2(2)	C(127)-Yb(6)-C(139)	96.4(3)
O(17)-Yb(4)-O(19)	123.0(3)	C(133)-Yb(6)-O(23)	88.1(2)
O(13)-Yb(4)-O(19)	85.3(3)	C(127)-Yb(6)-O(23)	160.5(3)
O(14)-Yb(4)-O(19)	76.3(2)	C(139)-Yb(6)-O(23)	87.8(3)
O(20)-Yb(4)-O(19)	66.1(2)	C(133)-Yb(6)-O(24)	153.8(2)
O(16)-Yb(4)-O(15)	64.3(3)	C(127)-Yb(6)-O(24)	94.8(3)
O(17)-Yb(4)-O(15)	77.0(3)	C(139)-Yb(6)-O(24)	77.8(3)
O(13)-Yb(4)-O(15)	154.9(3)	O(23)-Yb(6)-O(24)	67.4(2)
O(14)-Yb(4)-O(15)	94.3(3)	C(133)-Yb(6)-C(121)	107.3(4)
O(20)-Yb(4)-O(15)	107.4(3)	C(127)-Yb(6)-C(121)	87.4(5)
O(19)-Yb(4)-O(15)	75.2(3)	C(139)-Yb(6)-C(121)	156.8(5)
O(16)-Yb(4)-O(18)	78.6(3)	O(23)-Yb(6)-C(121)	81.6(5)
O(17)-Yb(4)-O(18)	64.2(3)	O(24)-Yb(6)-C(121)	79.1(4)
O(13)-Yb(4)-O(18)	72.2(3)	C(133)-Yb(6)-C(158)	98.0(4)
O(14)-Yb(4)-O(18)	107.5(3)	C(127)-Yb(6)-C(158)	94.1(5)
O(20)-Yb(4)-O(18)	92.6(3)	C(139)-Yb(6)-C(158)	161.3(5)
O(19)-Yb(4)-O(18)	152.1(3)	O(23)-Yb(6)-C(158)	77.3(5)
O(15)-Yb(4)-O(18)	130.7(3)	O(24)-Yb(6)-C(158)	85.9(4)
C(99)-Yb(5)-O(22)	95.1(2)	C(121)-Yb(6)-C(158)	9.9(4)

C(2)-O(1)-C(1)	113.8(7)	C(47)-O(12)-Yb(3)	114.8(5)
C(2)-O(1)-Yb(1)	113.0(6)	C(73)-O(13)-C(74)	113.9(9)
C(1)-O(1)-Yb(1)	124.7(5)	C(73)-O(13)-Yb(4)	123.4(7)
C(4)-O(2)-C(3)	111.2(7)	C(74)-O(13)-Yb(4)	112.7(6)
C(4)-O(2)-Yb(1)	127.0(5)	C(75)-O(14)-C(76)	109.4(8)
C(3)-O(2)-Yb(1)	121.5(5)	C(75)-O(14)-Yb(4)	121.3(6)
C(6)-O(3)-C(5)	110.2(6)	C(76)-O(14)-Yb(4)	127.5(6)
C(6)-O(3)-Yb(1)	112.1(5)	C(77)-O(15)-C(78)	112.9(10)
C(5)-O(3)-Yb(1)	122.8(5)	C(77)-O(15)-Yb(4)	128.1(8)
C(7)-O(4)-C(8)	111.3(7)	C(78)-O(15)-Yb(4)	117.1(7)
C(7)-O(4)-Yb(1)	115.2(5)	C(80)-O(16)-C(79)	112.9(9)
C(8)-O(4)-Yb(1)	123.9(5)	C(80)-O(16)-Yb(4)	129.3(7)
C(10)-O(5)-C(9)	109.5(7)	C(79)-O(16)-Yb(4)	116.5(6)
C(10)-O(5)-Yb(1)	118.2(5)	C(81)-O(17)-C(82)	113.5(10)
C(9)-O(5)-Yb(1)	125.0(5)	C(81)-O(17)-Yb(4)	124.5(9)
C(11)-O(6)-C(12)	110.4(6)	C(82)-O(17)-Yb(4)	120.6(9)
C(11)-O(6)-Yb(1)	114.0(5)	C(84)-O(18)-C(83)	112.6(11)
C(12)-O(6)-Yb(1)	123.6(5)	C(84)-O(18)-Yb(4)	123.4(9)
C(13)-O(7)-C(14)	109.6(6)	C(83)-O(18)-Yb(4)	113.8(9)
C(13)-O(7)-Yb(1)	129.3(5)	C(85)-O(19)-C(86)	112.5(9)
C(14)-O(7)-Yb(1)	120.1(5)	C(85)-O(19)-Yb(4)	124.4(7)
C(16)-O(8)-C(15)	113.0(7)	C(86)-O(19)-Yb(4)	117.3(7)
C(16)-O(8)-Yb(1)	131.0(5)	C(87)-O(20)-C(88)	113.9(9)
C(15)-O(8)-Yb(1)	112.6(5)	C(87)-O(20)-Yb(4)	117.6(7)
C(17)-O(9)-C(18)	111.7(6)	C(88)-O(20)-Yb(4)	127.1(7)
C(17)-O(9)-Yb(2)	119.3(5)	C(90)-O(21)-C(89)	111.3(7)
C(18)-O(9)-Yb(2)	113.6(5)	C(90)-O(21)-Yb(5)	115.1(5)
C(20)-O(10)-C(19)	110.5(7)	C(89)-O(21)-Yb(5)	119.3(5)
C(20)-O(10)-Yb(2)	120.3(5)	C(91)-O(22)-C(92)	111.8(6)
C(19)-O(10)-Yb(2)	115.1(5)	C(91)-O(22)-Yb(5)	112.6(5)
C(45)-O(11)-C(46)	110.0(6)	C(92)-O(22)-Yb(5)	122.2(5)
C(45)-O(11)-Yb(3)	119.5(5)	C(118)-O(23)-C(117)	110.8(7)
C(46)-O(11)-Yb(3)	112.5(5)	C(118)-O(23)-Yb(6)	113.6(5)
C(48)-O(12)-C(47)	113.0(7)	C(117)-O(23)-Yb(6)	120.3(5)
C(48)-O(12)-Yb(3)	121.7(5)	C(119)-O(24)-C(120)	110.7(7)

C(119)-O(24)-Yb(6)	113.3(5)	C(35)-C(34)-C(33)	123.9(9)
C(120)-O(24)-Yb(6)	117.0(5)	C(34)-C(35)-C(36)	119.7(8)
C(146)-O(25)-C(145)	110.5(15)	C(37)-C(36)-C(35)	119.0(8)
C(147)-O(26)-C(148)	118.3(17)	C(38)-C(37)-C(36)	120.0(9)
C(152)-O(29)-C(151)	137(3)	C(37)-C(38)-C(33)	123.7(8)
C(153)-O(30)-C(154)	103(3)	C(44)-C(39)-C(40)	112.8(8)
O(1)-C(2)-C(3)	111.9(8)	C(44)-C(39)-Yb(2)	121.5(7)
O(2)-C(3)-C(2)	111.4(8)	C(40)-C(39)-Yb(2)	125.3(7)
O(3)-C(6)-C(7)	109.6(6)	C(39)-C(40)-C(41)	123.6(9)
O(4)-C(7)-C(6)	107.9(7)	C(42)-C(41)-C(40)	119.4(9)
O(5)-C(10)-C(11)	107.7(8)	C(41)-C(42)-C(43)	121.1(10)
O(6)-C(11)-C(10)	110.1(7)	C(42)-C(43)-C(44)	117.9(10)
O(7)-C(14)-C(15)	108.6(7)	C(39)-C(44)-C(43)	125.2(9)
O(8)-C(15)-C(14)	110.1(7)	O(11)-C(46)-C(47)	107.7(7)
O(9)-C(18)-C(19)	107.9(7)	O(12)-C(47)-C(46)	109.3(7)
O(10)-C(19)-C(18)	107.7(7)	C(54)-C(49)-C(50)	112.8(8)
C(22)-C(21)-C(26)	112.5(8)	C(54)-C(49)-Yb(3)	125.4(7)
C(22)-C(21)-Yb(2)	124.4(7)	C(50)-C(49)-Yb(3)	121.7(6)
C(26)-C(21)-Yb(2)	123.0(6)	C(51)-C(50)-C(49)	123.3(9)
C(21)-C(22)-C(23)	124.4(9)	C(52)-C(51)-C(50)	120.1(10)
C(24)-C(23)-C(22)	120.7(9)	C(51)-C(52)-C(53)	120.0(10)
C(23)-C(24)-C(25)	117.7(9)	C(54)-C(53)-C(52)	119.8(10)
C(24)-C(25)-C(26)	120.3(10)	C(53)-C(54)-C(49)	123.9(9)
C(25)-C(26)-C(21)	124.3(9)	C(60A)-C(55)-C(56B)	103.4(7)
C(32)-C(27)-C(28)	111.1(8)	C(60A)-C(55)-C(56A)	120.6(7)
C(32)-C(27)-Yb(2)	126.8(7)	C(56B)-C(55)-C(56A)	17.3(6)
C(28)-C(27)-Yb(2)	121.5(6)	C(60A)-C(55)-C(60B)	15.4(10)
C(29)-C(28)-C(27)	124.5(8)	C(56B)-C(55)-C(60B)	117.6(6)
C(30)-C(29)-C(28)	120.2(9)	C(56A)-C(55)-C(60B)	134.8(7)
C(29)-C(30)-C(31)	119.0(9)	C(60A)-C(55)-Yb(3)	123.1(6)
C(30)-C(31)-C(32)	119.4(8)	C(56B)-C(55)-Yb(3)	133.1(7)
C(31)-C(32)-C(27)	125.7(9)	C(56A)-C(55)-Yb(3)	116.2(6)
C(34)-C(33)-C(38)	113.7(7)	C(60B)-C(55)-Yb(3)	108.2(6)
C(34)-C(33)-Yb(2)	120.3(6)	C(57A)-C(56A)-C(55)	119.5(7)
C(38)-C(33)-Yb(2)	125.6(6)	C(57B)-C(56B)-C(55)	121.2(7)

C(58A)-C(57A)-C(56A)	119.4(7)	C(98)-C(93)-Yb(5)	121.2(6)
C(58B)-C(57B)-C(56B)	120.6(7)	C(94)-C(93)-Yb(5)	125.3(6)
C(57A)-C(58A)-C(59A)	120.8(7)	C(95)-C(94)-C(93)	124.1(8)
C(57B)-C(58B)-C(59B)	119.2(7)	C(96)-C(95)-C(94)	120.5(9)
C(58A)-C(59A)-C(60A)	119.5(7)	C(95)-C(96)-C(97)	118.3(9)
C(60B)-C(59B)-C(58B)	120.1(7)	C(96)-C(97)-C(98)	121.0(9)
C(55)-C(60A)-C(59A)	120.0(7)	C(97)-C(98)-C(93)	123.0(9)
C(59B)-C(60B)-C(55)	121.2(7)	C(104)-C(99)-C(100)	112.8(9)
C(66)-C(61)-C(62)	113.1(8)	C(104)-C(99)-Yb(5)	121.1(7)
C(66)-C(61)-Yb(3)	125.6(6)	C(100)-C(99)-Yb(5)	126.0(7)
C(62)-C(61)-Yb(3)	121.3(7)	C(101)-C(100)-C(99)	123.5(11)
C(61)-C(62)-C(63)	123.8(10)	C(102)-C(101)-C(100)	121.3(11)
C(64)-C(63)-C(62)	119.2(9)	C(101)-C(102)-C(103)	118.5(11)
C(65)-C(64)-C(63)	119.6(9)	C(102)-C(103)-C(104)	119.0(12)
C(64)-C(65)-C(66)	119.8(10)	C(99)-C(104)-C(103)	124.8(11)
C(61)-C(66)-C(65)	124.5(9)	C(106)-C(105)-C(110)	110.8(8)
C(68)-C(67)-C(72)	112.6(8)	C(106)-C(105)-Yb(5)	124.6(7)
C(68)-C(67)-Yb(3)	122.1(6)	C(110)-C(105)-Yb(5)	124.3(6)
C(72)-C(67)-Yb(3)	125.0(6)	C(107)-C(106)-C(105)	126.0(10)
C(67)-C(68)-C(69)	125.5(8)	C(106)-C(107)-C(108)	119.2(9)
C(68)-C(69)-C(70)	119.4(8)	C(109)-C(108)-C(107)	119.3(10)
C(71)-C(70)-C(69)	118.9(8)	C(108)-C(109)-C(110)	117.8(10)
C(70)-C(71)-C(72)	119.4(9)	C(109)-C(110)-C(105)	126.9(9)
C(71)-C(72)-C(67)	124.1(8)	C(116)-C(111)-C(112)	112.4(8)
C(75)-C(74)-O(13)	112.1(11)	C(116)-C(111)-Yb(5)	121.3(7)
O(14)-C(75)-C(74)	109.6(10)	C(112)-C(111)-Yb(5)	126.3(6)
O(15)-C(78)-C(79)	109.2(9)	C(113)-C(112)-C(111)	124.1(9)
O(16)-C(79)-C(78)	103.6(9)	C(114)-C(113)-C(112)	119.1(9)
C(83)-C(82)-O(17)	107.7(10)	C(115)-C(114)-C(113)	119.4(9)
C(82)-C(83)-O(18)	112.7(11)	C(114)-C(115)-C(116)	119.2(10)
O(19)-C(86)-C(87)	112.1(11)	C(111)-C(116)-C(115)	125.8(10)
O(20)-C(87)-C(86)	115.3(12)	O(23)-C(118)-C(119)	109.4(8)
O(21)-C(90)-C(91)	108.2(8)	O(24)-C(119)-C(118)	106.9(7)
O(22)-C(91)-C(90)	107.8(8)	C(122)-C(121)-C(126)	118.5(7)
C(98)-C(93)-C(94)	113.1(8)	C(122)-C(121)-Yb(6)	119.0(7)

C(126)-C(121)-Yb(6)	122.3(7)
C(123)-C(122)-C(121)	120.7(7)
C(122)-C(123)-C(124)	120.0(7)
C(125)-C(124)-C(123)	119.8(7)
C(124)-C(125)-C(126)	119.7(7)
C(125)-C(126)-C(121)	120.9(7)
C(132)-C(127)-C(128)	113.9(9)
C(132)-C(127)-Yb(6)	120.2(7)
C(128)-C(127)-Yb(6)	125.7(8)
C(129)-C(128)-C(127)	123.2(12)
C(130)-C(129)-C(128)	120.6(14)
C(129)-C(130)-C(131)	120.9(11)
C(130)-C(131)-C(132)	117.5(12)
C(127)-C(132)-C(131)	123.9(11)
C(134)-C(133)-C(138)	112.6(9)
C(134)-C(133)-Yb(6)	125.6(7)
C(138)-C(133)-Yb(6)	121.8(7)
C(133)-C(134)-C(135)	125.2(9)
C(136)-C(135)-C(134)	119.6(10)
C(137)-C(136)-C(135)	118.8(10)
C(136)-C(137)-C(138)	121.3(10)
C(137)-C(138)-C(133)	122.5(10)
C(144)-C(139)-C(140)	113.6(10)
C(144)-C(139)-Yb(6)	123.6(8)
C(140)-C(139)-Yb(6)	122.8(8)
C(139)-C(140)-C(141)	123.8(13)
C(142)-C(141)-C(140)	117.1(14)
C(143)-C(142)-C(141)	121.6(14)
C(142)-C(143)-C(144)	119.6(15)
C(143)-C(144)-C(139)	124.2(13)
O(25)-C(146)-C(147)	109.8(15)
O(26)-C(147)-C(146)	118(2)
C(163)-C(158)-C(159)	119.0(7)
C(163)-C(158)-Yb(6)	120.0(8)
C(159)-C(158)-Yb(6)	120.8(8)
C(160)-C(159)-C(158)	120.3(7)
C(159)-C(160)-C(161)	120.0(7)
C(162)-C(161)-C(160)	120.2(7)
C(161)-C(162)-C(163)	119.9(7)
C(162)-C(163)-C(158)	120.4(7)
O(29)-C(152)-C(153)	141(3)
O(30)-C(153)-C(152)	124(3)

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