

# Supporting Information For

## Surface-grafted Europium and Erbium complexes of the 12-tungstosilicate heteropolyoxometalate: A synthetic and structural investigations

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## Contents

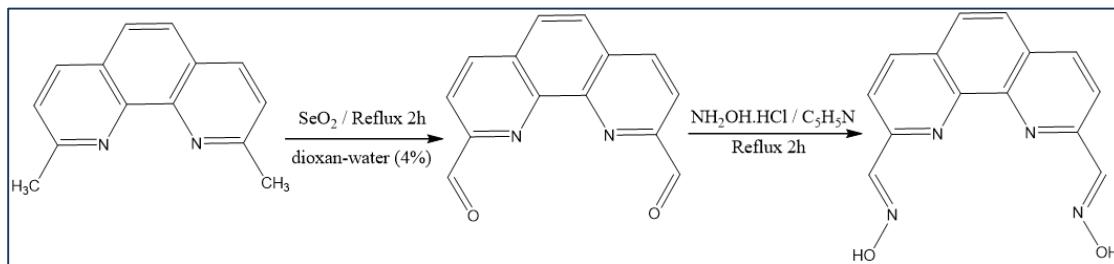
S1. Synthesis and Characterization of 1,10-phenanthroline-2,9-dicarbaldehyde dioxime Ligand (PDOX)

S2. Characterization for compounds **1** and **2**

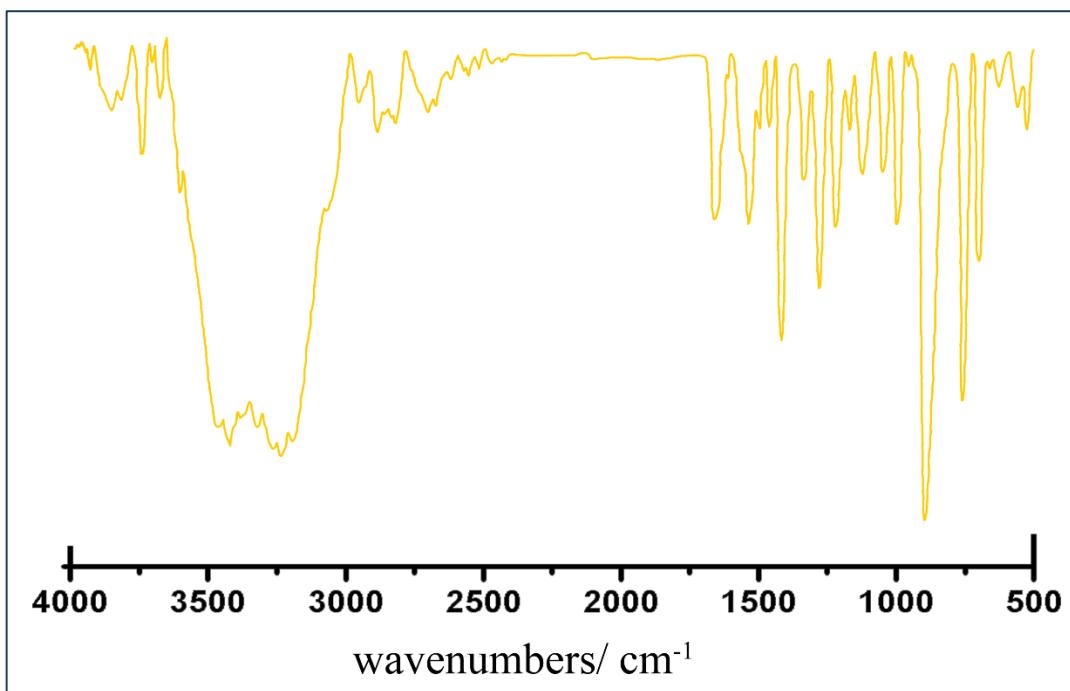
S3. Crystallographic characteristic data for compounds **1** and **2**

## S1. Synthesis and Characterization of 1,10-phenanthroline-2,9-dicarbaldehyde dioxime Ligand (PDOX)

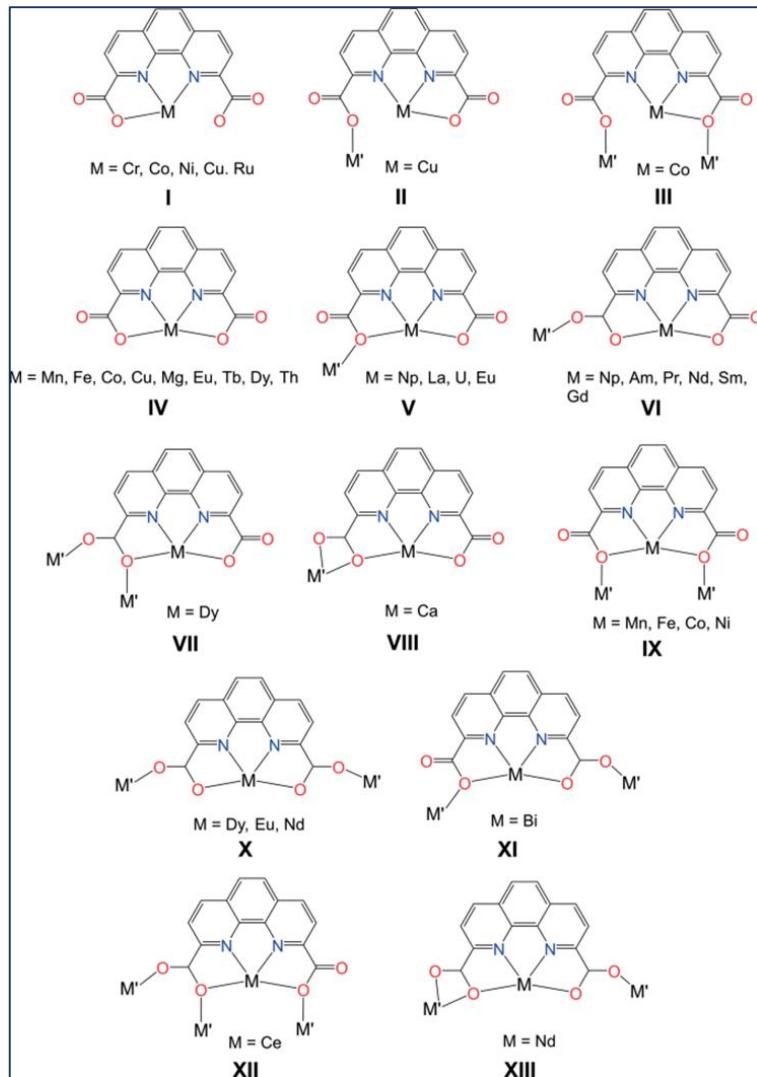
Synthesis procedure of ligand PDOX is illustrated in Scheme 3. A mixture of neocuproin (3 g) and selenium dioxide (7.5 g) in dioxane containing 4% water (200 ml) was heated under reflux for 3 hours and then filtered through celite while hot. The dialdehyde (2.4 g, 70%) was separated from the cold filterate. A suspension of 1,10-phenanthroline-2,9-dicarbaldehyde (400 mg, 1.69 mmol) in 10 ml of absolute ethanol was stirred at 60 °C for 10 min. NH<sub>2</sub>OH.HCl was then progressively added (622 mg, 8.8 mmol). The addition of about 400 mg of hydroxylamine dissolved the dialdehyde within a few minutes to give a brown solution, after which a brown precipitate was obtained (after the complete addition of NH<sub>2</sub>OH.HCl). The reaction mixture, in 30 ml of absolute EtOH, was warmed to 80 °C and stirred for 20 minutes. The mixture was stirred at reflux (95°C) for 2 hours after the addition of pyridine (1.64 ml, 20.3 mmol). The reaction mixture was then allowed to cool at room temperature. After removal of the liquid phase, the precipitate was washed with 30 ml of water to eliminate the excess of NH<sub>2</sub>OH.HCl (352 mg, yield 78%). IR (KBr)  $\tilde{\nu}$ : 1617 cm<sup>-1</sup> (C=N oxime).<sup>1</sup>



**Figure S1.** Ligand (PDOX) synthesis procedure.

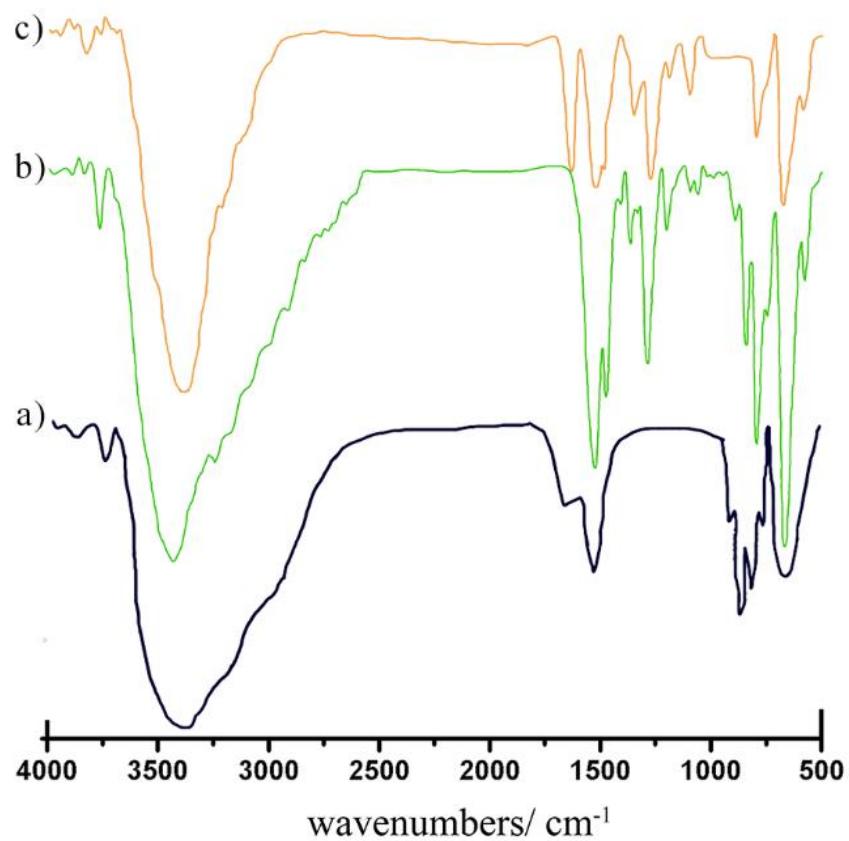


**Figure S2.** Infrared spectrum of the Ligand (PDOX).



**Figure S3.** Classification of the coordination modes found for PDA ligands in the CSD.

## S2. Characterizations for **1** and **2**



**Figure S4.** IR spectra of POM a) H<sub>4</sub>[SiW<sub>12</sub>O<sub>40</sub>], and Hybrids b) **1** and c) **2**.

## S3. Crystallographic characteristic data for compounds 1 and 2

### S3.1- Crystal structure report for 1

A specimen of  $C_{112}H_{98}Eu_8N_{16}O_{137}Si_2W_{24}$ , approximate dimensions 0.071 mm x 0.204 mm x 0.244 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart APEX CCD system equipped with a graphite monochromator and a Mo-K $\alpha$  fine-focus sealed tube ( $\lambda = 0.71073 \text{ \AA}$ ).

The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 180000 reflections to a maximum  $\theta$  angle of  $29.32^\circ$  ( $0.73 \text{ \AA}$  resolution), of which 25583 were independent (average redundancy 7.036, completeness = 96.9%,  $R_{\text{int}} = 8.27\%$ ,  $R_{\text{sig}} = 7.18\%$ ) and 19719 (77.08%) were greater than  $2\sigma(F^2)$ . The final cell constants of  $a = 33.656(3) \text{ \AA}$ ,  $b = 13.9520(11) \text{ \AA}$ ,  $c = 20.7047(16) \text{ \AA}$ ,  $\beta = 97.6360(10)^\circ$ , volume =  $9636.1(13) \text{ \AA}^3$ , are based upon the refinement of the XYZ-centroids of reflections above  $20 \sigma(I)$ . Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.1040 and 0.3790.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with  $Z = 2$  for the formula unit,  $C_{112}H_{98}Eu_8N_{16}O_{137}Si_2W_{24}$ . The final anisotropic full-matrix least-squares refinement on  $F^2$  with 1416 variables converged at  $R1 = 7.89\%$ , for the observed data and  $wR2 = 19.30\%$  for all data. The goodness-of-fit was 1.193. The largest peak in the final difference electron density synthesis was  $3.331 \text{ e}^-/\text{\AA}^3$  and the largest hole was  $-2.842 \text{ e}^-/\text{\AA}^3$  with an RMS deviation of  $0.403 \text{ e}^-/\text{\AA}^3$ . On the basis of the final model, the calculated density was  $3.289 \text{ g/cm}^3$  and  $F(000), 8572 \text{ e}^-$ .

**Table S1** Experimental details, data collection and structure refinement for **1**.

Compound <b>1</b>	JTM1081a
Crystal data	
Chemical formula	$2(\text{C}_{56}\text{H}_{43}\text{Eu}_4\text{N}_8\text{O}_{25.50}) \cdot 2(\text{O}_{40}\text{SiW}_{12}) \cdot 5.5(\text{H}_2\text{O})$
$M_r$	9544.32
Crystal system, space group	monoclinic, P 1 21/c 1
Temperature (K)	150
$a, b, c$ (Å)	33.656 (3), 13.9520 (11), 20.7047 (16)
$\beta$ (°)	97.636 (1)
$V$ (Å <sup>3</sup> )	9636.2 (13)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	16.94
Crystal size (mm)	0.071 × 0.204 × 0.244
Data collection	
Diffractometer	Bruker Smart <i>APEX</i> CCD
Absorption correction	Multi-scan <i>SADABS</i> (Krause <i>et al.</i> , 2015)
$T_{\min}, T_{\max}$	0.10, 0.38
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	180000, 25583, 19719
$R_{\text{int}}$	0.083
(sin $\theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.689
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.079, 0.193, 1.19
No. of reflections	25583
No. of parameters	1416
No. of restraints	842
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å <sup>-3</sup> )	3.33, -2.84
Absolute structure	Flack x determined using 3567 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	0.015 (6)
CCDC no.	1934958

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL-2018/1* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Bruker, 2016).

**Table S2** The bond lengths ( $\text{\AA}$ ) for **1**.

Bond	Lengths	Bond	Lengths
Eu1-O5	2.378(12)	Eu1-O3	2.386(13)
Eu1-O6	2.404(14)	Eu1-O15	2.412(12)
Eu1-O1	2.424(13)	Eu1-O23	2.430(13)
Eu1-N2	2.536(15)	Eu1-N1	2.536(15)
Eu1-C54	3.15(2)	Eu1-Eu4	4.1322(15)
Eu1-H5A	2.7023	Eu1-H5B	2.7025
Eu1-H6A	2.7006	Eu1-H6B	2.7003
Eu2-O11	2.36(2)	Eu2-O13	2.40(2)
Eu2-O4	2.417(16)	Eu2-O7	2.422(18)
Eu2-O9A	2.47(2)	Eu2-O9	2.47(2)
Eu2-O12	2.53(2)	Eu2-N3	2.545(19)
Eu2-N4	2.550(18)	Eu2-O11A	2.62(3)
Eu2-C26	3.24(3)	Eu2-H11A	2.6987
Eu2-H11B	2.699	Eu2-H12A	2.6983
Eu2-H12B	2.6987	Eu2-H13A	2.6991
Eu2-H13B	2.6994	Eu3-O8	2.342(14)
Eu3-O18	2.359(18)	Eu3-O14	2.365(15)
Eu3-O16	2.410(17)	Eu3-O20	2.422(15)
Eu3-O19	2.44(2)	Eu3-N8	2.525(14)
Eu3-N5	2.537(18)	Eu3-H18A	2.7016
Eu3-H18B	2.7014	Eu3-H19A	2.7003
Eu3-H19B	2.6999	Eu3-H20A	2.6997
Eu3-H20B	2.6997	Eu4-O10	2.344(16)
Eu4-O23	2.411(14)	Eu4-O21	2.418(19)
Eu4-O25	2.447(15)	Eu4-O17	2.474(19)
Eu4-O72	2.47(3)	Eu4-N6	2.566(15)

<b>Bond</b>	<b>Lengths</b>	<b>Bond</b>	<b>Lengths</b>
Eu4-O1	2.566(12)	Eu4-N7	2.582(17)
Eu4-H25A	2.6999	Eu4-H25B	2.7
Eu4-H72B	2.52(3)	Eu4A-O72	1.78(4)
Eu4A-O10	2.15(3)	Eu4A-O17	2.22(3)
Eu4A-O21	2.28(3)	Eu4A-N7	2.46(3)
Eu4A-N6	2.78(3)	Eu4A-O23	2.92(3)
Eu4A-C26	2.94(4)	Eu4A-O25	3.05(3)
Eu4A-O9A	3.07(4)	Eu4A-O1	3.10(3)
Eu4A-C44	3.20(3)	Eu4A-H72A	2.14(4)
Eu4A-H72B	1.87(4)	O1-C1	1.32(2)
O2-C1	1.22(2)	O3-C12	1.28(2)
O4-C12	1.26(3)	O5-H5A	0.87
O5-H5B	0.87	O6-H6A	0.87
O6-H6B	0.87	O7-C15	1.26(3)
O8-C15	1.32(3)	O9-C26	1.31(3)
O9A-C26	1.31(3)	O10-C26	1.27(3)
O11-H11A	0.87	O11-H11B	0.87
O11A-H11C	0.87	O11A-H11D	0.87
O12-H12A	0.87	O12-H12B	0.87
O13-H13A	0.87	O13-H13B	0.87
O14-C29	1.30(2)	O15-C29	1.23(2)
O16-C40	1.30(3)	O17-C40	1.30(3)
O18-H18A	0.87	O18-H18B	0.87
O19-H19A	0.87	O19-H19B	0.87
O20-H20A	0.87	O20-H20B	0.87
O21-C43	1.30(3)	O22-C43	1.25(3)
O23-C54	1.32(2)	O24-C54	1.16(3)

<b>Bond</b>	<b>Lengths</b>	<b>Bond</b>	<b>Lengths</b>
O25-H25A	0.87	O25-H25B	0.87
N1-C14	1.35(2)	N1-C2	1.35(2)
N2-C13	1.34(2)	N2-C11	1.36(2)
N3-C16	1.35(3)	N3-C28	1.41(3)
N4-C25	1.33(3)	N4-C27	1.35(2)
N5-C41	1.34(3)	N5-C39	1.36(3)
N6-C53	1.32(3)	N6-C56	1.38(2)
N7-C44	1.30(3)	N7-C55	1.36(2)
N8-C30	1.32(3)	N8-C42	1.35(2)
C1-C2	1.54(3)	C2-C3	1.41(3)
C3-C4	1.44(3)	C3-H3	0.95
C4-C5	1.38(3)	C4-H4	0.95
C5-C14	1.43(3)	C5-C6	1.43(3)
C6-C7	1.32(3)	C6-H6	0.95
C7-C8	1.43(3)	C7-H7	0.95
C8-C13	1.41(2)	C8-C9	1.47(3)
C9-C10	1.33(3)	C9-H9	0.95
C10-C11	1.37(3)	C10-H10	0.95
C11-C12	1.54(3)	C13-C14	1.47(3)
C15-C16	1.50(3)	C16-C17	1.38(3)
C17-C18	1.39(4)	C17-H17	0.95
C18-C19	1.38(3)	C18-H18	0.95
C19-C28	1.42(3)	C19-C20	1.51(3)
C20-C21	1.28(3)	C20-H20	0.95
C21-C22	1.48(3)	C21-H21	0.95
C22-C23	1.38(3)	C22-C27	1.42(3)
C23-C24	1.44(3)	C23-H23	0.95

<b>Bond</b>	<b>Lengths</b>	<b>Bond</b>	<b>Lengths</b>
C24-C25	1.40(3)	C24-H24	0.95
C25-C26	1.53(4)	C27-C28	1.46(3)
C29-C30	1.55(3)	C30-C31	1.40(3)
C31-C32	1.40(3)	C31-H31	0.95
C32-C33	1.41(2)	C32-H32	0.95
C33-C42	1.40(2)	C33-C34	1.43(2)
C34-C35	1.35(3)	C34-H34	0.95
C35-C36	1.45(3)	C35-H35	0.95
C36-C37	1.41(3)	C36-C41	1.43(3)
C37-C38	1.41(3)	C37-H37	0.95
C38-C39	1.40(3)	C38-H38	0.95
C39-C40	1.48(3)	C41-C42	1.45(3)
C43-C44	1.48(3)	C44-C45	1.42(3)
C45-C46	1.43(3)	C45-H45	0.95
C46-C47	1.34(3)	C46-H46	0.95
C47-C55	1.45(2)	C47-C48	1.45(3)
C48-C49	1.32(3)	C48-H48	0.95
C49-C50	1.47(3)	C49-H49	0.95
C50-C51	1.41(3)	C50-C56	1.44(2)
C51-C52	1.38(3)	C51-H51	0.95
C52-C53	1.42(3)	C52-H52	0.95
C53-C54	1.55(3)	C55-C56	1.44(3)
W1-O26	1.699(14)	W1-O31	1.846(19)
W1-O33	1.87(2)	W1-O39	1.90(2)
W1-O38	1.912(18)	W1-O46	2.42(2)
W1-O45	2.43(2)	W2-O27	1.694(15)
W2-O32	1.86(2)	W2-O34	1.879(19)

Bond	Lengths	Bond	Lengths
W2-O31	1.907(19)	W2-O36	1.91(2)
W2-O46	2.37(2)	W2-O47	2.40(2)
W3-O28	1.671(13)	W3-O35	1.855(19)
W3-O38	1.898(19)	W3-O34	1.92(2)
W3-O37	1.945(19)	W3-O47	2.40(2)
W3-O45	2.41(2)	W4-O42	1.661(16)
W4-O43	1.872(19)	W4-O36	1.88(2)
W4-O41	1.892(17)	W4-O35	1.930(18)
W4-O47	2.37(2)	W4-O44	2.40(2)
W5-O29	1.667(15)	W5-O41	1.884(16)
W5-O39	1.912(19)	W5-O32	1.93(2)
W5-O40	1.938(18)	W5-O46	2.35(2)
W5-O44	2.45(2)	W6-O30	1.678(16)
W6-O40	1.840(19)	W6-O37	1.859(18)
W6-O43	1.921(18)	W6-O33	1.933(19)
W6-O44	2.35(2)	W6-O45	2.37(2)
Si1-O45	1.61(2)	Si1-O45	1.61(2)
Si1-O44	1.62(2)	Si1-O44	1.62(2)
Si1-O47	1.63(2)	Si1-O47	1.63(2)
Si1-O46	1.67(2)	Si1-O46	1.67(2)
O44-O45	1.80(3)	O48-W7	1.646(15)
W7-O55	1.85(2)	W7-O53	1.879(19)
W7-O56	1.933(15)	W7-O54	1.947(17)
W7-O69	2.31(2)	W7-O65	2.45(2)
W8-O49	1.683(15)	W8-O57	1.87(2)
W8-O56	1.880(16)	W8-O64	1.881(16)
W8-O61	1.91(2)	W8-O68	2.32(2)

<b>Bond</b>	<b>Lengths</b>	<b>Bond</b>	<b>Lengths</b>
W8-O65	2.45(2)	W9-O50	1.677(15)
W9-O59	1.901(19)	W9-O57	1.91(2)
W9-O58	1.93(2)	W9-O53	1.93(2)
W9-O68	2.39(3)	W9-O69	2.43(2)
W10-O51	1.663(15)	W10-O67	1.88(2)
W10-O59	1.878(18)	W10-O60	1.93(2)
W10-O55	1.97(2)	W10-O69	2.44(2)
W10-O66	2.47(2)	W11-O52	1.670(15)
W11-O60	1.88(2)	W11-O58	1.879(19)
W11-O61	1.90(2)	W11-O62	1.92(2)
W11-O68	2.38(3)	W11-O66	2.43(2)
W12-O63	1.656(17)	W12-O54	1.868(18)
W12-O62	1.88(2)	W12-O67	1.89(2)
W12-O64	1.916(16)	W12-O66	2.28(2)
W12-O65	2.42(2)	Si2-O65	1.55(2)
Si2-O65	1.55(2)	Si2-O69	1.64(2)
Si2-O69	1.64(2)	Si2-O66	1.64(2)
Si2-O66	1.64(2)	Si2-O68	1.70(3)
Si2-O68	1.70(3)	O65-O66	1.75(3)
O65-O69	1.78(3)	O70-H70A	0.8702
O70-H70B	0.87	O71-H71A	0.87
O71-H71B	0.87	O72-H72A	0.8701
O72-H72B	0.8702	O73-H73A	0.87
O73-H73B	0.8701	O74-H74A	0.87
O74-H74B	0.8701		

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S3** The bond angles ( $^{\circ}$ ) for **1**.

Bond	Angles	Bond	Angles
O5-Eu1-O3	98.3(5)	O5-Eu1-O6	144.2(4)
O3-Eu1-O6	84.2(5)	O5-Eu1-O15	142.4(5)
O3-Eu1-O15	78.7(5)	O6-Eu1-O15	73.3(5)
O5-Eu1-O1	92.2(4)	O3-Eu1-O1	166.2(4)
O6-Eu1-O1	92.4(5)	O15-Eu1-O1	87.5(5)
O5-Eu1-O23	74.2(4)	O3-Eu1-O23	107.9(5)
O6-Eu1-O23	139.0(4)	O15-Eu1-O23	71.3(5)
O1-Eu1-O23	66.5(4)	O5-Eu1-N2	75.0(4)
O3-Eu1-N2	64.2(5)	O6-Eu1-N2	74.2(5)
O15-Eu1-N2	132.4(5)	O1-Eu1-N2	127.7(5)
O23-Eu1-N2	146.6(5)	O5-Eu1-N1	75.4(5)
O3-Eu1-N1	126.8(5)	O6-Eu1-N1	74.8(5)
O15-Eu1-N1	136.0(5)	O1-Eu1-N1	64.5(5)
O23-Eu1-N1	120.0(5)	N2-Eu1-N1	63.2(5)
O5-Eu1-C54	77.9(5)	O3-Eu1-C54	85.0(5)
O6-Eu1-C54	137.7(5)	O15-Eu1-C54	64.5(5)
O1-Eu1-C54	88.6(5)	O23-Eu1-C54	22.9(5)
N2-Eu1-C54	134.8(5)	N1-Eu1-C54	140.7(5)
O5-Eu1-Eu4	81.2(3)	O3-Eu1-Eu4	138.1(3)
O6-Eu1-Eu4	120.1(3)	O15-Eu1-Eu4	77.1(4)
O1-Eu1-Eu4	35.2(3)	O23-Eu1-Eu4	31.2(3)
N2-Eu1-Eu4	150.3(3)	N1-Eu1-Eu4	93.9(4)
C54-Eu1-Eu4	53.6(4)	O5-Eu1-H5A	18.3
O3-Eu1-H5A	86.6	O6-Eu1-H5A	129.2
O15-Eu1-H5A	152.0	O1-Eu1-H5A	105.8
O23-Eu1-H5A	91.2	N2-Eu1-H5A	57.0

Bond	Angles	Bond	Angles
N1-Eu1-H5A	71.6	C54-Eu1-H5A	90.7
Eu4-Eu1-H5A	99.3	O5-Eu1-H5B	18.3
O3-Eu1-H5B	88.2	O6-Eu1-H5B	158.0
O15-Eu1-H5B	125.4	O1-Eu1-H5B	99.5
O23-Eu1-H5B	62.9	N2-Eu1-H5B	83.9
N1-Eu1-H5B	93.7	C54-Eu1-H5B	61.6
Eu4-Eu1-H5B	78.6	H5A-Eu1-H5B	29.4
O5-Eu1-H6A	128.2	O3-Eu1-H6A	75.6
O6-Eu1-H6A	18.5	O15-Eu1-H6A	87.8
O1-Eu1-H6A	104.7	O23-Eu1-H6A	157.2
N2-Eu1-H6A	55.8	N1-Eu1-H6A	69.3
C54-Eu1-H6A	149.0	Eu4-Eu1-H6A	136.4
H5A-Eu1-H6A	111.6	H5B-Eu1-H6A	139.7
O5-Eu1-H6B	156.3	O3-Eu1-H6B	71.6
O6-Eu1-H6B	18.5	O15-Eu1-H6B	58.4
O1-Eu1-H6B	101.6	O23-Eu1-H6B	128.9
N2-Eu1-H6B	81.3	N1-Eu1-H6B	93.2
C54-Eu1-H6B	121.1	Eu4-Eu1-H6B	120.8
H5A-Eu1-H6B	138.2	H5B-Eu1-H6B	158.8
H6A-Eu1-H6B	29.4	O11-Eu2-O13	132.6(8)
O11-Eu2-O4	142.1(6)	O13-Eu2-O4	75.9(7)
O11-Eu2-O7	82.4(7)	O13-Eu2-O7	75.4(7)
O4-Eu2-O7	82.8(6)	O11-Eu2-O9A	97.2(10)
O13-Eu2-O9A	96.0(8)	O4-Eu2-O9A	104.5(10)
O7-Eu2-O9A	167.2(9)	O11-Eu2-O9	73.4(8)
O13-Eu2-O9	112.0(8)	O4-Eu2-O9	124.3(7)
O7-Eu2-O9	152.6(7)	O11-Eu2-O12	71.3(7)

Bond	Angles	Bond	Angles
O13-Eu2-O12	67.6(8)	O4-Eu2-O12	143.4(6)
O7-Eu2-O12	90.2(7)	O9A-Eu2-O12	77.7(10)
O9-Eu2-O12	70.2(8)	O11-Eu2-N3	75.3(7)
O13-Eu2-N3	126.0(7)	O4-Eu2-N3	66.9(6)
O7-Eu2-N3	62.7(6)	O9A-Eu2-N3	129.7(8)
O9-Eu2-N3	121.0(8)	O12-Eu2-N3	139.3(7)
O11-Eu2-N4	80.1(6)	O13-Eu2-N4	146.2(8)
O4-Eu2-N4	80.5(5)	O7-Eu2-N4	125.3(6)
O9A-Eu2-N4	66.8(8)	O9-Eu2-N4	63.4(7)
O12-Eu2-N4	130.6(7)	N3-Eu2-N4	62.9(6)
O11-Eu2-O11A	135.9(8)	O13-Eu2-O11A	71.6(10)
O4-Eu2-O11A	69.5(8)	O7-Eu2-O11A	141.0(8)
O9A-Eu2-O11A	38.9(11)	O9-Eu2-O11A	62.6(9)
O12-Eu2-O11A	95.9(9)	N3-Eu2-O11A	124.4(8)
N4-Eu2-O11A	77.6(8)	O11-Eu2-C26	85.5(7)
O13-Eu2-C26	117.0(8)	O4-Eu2-C26	104.0(6)
O7-Eu2-C26	166.8(7)	O9A-Eu2-C26	21.5(6)
O9-Eu2-C26	21.5(6)	O12-Eu2-C26	90.7(8)
N3-Eu2-C26	109.2(7)	N4-Eu2-C26	46.8(6)
O11A-Eu2-C26	51.9(8)	O11-Eu2-H11A	18.3
O13-Eu2-H11A	147.2	O4-Eu2-H11A	136.0
O7-Eu2-H11A	98.0	O9A-Eu2-H11A	84.0
O9-Eu2-H11A	60.9	O12-Eu2-H11A	80.6
N3-Eu2-H11A	74.6	N4-Eu2-H11A	63.1
O11A-Eu2-H11A	120.9	C26-Eu2-H11A	69.2
O11-Eu2-H11B	18.3	O13-Eu2-H11B	117.9
O4-Eu2-H11B	159.9	O7-Eu2-H11B	86.7

Bond	Angles	Bond	Angles
O9A-Eu2-H11B	89.1	O9-Eu2-H11B	66.3
O12-Eu2-H11B	53.3	N3-Eu2-H11B	93.1
N4-Eu2-H11B	91.8	O11A-Eu2-H11B	127.1
C26-Eu2-H11B	83.3	H11A-Eu2-H11B	29.5
O11-Eu2-H12A	53.0	O13-Eu2-H12A	86.1
O4-Eu2-H12A	161.9	O7-Eu2-H12A	91.8
O9A-Eu2-H12A	78.0	O9-Eu2-H12A	63.5
O12-Eu2-H12A	18.8	N3-Eu2-H12A	125.6
N4-Eu2-H12A	116.2	O11A-Eu2-H12A	105.9
C26-Eu2-H12A	84.9	H11A-Eu2-H12A	61.8
H11B-Eu2-H12A	34.9	O11-Eu2-H12B	80.6
O13-Eu2-H12B	67.8	O4-Eu2-H12B	137.3
O7-Eu2-H12B	107.9	O9A-Eu2-H12B	59.6
O9-Eu2-H12B	56.2	O12-Eu2-H12B	18.8
N3-Eu2-H12B	155.0	N4-Eu2-H12B	119.4
O11A-Eu2-H12B	78.2	C26-Eu2-H12B	74.9
H11A-Eu2-H12B	84.6	H11B-Eu2-H12B	62.4
H12A-Eu2-H12B	29.5	O11-Eu2-H13A	121.7
O13-Eu2-H13A	18.5	O4-Eu2-H13A	91.9
O7-Eu2-H13A	86.4	O9A-Eu2-H13A	83.0
O9-Eu2-H13A	95.4	O12-Eu2-H13A	51.7
N3-Eu2-H13A	143.5	N4-Eu2-H13A	145.5
O11A-Eu2-H13A	68.3	C26-Eu2-H13A	104.5
H11A-Eu2-H13A	132.2	H11B-Eu2-H13A	104.6
H12A-Eu2-H13A	70.5	H12B-Eu2-H13A	49.5
O11-Eu2-H13B	150.3	O13-Eu2-H13B	18.5
O4-Eu2-H13B	62.7	O7-Eu2-H13B	87.3

Bond	Angles	Bond	Angles
O9A-Eu2-H13B	86.9	O9-Eu2-H13B	107.5
O12-Eu2-H13B	81.1	N3-Eu2-H13B	123.7
N4-Eu2-H13B	127.7	O11A-Eu2-H13B	56.0
C26-Eu2-H13B	105.8	H11A-Eu2-H13B	160.9
H11B-Eu2-H13B	133.9	H12A-Eu2-H13B	99.9
H12B-Eu2-H13B	76.3	H13A-Eu2-H13B	29.4
O8-Eu3-O18	142.0(6)	O8-Eu3-O14	75.4(5)
O18-Eu3-O14	96.5(7)	O8-Eu3-O16	91.5(6)
O18-Eu3-O16	92.4(7)	O14-Eu3-O16	166.7(5)
O8-Eu3-O20	73.8(5)	O18-Eu3-O20	144.0(5)
O14-Eu3-O20	89.6(5)	O16-Eu3-O20	88.9(6)
O8-Eu3-O19	73.3(6)	O18-Eu3-O19	69.1(7)
O14-Eu3-O19	86.8(7)	O16-Eu3-O19	87.2(8)
O20-Eu3-O19	146.8(6)	O8-Eu3-N8	125.7(5)
O18-Eu3-N8	80.0(6)	O14-Eu3-N8	65.0(5)
O16-Eu3-N8	126.6(5)	O20-Eu3-N8	70.5(5)
O19-Eu3-N8	135.4(7)	O8-Eu3-N5	137.3(6)
O18-Eu3-N5	76.9(6)	O14-Eu3-N5	127.8(5)
O16-Eu3-N5	63.9(6)	O20-Eu3-N5	71.5(5)
O19-Eu3-N5	134.1(7)	N8-Eu3-N5	62.9(5)
O8-Eu3-H18A	123.8	O18-Eu3-H18A	18.2
O14-Eu3-H18A	90.5	O16-Eu3-H18A	95.0
O20-Eu3-H18A	161.7	O19-Eu3-H18A	51.4
N8-Eu3-H18A	93.0	N5-Eu3-H18A	94.2
O8-Eu3-H18B	145.0	O18-Eu3-H18B	18.2
O14-Eu3-H18B	81.9	O16-Eu3-H18B	108.5
O20-Eu3-H18B	132.8	O19-Eu3-H18B	79.2

Bond	Angles	Bond	Angles
N8-Eu3-H18B	63.8	N5-Eu3-H18B	77.7
H18A-Eu3-H18B	29.4	O8-Eu3-H19A	90.4
O18-Eu3-H19A	53.5	O14-Eu3-H19A	98.4
O16-Eu3-H19A	79.1	O20-Eu3-H19A	160.1
O19-Eu3-H19A	18.6	N8-Eu3-H19A	129.4
N5-Eu3-H19A	115.9	H18A-Eu3-H19A	37.4
H18B-Eu3-H19A	66.7	O8-Eu3-H19B	62.2
O18-Eu3-H19B	82.9	O14-Eu3-H19B	97.8
O16-Eu3-H19B	73.6	O20-Eu3-H19B	131.5
O19-Eu3-H19B	18.6	N8-Eu3-H19B	153.9
N5-Eu3-H19B	131.4	H18A-Eu3-H19B	66.6
H18B-Eu3-H19B	95.7	H19A-Eu3-H19B	29.4
O8-Eu3-H20A	57.2	O18-Eu3-H20A	160.5
O14-Eu3-H20A	92.7	O16-Eu3-H20A	81.9
O20-Eu3-H20A	18.6	O19-Eu3-H20A	128.8
N8-Eu3-H20A	88.3	N5-Eu3-H20A	83.8
H18A-Eu3-H20A	176.8	H18B-Eu3-H20A	151.4
H19A-Eu3-H20A	141.8	H19B-Eu3-H20A	113.0
O8-Eu3-H20B	86.3	O18-Eu3-H20B	131.0
O14-Eu3-H20B	106.3	O16-Eu3-H20B	74.6
O20-Eu3-H20B	18.6	O19-Eu3-H20B	152.4
N8-Eu3-H20B	71.9	N5-Eu3-H20B	54.8
H18A-Eu3-H20B	148.9	H18B-Eu3-H20B	126.0
H19A-Eu3-H20B	153.4	H19B-Eu3-H20B	133.8
H20A-Eu3-H20B	29.4	O10-Eu4-O23	98.6(6)
O10-Eu4-O21	85.4(7)	O23-Eu4-O21	159.2(6)
O10-Eu4-O25	135.4(6)	O23-Eu4-O25	81.3(5)

Bond	Angles	Bond	Angles
O21-Eu4-O25	81.6(7)	O10-Eu4-O17	69.6(7)
O23-Eu4-O17	68.6(6)	O21-Eu4-O17	131.1(7)
O25-Eu4-O17	144.7(6)	O10-Eu4-O72	76.3(8)
O23-Eu4-O72	130.2(7)	O21-Eu4-O72	70.6(8)
O25-Eu4-O72	136.2(7)	O17-Eu4-O72	63.2(8)
O10-Eu4-N6	142.0(6)	O23-Eu4-N6	62.7(5)
O21-Eu4-N6	124.3(6)	O25-Eu4-N6	77.3(5)
O17-Eu4-N6	72.7(6)	O72-Eu4-N6	90.9(7)
O10-Eu4-O1	68.9(5)	O23-Eu4-O1	64.5(4)
O21-Eu4-O1	98.6(5)	O25-Eu4-O1	71.2(4)
O17-Eu4-O1	109.4(5)	O72-Eu4-O1	144.4(7)
N6-Eu4-O1	121.3(4)	O10-Eu4-N7	133.2(6)
O23-Eu4-N7	123.9(5)	O21-Eu4-N7	62.1(6)
O25-Eu4-N7	75.3(5)	O17-Eu4-N7	106.2(6)
O72-Eu4-N7	62.1(7)	N6-Eu4-N7	62.8(5)
O1-Eu4-N7	143.5(5)	O10-Eu4-Eu1	83.0(5)
O23-Eu4-Eu1	31.5(3)	O21-Eu4-Eu1	130.7(4)
O25-Eu4-Eu1	74.1(4)	O17-Eu4-Eu1	88.2(5)
O72-Eu4-Eu1	149.1(6)	N6-Eu4-Eu1	91.5(3)
O1-Eu4-Eu1	33.0(3)	N7-Eu4-Eu1	143.6(4)
O10-Eu4-H25A	121.6	O23-Eu4-H25A	68.6
O21-Eu4-H25A	91.9	O25-Eu4-H25A	18.6
O17-Eu4-H25A	137.0	O72-Eu4-H25A	154.6
N6-Eu4-H25A	84.0	O1-Eu4-H25A	53.9
N7-Eu4-H25A	93.8	Eu1-Eu4-H25A	56.1
O10-Eu4-H25B	123.6	O23-Eu4-H25B	97.6
O21-Eu4-H25B	63.9	O25-Eu4-H25B	18.6

Bond	Angles	Bond	Angles
O17-Eu4-H25B	163.3	O72-Eu4-H25B	126.9
N6-Eu4-H25B	92.8	O1-Eu4-H25B	70.5
N7-Eu4-H25B	73.1	Eu1-Eu4-H25B	83.7
H25A-Eu4-H25B	29.4	O10-Eu4-H72B	73.3(7)
O23-Eu4-H72B	110.4(7)	O21-Eu4-H72B	90.3(8)
O25-Eu4-H72B	148.6(7)	O17-Eu4-H72B	43.3(8)
O72-Eu4-H72B	20.1(2)	N6-Eu4-H72B	82.6(7)
O1-Eu4-H72B	140.2(6)	N7-Eu4-H72B	74.1(7)
Eu1-Eu4-H72B	130.8(6)	H25A-Eu4-H72B	165.0
H25B-Eu4-H72B	145.1	O72-Eu4A-O10	98.2(15)
O72-Eu4A-O17	80.1(14)	O10-Eu4A-O17	78.1(10)
O72-Eu4A-O21	87.3(14)	O10-Eu4A-O21	93.5(11)
O17-Eu4A-O21	163.5(16)	O72-Eu4A-N7	74.1(12)
O10-Eu4A-N7	158.0(13)	O17-Eu4A-N7	119.6(11)
O21-Eu4A-N7	65.9(8)	O72-Eu4A-N6	101.9(13)
O10-Eu4A-N6	140.6(12)	O17-Eu4A-N6	72.5(8)
O21-Eu4A-N6	120.8(11)	N7-Eu4A-N6	61.3(7)
O72-Eu4A-O23	140.1(14)	O10-Eu4A-O23	89.4(10)
O17-Eu4A-O23	63.2(8)	O21-Eu4A-O23	131.6(13)
N7-Eu4A-O23	109.9(10)	N6-Eu4A-O23	54.1(6)
O72-Eu4A-C26	75.7(13)	O10-Eu4A-C26	23.0(8)
O17-Eu4A-C26	78.9(10)	O21-Eu4A-C26	87.8(10)
N7-Eu4A-C26	140.5(13)	N6-Eu4A-C26	151.3(11)
O23-Eu4A-C26	109.6(9)	O72-Eu4A-O25	140.3(13)
O10-Eu4A-O25	115.8(11)	O17-Eu4A-O25	124.9(12)
O21-Eu4A-O25	71.5(9)	N7-Eu4A-O25	66.7(8)
N6-Eu4A-O25	64.8(7)	O23-Eu4A-O25	64.0(7)

Bond	Angles	Bond	Angles
C26-Eu4A-O25	134.1(10)	O72-Eu4A-O9A	58.3(13)
O10-Eu4A-O9A	46.2(9)	O17-Eu4A-O9A	93.7(12)
O21-Eu4A-O9A	70.6(10)	N7-Eu4A-O9A	115.4(11)
N6-Eu4A-O9A	158.2(13)	O23-Eu4A-O9A	134.7(9)
C26-Eu4A-O9A	25.0(7)	O25-Eu4A-O9A	135.8(11)
O72-Eu4A-O1	158.1(14)	O10-Eu4A-O1	60.9(8)
O17-Eu4A-O1	100.0(10)	O21-Eu4A-O1	87.8(9)
N7-Eu4A-O1	122.7(11)	N6-Eu4A-O1	98.9(9)
O23-Eu4A-O1	52.3(6)	C26-Eu4A-O1	82.8(8)
O25-Eu4A-O1	56.6(6)	O9A-Eu4A-O1	100.0(9)
O72-Eu4A-C44	66.2(12)	O10-Eu4A-C44	136.0(12)
O17-Eu4A-C44	133.2(11)	O21-Eu4A-C44	47.3(7)
N7-Eu4A-C44	22.1(6)	N6-Eu4A-C44	83.4(7)
O23-Eu4A-C44	129.7(10)	C26-Eu4A-C44	119.7(11)
O25-Eu4A-C44	74.9(7)	O9A-Eu4A-C44	95.0(10)
O1-Eu4A-C44	123.4(9)	O72-Eu4A-H72A	23.5(5)
O10-Eu4A-H72A	76.7(12)	O17-Eu4A-H72A	84.8(13)
O21-Eu4A-H72A	79.5(12)	N7-Eu4A-H72A	91.2(12)
N6-Eu4A-H72A	124.9(12)	O23-Eu4A-H72A	147.2(13)
C26-Eu4A-H72A	53.7(10)	O25-Eu4A-H72A	148.7(12)
O1-Eu4A-H72A	134.8(11)	C44-Eu4A-H72A	76.9(11)
O72-Eu4A-H72B	27.4(6)	O10-Eu4A-H72B	92.4(14)
O17-Eu4A-H72B	52.7(11)	O21-Eu4A-H72B	114.4(16)
N7-Eu4A-H72B	89.4(12)	N6-Eu4A-H72B	90.2(12)
O23-Eu4A-H72B	113.7(13)	C26-Eu4A-H72B	74.5(13)
O25-Eu4A-H72B	151.3(12)	O9A-Eu4A-H72B	68.0(14)
O1-Eu4A-H72B	147.1(13)	C44-Eu4A-H72B	88.9(12)

Bond	Angles	Bond	Angles
H72A-Eu4A-H72B	39.3	C1-O1-Eu1	125.0(11)
C1-O1-Eu4	117.7(11)	Eu1-O1-Eu4	111.8(5)
C1-O1-Eu4A	109.8(12)	Eu1-O1-Eu4A	116.4(6)
C12-O3-Eu1	125.5(12)	C12-O4-Eu2	130.0(14)
Eu1-O5-H5A	102.4	Eu1-O5-H5B	102.4
H5A-O5-H5B	104.1	Eu1-O6-H6A	100.4
Eu1-O6-H6B	100.4	H6A-O6-H6B	104.1
C15-O7-Eu2	124.4(15)	C15-O8-Eu3	139.6(14)
C26-O9-Eu2	114.8(17)	C26-O9A-Eu2	114.9(17)
C26-O9A-Eu4A	71.8(17)	Eu2-O9A-Eu4A	158.8(17)
C26-O10-Eu4A	116.(2)	C26-O10-Eu4	132.9(18)
Eu2-O11-H11A	103.5	Eu2-O11-H11B	103.5
H11A-O11-H11B	104.1	Eu2-O11A-H11C	104.1
Eu2-O11A-H11D	104.1	H11C-O11A-H11D	104.1
Eu2-O12-H12A	91.9	Eu2-O12-H12B	91.9
H12A-O12-H12B	104.1	Eu2-O13-H13A	100.3
Eu2-O13-H13B	100.3	H13A-O13-H13B	104.1
C29-O14-Eu3	126.7(13)	C29-O15-Eu1	134.9(13)
C40-O16-Eu3	125.3(16)	C40-O17-Eu4A	164.(2)
C40-O17-Eu4	148.1(18)	Eu3-O18-H18A	103.8
Eu3-O18-H18B	103.7	H18A-O18-H18B	104.1
Eu3-O19-H19A	97.6	Eu3-O19-H19B	97.5
H19A-O19-H19B	104.1	Eu3-O20-H20A	99.1
Eu3-O20-H20B	99.1	H20A-O20-H20B	104.1
C43-O21-Eu4A	117.0(16)	C43-O21-Eu4	125.6(15)
C54-O23-Eu4	129.4(13)	C54-O23-Eu1	111.1(13)
Eu4-O23-Eu1	117.2(5)	C54-O23-Eu4A	125.4(13)

Bond	Angles	Bond	Angles
Eu1-O23-Eu4A	123.3(7)	Eu4-O25-H25A	97.3
Eu4A-O25-H25A	104.8	Eu4-O25-H25B	97.3
Eu4A-O25-H25B	93.0	H25A-O25-H25B	104.1
C14-N1-C2	117.8(16)	C14-N1-Eu1	121.5(13)
C2-N1-Eu1	120.6(12)	C13-N2-C11	116.0(16)
C13-N2-Eu1	122.6(12)	C11-N2-Eu1	121.3(12)
C16-N3-C28	115.(2)	C16-N3-Eu2	123.1(15)
C28-N3-Eu2	121.2(15)	C25-N4-C27	118.4(19)
C25-N4-Eu2	118.3(14)	C27-N4-Eu2	123.3(14)
C41-N5-C39	117.8(18)	C41-N5-Eu3	121.9(13)
C39-N5-Eu3	120.0(14)	C53-N6-C56	117.8(16)
C53-N6-Eu4	120.5(11)	C56-N6-Eu4	121.6(12)
C53-N6-Eu4A	126.9(12)	C56-N6-Eu4A	112.8(13)
C44-N7-C55	118.6(18)	C44-N7-Eu4A	112.8(16)
C55-N7-Eu4A	123.7(13)	C44-N7-Eu4	120.1(15)
C55-N7-Eu4	120.8(12)	C30-N8-C42	117.3(16)
C30-N8-Eu3	119.5(12)	C42-N8-Eu3	122.6(11)
O2-C1-O1	123.9(18)	O2-C1-C2	121.2(17)
O1-C1-C2	114.8(16)	N1-C2-C3	124.1(18)
N1-C2-C1	114.0(15)	C3-C2-C1	121.6(18)
C2-C3-C4	117.(2)	C2-C3-H3	121.3
C4-C3-H3	121.3	C5-C4-C3	119.(2)
C5-C4-H4	120.7	C3-C4-H4	120.7
C4-C5-C14	119.(2)	C4-C5-C6	123.(2)
C14-C5-C6	117.5(19)	C7-C6-C5	122.9(18)
C7-C6-H6	118.5	C5-C6-H6	118.5
C6-C7-C8	121.4(19)	C6-C7-H7	119.3

Bond	Angles	Bond	Angles
C8-C7-H7	119.3	C13-C8-C7	120.3(18)
C13-C8-C9	112.2(17)	C7-C8-C9	127.4(18)
C10-C9-C8	121.0(18)	C10-C9-H9	119.5
C8-C9-H9	119.5	C9-C10-C11	121.(2)
C9-C10-H10	119.7	C11-C10-H10	119.7
N2-C11-C10	123.0(18)	N2-C11-C12	110.5(16)
C10-C11-C12	126.5(19)	O4-C12-O3	123.9(19)
O4-C12-C11	118.3(19)	O3-C12-C11	117.8(18)
N2-C13-C8	127.1(17)	N2-C13-C14	115.4(15)
C8-C13-C14	117.5(16)	N1-C14-C5	122.8(19)
N1-C14-C13	117.0(16)	C5-C14-C13	120.3(17)
O7-C15-O8	124.(2)	O7-C15-C16	121.(2)
O8-C15-C16	115.(2)	N3-C16-C17	124.(2)
N3-C16-C15	109.(2)	C17-C16-C15	127.(2)
C16-C17-C18	120.(3)	C16-C17-H17	119.8
C18-C17-H17	119.8	C19-C18-C17	119.(2)
C19-C18-H18	120.5	C17-C18-H18	120.5
C18-C19-C28	118.(2)	C18-C19-C20	125.(2)
C28-C19-C20	117.(2)	C21-C20-C19	121.(2)
C21-C20-H20	119.6	C19-C20-H20	119.6
C20-C21-C22	125.(2)	C20-C21-H21	117.5
C22-C21-H21	117.5	C23-C22-C27	116.(2)
C23-C22-C21	127.(2)	C27-C22-C21	116.4(19)
C22-C23-C24	120.(2)	C22-C23-H23	120.0
C24-C23-H23	120.0	C25-C24-C23	118.(2)
C25-C24-H24	121.1	C23-C24-H24	121.1
N4-C25-C24	122.(2)	N4-C25-C26	113.(2)

Bond	Angles	Bond	Angles
C24-C25-C26	124.(2)	O10-C26-O9A	118.(2)
O10-C26-O9	128.(3)	O10-C26-C25	114.(3)
O9A-C26-C25	121.(3)	O9-C26-C25	113.(2)
O10-C26-Eu4A	41.2(14)	O9-C26-Eu4A	88.5(18)
C25-C26-Eu4A	155.(2)	O10-C26-Eu2	162.(2)
O9A-C26-Eu2	43.7(13)	O9-C26-Eu2	43.7(13)
C25-C26-Eu2	82.0(15)	Eu4A-C26-Eu2	123.5(11)
N4-C27-C22	124.6(19)	N4-C27-C28	115.4(18)
C22-C27-C28	119.9(19)	N3-C28-C19	123.(2)
N3-C28-C27	116.(2)	C19-C28-C27	121.(2)
O15-C29-O14	127.3(19)	O15-C29-C30	119.2(18)
O14-C29-C30	113.5(17)	N8-C30-C31	123.4(19)
N8-C30-C29	115.0(17)	C31-C30-C29	121.5(18)
C32-C31-C30	119.2(17)	C32-C31-H31	120.4
C30-C31-H31	120.4	C31-C32-C33	118.8(17)
C31-C32-H32	120.6	C33-C32-H32	120.6
C42-C33-C32	116.4(16)	C42-C33-C34	119.4(16)
C32-C33-C34	123.9(17)	C35-C34-C33	121.7(18)
C35-C34-H34	119.2	C33-C34-H34	119.2
C34-C35-C36	121.3(19)	C34-C35-H35	119.3
C36-C35-H35	119.3	C37-C36-C41	118.4(18)
C37-C36-C35	123.4(19)	C41-C36-C35	118.1(18)
C38-C37-C36	118.(2)	C38-C37-H37	120.8
C36-C37-H37	120.8	C39-C38-C37	118.(2)
C39-C38-H38	120.8	C37-C38-H38	120.8
N5-C39-C38	124.(2)	N5-C39-C40	114.(2)
C38-C39-C40	122.(2)	O16-C40-O17	127.(3)

Bond	Angles	Bond	Angles
O16-C40-C39	117.(2)	O17-C40-C39	117.(2)
N5-C41-C36	123.0(18)	N5-C41-C42	117.0(17)
C36-C41-C42	119.6(17)	N8-C42-C33	124.7(16)
N8-C42-C41	115.5(15)	C33-C42-C41	119.8(16)
O22-C43-O21	123.(2)	O22-C43-C44	122.(2)
O21-C43-C44	115.(2)	N7-C44-C45	125.(2)
N7-C44-C43	115.(2)	C45-C44-C43	121.(2)
N7-C44-Eu4A	45.1(12)	C45-C44-Eu4A	158.6(16)
C43-C44-Eu4A	72.6(13)	C44-C45-C46	116.(2)
C44-C45-H45	122.1	C46-C45-H45	122.1
C47-C46-C45	121.2(19)	C47-C46-H46	119.4
C45-C46-H46	119.4	C46-C47-C55	117.8(19)
C46-C47-C48	125.7(18)	C55-C47-C48	116.4(18)
C49-C48-C47	124.5(19)	C49-C48-H48	117.7
C47-C48-H48	117.7	C48-C49-C50	121.3(18)
C48-C49-H49	119.4	C50-C49-H49	119.4
C51-C50-C56	115.0(18)	C51-C50-C49	128.1(18)
C56-C50-C49	116.9(17)	C52-C51-C50	122.6(19)
C52-C51-H51	118.7	C50-C51-H51	118.7
C51-C52-C53	117.(2)	C51-C52-H52	121.3
C53-C52-H52	121.3	N6-C53-C52	124.0(17)
N6-C53-C54	115.2(16)	C52-C53-C54	120.6(18)
O24-C54-O23	125.(2)	O24-C54-C53	124.4(19)
O23-C54-C53	111.1(17)	O24-C54-Eu1	81.2(14)
O23-C54-Eu1	46.0(10)	C53-C54-Eu1	150.3(13)
N7-C55-C56	118.1(16)	N7-C55-C47	122.0(17)
C56-C55-C47	119.9(17)	N6-C56-C55	116.0(16)

Bond	Angles	Bond	Angles
N6-C56-C50	123.1(18)	C55-C56-C50	120.9(17)
O26-W1-O31	101.8(9)	O26-W1-O33	101.6(9)
O31-W1-O33	87.7(9)	O26-W1-O39	99.9(9)
O31-W1-O39	88.5(8)	O33-W1-O39	158.5(10)
O26-W1-O38	101.1(8)	O31-W1-O38	157.2(10)
O33-W1-O38	88.1(7)	O39-W1-O38	87.3(8)
O26-W1-O46	154.7(8)	O31-W1-O46	62.5(8)
O33-W1-O46	97.6(9)	O39-W1-O46	62.1(8)
O38-W1-O46	95.9(9)	O26-W1-O45	158.5(7)
O31-W1-O45	93.6(9)	O33-W1-O45	63.7(8)
O39-W1-O45	95.5(9)	O38-W1-O45	64.5(8)
O46-W1-O45	46.8(7)	O27-W2-O32	101.4(9)
O27-W2-O34	98.8(9)	O32-W2-O34	89.5(9)
O27-W2-O31	103.5(9)	O32-W2-O31	90.5(8)
O34-W2-O31	157.3(10)	O27-W2-O36	100.0(9)
O32-W2-O36	158.5(10)	O34-W2-O36	88.0(8)
O31-W2-O36	83.8(9)	O27-W2-O46	157.5(9)
O32-W2-O46	63.0(8)	O34-W2-O46	97.2(9)
O31-W2-O46	62.9(9)	O36-W2-O46	96.2(9)
O27-W2-O47	154.4(8)	O32-W2-O47	97.3(9)
O34-W2-O47	63.9(8)	O31-W2-O47	93.6(9)
O36-W2-O47	62.7(8)	O46-W2-O47	48.0(7)
O28-W3-O35	100.5(9)	O28-W3-O38	100.0(8)
O35-W3-O38	89.9(8)	O28-W3-O34	100.7(8)
O35-W3-O34	88.1(8)	O38-W3-O34	159.3(9)
O28-W3-O37	101.6(9)	O35-W3-O37	157.9(10)
O38-W3-O37	87.4(8)	O34-W3-O37	86.8(9)

Bond	Angles	Bond	Angles
O28-W3-O47	155.4(7)	O35-W3-O47	62.3(9)
O38-W3-O47	97.5(9)	O34-W3-O47	63.4(8)
O37-W3-O47	96.3(9)	O28-W3-O45	158.3(7)
O35-W3-O45	95.4(9)	O38-W3-O45	65.2(8)
O34-W3-O45	94.4(9)	O37-W3-O45	63.6(8)
O47-W3-O45	46.3(7)	O42-W4-O43	99.7(9)
O42-W4-O36	101.1(10)	O43-W4-O36	89.1(9)
O42-W4-O41	101.4(9)	O43-W4-O41	88.0(8)
O36-W4-O41	157.5(9)	O42-W4-O35	103.1(9)
O43-W4-O35	157.0(10)	O36-W4-O35	89.4(8)
O41-W4-O35	84.7(8)	O42-W4-O47	157.4(8)
O43-W4-O47	96.9(9)	O36-W4-O47	63.8(9)
O41-W4-O47	94.4(8)	O35-W4-O47	62.1(8)
O42-W4-O44	156.8(8)	O43-W4-O44	63.1(8)
O36-W4-O44	94.4(9)	O41-W4-O44	64.5(7)
O35-W4-O44	94.1(9)	O47-W4-O44	45.8(7)
O29-W5-O41	102.6(9)	O29-W5-O39	100.8(9)
O41-W5-O39	90.9(8)	O29-W5-O32	100.6(9)
O41-W5-O32	156.5(9)	O39-W5-O32	87.9(8)
O29-W5-O40	101.9(9)	O41-W5-O40	86.5(7)
O39-W5-O40	157.1(9)	O32-W5-O40	85.6(8)
O29-W5-O46	156.0(9)	O41-W5-O46	96.0(8)
O39-W5-O46	63.5(9)	O32-W5-O46	62.7(8)
O40-W5-O46	94.2(8)	O29-W5-O44	157.2(8)
O41-W5-O44	63.4(8)	O39-W5-O44	97.5(8)
O32-W5-O44	93.5(9)	O40-W5-O44	61.2(8)
O46-W5-O44	46.7(7)	O30-W6-O40	101.3(9)

Bond	Angles	Bond	Angles
O30-W6-O37	101.0(10)	O40-W6-O37	91.0(9)
O30-W6-O43	98.8(9)	O40-W6-O43	86.9(8)
O37-W6-O43	160.1(10)	O30-W6-O33	99.9(9)
O40-W6-O33	158.4(9)	O37-W6-O33	89.1(8)
O43-W6-O33	85.7(8)	O30-W6-O44	156.8(9)
O40-W6-O44	64.5(8)	O37-W6-O44	97.6(9)
O43-W6-O44	63.6(8)	O33-W6-O44	94.0(9)
O30-W6-O45	158.2(9)	O40-W6-O45	96.2(9)
O37-W6-O45	65.5(9)	O43-W6-O45	95.0(9)
O33-W6-O45	64.3(8)	O44-W6-O45	44.7(7)
O45-Si1-O45	180.0	O45-Si1-O44	112.5(11)
O45-Si1-O44	67.5(11)	O45-Si1-O44	67.5(11)
O45-Si1-O44	112.5(11)	O44-Si1-O44	180.0
O45-Si1-O47	108.7(10)	O45-Si1-O47	71.3(10)
O44-Si1-O47	110.4(11)	O44-Si1-O47	69.6(11)
O45-Si1-O47	71.3(10)	O45-Si1-O47	108.7(10)
O44-Si1-O47	69.6(11)	O44-Si1-O47	110.4(11)
O47-Si1-O47	180.0	O45-Si1-O46	108.0(11)
O45-Si1-O46	72.0(11)	O44-Si1-O46	109.3(11)
O44-Si1-O46	70.7(11)	O47-Si1-O46	107.7(11)
O47-Si1-O46	72.3(11)	O45-Si1-O46	72.0(11)
O45-Si1-O46	108.0(11)	O44-Si1-O46	70.7(11)
O44-Si1-O46	109.3(11)	O47-Si1-O46	72.3(11)
O47-Si1-O46	107.7(11)	O46-Si1-O46	180.0
W1-O31-W2	139.5(12)	W2-O32-W5	137.0(12)
W1-O33-W6	136.8(11)	W2-O34-W3	137.6(11)
W3-O35-W4	139.0(13)	W4-O36-W2	137.6(12)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
W6-O37-W3	135.7(12)	W3-O38-W1	136.4(12)
W1-O39-W5	137.8(12)	W6-O40-W5	139.1(11)
W5-O41-W4	138.6(10)	W4-O43-W6	137.0(12)
Si1-O44-O45	56.0(10)	Si1-O44-W6	124.2(11)
O45-O44-W6	68.3(9)	Si1-O44-W4	121.6(11)
O45-O44-W4	131.9(13)	W6-O44-W4	95.9(8)
Si1-O44-W5	119.4(11)	O45-O44-W5	131.6(13)
W6-O44-W5	94.9(7)	W4-O44-W5	93.4(8)
Si1-O45-O44	56.5(10)	Si1-O45-W6	123.5(11)
O44-O45-W6	67.0(9)	Si1-O45-W3	121.3(11)
O44-O45-W3	133.0(13)	W6-O45-W3	94.8(7)
Si1-O45-W1	121.4(11)	O44-O45-W1	129.1(12)
W6-O45-W1	94.7(7)	W3-O45-W1	93.7(7)
Si1-O46-W5	123.2(11)	Si1-O46-W2	119.9(11)
W5-O46-W2	96.7(8)	Si1-O46-W1	119.7(11)
W5-O46-W1	96.4(8)	W2-O46-W1	94.6(8)
Si1-O47-W4	123.0(11)	Si1-O47-W3	121.1(11)
W4-O47-W3	95.9(8)	Si1-O47-W2	119.9(11)
W4-O47-W2	95.5(7)	W3-O47-W2	95.0(7)
O48-W7-O55	100.0(10)	O48-W7-O53	101.5(9)
O55-W7-O53	89.8(9)	O48-W7-O56	98.8(8)
O55-W7-O56	88.6(8)	O53-W7-O56	159.6(9)
O48-W7-O54	100.2(9)	O55-W7-O54	159.9(10)
O53-W7-O54	86.7(8)	O56-W7-O54	87.8(7)
O48-W7-O69	159.7(9)	O55-W7-O69	65.7(10)
O53-W7-O69	65.7(9)	O56-W7-O69	95.2(8)
O54-W7-O69	94.9(8)	O48-W7-O65	156.6(8)

Bond	Angles	Bond	Angles
O55-W7-O65	96.6(10)	O53-W7-O65	94.9(9)
O56-W7-O65	65.1(7)	O54-W7-O65	64.0(8)
O69-W7-O65	43.7(8)	O49-W8-O57	101.1(10)
O49-W8-O56	99.7(8)	O57-W8-O56	159.1(9)
O49-W8-O64	102.7(8)	O57-W8-O64	89.5(8)
O56-W8-O64	88.0(7)	O49-W8-O61	99.1(10)
O57-W8-O61	88.3(9)	O56-W8-O61	86.4(8)
O64-W8-O61	158.1(10)	O49-W8-O68	155.4(10)
O57-W8-O68	63.9(10)	O56-W8-O68	95.7(8)
O64-W8-O68	96.8(9)	O61-W8-O68	62.8(10)
O49-W8-O65	159.4(9)	O57-W8-O65	94.7(10)
O56-W8-O65	65.7(7)	O64-W8-O65	64.0(8)
O61-W8-O65	94.5(10)	O68-W8-O65	45.0(9)
O50-W9-O59	103.0(9)	O50-W9-O57	100.3(9)
O59-W9-O57	88.4(9)	O50-W9-O58	98.8(9)
O59-W9-O58	158.2(10)	O57-W9-O58	87.0(8)
O50-W9-O53	99.3(8)	O59-W9-O53	88.2(8)
O57-W9-O53	160.3(10)	O58-W9-O53	89.0(9)
O50-W9-O68	153.6(8)	O59-W9-O68	96.3(10)
O57-W9-O68	62.0(9)	O58-W9-O68	62.9(9)
O53-W9-O68	99.2(9)	O50-W9-O69	156.2(7)
O59-W9-O69	63.5(8)	O57-W9-O69	98.8(10)
O58-W9-O69	96.3(9)	O53-W9-O69	62.5(8)
O68-W9-O69	50.1(8)	O51-W10-O67	104.4(9)
O51-W10-O59	102.8(9)	O67-W10-O59	88.0(9)
O51-W10-O60	99.3(9)	O67-W10-O60	88.6(8)
O59-W10-O60	157.8(9)	O51-W10-O55	97.8(9)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O67-W10-O55	157.8(10)	O59-W10-O55	87.6(9)
O60-W10-O55	87.4(9)	O51-W10-O69	154.2(8)
O67-W10-O69	97.1(9)	O59-W10-O69	63.5(8)
O60-W10-O69	95.2(9)	O55-W10-O69	61.6(9)
O51-W10-O66	157.8(8)	O67-W10-O66	60.9(9)
O59-W10-O66	93.7(9)	O60-W10-O66	65.6(8)
O55-W10-O66	97.7(9)	O69-W10-O66	47.8(8)
O52-W11-O60	100.4(9)	O52-W11-O58	100.1(9)
O60-W11-O58	159.5(10)	O52-W11-O61	98.9(10)
O60-W11-O61	88.1(9)	O58-W11-O61	88.3(9)
O52-W11-O62	102.5(9)	O60-W11-O62	88.8(8)
O58-W11-O62	87.2(9)	O61-W11-O62	158.6(11)
O52-W11-O68	153.6(8)	O60-W11-O68	97.0(10)
O58-W11-O68	63.7(9)	O61-W11-O68	61.9(9)
O62-W11-O68	97.6(10)	O52-W11-O66	158.4(8)
O60-W11-O66	67.0(9)	O58-W11-O66	93.5(9)
O61-W11-O66	98.1(10)	O62-W11-O66	61.4(9)
O68-W11-O66	47.9(8)	O63-W12-O54	99.4(9)
O63-W12-O62	101.3(10)	O54-W12-O62	89.3(8)
O63-W12-O67	101.0(10)	O54-W12-O67	159.6(10)
O62-W12-O67	87.7(9)	O63-W12-O64	98.6(9)
O54-W12-O64	87.4(7)	O62-W12-O64	160.1(10)
O67-W12-O64	88.6(8)	O63-W12-O66	159.5(9)
O54-W12-O66	95.8(9)	O62-W12-O66	65.1(10)
O67-W12-O66	64.7(10)	O64-W12-O66	95.7(8)
O63-W12-O65	156.8(9)	O54-W12-O65	65.7(8)
O62-W12-O65	96.4(9)	O67-W12-O65	94.6(10)

Bond	Angles	Bond	Angles
O64-W12-O65	64.4(7)	O66-W12-O65	43.6(8)
O65-Si2-O65	180.0	O65-Si2-O69	67.6(12)
O65-Si2-O69	112.4(12)	O65-Si2-O69	112.4(12)
O65-Si2-O69	67.6(12)	O69-Si2-O69	180.0
O65-Si2-O66	113.6(12)	O65-Si2-O66	66.4(12)
O69-Si2-O66	74.3(12)	O69-Si2-O66	105.7(12)
O65-Si2-O66	66.4(12)	O65-Si2-O66	113.6(12)
O69-Si2-O66	105.7(12)	O69-Si2-O66	74.3(12)
O66-Si2-O66	180.0	O65-Si2-O68	111.5(12)
O65-Si2-O68	68.5(12)	O69-Si2-O68	75.3(12)
O69-Si2-O68	104.7(12)	O66-Si2-O68	108.4(12)
O66-Si2-O68	71.6(12)	O65-Si2-O68	68.5(12)
O65-Si2-O68	111.5(12)	O69-Si2-O68	104.7(12)
O69-Si2-O68	75.3(12)	O66-Si2-O68	71.6(12)
O66-Si2-O68	108.4(12)	O68-Si2-O68	180.0
W7-O53-W9	135.2(13)	W12-O54-W7	136.5(11)
W7-O55-W10	135.9(14)	W8-O56-W7	136.5(9)
W8-O57-W9	137.3(13)	W11-O58-W9	137.3(12)
W10-O59-W9	139.3(11)	W11-O60-W10	135.4(12)
W11-O61-W8	137.0(14)	W12-O62-W11	136.2(13)
W8-O64-W12	138.0(10)	Si2-O65-O66	59.4(10)
Si2-O65-O69	58.7(11)	O66-O65-O69	95.9(14)
Si2-O65-W12	123.4(11)	O66-O65-W12	64.0(10)
O69-O65-W12	130.3(14)	Si2-O65-W7	122.5(12)
O66-O65-W7	129.5(15)	O69-O65-W7	63.9(10)
W12-O65-W7	93.4(8)	Si2-O65-W8	123.2(13)
O66-O65-W8	130.9(14)	O69-O65-W8	128.7(13)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
W12-O65-W8	93.4(8)	W7-O65-W8	92.4(7)
Si2-O66-O65	54.3(11)	Si2-O66-W12	126.6(13)
O65-O66-W12	72.3(11)	Si2-O66-W11	120.0(11)
O65-O66-W11	135.3(15)	W12-O66-W11	96.9(9)
Si2-O66-W10	118.1(13)	O65-O66-W10	131.6(14)
W12-O66-W10	95.7(8)	W11-O66-W10	91.9(8)
W10-O67-W12	138.3(13)	Si2-O68-W8	123.2(14)
Si2-O68-W11	120.4(12)	W8-O68-W11	97.9(10)
Si2-O68-W9	116.9(12)	W8-O68-W9	96.7(9)
W11-O68-W9	96.0(10)	Si2-O69-O65	53.8(10)
Si2-O69-W7	126.2(13)	O65-O69-W7	72.4(11)
Si2-O69-W9	117.6(11)	O65-O69-W9	131.0(14)
W7-O69-W9	96.2(9)	Si2-O69-W10	119.8(12)
O65-O69-W10	134.4(14)	W7-O69-W10	96.4(8)
W9-O69-W10	93.5(8)	H70A-O70-H70B	104.1
H71A-O71-H71B	104.1	Eu4A-O72-H72A	102.0
Eu4-O72-H72A	106.0	Eu4A-O72-H72B	82.1
Eu4-O72-H72B	82.8	H72A-O72-H72B	104.1
H73A-O73-H73B	104.1	H74A-O74-H74B	104.1

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S4** The torsion angles ( $^{\circ}$ ) for **1**.

Bond	Angles	Bond	Angles
Eu1-O1-C1-O2	168.0(17)	Eu4-O1-C1-O2	-40.(3)
Eu4A-O1-C1-O2	-46.(2)	Eu1-O1-C1-C2	-12.(2)
Eu4-O1-C1-C2	139.8(13)	Eu4A-O1-C1-C2	134.1(14)
C14-N1-C2-C3	-6.(3)	Eu1-N1-C2-C3	175.5(16)
C14-N1-C2-C1	-179.6(16)	Eu1-N1-C2-C1	1.(2)
O2-C1-C2-N1	-173.7(19)	O1-C1-C2-N1	6.(2)
O2-C1-C2-C3	12.(3)	O1-C1-C2-C3	-168.1(18)
N1-C2-C3-C4	4.(3)	C1-C2-C3-C4	177.7(19)
C2-C3-C4-C5	-2.(3)	C3-C4-C5-C14	1.(3)
C3-C4-C5-C6	178.(2)	C4-C5-C6-C7	-179.(2)
C14-C5-C6-C7	-3.(3)	C5-C6-C7-C8	1.(3)
C6-C7-C8-C13	2.(3)	C6-C7-C8-C9	177.(2)
C13-C8-C9-C10	2.(3)	C7-C8-C9-C10	-173.(2)
C8-C9-C10-C11	-5.(3)	C13-N2-C11-C10	2.(3)
Eu1-N2-C11-C10	-176.4(14)	C13-N2-C11-C12	-178.3(16)
Eu1-N2-C11-C12	4.(2)	C9-C10-C11-N2	3.(3)
C9-C10-C11-C12	-177.4(19)	Eu2-O4-C12-O3	-49.(3)
Eu2-O4-C12-C11	133.9(15)	Eu1-O3-C12-O4	173.9(16)
Eu1-O3-C12-C11	-9.(3)	N2-C11-C12-O4	-179.8(18)
C10-C11-C12-O4	0.(3)	N2-C11-C12-O3	3.(3)
C10-C11-C12-O3	-177.(2)	C11-N2-C13-C8	-4.(3)
Eu1-N2-C13-C8	173.8(14)	C11-N2-C13-C14	177.0(16)
Eu1-N2-C13-C14	-5.(2)	C7-C8-C13-N2	177.6(18)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
C9-C8-C13-N2	2.(3)	C7-C8-C13-C14	-4.(3)
C9-C8-C13-C14	-178.9(16)	C2-N1-C14-C5	5.(3)
Eu1-N1-C14-C5	-176.5(14)	C2-N1-C14-C13	-175.8(16)
Eu1-N1-C14-C13	3.(2)	C4-C5-C14-N1	-2.(3)
C6-C5-C14-N1	-179.3(18)	C4-C5-C14-C13	178.0(19)
C6-C5-C14-C13	1.(3)	N2-C13-C14-N1	1.(2)
C8-C13-C14-N1	-177.8(16)	N2-C13-C14-C5	-179.2(17)
C8-C13-C14-C5	2.(3)	Eu2-O7-C15-O8	172.8(15)
Eu2-O7-C15-C16	-5.(3)	Eu3-O8-C15-O7	42.(4)
Eu3-O8-C15-C16	-139.3(19)	C28-N3-C16-C17	-4.(4)
Eu2-N3-C16-C17	-174.5(19)	C28-N3-C16-C15	176.3(19)
Eu2-N3-C16-C15	6.(3)	O7-C15-C16-N3	-1.(3)
O8-C15-C16-N3	-179.0(19)	O7-C15-C16-C17	180.(2)
O8-C15-C16-C17	2.(4)	N3-C16-C17-C18	2.(4)
C15-C16-C17-C18	-178.(2)	C16-C17-C18-C19	3.(4)
C17-C18-C19-C28	-6.(4)	C17-C18-C19-C20	175.(2)
C18-C19-C20-C21	177.(3)	C28-C19-C20-C21	-2.(4)
C19-C20-C21-C22	-1.(4)	C20-C21-C22-C23	-176.(3)
C20-C21-C22-C27	4.(4)	C27-C22-C23-C24	-3.(4)
C21-C22-C23-C24	178.(2)	C22-C23-C24-C25	3.(4)
C27-N4-C25-C24	-5.(4)	Eu2-N4-C25-C24	171.7(18)
C27-N4-C25-C26	-179.(2)	Eu2-N4-C25-C26	-2.(3)
C23-C24-C25-N4	1.(4)	C23-C24-C25-C26	174.(2)
Eu4A-O10-C26-O9A	-35.(4)	Eu4-O10-C26-O9	24.(5)

Bond	Angles	Bond	Angles
Eu4A-O10-C26-C25	172.1(18)	Eu4-O10-C26-C25	176.8(17)
Eu4A-O10-C26-Eu2	-37.(7)	Eu4-O10-C26-Eu2	-32.(8)
Eu2-O9A-C26-O10	-179.(2)	Eu4A-O9A-C26-O10	22.(2)
Eu2-O9A-C26-C25	-29.(4)	Eu4A-O9A-C26-C25	173.(3)
Eu2-O9A-C26-Eu4A	158.(2)	Eu4A-O9A-C26-Eu2	-158.(2)
Eu2-O9-C26-O10	-158.(3)	Eu2-O9-C26-C25	49.(3)
N4-C25-C26-O10	172.(2)	C24-C25-C26-O10	-1.(4)
N4-C25-C26-O9A	21.(4)	C24-C25-C26-O9A	-153.(3)
N4-C25-C26-O9	-30.(3)	C24-C25-C26-O9	156.(3)
N4-C25-C26-Eu4A	-176.(3)	C24-C25-C26-Eu4A	11.(6)
N4-C25-C26-Eu2	1.1(19)	C24-C25-C26-Eu2	-172.(2)
C25-N4-C27-C22	5.(3)	Eu2-N4-C27-C22	-171.5(16)
C25-N4-C27-C28	-172.(2)	Eu2-N4-C27-C28	11.(3)
C23-C22-C27-N4	-1.(3)	C21-C22-C27-N4	178.(2)
C23-C22-C27-C28	176.(2)	C21-C22-C27-C28	-4.(3)
C16-N3-C28-C19	1.(3)	Eu2-N3-C28-C19	171.4(17)
C16-N3-C28-C27	-178.(2)	Eu2-N3-C28-C27	-7.(3)
C18-C19-C28-N3	4.(4)	C20-C19-C28-N3	-177.(2)
C18-C19-C28-C27	-177.(2)	C20-C19-C28-C27	2.(3)
N4-C27-C28-N3	-2.(3)	C22-C27-C28-N3	-180.(2)
N4-C27-C28-C19	179.(2)	C22-C27-C28-C19	1.(3)
Eu1-O15-C29-O14	39.(3)	Eu1-O15-C29-C30	-139.9(15)
Eu3-O14-C29-O15	177.5(16)	Eu3-O14-C29-C30	-4.(2)
C42-N8-C30-C31	-5.(3)	Eu3-N8-C30-C31	-175.5(15)

Bond	Angles	Bond	Angles
C42-N8-C30-C29	175.9(16)	Eu3-N8-C30-C29	5.(2)
O15-C29-C30-N8	177.7(18)	O14-C29-C30-N8	-1.(3)
O15-C29-C30-C31	-2.(3)	O14-C29-C30-C31	179.3(19)
N8-C30-C31-C32	2.(3)	C29-C30-C31-C32	-179.0(18)
C30-C31-C32-C33	0.(3)	C31-C32-C33-C42	1.(2)
C31-C32-C33-C34	174.2(18)	C42-C33-C34-C35	-1.(3)
C32-C33-C34-C35	-174.0(19)	C33-C34-C35-C36	0.(3)
C34-C35-C36-C37	174.(2)	C34-C35-C36-C41	-1.(3)
C41-C36-C37-C38	-2.(3)	C35-C36-C37-C38	-178.(2)
C36-C37-C38-C39	4.(4)	C41-N5-C39-C38	4.(3)
Eu3-N5-C39-C38	177.4(19)	C41-N5-C39-C40	-173.(2)
Eu3-N5-C39-C40	1.(3)	C37-C38-C39-N5	-5.(4)
C37-C38-C39-C40	171.(2)	Eu3-O16-C40-O17	-176.(2)
Eu3-O16-C40-C39	6.(4)	Eu4A-O17-C40-O16	76.(8)
Eu4-O17-C40-O16	69.(5)	Eu4A-O17-C40-C39	-105.(7)
Eu4-O17-C40-C39	-113.(3)	N5-C39-C40-O16	-4.(4)
C38-C39-C40-O16	179.(2)	N5-C39-C40-O17	177.(2)
C38-C39-C40-O17	1.(4)	C39-N5-C41-C36	-1.(3)
Eu3-N5-C41-C36	-174.6(14)	C39-N5-C41-C42	172.3(18)
Eu3-N5-C41-C42	-1.(2)	C37-C36-C41-N5	0.(3)
C35-C36-C41-N5	176.2(19)	C37-C36-C41-C42	-172.9(19)
C35-C36-C41-C42	3.(3)	C30-N8-C42-C33	6.(3)
Eu3-N8-C42-C33	176.8(13)	C30-N8-C42-C41	-174.4(17)
Eu3-N8-C42-C41	-4.(2)	C32-C33-C42-N8	-4.(3)

Bond	Angles	Bond	Angles
C34-C33-C42-N8	-178.0(17)	C32-C33-C42-C41	176.3(16)
C34-C33-C42-C41	3.(3)	N5-C41-C42-N8	3.(3)
C36-C41-C42-N8	176.8(17)	N5-C41-C42-C33	-177.4(17)
C36-C41-C42-C33	-4.(3)	Eu4A-O21-C43-O22	145.(2)
Eu4-O21-C43-O22	162.6(19)	Eu4A-O21-C43-C44	-34.(3)
Eu4-O21-C43-C44	-17.(3)	C55-N7-C44-C45	1.(3)
Eu4A-N7-C44-C45	-155.(2)	Eu4-N7-C44-C45	-171.4(18)
C55-N7-C44-C43	178.8(19)	Eu4A-N7-C44-C43	23.(3)
Eu4-N7-C44-C43	7.(3)	C55-N7-C44-Eu4A	156.(2)
O22-C43-C44-N7	-174.(2)	O21-C43-C44-N7	5.(3)
O22-C43-C44-C45	4.(4)	O21-C43-C44-C45	-176.(2)
O22-C43-C44-Eu4A	-157.(3)	O21-C43-C44-Eu4A	22.(2)
N7-C44-C45-C46	-2.(3)	C43-C44-C45-C46	-179.(2)
Eu4A-C44-C45-C46	-55.(6)	C44-C45-C46-C47	3.(3)
C45-C46-C47-C55	-3.(3)	C45-C46-C47-C48	-179.0(19)
C46-C47-C48-C49	-179.8(19)	C55-C47-C48-C49	4.(3)
C47-C48-C49-C50	-2.(3)	C48-C49-C50-C51	-177.(2)
C48-C49-C50-C56	0.(3)	C56-C50-C51-C52	0.(3)
C49-C50-C51-C52	177.2(19)	C50-C51-C52-C53	0.(3)
C56-N6-C53-C52	-2.(3)	Eu4-N6-C53-C52	174.2(14)
Eu4A-N6-C53-C52	158.4(16)	C56-N6-C53-C54	172.6(15)
Eu4-N6-C53-C54	-11.(2)	Eu4A-N6-C53-C54	-27.(2)
C51-C52-C53-N6	1.(3)	C51-C52-C53-C54	-173.5(18)
Eu4-O23-C54-O24	-175.1(16)	Eu1-O23-C54-O24	23.(3)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
Eu4A-O23-C54-O24	-162.4(18)	Eu4-O23-C54-C53	5.(2)
Eu1-O23-C54-C53	-157.3(12)	Eu4A-O23-C54-C53	18.(2)
Eu4-O23-C54-Eu1	162.3(18)	Eu4A-O23-C54-Eu1	175.0(17)
N6-C53-C54-O24	-176.(2)	C52-C53-C54-O24	0.(3)
N6-C53-C54-O23	4.(2)	C52-C53-C54-O23	179.6(17)
N6-C53-C54-Eu1	-30.(3)	C52-C53-C54-Eu1	146.(2)
C44-N7-C55-C56	-177.1(18)	Eu4A-N7-C55-C56	-24.(2)
Eu4-N7-C55-C56	-5.(2)	C44-N7-C55-C47	-1.(3)
Eu4A-N7-C55-C47	152.3(16)	Eu4-N7-C55-C47	170.9(13)
C46-C47-C55-N7	2.(3)	C48-C47-C55-N7	178.5(17)
C46-C47-C55-C56	178.4(17)	C48-C47-C55-C56	-6.(2)
C53-N6-C56-C55	-174.9(15)	Eu4-N6-C56-C55	8.(2)
Eu4A-N6-C56-C55	21.6(19)	C53-N6-C56-C50	3.(3)
Eu4-N6-C56-C50	-174.1(13)	Eu4A-N6-C56-C50	-160.9(15)
N7-C55-C56-N6	-2.(2)	C47-C55-C56-N6	-178.2(15)
N7-C55-C56-C50	-179.6(16)	C47-C55-C56-C50	4.(3)
C51-C50-C56-N6	-1.(3)	C49-C50-C56-N6	-178.8(16)
C51-C50-C56-C55	175.9(17)	C49-C50-C56-C55	-1.(3)
O26-W1-O31-W2	150.7(19)	O33-W1-O31-W2	-108.(2)
O39-W1-O31-W2	51.(2)	O38-W1-O31-W2	-28.(4)
O46-W1-O31-W2	-8.2(17)	O45-W1-O31-W2	-45.(2)
O27-W2-O32-W5	154.7(16)	O34-W2-O32-W5	-106.4(17)
O31-W2-O32-W5	50.8(18)	O36-W2-O32-W5	-23.(3)
O46-W2-O32-W5	-8.1(14)	O47-W2-O32-W5	-42.9(17)

Bond	Angles	Bond	Angles
O26-W1-O33-W6	-155.7(15)	O31-W1-O33-W6	102.8(17)
O39-W1-O33-W6	23.(3)	O38-W1-O33-W6	-54.8(17)
O46-W1-O33-W6	40.9(17)	O45-W1-O33-W6	7.6(14)
O27-W2-O34-W3	-156.9(18)	O32-W2-O34-W3	101.6(19)
O31-W2-O34-W3	12.(4)	O36-W2-O34-W3	-57.1(19)
O46-W2-O34-W3	38.9(19)	O47-W2-O34-W3	3.3(15)
O28-W3-O35-W4	-152.1(17)	O38-W3-O35-W4	107.7(18)
O34-W3-O35-W4	-51.6(18)	O37-W3-O35-W4	25.(3)
O47-W3-O35-W4	9.2(15)	O45-W3-O35-W4	42.7(18)
O42-W4-O36-W2	-154.8(17)	O43-W4-O36-W2	105.6(18)
O41-W4-O36-W2	23.(3)	O35-W4-O36-W2	-51.5(18)
O47-W4-O36-W2	7.4(15)	O44-W4-O36-W2	42.6(18)
O28-W3-O38-W1	160.0(15)	O35-W3-O38-W1	-99.3(17)
O34-W3-O38-W1	-15.(3)	O37-W3-O38-W1	58.8(16)
O47-W3-O38-W1	-37.3(16)	O45-W3-O38-W1	-3.3(13)
O30-W6-O40-W5	155.7(16)	O37-W6-O40-W5	-102.8(17)
O43-W6-O40-W5	57.3(17)	O33-W6-O40-W5	-13.(3)
O44-W6-O40-W5	-4.8(14)	O45-W6-O40-W5	-37.3(17)
O29-W5-O41-W4	155.7(14)	O39-W5-O41-W4	-103.0(15)
O32-W5-O41-W4	-16.(3)	O40-W5-O41-W4	54.3(15)
O46-W5-O41-W4	-39.6(15)	O44-W5-O41-W4	-5.1(13)
O42-W4-O41-W5	-155.3(14)	O43-W4-O41-W5	-55.8(15)
O36-W4-O41-W5	27.(3)	O35-W4-O41-W5	102.4(16)
O47-W4-O41-W5	40.9(15)	O44-W4-O41-W5	5.2(13)

Bond	Angles	Bond	Angles
O42-W4-O43-W6	157.4(17)	O36-W4-O43-W6	-101.5(18)
O41-W4-O43-W6	56.1(18)	O35-W4-O43-W6	-15.(3)
O47-W4-O43-W6	-38.1(18)	O44-W4-O43-W6	-6.1(15)
O45-Si1-O44-O45	180.002(5)	O47-Si1-O44-O45	58.4(13)
O47-Si1-O44-O45	-121.6(13)	O46-Si1-O44-O45	-60.0(12)
O46-Si1-O44-O45	120.0(12)	O45-Si1-O44-W6	177.5(11)
O45-Si1-O44-W6	-2.5(11)	O47-Si1-O44-W6	55.9(15)
O47-Si1-O44-W6	-124.1(15)	O46-Si1-O44-W6	-62.4(15)
O46-Si1-O44-W6	117.6(15)	O45-Si1-O44-W4	-57.9(15)
O45-Si1-O44-W4	122.0(15)	O47-Si1-O44-W4	-179.5(11)
O47-Si1-O44-W4	0.5(11)	O46-Si1-O44-W4	62.1(14)
O46-Si1-O44-W4	-117.9(14)	O45-Si1-O44-W5	57.3(14)
O45-Si1-O44-W5	-122.7(14)	O47-Si1-O44-W5	-64.3(14)
O47-Si1-O44-W5	115.7(14)	O46-Si1-O44-W5	177.4(11)
O46-Si1-O44-W5	-2.6(11)	O44-Si1-O45-O44	180.004(5)
O47-Si1-O45-O44	-57.4(13)	O47-Si1-O45-O44	122.6(13)
O46-Si1-O45-O44	59.2(12)	O46-Si1-O45-O44	-120.8(12)
O44-Si1-O45-W6	177.6(11)	O44-Si1-O45-W6	-2.4(11)
O47-Si1-O45-W6	-59.8(15)	O47-Si1-O45-W6	120.2(15)
O46-Si1-O45-W6	56.8(15)	O46-Si1-O45-W6	-123.2(15)
O44-Si1-O45-W3	56.3(15)	O44-Si1-O45-W3	-123.7(15)
O47-Si1-O45-W3	178.9(12)	O47-Si1-O45-W3	-1.1(12)
O46-Si1-O45-W3	-64.5(14)	O46-Si1-O45-W3	115.5(14)
O44-Si1-O45-W1	-61.2(14)	O44-Si1-O45-W1	118.8(14)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O47-Si1-O45-W1	61.4(14)	O47-Si1-O45-W1	-118.6(14)
O46-Si1-O45-W1	178.1(11)	O46-Si1-O45-W1	-1.9(11)
O45-Si1-O46-W5	-119.9(15)	O45-Si1-O46-W5	60.1(15)
O44-Si1-O46-W5	2.9(12)	O44-Si1-O46-W5	-177.1(12)
O47-Si1-O46-W5	122.9(15)	O47-Si1-O46-W5	-57.1(15)
O45-Si1-O46-W2	117.6(14)	O45-Si1-O46-W2	-62.4(14)
O44-Si1-O46-W2	-119.6(14)	O44-Si1-O46-W2	60.4(14)
O47-Si1-O46-W2	0.4(11)	O47-Si1-O46-W2	-179.6(11)
O45-Si1-O46-W1	1.9(11)	O45-Si1-O46-W1	-178.1(11)
O44-Si1-O46-W1	124.7(14)	O44-Si1-O46-W1	-55.3(14)
O47-Si1-O46-W1	-115.3(14)	O47-Si1-O46-W1	64.7(14)
O45-Si1-O47-W4	123.4(15)	O45-Si1-O47-W4	-56.6(15)
O44-Si1-O47-W4	-0.5(11)	O44-Si1-O47-W4	179.5(11)
O46-Si1-O47-W4	-119.8(15)	O46-Si1-O47-W4	60.2(15)
O45-Si1-O47-W3	1.1(12)	O45-Si1-O47-W3	-178.9(12)
O44-Si1-O47-W3	-122.7(15)	O44-Si1-O47-W3	57.3(15)
O46-Si1-O47-W3	118.0(15)	O46-Si1-O47-W3	-62.1(15)
O45-Si1-O47-W2	-116.4(14)	O45-Si1-O47-W2	63.6(14)
O44-Si1-O47-W2	119.7(14)	O44-Si1-O47-W2	-60.3(14)
O46-Si1-O47-W2	0.4(11)	O46-Si1-O47-W2	-179.6(11)
O48-W7-O53-W9	-157.0(16)	O55-W7-O53-W9	-56.9(18)
O56-W7-O53-W9	29.(3)	O54-W7-O53-W9	103.3(17)
O69-W7-O53-W9	6.4(14)	O65-W7-O53-W9	39.8(17)
O63-W12-O54-W7	-154.8(14)	O62-W12-O54-W7	103.8(15)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O67-W12-O54-W7	22.(3)	O64-W12-O54-W7	-56.6(14)
O66-W12-O54-W7	38.9(14)	O65-W12-O54-W7	6.5(12)
O48-W7-O55-W10	158.5(16)	O53-W7-O55-W10	56.8(18)
O56-W7-O55-W10	-102.8(17)	O54-W7-O55-W10	-23.(3)
O69-W7-O55-W10	-6.5(15)	O65-W7-O55-W10	-38.2(18)
O49-W8-O56-W7	158.3(13)	O57-W8-O56-W7	-27.(3)
O64-W8-O56-W7	55.8(14)	O61-W8-O56-W7	-103.0(15)
O68-W8-O56-W7	-40.8(15)	O65-W8-O56-W7	-6.4(12)
O49-W8-O57-W9	156.5(18)	O56-W8-O57-W9	-18.(4)
O64-W8-O57-W9	-100.6(19)	O61-W8-O57-W9	57.6(19)
O68-W8-O57-W9	-2.8(16)	O65-W8-O57-W9	-36.8(19)
O51-W10-O59-W9	-152.2(18)	O67-W10-O59-W9	103.(2)
O60-W10-O59-W9	22.(4)	O55-W10-O59-W9	-54.8(19)
O69-W10-O59-W9	4.5(16)	O66-W10-O59-W9	42.8(19)
O52-W11-O60-W10	157.9(16)	O58-W11-O60-W10	-23.(4)
O61-W11-O60-W10	-103.3(18)	O62-W11-O60-W10	55.5(18)
O68-W11-O60-W10	-42.0(18)	O66-W11-O60-W10	-3.7(15)
O52-W11-O61-W8	-154.1(18)	O60-W11-O61-W8	105.7(19)
O58-W11-O61-W8	-54.1(19)	O62-W11-O61-W8	24.(4)
O68-W11-O61-W8	6.7(16)	O66-W11-O61-W8	39.2(19)
O63-W12-O62-W11	157.0(17)	O54-W12-O62-W11	-103.5(18)
O67-W12-O62-W11	56.3(18)	O64-W12-O62-W11	-23.(4)
O66-W12-O62-W11	-6.8(15)	O65-W12-O62-W11	-38.0(18)
O49-W8-O64-W12	-157.3(14)	O57-W8-O64-W12	101.4(15)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O56-W8-O64-W12	-57.8(14)	O61-W8-O64-W12	17.(3)
O68-W8-O64-W12	37.7(15)	O65-W8-O64-W12	6.0(12)
O69-Si2-O65-O66	-120.0(14)	O69-Si2-O65-O66	60.0(14)
O66-Si2-O65-O66	180.001(2)	O68-Si2-O65-O66	-57.2(14)
O68-Si2-O65-O66	122.8(14)	O69-Si2-O65-O69	180.002(2)
O66-Si2-O65-O69	-60.0(14)	O66-Si2-O65-O69	120.0(14)
O68-Si2-O65-O69	62.8(14)	O68-Si2-O65-O69	-117.2(14)
O69-Si2-O65-W12	-120.4(17)	O69-Si2-O65-W12	59.6(17)
O66-Si2-O65-W12	179.6(13)	O66-Si2-O65-W12	-0.4(13)
O68-Si2-O65-W12	-57.6(17)	O68-Si2-O65-W12	122.4(17)
O69-Si2-O65-W7	-0.1(12)	O69-Si2-O65-W7	180.0(12)
O66-Si2-O65-W7	-60.0(17)	O66-Si2-O65-W7	120.0(17)
O68-Si2-O65-W7	62.8(16)	O68-Si2-O65-W7	-117.2(16)
O69-Si2-O65-W8	118.5(16)	O69-Si2-O65-W8	-61.5(16)
O66-Si2-O65-W8	58.5(17)	O66-Si2-O65-W8	-121.5(17)
O68-Si2-O65-W8	-178.7(12)	O68-Si2-O65-W8	1.3(12)
O65-Si2-O66-O65	179.998(3)	O69-Si2-O66-O65	56.2(14)
O69-Si2-O66-O65	-123.8(14)	O68-Si2-O66-O65	124.5(15)
O68-Si2-O66-O65	-55.5(15)	O65-Si2-O66-W12	0.4(14)
O65-Si2-O66-W12	-179.6(14)	O69-Si2-O66-W12	56.7(17)
O69-Si2-O66-W12	-123.3(17)	O68-Si2-O66-W12	124.9(18)
O68-Si2-O66-W12	-55.1(18)	O65-Si2-O66-W11	-126.6(17)
O65-Si2-O66-W11	53.4(17)	O69-Si2-O66-W11	-70.3(15)
O69-Si2-O66-W11	109.7(15)	O68-Si2-O66-W11	-2.1(13)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O68-Si2-O66-W11	177.9(13)	O65-Si2-O66-W10	122.9(16)
O65-Si2-O66-W10	-57.1(16)	O69-Si2-O66-W10	179.2(12)
O69-Si2-O66-W10	-0.8(12)	O68-Si2-O66-W10	-112.6(15)
O68-Si2-O66-W10	67.4(15)	O69-O65-O66-Si2	-48.0(11)
W12-O65-O66-Si2	179.6(12)	W7-O65-O66-Si2	-108.8(17)
W8-O65-O66-Si2	109.3(18)	Si2-O65-O66-W12	-179.6(12)
O69-O65-O66-W12	132.3(14)	W7-O65-O66-W12	71.6(15)
W8-O65-O66-W12	-70.4(16)	Si2-O65-O66-W11	98.5(18)
O69-O65-O66-W11	50.(2)	W12-O65-O66-W11	-81.9(17)
W7-O65-O66-W11	-10.(3)	W8-O65-O66-W11	-152.2(13)
Si2-O65-O66-W10	-97.8(18)	O69-O65-O66-W10	-145.9(16)
W12-O65-O66-W10	81.8(16)	W7-O65-O66-W10	153.4(12)
W8-O65-O66-W10	11.(3)	O51-W10-O67-W12	155.5(18)
O59-W10-O67-W12	-101.8(19)	O60-W10-O67-W12	56.2(19)
O55-W10-O67-W12	-23.(4)	O69-W10-O67-W12	-38.8(19)
O66-W10-O67-W12	-6.5(16)	O63-W12-O67-W10	-157.8(18)
O54-W12-O67-W10	25.(4)	O62-W12-O67-W10	-57.(2)
O64-W12-O67-W10	103.8(19)	O66-W12-O67-W10	6.8(16)
O65-W12-O67-W10	39.6(19)	O65-Si2-O68-W8	-1.4(13)
O65-Si2-O68-W8	178.6(13)	O69-Si2-O68-W8	-59.6(16)
O69-Si2-O68-W8	120.4(16)	O66-Si2-O68-W8	-127.2(17)
O66-Si2-O68-W8	52.8(17)	O65-Si2-O68-W11	123.6(17)
O65-Si2-O68-W11	-56.4(17)	O69-Si2-O68-W11	65.4(16)
O69-Si2-O68-W11	-114.6(16)	O66-Si2-O68-W11	-2.1(13)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
O66-Si2-O68-W11	177.9(13)	O65-Si2-O68-W9	-120.7(16)
O65-Si2-O68-W9	59.3(16)	O69-Si2-O68-W9	-178.9(13)
O69-Si2-O68-W9	1.1(13)	O66-Si2-O68-W9	113.6(16)
O66-Si2-O68-W9	-66.4(16)	O65-Si2-O69-O65	180.002(4)
O66-Si2-O69-O65	55.5(13)	O66-Si2-O69-O65	-124.5(13)
O68-Si2-O69-O65	-58.8(14)	O68-Si2-O69-O65	121.2(14)
O65-Si2-O69-W7	179.9(13)	O65-Si2-O69-W7	-0.1(13)
O66-Si2-O69-W7	55.4(17)	O66-Si2-O69-W7	-124.6(17)
O68-Si2-O69-W7	-58.9(17)	O68-Si2-O69-W7	121.1(17)
O65-Si2-O69-W9	57.7(16)	O65-Si2-O69-W9	-122.3(16)
O66-Si2-O69-W9	-66.8(15)	O66-Si2-O69-W9	113.2(15)
O68-Si2-O69-W9	178.9(12)	O68-Si2-O69-W9	-1.1(12)
O65-Si2-O69-W10	-54.6(16)	O65-Si2-O69-W10	125.4(16)
O66-Si2-O69-W10	-179.1(12)	O66-Si2-O69-W10	0.9(12)
O68-Si2-O69-W10	66.5(15)	O68-Si2-O69-W10	-113.5(15)

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S5** Hydrogen bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) for **1**.

	<b>Donor-H</b>	<b>Acceptor-H</b>	<b>Donor-Acceptor</b>	<b>Angle</b>
O11A-H11C $\cdots$ O21	0.87	2.56	3.27(4)	139.2
C17-H17 $\cdots$ O56	0.95	2.53	3.36(3)	146.7
C38-H38 $\cdots$ O42	0.95	2.42	3.25(3)	146.6
O70-H70B $\cdots$ O2	0.87	2.12	2.95(3)	159.2
O71-H71A $\cdots$ O33	0.87	2.49	3.13(4)	130.4
O71-H71B $\cdots$ O25	0.87	2.33	3.04(3)	139.0
O72-H72A $\cdots$ O9 <sup>a</sup>	0.87	1.72	2.50(4)	147.7
O72-H72B $\cdots$ O17	0.87	1.84	2.59(3)	143.6
O73-H73A $\cdots$ O17	0.87	2.60	3.45(4)	169.7
O74-H74A $\cdots$ O22	0.87	1.91	2.77(3)	168.4

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S6** Atomic coordinates and equivalent isotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **1**.(U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
Eu1	0.28872(3)	0.10464(7)	0.27989(5)	0.02448(19)
Eu2	0.26174(3)	0.49228(9)	0.15326(7)	0.0471(3)
Eu3	0.24302(3)	0.10831(8)	0.98657(5)	0.0334(2)
Eu4	0.21184(3)	0.87262(8)	0.25643(5)	0.0234(3)
Eu4A	0.2069(6)	0.8322(19)	0.2359(12)	0.0234(3)
O1	0.2779(4)	0.9416(9)	0.3140(6)	0.026(3)
O2	0.3006(5)	0.8051(12)	0.3622(9)	0.052(4)
O3	0.2861(4)	0.2732(10)	0.2602(7)	0.032(3)
O4	0.3116(4)	0.4117(10)	0.2290(8)	0.040(3)
O5	0.3017(4)	0.0537(10)	0.1751(6)	0.028(3)
O6	0.3195(4)	0.1500(11)	0.3870(7)	0.036(3)
O7	0.2580(5)	0.3380(13)	0.0992(9)	0.053(4)
O8	0.2862(4)	0.2106(11)	0.0525(7)	0.038(3)
O9	0.2444(7)	0.6637(16)	0.1597(13)	0.048(6)
O9A	0.2492(10)	0.6448(17)	0.2076(17)	0.048(6)
O10	0.2672(5)	0.7971(14)	0.2206(9)	0.058(5)
O11	0.2497(6)	0.5490(14)	0.0450(10)	0.064(5)
O11A	0.2650(10)	0.568(2)	0.2695(15)	0.044(7)
O12	0.1871(6)	0.5144(17)	0.1223(12)	0.079(6)
O13	0.2232(7)	0.3938(15)	0.2172(13)	0.086(7)
O14	0.2555(4)	0.2362(12)	0.9171(8)	0.041(4)
O15	0.2353(4)	0.3479(11)	0.8399(7)	0.036(3)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
O16	0.2425(5)	0.9949(12)	0.0743(9)	0.055(4)
O17	0.2097(6)	0.8913(14)	0.1372(9)	0.059(5)
O18	0.2429(5)	0.9856(14)	0.9082(10)	0.065(5)
O19	0.3112(6)	0.0543(16)	0.9782(13)	0.087(7)
O20	0.2005(4)	0.2127(11)	0.0409(7)	0.039(3)
O21	0.2079(6)	0.7314(15)	0.3230(10)	0.064(5)
O22	0.1767(5)	0.5981(12)	0.3490(9)	0.047(4)
O23	0.2264(4)	0.0352(10)	0.2278(7)	0.032(3)
O24	0.2122(5)	0.1767(14)	0.1849(8)	0.050(4)
O25	0.1988(4)	0.9518(12)	0.3570(7)	0.039(3)
N1	0.3511(5)	0.0017(12)	0.3020(7)	0.027(3)
N2	0.3547(5)	0.1831(11)	0.2641(7)	0.025(3)
N3	0.3227(6)	0.4389(14)	0.1017(10)	0.044(4)
N4	0.3192(5)	0.6116(13)	0.1548(9)	0.036(4)
N5	0.1771(6)	0.0230(13)	0.9929(9)	0.037(4)
N6	0.1521(4)	0.9815(12)	0.2171(7)	0.026(3)
N7	0.1416(5)	0.8133(13)	0.2752(8)	0.032(4)
N8	0.1836(4)	0.1598(11)	0.9068(7)	0.024(3)
C1	0.3065(6)	0.8807(14)	0.3359(9)	0.029(4)
C2	0.3491(5)	0.9122(13)	0.3259(9)	0.026(4)
C3	0.3819(7)	0.8481(17)	0.3353(11)	0.041(5)
C4	0.4202(7)	0.8835(17)	0.3224(11)	0.040(5)
C5	0.4226(6)	0.9765(16)	0.3000(10)	0.037(5)
C6	0.4594(5)	0.0201(15)	0.2880(10)	0.031(4)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
C7	0.4616(6)	0.1093(17)	0.2672(10)	0.038(5)
C8	0.4268(5)	0.1691(15)	0.2563(9)	0.028(4)
C9	0.4250(6)	0.2701(15)	0.2365(9)	0.031(4)
C10	0.3912(6)	0.3203(16)	0.2348(10)	0.034(4)
C11	0.3565(5)	0.2768(14)	0.2471(9)	0.027(4)
C12	0.3149(6)	0.3242(15)	0.2444(11)	0.036(4)
C13	0.3894(5)	0.1348(13)	0.2698(8)	0.023(3)
C14	0.3873(5)	0.0346(15)	0.2915(9)	0.027(4)
C15	0.2869(7)	0.2989(17)	0.0761(11)	0.042(5)
C16	0.3259(7)	0.3510(17)	0.0755(12)	0.045(5)
C17	0.3597(8)	0.317(2)	0.0521(13)	0.051(6)
C18	0.3940(7)	0.3734(19)	0.0565(13)	0.050(6)
C19	0.3943(7)	0.4610(17)	0.0876(11)	0.041(5)
C20	0.4301(7)	0.5264(17)	0.1008(12)	0.044(5)
C21	0.4270(6)	0.6088(17)	0.1274(12)	0.041(5)
C22	0.3895(7)	0.6488(16)	0.1467(11)	0.038(5)
C23	0.3841(7)	0.7382(19)	0.1720(13)	0.050(6)
C24	0.3450(6)	0.7673(17)	0.1859(11)	0.040(5)
C25	0.3137(7)	0.7002(19)	0.1754(12)	0.048(6)
C26	0.2717(9)	0.716(2)	0.1938(13)	0.060(7)
C27	0.3555(6)	0.5881(15)	0.1384(10)	0.031(4)
C28	0.3579(7)	0.4940(17)	0.1080(12)	0.043(5)
C29	0.2294(6)	0.2794(15)	0.8748(10)	0.033(4)
C30	0.1868(6)	0.2349(15)	0.8693(10)	0.034(4)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
C31	0.1547(6)	0.2725(14)	0.8269(9)	0.029(4)
C32	0.1169(6)	0.2305(14)	0.8247(9)	0.027(4)
C33	0.1122(5)	0.1516(13)	0.8656(8)	0.021(3)
C34	0.0745(6)	0.1083(14)	0.8719(9)	0.029(4)
C35	0.0710(6)	0.0384(15)	0.9160(10)	0.034(4)
C36	0.1055(6)	0.0043(14)	0.9592(10)	0.031(4)
C37	0.1029(8)	0.9374(18)	0.0098(12)	0.048(6)
C38	0.1383(8)	0.9121(19)	0.0504(13)	0.051(6)
C39	0.1739(7)	0.9594(16)	0.0418(11)	0.038(5)
C40	0.2113(9)	0.948(2)	0.0878(13)	0.058(7)
C41	0.1437(6)	0.0454(14)	0.9532(9)	0.029(4)
C42	0.1465(5)	0.1222(13)	0.9068(8)	0.022(3)
C43	0.1758(7)	0.6815(18)	0.3269(12)	0.045(5)
C44	0.1375(7)	0.7301(17)	0.3023(11)	0.042(5)
C45	0.1002(6)	0.6852(17)	0.3072(11)	0.038(5)
C46	0.0653(6)	0.7383(15)	0.2814(9)	0.030(4)
C47	0.0684(6)	0.8234(15)	0.2520(9)	0.031(4)
C48	0.0352(6)	0.8838(15)	0.2251(10)	0.033(4)
C49	0.0390(6)	0.9667(15)	0.1964(9)	0.031(4)
C50	0.0787(6)	0.0071(14)	0.1907(9)	0.027(4)
C51	0.0878(6)	0.0961(16)	0.1643(10)	0.035(4)
C52	0.1265(6)	0.1277(16)	0.1641(10)	0.034(4)
C53	0.1578(5)	0.0670(14)	0.1922(9)	0.026(4)
C54	0.2020(6)	0.1018(16)	0.2006(10)	0.033(4)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
C55	0.1081(5)	0.8619(13)	0.2503(8)	0.022(3)
C56	0.1131(6)	0.9515(14)	0.2179(9)	0.027(4)
W1	0.07991(2)	0.16745(6)	0.50481(4)	0.02897(17)
W2	0.05394(2)	0.06846(7)	0.64993(3)	0.03110(18)
W3	0.97674(3)	0.89502(6)	0.64560(4)	0.03248(19)
W4	0.06797(2)	0.83750(6)	0.58650(4)	0.02887(17)
W5	0.01132(3)	0.76587(6)	0.43846(4)	0.03222(18)
W6	0.08914(2)	0.93653(6)	0.43796(3)	0.02501(16)
Si1	0.0	0.0	0.5	0.0153(11)
O26	0.1178(4)	0.2485(11)	0.5087(8)	0.039(4)
O27	0.0797(5)	0.0979(14)	0.7231(8)	0.049(4)
O28	0.9669(5)	0.8444(10)	0.7148(6)	0.035(3)
O29	0.0162(6)	0.6566(11)	0.4079(8)	0.051(4)
O30	0.1323(5)	0.9059(15)	0.4110(8)	0.054(5)
O31	0.0858(6)	0.1209(16)	0.5890(10)	0.071(5)
O32	0.0184(6)	0.1706(16)	0.6357(10)	0.068(5)
O33	0.1052(6)	0.0560(14)	0.4811(9)	0.066(5)
O34	0.0132(6)	0.9944(15)	0.6792(11)	0.069(5)
O35	0.0208(6)	0.8234(15)	0.6294(11)	0.068(5)
O36	0.0804(6)	0.9514(15)	0.6332(11)	0.071(5)
O37	0.9358(6)	0.9941(14)	0.6327(10)	0.069(5)
O38	0.9433(6)	0.8198(13)	0.5842(9)	0.064(5)
O39	0.9619(6)	0.7523(16)	0.4735(9)	0.067(5)
O40	0.0578(6)	0.8312(15)	0.4136(8)	0.061(5)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
O41	0.0405(5)	0.7561(13)	0.5224(8)	0.051(4)
O42	0.1003(5)	0.7618(13)	0.6270(8)	0.052(4)
O43	0.0988(6)	0.8801(15)	0.5233(9)	0.066(5)
O44	0.0329(6)	0.9168(16)	0.4929(10)	0.016(4)
O45	0.9639(6)	0.9632(15)	0.5378(10)	0.014(4)
O46	0.9777(7)	0.9081(16)	0.4583(10)	0.017(4)
O47	0.0189(6)	0.9604(16)	0.5716(10)	0.016(4)
O48	0.6056(5)	0.7526(13)	0.5915(9)	0.051(4)
W7	0.57177(2)	0.67224(6)	0.56399(4)	0.02882(17)
W8	0.58470(2)	0.54706(6)	0.41944(4)	0.02717(16)
W9	0.51327(3)	0.37385(8)	0.35809(4)	0.0468(2)
W10	0.43602(2)	0.54727(8)	0.35291(4)	0.0384(2)
W11	0.42187(3)	0.67215(7)	0.49590(5)	0.0386(2)
W12	0.50702(2)	0.71890(7)	0.41800(4)	0.03499(19)
Si2	0.5	0.5	0.5	0.0140(11)
O49	0.6256(4)	0.5671(14)	0.3827(7)	0.050(4)
O50	0.5203(4)	0.3110(11)	0.2915(7)	0.039(3)
O51	0.4045(4)	0.5649(12)	0.2850(8)	0.042(4)
O52	0.3847(5)	0.7513(12)	0.4964(8)	0.046(4)
O53	0.5309(6)	0.6981(15)	0.6151(10)	0.070(5)
O54	0.5404(5)	0.7459(14)	0.4954(8)	0.053(4)
O55	0.5886(7)	0.5703(17)	0.6178(11)	0.080(6)
O56	0.5993(5)	0.6150(12)	0.4974(8)	0.046(4)
O57	0.5547(7)	0.4678(16)	0.3584(11)	0.080(6)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
O58	0.5494(7)	0.3045(14)	0.4214(10)	0.071(5)
O59	0.4757(6)	0.4691(15)	0.3246(10)	0.065(5)
O60	0.4078(6)	0.6166(16)	0.4135(10)	0.070(5)
O61	0.3977(7)	0.5655(17)	0.5322(11)	0.083(6)
O62	0.4621(6)	0.7457(17)	0.4604(11)	0.075(6)
O63	0.5118(6)	0.8206(13)	0.3785(8)	0.058(5)
O64	0.5512(5)	0.6505(13)	0.3904(8)	0.048(4)
O65	0.5290(6)	0.5790(17)	0.4818(11)	0.020(5)
O66	0.4773(7)	0.5878(17)	0.4568(11)	0.023(5)
O67	0.4722(6)	0.6498(18)	0.3553(11)	0.078(6)
O68	0.5358(8)	0.4539(19)	0.4584(12)	0.027(5)
O69	0.4749(7)	0.4490(18)	0.4356(11)	0.021(5)
O70	0.3184(8)	0.901(2)	0.8809(15)	0.038(7)
O71	0.1966(8)	0.4165(19)	0.9736(12)	0.029(6)
O72	0.1816(8)	0.740(2)	0.1876(13)	0.030(6)
O73	0.1851(10)	0.809(2)	0.5426(17)	0.048(8)
O74	0.1574(6)	0.4700(16)	0.2475(10)	0.068(5)

**Table S7** Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **1**.

The anisotropic atomic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
Eu1	0.0161(4)	0.0256(4)	0.0327(5)	-0.0017(4)	0.0067(3)	0.0016(3)
Eu2	0.0259(5)	0.0447(7)	0.0730(9)	0.0133(6)	0.0147(5)	-0.0022(5)
Eu3	0.0240(5)	0.0306(5)	0.0417(6)	0.0023(4)	-0.0096(4)	0.0011(4)
Eu4	0.0175(4)	0.0232(6)	0.0283(5)	-0.0040(5)	-0.0012(3)	0.0024(4)
Eu4A	0.0175(4)	0.0232(6)	0.0283(5)	-0.0040(5)	-0.0012(3)	0.0024(4)
O1	0.019(5)	0.028(6)	0.028(6)	0.001(5)	-0.002(4)	0.002(5)
O2	0.035(8)	0.046(9)	0.075(11)	0.022(8)	0.012(7)	-0.005(7)
O3	0.023(5)	0.026(6)	0.049(7)	0.005(5)	0.016(5)	-0.002(5)
O4	0.038(6)	0.028(6)	0.058(7)	0.001(6)	0.017(6)	0.001(5)
O5	0.021(6)	0.044(8)	0.019(6)	0.002(5)	0.008(5)	-0.004(5)
O6	0.021(6)	0.044(8)	0.043(8)	-0.006(6)	0.004(5)	-0.006(6)
O7	0.047(7)	0.052(8)	0.060(8)	-0.002(7)	0.009(6)	-0.011(6)
O8	0.035(6)	0.037(7)	0.039(7)	-0.003(6)	-0.010(5)	0.005(5)
O9	0.038(7)	0.053(8)	0.053(8)	-0.002(6)	0.008(6)	0.003(6)
O9A	0.038(7)	0.053(8)	0.053(8)	-0.002(6)	0.008(6)	0.003(6)
O10	0.052(8)	0.061(8)	0.063(8)	-0.023(7)	0.014(7)	0.014(7)
O11	0.055(10)	0.058(10)	0.080(12)	0.006(9)	0.010(9)	-0.010(9)
O11A	0.050(14)	0.043(14)	0.042(13)	0.005(12)	0.022(12)	0.012(12)
O12	0.048(10)	0.085(13)	0.103(14)	0.011(11)	0.011(10)	-0.001(10)
O13	0.080(12)	0.060(11)	0.129(15)	0.025(11)	0.052(12)	0.018(10)
O14	0.025(6)	0.049(7)	0.048(7)	0.010(6)	-0.001(5)	-0.002(6)
O15	0.025(6)	0.049(7)	0.036(6)	0.013(6)	0.016(5)	0.000(5)
O16	0.056(8)	0.041(7)	0.063(8)	0.015(7)	-0.014(7)	-0.007(6)
O17	0.071(9)	0.052(8)	0.053(8)	-0.005(7)	0.008(7)	0.002(7)
O18	0.037(8)	0.067(11)	0.091(12)	-0.029(10)	0.009(8)	0.003(8)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
O19	0.045(10)	0.075(12)	0.135(16)	-0.038(12)	-0.013(10)	0.003(9)
O20	0.029(7)	0.048(8)	0.038(8)	0.002(7)	-0.002(6)	-0.004(6)
O21	0.051(8)	0.069(9)	0.070(9)	0.026(7)	-0.007(7)	-0.010(7)
O22	0.035(8)	0.040(8)	0.063(10)	0.013(7)	-0.006(7)	-0.002(7)
O23	0.023(5)	0.041(6)	0.032(6)	0.010(5)	0.005(5)	-0.003(5)
O24	0.034(8)	0.066(10)	0.053(9)	0.001(8)	0.011(7)	-0.011(7)
O25	0.034(6)	0.050(7)	0.033(6)	0.002(6)	0.005(5)	-0.002(6)
N1	0.025(6)	0.034(7)	0.022(6)	0.001(5)	-0.001(5)	0.007(6)
N2	0.028(6)	0.025(6)	0.022(6)	-0.004(5)	0.002(5)	0.000(5)
N3	0.039(8)	0.043(8)	0.050(8)	0.004(7)	0.008(7)	-0.001(7)
N4	0.030(7)	0.038(7)	0.039(7)	-0.005(6)	0.003(6)	-0.001(6)
N5	0.045(8)	0.030(7)	0.035(7)	0.003(6)	0.002(6)	-0.006(6)
N6	0.019(6)	0.035(7)	0.022(6)	-0.007(5)	-0.002(5)	-0.001(5)
N7	0.032(7)	0.036(7)	0.029(7)	0.007(6)	0.002(6)	-0.002(6)
N8	0.020(6)	0.029(6)	0.022(6)	0.001(5)	-0.002(5)	-0.003(5)
C1	0.026(7)	0.030(7)	0.031(7)	0.003(6)	-0.002(6)	0.002(6)
C2	0.026(7)	0.025(7)	0.028(7)	0.000(6)	0.007(6)	0.008(6)
C3	0.038(8)	0.041(8)	0.043(8)	0.013(7)	-0.002(7)	0.005(7)
C4	0.035(8)	0.045(9)	0.038(8)	0.000(7)	0.001(7)	0.015(7)
C5	0.035(8)	0.041(8)	0.033(8)	0.002(7)	-0.002(6)	0.001(7)
C6	0.015(6)	0.041(8)	0.036(8)	-0.005(7)	0.004(6)	0.010(6)
C7	0.030(7)	0.050(9)	0.037(8)	0.001(7)	0.009(6)	0.002(7)
C8	0.023(7)	0.037(8)	0.023(7)	0.001(6)	-0.002(6)	0.000(6)
C9	0.030(7)	0.035(8)	0.031(7)	-0.009(6)	0.010(6)	-0.004(6)
C10	0.033(8)	0.035(8)	0.034(8)	-0.003(7)	0.003(6)	-0.001(7)
C11	0.021(7)	0.030(7)	0.029(7)	-0.003(6)	-0.001(6)	-0.002(6)
C12	0.035(8)	0.030(8)	0.042(8)	-0.004(7)	0.004(7)	0.002(7)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
C13	0.016(6)	0.029(7)	0.023(7)	0.001(6)	0.002(5)	0.003(6)
C14	0.020(6)	0.037(8)	0.025(7)	-0.002(6)	0.006(6)	0.003(6)
C15	0.041(8)	0.042(9)	0.042(8)	0.004(7)	0.000(7)	-0.004(7)
C16	0.041(8)	0.040(9)	0.052(9)	0.003(7)	0.004(7)	0.002(7)
C17	0.048(9)	0.053(10)	0.053(9)	0.001(8)	0.006(8)	0.004(8)
C18	0.041(9)	0.055(10)	0.055(9)	-0.002(8)	0.010(7)	0.011(8)
C19	0.042(8)	0.040(9)	0.043(8)	0.006(7)	0.009(7)	0.002(7)
C20	0.031(8)	0.044(9)	0.058(9)	-0.003(8)	0.011(7)	0.002(7)
C21	0.027(7)	0.045(9)	0.054(9)	0.002(7)	0.015(7)	-0.002(7)
C22	0.037(8)	0.032(8)	0.046(8)	0.002(7)	0.008(7)	0.000(7)
C23	0.040(9)	0.053(9)	0.058(9)	-0.009(8)	0.009(7)	0.004(8)
C24	0.032(8)	0.045(9)	0.046(8)	-0.013(7)	0.012(7)	0.006(7)
C25	0.042(9)	0.055(9)	0.051(9)	-0.004(8)	0.018(7)	-0.004(8)
C26	0.055(10)	0.062(10)	0.065(10)	-0.016(8)	0.010(8)	0.004(8)
C27	0.024(7)	0.032(8)	0.039(8)	0.002(7)	0.007(6)	-0.003(6)
C28	0.043(8)	0.040(9)	0.047(9)	0.008(7)	0.006(7)	-0.004(7)
C29	0.030(7)	0.037(8)	0.033(7)	0.003(7)	0.011(6)	0.007(6)
C30	0.035(8)	0.036(8)	0.030(7)	-0.003(7)	0.006(6)	0.004(7)
C31	0.028(7)	0.033(8)	0.025(7)	0.011(6)	0.005(6)	-0.005(6)
C32	0.027(7)	0.031(7)	0.023(7)	0.002(6)	0.008(6)	0.012(6)
C33	0.025(7)	0.024(7)	0.015(6)	0.000(5)	0.006(5)	-0.001(6)
C34	0.026(7)	0.033(8)	0.025(7)	0.002(6)	-0.001(6)	-0.005(6)
C35	0.032(7)	0.035(8)	0.035(8)	0.001(7)	0.002(6)	-0.009(7)
C36	0.025(7)	0.028(7)	0.036(8)	0.002(6)	-0.007(6)	0.004(6)
C37	0.051(9)	0.047(9)	0.046(9)	0.006(8)	0.003(7)	-0.010(8)
C38	0.053(9)	0.045(9)	0.053(9)	0.009(8)	0.001(8)	-0.015(8)
C39	0.038(8)	0.034(8)	0.040(8)	0.007(7)	-0.001(7)	-0.002(7)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
C40	0.065(10)	0.060(10)	0.049(10)	0.006(8)	0.004(8)	0.000(8)
C41	0.032(7)	0.023(7)	0.030(7)	0.000(6)	0.001(6)	-0.004(6)
C42	0.014(6)	0.026(7)	0.024(7)	-0.002(6)	-0.004(5)	0.000(5)
C43	0.040(8)	0.046(9)	0.046(9)	0.010(7)	0.000(7)	-0.008(7)
C44	0.042(8)	0.044(9)	0.038(8)	0.008(7)	-0.004(7)	-0.004(7)
C45	0.028(7)	0.046(9)	0.040(8)	-0.001(7)	0.001(6)	-0.004(7)
C46	0.032(7)	0.036(8)	0.025(7)	-0.003(6)	0.013(6)	-0.006(6)
C47	0.029(7)	0.039(8)	0.027(7)	-0.005(6)	0.014(6)	-0.002(6)
C48	0.030(7)	0.034(8)	0.032(7)	-0.015(6)	-0.002(6)	-0.012(6)
C49	0.025(7)	0.037(8)	0.029(7)	-0.011(6)	-0.002(6)	0.005(6)
C50	0.029(7)	0.028(7)	0.023(7)	0.000(6)	0.001(6)	0.007(6)
C51	0.031(7)	0.038(8)	0.035(8)	-0.001(7)	0.001(6)	0.004(7)
C52	0.029(7)	0.038(8)	0.036(8)	0.005(7)	0.002(6)	0.007(7)
C53	0.018(6)	0.037(8)	0.022(7)	-0.001(6)	-0.001(5)	0.000(6)
C54	0.036(8)	0.034(8)	0.032(8)	0.004(7)	0.009(6)	0.008(7)
C55	0.024(7)	0.024(7)	0.020(6)	-0.008(6)	0.008(5)	-0.002(6)
C56	0.030(7)	0.028(7)	0.022(7)	-0.008(6)	-0.004(6)	0.005(6)
W1	0.0270(4)	0.0292(4)	0.0289(4)	0.0071(3)	-0.0030(3)	-0.0118(3)
W2	0.0278(4)	0.0492(5)	0.0158(3)	-0.0091(3)	0.0010(3)	-0.0079(3)
W3	0.0522(5)	0.0283(4)	0.0191(3)	0.0010(3)	0.0128(3)	-0.0075(4)
W4	0.0265(4)	0.0277(4)	0.0323(4)	0.0062(3)	0.0034(3)	0.0063(3)
W5	0.0470(5)	0.0231(4)	0.0279(4)	-0.0039(3)	0.0103(3)	0.0026(3)
W6	0.0223(3)	0.0336(4)	0.0197(3)	-0.0027(3)	0.0048(3)	0.0037(3)
Si1	0.017(3)	0.017(3)	0.011(3)	0.001(2)	-0.002(2)	-0.002(2)
O26	0.028(7)	0.039(8)	0.049(8)	0.017(7)	-0.003(6)	-0.011(6)
O27	0.031(7)	0.073(11)	0.039(8)	-0.018(8)	-0.004(6)	0.001(7)
O28	0.055(8)	0.029(7)	0.023(6)	-0.001(5)	0.008(6)	-0.004(6)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
O29	0.086(11)	0.036(8)	0.036(8)	-0.014(7)	0.026(8)	-0.012(8)
O30	0.043(8)	0.082(11)	0.038(8)	-0.022(8)	0.009(7)	-0.004(8)
O31	0.065(9)	0.084(9)	0.069(9)	0.026(8)	0.027(7)	0.017(7)
O32	0.055(8)	0.088(9)	0.067(8)	0.028(7)	0.031(7)	0.015(7)
O33	0.084(9)	0.055(8)	0.050(8)	-0.002(7)	-0.029(7)	0.016(7)
O34	0.055(8)	0.070(9)	0.092(9)	-0.020(8)	0.046(7)	-0.005(7)
O35	0.059(8)	0.066(9)	0.086(9)	-0.031(7)	0.033(7)	-0.011(7)
O36	0.060(8)	0.067(9)	0.093(9)	-0.021(8)	0.037(7)	-0.007(7)
O37	0.081(9)	0.055(8)	0.062(8)	-0.003(7)	-0.026(7)	0.015(7)
O38	0.078(9)	0.050(8)	0.056(8)	-0.007(7)	-0.018(7)	0.025(7)
O39	0.071(9)	0.084(9)	0.049(8)	0.024(7)	0.022(7)	0.016(7)
O40	0.072(9)	0.071(9)	0.040(7)	0.011(7)	0.007(7)	-0.021(7)
O41	0.050(7)	0.062(8)	0.040(7)	0.005(6)	0.006(6)	-0.023(6)
O42	0.042(8)	0.057(10)	0.054(9)	0.029(8)	-0.002(7)	0.000(7)
O43	0.074(9)	0.073(9)	0.048(8)	0.015(7)	0.000(7)	-0.028(7)
O44	0.017(8)	0.016(8)	0.014(8)	-0.003(6)	0.004(6)	-0.003(6)
O45	0.011(7)	0.016(8)	0.016(8)	0.001(6)	0.001(6)	0.001(6)
O46	0.019(8)	0.014(8)	0.016(8)	0.000(7)	0.001(6)	0.003(7)
O47	0.014(7)	0.019(8)	0.013(7)	0.004(7)	0.000(6)	0.000(6)
O48	0.034(8)	0.052(9)	0.063(10)	-0.025(8)	-0.005(7)	-0.006(7)
W7	0.0185(3)	0.0313(4)	0.0373(4)	-0.0002(3)	0.0062(3)	-0.0049(3)
W8	0.0167(3)	0.0387(4)	0.0257(4)	0.0042(3)	0.0015(3)	-0.0068(3)
W9	0.0680(7)	0.0441(5)	0.0291(4)	-0.0050(4)	0.0094(4)	0.0113(5)
W10	0.0246(4)	0.0658(6)	0.0241(4)	0.0064(4)	0.0006(3)	0.0098(4)
W11	0.0262(4)	0.0384(5)	0.0475(5)	-0.0096(4)	-0.0089(3)	0.0117(3)
W12	0.0275(4)	0.0377(5)	0.0403(5)	0.0082(4)	0.0064(3)	-0.0054(3)
Si2	0.009(2)	0.017(3)	0.016(3)	0.000(2)	0.001(2)	0.001(2)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
O49	0.028(7)	0.087(12)	0.034(8)	0.018(8)	0.005(6)	0.009(8)
O50	0.038(7)	0.045(8)	0.037(7)	-0.006(6)	0.013(6)	-0.017(6)
O51	0.025(7)	0.055(9)	0.045(8)	0.016(7)	0.002(6)	-0.008(6)
O52	0.035(8)	0.043(8)	0.061(9)	0.002(7)	0.011(7)	0.008(7)
O53	0.066(9)	0.069(9)	0.080(9)	0.019(7)	0.032(7)	0.019(7)
O54	0.045(7)	0.067(8)	0.048(7)	-0.004(7)	0.007(6)	0.019(7)
O55	0.081(9)	0.088(10)	0.082(9)	0.017(8)	0.046(8)	0.013(8)
O56	0.050(7)	0.049(7)	0.039(7)	-0.004(6)	0.000(6)	0.027(6)
O57	0.091(10)	0.067(9)	0.071(9)	0.024(8)	-0.028(8)	-0.009(8)
O58	0.085(9)	0.053(8)	0.067(9)	0.015(7)	-0.020(7)	-0.023(7)
O59	0.056(8)	0.072(9)	0.076(9)	0.024(7)	0.038(7)	0.020(7)
O60	0.058(8)	0.079(9)	0.075(9)	-0.025(8)	0.021(7)	-0.023(7)
O61	0.093(10)	0.074(9)	0.072(9)	-0.004(8)	-0.024(8)	-0.020(8)
O62	0.060(9)	0.093(10)	0.076(9)	-0.033(8)	0.022(7)	-0.022(8)
O63	0.086(12)	0.043(9)	0.044(9)	0.012(7)	0.006(8)	0.004(9)
O64	0.046(7)	0.060(8)	0.035(7)	-0.009(6)	-0.009(6)	0.017(6)
O65	0.008(7)	0.025(8)	0.026(8)	0.005(7)	0.003(6)	-0.002(7)
O66	0.027(8)	0.022(8)	0.020(8)	0.009(7)	0.006(7)	0.001(7)
O67	0.064(9)	0.099(10)	0.075(9)	-0.026(8)	0.023(7)	-0.008(8)
O68	0.030(9)	0.032(9)	0.020(8)	0.005(7)	0.001(7)	-0.010(8)
O69	0.014(8)	0.025(9)	0.023(8)	-0.002(7)	-0.003(7)	0.000(7)
O70	0.035(11)	0.034(11)	0.047(12)	-0.008(10)	0.011(10)	0.015(9)
O71	0.035(10)	0.026(10)	0.023(10)	0.007(8)	-0.005(8)	-0.010(9)
O72	0.023(8)	0.036(8)	0.032(8)	-0.005(6)	0.003(6)	-0.004(6)
O73	0.044(14)	0.039(14)	0.058(15)	-0.004(12)	-0.005(12)	0.013(12)
O74	0.049(10)	0.085(13)	0.071(11)	-0.011(10)	0.010(9)	-0.004(9)

**Table S8** Hydrogen atomic coordinates and isotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **1**.

	x/a	y/b	z/c	U(eq)
H5A	0.3219	0.0896	0.1684	0.041
H5B	0.2816	0.0779	0.1496	0.041
H6A	0.3407	0.1797	0.3774	0.054
H6B	0.3035	0.1959	0.3956	0.054
H11A	0.2622	0.6037	0.0468	0.096
H11B	0.2244	0.5647	0.0403	0.096
H11C	0.2413	0.5924	0.2701	0.066
H11D	0.2805	0.6179	0.2680	0.066
H12A	0.1907	0.5469	0.0877	0.118
H12B	0.1862	0.5578	0.1522	0.118
H13A	0.2017	0.4287	0.2165	0.129
H13B	0.2361	0.4033	0.2559	0.129
H18A	0.2679	-0.0192	-0.0977	0.097
H18B	0.2314	0.0120	-0.1276	0.097
H19A	0.3055	-0.0048	-0.0327	0.131
H19B	0.3197	0.0513	0.0197	0.131
H20A	0.2174	0.2276	0.0750	0.059
H20B	0.1851	0.1696	0.0552	0.059
H25A	0.2200	-0.0119	0.3620	0.058
H25B	0.2051	-0.0961	0.3832	0.058

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
H3	0.3788	-0.2158	0.3497	0.05
H4	0.4434	-0.1562	0.3290	0.048
H6	0.4833	-0.0167	0.2952	0.037
H7	0.4868	0.1343	0.2595	0.046
H9	0.4483	0.3002	0.2246	0.037
H10	0.3911	0.3869	0.2250	0.041
H17	0.3596	0.2556	0.0329	0.062
H18	0.4169	0.3519	0.0383	0.06
H20	0.4553	0.5065	0.0894	0.053
H21	0.4505	0.6469	0.1353	0.049
H23	0.4062	0.7810	0.1805	0.06
H24	0.3405	0.8299	0.2016	0.048
H31	0.1587	0.3259	-0.2000	0.034
H32	0.0947	0.2547	-0.2039	0.032
H34	0.0512	0.1292	-0.1557	0.034
H35	0.0454	0.0111	-0.0814	0.041
H37	0.0779	-0.0899	0.0162	0.058
H38	0.1380	-0.1359	0.0829	0.061
H45	0.0984	-0.3763	0.3263	0.046
H46	0.0395	-0.2869	0.2852	0.036
H48	0.0088	-0.1381	0.2286	0.039
H49	0.0157	0.0012	0.1789	0.038

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
H51	0.0664	0.1359	0.1458	0.042
H52	0.1320	0.1880	0.1460	0.041
H70A	0.3239	-0.0669	-0.1528	0.057
H70B	0.3172	-0.1583	-0.1323	0.057
H71A	0.1774	0.3988	-0.0047	0.044
H71B	0.1843	0.4448	-0.0607	0.044
H72A	0.2004	0.6968	0.1873	0.046
H72B	0.1854	0.7784	0.1561	0.046
H73A	0.1942	0.7585	0.5640	0.072
H73B	0.1648	0.7885	0.5159	0.072
H74A	0.1642	-0.4968	0.2828	0.102
H74B	0.1390	-0.4954	0.2250	0.102

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### S3.2 - Crystal structure report for 2

A specimen of  $C_{42}H_{51}Er_3N_6NaO_{70}SiW_{12}$ , approximate dimensions 0.063 mm x 0.082 mm x 0.153 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart APEX CCD system equipped with a graphite monochromator and a Mo-K $\alpha$  fine-focus sealed tube ( $\lambda = 0.71073 \text{ \AA}$ ).

The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a trigonal unit cell yielded a total of 44023 reflections to a maximum  $\theta$  angle of  $30.24^\circ$  ( $0.71 \text{ \AA}$  resolution), of which 8463 were independent (average redundancy 5.202, completeness = 96.8%,  $R_{\text{int}} = 4.57\%$ ,  $R_{\text{sig}} = 4.59\%$ ) and 7801 (92.18%) were greater than  $2\sigma(F^2)$ . The final cell constants of  $a = 20.288(5) \text{ \AA}$ ,  $b = 20.288(5) \text{ \AA}$ ,  $c = 18.818(5) \text{ \AA}$ , volume =  $6708.(4) \text{ \AA}^3$ , are based upon the refinement of the XYZ-centroids of reflections above  $20 \sigma(I)$ . Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.1660 and 0.3920.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group R 3, with  $Z = 3$  for the formula unit,  $C_{42}H_{51}Er_3N_6NaO_{70}SiW_{12}$ . The final anisotropic full-matrix least-squares refinement on  $F^2$  with 431 variables converged at  $R1 = 2.76\%$ , for the observed data and  $wR2 = 7.27\%$  for all data. The goodness-of-fit was 1.016. The largest peak in the final difference electron density synthesis was  $2.249 \text{ e}^-/\text{\AA}^3$  and the largest hole was -  $1.493 \text{ e}^-/\text{\AA}^3$  with an RMS deviation of  $0.269 \text{ e}^-/\text{\AA}^3$ . On the basis of the final model, the calculated density was  $3.356 \text{ g/cm}^3$  and  $F(000), 6066 \text{ e}^-$ .

**Table S9** Experimental details, data collection and structure refinement for **2**.

Compound 2	JTM1074
Crystal data	
Chemical formula	C <sub>42</sub> H <sub>36</sub> Er <sub>3</sub> N <sub>6</sub> NaO <sub>61</sub> SiW <sub>12</sub> ·1.5(O)·7.5(H <sub>2</sub> O)
M <sub>r</sub>	4518.94
Crystal system, space group	Trigonal, R3
Temperature (K)	150
a, c (Å)	20.288 (5), 18.818 (5)
V (Å <sup>3</sup> )	6708 (4)
Z	3
Radiation type	Mo Kα
μ (mm <sup>-1</sup> )	18.28
Crystal size (mm)	0.15 × 0.08 × 0.06
Data collection	
Diffractometer	Bruker Smart APEX CCD
Absorption correction	Multi-scan SADABS (Krause <i>et al.</i> , 2015)
T <sub>min</sub> , T <sub>max</sub>	0.17, 0.39
No. of measured, independent and observed [I > 2σ(I)] reflections	44023, 8463, 7801
R <sub>int</sub>	0.046
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.709
Refinement	
R[F <sup>2</sup> > 2σ(F <sup>2</sup> )], wR(F <sup>2</sup> ), S	0.028, 0.073, 1.02
No. of reflections	8463
No. of parameters	431
No. of restraints	259
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	2.25, -1.49
Absolute structure	Flack x determined using 3567 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	0.015 (6)
CCDC no.	1934951

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL-2018/1* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Bruker, 2016).

**Table S10** The bond lengths ( $\text{\AA}$ ) for **2**.

Bond	Lengths	Bond	Lengths
Si1-O20	1.609(14)	Si1-O19	1.616(7)
Si1-O19	1.616(7)	Si1-O19	1.616(7)
W1-O7	1.726(8)	W1-O13	1.866(7)
W1-O8	1.870(7)	W1-O8	1.935(7)
W1-O9	1.948(7)	W1-O19	2.301(7)
W2-O15	1.685(8)	W2-O16	1.873(7)
W2-O14	1.902(8)	W2-O12	1.925(7)
W2-O13	1.951(8)	W2-O19	2.355(7)
W3-O10	1.708(8)	W3-O12	1.861(7)
W3-O9	1.906(8)	W3-O11	1.913(8)
W3-O14	1.976(8)	W3-O19	2.354(7)
W4-O18	1.704(8)	W4-O11	1.886(8)
W4-O17	1.914(8)	W4-O16	1.919(8)
W4-O17	1.959(8)	W4-O20	2.346(7)
Er1-O1	2.285(8)	Er1-O3	2.314(9)
Er1-O6	2.344(9)	Er1-O2	2.348(8)
Er1-O5	2.349(9)	Er1-O7	2.358(8)
Er1-N1	2.446(9)	Er1-N2	2.449(10)
Na1-O21	2.414(13)	Na1-O21	2.414(13)
Na1-O21	2.414(13)	Na1-O2	2.470(10)
Na1-O2	2.470(10)	Na1-O2	2.470(10)
O1-C1	1.260(14)	O2-C1	1.263(14)

<b>Bond</b>	<b>Lengths</b>	<b>Bond</b>	<b>Lengths</b>
O3-C12	1.278(18)	O4-C12	1.223(18)
O5-H5A	0.87	O5-H5B	0.87
O6-H6A	0.8699	O6-H6B	0.8701
O21-H21A	0.87	O21-H21B	0.87
N1-C2	1.321(15)	N1-C6	1.364(15)
N2-C10	1.332(16)	N2-C11	1.348(16)
C1-C2	1.492(16)	C2-C3	1.396(16)
C3-C4	1.364(18)	C3-H3	0.95
C4-C5	1.395(18)	C4-H4	0.95
C5-C7	1.419(19)	C5-C6	1.429(18)
C6-C10	1.420(17)	C7-C8	1.37(2)
C7-H7A	0.95	C8-C9	1.38(2)
C8-H8	0.95	C9-C10	1.435(18)
C9-C13	1.45(2)	C11-C14	1.38(2)
C11-C12	1.50(2)	C13-C14	1.38(2)
C13-H13	0.95	C14-H14	0.95
O23-H23A	0.87	O23-H23B	0.87
O24-H24A	0.8701	O24-H24B	0.8701
O25-H25A	0.8699	O25-H25B	0.8701
O26-H26A	0.8701	O26-H26B	0.87
O27-H27A	0.87	O27-H27B	0.87

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S11** The bond angles ( $^{\circ}$ ) for **2**.

Bond	Angles	Bond	Angles
O20-Si1-O19	109.9(3)	O20-Si1-O19	109.9(3)
O19-Si1-O19	109.1(3)	O20-Si1-O19	109.9(3)
O19-Si1-O19	109.1(3)	O19-Si1-O19	109.1(3)
O7-W1-O13	99.6(4)	O7-W1-O8	100.8(3)
O13-W1-O8	92.7(3)	O7-W1-O8	102.2(3)
O13-W1-O8	158.1(3)	O8-W1-O8	84.9(4)
O7-W1-O9	100.1(3)	O13-W1-O9	89.2(3)
O8-W1-O9	158.4(3)	O8-W1-O9	85.4(3)
O7-W1-O19	172.7(3)	O13-W1-O19	75.5(3)
O8-W1-O19	85.0(3)	O8-W1-O19	82.7(3)
O9-W1-O19	74.6(3)	O15-W2-O16	102.6(4)
O15-W2-O14	100.1(4)	O16-W2-O14	93.7(3)
O15-W2-O12	102.1(3)	O16-W2-O12	85.0(3)
O14-W2-O12	157.6(3)	O15-W2-O13	99.6(4)
O16-W2-O13	157.1(3)	O14-W2-O13	87.7(3)
O12-W2-O13	85.1(3)	O15-W2-O19	170.7(3)
O16-W2-O19	85.6(3)	O14-W2-O19	74.9(3)
O12-W2-O19	82.7(3)	O13-W2-O19	72.7(3)
O10-W3-O12	101.2(3)	O10-W3-O9	99.8(4)
O12-W3-O9	94.3(3)	O10-W3-O11	102.2(4)
O12-W3-O11	85.7(3)	O9-W3-O11	157.6(3)
O10-W3-O14	99.3(4)	O12-W3-O14	159.2(3)
O9-W3-O14	85.7(3)	O11-W3-O14	86.4(3)
O10-W3-O19	170.7(3)	O12-W3-O19	86.3(3)
O9-W3-O19	74.1(3)	O11-W3-O19	83.5(3)
O14-W3-O19	73.6(3)	O18-W4-O11	103.2(4)

Bond	Angles	Bond	Angles
O18-W4-O17	99.2(4)	O11-W4-O17	91.7(3)
O18-W4-O16	102.1(4)	O11-W4-O16	86.4(3)
O17-W4-O16	158.5(3)	O18-W4-O17	98.3(4)
O11-W4-O17	158.2(3)	O17-W4-O17	87.9(5)
O16-W4-O17	86.1(3)	O18-W4-O20	170.0(4)
O11-W4-O20	85.0(3)	O17-W4-O20	74.6(3)
O16-W4-O20	83.9(3)	O17-W4-O20	73.9(3)
O1-Er1-O3	83.7(3)	O1-Er1-O6	140.8(3)
O3-Er1-O6	89.4(4)	O1-Er1-O2	81.1(3)
O3-Er1-O2	164.3(3)	O6-Er1-O2	99.6(4)
O1-Er1-O5	71.3(3)	O3-Er1-O5	93.5(3)
O6-Er1-O5	70.6(3)	O2-Er1-O5	77.5(3)
O1-Er1-O7	72.6(3)	O3-Er1-O7	90.3(3)
O6-Er1-O7	146.2(3)	O2-Er1-O7	89.4(3)
O5-Er1-O7	143.1(3)	O1-Er1-N1	133.3(3)
O3-Er1-N1	130.1(3)	O6-Er1-N1	78.8(3)
O2-Er1-N1	64.9(3)	O5-Er1-N1	126.0(3)
O7-Er1-N1	75.7(3)	O1-Er1-N2	134.0(3)
O3-Er1-N2	65.0(3)	O6-Er1-N2	74.6(3)
O2-Er1-N2	129.9(3)	O5-Er1-N2	139.1(3)
O7-Er1-N2	74.7(3)	N1-Er1-N2	65.1(3)
O21-Na1-O21	87.5(5)	O21-Na1-O21	87.5(5)
O21-Na1-O21	87.5(5)	O21-Na1-O2	80.2(4)
O21-Na1-O2	163.1(3)	O21-Na1-O2	103.4(3)
O21-Na1-O2	163.1(3)	O21-Na1-O2	103.4(3)
O21-Na1-O2	80.2(4)	O2-Na1-O2	91.4(4)
O21-Na1-O2	103.4(3)	O21-Na1-O2	80.2(4)

Bond	Angles	Bond	Angles
O21-Na1-O2	163.1(3)	O2-Na1-O2	91.4(4)
O2-Na1-O2	91.4(4)	C1-O1-Er1	140.4(8)
C1-O2-Er1	124.4(7)	C1-O2-Na1	116.4(7)
Er1-O2-Na1	119.0(4)	C12-O3-Er1	126.9(9)
Er1-O5-H5A	109.4	Er1-O5-H5B	109.2
H5A-O5-H5B	104.5	Er1-O6-H6A	109.2
Er1-O6-H6B	109.3	H6A-O6-H6B	104.5
W1-O7-Er1	157.8(4)	W1-O8-W1	152.6(4)
W3-O9-W1	119.8(4)	W4-O11-W3	150.8(5)
W3-O12-W2	152.7(4)	W1-O13-W2	120.8(4)
W2-O14-W3	120.3(4)	W2-O16-W4	151.6(4)
W4-O17-W4	120.1(4)	Si1-O19-W1	125.3(4)
Si1-O19-W3	123.2(4)	W1-O19-W3	91.5(3)
Si1-O19-W2	124.7(4)	W1-O19-W2	90.9(2)
W3-O19-W2	91.2(2)	Si1-O20-W4	124.3(3)
Si1-O20-W4	124.3(3)	W4-O20-W4	91.4(4)
Si1-O20-W4	124.3(3)	W4-O20-W4	91.4(4)
W4-O20-W4	91.4(4)	Na1-O21-H21A	109.2
Na1-O21-H21B	109.2	H21A-O21-H21B	104.5
C2-N1-C6	119.2(10)	C2-N1-Er1	120.7(8)
C6-N1-Er1	120.1(7)	C10-N2-C11	118.1(11)
C10-N2-Er1	121.3(7)	C11-N2-Er1	120.6(9)
O1-C1-O2	124.7(10)	O1-C1-C2	118.7(10)
O2-C1-C2	116.6(10)	N1-C2-C3	122.6(11)
N1-C2-C1	112.9(10)	C3-C2-C1	124.5(11)
C4-C3-C2	118.7(12)	C4-C3-H3	120.6
C2-C3-H3	120.6	C3-C4-C5	121.3(12)

<b>Bond</b>	<b>Angles</b>	<b>Bond</b>	<b>Angles</b>
C3-C4-H4	119.4	C5-C4-H4	119.4
C4-C5-C7	125.4(13)	C4-C5-C6	116.3(12)
C7-C5-C6	118.3(12)	N1-C6-C10	116.8(11)
N1-C6-C5	121.8(11)	C10-C6-C5	121.4(11)
C8-C7-C5	119.5(14)	C8-C7-H7A	120.2
C5-C7-H7A	120.2	C7-C8-C9	123.8(14)
C7-C8-H8	118.1	C9-C8-H8	118.1
C8-C9-C10	118.9(13)	C8-C9-C13	126.9(13)
C10-C9-C13	114.1(12)	N2-C10-C6	116.7(11)
N2-C10-C9	125.3(11)	C6-C10-C9	118.0(12)
N2-C11-C14	122.2(13)	N2-C11-C12	112.3(12)
C14-C11-C12	125.5(13)	O4-C12-O3	126.3(16)
O4-C12-C11	118.5(16)	O3-C12-C11	115.1(12)
C14-C13-C9	119.1(13)	C14-C13-H13	120.4
C9-C13-H13	120.4	C11-C14-C13	121.1(13)
C11-C14-H14	119.4	C13-C14-H14	119.4
H23A-O23-H23B	104.5	H24A-O24-H24B	104.5
H25A-O25-H25B	109.5	H26A-O26-H26B	109.5
H27A-O27-H27B	109.5		

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S12** Hydrogen atomic coordinates and isotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **2**.

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
H5A	0.3447	0.8829	0.2354	0.034
H5B	0.2777	0.8153	0.2447	0.034
H6A	0.4264	1.0050	0.3473	0.042
H6B	0.4081	0.9697	0.2821	0.042
H21A	0.2271	0.6560	0.1740	0.055
H21B	0.2855	0.7301	0.1688	0.055
H3	0.1431	0.7426	0.4507	0.023
H4	0.0562	0.6939	0.5430	0.024
H7A	-0.0351	0.5779	0.6194	0.032
H8	-0.0900	0.4492	0.6376	0.038
H13	-0.0989	0.3183	0.6090	0.031
H14	-0.0516	0.2566	0.5395	0.035
H23A	0.5144	0.9284	0.2363	0.048
H23B	0.4895	0.9133	0.1670	0.048
H24A	0.0442	0.7806	0.5990	0.088
H24B	-0.0327	0.7326	0.6083	0.088
H25A	-0.1316	0.6851	0.6657	0.087
H25B	-0.1270	0.6965	0.5910	0.087
H26A	-0.1703	0.5471	0.7860	0.094
H26B	-0.1595	0.5485	0.7113	0.094
H27A	0.0028	0.5673	0.8138	0.111
H27B	0.0137	0.5686	0.7391	0.111

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S13** Hydrogen bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) for **2**.

	<b>Donor-H</b>	<b>Acceptor-H</b>	<b>Donor-Acceptor</b>	<b>Angle</b>
O5-H5A $\cdots$ O4	0.87	2.45	3.057(19)	127.2
O6-H6A $\cdots$ O14	0.87	2.15	2.862(13)	139.3
O21-H21B $\cdots$ O22	0.87	2.02	2.81(2)	150.1
C14-H14 $\cdots$ O5	0.95	2.48	3.259(16)	138.7
O23-H23A $\cdots$ O24	0.87	1.81	2.68(4)	179.1
O23-H23B $\cdots$ O26	0.87	1.93	2.79(4)	168.8
O24-H24A $\cdots$ O23	0.87	1.81	2.68(4)	179.1
O24-H24B $\cdots$ O25	0.87	1.95	2.67(4)	139.9
O26-H26A $\cdots$ O23	0.87	2.02	2.79(4)	147.0
O26-H26B $\cdots$ O18	0.87	2.20	3.03(3)	158.7
O27-H27B $\cdots$ O12	0.87	2.57	3.34(3)	149.4

Symmetry code(s): (i)  $-x+y, -x+1, z$ ; (ii)  $-y+1, x-y+1, z$ .

**Table S14** Atomic coordinates and equivalent isotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **2**.(U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
Si1	0.333333	0.666667	0.7184(3)	0.004
W1	0.30678(2)	0.75603(3)	0.57142(2)	0.00979(10)
W2	0.37577(3)	0.85817(3)	0.71855(3)	0.01588(11)
W3	0.52625(3)	0.80742(3)	0.71126(2)	0.01289(10)
W4	0.41341(3)	0.77239(3)	0.87416(2)	0.01327(10)
Er1	0.34143(3)	0.85212(3)	0.37873(3)	0.01079(11)
Na1	0.333333	0.666667	0.2768(6)	0.034(2)
O1	0.2359(5)	0.7375(4)	0.3546(5)	0.0165(17)
O2	0.2178(5)	0.6194(5)	0.3507(5)	0.0155(17)
O3	0.1067(6)	0.3610(5)	0.3909(6)	0.027(2)
O4	0.0376(8)	0.2474(7)	0.4423(10)	0.069(4)
O5	0.3260(6)	0.8382(5)	0.2549(5)	0.023(2)
O6	0.4258(5)	0.9678(5)	0.3237(5)	0.028(2)
O7	0.2998(4)	0.7851(4)	0.4869(4)	0.0108(15)
O8	0.3941(4)	0.7477(4)	0.5621(4)	0.0104(15)
O9	0.5298(4)	0.7871(4)	0.6129(4)	0.0085(14)
O10	0.6134(5)	0.8873(4)	0.7204(5)	0.0143(16)
O11	0.4890(4)	0.7889(5)	0.8068(4)	0.0120(15)
O12	0.4641(4)	0.8496(4)	0.6978(4)	0.0079(14)
O13	0.3601(4)	0.8507(4)	0.6159(4)	0.0110(15)
O14	0.2707(4)	0.8262(4)	0.7284(4)	0.0111(15)
O15	0.4138(5)	0.9528(4)	0.7289(4)	0.0128(16)
O16	0.3834(4)	0.8261(4)	0.8100(4)	0.0098(15)
O17	0.3113(5)	0.7298(5)	0.9151(4)	0.0147(17)
O18	0.4625(5)	0.8395(5)	0.9373(4)	0.0167(17)

	<b>x/a</b>	<b>y/b</b>	<b>z/c</b>	<b>U(eq)</b>
O19	0.4168(4)	0.6890(4)	0.6892(4)	0.0058(14)
O20	0.333333	0.666667	0.8039(7)	0.009(2)
O21	0.2563(6)	0.6958(6)	0.1996(6)	0.037(3)
N1	0.1110(5)	0.5700(5)	0.4443(5)	0.0105(18)
N2	0.0503(5)	0.4232(5)	0.4698(5)	0.0133(19)
C1	0.2033(6)	0.6690(7)	0.3746(6)	0.012(2)
C2	0.1435(7)	0.6435(6)	0.4306(6)	0.015(2)
C3	0.1218(7)	0.6909(8)	0.4645(7)	0.019(2)
C4	0.0693(7)	0.6615(7)	0.5178(7)	0.020(3)
C5	0.0345(7)	0.5847(7)	0.5362(7)	0.021(3)
C6	0.0570(7)	0.5393(7)	0.4962(7)	0.016(2)
C7	0.9796(8)	0.5489(9)	0.5908(8)	0.027(3)
C8	0.9481(8)	0.4723(9)	0.6019(8)	0.032(3)
C9	0.9683(7)	0.4266(8)	0.5642(7)	0.022(3)
C10	0.0244(7)	0.4601(7)	0.5091(7)	0.016(2)
C11	0.0222(7)	0.3485(7)	0.4823(8)	0.024(3)
C12	0.0565(9)	0.3144(9)	0.4343(9)	0.036(4)
C13	0.9391(8)	0.3458(8)	0.5743(7)	0.026(3)
C14	0.9672(8)	0.3095(8)	0.5329(8)	0.029(3)
O22	0.3142(12)	0.7637(12)	0.0668(12)	0.033(5)
O23	0.4797(12)	0.9266(11)	0.2079(11)	0.032(5)
O24	0.0112(16)	0.7459(16)	0.6274(16)	0.058(7)
O25	0.8593(14)	0.6627(15)	0.6245(16)	0.058(7)
O26	0.8610(16)	0.5510(17)	0.7525(14)	0.063(8)
O27	0.9823(17)	0.5648(19)	0.7726(18)	0.074(9)

**Table S15** Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for **2**.

The anisotropic atomic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
Si1	0.005	0.005	0.005	0	0	0.004
W1	0.0102(2)	0.0100(2)	0.0101(2)	0.00187(16)	0.00073(16)	0.00579(17)
W2	0.0167(2)	0.0129(2)	0.0182(3)	-0.00094(18)	0.00093(19)	0.00749(19)
W3	0.0089(2)	0.0118(2)	0.0156(2)	-0.00238(17)	-0.00108(17)	0.00338(17)
W4	0.0144(2)	0.0129(2)	0.0108(2)	-0.00370(17)	-0.00151(17)	0.00559(18)
Er1	0.0102(2)	0.0081(2)	0.0137(2)	0.00249(18)	-0.00054(19)	0.00429(18)
Na1	0.033(3)	0.033(3)	0.035(6)	0	0	0.0165(17)
O1	0.016(4)	0.008(3)	0.020(4)	0.003(3)	-0.006(3)	0.002(3)
O2	0.015(4)	0.009(3)	0.019(4)	0.004(3)	0.004(3)	0.003(3)
O3	0.029(4)	0.019(4)	0.038(5)	-0.003(3)	0.004(4)	0.017(3)
O4	0.060(8)	0.028(6)	0.126(10)	0.007(7)	0.021(7)	0.029(6)
O5	0.036(5)	0.016(4)	0.016(4)	0.005(3)	0.001(4)	0.013(4)
O6	0.022(5)	0.016(4)	0.028(5)	0.012(4)	-0.007(4)	-0.004(4)
O7	0.016(3)	0.011(3)	0.010(3)	-0.002(3)	0.002(3)	0.011(3)
O8	0.012(3)	0.007(3)	0.015(4)	0.003(3)	0.004(3)	0.007(3)
O9	0.007(3)	0.010(3)	0.013(3)	-0.002(3)	-0.004(3)	0.007(3)
O10	0.015(4)	0.010(4)	0.017(4)	-0.004(3)	-0.003(3)	0.005(3)
O11	0.011(3)	0.015(3)	0.007(3)	-0.003(3)	0.002(3)	0.004(3)
O12	0.009(3)	0.006(3)	0.012(3)	-0.002(3)	0.001(3)	0.006(3)
O13	0.012(3)	0.009(3)	0.014(4)	-0.002(3)	0.000(3)	0.006(3)
O14	0.011(3)	0.012(3)	0.011(3)	0.000(3)	0.002(3)	0.006(3)
O15	0.016(4)	0.006(3)	0.014(4)	-0.002(3)	0.003(3)	0.004(3)
O16	0.009(3)	0.012(3)	0.008(3)	0.001(3)	0.001(3)	0.005(3)
O17	0.019(4)	0.016(4)	0.014(4)	-0.004(3)	-0.004(3)	0.012(3)
O18	0.023(4)	0.017(4)	0.010(4)	-0.003(3)	-0.002(3)	0.010(3)

	<b>U<sub>11</sub></b>	<b>U<sub>22</sub></b>	<b>U<sub>33</sub></b>	<b>U<sub>23</sub></b>	<b>U<sub>13</sub></b>	<b>U<sub>12</sub></b>
O19	0.007(3)	0.004(3)	0.007(3)	-0.002(2)	0.000(3)	0.003(3)
O20	0.010(3)	0.010(3)	0.006(5)	0	0	0.0049(15)
O21	0.042(6)	0.028(5)	0.040(6)	-0.009(4)	-0.009(5)	0.016(5)
N1	0.010(4)	0.011(4)	0.010(4)	0.000(3)	-0.002(3)	0.005(3)
N2	0.010(4)	0.009(4)	0.015(4)	0.005(3)	-0.003(3)	0.001(3)
C1	0.009(4)	0.017(4)	0.010(4)	-0.002(4)	0.003(3)	0.005(4)
C2	0.015(4)	0.014(4)	0.013(5)	-0.005(4)	-0.003(4)	0.005(4)
C3	0.018(5)	0.023(5)	0.023(5)	-0.003(4)	-0.004(4)	0.015(4)
C4	0.018(5)	0.020(5)	0.026(5)	-0.009(4)	-0.007(4)	0.013(4)
C5	0.017(5)	0.024(5)	0.022(5)	-0.001(4)	0.003(4)	0.011(4)
C6	0.012(4)	0.017(5)	0.017(5)	0.004(4)	-0.002(4)	0.006(4)
C7	0.019(5)	0.038(6)	0.025(5)	-0.005(5)	-0.001(4)	0.015(4)
C8	0.022(5)	0.041(6)	0.022(5)	-0.003(5)	0.001(4)	0.009(5)
C9	0.010(4)	0.028(5)	0.023(5)	0.005(4)	0.001(4)	0.007(4)
C10	0.010(4)	0.015(4)	0.014(5)	0.002(4)	-0.006(4)	0.000(4)
C11	0.020(5)	0.020(5)	0.029(6)	0.003(4)	-0.001(4)	0.009(4)
C12	0.034(6)	0.026(6)	0.053(7)	-0.001(5)	0.001(5)	0.018(5)
C13	0.022(5)	0.029(5)	0.019(5)	0.011(4)	-0.004(4)	0.008(4)
C14	0.033(6)	0.019(5)	0.029(6)	0.014(4)	-0.007(5)	0.009(4)
O22	0.037(5)	0.030(5)	0.031(5)	0.001(3)	0.000(3)	0.016(3)
O23	0.032(5)	0.031(5)	0.030(5)	0.001(3)	0.001(3)	0.013(3)
O24	0.060(12)	0.064(12)	0.073(13)	-0.010(10)	0.006(10)	0.047(10)
O25	0.046(11)	0.039(11)	0.082(13)	-0.022(9)	0.020(10)	0.016(9)
O26	0.059(12)	0.075(13)	0.045(12)	0.013(10)	-0.019(10)	0.027(10)
O27	0.065(13)	0.087(15)	0.070(14)	-0.028(11)	0.011(10)	0.038(11)