

Supplementary Material (ESI) for Dalton Transactions

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Lutetium alkyl and hydride complexes in a non-cyclopentadienyl coordination environment

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Table 1.1 Crystal data and structure refinement for [Lu(tbmp)(CH₂SiMe₃)(THF)₂] (1).

Identification code	mk1	
Empirical formula	C ₃₄ H ₅₅ LuO ₄ SSi	
Formula weight	762.90	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 17.657(3) Å	α = 90°
	b = 18.687(3) Å	β = 90°
	c = 22.178(4) Å	γ = 90°
Volume	7318(2) Å ³	
Z	8	
Density (calculated)	1.385 Mg/m ³	
Absorption coefficient	2.820 mm ⁻¹	
F(000)	3136	
Crystal size	0.25×0.12×0.10 mm ³	
Theta range for data collection	2.17 to 28.42°	
Index ranges	-23≤h≤23, -24≤k≤25, -29≤l≤29	
Reflections collected	81995	
Independent reflections	9170 [R(int) = 0.1015]	

Completeness to theta = 28.42°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.7657 and 0.5391
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9170 / 0 / 381
Goodness-of-fit on F ²	1.570
Final R indices [I>2sigma(I)]	R1 = 0.0848, wR2 = 0.1504
R indices (all data)	R1 = 0.1013, wR2 = 0.1552
Largest diff. peak and hole	1.994 and -4.259 e.Å ⁻³

Table 1.2 Bond lengths [Å] and angles [°] for mk1.

Lu-O(1)	2.098(5)
Lu-O(2)	2.099(4)
Lu-O(3)	2.332(5)
Lu-O(4)	2.334(5)
Lu-C(23)	2.348(7)
Lu-S	2.9553(17)
Si-C(23)	1.821(7)
Si-C(25)	1.864(11)
Si-C(24)	1.879(8)
Si-C(26)	1.882(9)
S-C(2)	1.794(7)
S-C(12)	1.794(7)
O(1)-C(1)	1.323(8)
O(2)-C(13)	1.332(8)
O(3)-C(30)	1.451(9)
O(3)-C(27)	1.461(9)
O(4)-C(34)	1.419(10)
O(4)-C(31)	1.459(8)
C(1)-C(2)	1.399(9)
C(1)-C(6)	1.420(9)
C(2)-C(3)	1.388(9)
C(3)-C(4)	1.386(10)

C(3)-H(3)	0.9500
C(4)-C(5)	1.389(10)
C(4)-C(7)	1.513(10)
C(5)-C(6)	1.395(9)
C(5)-H(5)	0.9500
C(6)-C(8)	1.529(9)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(9)	1.525(10)
C(8)-C(11)	1.533(10)
C(8)-C(10)	1.548(10)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.395(9)
C(12)-C(13)	1.399(9)
C(13)-C(14)	1.426(9)
C(14)-C(15)	1.386(9)
C(14)-C(19)	1.526(10)
C(15)-C(16)	1.403(10)
C(15)-H(15)	0.9500
C(16)-C(17)	1.380(10)
C(16)-C(18)	1.514(10)
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800

C(19)-C(20)	1.531(11)
C(19)-C(21)	1.543(10)
C(19)-C(22)	1.540(10)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.497(12)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.505(13)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.506(12)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900

C(31)-C(32)	1.500(11)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.532(11)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.513(12)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900

O(1)-Lu-O(2)	97.26(18)
O(1)-Lu-O(3)	150.02(18)
O(2)-Lu-O(3)	85.74(17)
O(1)-Lu-O(4)	86.10(18)
O(2)-Lu-O(4)	156.49(18)
O(3)-Lu-O(4)	80.16(17)
O(1)-Lu-C(23)	104.4(2)
O(2)-Lu-C(23)	108.3(2)
O(3)-Lu-C(23)	102.9(2)
O(4)-Lu-C(23)	93.2(2)
O(1)-Lu-S	69.48(13)
O(2)-Lu-S	70.51(13)
O(3)-Lu-S	83.73(14)
O(4)-Lu-S	89.22(13)
C(23)-Lu-S	173.23(19)
C(23)-Si-C(25)	111.1(5)
C(23)-Si-C(24)	110.3(4)
C(25)-Si-C(24)	109.6(5)
C(23)-Si-C(26)	113.6(4)
C(25)-Si-C(26)	108.0(6)
C(24)-Si-C(26)	103.9(4)
C(2)-S-C(12)	103.5(3)

C(2)-S-Lu	94.5(2)
C(12)-S-Lu	93.6(2)
C(1)-O(1)-Lu	136.0(4)
C(13)-O(2)-Lu	133.7(4)
C(30)-O(3)-C(27)	108.6(6)
C(30)-O(3)-Lu	126.0(4)
C(27)-O(3)-Lu	121.7(4)
C(34)-O(4)-C(31)	108.5(6)
C(34)-O(4)-Lu	126.6(5)
C(31)-O(4)-Lu	123.9(4)
O(1)-C(1)-C(2)	121.2(6)
O(1)-C(1)-C(6)	120.9(6)
C(2)-C(1)-C(6)	117.9(6)
C(3)-C(2)-C(1)	122.9(6)
C(3)-C(2)-S	118.9(5)
C(1)-C(2)-S	118.1(5)
C(2)-C(3)-C(4)	119.5(6)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	118.2(6)
C(5)-C(4)-C(7)	120.6(7)
C(3)-C(4)-C(7)	121.3(7)
C(4)-C(5)-C(6)	123.7(6)
C(4)-C(5)-H(5)	118.1
C(6)-C(5)-H(5)	118.1
C(5)-C(6)-C(1)	117.8(6)
C(5)-C(6)-C(8)	121.5(6)
C(1)-C(6)-C(8)	120.7(6)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5

C(9)-C(8)-C(6)	109.9(6)
C(9)-C(8)-C(11)	108.6(6)
C(6)-C(8)-C(11)	112.5(6)
C(9)-C(8)-C(10)	109.8(6)
C(6)-C(8)-C(10)	109.9(6)
C(11)-C(8)-C(10)	106.1(6)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	122.7(6)
C(17)-C(12)-S	118.5(5)
C(13)-C(12)-S	118.8(5)
O(2)-C(13)-C(12)	121.8(6)
O(2)-C(13)-C(14)	120.7(6)
C(12)-C(13)-C(14)	117.5(6)
C(15)-C(14)-C(13)	118.0(6)
C(15)-C(14)-C(19)	121.2(6)
C(13)-C(14)-C(19)	120.8(6)
C(14)-C(15)-C(16)	124.5(6)

C(14)-C(15)-H(15)	117.8
C(16)-C(15)-H(15)	117.8
C(17)-C(16)-C(15)	116.8(6)
C(17)-C(16)-C(18)	122.4(7)
C(15)-C(16)-C(18)	120.7(7)
C(16)-C(17)-C(12)	120.5(7)
C(16)-C(17)-H(17)	119.7
C(12)-C(17)-H(17)	119.7
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(14)-C(19)-C(20)	109.8(6)
C(14)-C(19)-C(21)	109.8(6)
C(20)-C(19)-C(21)	110.5(6)
C(14)-C(19)-C(22)	113.6(6)
C(20)-C(19)-C(22)	106.8(7)
C(21)-C(19)-C(22)	106.2(7)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5

H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
Si-C(23)-Lu	129.5(4)
Si-C(23)-H(23A)	104.9
Lu-C(23)-H(23A)	104.9
Si-C(23)-H(23B)	104.9
Lu-C(23)-H(23B)	104.9
H(23A)-C(23)-H(23B)	105.8
Si-C(24)-H(24A)	109.5
Si-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
Si-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
Si-C(25)-H(25A)	109.5
Si-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
Si-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si-C(26)-H(26A)	109.5
Si-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(3)-C(27)-C(28)	105.2(7)
O(3)-C(27)-H(27A)	110.7
C(28)-C(27)-H(27A)	110.7
O(3)-C(27)-H(27B)	110.7
C(28)-C(27)-H(27B)	110.7
H(27A)-C(27)-H(27B)	108.8

C(27)-C(28)-C(29)	101.9(7)
C(27)-C(28)-H(28A)	111.4
C(29)-C(28)-H(28A)	111.4
C(27)-C(28)-H(28B)	111.4
C(29)-C(28)-H(28B)	111.4
H(28A)-C(28)-H(28B)	109.3
C(30)-C(29)-C(28)	103.8(7)
C(30)-C(29)-H(29A)	111.0
C(28)-C(29)-H(29A)	111.0
C(30)-C(29)-H(29B)	111.0
C(28)-C(29)-H(29B)	111.0
H(29A)-C(29)-H(29B)	109.0
O(3)-C(30)-C(29)	105.8(7)
O(3)-C(30)-H(30A)	110.6
C(29)-C(30)-H(30A)	110.6
O(3)-C(30)-H(30B)	110.6
C(29)-C(30)-H(30B)	110.6
H(30A)-C(30)-H(30B)	108.7
O(4)-C(31)-C(32)	105.2(6)
O(4)-C(31)-H(31A)	110.7
C(32)-C(31)-H(31A)	110.7
O(4)-C(31)-H(31B)	110.7
C(32)-C(31)-H(31B)	110.7
H(31A)-C(31)-H(31B)	108.8
C(31)-C(32)-C(33)	103.4(6)
C(31)-C(32)-H(32A)	111.1
C(33)-C(32)-H(32A)	111.1
C(31)-C(32)-H(32B)	111.1
C(33)-C(32)-H(32B)	111.1
H(32A)-C(32)-H(32B)	109.1
C(34)-C(33)-C(32)	98.8(6)
C(34)-C(33)-H(33A)	112.0
C(32)-C(33)-H(33A)	112.0
C(34)-C(33)-H(33B)	112.0

C(32)-C(33)-H(33B)	112.0
H(33A)-C(33)-H(33B)	109.7
O(4)-C(34)-C(33)	107.2(7)
O(4)-C(34)-H(34A)	110.3
C(33)-C(34)-H(34A)	110.3
O(4)-C(34)-H(34B)	110.3
C(33)-C(34)-H(34B)	110.3
H(34A)-C(34)-H(34B)	108.5

Table 2.1 Crystal data and structure refinement for [Lu(tbbp)(CH₂SiMe₃)(THF)₂] (1^{tBu}).

Identification code	mk1_tBu	
Empirical formula	C ₄₀ H ₆₇ LuO ₄ SSi	
Formula weight	847.06	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.820(3) Å	α = 90°
	b = 23.858(6) Å	β = 93.261(4)°
	c = 16.458(4) Å	γ = 90°
Volume	4241.6(19) Å ³	
Z	4	
Density (calculated)	1.326 Mg/m ³	
Absorption coefficient	2.440 mm ⁻¹	
F(000)	1760	
Crystal size	0.53×0.21×0.12 mm ³	
Theta range for data collection	2.36 to 28.37°	
Index ranges	-14≤h≤13, -31≤k≤31, -21≤l≤21	
Reflections collected	43156	
Independent reflections	10572 [R(int) = 0.0563]	
Completeness to theta = 28.37°	99.7 %	
Absorption correction	Empirical	
Max. and min. transmission	1.0000 and 0.6637	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10572 / 0 / 439
Goodness-of-fit on F^2	1.014
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0313, wR2 = 0.0697
R indices (all data)	R1 = 0.0448, wR2 = 0.0748
Largest diff. peak and hole	1.191 and -0.907 e.Å ⁻³

Table 2.2 Bond lengths [Å] and angles [°] for mk1_tBu.

Si-C(29)	1.841(3)
Si-C(31)	1.868(3)
Si-C(30)	1.880(4)
Si-C(32)	1.882(3)
S-C(2)	1.793(3)
S-C(15)	1.793(3)
S-Lu	2.9066(10)
Lu-O(2)	2.103(2)
Lu-O(1)	2.118(2)
Lu-O(3)	2.325(2)
Lu-O(4)	2.368(2)
Lu-C(29)	2.375(3)
O(1)-C(1)	1.337(3)
O(2)-C(16)	1.334(3)
O(3)-C(36)	1.447(4)
O(3)-C(33)	1.455(4)
O(4)-C(40)	1.462(4)
O(4)-C(37)	1.479(3)
C(1)-C(2)	1.414(4)
C(1)-C(6)	1.430(4)
C(2)-C(3)	1.399(4)
C(3)-C(4)	1.385(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.411(4)
C(4)-C(7)	1.533(4)

C(5)-C(6)	1.393(4)
C(5)-H(5)	0.9300
C(6)-C(11)	1.544(4)
C(7)-C(8)	1.529(4)
C(7)-C(9)	1.534(4)
C(7)-C(10)	1.545(4)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(14)	1.538(4)
C(11)-C(12)	1.539(4)
C(11)-C(13)	1.543(4)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-C(20)	1.392(4)
C(15)-C(16)	1.412(4)
C(16)-C(17)	1.426(4)
C(17)-C(18)	1.397(4)
C(17)-C(25)	1.539(4)
C(18)-C(19)	1.413(4)
C(18)-H(18)	0.9300

C(19)-C(20)	1.392(4)
C(19)-C(21)	1.536(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.534(5)
C(21)-C(24)	1.539(4)
C(21)-C(23)	1.541(4)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(27)	1.538(4)
C(25)-C(26)	1.539(4)
C(25)-C(28)	1.546(4)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600

C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(34)	1.519(5)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-C(35)	1.515(5)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(35)-C(36)	1.513(5)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-C(38)	1.483(5)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-C(39)	1.452(6)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-C(40)	1.502(4)
C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(29)-Si-C(31)	108.37(16)
C(29)-Si-C(30)	110.97(17)
C(31)-Si-C(30)	109.56(18)
C(29)-Si-C(32)	116.02(15)
C(31)-Si-C(32)	107.16(16)
C(30)-Si-C(32)	104.56(18)
C(2)-S-C(15)	103.54(12)

C(2)-S-Lu	94.27(10)
C(15)-S-Lu	94.68(10)
O(2)-Lu-O(1)	98.43(8)
O(2)-Lu-O(3)	85.13(8)
O(1)-Lu-O(3)	158.10(8)
O(2)-Lu-O(4)	145.53(8)
O(1)-Lu-O(4)	86.42(7)
O(3)-Lu-O(4)	78.90(7)
O(2)-Lu-C(29)	99.96(9)
O(1)-Lu-C(29)	108.00(10)
O(3)-Lu-C(29)	92.50(10)
O(4)-Lu-C(29)	110.99(9)
O(2)-Lu-S	71.05(6)
O(1)-Lu-S	71.77(6)
O(3)-Lu-S	89.27(6)
O(4)-Lu-S	78.34(5)
C(29)-Lu-S	170.67(8)
C(1)-O(1)-Lu	133.37(18)
C(16)-O(2)-Lu	134.31(17)
C(36)-O(3)-C(33)	106.1(2)
C(36)-O(3)-Lu	123.28(19)
C(33)-O(3)-Lu	129.33(18)
C(40)-O(4)-C(37)	106.9(2)
C(40)-O(4)-Lu	125.04(17)
C(37)-O(4)-Lu	122.41(16)
O(1)-C(1)-C(2)	120.6(2)
O(1)-C(1)-C(6)	121.7(3)
C(2)-C(1)-C(6)	117.7(3)
C(3)-C(2)-C(1)	121.9(3)
C(3)-C(2)-S	118.3(2)
C(1)-C(2)-S	119.8(2)
C(4)-C(3)-C(2)	121.5(3)
C(4)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2

C(3)-C(4)-C(5)	116.2(3)
C(3)-C(4)-C(7)	123.9(3)
C(5)-C(4)-C(7)	119.9(2)
C(6)-C(5)-C(4)	124.8(3)
C(6)-C(5)-H(5)	117.6
C(4)-C(5)-H(5)	117.6
C(5)-C(6)-C(1)	117.9(3)
C(5)-C(6)-C(11)	121.3(3)
C(1)-C(6)-C(11)	120.8(3)
C(8)-C(7)-C(4)	112.5(2)
C(8)-C(7)-C(9)	108.4(3)
C(4)-C(7)-C(9)	110.4(2)
C(8)-C(7)-C(10)	108.4(3)
C(4)-C(7)-C(10)	108.4(2)
C(9)-C(7)-C(10)	108.7(3)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(14)-C(11)-C(12)	106.9(3)

C(14)-C(11)-C(13)	110.3(3)
C(12)-C(11)-C(13)	107.8(3)
C(14)-C(11)-C(6)	109.9(2)
C(12)-C(11)-C(6)	112.2(3)
C(13)-C(11)-C(6)	109.7(2)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	122.5(3)
C(20)-C(15)-S	118.6(2)
C(16)-C(15)-S	118.9(2)
O(2)-C(16)-C(15)	120.4(2)
O(2)-C(16)-C(17)	122.1(3)
C(15)-C(16)-C(17)	117.5(3)
C(18)-C(17)-C(16)	117.9(3)
C(18)-C(17)-C(25)	121.5(3)
C(16)-C(17)-C(25)	120.6(3)
C(17)-C(18)-C(19)	124.7(3)
C(17)-C(18)-H(18)	117.6

C(19)-C(18)-H(18)	117.6
C(20)-C(19)-C(18)	116.1(3)
C(20)-C(19)-C(21)	123.3(3)
C(18)-C(19)-C(21)	120.7(3)
C(15)-C(20)-C(19)	121.2(3)
C(15)-C(20)-H(20)	119.4
C(19)-C(20)-H(20)	119.4
C(22)-C(21)-C(19)	112.2(3)
C(22)-C(21)-C(24)	107.9(3)
C(19)-C(21)-C(24)	110.7(3)
C(22)-C(21)-C(23)	108.9(3)
C(19)-C(21)-C(23)	108.4(3)
C(24)-C(21)-C(23)	108.8(3)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(27)-C(25)-C(26)	107.9(3)
C(27)-C(25)-C(17)	109.1(2)
C(26)-C(25)-C(17)	112.5(3)

C(27)-C(25)-C(28)	109.6(3)
C(26)-C(25)-C(28)	106.7(3)
C(17)-C(25)-C(28)	111.0(2)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
Si-C(29)-Lu	125.59(16)
Si-C(29)-H(29A)	105.9
Lu-C(29)-H(29A)	105.9
Si-C(29)-H(29B)	105.9
Lu-C(29)-H(29B)	105.9
H(29A)-C(29)-H(29B)	106.2
Si-C(30)-H(30A)	109.5
Si-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si-C(31)-H(31A)	109.5

Si-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Si-C(32)-H(32A)	109.5
Si-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(3)-C(33)-C(34)	104.4(3)
O(3)-C(33)-H(33A)	110.9
C(34)-C(33)-H(33A)	110.9
O(3)-C(33)-H(33B)	110.9
C(34)-C(33)-H(33B)	110.9
H(33A)-C(33)-H(33B)	108.9
C(35)-C(34)-C(33)	105.5(3)
C(35)-C(34)-H(34A)	110.6
C(33)-C(34)-H(34A)	110.6
C(35)-C(34)-H(34B)	110.6
C(33)-C(34)-H(34B)	110.6
H(34A)-C(34)-H(34B)	108.8
C(36)-C(35)-C(34)	105.1(3)
C(36)-C(35)-H(35A)	110.7
C(34)-C(35)-H(35A)	110.7
C(36)-C(35)-H(35B)	110.7
C(34)-C(35)-H(35B)	110.7
H(35A)-C(35)-H(35B)	108.8
O(3)-C(36)-C(35)	105.9(3)
O(3)-C(36)-H(36A)	110.5
C(35)-C(36)-H(36A)	110.5
O(3)-C(36)-H(36B)	110.5
C(35)-C(36)-H(36B)	110.5

H(36A)-C(36)-H(36B)	108.7
O(4)-C(37)-C(38)	106.4(3)
O(4)-C(37)-H(37A)	110.5
C(38)-C(37)-H(37A)	110.5
O(4)-C(37)-H(37B)	110.5
C(38)-C(37)-H(37B)	110.5
H(37A)-C(37)-H(37B)	108.6
C(39)-C(38)-C(37)	107.6(3)
C(39)-C(38)-H(38A)	110.2
C(37)-C(38)-H(38A)	110.2
C(39)-C(38)-H(38B)	110.2
C(37)-C(38)-H(38B)	110.2
H(38A)-C(38)-H(38B)	108.5
C(38)-C(39)-C(40)	103.9(3)
C(38)-C(39)-H(39A)	111.0
C(40)-C(39)-H(39A)	111.0
C(38)-C(39)-H(39B)	111.0
C(40)-C(39)-H(39B)	111.0
H(39A)-C(39)-H(39B)	109.0
O(4)-C(40)-C(39)	105.6(3)
O(4)-C(40)-H(40A)	110.6
C(39)-C(40)-H(40A)	110.6
O(4)-C(40)-H(40B)	110.6
C(39)-C(40)-H(40B)	110.6
H(40A)-C(40)-H(40B)	108.8

Table 3.1 Crystal data and structure refinement for [Lu(etbmp)(CH₂SiMe₃)(THF)] (2).

Identification code	mk2
Empirical formula	C ₃₂ H ₅₁ LuO ₃ S ₂ Si
Formula weight	750.94
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1

Unit cell dimensions	a = 8.7517(17) Å	$\alpha = 75.023(4)^\circ$
	b = 12.703(2) Å	$\beta = 82.049(5)^\circ$
	c = 16.986(3) Å	$\gamma = 75.436(4)^\circ$
Volume	1760.1(6) Å ³	
Z	2	
Density (calculated)	1.417 Mg/m ³	
Absorption coefficient	2.985 mm ⁻¹	
F(000)	768	
Crystal size	0.29×0.21×0.05 mm ³	
Theta range for data collection	2.33 to 28.35°.	
Index ranges	-11≤h≤11, -16≤k≤16, -22≤l≤22	
Reflections collected	24117	
Independent reflections	8702 [R(int) = 0.0503]	
Completeness to theta = 28.35°	99.2 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8651 and 0.4781	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8702 / 0 / 363	
Goodness-of-fit on F ²	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.0843	
R indices (all data)	R1 = 0.0482, wR2 = 0.0873	
Largest diff. peak and hole	1.379 and -1.011 e.Å ⁻³	

Table 3.2 Bond lengths [Å] and angles [°] for mk2.

Si-C(25)	1.844(5)
Si-C(26)	1.867(5)
Si-C(28)	1.870(5)
Si-C(27)	1.879(5)
S(1)-C(2)	1.777(4)
S(1)-C(12)	1.815(5)
S(1)-Lu	2.9619(12)
S(2)-C(14)	1.779(4)

S(2)-C(13)	1.825(5)
S(2)-Lu	2.8461(12)
Lu-O(1)	2.101(3)
Lu-O(2)	2.115(3)
Lu-O(3)	2.234(3)
Lu-C(25)	2.335(4)
O(1)-C(1)	1.333(5)
O(2)-C(15)	1.327(5)
O(3)-C(32)	1.440(6)
O(3)-C(29)	1.446(5)
C(1)-C(2)	1.412(6)
C(1)-C(6)	1.420(5)
C(2)-C(3)	1.391(6)
C(3)-C(4)	1.374(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.388(6)
C(4)-C(7)	1.512(6)
C(5)-C(6)	1.390(6)
C(5)-H(5)	0.9500
C(6)-C(8)	1.540(6)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(10)	1.530(6)
C(8)-C(11)	1.535(6)
C(8)-C(9)	1.535(6)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800

C(11)-H(11C)	0.9800
C(12)-C(13)	1.498(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.393(5)
C(14)-C(15)	1.412(5)
C(15)-C(16)	1.431(5)
C(16)-C(17)	1.382(6)
C(16)-C(21)	1.531(6)
C(17)-C(18)	1.404(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.378(6)
C(18)-C(20)	1.505(6)
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(23)	1.532(6)
C(21)-C(24)	1.533(5)
C(21)-C(22)	1.537(6)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9800

C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.489(7)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(31)	1.497(8)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.427(7)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(25)-Si-C(26)	110.7(2)
C(25)-Si-C(28)	110.9(2)
C(26)-Si-C(28)	108.4(2)
C(25)-Si-C(27)	113.2(2)
C(26)-Si-C(27)	106.6(3)
C(28)-Si-C(27)	106.8(2)
C(2)-S(1)-C(12)	101.2(2)
C(2)-S(1)-Lu	95.44(14)
C(12)-S(1)-Lu	104.10(15)
C(14)-S(2)-C(13)	102.1(2)
C(14)-S(2)-Lu	96.36(14)
C(13)-S(2)-Lu	103.31(16)
O(1)-Lu-O(2)	147.93(11)
O(1)-Lu-O(3)	92.55(11)

O(2)-Lu-O(3)	94.76(11)
O(1)-Lu-C(25)	108.71(13)
O(2)-Lu-C(25)	101.10(13)
O(3)-Lu-C(25)	98.08(14)
O(1)-Lu-S(2)	91.15(8)
O(2)-Lu-S(2)	71.07(8)
O(3)-Lu-S(2)	157.46(8)
C(25)-Lu-S(2)	101.76(12)
O(1)-Lu-S(1)	68.62(8)
O(2)-Lu-S(1)	80.72(8)
O(3)-Lu-S(1)	86.42(8)
C(25)-Lu-S(1)	174.95(11)
S(2)-Lu-S(1)	74.28(3)
C(1)-O(1)-Lu	137.9(2)
C(15)-O(2)-Lu	134.3(2)
C(32)-O(3)-C(29)	108.3(4)
C(32)-O(3)-Lu	127.3(3)
C(29)-O(3)-Lu	123.6(3)
O(1)-C(1)-C(2)	119.7(4)
O(1)-C(1)-C(6)	122.5(4)
C(2)-C(1)-C(6)	117.9(4)
C(3)-C(2)-C(1)	121.9(4)
C(3)-C(2)-S(1)	119.9(3)
C(1)-C(2)-S(1)	118.3(3)
C(4)-C(3)-C(2)	120.6(4)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	117.6(4)
C(3)-C(4)-C(7)	121.6(4)
C(5)-C(4)-C(7)	120.8(4)
C(4)-C(5)-C(6)	124.5(4)
C(4)-C(5)-H(5)	117.8
C(6)-C(5)-H(5)	117.8
C(5)-C(6)-C(1)	117.6(4)

C(5)-C(6)-C(8)	122.0(4)
C(1)-C(6)-C(8)	120.4(4)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(10)-C(8)-C(11)	107.6(4)
C(10)-C(8)-C(9)	110.9(4)
C(11)-C(8)-C(9)	107.3(4)
C(10)-C(8)-C(6)	109.4(3)
C(11)-C(8)-C(6)	111.6(4)
C(9)-C(8)-C(6)	110.1(3)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-S(1)	115.6(3)
C(13)-C(12)-H(12A)	108.4

S(1)-C(12)-H(12A)	108.4
C(13)-C(12)-H(12B)	108.4
S(1)-C(12)-H(12B)	108.4
H(12A)-C(12)-H(12B)	107.4
C(12)-C(13)-S(2)	115.2(3)
C(12)-C(13)-H(13A)	108.5
S(2)-C(13)-H(13A)	108.5
C(12)-C(13)-H(13B)	108.5
S(2)-C(13)-H(13B)	108.5
H(13A)-C(13)-H(13B)	107.5
C(19)-C(14)-C(15)	122.1(4)
C(19)-C(14)-S(2)	119.6(3)
C(15)-C(14)-S(2)	118.3(3)
O(2)-C(15)-C(14)	119.8(3)
O(2)-C(15)-C(16)	122.4(4)
C(14)-C(15)-C(16)	117.8(4)
C(17)-C(16)-C(15)	117.7(4)
C(17)-C(16)-C(21)	122.2(4)
C(15)-C(16)-C(21)	120.1(4)
C(16)-C(17)-C(18)	124.4(4)
C(16)-C(17)-H(17)	117.8
C(18)-C(17)-H(17)	117.8
C(19)-C(18)-C(17)	117.4(4)
C(19)-C(18)-C(20)	121.6(4)
C(17)-C(18)-C(20)	120.9(4)
C(18)-C(19)-C(14)	120.5(4)
C(18)-C(19)-H(19)	119.8
C(14)-C(19)-H(19)	119.8
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

C(16)-C(21)-C(23)	109.6(3)
C(16)-C(21)-C(24)	112.1(4)
C(23)-C(21)-C(24)	107.7(3)
C(16)-C(21)-C(22)	110.2(3)
C(23)-C(21)-C(22)	110.5(4)
C(24)-C(21)-C(22)	106.7(3)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
Si-C(25)-Lu	127.9(2)
Si-C(25)-H(25A)	105.3
Lu-C(25)-H(25A)	105.3
Si-C(25)-H(25B)	105.3
Lu-C(25)-H(25B)	105.3
H(25A)-C(25)-H(25B)	106.0
Si-C(26)-H(26A)	109.5
Si-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si-C(26)-H(26C)	109.5

H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si-C(27)-H(27A)	109.5
Si-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si-C(28)-H(28A)	109.5
Si-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(3)-C(29)-C(30)	107.0(4)
O(3)-C(29)-H(29A)	110.3
C(30)-C(29)-H(29A)	110.3
O(3)-C(29)-H(29B)	110.3
C(30)-C(29)-H(29B)	110.3
H(29A)-C(29)-H(29B)	108.6
C(29)-C(30)-C(31)	103.8(4)
C(29)-C(30)-H(30A)	111.0
C(31)-C(30)-H(30A)	111.0
C(29)-C(30)-H(30B)	111.0
C(31)-C(30)-H(30B)	111.0
H(30A)-C(30)-H(30B)	109.0
C(32)-C(31)-C(30)	106.3(5)
C(32)-C(31)-H(31A)	110.5
C(30)-C(31)-H(31A)	110.5
C(32)-C(31)-H(31B)	110.5
C(30)-C(31)-H(31B)	110.5
H(31A)-C(31)-H(31B)	108.7
C(31)-C(32)-O(3)	108.3(5)
C(31)-C(32)-H(32A)	110.0

O(3)-C(32)-H(32A)	110.0
C(31)-C(32)-H(32B)	110.0
O(3)-C(32)-H(32B)	110.0
H(32A)-C(32)-H(32B)	108.4

Table 4.1 Crystal data and structure refinement for [Lu(tbmp)(OCPh₃)(THF)₂] (5).

Identification code	mk5	
Empirical formula	C _{55.75} H ₇₄ LuO _{5.75} S	
Formula weight	1043.18	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 33.017(5) Å	α b = 90°
	b = 18.291(3) Å	β = 108.832(3)°
	c = 20.635(3) Å	γ = 90°
Volume	11794(3) Å ³	
Z	8	
Density (calculated)	1.175 Mg/m ³	
Absorption coefficient	1.750 mm ⁻¹	
F(000)	4332	
Crystal size	0.67×0.18×0.13 mm ³	
Theta range for data collection	1.52 to 28.40°.	
Index ranges	-44 ≤ h ≤ 44, -24 ≤ k ≤ 24, -27 ≤ l ≤ 27	
Reflections collected	80196	
Independent reflections	14774 [R(int) = 0.0954]	
Completeness to theta = 28.40°	99.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8044 and 0.3868	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14774 / 27 / 573	
Goodness-of-fit on F ²	1.057	
Final R indices [I > 2σ(I)]	R1 = 0.0501, wR2 = 0.1294	

R indices (all data)

R1 = 0.0936, wR2 = 0.1488

Largest diff. peak and hole

1.116 and -0.547 e.Å⁻³

Table 4.2 Bond lengths [Å] and angles [°] for mk5.

Lu-O(5)	2.016(3)
Lu-O(2)	2.105(4)
Lu-O(1)	2.116(4)
Lu-O(3)	2.303(4)
Lu-O(4)	2.319(4)
Lu-S	2.8961(14)
S-C(2)	1.776(7)
S-C(12)	1.793(6)
O(1)-C(1)	1.324(6)
O(2)-C(13)	1.334(6)
O(3)-C(45)	1.386(9)
O(3)-C(42)	1.448(9)
O(4)-C(49)	1.429(8)
O(4)-C(46)	1.442(8)
O(5)-C(23)	1.394(6)
C(1)-C(2)	1.399(8)
C(1)-C(6)	1.422(8)
C(2)-C(3)	1.402(8)
C(3)-C(4)	1.376(11)
C(3)-H(3)	0.9500
C(4)-C(5)	1.398(12)
C(4)-C(7)	1.507(10)
C(5)-C(6)	1.399(9)
C(5)-H(5)	0.9500
C(6)-C(8)	1.517(10)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(11)	1.523(10)

C(8)-C(9)	1.541(10)
C(8)-C(10)	1.543(9)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.382(8)
C(12)-C(13)	1.389(8)
C(13)-C(14)	1.414(8)
C(14)-C(15)	1.377(8)
C(14)-C(19)	1.529(9)
C(15)-C(16)	1.387(9)
C(15)-H(15)	0.9500
C(16)-C(17)	1.381(9)
C(16)-C(18)	1.522(9)
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(21)	1.525(10)
C(19)-C(22)	1.551(9)
C(19)-C(20)	1.573(9)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800

C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.533(7)
C(23)-C(36)	1.534(7)
C(23)-C(30)	1.549(7)
C(24)-C(25)	1.371(8)
C(24)-C(29)	1.391(8)
C(25)-C(26)	1.385(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.368(9)
C(26)-H(26)	0.9500
C(27)-C(28)	1.372(10)
C(27)-H(27)	0.9500
C(28)-C(29)	1.385(8)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(35)	1.374(8)
C(30)-C(31)	1.386(8)
C(31)-C(32)	1.387(8)
C(31)-H(31)	0.9500
C(32)-C(33)	1.366(9)
C(32)-H(32)	0.9500
C(33)-C(34)	1.353(10)
C(33)-H(33)	0.9500
C(34)-C(35)	1.391(9)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-C(37)	1.386(8)
C(36)-C(41)	1.393(8)
C(37)-C(38)	1.395(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.374(10)
C(38)-H(38)	0.9500
C(39)-C(40)	1.374(10)

C(39)-H(39)	0.9500
C(40)-C(41)	1.376(8)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-C(43)	1.429(12)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.502(14)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.464(11)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.482(11)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.400(15)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.441(12)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(54)	1.508(19)
C(50)-C(51)	1.521(19)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-C(52)	1.592(19)
C(51)-C(54)	1.93(4)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900

C(52)-C(53)	1.607(19)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.574(19)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)#1	1.523(13)
C(55)-C(56)	1.523(13)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-C(57)	1.534(19)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(57)#1	1.53(2)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-C(59)	1.540(18)
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-C(60)	1.481(18)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.544(17)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-C(62)	1.542(18)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800

C(63)-C(64)	1.448(13)
C(63)-C(64)#1	1.448(13)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-C(65)	1.520(17)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
O(5)-Lu-O(2)	103.01(15)
O(5)-Lu-O(1)	104.02(14)
O(2)-Lu-O(1)	97.77(16)
O(5)-Lu-O(3)	100.66(15)
O(2)-Lu-O(3)	88.58(15)
O(1)-Lu-O(3)	152.34(15)
O(5)-Lu-O(4)	100.14(15)
O(2)-Lu-O(4)	154.92(15)
O(1)-Lu-O(4)	85.76(15)
O(3)-Lu-O(4)	77.73(15)
O(5)-Lu-S	171.34(11)
O(2)-Lu-S	71.33(11)
O(1)-Lu-S	70.92(11)
O(3)-Lu-S	85.95(11)
O(4)-Lu-S	86.66(11)
C(2)-S-C(12)	103.8(3)
C(2)-S-Lu	94.4(2)
C(12)-S-Lu	94.09(19)
C(1)-O(1)-Lu	133.7(4)
C(13)-O(2)-Lu	132.8(4)
C(45)-O(3)-C(42)	106.1(6)
C(45)-O(3)-Lu	122.1(4)
C(42)-O(3)-Lu	128.6(5)

C(49)-O(4)-C(46)	108.3(5)
C(49)-O(4)-Lu	124.7(4)
C(46)-O(4)-Lu	126.3(4)
C(23)-O(5)-Lu	166.4(3)
O(1)-C(1)-C(2)	120.1(5)
O(1)-C(1)-C(6)	120.3(6)
C(2)-C(1)-C(6)	119.5(6)
C(1)-C(2)-C(3)	121.3(6)
C(1)-C(2)-S	120.0(4)
C(3)-C(2)-S	118.8(5)
C(4)-C(3)-C(2)	120.4(7)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	118.0(6)
C(3)-C(4)-C(7)	120.7(8)
C(5)-C(4)-C(7)	121.3(8)
C(4)-C(5)-C(6)	124.0(7)
C(4)-C(5)-H(5)	118.0
C(6)-C(5)-H(5)	118.0
C(5)-C(6)-C(1)	116.8(7)
C(5)-C(6)-C(8)	121.2(6)
C(1)-C(6)-C(8)	122.0(6)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-C(11)	111.6(6)
C(6)-C(8)-C(9)	107.1(6)
C(11)-C(8)-C(9)	109.6(7)
C(6)-C(8)-C(10)	112.5(6)
C(11)-C(8)-C(10)	108.6(7)
C(9)-C(8)-C(10)	107.3(6)

C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	122.2(6)
C(17)-C(12)-S	118.4(5)
C(13)-C(12)-S	119.4(4)
O(2)-C(13)-C(12)	121.0(5)
O(2)-C(13)-C(14)	120.8(5)
C(12)-C(13)-C(14)	118.2(5)
C(15)-C(14)-C(13)	117.4(6)
C(15)-C(14)-C(19)	122.5(6)
C(13)-C(14)-C(19)	120.0(5)
C(14)-C(15)-C(16)	124.9(6)
C(14)-C(15)-H(15)	117.5
C(16)-C(15)-H(15)	117.5
C(17)-C(16)-C(15)	116.6(6)
C(17)-C(16)-C(18)	122.0(6)
C(15)-C(16)-C(18)	121.4(6)
C(16)-C(17)-C(12)	120.5(6)

C(16)-C(17)-H(17)	119.7
C(12)-C(17)-H(17)	119.7
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(21)-C(19)-C(14)	111.1(5)
C(21)-C(19)-C(22)	109.4(6)
C(14)-C(19)-C(22)	110.2(6)
C(21)-C(19)-C(20)	108.4(6)
C(14)-C(19)-C(20)	111.6(6)
C(22)-C(19)-C(20)	106.0(6)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(5)-C(23)-C(24)	110.0(4)
O(5)-C(23)-C(36)	109.9(4)

C(24)-C(23)-C(36)	107.2(4)
O(5)-C(23)-C(30)	105.9(4)
C(24)-C(23)-C(30)	111.5(4)
C(36)-C(23)-C(30)	112.3(4)
C(25)-C(24)-C(29)	117.2(5)
C(25)-C(24)-C(23)	120.9(5)
C(29)-C(24)-C(23)	121.9(5)
C(24)-C(25)-C(26)	121.4(6)
C(24)-C(25)-H(25)	119.3
C(26)-C(25)-H(25)	119.3
C(27)-C(26)-C(25)	121.0(6)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	118.6(6)
C(26)-C(27)-H(27)	120.7
C(28)-C(27)-H(27)	120.7
C(27)-C(28)-C(29)	120.4(6)
C(27)-C(28)-H(28)	119.8
C(29)-C(28)-H(28)	119.8
C(28)-C(29)-C(24)	121.4(6)
C(28)-C(29)-H(29)	119.3
C(24)-C(29)-H(29)	119.3
C(35)-C(30)-C(31)	117.6(5)
C(35)-C(30)-C(23)	123.3(5)
C(31)-C(30)-C(23)	118.7(5)
C(30)-C(31)-C(32)	120.8(6)
C(30)-C(31)-H(31)	119.6
C(32)-C(31)-H(31)	119.6
C(33)-C(32)-C(31)	120.6(6)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(34)-C(33)-C(32)	119.1(6)
C(34)-C(33)-H(33)	120.4
C(32)-C(33)-H(33)	120.4

C(33)-C(34)-C(35)	121.0(6)
C(33)-C(34)-H(34)	119.5
C(35)-C(34)-H(34)	119.5
C(30)-C(35)-C(34)	120.8(6)
C(30)-C(35)-H(35)	119.6
C(34)-C(35)-H(35)	119.6
C(37)-C(36)-C(41)	117.8(5)
C(37)-C(36)-C(23)	120.4(5)
C(41)-C(36)-C(23)	121.7(5)
C(36)-C(37)-C(38)	121.1(6)
C(36)-C(37)-H(37)	119.5
C(38)-C(37)-H(37)	119.5
C(39)-C(38)-C(37)	120.0(6)
C(39)-C(38)-H(38)	120.0
C(37)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	119.1(6)
C(40)-C(39)-H(39)	120.4
C(38)-C(39)-H(39)	120.4
C(39)-C(40)-C(41)	121.3(7)
C(39)-C(40)-H(40)	119.4
C(41)-C(40)-H(40)	119.4
C(40)-C(41)-C(36)	120.6(6)
C(40)-C(41)-H(41)	119.7
C(36)-C(41)-H(41)	119.7
C(43)-C(42)-O(3)	109.4(8)
C(43)-C(42)-H(42A)	109.8
O(3)-C(42)-H(42A)	109.8
C(43)-C(42)-H(42B)	109.8
O(3)-C(42)-H(42B)	109.8
H(42A)-C(42)-H(42B)	108.2
C(42)-C(43)-C(44)	105.5(7)
C(42)-C(43)-H(43A)	110.6
C(44)-C(43)-H(43A)	110.6
C(42)-C(43)-H(43B)	110.6

C(44)-C(43)-H(43B)	110.6
H(43A)-C(43)-H(43B)	108.8
C(45)-C(44)-C(43)	104.6(8)
C(45)-C(44)-H(44A)	110.8
C(43)-C(44)-H(44A)	110.8
C(45)-C(44)-H(44B)	110.8
C(43)-C(44)-H(44B)	110.8
H(44A)-C(44)-H(44B)	108.9
O(3)-C(45)-C(44)	108.6(8)
O(3)-C(45)-H(45A)	110.0
C(44)-C(45)-H(45A)	110.0
O(3)-C(45)-H(45B)	110.0
C(44)-C(45)-H(45B)	110.0
H(45A)-C(45)-H(45B)	108.3
O(4)-C(46)-C(47)	106.3(7)
O(4)-C(46)-H(46A)	110.5
C(47)-C(46)-H(46A)	110.5
O(4)-C(46)-H(46B)	110.5
C(47)-C(46)-H(46B)	110.5
H(46A)-C(46)-H(46B)	108.7
C(48)-C(47)-C(46)	107.2(8)
C(48)-C(47)-H(47A)	110.3
C(46)-C(47)-H(47A)	110.3
C(48)-C(47)-H(47B)	110.3
C(46)-C(47)-H(47B)	110.3
H(47A)-C(47)-H(47B)	108.5
C(47)-C(48)-C(49)	108.8(9)
C(47)-C(48)-H(48A)	109.9
C(49)-C(48)-H(48A)	109.9
C(47)-C(48)-H(48B)	109.9
C(49)-C(48)-H(48B)	109.9
H(48A)-C(48)-H(48B)	108.3
O(4)-C(49)-C(48)	107.5(7)
O(4)-C(49)-H(49A)	110.2

C(48)-C(49)-H(49A)	110.2
O(4)-C(49)-H(49B)	110.2
C(48)-C(49)-H(49B)	110.2
H(49A)-C(49)-H(49B)	108.5
C(54)-C(50)-C(51)	79(2)
C(54)-C(50)-H(50A)	115.3
C(51)-C(50)-H(50A)	115.4
C(54)-C(50)-H(50B)	115.3
C(51)-C(50)-H(50B)	115.4
H(50A)-C(50)-H(50B)	112.4
C(50)-C(51)-C(52)	104.9(16)
C(50)-C(51)-C(54)	50.0(12)
C(52)-C(51)-C(54)	84.8(12)
C(50)-C(51)-H(51A)	110.7
C(52)-C(51)-H(51A)	110.8
C(54)-C(51)-H(51A)	159.2
C(50)-C(51)-H(51B)	110.8
C(52)-C(51)-H(51B)	110.8
C(54)-C(51)-H(51B)	76.5
H(51A)-C(51)-H(51B)	108.8
C(51)-C(52)-C(53)	94.3(12)
C(51)-C(52)-H(52A)	112.9
C(53)-C(52)-H(52A)	112.9
C(51)-C(52)-H(52B)	112.8
C(53)-C(52)-H(52B)	112.9
H(52A)-C(52)-H(52B)	110.3
C(54)-C(53)-C(52)	97.4(13)
C(54)-C(53)-H(53A)	112.3
C(52)-C(53)-H(53A)	112.3
C(54)-C(53)-H(53B)	112.2
C(52)-C(53)-H(53B)	112.2
H(53A)-C(53)-H(53B)	109.9
C(50)-C(54)-C(53)	101(3)
C(50)-C(54)-C(51)	50.6(12)

C(53)-C(54)-C(51)	83.2(12)
C(50)-C(54)-H(54A)	111.6
C(53)-C(54)-H(54A)	111.6
C(51)-C(54)-H(54A)	75.0
C(50)-C(54)-H(54B)	111.7
C(53)-C(54)-H(54B)	111.6
C(51)-C(54)-H(54B)	160.1
H(54A)-C(54)-H(54B)	109.4
C(56)#1-C(55)-C(56)	107.7(16)
C(56)#1-C(55)-H(55A)	110.2
C(56)-C(55)-H(55A)	110.2
C(56)#1-C(55)-H(55B)	110.2
C(56)-C(55)-H(55B)	110.2
H(55A)-C(55)-H(55B)	108.5
C(55)-C(56)-C(57)	105.6(14)
C(55)-C(56)-H(56A)	110.6
C(57)-C(56)-H(56A)	110.6
C(55)-C(56)-H(56B)	110.6
C(57)-C(56)-H(56B)	110.6
H(56A)-C(56)-H(56B)	108.7
C(57)#1-C(57)-C(56)	104(2)
C(57)#1-C(57)-H(57A)	110.9
C(56)-C(57)-H(57A)	110.9
C(57)#1-C(57)-H(57B)	110.9
C(56)-C(57)-H(57B)	110.9
H(57A)-C(57)-H(57B)	108.9
C(59)-C(58)-H(58A)	109.5
C(59)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(59)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(60)-C(59)-C(58)	110.8(18)
C(60)-C(59)-H(59A)	109.5

C(58)-C(59)-H(59A)	109.5
C(60)-C(59)-H(59B)	109.5
C(58)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	108.1
C(59)-C(60)-C(61)	111.7(15)
C(59)-C(60)-H(60A)	109.2
C(61)-C(60)-H(60A)	109.3
C(59)-C(60)-H(60B)	109.3
C(61)-C(60)-H(60B)	109.3
H(60A)-C(60)-H(60B)	107.9
C(60)-C(61)-C(62)	99.9(12)
C(60)-C(61)-H(61A)	111.7
C(62)-C(61)-H(61A)	111.8
C(60)-C(61)-H(61B)	111.8
C(62)-C(61)-H(61B)	111.9
H(61A)-C(61)-H(61B)	109.5
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.4
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(64)-C(63)-C(64)#1	123(2)
C(64)-C(63)-H(63A)	106.5
C(64)#1-C(63)-H(63A)	106.5
C(64)-C(63)-H(63B)	106.5
C(64)#1-C(63)-H(63B)	106.5
H(63A)-C(63)-H(63B)	106.5
C(63)-C(64)-C(65)	113.2(16)
C(63)-C(64)-H(64A)	108.9
C(65)-C(64)-H(64A)	108.9
C(63)-C(64)-H(64B)	108.9
C(65)-C(64)-H(64B)	108.9
H(64A)-C(64)-H(64B)	107.8

C(64)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(64)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5

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

Table 5.1 Crystal data and structure refinement for [Lu(tbmp)(OCHPh₂)(THF)₃] (6).

Identification code	mk6	
Empirical formula	C ₄₇ H ₆₃ LuO ₆ S	
Formula weight	931.00	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 14.710(3) Å	α = 90°
	b = 13.582(3) Å	β = 108.290(4)°
	c = 22.910(4) Å	γ = 90°
Volume	4346.0(14) Å ³	
Z	4	
Density (calculated)	1.423 Mg/m ³	
Absorption coefficient	2.366 mm ⁻¹	
F(000)	1920	
Crystal size	0.28×0.21×0.08 mm ³	
Theta range for data collection	1.96 to 28.38°	
Index ranges	-19≤h≤19, -18≤k≤18, -30≤l≤30	
Reflections collected	57519	
Independent reflections	10862 [R(int) = 0.0947]	
Completeness to theta = 28.38°	99.7 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8333 and 0.5571	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10862 / 0 / 496
Goodness-of-fit on F^2	1.015
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0420, wR2 = 0.0884
R indices (all data)	R1 = 0.0700, wR2 = 0.0973
Largest diff. peak and hole	1.488 and -0.812 e.Å ⁻³

Table 5.2 Bond lengths [Å] and angles [°] for mk6.

Lu(1)-O(3)	2.045(3)
Lu(1)-O(1)	2.151(3)
Lu(1)-O(2)	2.176(3)
Lu(1)-O(6)	2.347(3)
Lu(1)-O(4)	2.389(3)
Lu(1)-O(5)	2.445(3)
Lu(1)-S(1)	2.8707(11)
S(1)-C(22)	1.765(4)
S(1)-C(11)	1.788(4)
O(1)-C(1)	1.326(4)
O(2)-C(12)	1.316(5)
O(3)-C(23)	1.383(5)
O(4)-C(36)	1.431(5)
O(4)-C(39)	1.442(5)
O(5)-C(40)	1.438(5)
O(5)-C(43)	1.450(5)
O(6)-C(47)	1.440(5)
O(6)-C(44)	1.444(6)
C(1)-C(11)	1.417(5)
C(1)-C(2)	1.427(6)
C(2)-C(7)	1.395(6)
C(2)-C(3)	1.522(6)
C(3)-C(4)	1.526(6)
C(3)-C(5)	1.528(6)
C(3)-C(6)	1.535(6)

C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.406(6)
C(7)-H(7)	0.9500
C(8)-C(10)	1.363(6)
C(8)-C(9)	1.512(6)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.383(5)
C(10)-H(10)	0.9500
C(12)-C(22)	1.406(6)
C(12)-C(13)	1.428(6)
C(13)-C(18)	1.394(6)
C(13)-C(14)	1.520(6)
C(14)-C(15)	1.513(7)
C(14)-C(17)	1.519(6)
C(14)-C(16)	1.534(7)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

C(18)-C(19)	1.402(6)
C(18)-H(18)	0.9500
C(19)-C(21)	1.367(6)
C(19)-C(20)	1.511(6)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.388(6)
C(21)-H(21)	0.9500
C(23)-C(24)	1.523(6)
C(23)-C(30)	1.528(6)
C(23)-H(23)	1.0000
C(24)-C(29)	1.372(6)
C(24)-C(25)	1.389(6)
C(25)-C(26)	1.378(7)
C(25)-H(25)	0.9500
C(26)-C(27)	1.370(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.362(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.393(6)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(31)	1.373(6)
C(30)-C(35)	1.391(6)
C(31)-C(32)	1.386(7)
C(31)-H(31)	0.9500
C(32)-C(33)	1.378(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.372(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.385(6)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500

C(36)-C(37)	1.504(7)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.500(7)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.505(7)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.482(7)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.519(6)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.525(6)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.499(7)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.475(8)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.504(8)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900

O(3)-Lu(1)-O(1)	162.89(12)
O(3)-Lu(1)-O(2)	96.59(11)
O(1)-Lu(1)-O(2)	95.81(11)
O(3)-Lu(1)-O(6)	100.07(11)
O(1)-Lu(1)-O(6)	94.00(11)
O(2)-Lu(1)-O(6)	78.08(10)
O(3)-Lu(1)-O(4)	87.67(11)
O(1)-Lu(1)-O(4)	87.33(11)
O(2)-Lu(1)-O(4)	150.56(11)
O(6)-Lu(1)-O(4)	72.50(11)
O(3)-Lu(1)-O(5)	80.85(11)
O(1)-Lu(1)-O(5)	82.04(10)
O(2)-Lu(1)-O(5)	137.47(10)
O(6)-Lu(1)-O(5)	144.39(10)
O(4)-Lu(1)-O(5)	71.97(10)
O(3)-Lu(1)-S(1)	102.42(9)
O(1)-Lu(1)-S(1)	71.33(7)
O(2)-Lu(1)-S(1)	68.77(7)
O(6)-Lu(1)-S(1)	141.59(8)
O(4)-Lu(1)-S(1)	138.74(8)
O(5)-Lu(1)-S(1)	70.41(7)
C(22)-S(1)-C(11)	105.01(19)
C(22)-S(1)-Lu(1)	97.73(14)
C(11)-S(1)-Lu(1)	95.41(13)
C(1)-O(1)-Lu(1)	132.2(2)
C(12)-O(2)-Lu(1)	132.3(3)
C(23)-O(3)-Lu(1)	170.2(3)
C(36)-O(4)-C(39)	109.9(4)
C(36)-O(4)-Lu(1)	123.5(3)
C(39)-O(4)-Lu(1)	126.6(3)
C(40)-O(5)-C(43)	107.9(3)
C(40)-O(5)-Lu(1)	126.5(3)
C(43)-O(5)-Lu(1)	123.2(2)
C(47)-O(6)-C(44)	108.6(4)

C(47)-O(6)-Lu(1)	123.0(3)
C(44)-O(6)-Lu(1)	127.5(3)
O(1)-C(1)-C(11)	120.6(4)
O(1)-C(1)-C(2)	122.4(4)
C(11)-C(1)-C(2)	116.9(4)
C(7)-C(2)-C(1)	118.1(4)
C(7)-C(2)-C(3)	121.0(4)
C(1)-C(2)-C(3)	120.8(4)
C(2)-C(3)-C(4)	113.2(4)
C(2)-C(3)-C(5)	110.1(4)
C(4)-C(3)-C(5)	107.9(4)
C(2)-C(3)-C(6)	108.7(3)
C(4)-C(3)-C(6)	106.7(4)
C(5)-C(3)-C(6)	110.2(4)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-C(8)	123.7(4)
C(2)-C(7)-H(7)	118.1

C(8)-C(7)-H(7)	118.1
C(10)-C(8)-C(7)	117.6(4)
C(10)-C(8)-C(9)	121.0(4)
C(7)-C(8)-C(9)	121.4(4)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-C(11)	121.0(4)
C(8)-C(10)-H(10)	119.5
C(11)-C(10)-H(10)	119.5
C(10)-C(11)-C(1)	122.6(4)
C(10)-C(11)-S(1)	118.5(3)
C(1)-C(11)-S(1)	118.8(3)
O(2)-C(12)-C(22)	120.5(4)
O(2)-C(12)-C(13)	122.2(4)
C(22)-C(12)-C(13)	117.3(4)
C(18)-C(13)-C(12)	117.3(4)
C(18)-C(13)-C(14)	122.2(4)
C(12)-C(13)-C(14)	120.5(4)
C(15)-C(14)-C(17)	106.8(4)
C(15)-C(14)-C(13)	112.3(4)
C(17)-C(14)-C(13)	110.8(4)
C(15)-C(14)-C(16)	108.6(5)
C(17)-C(14)-C(16)	108.9(4)
C(13)-C(14)-C(16)	109.4(4)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(13)-C(18)-C(19)	124.5(4)
C(13)-C(18)-H(18)	117.7
C(19)-C(18)-H(18)	117.7
C(21)-C(19)-C(18)	117.3(4)
C(21)-C(19)-C(20)	122.5(4)
C(18)-C(19)-C(20)	120.2(4)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-C(22)	120.4(4)
C(19)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(21)-C(22)-C(12)	123.0(4)
C(21)-C(22)-S(1)	119.9(3)
C(12)-C(22)-S(1)	116.8(3)
O(3)-C(23)-C(24)	111.2(4)
O(3)-C(23)-C(30)	112.1(3)
C(24)-C(23)-C(30)	112.2(3)
O(3)-C(23)-H(23)	107.0

C(24)-C(23)-H(23)	107.0
C(30)-C(23)-H(23)	107.0
C(29)-C(24)-C(25)	119.0(4)
C(29)-C(24)-C(23)	121.0(4)
C(25)-C(24)-C(23)	120.0(4)
C(26)-C(25)-C(24)	120.2(4)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	120.2(5)
C(27)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(28)-C(27)-C(26)	120.3(5)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(29)	119.9(4)
C(27)-C(28)-H(28)	120.0
C(29)-C(28)-H(28)	120.0
C(24)-C(29)-C(28)	120.3(5)
C(24)-C(29)-H(29)	119.8
C(28)-C(29)-H(29)	119.8
C(31)-C(30)-C(35)	117.8(4)
C(31)-C(30)-C(23)	121.2(4)
C(35)-C(30)-C(23)	121.0(4)
C(30)-C(31)-C(32)	121.5(4)
C(30)-C(31)-H(31)	119.2
C(32)-C(31)-H(31)	119.2
C(33)-C(32)-C(31)	119.8(5)
C(33)-C(32)-H(32)	120.1
C(31)-C(32)-H(32)	120.1
C(34)-C(33)-C(32)	119.8(5)
C(34)-C(33)-H(33)	120.1
C(32)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	119.9(4)
C(33)-C(34)-H(34)	120.1

C(35)-C(34)-H(34)	120.1
C(34)-C(35)-C(30)	121.2(4)
C(34)-C(35)-H(35)	119.4
C(30)-C(35)-H(35)	119.4
O(4)-C(36)-C(37)	105.6(4)
O(4)-C(36)-H(36A)	110.6
C(37)-C(36)-H(36A)	110.6
O(4)-C(36)-H(36B)	110.6
C(37)-C(36)-H(36B)	110.6
H(36A)-C(36)-H(36B)	108.7
C(38)-C(37)-C(36)	102.3(4)
C(38)-C(37)-H(37A)	111.3
C(36)-C(37)-H(37A)	111.3
C(38)-C(37)-H(37B)	111.3
C(36)-C(37)-H(37B)	111.3
H(37A)-C(37)-H(37B)	109.2
C(37)-C(38)-C(39)	103.1(4)
C(37)-C(38)-H(38A)	111.2
C(39)-C(38)-H(38A)	111.2
C(37)-C(38)-H(38B)	111.2
C(39)-C(38)-H(38B)	111.2
H(38A)-C(38)-H(38B)	109.1
O(4)-C(39)-C(38)	105.2(4)
O(4)-C(39)-H(39A)	110.7
C(38)-C(39)-H(39A)	110.7
O(4)-C(39)-H(39B)	110.7
C(38)-C(39)-H(39B)	110.7
H(39A)-C(39)-H(39B)	108.8
O(5)-C(40)-C(41)	105.5(4)
O(5)-C(40)-H(40A)	110.6
C(41)-C(40)-H(40A)	110.6
O(5)-C(40)-H(40B)	110.6
C(41)-C(40)-H(40B)	110.6
H(40A)-C(40)-H(40B)	108.8

C(40)-C(41)-C(42)	103.9(4)
C(40)-C(41)-H(41A)	111.0
C(42)-C(41)-H(41A)	111.0
C(40)-C(41)-H(41B)	111.0
C(42)-C(41)-H(41B)	111.0
H(41A)-C(41)-H(41B)	109.0
C(41)-C(42)-C(43)	104.7(4)
C(41)-C(42)-H(42A)	110.8
C(43)-C(42)-H(42A)	110.8
C(41)-C(42)-H(42B)	110.8
C(43)-C(42)-H(42B)	110.8
H(42A)-C(42)-H(42B)	108.9
O(5)-C(43)-C(42)	106.4(3)
O(5)-C(43)-H(43A)	110.4
C(42)-C(43)-H(43A)	110.4
O(5)-C(43)-H(43B)	110.4
C(42)-C(43)-H(43B)	110.4
H(43A)-C(43)-H(43B)	108.6
O(6)-C(44)-C(45)	106.5(4)
O(6)-C(44)-H(44A)	110.4
C(45)-C(44)-H(44A)	110.4
O(6)-C(44)-H(44B)	110.4
C(45)-C(44)-H(44B)	110.4
H(44A)-C(44)-H(44B)	108.6
C(46)-C(45)-C(44)	105.2(5)
C(46)-C(45)-H(45A)	110.7
C(44)-C(45)-H(45A)	110.7
C(46)-C(45)-H(45B)	110.7
C(44)-C(45)-H(45B)	110.7
H(45A)-C(45)-H(45B)	108.8
C(45)-C(46)-C(47)	103.4(5)
C(45)-C(46)-H(46A)	111.1
C(47)-C(46)-H(46A)	111.1
C(45)-C(46)-H(46B)	111.1

C(47)-C(46)-H(46B)	111.1
H(46A)-C(46)-H(46B)	109.0
O(6)-C(47)-C(46)	104.2(5)
O(6)-C(47)-H(47A)	110.9
C(46)-C(47)-H(47A)	110.9
O(6)-C(47)-H(47B)	110.9
C(46)-C(47)-H(47B)	110.9
H(47A)-C(47)-H(47B)	108.9

Table 6.1 Crystal data and structure refinement for [Lu(tbmp)(μ -H)(THF)₂]₂ (7).

Identification code	mk7	
Empirical formula	C ₃₉ H ₆₅ LuO ₅ S	
Formula weight	820.98	
Temperature	140(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 29.835(9) Å	$\alpha = 90^\circ$
	b = 17.805(6) Å	$\beta = 121.466(5)^\circ$
	c = 18.098(6) Å	$\gamma = 90^\circ$
Volume	8200(5) Å ³	
Z	8	
Density (calculated)	1.330 Mg/m ³	
Absorption coefficient	2.496 mm ⁻¹	
F(000)	3407	
Crystal size	0.60×0.30×0.30 mm ³	
Theta range for data collection	2.26 to 28.36°	
Index ranges	-39≤h≤39, -23≤k≤23, -24≤l≤23	
Reflections collected	42018	
Independent reflections	10147 [R(int) = 0.0280]	
Completeness to theta = 28.36°	99.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.5214 and 0.3159	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10147 / 14 / 414
Goodness-of-fit on F^2	0.987
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0256, wR2 = 0.0633
R indices (all data)	R1 = 0.0332, wR2 = 0.0682
Largest diff. peak and hole	1.783 and -0.513 e.Å ⁻³

Table 6.2 Bond lengths [Å] and angles [°] for mk7.

Lu-O(1)	2.1229(18)
Lu-O(2)	2.1245(19)
Lu-O(4)	2.3456(19)
Lu-O(3)	2.379(2)
Lu-S	2.9191(12)
Lu-Lu#1	3.5530(13)
Lu-H(1)	2.09(3)
S-C(12)	1.779(3)
S-C(2)	1.782(3)
O(1)-C(1)	1.323(3)
O(2)-C(13)	1.329(3)
O(3)-C(26)	1.441(3)
O(3)-C(23)	1.448(3)
O(4)-C(27)	1.451(3)
O(4)-C(30)	1.452(3)
C(1)-C(2)	1.419(3)
C(1)-C(6)	1.421(4)
C(2)-C(3)	1.393(3)
C(3)-C(4)	1.388(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.391(4)
C(4)-C(7)	1.514(4)
C(5)-C(6)	1.395(3)
C(5)-H(5)	0.9500
C(6)-C(8)	1.541(4)

C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(10)	1.536(4)
C(8)-C(11)	1.537(4)
C(8)-C(9)	1.543(4)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.400(3)
C(12)-C(13)	1.418(4)
C(13)-C(14)	1.423(4)
C(14)-C(15)	1.393(4)
C(14)-C(19)	1.533(4)
C(15)-C(16)	1.399(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.381(4)
C(16)-C(18)	1.516(4)
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(22)	1.531(4)
C(19)-C(20)	1.535(4)
C(19)-C(21)	1.543(4)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.524(5)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.530(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.514(5)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.461(5)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.427(5)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.463(5)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
O(5)-C(34)	1.422(5)
O(5)-C(31)	1.423(5)
C(31)-C(32)	1.482(6)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.487(6)

C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.506(6)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.461(15)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.558(15)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.500(13)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.515(14)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(41)	1.301(15)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(42)	1.318(14)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.487(16)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.506(16)

C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
O(1)-Lu-O(2)	99.00(8)
O(1)-Lu-O(4)	147.77(7)
O(2)-Lu-O(4)	83.02(7)
O(1)-Lu-O(3)	82.96(7)
O(2)-Lu-O(3)	144.13(7)
O(4)-Lu-O(3)	77.45(8)
O(1)-Lu-S	70.43(5)
O(2)-Lu-S	69.95(5)
O(4)-Lu-S	80.38(5)
O(3)-Lu-S	77.26(5)
O(1)-Lu-Lu#1	107.31(5)
O(2)-Lu-Lu#1	110.03(5)
O(4)-Lu-Lu#1	101.99(5)
O(3)-Lu-Lu#1	103.32(5)
S-Lu-Lu#1	177.633(13)
O(1)-Lu-H(1)	86.4(9)
O(2)-Lu-H(1)	87.4(9)
O(4)-Lu-H(1)	125.8(9)
O(3)-Lu-H(1)	128.3(9)
S-Lu-H(1)	143.8(9)
Lu#1-Lu-H(1)	34.3(9)
C(12)-S-C(2)	103.36(12)
C(12)-S-Lu	95.56(8)
C(2)-S-Lu	95.17(8)
C(1)-O(1)-Lu	135.07(16)
C(13)-O(2)-Lu	135.32(17)
C(26)-O(3)-C(23)	104.6(2)
C(26)-O(3)-Lu	116.82(17)

C(23)-O(3)-Lu	133.70(17)
C(27)-O(4)-C(30)	108.7(2)
C(27)-O(4)-Lu	124.62(17)
C(30)-O(4)-Lu	126.59(16)
O(1)-C(1)-C(2)	120.4(2)
O(1)-C(1)-C(6)	122.0(2)
C(2)-C(1)-C(6)	117.6(2)
C(3)-C(2)-C(1)	122.2(2)
C(3)-C(2)-S	118.9(2)
C(1)-C(2)-S	118.91(18)
C(4)-C(3)-C(2)	120.0(2)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	118.1(2)
C(3)-C(4)-C(7)	120.9(3)
C(5)-C(4)-C(7)	121.0(3)
C(4)-C(5)-C(6)	123.8(3)
C(4)-C(5)-H(5)	118.1
C(6)-C(5)-H(5)	118.1
C(5)-C(6)-C(1)	118.2(2)
C(5)-C(6)-C(8)	121.3(2)
C(1)-C(6)-C(8)	120.4(2)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(10)-C(8)-C(11)	107.9(2)
C(10)-C(8)-C(6)	110.8(2)
C(11)-C(8)-C(6)	112.1(2)
C(10)-C(8)-C(9)	110.3(2)
C(11)-C(8)-C(9)	107.4(2)
C(6)-C(8)-C(9)	108.3(2)

C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	122.0(2)
C(17)-C(12)-S	119.3(2)
C(13)-C(12)-S	118.66(18)
O(2)-C(13)-C(12)	120.0(2)
O(2)-C(13)-C(14)	122.3(2)
C(12)-C(13)-C(14)	117.7(2)
C(15)-C(14)-C(13)	118.2(2)
C(15)-C(14)-C(19)	121.2(2)
C(13)-C(14)-C(19)	120.6(2)
C(14)-C(15)-C(16)	124.0(3)
C(14)-C(15)-H(15)	118.0
C(16)-C(15)-H(15)	118.0
C(17)-C(16)-C(15)	117.8(2)
C(17)-C(16)-C(18)	121.4(3)
C(15)-C(16)-C(18)	120.8(3)
C(16)-C(17)-C(12)	120.3(3)

C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(19)-C(14)	108.5(2)
C(22)-C(19)-C(20)	107.7(3)
C(14)-C(19)-C(20)	112.3(2)
C(22)-C(19)-C(21)	110.1(2)
C(14)-C(19)-C(21)	110.8(2)
C(20)-C(19)-C(21)	107.3(3)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(3)-C(23)-C(24)	104.7(3)
O(3)-C(23)-H(23A)	110.8

C(24)-C(23)-H(23A)	110.8
O(3)-C(23)-H(23B)	110.8
C(24)-C(23)-H(23B)	110.8
H(23A)-C(23)-H(23B)	108.9
C(23)-C(24)-C(25)	104.7(3)
C(23)-C(24)-H(24A)	110.8
C(25)-C(24)-H(24A)	110.8
C(23)-C(24)-H(24B)	110.8
C(25)-C(24)-H(24B)	110.8
H(24A)-C(24)-H(24B)	108.9
C(26)-C(25)-C(24)	104.1(3)
C(26)-C(25)-H(25A)	110.9
C(24)-C(25)-H(25A)	110.9
C(26)-C(25)-H(25B)	110.9
C(24)-C(25)-H(25B)	110.9
H(25A)-C(25)-H(25B)	109.0
O(3)-C(26)-C(25)	104.8(3)
O(3)-C(26)-H(26A)	110.8
C(25)-C(26)-H(26A)	110.8
O(3)-C(26)-H(26B)	110.8
C(25)-C(26)-H(26B)	110.8
H(26A)-C(26)-H(26B)	108.9
O(4)-C(27)-C(28)	106.6(3)
O(4)-C(27)-H(27A)	110.4
C(28)-C(27)-H(27A)	110.4
O(4)-C(27)-H(27B)	110.4
C(28)-C(27)-H(27B)	110.4
H(27A)-C(27)-H(27B)	108.6
C(29)-C(28)-C(27)	108.1(3)
C(29)-C(28)-H(28A)	110.1
C(27)-C(28)-H(28A)	110.1
C(29)-C(28)-H(28B)	110.1
C(27)-C(28)-H(28B)	110.1
H(28A)-C(28)-H(28B)	108.4

C(28)-C(29)-C(30)	108.1(3)
C(28)-C(29)-H(29A)	110.1
C(30)-C(29)-H(29A)	110.1
C(28)-C(29)-H(29B)	110.1
C(30)-C(29)-H(29B)	110.1
H(29A)-C(29)-H(29B)	108.4
O(4)-C(30)-C(29)	106.7(3)
O(4)-C(30)-H(30A)	110.4
C(29)-C(30)-H(30A)	110.4
O(4)-C(30)-H(30B)	110.4
C(29)-C(30)-H(30B)	110.4
H(30A)-C(30)-H(30B)	108.6
C(34)-O(5)-C(31)	108.9(3)
O(5)-C(31)-C(32)	106.0(3)
O(5)-C(31)-H(31A)	110.5
C(32)-C(31)-H(31A)	110.5
O(5)-C(31)-H(31B)	110.5
C(32)-C(31)-H(31B)	110.5
H(31A)-C(31)-H(31B)	108.7
C(31)-C(32)-C(33)	102.7(3)
C(31)-C(32)-H(32A)	111.2
C(33)-C(32)-H(32A)	111.2
C(31)-C(32)-H(32B)	111.2
C(33)-C(32)-H(32B)	111.2
H(32A)-C(32)-H(32B)	109.1
C(32)-C(33)-C(34)	103.9(3)
C(32)-C(33)-H(33A)	111.0
C(34)-C(33)-H(33A)	111.0
C(32)-C(33)-H(33B)	111.0
C(34)-C(33)-H(33B)	111.0
H(33A)-C(33)-H(33B)	109.0
O(5)-C(34)-C(33)	106.8(3)
O(5)-C(34)-H(34A)	110.4
C(33)-C(34)-H(34A)	110.4

O(5)-C(34)-H(34B)	110.4
C(33)-C(34)-H(34B)	110.4
H(34A)-C(34)-H(34B)	108.6
C(36)-C(35)-H(35A)	109.5
C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(35)-C(36)-C(37)	115.7(13)
C(35)-C(36)-H(36A)	108.4
C(37)-C(36)-H(36A)	108.4
C(35)-C(36)-H(36B)	108.4
C(37)-C(36)-H(36B)	108.4
H(36A)-C(36)-H(36B)	107.4
C(38)-C(37)-C(36)	107.3(12)
C(38)-C(37)-H(37A)	110.2
C(36)-C(37)-H(37A)	110.2
C(38)-C(37)-H(37B)	110.2
C(36)-C(37)-H(37B)	110.2
H(37A)-C(37)-H(37B)	108.5
C(37)-C(38)-C(39)	112.4(13)
C(37)-C(38)-H(38A)	109.1
C(39)-C(38)-H(38A)	109.1
C(37)-C(38)-H(38B)	109.1
C(39)-C(38)-H(38B)	109.1
H(38A)-C(38)-H(38B)	107.9
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-H(40A)	109.5

C(41)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(41)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(40)-C(41)-C(42)	155(3)
C(40)-C(41)-H(41A)	97.6
C(42)-C(41)-H(41A)	97.6
C(40)-C(41)-H(41B)	97.6
C(42)-C(41)-H(41B)	97.6
H(41A)-C(41)-H(41B)	103.6
C(41)-C(42)-C(43)	124.3(16)
C(41)-C(42)-H(42A)	106.3
C(43)-C(42)-H(42A)	106.3
C(41)-C(42)-H(42B)	106.3
C(43)-C(42)-H(42B)	106.3
H(42A)-C(42)-H(42B)	106.4
C(42)-C(43)-C(44)	109.1(15)
C(42)-C(43)-H(43A)	109.9
C(44)-C(43)-H(43A)	109.9
C(42)-C(43)-H(43B)	109.9
C(44)-C(43)-H(43B)	109.9
H(43A)-C(43)-H(43B)	108.3
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5

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