

Supplementary Materials

Table S1. Crystal data and structure refinement for apx539_fulla.

Identification Code	apx539_fulla
Empirical formula	C ₃₀ H ₆₀ Ce O ₂ Si ₄
Formula weight	705.26
Temperature	140(1) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	$a = 11.199(6) \text{ Å}$
	$b = 34.737(18) \text{ Å}$
	$c = 10.931(6) \text{ Å}$
Volume	3795(3) Å ³
Z	4
Density (calculated)	1.234 Mg/m ³
Absorption coefficient	1.348 mm ⁻¹
$F(000)$	1480
Crystal size	0.120 × 0.100 × 0.080 mm ³
Theta range for data collection	2.037 to 25.782°
Index ranges	$-13 \leq h \leq 13, -42 \leq k \leq 42, -13 \leq l \leq 13$
Reflections collected	36,532
Independent reflections	7265 [R(int) = 0.2058]
Completeness to theta = 25.000°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.898 and 0.874
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7265/31/352
Goodness-of-fit on F^2	0.966
Final R indices [I > 2sigma(I)]	$R1 = 0.0696, wR2 = 0.1389$
R indices (all data)	$R1 = 0.1595, wR2 = 0.1775$
Extinction coefficient	n/a
Largest diff. peak and hole	1.027 and -1.839 e·Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for apx539_fulla. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
Ce(1)	7318(1)	1272(1)	9469(1)	32(1)
Si(1)	4078(3)	1148(1)	10,387(4)	59(1)
Si(2)	9288(3)	437(1)	12,547(3)	42(1)
Si(3)	10,517(2)	1975(1)	11,906(3)	37(1)
Si(4)	8495(3)	1379(1)	6371(3)	41(1)
O(1)	6218(5)	1772(2)	8700(6)	36(2)
O(2)	6263(6)	855(2)	7984(7)	50(2)
C(1)	6637(9)	778(3)	11,079(10)	43(2)
C(2)	5909(9)	1117(3)	10,989(10)	43(2)
C(3)	6917(8)	1393(3)	11,737(9)	39(2)
C(4)	8173(8)	1224(2)	12,234(9)	36(2)
C(5)	8027(8)	834(2)	11,858(8)	31(2)
C(6)	3524(15)	690(4)	10,775(16)	133(6)
C(7)	3732(10)	1546(4)	11,265(12)	82(4)
C(8)	3098(11)	1225(4)	8527(13)	100(5)
C(9)	8580(9)	73(2)	13,262(9)	46(3)
C(10)	9586(11)	195(3)	11,196(11)	65(3)
C(11)	10,902(9)	620(3)	13,900(10)	53(3)
C(12)	9211(8)	1708(2)	9067(8)	31(2)
C(13)	9829(8)	1621(2)	10,488(9)	31(2)
C(14)	10,067(8)	1214(2)	10,524(9)	35(2)
C(15)	9588(8)	1068(2)	9209(9)	32(2)
C(16)	9032(8)	1380(2)	8249(9)	36(2)
C(17)	11,374(9)	2353(3)	11,397(10)	56(3)
C(18)	11,741(9)	1735(3)	13,519(9)	50(3)
C(19)	9211(8)	2213(2)	12,253(9)	40(2)
C(20)	9606(12)	1711(3)	6041(10)	67(3)
C(21)	6772(11)	1573(4)	5386(10)	93(5)
C(22)	8678(13)	895(3)	5809(11)	70(4)
C(23)	5555(8)	2128(3)	8199(9)	39(2)
C(24)	6549(9)	2415(3)	8113(10)	51(3)
C(25)	4407(9)	2062(3)	6791(9)	55(3)
C(26)	5066(8)	2280(3)	9182(9)	43(2)
C(27)	5618(11)	542(3)	7068(11)	65(3)
C(28)	4570(20)	379(6)	7330(30)	76(6)
C(28')	5290(50)	274(10)	7980(40)	76(6)
C(29)	4959(18)	701(5)	5573(13)	71(5)
C(29')	4300(30)	671(12)	6060(40)	71(5)
C(30)	6665(17)	267(4)	7150(20)	86(6)
C(30')	5930(160)	250(30)	6300(160)	86(6)

Table S3. Bond lengths [Å] and angles [°] for apx539_fulla.

Ce(1)–O(1)	2.077(5)
Ce(1)–O(2)	2.097(6)
Ce(1)–C(4)	2.733(9)
Ce(1)–C(3)	2.743(9)
Ce(1)–C(14)	2.764(8)
Ce(1)–C(15)	2.774(8)
Ce(1)–C(13)	2.791(8)
Ce(1)–C(12)	2.798(8)
Ce(1)–C(1)	2.799(9)
Ce(1)–C(5)	2.810(8)
Ce(1)–C(2)	2.811(9)
Ce(1)–C(16)	2.812(9)
Si(1)–C(7)	1.821(11)
Si(1)–C(6)	1.826(11)
Si(1)–C(8)	1.844(13)
Si(1)–C(2)	1.853(9)
Si(2)–C(9)	1.844(9)
Si(2)–C(10)	1.855(10)
Si(2)–C(11)	1.856(10)
Si(2)–C(5)	1.870(9)
Si(3)–C(13)	1.852(9)
Si(3)–C(17)	1.854(9)
Si(3)–C(19)	1.863(8)
Si(3)–C(18)	1.871(9)
Si(4)–C(22)	1.833(10)
Si(4)–C(20)	1.847(10)
Si(4)–C(16)	1.861(9)
Si(4)–C(21)	1.861(11)
O(1)–C(23)	1.417(10)
O(2)–C(27)	1.432(12)
C(1)–C(5)	1.410(11)
C(1)–C(2)	1.411(11)
C(2)–C(3)	1.425(12)
C(3)–C(4)	1.388(11)
C(4)–C(5)	1.406(11)
C(12)–C(16)	1.407(11)
C(12)–C(13)	1.420(11)
C(13)–C(14)	1.433(11)
C(14)–C(15)	1.385(11)
C(15)–C(16)	1.438(11)
C(23)–C(26)	1.505(12)
C(23)–C(25)	1.513(12)
C(23)–C(24)	1.529(12)
C(27)–C(28)	1.446(14)
C(27)–C(29')	1.455(18)

Table S3. *Cont.*

C(27)–C(30')	1.46(2)
C(27)–C(30)	1.485(13)
C(27)–C(28')	1.523(18)
C(27)–C(29)	1.558(14)
O(1)–Ce(1)–O(2)	103.9(2)
O(1)–Ce(1)–C(4)	110.2(2)
O(2)–Ce(1)–C(4)	127.5(3)
O(1)–Ce(1)–C(3)	85.9(2)
O(2)–Ce(1)–C(3)	122.7(3)
C(4)–Ce(1)–C(3)	29.4(2)
O(1)–Ce(1)–C(14)	125.1(2)
O(2)–Ce(1)–C(14)	113.9(2)
C(4)–Ce(1)–C(14)	76.4(3)
C(3)–Ce(1)–C(14)	103.8(3)
O(1)–Ce(1)–C(15)	125.1(2)
O(2)–Ce(1)–C(15)	88.1(2)
C(4)–Ce(1)–C(15)	102.6(2)
C(3)–Ce(1)–C(15)	131.5(2)
C(14)–Ce(1)–C(15)	29.0(2)
O(1)–Ce(1)–C(13)	96.1(2)
O(2)–Ce(1)–C(13)	136.3(2)
C(4)–Ce(1)–C(13)	78.3(2)
C(3)–Ce(1)–C(13)	96.8(3)
C(14)–Ce(1)–C(13)	29.9(2)
C(15)–Ce(1)–C(13)	49.2(2)
O(1)–Ce(1)–C(12)	80.6(2)
O(2)–Ce(1)–C(12)	117.1(2)
C(4)–Ce(1)–C(12)	107.1(2)
C(3)–Ce(1)–C(12)	120.2(3)
C(14)–Ce(1)–C(12)	47.5(3)
C(15)–Ce(1)–C(12)	47.7(2)
C(13)–Ce(1)–C(12)	29.4(2)
O(1)–Ce(1)–C(1)	119.2(2)
O(2)–Ce(1)–C(1)	81.1(3)
C(4)–Ce(1)–C(1)	47.7(3)
C(3)–Ce(1)–C(1)	47.5(3)
C(14)–Ce(1)–C(1)	105.1(3)
C(15)–Ce(1)–C(1)	115.5(2)
C(13)–Ce(1)–C(1)	121.7(3)
C(12)–Ce(1)–C(1)	150.7(3)
O(1)–Ce(1)–C(5)	134.2(2)
O(2)–Ce(1)–C(5)	99.8(2)
C(4)–Ce(1)–C(5)	29.4(2)
C(3)–Ce(1)–C(5)	48.4(2)
C(14)–Ce(1)–C(5)	77.2(2)

Table S3. *Cont.*

C(15)–Ce(1)–C(5)	94.0(2)
C(13)–Ce(1)–C(5)	93.0(2)
C(12)–Ce(1)–C(5)	121.5(2)
C(1)–Ce(1)–C(5)	29.1(2)
O(1)–Ce(1)–C(2)	90.6(2)
O(2)–Ce(1)–C(2)	93.1(3)
C(4)–Ce(1)–C(2)	49.1(3)
C(3)–Ce(1)–C(2)	29.7(3)
C(14)–Ce(1)–C(2)	123.7(3)
C(15)–Ce(1)–C(2)	142.8(3)
C(13)–Ce(1)–C(2)	125.5(3)
C(12)–Ce(1)–C(2)	149.7(3)
C(1)–Ce(1)–C(2)	29.1(2)
C(5)–Ce(1)–C(2)	49.1(2)
O(1)–Ce(1)–C(16)	95.9(2)
O(2)–Ce(1)–C(16)	89.5(3)
C(4)–Ce(1)–C(16)	124.0(3)
C(3)–Ce(1)–C(16)	146.4(3)
C(14)–Ce(1)–C(16)	48.6(3)
C(15)–Ce(1)–C(16)	29.8(2)
C(13)–Ce(1)–C(16)	49.6(2)
C(12)–Ce(1)–C(16)	29.0(2)
C(1)–Ce(1)–C(16)	144.8(2)
C(5)–Ce(1)–C(16)	123.1(2)
C(2)–Ce(1)–C(16)	172.1(3)
C(7)–Si(1)–C(6)	111.3(7)
C(7)–Si(1)–C(8)	108.0(5)
C(6)–Si(1)–C(8)	106.7(7)
C(7)–Si(1)–C(2)	108.8(5)
C(6)–Si(1)–C(2)	107.7(6)
C(8)–Si(1)–C(2)	114.4(5)
C(9)–Si(2)–C(10)	107.0(5)
C(9)–Si(2)–C(11)	110.3(4)
C(10)–Si(2)–C(11)	109.2(5)
C(9)–Si(2)–C(5)	106.6(4)
C(10)–Si(2)–C(5)	112.8(4)
C(11)–Si(2)–C(5)	110.9(4)
C(13)–Si(3)–C(17)	107.2(4)
C(13)–Si(3)–C(19)	113.4(4)
C(17)–Si(3)–C(19)	107.8(4)
C(13)–Si(3)–C(18)	110.1(4)
C(17)–Si(3)–C(18)	109.9(5)
C(19)–Si(3)–C(18)	108.4(4)
C(22)–Si(4)–C(20)	108.6(5)
C(22)–Si(4)–C(16)	110.0(4)

Table S3. *Cont.*

C(20)–Si(4)–C(16)	107.7(4)
C(22)–Si(4)–C(21)	112.4(6)
C(20)–Si(4)–C(21)	106.0(6)
C(16)–Si(4)–C(21)	111.9(4)
C(23)–O(1)–Ce(1)	175.9(5)
C(27)–O(2)–Ce(1)	174.4(6)
C(5)–C(1)–C(2)	111.9(8)
C(5)–C(1)–Ce(1)	75.9(5)
C(2)–C(1)–Ce(1)	75.9(5)
C(1)–C(2)–C(3)	103.8(8)
C(1)–C(2)–Si(1)	125.9(7)
C(3)–C(2)–Si(1)	128.9(7)
C(1)–C(2)–Ce(1)	75.0(5)
C(3)–C(2)–Ce(1)	72.5(5)
Si(1)–C(2)–Ce(1)	127.2(5)
C(4)–C(3)–C(2)	110.0(8)
C(4)–C(3)–Ce(1)	74.9(5)
C(2)–C(3)–Ce(1)	77.8(5)
C(3)–C(4)–C(5)	109.2(8)
C(3)–C(4)–Ce(1)	75.7(5)
C(5)–C(4)–Ce(1)	78.4(5)
C(4)–C(5)–C(1)	105.1(7)
C(4)–C(5)–Si(2)	128.7(6)
C(1)–C(5)–Si(2)	124.7(7)
C(4)–C(5)–Ce(1)	72.3(5)
C(1)–C(5)–Ce(1)	75.0(5)
Si(2)–C(5)–Ce(1)	128.2(4)
C(16)–C(12)–C(13)	112.4(8)
C(16)–C(12)–Ce(1)	76.0(5)
C(13)–C(12)–Ce(1)	75.0(4)
C(12)–C(13)–C(14)	103.5(7)
C(12)–C(13)–Si(3)	125.9(6)
C(14)–C(13)–Si(3)	129.0(6)
C(12)–C(13)–Ce(1)	75.5(5)
C(14)–C(13)–Ce(1)	74.0(4)
Si(3)–C(13)–Ce(1)	125.9(4)
C(15)–C(14)–C(13)	110.6(7)
C(15)–C(14)–Ce(1)	75.9(5)
C(13)–C(14)–Ce(1)	76.1(4)
C(14)–C(15)–C(16)	108.6(7)
C(14)–C(15)–Ce(1)	75.1(5)
C(16)–C(15)–Ce(1)	76.5(5)
C(12)–C(16)–C(15)	104.8(7)
C(12)–C(16)–Si(4)	125.8(7)
C(15)–C(16)–Si(4)	128.4(7)

Table S3. *Cont.*

C(12)–C(16)–Ce(1)	74.9(5)
C(15)–C(16)–Ce(1)	73.6(5)
Si(4)–C(16)–Ce(1)	125.0(4)
O(1)–C(23)–C(26)	109.1(7)
O(1)–C(23)–C(25)	108.6(7)
C(26)–C(23)–C(25)	111.3(8)
O(1)–C(23)–C(24)	108.8(7)
C(26)–C(23)–C(24)	108.9(7)
C(25)–C(23)–C(24)	110.1(8)
O(2)–C(27)–C(28)	110.9(11)
O(2)–C(27)–C(29')	108.3(19)
O(2)–C(27)–C(30')	139(6)
C(29')–C(27)–C(30')	102(7)
O(2)–C(27)–C(30)	108.2(11)
C(28)–C(27)–C(30)	115.1(14)
O(2)–C(27)–C(28')	101.7(17)
C(29')–C(27)–C(28')	103(3)
C(30')–C(27)–C(28')	98(6)
O(2)–C(27)–C(29)	108.5(10)
C(28)–C(27)–C(29)	107.7(15)
C(30)–C(27)–C(29)	106.1(13)

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for apx539_fulla. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ce(1)	21(1)	34(1)	39(1)	−1(1)	11(1)	−1(1)
Si(1)	30(2)	47(2)	106(3)	14(2)	36(2)	4(1)
Si(2)	41(2)	39(2)	52(2)	12(1)	27(1)	17(1)
Si(3)	24(1)	40(2)	43(2)	−8(1)	13(1)	−4(1)
Si(4)	44(2)	47(2)	36(2)	−4(1)	21(1)	5(1)
O(1)	27(3)	35(3)	39(4)	5(3)	8(3)	11(3)
O(2)	43(4)	43(4)	60(4)	−16(3)	19(3)	−7(3)
C(1)	38(6)	30(5)	72(7)	6(5)	35(5)	5(4)
C(2)	38(6)	37(5)	67(7)	7(5)	34(5)	5(5)
C(3)	28(5)	42(6)	48(6)	6(5)	19(4)	7(4)
C(4)	30(5)	36(5)	44(5)	−1(5)	19(4)	1(4)
C(5)	31(5)	36(5)	32(5)	−3(4)	19(4)	−1(4)
C(6)	101(9)	111(9)	181(10)	35(8)	59(7)	−18(7)
C(7)	47(7)	118(11)	93(9)	−1(8)	43(7)	23(7)
C(8)	35(6)	127(12)	116(11)	−26(9)	15(7)	10(8)
C(9)	50(6)	40(6)	45(6)	1(5)	19(5)	−1(5)
C(10)	84(9)	53(7)	72(8)	16(6)	46(7)	37(6)
C(11)	47(6)	46(6)	63(7)	15(5)	24(5)	3(5)
C(12)	31(5)	33(5)	37(5)	−2(4)	23(4)	−3(4)

Table S4. *Cont.*

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(13)	27(5)	35(5)	38(5)	−1(4)	21(4)	−6(4)
C(14)	21(4)	42(6)	41(6)	1(5)	11(4)	−1(4)
C(15)	27(5)	27(5)	41(6)	7(4)	15(4)	10(4)
C(16)	32(5)	43(6)	35(5)	0(4)	17(4)	5(4)
C(17)	42(6)	53(7)	72(7)	−20(6)	26(6)	−21(5)
C(18)	32(5)	59(7)	41(6)	−4(5)	2(4)	3(5)
C(19)	38(5)	40(6)	37(6)	−14(4)	13(4)	−2(4)
C(20)	91(9)	61(7)	55(7)	−13(6)	37(7)	−20(7)
C(21)	68(9)	165(14)	39(7)	15(8)	18(6)	42(9)
C(22)	122(11)	45(6)	63(8)	−17(6)	59(8)	−10(7)
C(23)	22(5)	45(6)	49(6)	−6(5)	15(4)	−3(4)
C(24)	47(6)	59(7)	42(6)	4(5)	15(5)	13(5)
C(25)	30(6)	72(7)	50(6)	−5(6)	7(5)	12(5)
C(26)	29(5)	39(6)	58(7)	5(5)	16(5)	5(4)
C(27)	56(7)	60(8)	86(9)	−12(7)	37(7)	−14(6)
C(28)	63(8)	77(8)	85(8)	−7(6)	31(6)	−4(6)
C(28')	63(8)	77(8)	85(8)	−7(6)	31(6)	−4(6)
C(29)	78(12)	78(10)	43(10)	3(8)	15(8)	−21(10)
C(29')	78(12)	78(10)	43(10)	3(8)	15(8)	−21(10)
C(30)	73(12)	70(9)	107(15)	−44(10)	34(11)	−17(9)
C(30')	73(12)	70(9)	107(15)	−44(10)	34(11)	−17(9)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for apx539_fulla.

	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H(1)	6248	545	10,673	52
H(3)	6758	1648	11,871	46
H(4)	8982	1350	12,736	43
H(6A)	3652	693	11,705	199
H(6B)	4036	484	10,660	199
H(6C)	2593	653	10,165	199
H(7A)	4034	1783	11,042	122
H(7B)	2787	1561	10,978	122
H(7C)	4194	1505	12,237	122
H(8A)	3265	1018	8042	150
H(8B)	2163	1233	8293	150
H(8C)	3356	1465	8277	150
H(9A)	8411	187	13,968	69
H(9B)	7757	−24	12,548	69
H(9C)	9203	−136	13,641	69
H(10A)	9956	377	10,798	98
H(10B)	10,201	−14	11,593	98
H(10C)	8755	98	10,499	98

Table S5. *Cont.*

	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H(11A)	11,259	809	13,515	79
H(11B)	10,759	734	14,623	79
H(11C)	11,522	410	14,262	79
H(12)	8954	1955	8716	37
H(14)	10,484	1069	11,321	43
H(15)	9621	812	8983	38
H(17A)	11,744	2542	12,112	84
H(17B)	12,079	2239	11,250	84
H(17C)	10,742	2474	10,567	84
H(18A)	12,092	1920	14,246	75
H(18B)	11,300	1533	13,758	75
H(18C)	12,461	1628	13,379	75
H(19A)	9628	2393	12,994	60
H(19B)	8597	2348	11,447	60
H(19C)	8736	2022	12,497	60
H(20A)	9520	1966	6332	101
H(20B)	10,516	1626	6541	101
H(20C)	9360	1713	5078	101
H(21A)	6723	1826	5715	140
H(21B)	6556	1586	4432	140
H(21C)	6147	1407	5504	140
H(22A)	8104	720	5975	105
H(22B)	8434	899	4846	105
H(22C)	9590	813	6309	105
H(23A)	6108	2657	7774	76
H(23B)	7281	2451	9008	76
H(23C)	6881	2317	7503	76
H(24A)	3948	2301	6439	82
H(24B)	4748	1965	6187	82
H(24C)	3796	1878	6854	82
H(25A)	4616	2521	8849	65
H(25B)	4457	2099	9260	65
H(25C)	5814	2318	10,065	65
H(28A)	4952	273	8241	114
H(28B)	4123	179	6678	114
H(28C)	3938	576	7253	114
H(28D)	6092	151	8627	114
H(28E)	4664	82	7417	114
H(28F)	4900	420	8453	114
H(29A)	4408	919	5516	106
H(29B)	4418	503	4958	106
H(29C)	5643	778	5325	106
H(29D)	4139	926	6296	106
H(29E)	3633	499	6065	106

Table S5. *Cont.*

	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H(29F)	4268	674	5171	106
H(30A)	7193	382	6756	129
H(30B)	6247	37	6650	129
H(30C)	7230	203	8089	129
H(30D)	5160	94	5798	129
H(30E)	6195	375	5672	129
H(30F)	6654	93	6923	129