Table 1. Crystal data and structure refinement for nn3clh.

Identification code	nn3clh
Empirical formula	$C_{24}H_{57}CeCl_{0.50}N_4Si_3$
Formula weight	643.85
Temperature	210(2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	P$\bar{3}$1c
Unit cell dimensions	*a* = 12.5843(5) Å alpha = 90°
	b = 12.5843(5) Å beta = 90°
	c = 25.433(2) Å gamma = 120°
Volume, Z	3488.1(3) Å^3, 4
Density (calculated)	1.226 Mg/m^3
Absorption coefficient	1.463 mm^{-1}
F(000)	1350
Crystal size	0.50 x 0.30 x 0.20 mm
θ range for data collection	1.60 to 28.53°
Limiting indices	$-16 \le h \le 16$, $-16 \le k \le 13$, $-34 \le l \le 23$
Reflections collected	20199
Independent reflections	2837 (R_{int} = 0.0382)
Completeness to θ = 28.53°	95.6 %
Absorption correction	SADABS
Max. and min. transmission	0.7585 and 0.5282
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2837 / 0 / 104
Goodness-of-fit on F^2	1.080
Final R indices [I>2σ(I)]	R1 = 0.0296, wR2 = 0.0587
R indices (all data)	R1 = 0.0422, wR2 = 0.0621
Largest diff. peak and hole	0.302 and -0.331 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for nn3clh. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ce1	6667	3333	3683(1)	33(1)
Cl1	6667	3333	2500	48(1)
Si1	3583(1)	1145(1)	3776(1)	57(1)
N1	5033(2)	1635(2)	4008(1)	46(1)
N4	6667	3333	4756(1)	43(1)
C1	7791(3)	3333(3)	4926(1)	54(1)
C2	5193(3)	1202(3)	4526(1)	54(1)
C3	2525(3)	1114(4)	4308(1)	92(1)
C4	3768(3)	2322(3)	3275(1)	70(1)
C5	2864(3)	-414(3)	3451(1)	79(1)
C6	3710(4)	-409(4)	3015(2)	90(1)
C7	2638(6)	-1406(4)	3855(2)	147(2)
C8	1629(4)	-709(5)	3194(2)	134(2)

Table 3. Selected bond lengths [Å] and angles [°] for nn3clh.

Ce1-N1	2.255(2)	Ce1-N4	2.730(3)
Ce1-Cl1	3.0080(3)	Ce1-Si1	3.4656(8)
N1#1-Ce1-N1#2	107.36(6)	N1-Ce1-N4	68.49(5)
N1-Ce1-Cl1	111.51(5)	N4-Ce1-Cl1	180.0
N1#1-Ce1-Si1#2	99.36(6)	N1-Ce1-Si1	25.01(5)
N4-Ce1-Si1	86.069(14)	Cl1-Ce1-Si1	93.931(14)
Ce1#3-Cl1-Ce1	180.0		

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -y+1,-x+1,-z+1/2

Table 4. Bond lengths [Å] and angles [°] for nn3clh.

Ce1-N1#1	2.255(2)	Ce1-N1#2	2.255(2)
Ce1-N1	2.255(2)	Ce1-N4	2.730(3)
Ce1-Cl1	3.0080(3)	Ce1-Si1#2	3.4656(8)
Ce1-Si1	3.4656(8)	Ce1-Si1#1	3.4657(8)
Cl1-Ce1#3	3.0080(3)	Si1-N1	1.712(2)
Si1-C4	1.877(3)	Si1-C3	1.886(3)
Si1-C5	1.892(4)	N1-C2	1.478(3)
N4-C1	1.479(3)	N4-C1#2	1.480(3)
N4-C1#1	1.480(3)	C1-C2#1	1.509(4)
C2-C1#2	1.509(4)	C5-C7	1.531(5)
C5-C6	1.534(5)	C5-C8	1.549(5)
N1#1-Ce1-N1#2	107.36(6)	N1#1-Ce1-N1	107.36(6)
N1#2-Ce1-N1	107.36(6)	N1#1-Ce1-N4	68.49(5)
N1#2-Ce1-N4	68.49(5)	N1-Ce1-N4	68.49(5)
N1#1-Ce1-Cl1	111.51(5)	N1#2-Ce1-Cl1	111.51(5)
N1-Ce1-Cl1	111.51(5)	N4-Ce1-Cl1	180.0
N1#1-Ce1-Si1#2	99.36(6)	N1#2-Ce1-Si1#2	25.01(5)
N1-Ce1-Si1#2	131.93(6)	N4-Ce1-Si1#2	86.070(14)
Cl1-Ce1-Si1#2	93.930(14)	N1#1-Ce1-Si1	131.92(6)
N1#2-Ce1-Si1	99.36(6)	N1-Ce1-Si1	25.01(5)
N4-Ce1-Si1	86.069(14)	Cl1-Ce1-Si1	93.931(14)
Si1#2-Ce1-Si1	119.535(3)	N1#1-Ce1-Si1#1	25.01(5)
N1#2-Ce1-Si1#1	131.93(6)	N1-Ce1-Si1#1	99.36(6)
N4-Ce1-Si1#1	86.070(14)	Cl1-Ce1-Si1#1	93.930(14)
Si1#2-Ce1-Si1#1	119.535(3)	Si1-Ce1-Si1#1	119.534(3)
Ce1#3-Cl1-Ce1	180.0	N1-Si1-C4	105.06(12)
N1-Si1-C3	112.02(15)	C4-Si1-C3	108.15(17)
N1-Si1-C5	113.28(15)	C4-Si1-C5	109.10(16)
C3-Si1-C5	109.01(19)	N1-Si1-Ce1	33.83(7)
C4-Si1-Ce1	71.26(10)	C3-Si1-Ce1	124.36(14)
C5-Si1-Ce1	124.00(13)	C2-N1-Si1	119.41(18)
C2-N1-Ce1	116.66(16)	Si1-N1-Ce1	121.16(11)
C1-N4-C1#2	111.82(15)	C1-N4-C1#1	111.82(15)
C1#2-N4-C1#1	111.81(15)	C1-N4-Ce1	107.01(16)
C1#2-N4-Ce1	107.01(16)	C1#1-N4-Ce1	107.01(16)
N4-C1-C2#1	110.1(2)	N1-C2-C1#2	109.2(2)
C7-C5-C6	109.5(4)	C7-C5-C8	109.4(4)
C6-C5-C8	108.0(3)	C7-C5-Si1	110.5(3)
C6-C5-Si1	109.9(2)	C8-C5-Si1	109.6(3)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z   #2 -x+y+1,-x+1,z   #3 -y+1,-x+1,-z+1/2

Table 5. Anisotropic displacement parameters [$Å^2 \times 10^3$] for nn3clh.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Ce1	37(1)	37(1)	26(1)	0	0	19(1)
Cl1	41(1)	41(1)	62(1)	0	0	21(1)
Si1	39(1)	76(1)	42(1)	21(1)	4(1)	19(1)
N1	45(1)	51(1)	38(1)	6(1)	-5(1)	22(1)
N4	50(1)	50(1)	29(2)	0	0	25(1)
C1	65(2)	69(2)	33(1)	-12(1)	-13(1)	36(2)
C2	59(2)	52(2)	45(2)	13(1)	-7(1)	22(1)
C3	61(2)	141(4)	71(2)	41(2)	28(2)	49(2)
C4	48(2)	106(3)	57(2)	33(2)	5(1)	40(2)
C5	59(2)	76(2)	56(2)	13(2)	-12(2)	0(2)
C6	83(3)	83(3)	87(3)	-12(2)	-15(2)	28(2)
C7	191(6)	62(3)	103(4)	23(3)	-23(4)	-1(3)
C8	55(2)	175(5)	99(3)	-20(3)	-18(2)	2(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for nn3clh.

	x	y	z	U(eq)
H1A	7616	2486	4966	65
H1B	8058	3742	5268	65
H2A	5836	982	4505	65
H2B	4427	472	4632	65
H3A	1703	783	4167	138
H3B	2816	1941	4436	138
H3C	2511	601	4596	138
H4B	2981	2077	3113	104
H4C	4347	2385	3008	104
H4D	4073	3111	3446	104
H6A	3317	-1197	2838	135
H6B	4478	-260	3168	135
H6C	3870	234	2764	135
H7A	2138	-2210	3698	221
H7B	2214	-1324	4157	221
H7C	3417	-1314	3966	221
H8A	1178	-1569	3096	201
H8B	1786	-206	2883	201
H8C	1149	-538	3443	201

Table 7. Selected torsion angles [°] for nn3clh.

N4-Ce1-Si1-N1	-43.78(14)
Cl1-Ce1-Si1-N1	136.22(14)
N1-Ce1-Si1-C4	177.8(2)
N4-Ce1-Si1-C4	134.01(13)
Cl1-Ce1-Si1-C4	-45.99(13)
N1-Ce1-Si1-C3	78.2(2)
N4-Ce1-Si1-C3	34.42(15)
Cl1-Ce1-Si1-C3	-145.58(15)
N1-Ce1-Si1-C5	-81.37(19)
N4-Ce1-Si1-C5	-125.15(13)
Cl1-Ce1-Si1-C5	54.85(13)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z   #2 -x+y+1,-x+1,z   #3 -y+1,-x+1,-z+1/2

Table 8. Torsion angles [°] for nn3clh.

N1#1-Ce1-Cl1-Ce1#3	-170(3)
N1#2-Ce1-Cl1-Ce1#3	-50(3)
N1-Ce1-Cl1-Ce1#3	70(3)
N4-Ce1-Cl1-Ce1#3	0(7)
Si1#2-Ce1-Cl1-Ce1#3	-68(3)
Si1-Ce1-Cl1-Ce1#3	52(3)
Si1#1-Ce1-Cl1-Ce1#3	172(3)
N1#1-Ce1-Si1-N1	12.46(14)
N1#2-Ce1-Si1-N1	-111.22(19)
N4-Ce1-Si1-N1	-43.78(14)
Cl1-Ce1-Si1-N1	136.22(14)
Si1#2-Ce1-Si1-N1	-127.01(14)
Si1#1-Ce1-Si1-N1	39.45(15)
N1#1-Ce1-Si1-C4	-169.74(15)
N1#2-Ce1-Si1-C4	66.58(14)
N1-Ce1-Si1-C4	177.8(2)
N4-Ce1-Si1-C4	134.01(13)
Cl1-Ce1-Si1-C4	-45.99(13)
Si1#2-Ce1-Si1-C4	50.78(14)
Si1#1-Ce1-Si1-C4	-142.76(13)
N1#1-Ce1-Si1-C3	90.67(16)
N1#2-Ce1-Si1-C3	-33.01(16)
N1-Ce1-Si1-C3	78.2(2)
N4-Ce1-Si1-C3	34.42(15)
Cl1-Ce1-Si1-C3	-145.58(15)
Si1#2-Ce1-Si1-C3	-48.81(15)
Si1#1-Ce1-Si1-C3	117.65(15)
N1#1-Ce1-Si1-C5	-68.90(15)
N1#2-Ce1-Si1-C5	167.42(14)
N1-Ce1-Si1-C5	-81.37(19)
N4-Ce1-Si1-C5	-125.15(13)
Cl1-Ce1-Si1-C5	54.85(13)
Si1#2-Ce1-Si1-C5	151.62(13)
Si1#1-Ce1-Si1-C5	-41.92(14)
C4-Si1-N1-C2	158.4(2)
C3-Si1-N1-C2	41.2(3)
C5-Si1-N1-C2	-82.6(2)
Ce1-Si1-N1-C2	160.5(3)
C4-Si1-N1-Ce1	-2.16(19)
C3-Si1-N1-Ce1	-119.35(18)
C5-Si1-N1-Ce1	116.84(15)
N1#1-Ce1-N1-C2	28.6(2)
N1#2-Ce1-N1-C2	-86.53(17)
N4-Ce1-N1-C2	-28.94(18)
Cl1-Ce1-N1-C2	151.06(18)
Si1#2-Ce1-N1-C2	-92.0(2)
Si1-Ce1-N1-C2	-161.0(3)
Si1#1-Ce1-N1-C2	53.0(2)
N1#1-Ce1-N1-Si1	-170.32(12)
N1#2-Ce1-N1-Si1	74.51(19)
N4-Ce1-N1-Si1	132.10(15)
Cl1-Ce1-N1-Si1	-47.90(15)
Si1#2-Ce1-N1-Si1	69.03(15)
Si1#1-Ce1-N1-Si1	-145.93(12)
N1#1-Ce1-N4-C1	-1.96(15)

N1#2-Ce1-N4-C1	-121.96(15)
N1-Ce1-N4-C1	118.04(15)
Cl1-Ce1-N4-C1	-63(69)
Si1#2-Ce1-N4-C1	-103.64(13)
Si1-Ce1-N4-C1	136.36(13)
Si1#1-Ce1-N4-C1	16.36(13)
N1#1-Ce1-N4-C1#2	-121.96(14)
N1#2-Ce1-N4-C1#2	118.04(14)
N1-Ce1-N4-C1#2	-1.96(14)
Cl1-Ce1-N4-C1#2	177(100)
Si1#2-Ce1-N4-C1#2	136.36(13)
Si1-Ce1-N4-C1#2	16.36(13)
Si1#1-Ce1-N4-C1#2	-103.64(13)
N1#1-Ce1-N4-C1#1	118.04(14)
N1#2-Ce1-N4-C1#1	-1.96(14)
N1-Ce1-N4-C1#1	-121.96(14)
Cl1-Ce1-N4-C1#1	57(39)
Si1#2-Ce1-N4-C1#1	16.37(13)
Si1-Ce1-N4-C1#1	-103.63(13)
Si1#1-Ce1-N4-C1#1	136.37(13)
C1#2-N4-C1-C2#1	147.3(3)
C1#1-N4-C1-C2#1	-86.5(3)
Ce1-N4-C1-C2#1	30.4(2)
Si1-N1-C2-C1#2	-102.9(2)
Ce1-N1-C2-C1#2	58.5(3)
N1-Si1-C5-C7	66.3(4)
C4-Si1-C5-C7	-177.0(3)
C3-Si1-C5-C7	-59.1(4)
Ce1-Si1-C5-C7	103.1(3)
N1-Si1-C5-C6	-54.6(3)
C4-Si1-C5-C6	62.0(3)
C3-Si1-C5-C6	180.0(3)
Ce1-Si1-C5-C6	-17.8(3)
N1-Si1-C5-C8	-173.1(2)
C4-Si1-C5-C8	-56.5(3)
C3-Si1-C5-C8	61.5(3)
Ce1-Si1-C5-C8	-136.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z   #2 -x+y+1,-x+1,z   #3 -y+1,-x+1,-z+1/2

Table 1. Crystal data and structure refinement for nn3br.

Identification code	nn3br
Empirical formula	C24 H57 Br Ce N4 Si3
Formula weight	706.04
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Trigonal, P-31c
Unit cell dimensions	a = 12.6070(19) A alpha = 90 deg. b = 12.6070(19) A beta = 90 deg. c = 25.557(3) A gamma = 120 deg.
Volume	3517.8(8) A^3
Z, Calculated density	4, 1.333 Mg/m^3
Absorption coefficient	2.549 mm^-1
F(000)	1456
Crystal size	0.3 x 0.3 x 0.2 mm
Theta range for data collection	1.59 to 28.44 deg.
Limiting indices	-16<=h<=9, -15<=k<=16, -33<=l<=33
Reflections collected / unique	20367 / 2879 [R(int) = 0.0515]
Completeness to theta = 28.44	97.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2879 / 0 / 104
Goodness-of-fit on F^2	1.584
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.0765
R indices (all data)	R1 = 0.0684, wR2 = 0.0795
Largest diff. peak and hole	0.547 and -0.827 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nn3br.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ce(1)	-3333	-6667	3719(1)	34(1)
N(1)	-4998(2)	-6647(3)	4037(1)	46(1)
N(4)	-3333	-6667	4775(2)	46(1)
Si(1)	-6433(1)	-7618(1)	3799(1)	57(1)
Br(1)	-3333	-6667	2500	48(1)
C(2)	-4848(3)	-6063(4)	4553(1)	56(1)
C(3)	-4476(3)	-6704(3)	4949(1)	56(1)
C(7)	-6237(3)	-8621(4)	3317(2)	72(1)
C(8)	-7495(4)	-8642(4)	4331(2)	93(2)
C(9)	-7138(4)	-6803(5)	3457(2)	81(1)
C(10)	-8354(4)	-7718(6)	3196(2)	130(2)
C(11)	-6271(4)	-5951(5)	3027(2)	92(2)
C(12)	-7403(6)	-6044(6)	3847(2)	131(2)

Table 3. Bond lengths [A] and angles [deg] for nn3br.

Ce(1)-N(1)#1	2.263(3)
Ce(1)-N(1)#2	2.263(3)
Ce(1)-N(1)	2.263(3)
Ce(1)-N(4)	2.700(4)
Ce(1)-Br(1)	3.1150(5)
Ce(1)-Si(1)#1	3.4734(11)
Ce(1)-Si(1)#2	3.4735(11)
Ce(1)-Si(1)	3.4735(11)
N(1)-C(2)	1.476(4)
N(1)-Si(1)	1.710(3)
N(4)-C(3)#1	1.485(4)
N(4)-C(3)#2	1.485(4)
N(4)-C(3)	1.485(4)
Si(1)-C(7)	1.869(4)
Si(1)-C(9)	1.877(5)
Si(1)-C(8)	1.892(4)
Br(1)-Ce(1)#3	3.1151(4)
C(2)-C(3)	1.509(5)
C(9)-C(12)	1.531(6)
C(9)-C(10)	1.535(6)
C(9)-C(11)	1.542(6)
N(1)#1-Ce(1)-N(1)#2	107.83(7)
N(1)#1-Ce(1)-N(1)	107.83(7)
N(1)#2-Ce(1)-N(1)	107.83(7)
N(1)#1-Ce(1)-N(4)	68.93(7)
N(1)#2-Ce(1)-N(4)	68.93(7)
N(1)-Ce(1)-N(4)	68.93(7)
N(1)#1-Ce(1)-Br(1)	111.07(7)
N(1)#2-Ce(1)-Br(1)	111.07(7)
N(1)-Ce(1)-Br(1)	111.07(7)
N(4)-Ce(1)-Br(1)	180.0
N(1)#1-Ce(1)-Si(1)#1	24.89(7)
N(1)#2-Ce(1)-Si(1)#1	99.93(7)
N(1)-Ce(1)-Si(1)#1	132.15(7)
N(4)-Ce(1)-Si(1)#1	86.613(17)
Br(1)-Ce(1)-Si(1)#1	93.387(17)
N(1)#1-Ce(1)-Si(1)#2	132.15(7)
N(1)#2-Ce(1)-Si(1)#2	24.88(7)
N(1)-Ce(1)-Si(1)#2	99.92(7)
N(4)-Ce(1)-Si(1)#2	86.613(17)
Br(1)-Ce(1)-Si(1)#2	93.387(17)
Si(1)#1-Ce(1)-Si(1)#2	119.655(4)
N(1)#1-Ce(1)-Si(1)	99.92(7)
N(1)#2-Ce(1)-Si(1)	132.15(7)
N(1)-Ce(1)-Si(1)	24.89(7)
N(4)-Ce(1)-Si(1)	86.613(17)
Br(1)-Ce(1)-Si(1)	93.387(17)
Si(1)#1-Ce(1)-Si(1)	119.654(4)
Si(1)#2-Ce(1)-Si(1)	119.654(4)
C(2)-N(1)-Si(1)	120.0(2)
C(2)-N(1)-Ce(1)	116.0(2)
Si(1)-N(1)-Ce(1)	121.29(13)
C(3)#1-N(4)-C(3)#2	111.5(2)
C(3)#1-N(4)-C(3)	111.5(2)
C(3)#2-N(4)-C(3)	111.5(2)
C(3)#1-N(4)-Ce(1)	107.4(2)
C(3)#2-N(4)-Ce(1)	107.4(2)
C(3)-N(4)-Ce(1)	107.4(2)
N(1)-Si(1)-C(7)	105.55(15)
N(1)-Si(1)-C(9)	113.26(19)
C(7)-Si(1)-C(9)	108.8(2)
N(1)-Si(1)-C(8)	111.53(17)

C(7)-Si(1)-C(8)	107.4(2)
C(9)-Si(1)-C(8)	110.0(2)
N(1)-Si(1)-Ce(1)	33.83(9)
C(7)-Si(1)-Ce(1)	71.81(12)
C(9)-Si(1)-Ce(1)	122.84(15)
C(8)-Si(1)-Ce(1)	124.62(16)
Ce(1)-Br(1)-Ce(1)#3	180.0
N(1)-C(2)-C(3)	109.2(3)
N(4)-C(3)-C(2)	109.8(3)
C(12)-C(9)-C(10)	107.7(4)
C(12)-C(9)-C(11)	109.2(5)
C(10)-C(9)-C(11)	108.0(4)
C(12)-C(9)-Si(1)	110.5(3)
C(10)-C(9)-Si(1)	111.1(4)
C(11)-C(9)-Si(1)	110.4(3)

Symmetry transformations used to generate equivalent atoms:
#1 -y-1,x-y-1,z   #2 -x+y,-x-1,z   #3 -y-1,-x-1,-z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for nn3br.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ce(1)	38(1)	38(1)	26(1)	0	0	19(1)
N(1)	46(2)	55(2)	37(2)	-11(1)	-3(1)	26(2)
N(4)	53(2)	53(2)	32(2)	0	0	27(1)
Si(1)	38(1)	76(1)	45(1)	-17(1)	5(1)	20(1)
Br(1)	44(1)	44(1)	54(1)	0	0	22(1)
C(2)	61(2)	71(3)	45(2)	-19(2)	-5(2)	40(2)
C(3)	60(2)	70(2)	37(2)	-11(2)	4(2)	31(2)
C(7)	47(2)	72(3)	64(3)	-30(2)	7(2)	5(2)
C(8)	65(3)	107(4)	76(3)	-15(3)	26(2)	19(3)
C(9)	56(3)	139(4)	59(3)	-27(3)	-13(2)	57(3)
C(10)	58(3)	220(7)	94(4)	-9(4)	-18(3)	56(4)
C(11)	86(3)	122(4)	81(3)	2(3)	-9(3)	62(3)
C(12)	163(6)	223(7)	90(4)	-32(4)	-11(4)	159(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for nn3br.

	x	y	z	U(eq)
H(2A)	-5629	-6119	4661	67
H(2B)	-4214	-5187	4532	67
H(3A)	-4341	-6296	5293	67
H(3B)	-5138	-7566	4988	67
H(7A)	-7040	-9235	3182	107
H(7B)	-5847	-9033	3489	107
H(7C)	-5720	-8121	3027	107
H(8A)	-8328	-9120	4192	140
H(8B)	-7491	-8138	4624	140
H(8C)	-7216	-9199	4454	140
H(10A)	-8790	-7293	3088	195
H(10B)	-8859	-8368	3446	195
H(10C)	-8191	-8079	2889	195
H(11A)	-6657	-5544	2848	137
H(11B)	-6105	-6435	2774	137
H(11C)	-5500	-5334	3187	137
H(12A)	-8022	-5876	3700	197
H(12B)	-6649	-5269	3916	197
H(12C)	-7709	-6502	4175	197

Table 1. Crystal data and structure refinement for nn3i.

Identification code	nn3i
Empirical formula	C24 H57 Ce I N4 Si3
Formula weight	753.03
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 9.7738(10) A alpha = 90 deg. b = 22.570(3) A beta = 97.680(5) deg. c = 16.122(2) A gamma = 90 deg.
Volume	3524.5(7) A^3
Z, Calculated density	4, 1.419 Mg/m^3
Absorption coefficient	2.287 mm^-1
F(000)	1528
Crystal size	0.4 x 0.15 x 0.05 mm
Theta range for data collection	1.56 to 28.45 deg.
Limiting indices	-12<=h<=7, -29<=k<=28, -19<=l<=20
Reflections collected / unique	20877 / 8219 [R(int) = 0.1139]
Completeness to theta = 28.45	92.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8219 / 0 / 298
Goodness-of-fit on F^2	0.858
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.0934
R indices (all data)	R1 = 0.1537, wR2 = 0.1173
Largest diff. peak and hole	1.635 and -1.346 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nn3i.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ce(1)	-2144(1)	12977(1)	5253(1)	26(1)
Si(1)	-437(2)	13914(1)	4047(1)	30(1)
Si(2)	-3551(2)	13614(1)	6930(1)	30(1)
Si(3)	-1669(2)	11481(1)	4933(1)	39(1)
N(1)	-416(6)	13247(2)	4586(3)	28(1)
N(2)	-2202(6)	13578(2)	6328(3)	29(2)
N(3)	-1735(6)	12057(2)	5647(3)	32(1)
N(4)	248(6)	12913(3)	6300(3)	32(2)
I(1)	-4962(1)	13006(1)	4077(1)	43(1)
C(1)	1355(7)	13091(4)	5797(4)	41(2)
C(2)	920(7)	12957(3)	4860(4)	35(2)
C(3)	115(7)	13327(3)	6985(4)	34(2)
C(4)	-856(7)	13821(3)	6681(4)	34(2)
C(5)	377(7)	12280(3)	6573(5)	36(2)
C(6)	-1044(7)	12000(3)	6524(4)	32(2)
C(7)	-2112(7)	14280(3)	4188(4)	38(2)
C(8)	1033(7)	14391(3)	4500(5)	43(2)
C(9)	-356(8)	13808(3)	2900(4)	33(2)
C(10)	1013(8)	13514(4)	2756(5)	50(2)
C(11)	-458(9)	14417(3)	2440(5)	54(2)
C(12)	-1566(8)	13417(3)	2494(5)	46(2)
C(21)	-2937(8)	13512(4)	8071(4)	55(2)
C(22)	-4738(8)	12982(3)	6584(5)	45(2)
C(23)	-4525(7)	14336(3)	6772(5)	36(2)
C(24)	-3551(10)	14860(4)	6986(6)	78(3)
C(25)	-5143(9)	14393(4)	5846(5)	62(3)
C(26)	-5698(9)	14373(4)	7319(5)	62(3)
C(31)	-1902(8)	11829(3)	3870(4)	44(2)
C(32)	46(8)	11092(4)	5098(5)	57(3)
C(33)	-3078(10)	10905(4)	4985(5)	56(3)
C(34)	-3156(11)	10488(4)	4205(6)	92(4)
C(35)	-4507(10)	11213(4)	4978(7)	89(4)
C(36)	-2776(10)	10521(4)	5780(6)	75(3)

Table 3. Bond lengths [A] and angles [deg] for nn3i.

Ce(1)-N(3)	2.192(6)
Ce(1)-N(1)	2.206(6)
Ce(1)-N(2)	2.208(5)
Ce(1)-N(4)	2.699(5)
Ce(1)-I(1)	3.1284(6)
Ce(1)-Si(1)	3.450(2)
Ce(1)-Si(3)	3.457(2)
Si(1)-N(1)	1.737(6)
Si(1)-C(8)	1.865(7)
Si(1)-C(7)	1.876(7)
Si(1)-C(9)	1.877(7)
Si(2)-N(2)	1.741(6)
Si(2)-C(21)	1.872(7)
Si(2)-C(22)	1.876(7)
Si(2)-C(23)	1.886(7)
Si(3)-N(3)	1.744(6)
Si(3)-C(31)	1.872(7)
Si(3)-C(32)	1.878(8)
Si(3)-C(33)	1.903(9)
N(1)-C(2)	1.474(8)
N(2)-C(4)	1.468(8)
N(3)-C(6)	1.490(7)
N(4)-C(3)	1.466(9)
N(4)-C(1)	1.492(9)
N(4)-C(5)	1.495(8)
C(1)-C(2)	1.544(9)
C(3)-C(4)	1.504(9)
C(5)-C(6)	1.518(9)
C(9)-C(10)	1.540(10)
C(9)-C(12)	1.549(9)
C(9)-C(11)	1.557(9)
C(23)-C(24)	1.529(11)
C(23)-C(26)	1.539(11)
C(23)-C(25)	1.540(9)
C(33)-C(36)	1.542(11)
C(33)-C(35)	1.559(12)
C(33)-C(34)	1.564(11)
N(3)-Ce(1)-N(1)	106.3(2)
N(3)-Ce(1)-N(2)	112.2(2)
N(1)-Ce(1)-N(2)	108.3(2)
N(3)-Ce(1)-N(4)	70.06(18)
N(1)-Ce(1)-N(4)	70.35(18)
N(2)-Ce(1)-N(4)	69.67(19)
N(3)-Ce(1)-I(1)	107.88(14)
N(1)-Ce(1)-I(1)	111.62(13)
N(2)-Ce(1)-I(1)	110.50(14)
N(4)-Ce(1)-I(1)	177.63(13)
N(3)-Ce(1)-Si(1)	131.33(17)
N(1)-Ce(1)-Si(1)	25.37(14)
N(2)-Ce(1)-Si(1)	97.51(16)
N(4)-Ce(1)-Si(1)	86.65(13)
I(1)-Ce(1)-Si(1)	95.66(3)
N(3)-Ce(1)-Si(3)	25.18(14)
N(1)-Ce(1)-Si(3)	94.04(15)
N(2)-Ce(1)-Si(3)	137.36(14)
N(4)-Ce(1)-Si(3)	85.34(13)
I(1)-Ce(1)-Si(3)	93.15(4)
Si(1)-Ce(1)-Si(3)	115.46(6)
N(1)-Si(1)-C(8)	110.4(3)
N(1)-Si(1)-C(7)	105.9(3)
C(8)-Si(1)-C(7)	109.7(3)
N(1)-Si(1)-C(9)	112.6(3)

C(8)-Si(1)-C(9)	109.1(3)
C(7)-Si(1)-C(9)	109.1(3)
N(1)-Si(1)-Ce(1)	33.0(2)
C(8)-Si(1)-Ce(1)	122.6(2)
C(7)-Si(1)-Ce(1)	72.9(2)
C(9)-Si(1)-Ce(1)	124.4(2)
N(2)-Si(2)-C(21)	112.0(3)
N(2)-Si(2)-C(22)	106.5(3)
C(21)-Si(2)-C(22)	107.6(4)
N(2)-Si(2)-C(23)	111.8(3)
C(21)-Si(2)-C(23)	109.2(4)
C(22)-Si(2)-C(23)	109.6(3)
N(3)-Si(3)-C(31)	106.2(3)
N(3)-Si(3)-C(32)	111.4(3)
C(31)-Si(3)-C(32)	108.9(4)
N(3)-Si(3)-C(33)	112.9(4)
C(31)-Si(3)-C(33)	109.1(4)
C(32)-Si(3)-C(33)	108.2(4)
N(3)-Si(3)-Ce(1)	32.34(18)
C(31)-Si(3)-Ce(1)	73.9(2)
C(32)-Si(3)-Ce(1)	124.7(3)
C(33)-Si(3)-Ce(1)	123.2(3)
C(2)-N(1)-Si(1)	119.1(5)
C(2)-N(1)-Ce(1)	115.9(4)
Si(1)-N(1)-Ce(1)	121.7(3)
C(4)-N(2)-Si(2)	118.2(4)
C(4)-N(2)-Ce(1)	114.7(4)
Si(2)-N(2)-Ce(1)	124.5(3)
C(6)-N(3)-Si(3)	120.7(4)
C(6)-N(3)-Ce(1)	113.5(4)
Si(3)-N(3)-Ce(1)	122.5(3)
C(3)-N(4)-C(1)	112.4(6)
C(3)-N(4)-C(5)	113.6(6)
C(1)-N(4)-C(5)	112.3(6)
C(3)-N(4)-Ce(1)	106.3(4)
C(1)-N(4)-Ce(1)	106.0(4)
C(5)-N(4)-Ce(1)	105.5(4)
N(4)-C(1)-C(2)	110.7(6)
N(1)-C(2)-C(1)	108.8(6)
N(4)-C(3)-C(4)	110.1(5)
N(2)-C(4)-C(3)	110.1(6)
N(4)-C(5)-C(6)	110.0(6)
N(3)-C(6)-C(5)	108.0(6)
C(10)-C(9)-C(12)	108.6(6)
C(10)-C(9)-C(11)	108.1(7)
C(12)-C(9)-C(11)	107.8(6)
C(10)-C(9)-Si(1)	110.8(5)
C(12)-C(9)-Si(1)	111.0(5)
C(11)-C(9)-Si(1)	110.5(5)
C(24)-C(23)-C(26)	108.5(7)
C(24)-C(23)-C(25)	107.8(7)
C(26)-C(23)-C(25)	109.0(6)
C(24)-C(23)-Si(2)	110.5(5)
C(26)-C(23)-Si(2)	111.8(5)
C(25)-C(23)-Si(2)	109.2(5)
C(36)-C(33)-C(35)	109.2(8)
C(36)-C(33)-C(34)	108.2(7)
C(35)-C(33)-C(34)	108.3(8)
C(36)-C(33)-Si(3)	111.2(6)
C(35)-C(33)-Si(3)	110.4(6)
C(34)-C(33)-Si(3)	109.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for nn3i.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ce(1)	23(1)	26(1)	27(1)	1(1)	2(1)	0(1)
Si(1)	33(1)	23(1)	34(1)	-1(1)	6(1)	-2(1)
Si(2)	32(1)	31(1)	30(1)	3(1)	7(1)	0(1)
Si(3)	57(2)	28(1)	34(1)	0(1)	12(1)	2(1)
N(1)	25(3)	25(3)	33(4)	6(3)	0(3)	1(3)
N(2)	34(4)	21(3)	31(4)	-4(3)	2(3)	2(3)
N(3)	39(4)	30(3)	26(3)	-3(3)	1(3)	4(3)
N(4)	31(4)	40(4)	24(3)	7(3)	3(3)	9(3)
I(1)	31(1)	57(1)	40(1)	-6(1)	-5(1)	0(1)
C(1)	19(4)	62(6)	42(5)	11(4)	9(3)	2(4)
C(2)	34(4)	41(5)	31(4)	5(4)	10(3)	-6(4)
C(3)	19(4)	50(5)	32(4)	-4(4)	-3(3)	3(4)
C(4)	35(5)	35(5)	36(5)	-8(4)	14(3)	-10(4)
C(5)	31(5)	36(5)	40(5)	7(4)	-2(4)	7(4)
C(6)	46(5)	29(4)	23(4)	2(4)	10(3)	5(4)
C(7)	37(5)	28(4)	48(5)	-4(4)	6(4)	6(4)
C(8)	35(5)	43(5)	54(6)	-2(4)	14(4)	-4(4)
C(9)	40(5)	24(4)	35(5)	7(3)	4(4)	-2(4)
C(10)	60(6)	47(5)	47(6)	-5(4)	23(4)	4(5)
C(11)	71(7)	44(5)	47(6)	9(4)	16(5)	3(5)
C(12)	54(6)	49(5)	34(5)	-3(4)	-1(4)	-7(5)
C(21)	52(6)	74(7)	38(5)	10(5)	6(4)	10(5)
C(22)	43(5)	39(5)	55(5)	7(5)	11(4)	-6(5)
C(23)	35(5)	36(5)	41(5)	6(4)	18(4)	6(4)
C(24)	78(8)	28(5)	134(10)	-8(6)	35(6)	3(5)
C(25)	85(7)	56(6)	50(6)	16(5)	23(5)	47(5)
C(26)	62(7)	59(6)	69(7)	17(5)	25(5)	25(5)
C(31)	60(6)	35(5)	41(5)	-12(4)	18(4)	-2(4)
C(32)	76(7)	52(6)	46(5)	5(5)	18(5)	21(5)
C(33)	87(8)	35(5)	54(6)	-14(5)	36(5)	-14(5)
C(34)	141(11)	60(7)	83(8)	-29(6)	47(7)	-40(7)
C(35)	75(8)	71(8)	124(10)	-28(7)	27(7)	-40(7)
C(36)	107(9)	38(6)	87(8)	10(5)	41(6)	-5(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for nn3i.

	x	y	z	U(eq)
H(1A)	2215	12874	5998	49
H(1B)	1542	13520	5872	49
H(2A)	1628	13107	4528	42
H(2B)	833	12523	4773	42
H(3A)	1032	13493	7199	41
H(3B)	-240	13115	7450	41
H(4A)	-974	14090	7152	41
H(4B)	-464	14054	6248	41
H(5A)	851	12257	7154	44
H(5B)	938	12059	6208	44
H(6A)	-960	11577	6686	38
H(6B)	-1593	12204	6912	38
H(7A)	-2177	14663	3899	56
H(7B)	-2153	14343	4786	56
H(7C)	-2882	14027	3953	56
H(8A)	1368	14621	4052	65
H(8B)	1781	14142	4774	65
H(8C)	722	14662	4912	65
H(10A)	1030	13459	2154	75
H(10B)	1095	13128	3036	75
H(10C)	1787	13767	2986	75
H(11A)	-418	14354	1842	80
H(11B)	312	14670	2674	80
H(11C)	-1333	14609	2513	80
H(12A)	-1497	13366	1897	69
H(12B)	-2445	13608	2560	69
H(12C)	-1519	13028	2769	69
H(21A)	-2316	13838	8271	82
H(21B)	-2443	13134	8157	82
H(21C)	-3731	13510	8384	82
H(22A)	-4230	12608	6665	68
H(22B)	-5097	13029	5990	68
H(22C)	-5509	12979	6916	68
H(24A)	-4072	15231	6902	118
H(24B)	-2825	14854	6621	118
H(24C)	-3130	14831	7571	118
H(25A)	-5649	14768	5761	93
H(25B)	-5775	14062	5692	93
H(25C)	-4398	14386	5495	93
H(26A)	-6176	14754	7222	93
H(26B)	-5311	14341	7910	93
H(26C)	-6353	14049	7172	93
H(31A)	-1842	11524	3444	67
H(31B)	-1178	12126	3839	67
H(31C)	-2808	12021	3770	67
H(32A)	-85	10671	4965	86
H(32B)	457	11136	5684	86
H(32C)	661	11268	4733	86
H(34A)	-3885	10193	4231	138
H(34B)	-2269	10286	4204	138
H(34C)	-3365	10723	3693	138
H(35A)	-5221	10911	5007	134
H(35B)	-4723	11442	4461	134
H(35C)	-4476	11478	5461	134
H(36A)	-3520	10231	5793	112
H(36B)	-2720	10774	6276	112
H(36C)	-1897	10312	5775	112