Rietveld refinement data from X-ray powder diffraction for $La_{8.9}Ce_{0.1}SrSi_6NO_{25}$

Crystal data

Space group	$P6_3/m$ (Nº 176), Z=1
a(Å)	9.7008(4)
c(Å)	7.2401(4)
Cell volume ($Å^3$)	590.06
Calculated density(g/cm^3)	5.459

Atomic coordinates and isotropic displacement parameters (in $Å^2$)

Atom	Wyckof site	x/a	y/b	z/c	occupancy[1]	B[2]
La(1)	4f	0.33330	0.66670	-0.0032(15)	0.493	0.5
Sr(1)	4f	0.33330	0.66670	-0.0032(15)	0.167	0.5
Ce(1)	4f	0.33330	0.66670	-0.0032(15)	0.007	0.5
La(2)	6h	0.0121(7)	0.2449(5)	0.25000	0.990	0.5
Ce(2)	6h	0.0121(7)	0.2449(5)	0.25000	0.110	0.5
Si	6h	0.403(2)	0.377(3)	0.25000	1.000	0.5
O(1)	6h	0.329(5)	0.479(5)	0.25000	0.962	0.5
N(1)	6h	0.329(5)	0.479(5)	0.25000	0.038	0.5
O(2)	6h	0.597(5)	0.473(5)	0.25000	0.962	0.5
N(2)	6h	0.597(5)	0.473(5)	0.25000	0.038	0.5
O(3)	12i	0.342(3)	0.261(3)	0.072(4)	1.922	0.5
N(3)	12i	0.342(3)	0.261(3)	0.072(4)	0.077	0.5
O(4)	2a	0.00000	0.00000	0.25000	0.320	0.5
N(4)	2a	0.00000	0.00000	0.25000	0.013	0.5

[1] Normalized to 1 Si according with the site multiplicity.
[2] The temperature factors were fixed to 0.5 $Å^2$ because of correlations with absorption effects.

Selected bond distances (Å)

La(1)/Sr(1)/Ce(1)-O(1)/N(1)	(x2)	2.57(3)
La(1)/Sr(1)/Ce(1)-O(1)/N(1)		2.57(4)
La(1)/Sr(1)/Ce(1)-O(2)/N(2)	(x2)	2.53(3)
La(1)/Sr(1)/Ce(1)-O(2)/N(2)		2.53(4)
La(1)/Sr(1)/Ce1-O(3)/N(3)	(x3)	2.91(3)
La(2)/Ce(2)-O(1)/N(1)		2.76(4)
La(2)/Ce(2)-O(2)/N(2))		2.47(6)
La(2)/Ce(2)-O(3)/N(3)	(x2)	2.48(3)
La(2)/Ce(2)-O(3)/N(3)	(x2)	2.64(3)
La(2)/Ce(2)-O(4)/N(4)		2.319(6)
Si-O(1)/N(1)		1.48(7)
Si-O(2)/N(2)		1.63(5)
Si-O(3)/N(3)	(x2)	1.62(3)

N_p, N_{refl}, N_{irefl} [a]	4750	502	252
P_p, P_i, P_g [b]	5	13	10
R_{Bragg}, R_F, χ^2	13.2	11.5	1.70
R_p, R_{wp} , R_{exp} [c]	33.2	36.8	28.17

(a) N_p, N_{refl}, N_{irefl} refer to the number of experimental points, total reflections and independent reflections respectively.
(b) Pp, Pi, Pg, refer to the number of profile, intensity-dependent and global refined parameters, respectively. The profile fitting of the data was performed with a pseudo-Voigt function, including asymmetry and preferred orientation corrections.
(c) Conventional Rietveld R-factors (R_p, R_{exp}) are calculated by using background corrected counts.

Observed and calculated X-ray diffraction patterns for the compound $La_{8.9}Ce_{0.1}SrSi_6NO_{25}$