Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Crystal structure and luminescence properties of the first lithium oxonitridolithosilicate $Li_3SiNO_2:Eu^{2+}$

Daniel S. Wimmer † [a], Kilian M. Rießbeck † [a], Markus Seibald[b], Dominik Baumann[b], Klaus Wurst[a], Gunter Heymann[a], and Hubert Huppertz*[a]

[a] Daniel S. Wimmer, Kilian M. Rießbeck, Klaus Wurst, Gunter Heymann, Hubert Huppertz:
Institut für Allgemeine, Anorganische und Theoretische Chemie,
Universität Innsbruck
Innrain 80-82, A-6020 Innsbruck, Austria
E-Mail: *Hubert.Huppertz@uibk.ac.at*
https://www.uibk.ac.at/aatc/mitarbeiter/hub/

[b] Markus Seibald, Dominik Baumann:
ams-OSRAM International GmbH,
Mittelstetter Weg 2, D-86830 Schwabmünchen, Germany

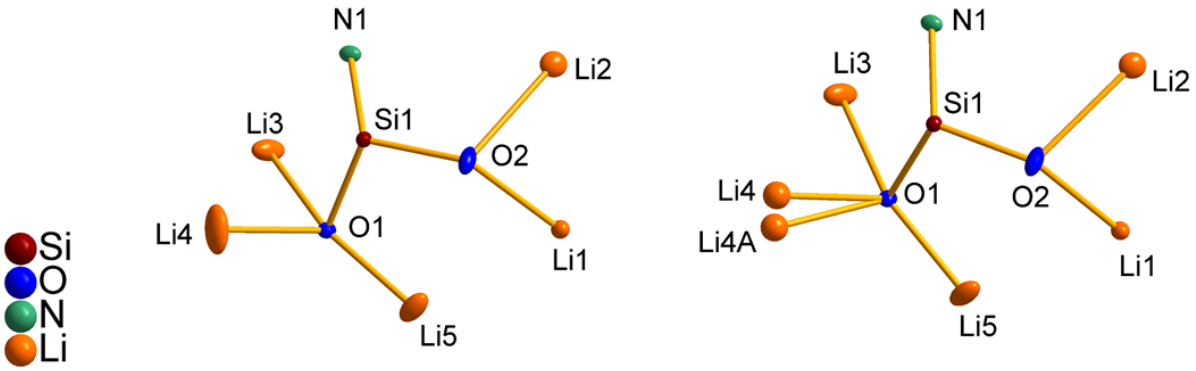

Figure S1: On the left, the asymmetric unit of Li_3SiNO_2 with the asymmetric displacement ellipsoids by describing the Li4 position with one Li site. On the right, the asymmetric unit of Li_3SiNO_2 with the asymmetric displacement ellipsoids by describing the Li4 position with two partially occupied Li sites (Li4 and Li4A). Li4 and Li4A are isotropically refined in the latter case.

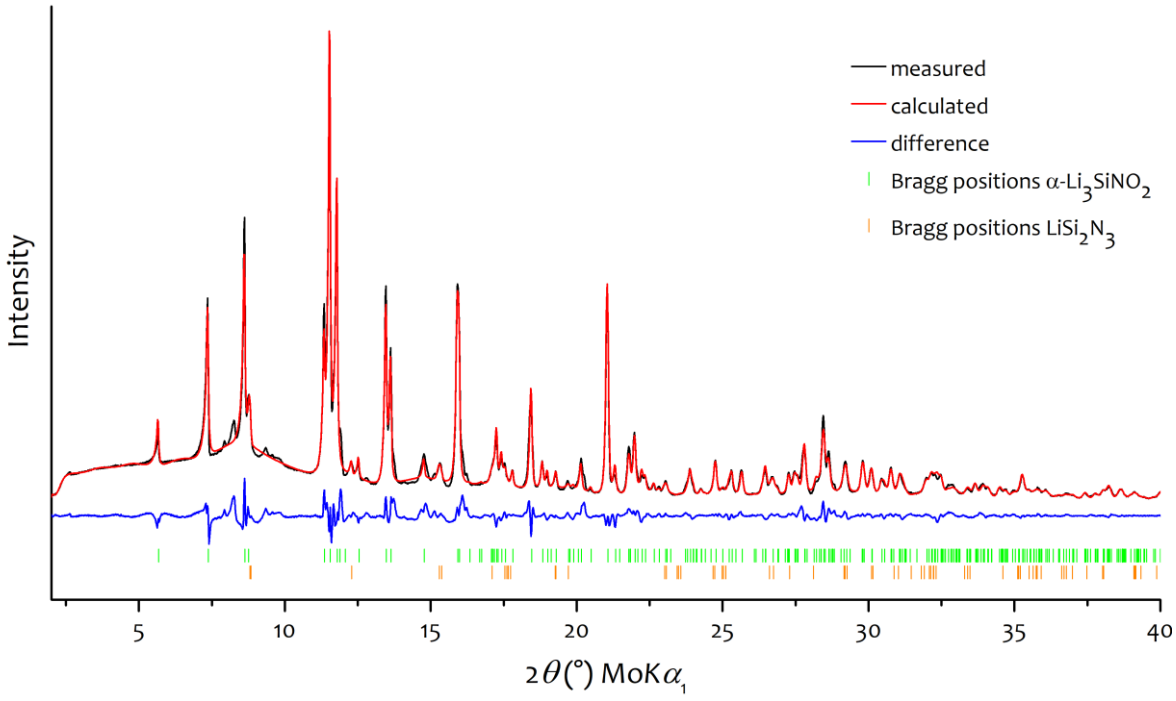

Figure S2: Rietveld fit of the measured powder diffraction data (black line), the calculated pattern based on single-crystal data of Li_3SiNO_2 (red line), and the difference plot (blue line). Tick marks represent the theoretical reflection position of Li_3SiNO_2 (green tick marks) and of the secondary phase $LiSi_2N_3$ (orange tick marks).

Table S1: Crystallographic data for Rietveld refinement of Li_3SiNO_2

Composition / Empirical formula	
Li_3SiNO_2 / wt%	97(1)
$LiSi_2N_3$ / wt%	3(1)
Crystallographic data	
Space group	*C*2/*c*
Powder diffractometer	STOE Stadi P
Radiation	Mo-$K\alpha_1$ (λ = 70.93 pm)
a / pm	1054.84(7)
b / pm	1103.05(8)
c / pm	512.54(4)
β / deg	116.66(1)
V / nm^3	0.53296(7)
Profile range	$2.0 \leq 2\Theta \leq 40.0$
2Θ step size / deg	0.015
R_{exp} / %	0.87
R_{wp} / %	7.80
R_p / %	5.35
R_{Bragg} / %	3.29

Table S2: Crystal data and structure refinement of single-crystal X-ray measurements at low temperature of Li_3SiNO_2.

Empirical formula	Li_3SiNO_2
Molar mass / g mol^{-1}	94.92
Crystal system	monoclinic
Space group	*C*2/*c*
Single-crystal data	
Single-crystal diffractometer	Bruker D8 Quest Kappa
Radiation	Mo-$K\alpha$ (λ = 71.073 pm)
a / pm	1048.47(4)
b / pm	1101.72(4)
c / pm	511.44(2)
β / deg	116.04(1)
V / nm^3	0.53083(4)
Formula units per cell Z	8
Calculated density / g cm^{-3}	2.375

Crystal size / mm^3	0.200 × 0.070 × 0.070
Temperature / K	183(2)
Detector distance / mm	40
Exposure time	0.5° / frame ; 40 s / frame
Absorption coefficient / mm^{-1}	0.605
$F(000)$ / e	368
Θ-range / deg	2.85 – 41.32
Range in *hkl*	± 19, ± 20, ± 9
Reflections total/independent	26737 / 1760
R_{int}	0.0295
Reflections with $I \geq 2\sigma(I)$	1722
Data / ref. parameters	1760 / 66
Absorption correction	MULTI-SCAN
Final R_1 / wR_2 [$I \geq 2\sigma(I)$]	0.0237 / 0.0726
Final R_1 / wR_2 (all data)	0.0240 / 0.0727
Goodness of fit on F^2	1.290
Largest diff. peak/hole / e·$Å^{-3}$	0.532 / -0.521

Table S3: Wyckoff positions, atomic coordinates, and equivalent isotropic displacement parameters U_{eq} ($Å^2$) of Li_3SiNO_2 (standard deviations in parentheses) of single-crystal X-ray measurements at low temperature.

Atom	Wyckoff-position	*x*	*y*	*z*	U_{eq}	Occ.
Si1	8*f*	0.22034(2)	0.43053(2)	0.25612(4)	0.00477(6)	1
Li1	4*e*	0	0.2019(2)	¾	0.0073(3)	1
Li2	4*e*	0	0.9746(2)	¾	0.0103(3)	1
Li3	4*e*	0	0.4334(2)	¾	0.0148(4)	1
Li4	4*e*	0	0.6813(3)	¾	0.0130(4)	0.84
Li4A	4*e*	0	0.725(2)	¾	0.014(2)	0.16
Li5	8*f*	0.2223(2)	0.3017(2)	0.7805(4)	0.0149(3)	1
O1	8*f*	0.12891(5)	0.31225(4)	0.0530(2)	0.00612(8)	1
O2	8*f*	0.38857(6)	0.39429(6)	0.3739(2)	0.0103(2)	1
N1	8*f*	0.16863(6)	0.44459(5)	0.5301(2)	0.00641(9)	1

Table S4: Anisotropic displacement parameters U_{ij} (Å²) of Li_3SiNO_2 (standard deviations in parentheses) of single-crystal X-ray measurements at low temperature. The displacement parameters of the atoms Li4 and Li4A were refined isotropically.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	0.00493(8)	0.00495(8)	0.00451(8)	-0.00049(5)	0.00214(6)	0.00005(5)
Li1	0.0074(7)	0.0064(7)	0.0092(7)	0	0.0046(6)	0
Li2	0.0106(8)	0.0121(8)	0.0064(7)	0	0.0020(6)	0
Li3	0.0126(9)	0.0096(8)	0.014(2)	0	-0.0011(7)	0
Li5	0.0182(7)	0.0149(7)	0.0152(7)	0.0070(5)	0.0107(6)	0.0083(5)
O1	0.0064(2)	0.0053(2)	0.0062(2)	-0.0007(2)	0.0025(2)	-0.0001(2)
O2	0.0061(2)	0.0136(2)	0.0103(2)	-0.0036(2)	0.0028(2)	0.0012(2)
N1	0.0090(2)	0.0055(2)	0.0056(2)	0.0001(2)	0.0039(2)	0.0004(2)

Table S5: Interatomic distances (Å) in Li_3SiNO_2 (standard deviations in parentheses) of single-crystal X-ray measurements at low temperature.

Si1–O2	1.6434(6)	Li3–O1	2.042(2) 2×	Li4A–O1	2.051(4) 2×
Si1–O1	1.6800(5)	**Ø Li3–O**	**2.042(2)**	Li4A–O2	2.56(2) 2×
Ø Si1–O	**1.6617(6)**			**Ø Li4A–O**	**2.31(2)**
		Li3–N1	2.182(2) 2×		
Si1–N1	1.7172(6)	Li3–N1	2.4802(6) 2×	Li4A–N1	2.54(2) 2×
Si1–N1	1.7242(6)	**Ø Li3–N**	**2.331(6)**	**Ø Li4A–N**	**2.54(2)**
Ø Si1–N	**1.7207(6)**				
		Li4–O1	2.0108(5) 2×	Li5–O1	1.889(2)
Li1–O2	1.881(2)	**Ø Li4–O**	**2.0108(5)**	Li5–O1	2.028(2)
Li1–O1	1.967(2) 3×			Li5–O2	2.415(2)
Ø Li1–O	**1.946(2)**	Li4–N1	2.209(2) 2×	**Ø Li5–O**	**2.111(2)**
		Ø Li4–N	**2.209(2)**		
Li2–O2	1.968(2) 2×			Li5–N1	1.950(2)
Li2–O2	2.122(2) 2×			**Ø Li5–N**	**1.950(2)**
Ø Li2–O	**2.045(2)**				