Highly Tenebrescent Hackmanites from Natural Nepheline

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SUPPORTING INFORMATION

Contents

1. SEM-EDS DATA

1.1. Nepheline

EDS results were averaged from spectra taken from four spots in the sample.

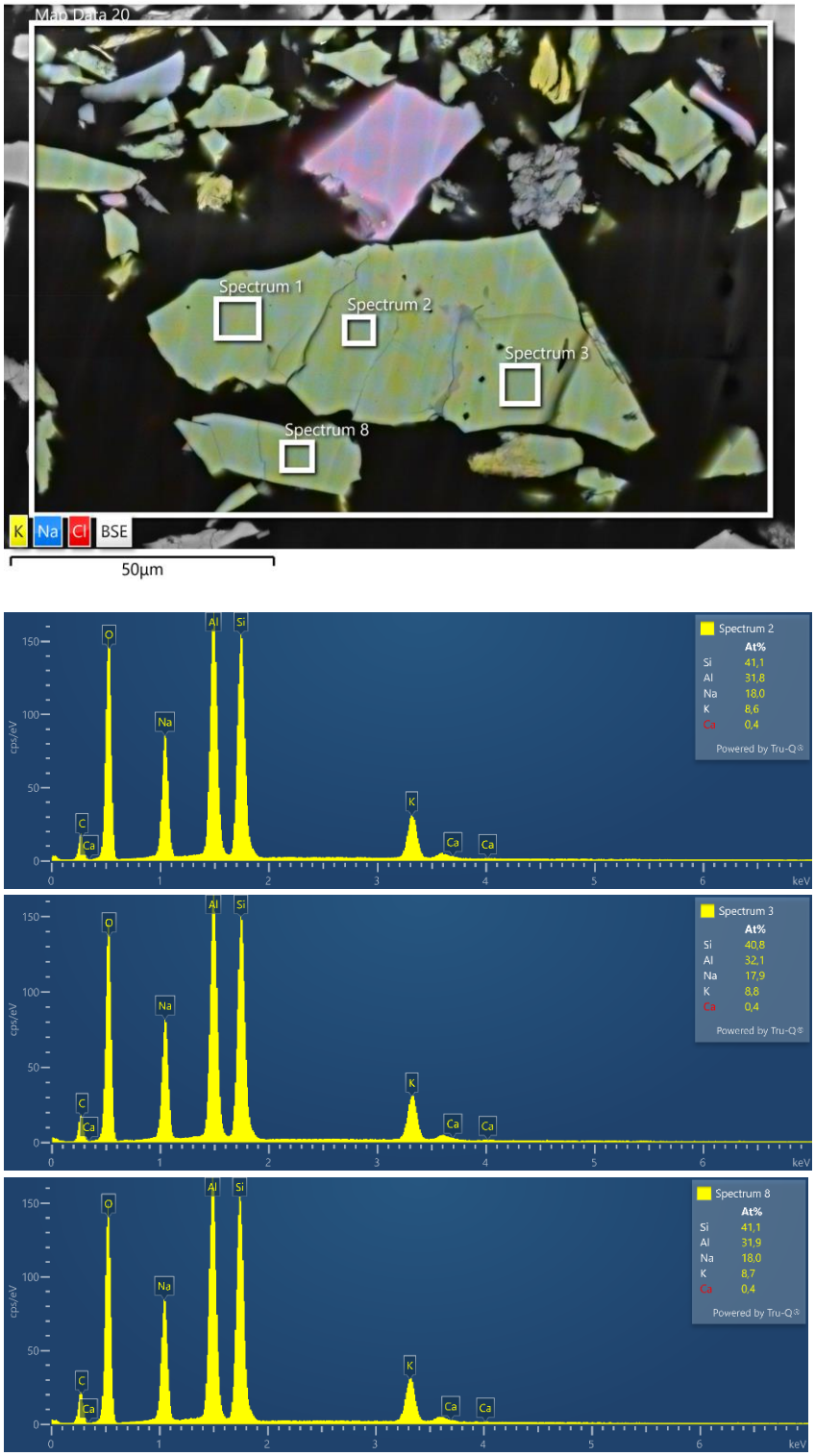

Figure S1. SEM-EDS image for nepheline together with spectra from spots 2, 3 and 8 (as marked in the image).

Table S1. Compositional data for nepheline (atom-%).

Label	Na	Al	Si	K	Ca
Spectrum 1	18.02	32	41.11	8.48	0.39
Spectrum 2	18.04	31.84	41.11	8.63	0.37
Spectrum 3	17.88	32.07	40.81	8.82	0.42
Spectrum 8	18.04	31.86	41.08	8.65	0.37
Statistic	**Na**	**Al**	**Si**	**K**	**Ca**
Max	18.04	32.07	41.11	8.82	0.42
Min	17.88	31.84	40.81	8.48	0.37
Average	18.0	31.9	41.0	8.7	0.4
Standard Deviation	0.08	0.11	0.14	0.14	0.02

1.2. Hackmanite (Na sample)

EDS results were averaged from spectra taken from three spots in the sample.

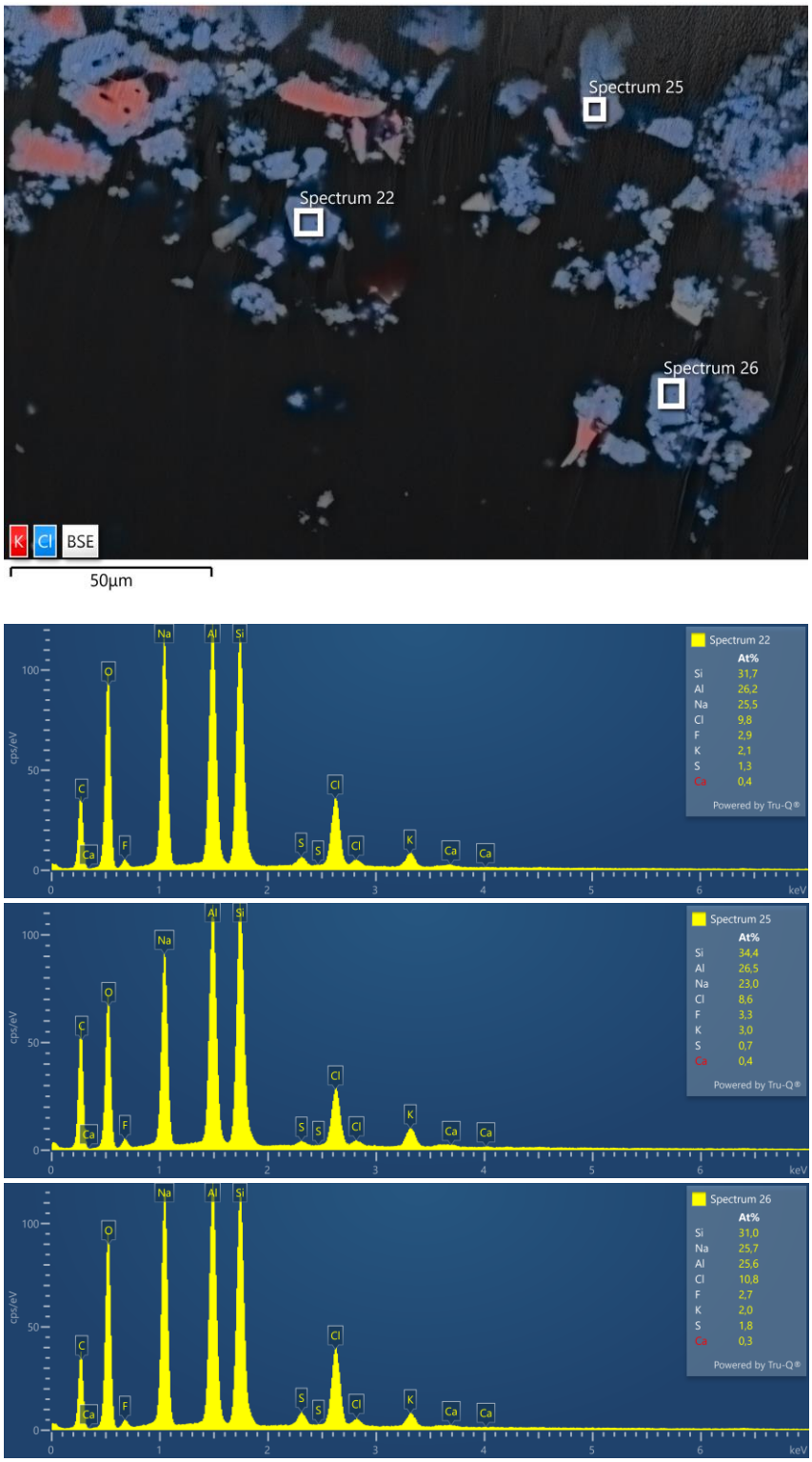

Figure S2. SEM-EDS image for nepheline together with spectra from spots 22, 25 and 26 (as marked in the image).

Table S2. Compositional data for Na sample (atom-%).

Label	F	Na	Al	Si	S	Cl	K	Ca
Spectrum 22	2.87	25.54	26.22	31.74	1.31	9.81	2.14	0.37
Spectrum 25	3.33	23.03	26.52	34.39	0.72	8.62	3.03	0.36
Spectrum 26	2.75	25.74	25.62	30.95	1.84	10.84	1.99	0.26
Statistic	**F**	**Na**	**Al**	**Si**	**S**	**Cl**	**K**	**Ca**
Max	3.33	25.74	26.52	34.39	1.84	10.84	3.03	0.37
Min	2.75	23.03	25.62	30.95	0.72	8.62	1.99	0.26
Average	3.0	24.8	26.1	32.4	1.3	9.8	2.4	0.3
Standard Deviation	0.31	1.51	0.45	1.8	0.56	1.11	0.56	0.06

2. SINGLE CRYSTAL X-RAY DATA FOR NEPHELINE

Table S3. List of fractional atomic coordinates, equivalent isotropic displacement parameters and atomic occupancies for single crystal X-ray structure of nepheline sample.

	x	***y***	***z***	U_{eq}	**Occupancy**
Si1	0.33427(13)	0.24094(13)	0.57670(11)	0.0098(3)	1
Si2	0.666667	0.333333	0.0856(3)	0.0101(4)	1
Al1	0.33277(15)	0.24014(14)	0.20336(13)	0.0096(3)	1
Al2	0.666667	0.333333	0.6970(3)	0.0099(4)	1
Na1	0.55680(12)	0.55473(13)	0.3907(4)	0.0177(2)	1
O1	0.5247(4)	0.3505(4)	0.1476(8)	0.0312(10)	1
O2	0.2267(4)	0.2864(3)	0.0742(5)	0.0127(6)	1
O3	0.2662(4)	0.0439(4)	0.1983(5)	0.0158(6)	1
O4	0.3166(3)	0.2910(2)	0.3986(6)	0.0240(5)	1
O5	0.5101(4)	0.3498(4)	0.6351(7)	0.0247(8)	1
O6	0.661(3)	0.2884(13)	0.9002(14)	0.0221(17)	0.3333
Ca1	0	0	0.434(7)	0.014(6)	0.0871
Na2	0	0	0.377(9)	0.015(6)	0.2726
K1	0	0	0.3991(15)	0.0095(19)	0.5532

3. RIETVELD REFINEMENT RESULTS FOR Na SAMPLE

A Rietveld refinement was carried out for the Na sample using the FullProf program assuming the cubic ($P\bar{4}3n$) sodalite crystal structure that has Na at 8e(x,x,x), Al at 6c(1/4, 1/2, 0), Si at 6d(1/4, 0, 1/2), O at 24i(x, y, z), Cl at 2a(0, 0, 0).

Table S4. Rietveld refinement results for the Na sample.

	Na sample
a/ Å	8.88877(4)
V / Å^3	702.30(1)
x(Na)	0.67928(8)
B(Na) / Å^2	0.70(3)
B(Al) / Å^2	0.59(20)
B(Si) / Å^2	0.17(18)
B(Cl) / Å^2	3.81(4)
x(O)	0.14274(34)
y(O)	0.14719(35)
z(O)	0.43894(11)
B(O) / Å^2	0.23(3)
R_{Bragg}/ %	4.6
χ^2	0.5
Na-Cl / Å	2.760(1)
Na-O / Å	2.348(1)
Al-O / Å	1.707(1)
Si-O / Å	1.655(1)

References

FullProf: Rodriguez-Carvajal, J., *FullProf.2k (Version 7.95 - Jan2023)*, Institut Laue-Langevin, France, **2023**, unpublished.

Crystal Structure: Hassan, I.; Antao, S.; Parise, J. Sodalite: High -Temperature Structures Obtained from Synchrotron Radiation and Rietveld Refinements. *Am. Miner.* **2004**, *89*, 5359–5364.

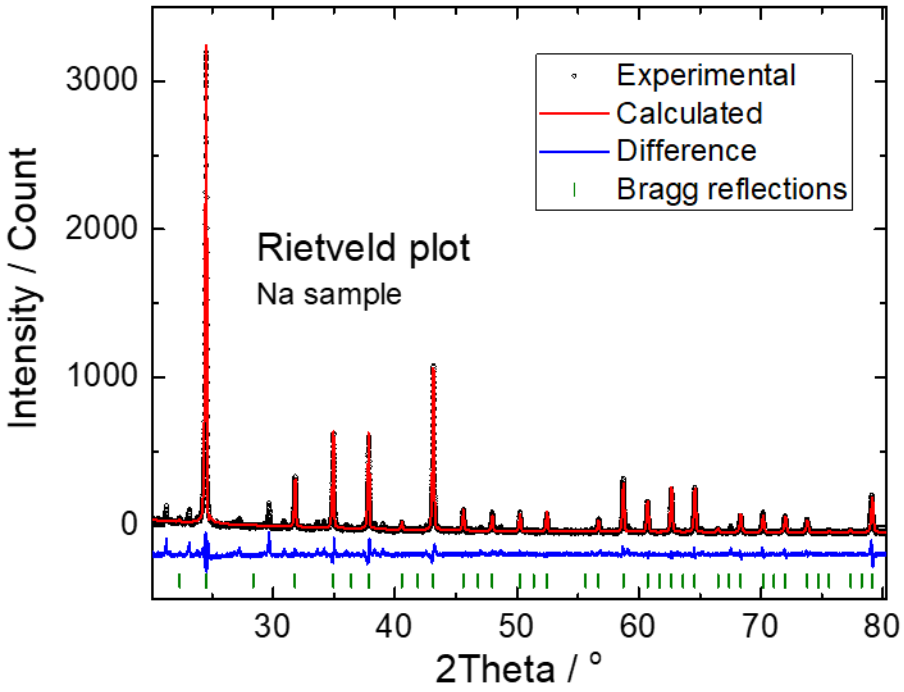

Figure S3. Rietveld plot for the Na sample.