Electronic Supplementary Material (ESI) for Journal of Analytical Atomic Spectrometry.

Supporting Information:

Approach to Using 3D Laser-Induced Breakdown Spectroscopy (LIBS) Data to Explore the Interaction of FLiNaK and FLiBe Molten Salts with Nuclear-Grade Graphite

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Supporting Information Figures

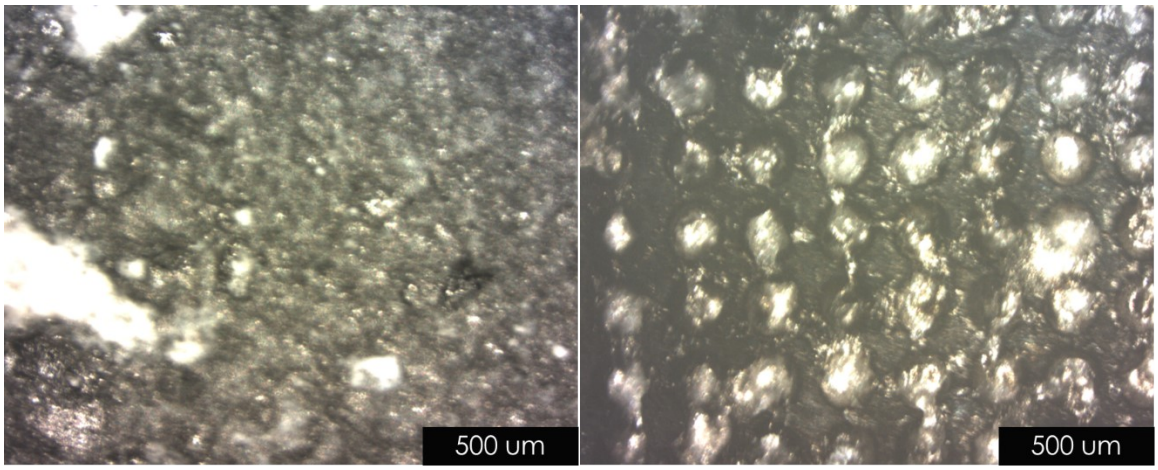

Figure S1: Images of a single area on a graphite sample exposed to FLiNaK before (*left*) and after (*right*) a 10 × 10 LIBS mapping measurement with 200 shots per spot. The center-to-center distance of each sample was 250 µm. The laser spot size was 200 µm in diameter. Note: The final sampling procedure used on 50 shots per spot.

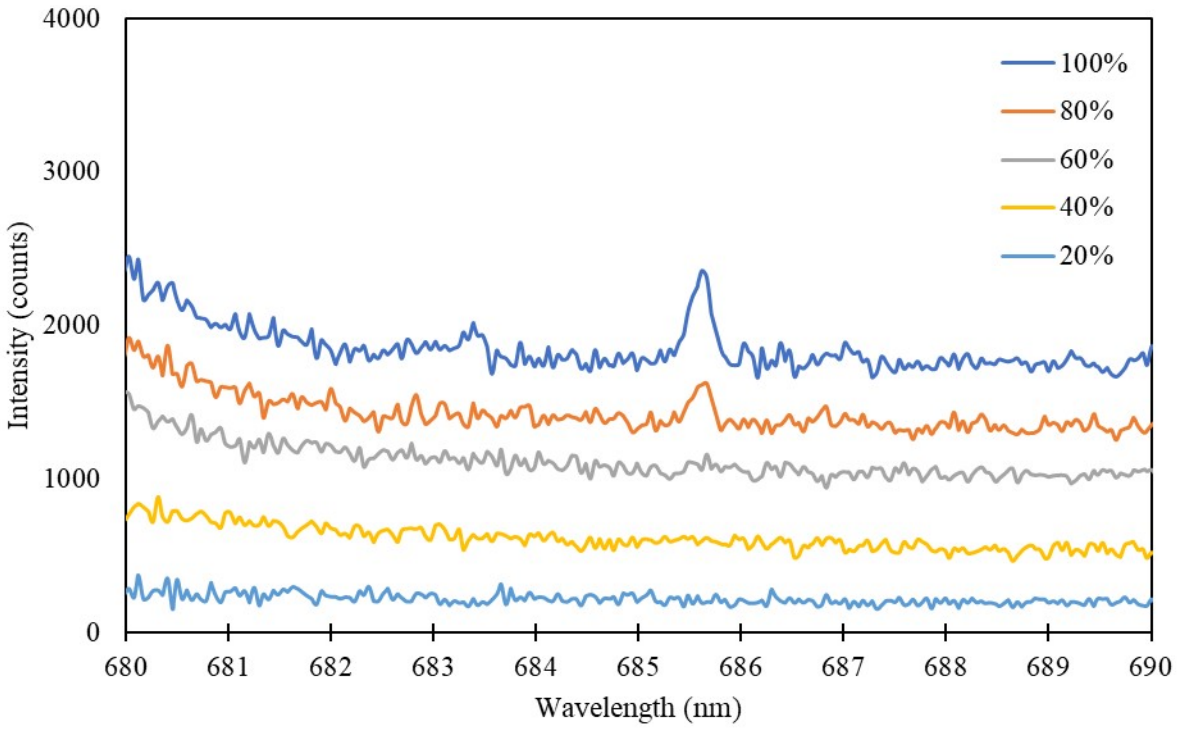

Figure S2: Optical emission spectra from 680 to 690 nm of a graphite sample exposed to molten FLiNaK at various energies (100%, 80%, 60%, 40%, and 20% of the maximum 16.4 mJ) performed with a delay time of 0.25 µs.

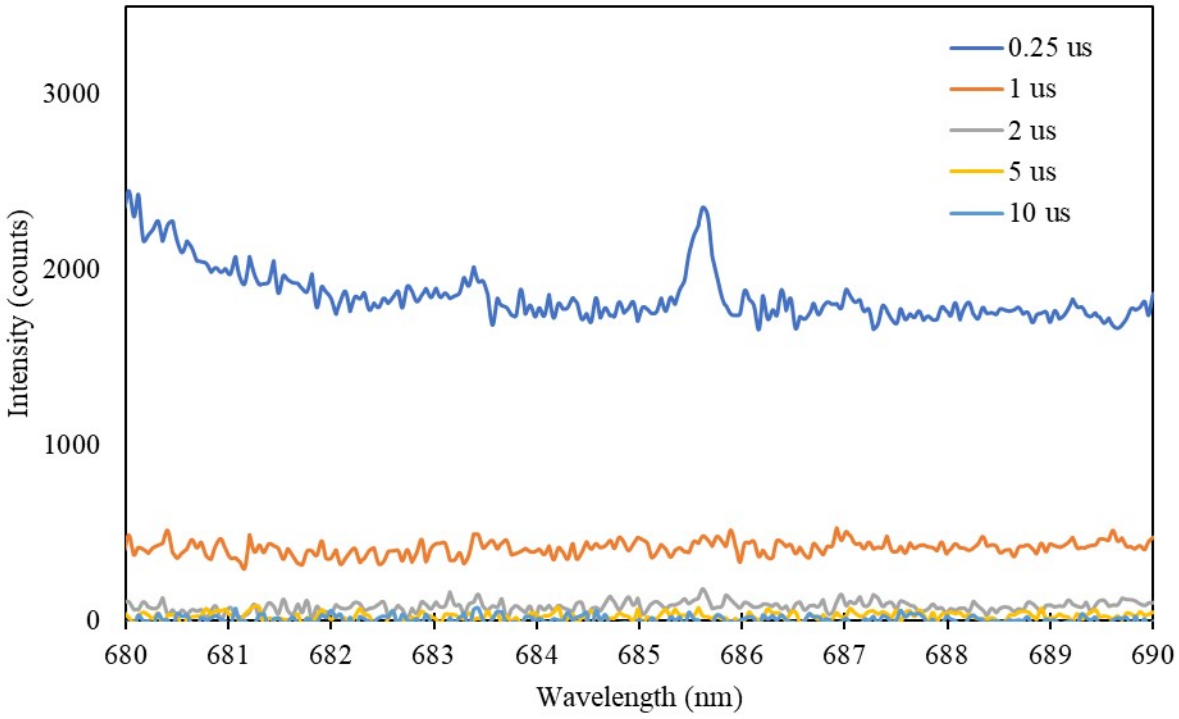

Figure S3: Optical emission spectra from 680 to 690 nm of a graphite sample exposed to molten FLiNaK at various delay times (0.25, 1, 2, 5, and 10 µs) performed at 100% laser pulse energy.

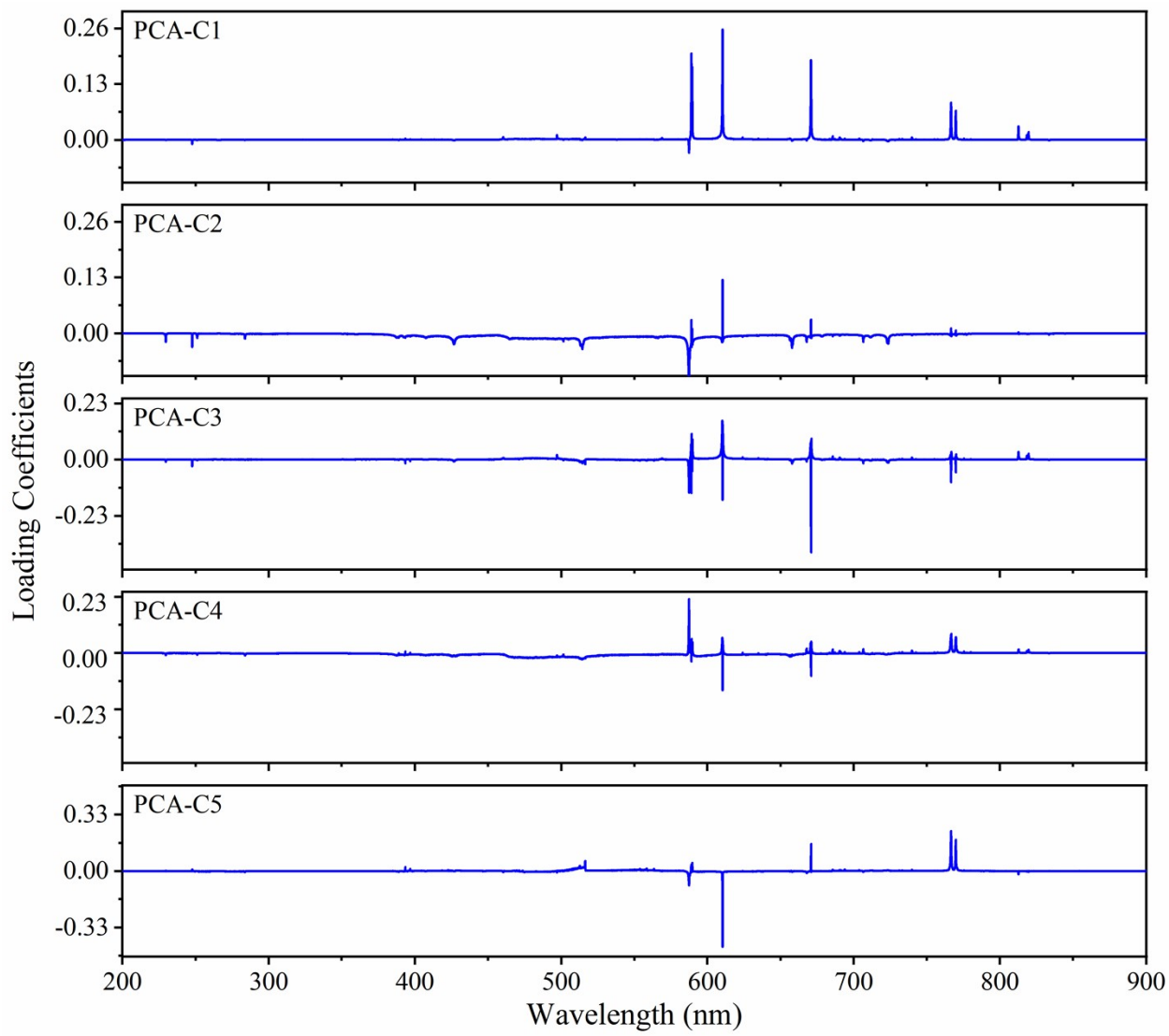

Figure S4. Loading plots of the first five components for PCA-based data segmentation for Sample K1.

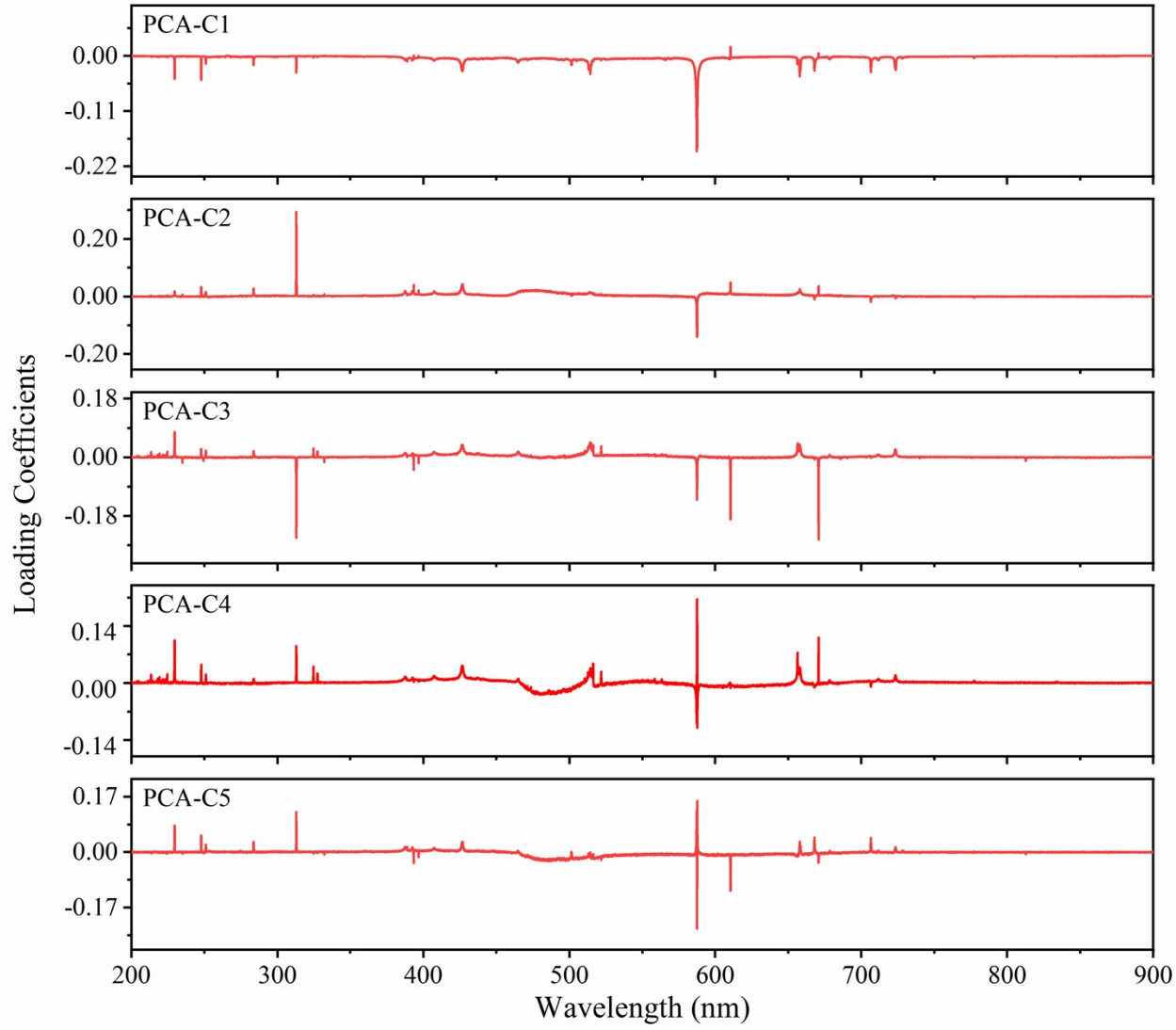

Figure S5. Loading plots of the first five components for PCA-based data segmentation for Sample B1.

Supporting Information Tables

Table S1: Correlation analysis between the 3D distributions of elements in Sample K1.

	H I	He I	Li I	C I	O I	F I	Na I	K I	C II	C_2 Swan
H I	1.00	0.09	0.10	−0.05	0.56	0.19	0.12	0.22	0.12	−0.14
He I	0.09	1.00	−0.48	0.48	0.22	−0.29	−0.51	−0.46	0.19	−0.14
Li I	0.10	-0.48	1.00	−0.48	0.06	0.64	0.95	0.87	−0.16	0.17
C I	−0.05	0.48	−0.48	1.00	−0.04	−0.40	−0.41	−0.37	0.66	0.15
O I	0.56	0.22	0.06	−0.04	1.00	0.11	0.03	0.09	0.08	−0.25
F I	0.19	−0.29	0.64	−0.40	0.11	1.00	0.56	0.70	−0.12	−0.03
Na I	0.12	−0.51	0.95	−0.41	0.03	0.56	1.00	0.88	−0.15	0.32
K I	0.22	−0.46	0.87	−0.37	0.09	0.70	0.88	1.00	−0.07	0.35
C II	0.12	0.19	−0.16	0.66	0.08	−0.12	−0.15	−0.07	1.00	0.09
C_2 Swan	−0.14	−0.14	0.17	0.15	−0.25	−0.03	0.32	0.35	0.09	1.00

Table S2: Correlation analysis between the 3D distributions of elements in Sample B1.

	H I	He I	Li I	C I	O I	F I	Be II	C II	C_2 Swan
H I	1.00	0.30	-0.25	0.35	0.53	-0.26	-0.30	0.54	0.70
He I	0.30	1.00	-0.22	0.23	0.57	-0.08	-0.33	0.55	0.05
Li I	-0.25	-0.22	1.00	-0.29	-0.04	0.82	0.57	-0.31	-0.20
C I	0.35	0.23	-0.29	1.00	0.01	-0.20	-0.06	0.74	0.46
O I	0.53	0.57	-0.04	0.01	1.00	-0.01	-0.08	0.19	0.02
F I	-0.26	-0.08	0.82	-0.20	-0.01	1.00	0.61	-0.16	-0.32
Be II	-0.30	-0.33	0.57	-0.06	-0.08	0.61	1.00	-0.21	-0.35
C II	0.54	0.55	-0.31	0.74	0.19	-0.16	-0.21	1.00	0.57
C_2 Swan	0.70	0.05	-0.20	0.46	0.02	-0.32	-0.35	0.57	1.00