**APPENDIX 2**

*PCA(2). Fossil and mineral sample type*

Two principal components account for 49%of the cumulative variance (Tables 1–3). The plots of the component loadings and component scores are shown in Fig. 1C, D. The first component explains 26.88% of the variance and has positive loadings on Mg, K, and Si and negative loadings on P and Al (Fig. 1.3). The A1, A2, A3, A4, B1, B3, B5, and B6 (carapace) specimens, along with margarite, variscite, ca-millisite, wavellite, augelite, and berlinite, exhibit the most negative scores (Fig. 1.4, x-axis) for PC 1, reflecting their high contents of P and Al. The A5, A6 (rock matrix), and B2, B4, B7, B8 (carapace) specimens, as well as limonite, albite, quartz, and biotite, show positive scores for the first component (Fig. 1.4, x-axis), indicating their high contents of Si, K, and Mg.

PC 2 (22.1%of variance explained) has high positive loadings on O and F and a high negative loading on Ca (Fig. 1.4). All of the carapace specimens, along with montmorillonite and muscovite, exhibit low positive scores (Fig. 1.4, y-axis) against PC 2, reflecting their relatively high contents of O and F. A5, A6 (rock matrix), fluorapatite, carbonate-fluorapatite, calcite, goethite, gypsum, and hematite show negative scores (Fig. 1.4 y-axis) against the second component according to their relatively high Ca concentrations.

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**Figure 1.** Principal component analysis (PCA) of EDS-derived data obtained from spinicaudatan carapaces and mineral samples (standard reference materials). (**1**) and (**2**) component loadings: PC1 vs. PC2 and PC1 vs. PC3, respectively. (3) and (4) component scores: PC1 vs. PC2 and PC1 vs. PC3, respectively.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **O** | **F** | **Mg** | **Al** | **Si** | **P** | **K** | **Ca** |
| **O** | 1 | 0.404472 | -0.071510 | 0.259911 | -0.145107 | 0.016994 | -0.231435 | -0.345530 |
| **F** | 0.404472 | 1 | 0.126527 | 0.101954 | -0.293694 | 0.026355 | 0.038171 | -0.152676 |
| **Mg** | -0.071510 | 0.126527 | 1 | 0.033959 | 0.115443 | -0.170267 | 0.095594 | -0.122177 |
| **Al** | 0.259911 | 0.101954 | 0.033959 | 1 | -0.251583 | 0.465773 | 0.011743 | -0.315901 |
| **Si** | -0.145107 | -0.293694 | 0.115443 | -0.251583 | 1 | -0.495894 | 0.301130 | -0.280374 |
| **P** | 0.016994 | 0.026355 | -0.170267 | 0.465773 | -0.495894 | 1 | -0.276138 | 0.265202 |
| **K** | -0.231435 | 0.038171 | 0.095594 | 0.011743 | 0.301130 | -0.276138 | 1 | -0.168073 |
| **Ca** | -0.345530 | -0.152676 | -0.122177 | -0.315901 | -0.280374 | 0.265202 | -0.168073 | 1 |

**Table 1.** Input correlation matrix of eight variables with unity in the principal diagonal. Data set includes (1) fossil carapace, (2) rock matrix, and (3) the following mineral specimens (high purity, 99.5%; included for comparisons purposes): albite, augelite, berlinite, biotite, calcite, ca-millisite, carbonate-fluorapatite, crandallite, fluorapatite, goethite, gypsum, hematite, limonite, margarite, montmorillonite, muscovite, quartz, variscite, and wavellite

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Variable** | **Component 1** | **Component 2** | **Component 3** | **Component 4** | **Component 5** | **Component 6** | **Component 7** | **Component 8** |  |
| **O** | -0.442347 | 0.623338 | 0.364171 | -0.308910 | 0.051746 | -0.286169 | 0.304491 | 0.102216 | 1 |
| **F** | -0.366336 | 0.517500 | 0.433165 | 0.419790 | -0.349564 | -0.055203 | -0.309177 | -0.115341 | 1 |
| **Mg** | 0.216114 | 0.303954 | -0.062684 | 0.723807 | 0.562541 | -0.063326 | 0.087304 | 0.070683 | 1 |
| **Al** | -0.566249 | 0.383266 | -0.653647 | -0.030682 | 0.062837 | -0.018446 | 0.072332 | -0.307820 | 1 |
| **Si** | 0.782983 | 0.200515 | -0.126071 | -0.277189 | 0.143425 | -0.402207 | -0.254062 | -0.084349 | 1 |
| **P** | -0.761277 | -0.306517 | -0.380214 | 0.058330 | 0.011998 | -0.234895 | -0.222634 | 0.271394 | 1 |
| **K** | 0.494944 | 0.250155 | -0.407395 | 0.282136 | -0.620278 | -0.096549 | 0.193241 | 0.124391 | 1 |
| **Ca** | -0.124624 | -0.822383 | 0.207862 | 0.279734 | -0.101727 | -0.323532 | 0.182031 | -0.196318 | 1 |
| Eigenvalue | 2.150320 | 1.76869 | 1.12107 | 1.03457 | 0.86108 | 0.42023 | 0.38575 | 0.25828 | 8 |
| Cumulative explainedvariance % | 26.879000 | 48.9876 | 63.001 | 75.9332 | 86.6967 | 91.9496 | 96.7714 | 100 |  |

**Table 2** . Solution of PCA.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Variable** | **Component 1** | **Component 2** | **Component 3** | **Variance \*** |
| **O** | -0.442347 | 0.623338 | 0.364171 | 71.684160 |
| **Na** | -0.366336 | 0.517500 | 0.433165 | 58.964020 |
| **Mg** | 0.216114 | 0.303954 | -0.062684 | 14.302260 |
| **Al** | -0.566249 | 0.383266 | -0.653647 | 89.478520 |
| **Si** | 0.782983 | 0.200515 | -0.126071 | 66.916250 |
| **K** | -0.761277 | -0.306517 | -0.380214 | 81.805800 |
| **Ca** | 0.494944 | 0.250155 | -0.407395 | 47.351780 |
| **Fe** | -0.124624 | -0.822383 | 0.207862 | 73.505160 |
| Eigenvalue | 2.150320 | 1.76869 | 1.12107 | 5.04008 |
| Cumulative explainedvariance % | 26.879000 | 48.9876 | 63.001 |  |

\* Variance explained by first 3 PC (%).

**Table 3**. Acceptable three-component solution of PCA.