

Johnson transformation method in geostatistic analysis— A case study in Tongling area, China

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Results of Transformation

When we carried out geostatistic analysis on the spatial variance structure and interpolation of As and Pb in soil in the Tongling ore concentration area, China, we found that these data couldn't obey the normal distribution which is a prerequisite hypothesis of geostatistics theory [1], meanwhile, it also couldn't obey the normal distribution after the Logarithm and Box-Cox transformation. The Johnson transformation includes a group of more complex mathematical functions, so it has more extensive and stronger adaptation ability [2]. Therefore, we tried transforming it by Johnson Transformation. After Johnson transformation, all the data could obey the normal distribution very well. The results are shown in the table below.

	Raw Data			Data After Johnson Transformation		
	skewness	kurtosis	P ^a	skewness	kurtosis	P ^a
As	5.79	38.32	<0.01	0.04	-0.34	>0.15
Pb	4.19	23.72	<0.01	-0.46	-0.63	>0.15

^a Single Sample Kolmogorov-Smirnov Test, $P < 0.05$ is not considered to obey normal distribution.

Table 1: The Johnson transformation of raw data and results of normality test.

Discussions

Johnson transformation can deal with a class of data which Logarithm and Box-Cox transformation failed, so it can be used as an alternative pre-processing method before geostatistic analysis. The variograms and interpolation maps which obtained by the Johnson transformation achieved good effect, and provided great importance for the future research.

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- [1] Gaus *et al.* (2003) *Environmental Geology* **44**, 939-948.
[2] Chou *et al.* (1998) *Journal of Quality Technology* **30**, 133-141.

The sinks of light Ge isotopes in global Ge cycling

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Although Ge isotope composition of seawater is unclear so far, the studies on igneous rocks and marine sediments [1, 2] suggested that seawater should be enriched in heavier Ge isotopes even more than that of opal sponges. It means seawater and the opal sponges will become huge reservoirs of heavy Ge isotopes. To balance the heavy Ge isotopes, therefore, would require fairly large reservoirs of light Ge isotopes. Where are these unknown reservoirs or sinks?

This study investigates the isotopic fractionations between the dominant Ge species in seawater, Ge-bearing sulfides, organic complexes and the species adsorbed on the surface of Fe oxy(hydro)oxides. Urey model or Bigeleisen-Mayer equation based theoretical method has been used to calculate the fractionation factors. The electronic structures and frequencies of the Ge species were obtained using quantum chemistry calculation at the B3LYP/6-311+G(d,p) level. Many different conformers are used to reduce the errors caused by configuration difference in solution. We find that the fractionations ($^{74/70}\text{Ge}$, 25) $\Delta_{\text{sphalerite-Ge(OH)}_4}$ and $\Delta_{\text{Ge-organic complexes-Ge(OH)}_4}$ are around -10‰, and -3~-4‰, respectively. Such large fractionations suggest these environments could be extremely enriched light Ge isotopes. Just as the observation of Galy *et al.* [3] and has been confirmed by Rouxel *et al.* [2], our results also show that the surface absorption processes between aqueous Ge species and Fe-oxyhydroxides could lead to a small Ge isotope fractionation, the fractionation $\Delta_{\text{Fe-oxyhydroxide - Ge(OH)}_4}$ is about -1.6‰. The results suggest that the sinks of light Ge isotopes, at least, include the environments of Ge-bearing sulfides and organic matters. Meanwhile, the Ge isotope compositions of heavy metal oxy(hydro)oxides can be 1-2‰ lighter than that of seawater.

- [1] Rouxel *et al.* (2006) *GCA* **70**, 3387-3400. [2] Rouxel *et al.* (2008) *Goldschmidt 2008*, A809. [3] Galy, *et al.* (2002). *GCA* **66**, 259.