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GEOCHEMISTRY

A Priori Estimates of Anomalously High $^{140, 142}$Ce and $^{148, 152, 154}$Sm Abundances and Anomalously Low ^{141}Pr and $^{151, 153}$Eu Abundances in Chondrites

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It is known that the graphic presentation of lanthanide abundances in terrestrial rocks and ores in the nucleus charge versus the logarithm of abundance coordinates has a Z-shaped pattern with deep minimums and sharp maximums and a general tendency of decreasing abundances with increase in the nucleus charge. The difference between any neighboring maximum and minimum is substantially reduced in the case of chondrite normalization. This method implies that the abundances of lanthanides in chondrites are regarded as reference values. Lanthanides of constant valence contained in chondrites demonstrate a clear abundance reduction tendency with increasing nucleus charge. In contrast, the abundances of lanthanides of variable valence are anomalous because high abundances atypical of the general tendency are inherent to Ce, Sm, and Yb, whereas Pr, Eu, and Tb are also characterized by anomalously low abundances atypical of the general tendency. Therefore, such anomalous abundances could not be described and certainly not estimated a priori.

This communication is an attempt to solve this problem for lanthanides of variable valence in two stages: (1) approximation of experimental data pertaining to a set of nuclides and (2) a priori estimation for another set of nuclides using the method applied to the first set.

The first stage begins with choice of the set of nuclides assigned for approximation of experimental data. The chosen nuclide set used for searching for a relationship between the content of the nuclide and its property should have the following properties:

the same p-evenness–oddness (either p^+ or p^-);

the same n-evenness–oddness (either n^+ or n^-);

constant valence;

p-evenness (p^+); and

n-evenness (n^+).

The last two requirements (the chosen nuclides must have both an even number of protons and an even number of neutrons) are dictated by reasons of accuracy of the expected results, because the sum of isotope shares related to the p^+n^+ set is greater than the sum of isotope shares belonging to the p^+n^- set and formal processing of more representative data is desirable.

The fulfillment of the aforementioned requirements during the choice of nuclides leads to the following set of 11 nuclides: $^{142; 144; 146}$Nd, $^{156; 158; 160}$Gd, $^{162; 164}$Dy, and $^{166; 168; 170}$Er.

The processing of experimental data as applied to the formula having a general view $\ln A = a_0 - a_1 \cdot m^{1/3}$ yields

$$\ln A_{calc} = 8.1449 - 4.6376 m^{1/3}, \qquad (1)$$

where A_{calc} is the weighted average abundance of the p^+n^+ set of the calculated isotope and m is the weighted average atomic mass of the calculated lanthanide.

Figure 1 shows approximation of experimental data based on formula (1). The presented graphs indicate that the experimental $\ln A_{exp}$ values for $^{142; 144; 146}$Nd, $^{156; 158; 160}$Gd, $^{162; 164}$Dy, and $^{166; 168; 170}$Er are satisfactorily described by formula (1). This is also supported by the fact that the maximum relative error is 2.1%. The figure also graphically illustrates the known fact that Ce, Sm, and Yb anomalies are positive.

Passing to the second stage (a priori estimation of abundances of nuclides of variable valence), let us emphasize that the absolute error is much smaller than the absolute value of the function, i.e., $|\delta_{abs}(\ln A)| < |\ln A|$. Therefore, one may suggest that introduction of a minor correction to function (1) may provide the desirable accuracy of prediction.

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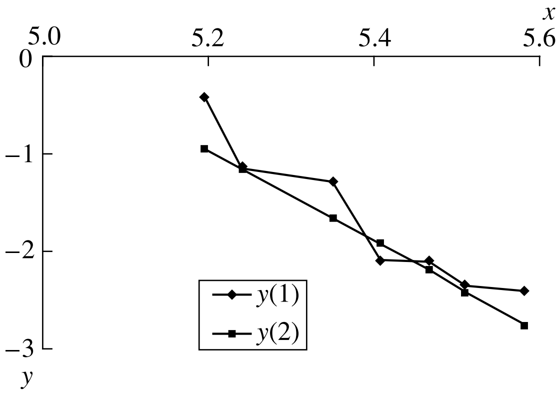

Fig. 1. Comparison of experimental $\ln A_{exp}$ values for $^{142; 144; 146}$Nd, $^{156; 158; 160}$Gd, $^{162; 164}$Dy, and $^{166; 168; 170}$Er (four points lying near the approximating straight line) and anomalous $\ln A_{exp}$ values for $^{140; 142}$Ce, $^{148; 152; 154}$Sm, and $^{172; 174; 176}$Yb (three points lying above the straight line). Coordinates: $x = m^{1/3}$; $y = \ln A + 5$. A is given in g-atom/t.

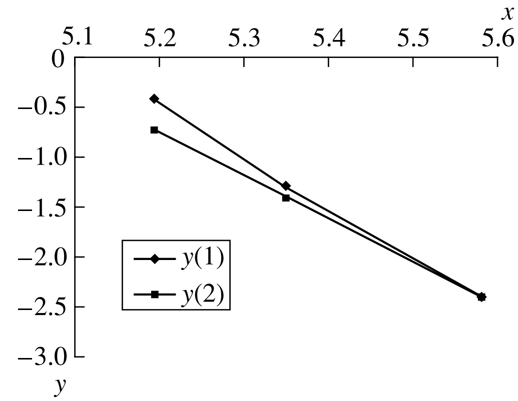

Fig. 2. Comparison of a priori $\ln A_{calc}$ estimates from formula (2) for $^{140; 142}$Ce and $^{148; 152; 154}$Sm with their experimental values. The maximum relative error $\delta|\ln A|$ is 3.9%. The coordinates are $x = m^{1/3}$; $y = \ln A + 5$. A is given in g-atom/t.

Let us introduce this minor correction to function (1) as a minor parameter α:

$$\ln A = (a_0 - a_1 m^{1/3})(1 - \alpha \cdot f(m))$$

or in a extended form

$$\ln A = (a_0 - a_1, m^{1/3})[1 - \alpha \cdot m(\mathrm{Yb})/m], \qquad (2)$$

where A is the weighted average abundance of the p^+n^+ set of isotopes of the calculated lanthanide, m(Yb) is the weighted average atomic mass of the p^+n^+ set of Yb isotopes, and m is the weighted average atomic mass of the calculated lanthanide.

Using the tabular data on Yb abundances [1] and shares of p^+n^+ Yb isotopes [2] for calculation $\ln A_{exp}$ and substituting this value in the left-hand side of formula (2), we obtain the value of the minor parameter α and, hence, expansion of formula (1) as the eventual calculation formula

$$\ln A_{calc} = (8.1449 - 4.6376 m^{1/3})(1 - 7.2094/m). \quad (3)$$

Figure 2 presents comparison of a priori estimates of Ce and Sm abundances based on formula (3) with the experimental data. It is evident that the experimental values of $\ln A_{exp}$ for $^{140; 142}$Ce and $^{148; 152; 154}$Sm are satisfactorily described by formula (3), which provides a maximum relative error not higher than 3%.

The efficiency of the proposed method as applied to the p-even lanthanides suggests that this method can also be used for p-odd lanthanides. Such expansion is also fulfilled in two stages. The first stage, i.e., the stage of approximation of experimental data on lanthanides

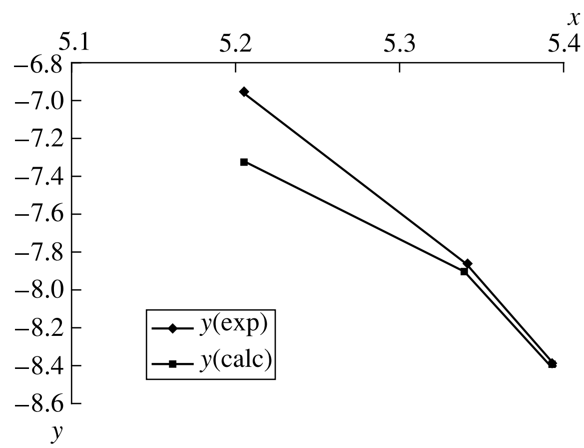

Fig. 3. Comparison of a priori $\ln A_{calc}$ estimates from formula (6) for ^{141}Pr and $^{151; 153}$Eu with their experimental values. The maximum relative error $\delta|\ln A|$ is 4.3%. The coordinates are $x = m^{1/3}$; $y = \ln A + 5$. A is given in g-atom/t.

of constant valence (La, Ho, Tm, and Lu), yields the formula

$$\ln A_{calc} = 26.2628 - 6.2959 m^{1/3}. \qquad (4)$$

The maximum relative error of experimental data approximation with formula (4) is 3.2%.

At the second stage of expansion, i.e., at the stage of a priori estimation of abundances of lanthanides of variable valence (Pr, Eu) with Tb as a reference lanthanide, we obtain the following formula:

$$\ln A_{calc} = (26.2628 - 6.2959 m^{1/3}) \times [1 + \alpha \cdot m(\mathrm{Tb})/m]. \qquad (5)$$

Using the tabular data on Tb abundances [1] for calculating $\ln A_{exp}$ and substituting this value in the left-hand side of formula (5), we obtain the value of the minor parameter α, and hence, expansion of formula (5) as the eventual design formula

$$\ln A_{\text{calc}} = (26.2628 - 6.2959 m^{1/3}) \times (1 + 11.0483/m). \quad (6)$$

Figure 3 shows the results of a priori estimates based on formula (6).

In summary, it may be stated that the problem of a priori estimation of abundances of three p^+n^+-lanthanides of variable valence has been solved for Ce and Sm and this solution provides a maximum relative error of 3.9%. The problem of a priori estimation of abundances of three p^-n^+-lanthanides of variable valence has been solved for Pr and Eu, and this solution provides a maximum relative error of 4.3%.

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