

The Concentration gradient theory simulations.

Based on the Zn isotope value formula:

$$\delta^{66}\text{Zn} = [({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{sample}} / ({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{IRMM-3702-1}} - 1] * 1000$$

In the following derivation equations,  $C_{\text{sp}}$  represents the sample concentration,  $C_{\text{st}}$  represents the specimen concentration, and  $k$  represents the sample-to-standard concentration ratio ( $k = C_{\text{sp}}/C_{\text{st}}$ ). And  $f$  symbolizes the ratio of interference signal intensity to isotope signal intensity within a specific concentration of Zn standard solution.

Model 1 Considering the isobaric interferences on  ${}^{64}\text{Zn}$ :

$$\begin{aligned}\delta^{66}\text{Zn} &= [({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{sample}} / ({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{IRMM-3702-1}} - 1] * 1000 \\ &= [({}^{66}\text{C}_{\text{sp}}/{}^{64}\text{C}_{\text{sp}}) / ({}^{66}\text{C}_{\text{st}}/{}^{64}\text{C}_{\text{sp}}) - 1] * 1000 \\ &= [(k{}^{66}\text{C}_{\text{st}} / (k{}^{64}\text{C}_{\text{st}} + f*{}^{64}\text{C}_{\text{st}})) / ({}^{66}\text{C}_{\text{st}} / ({}^{64}\text{C}_{\text{st}} + f*{}^{64}\text{C}_{\text{st}})) - 1] * 1000 \\ &= [k(1+f) / (k+f) - 1] * 1000 \\ &= [f(k-1) / (k+f)] * 1000\end{aligned}$$

Model 2 Considering isobaric interferences on  ${}^{66}\text{Zn}$ ,  ${}^{68}\text{Zn}$ , and  ${}^{70}\text{Zn}$ .

$$\begin{aligned}\delta^{66}\text{Zn} &= [({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{sample}} / ({}^{66}\text{Zn}/{}^{64}\text{Zn})_{\text{IRMM-3702-1}} - 1] * 1000 \\ &= [({}^{66}\text{C}_{\text{sp}}/{}^{64}\text{C}_{\text{sp}}) / ({}^{66}\text{C}_{\text{st}}/{}^{64}\text{C}_{\text{sp}}) - 1] * 1000 \\ &= [((k*{}^{66}\text{C}_{\text{st}} + f*{}^{66}\text{C}_{\text{st}}) / k*{}^{64}\text{C}_{\text{st}}) / (({}^{66}\text{C}_{\text{st}} + f*{}^{66}\text{C}_{\text{st}}) / {}^{64}\text{C}_{\text{st}}) - 1] * 1000 \\ &= [(k+f) / (k+k*f) - 1] * 1000 \\ &= [(f - f*k) / (k+k*f)] * 1000\end{aligned}$$