Algorithm 1: Generalization Algorithm for a wide range of inputs

Inputs:

Read ***y***

Where y is the percentage of A in Fe_xA_yB.

Constraints:

i. A ∈ {Ni, Cr, Co,Mn}, B ∈ {S, Se, Te}

ii. x+y ← 100, where x is the percentage of Fe in Fe_xA_yB.

iii. $0 < y \leq 62.5$.

Read $\boldsymbol{S_i}$ for i ← 1 to 4

Where $\boldsymbol{S_i}$ is the percentage of element ***A*** on i^{th} site of the structure Fe_xA_yB.

Constraints:

i. $S_i \leq \frac{1}{4*y} \times 100 \times 100$

ii. $\sum_{i\leftarrow 1}^{4} S_i = 100$

Step 1:

Convert percentage into real number to fit on our pretrained model

$y' \leftarrow y \times \frac{16}{100}$

$x' \leftarrow 16 - y'$

Step 2 (Reduction step):

Convert percentage values to the original range of 16

for i ← 1 to 4

$S_i' \leftarrow y' \times \frac{S_i}{100}$

Step 3:

Input $\frac{x'}{16}$, $\frac{y'}{16}$, and S_i' as the concentration of Fe, the concentration of A, and the number of atoms A on sites i=1 to 4.