

EXERCISE 1.1.

- A. Describe shortly the following terminologies: oxygen vacancy, oxygen vacancy ordering, antisite defect, A-site ordered double perovskite, B-site ordered double perovskite.
- B. Why the same transition metal is smaller as a trivalent cation than as a divalent ion?
- C. What happens to the bond valence when the bond length gets smaller?
- D. Looking at the formula to calculate the bond valence, can you see what kind of evident meaning the R^0 value has?

EXERCISE 1.2.

- A. Search for the ionic radius values for Ca^{2+} , Ti^{4+} and O^{2-} ions, relevant to the perovskite structure (HINT: consider the coordination numbers).
- B. Calculate the Tolerance factor for the mineral perovskite CaTiO_3 .
- C. How well Ca and Ti match size-wise with each other considering the ideal cubic perovskite structure?
- D. To improve the match, you could as a chemist consider different modifications, e.g., to control the oxygen content or replacing Ca (partly) with other alkaline earth metals. Which option you would select and why?

You can find ionic radius values at:

<http://abulafia.mt.ic.ac.uk/shannon/ptable.php>

EXERCISE 1.3.

- A. Below given are the bond lengths determined for the Cu-O bonds in a superconducting $\text{Cu(1)Ba}_2\text{YCu(2)}_2\text{O}_{7-\delta}$ sample. Calculate the bond valences and bond-valence-sums for Cu(1) and Cu(2) atoms.
- B. Assume that these are the true valence values for Cu(1) and Cu(2), and estimate the δ value in the $\text{Cu(1)Ba}_2\text{YCu(2)}_2\text{O}_{7-\delta}$ formula.

Cu(1)	2 x 1.86 Å
	2 x 1.91 Å
Cu(2)	2 x 1.92 Å
	2 x 1.94 Å
	1 x 2.26 Å

$$s_{ij} = \exp \left[\frac{(R_{ij}^0 - d_{ij})}{0.37} \right]$$

$$V_i = \pm \sum_j s_{ij}$$

$$R^0: \text{Cu}^{2+}-\text{O}^{2-}: 1.679 \text{ \AA}$$

