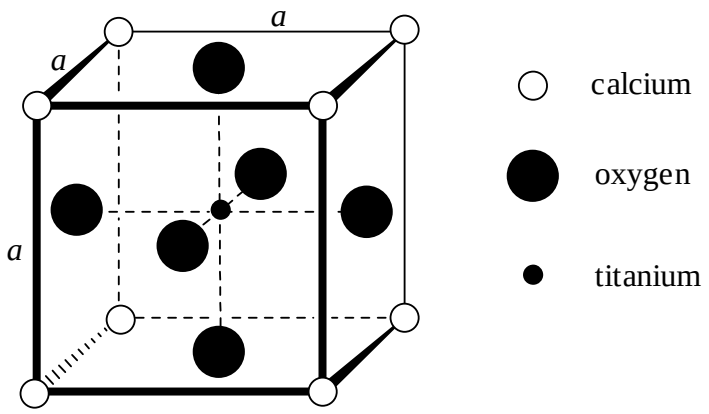
Marks 5

- The diagram below shows the structure of perovskite, a mineral made up of calcium (at each of the corners), oxygen (in the centre of each of the faces), and titanium (at the centre of the cube). The unit cell dimension (edge length, *a*) for perovskite is 0.38 nm.



What is the chemical formula of perovskite?

There are eight Ca^{2+} ions on the corners of the cube. These are each shared between eight unit cells: number of Ca^{2+} ions = 8 × 1/8 = 1.

There is a single, unshared Ti^{4+} ion at the cube centre.

There are six O^{2-} ions at the centres of the faces of the cube. These are each shared between two cubes: number of O^{2-} ions = 6 × 1/2 =3.

Overall, Ca^{2+} : Ti^{4+} : O^{2-} = 1 : 1 : 3. The formula is $CaTiO_3$.

Answer: **$CaTiO_3$**

What is the volume of the unit cell?

The length of the side of the cube = *a* = 0.38 nm. As $V = a^3$,

$V = (0.38 \times 10^{-9}\ m)^3 = 5.5 \times 10^{-29}\ m^3$

Answer: **$5.5 \times 10^{-29}\ m^3$**

What is the density of perovskite? Give your answer in g cm^{-3}.

As the atomic mass is the mass of a mole, the mass of one atom is $\frac{M}{N_a}$. From above, each unit cell contains 1 Ca^{2+}, 1 Ti^{4+} and 3 O^{2-}. The mass of one cell is therefore:

$$\text{mass of cell} = \frac{M_{Ca}}{N_a} + \frac{M_{Ti}}{N_a} + 3\frac{M_O}{N_a} = \frac{1}{N_a}(40.08 + 47.88 + 16.00)\ \text{g}$$

$$= \frac{1}{N_a} \times 135.96\ \text{g} = 2.258 \times 10^{-22}\ \text{g}$$

As 1 cm = 0.01 m, 1 cm^3 = $(0.01)^3$ m^3 = 1×10^{-6} m^3. From above, V = 5.5×10^{-29} m^3 so,

$$\text{volume} = 5.5 \times 10^{-29} / 1 \times 10^{-6}\ \text{cm}^3 = 5.5 \times 10^{-23}\ \text{cm}^3.$$

Hence,

$$\text{density} = \frac{\text{mass (g)}}{\text{volume}\,(\text{cm}^3)} = \frac{2.258 \times 10^{-22}\ \text{g}}{5.5 \times 10^{-23}\ \text{cm}^3} = 4.1\ \text{g cm}^{-3}$$

Answer: **4.1 g cm^{-3}**

ANSWER CONTINUES ON THE NEXT PAGE

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