• The cubic form of boron nitride (borazon) is the second-hardest material after diamond and it crystallizes with the structure shown below. The large spheres represent the nitrogen atoms and the smaller spheres represent boron atoms.



From the unit-cell shown above, determine the empirical formula of boron nitride.

There are N atoms on the corners and on the faces of the unit cell:

- There are 8 N atoms on the corners. These contribute 1/8 to the unit cell giving a total of $8 \times 1/8 = 1$ N atom.
- There are 6 N atoms on the faces. These contribute 1/2 to the unit cell giving a total of $6 \times 1/2 = 3$ N atoms.
- There are a total of 1 + 3 = 4 N atoms in the unit cell.

There are B atoms inside the unit cell:

• There are 4 B atoms completely inside the cell. These contribute only to this unit cell giving a total of $4 \times 1 = 4$ B atoms.

The formula is therefore B₄N₄ which simplifies to BN.

Answer: **BN**

Determine the oxidation state of the boron atoms.

Nitrogen has an oxidation number of –III (or -3) to complete its octet. To ensure neutrality, boron must be +III (or +3).

Answer: +III (or +3)

ANSWER CONTINUES ON THE NEXT PAGE

Marks 5 The cubic form of boron nitride is more thermally stable in air than diamond. Provide a reasonable explanation for this observation.

Boron and nitrogen have different electronegativities, with N more electronegative than B. This leads to partial δ + and δ - charges on B and N respectively. These charges give the bonds partial ionic character and this acts to increase the strength of the bonds.

A protective layer of B_2O_3 forms on the surface of BN in the presence of air. For diamond, gaseous CO_2 forms at high temperatures which leads to thermal degradation rather than protection.