

Exam Solutions in mineral chemistry

Exercise 1 (3pts)

1. The main steps of the Haber–Bosch process for producing ammonia are:

1. Production of reactants:

0.5

- **Nitrogen (N₂):** Obtained by fractional distillation of air (air contains about 78% nitrogen).
- **Hydrogen (H₂):** Obtained by methane reforming (CH₄):

$$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$$
 Carbon monoxide (CO) is then converted into carbon dioxide (CO₂) and removed.

2. Compression and heating of gases:

0.5

Nitrogen and hydrogen gases are compressed to high pressure and heated to 400–500 °C.

3. Synthesis in the reactor:

0.5

The gases pass over an iron catalyst bed. The reaction is partial, but the produced ammonia is rapidly liquefied to promote conversion.

4. Recovery and recycling:

0.5

Ammonia is separated by cooling, and the unreacted gases (N₂, H₂) are recycled back into the reactor.

2. Application of ammonia in industry:

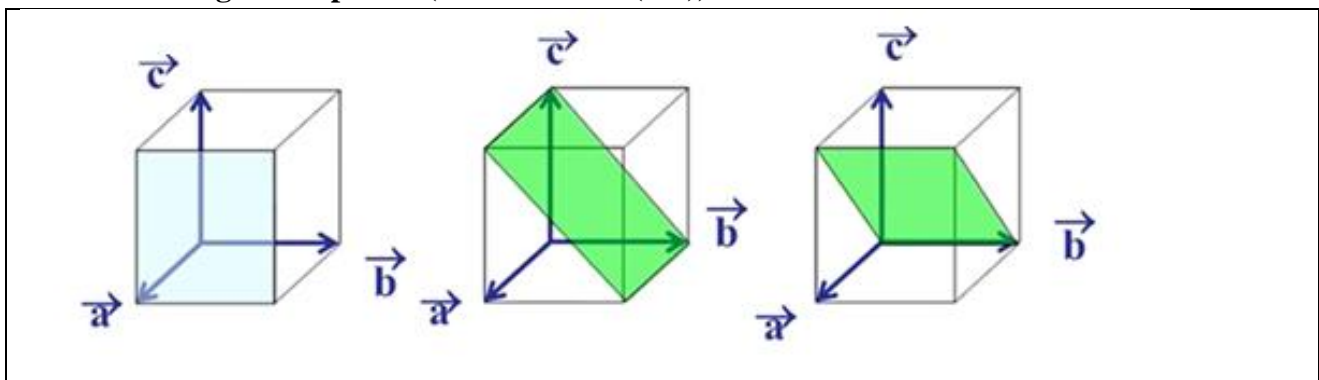
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Ammonia is used to manufacture fertilizers such as ammonium nitrate.

Exercise 2 (7pts)

I. The following lattice planes (Miller indices (hkl)). The unit cells are cubic.

1x3



a= 1	h= 1	a= ∞	h= 0	a= 1	h= 1
b= ∞	k= 0	b= 1	k= 1	b=∞	k= 0
c= ∞	l= 0	c= 1	l= 1	c=1	l= 1
donc le plan est : (1 0 0)		donc le plan est : (0 1 1)		donc le plan est : (1 0 1)	

II.

1. Calculation of the total number of atoms present in the crystal

$$n = \frac{m}{M} = \frac{N}{N_A}$$

$$N = \frac{mN_A}{M}$$

$$N = \frac{100 \times 6,023 \times 10^{23}}{183,84}$$

$$N = 3,28 \times 10^{23} \text{ atoms} \quad \mathbf{0.5}$$

2. Determination of the total number of unit cells forming the crystal
- Calculation of the number of atoms in one unit cell (multiplicity calculation)

$$M = NS \cdot 1/8 + NA \cdot 1/4 + NF \cdot 1/2 + NI \cdot 1 \quad \mathbf{0.5}$$

$$M = NS \frac{1}{8} + NA \frac{1}{4} + NF \frac{1}{2} + NI$$

$$M = 8 \times \frac{1}{8} + 1 = 2 \text{ atomes/maille} \quad \mathbf{0.5}$$

Each unit cell contains **2 atoms**.

1 unit cells \longrightarrow 2 atoms

N unit cells \longrightarrow $4,738 \times 10^{22}$ atoms

$$N_{\text{maille}} = \frac{1 \times 3,28 \times 10^{23}}{2}$$

$$N_{\text{maille}} = 1,64 \times 10^{23} \text{ unit cell} \quad \mathbf{0.5}$$

3. Calculation of the packing efficiency (compacity, C)

$$C = \frac{V_{\text{occupied by atoms in the unit cell}}}{V_{\text{unit cell}}} \quad \mathbf{0.5}$$

$$C = \frac{z \frac{4}{3} \pi r^3}{a^3}$$

$$C = \frac{4 \times \frac{4}{3} \times 3,14 \times r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$C = 0,68 \quad \mathbf{0.5}$$

4. Calculation of the packing fraction (τ)

$$\tau = C \times 100 \quad \mathbf{0.25}$$

$$\tau = 0,68 \times 100$$

$$\tau = 68\% \quad \mathbf{0.25}$$

The percentage of void in the unit cell.

$$\% \text{ de vide} = 100 - \tau \quad \mathbf{0.25}$$

$$\% \text{ de vide} = 100 - 68$$

$$\% \text{ de vide} = 32\% \quad \mathbf{0.25}$$

Exercise 3 (5pts)

1. Cesium Bromide (CsBr) – Cubic Crystal Structure

Nature of the bonding: The bonds between Cs and Br atoms are **ionic**.

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2. Representation of the unit cell:

Since $r^+ = 196\text{pm} < r^- = 265\text{pm}$, the Br^- ions occupy the corners of the cube, and the Cs^+ ions occupy the center of the cube.

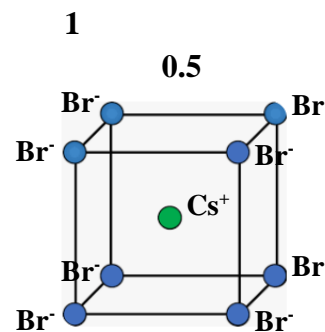
Calculation of the radius ratio:

$$\frac{r^+}{r^-} = \frac{196}{265} = 0,739 > 0,732 \quad 0.5$$

According to Pauling's rules, the crystal site of Cs^+ is **cubic**. 1

3. Coordination number (CN) of ions:

- For Br^- : $\text{Br}^- / \text{Cs}^+ = 8$ 0.5
- For Cs^+ : $\text{Cs}^+ / \text{Br}^- = 8$ 0.5



Exercise 4 (5pts)

Consider the following two atoms: ${}_5\text{B}$ and ${}_{13}\text{Al}$.

1. Position in the periodic table (column, period, group):

- Boron (B, Z = 5): $1s^2 2s^2 2p^1$ 0.25
 - Period: 2 0.25
 - Group: III_A 0.25
 - Column: 13 0.25
- Aluminum (Al, Z = 13): $1s^2 2s^2 2p^6 3s^2 3p^1$ 0.25
 - Period: 3 0.25
 - Group: III_A 0.25
 - Column: 13 0.25

2. Family of the elements:

Both boron and aluminum belong to the **boron family** 1

3. Possible oxidation states of boron in compounds:

B_2O_3 (boron trioxide): Boron has an oxidation state of +3 0.5

BF_3 (boron trifluoride): Boron has an oxidation state of +3 0.5

4. Applications of aluminum (Al) and boron (B):

- Aluminum (Al): 0.5
 - 1. Used in making **lightweight materials for the aerospace and automotive industries**
 - 2. Used in **packaging materials**, such as aluminum foil and cans
- Boron (B): 0.5
 - 1. Used in **borosilicate glass** (heat-resistant glass)
 - 2. Used as a **doping element in semiconductors** or in **boron-containing detergents and fertilizers**