''Abbes Laghrour'' University, Khenchela
Faculty of Sciences and Technology
Department of Matter Sciences

1st year Master of Materials Chemistry *Mai 2025*

ENGLISH EXAM

Text:

Liquids and gases lack three-dimensional order and cannot be used in [diffraction experiments] in the same way as are crystals. Certain information about the radial [distribution of electron density] can be obtained, but it lacks the distinctive detail of **crystal analysis**. It is not easy to locate light atoms in the presence of heavy atoms. **Difference-Fourier maps** alleviate the situation to some extent, but the [atomic positions] are not necessarily precise. **Least-squares refinement** of light-atom parameters is not always successful, because the contributions to the **structure factor** from these atoms are relatively small.

Hydrogen atoms are particularly difficult to localize with precision because of their small scattering power and the fact that the center of the hydrogen atom does not, in general, coincide with the maximum of its electron density. Terminal hydrogen atoms have a more aspherical **electron density distribution** than do hydrogen-bonded hydrogen atoms, and their bond distances, from X-ray studies, often appear short when compared with spectroscopic or neutron diffraction values. For similar reasons, [refinement of hydrogen-atom parameters] in a structure analysis may be imprecise and the standard deviations in their coordinate values may be as much as ten times greater than those for a carbon atom in the same structure. It is, nevertheless, very desirable to include hydrogen-atom positions in the [final structure model]. They lead to a best fit and are useful when comparing the results of [X-ray structure determination] with those of other techniques, notably nuclear magnetic resonance.

In general, **bond lengths** determined by X-ray methods represent distances between the centers of gravity of the electron clouds, which may not be the same as the internuclear separations. Internuclear distances can be found from [neutron diffraction] data, because neutrons are scattered by the **atomic nuclei**. If, for a given crystal, the synthesized neutron scattering density is subtracted from that of the X-ray scattering density, a much truer picture of the electron density can be obtained.

Questions:

1. Give an appropriate title for the text.
2. Why do liquids and gases cannot be used in diffraction experiments?
3. Explain why it is not successful to refine light-atom parameters?
4. Is it possible to localize hydrogen atoms with precision? Why?
5. What do bond lengths represent?
6. Give synonyms for the underlined words from the text.
7. What is the French translation for the words given in **bold**?
8. Use the words between [brackets] to make sentences.
9. Translate the last paragraph to French.

Good Luck

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Solution of the English exam

1. Crystal structure analysis/structural analysis/crystal structure refinement …(**1.5**)
2. The liquids and gases cannot be used in diffraction experiments because they lack three-dimensional order. …(**1.5**)

3. It is not successful to refine light-atom parameters because the standard deviations in their coordinate values may be as much as ten times greater than those for a carbon atom in the same structure. …(**1.5**)

4. Hydrogen atoms are particularly difficult to localize with precision (because of their small scattering power and the fact that their center does not coincide with the maximum of the electron density). …(**02**)

5. The bond lengths represent the distances between the centers of gravity of the electron clouds. …(**1.5**)

6. Locate = localize …(**0.5**)
   Small = light …(**0.5**)
   Distances = lengths …(**0.5**)
   Electron clouds = electron density distribution …(**0.5**)

7. **Crystal analysis** → analyse du cristal/cristallographique …(**0.5**)
   Difference-Fourier maps → cartes de Fourier difference …(**0.5**)
   Least-squares refinement → affinement par moindres carrés …(**0.5**)
   Structure factor → facteur de structure …(**0.5**)
   Electron density distribution → distribution de la densité électronique/nuage électronique …(**0.5**)
   Bond lengths → longueurs de liaison …(**0.5**)
   atomic nuclei → noyaux atomiques …(**0.5**)

8. [diffraction experiments] …(**0.5**)
   [distribution of electron density] …(**0.5**)
   [atomic positions] …(**0.5**)
   [refinement of hydrogen-atom parameters] …(**0.5**)
   [final structure model] …(**0.5**)
   [X-ray structure determination] …(**0.5**)
   [neutron diffraction] …(**0.5**)

9. Translation of the last paragraph. …(**03**)