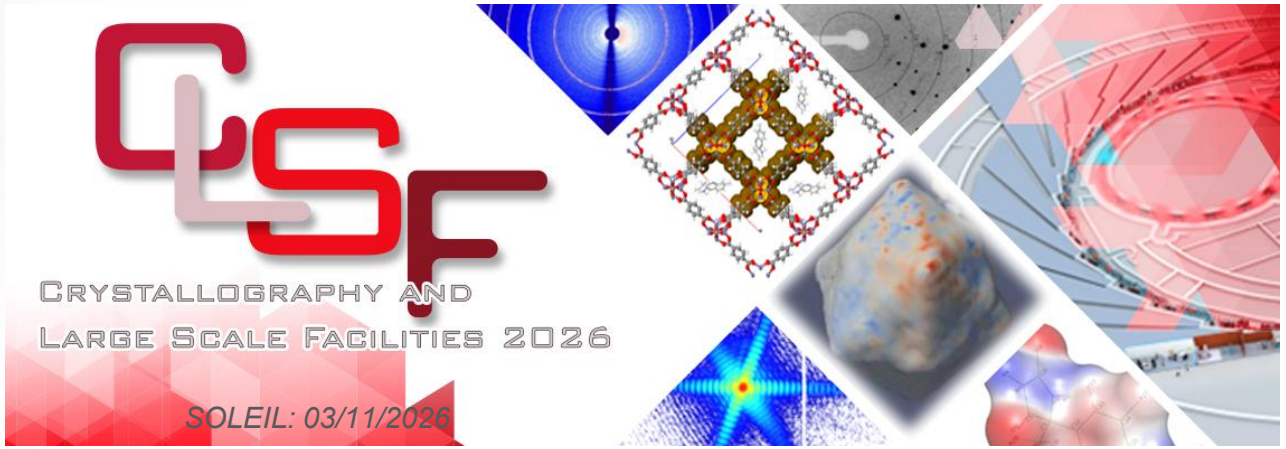
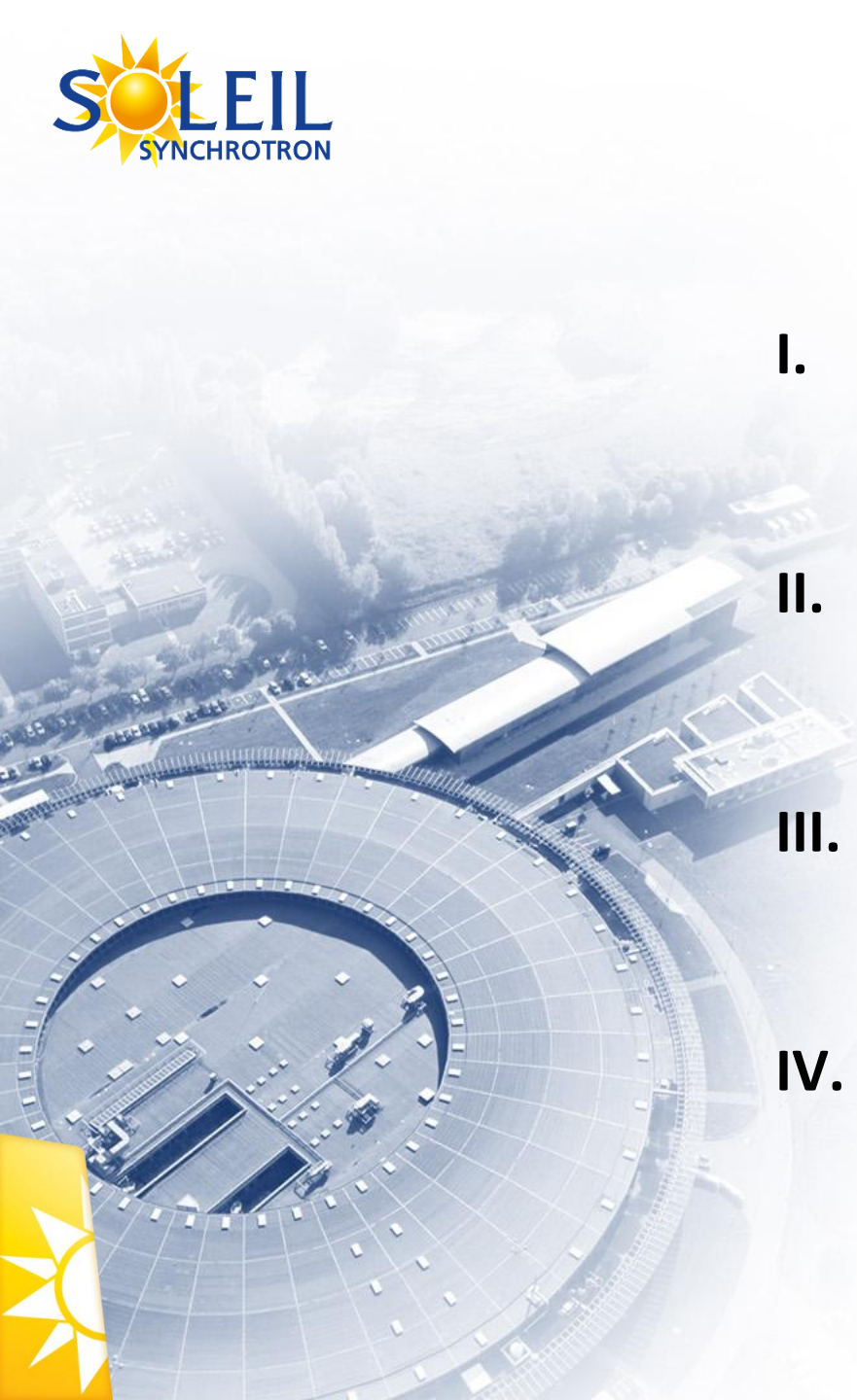
Symmetry elements & Crystal structures

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Outline



I. Symmetry elements and point groups

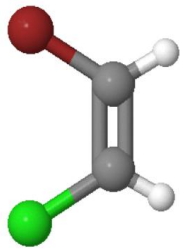
II. Symmetry and point group of a square-based pyramid

III. Crystal structure of marcasite FeS_2

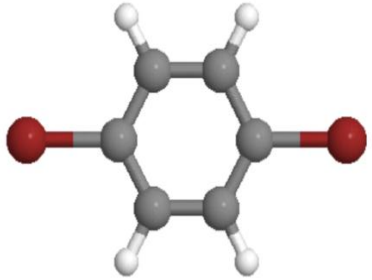
IV. Symmetry and Space Group

Represent the symmetry elements and give the point group of the following molecules, considered to be purely two-dimensional.

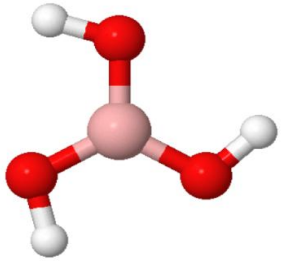
N.B.: *grayscale and atomic radii differentiate chemical species.*



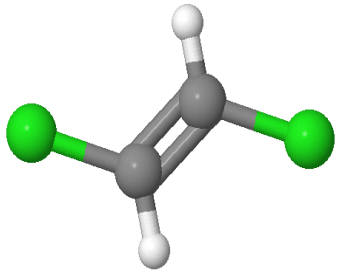
Ethylene BrCl



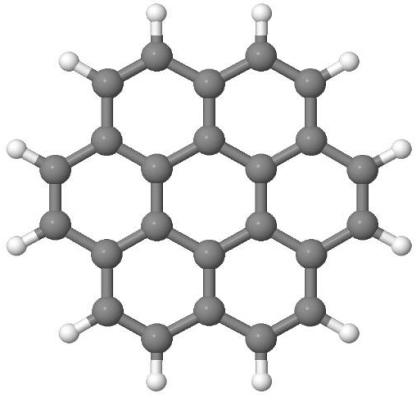
Dibromobenzene



Boric acid



Dichloroethene



Coronene

What are the symmetry elements of these figures?











2. Symmetry and point group of a square-based pyramid

Consider the square-based pyramid shown in the following figure.

a) Determine the symmetry elements of this pyramid.

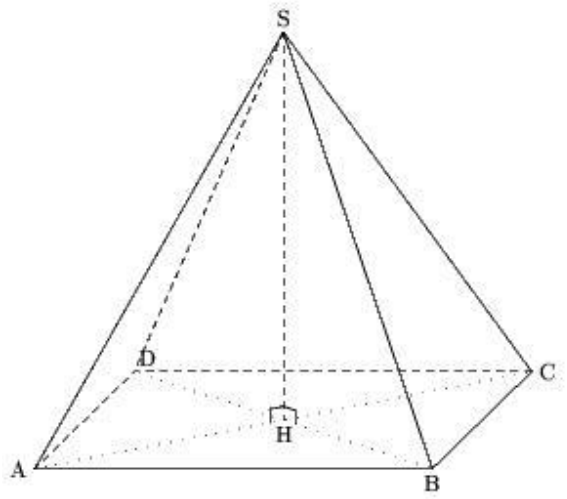
b) Give the corresponding point group. Which crystal system does it refer to?

c) Draw the stereographic projection of the equivalent directions.

d) Deduce the group order.

e) Determine in this system by calculation the intersection of the planes (110) and (-110)

N. B. *: **a** and **b** will be placed along the horizontal and vertical axes of the projection respectively.*



3. Crystal structure of marcasite FeS_2

The X-ray diffraction experiment performed on marcasite (**FeS_2**) shows as symmetry only the existence of **3 mutually perpendicular mirrors**.

1- What is the **Laue group** of the crystal, and what are the possible **point groups**?

2- Give stereographic projections of the Laue class and possible point groups

3- What are the possible **space groups** if we identify the following systematic extinctions :

On (0Kl): K+ l= 2n+1; On (h0l): h+l=2n+1.

The marcasite is centrosymmetric and has the following unit-cell parameters:

a= 4.45 Å, **b**= 5.40 Å et **c**= 3.38 Å. Knowing that the density of marcasite is 4.9 g/cm^3 and that the atomic masses of Fe and S are respectively 55.7 and 32.1 g.

4- Calculate the number of molecules (Z) per unit-cell.

Determine the space group of the ***IrAs2*** structure

- Unit-Cell : (a=6.05490 Å, b=6.07170 Å , c= 6.15870 Å, $\alpha=\gamma=90°$, $\beta=113.1970°$)
- What is the point group of symmetry and the Laue class

	x	y	z
Ir	0.28200	0.00000	0.29300
As1	0.33800	0.36600	0.18200
As2	0.15100	0.62500	0.37000

