

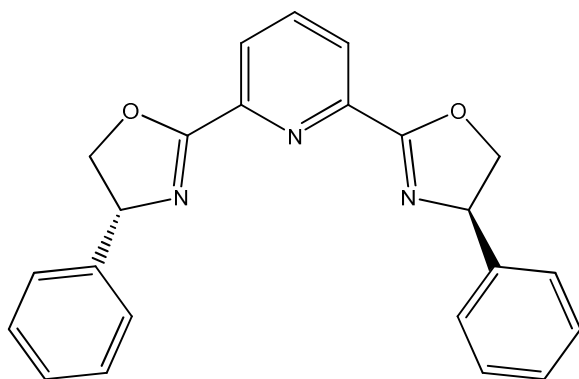
1. Below are six reflections from a structure in space group $Pbca$:

(h,k,l)	$ E $
(3,0,-4)	4.1
(2,3,6)	2.7
(2,-2,2)	3.6
(5,0,1)	2.4
(4, -5, -3)	1.9
(6, -2, 3)	3.1

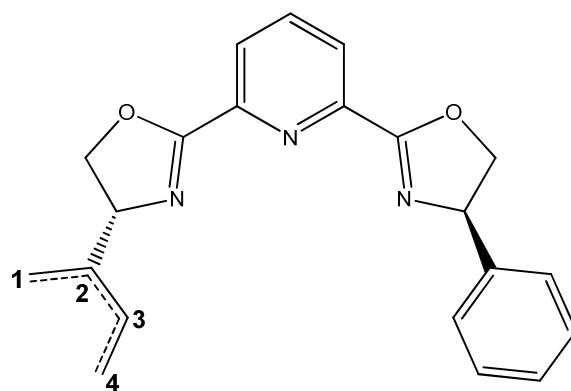
a) Choose three of these reflections which allow you to fix the origin of this space group, and justify your choice.

b) Do any three reflections meet the requirements for the Sayre equation? What is the significance of the Sayre equation in crystallography?

2. You are solving a crystal structure of a simple organic ligand. You have found 4 of the six carbons (which are numbered, 1-4) in what should be a phenyl ring – is it possible to use their coordinates to make accurate predictions for the coordinates of the other two carbons? If so, give the equations relating the xyz coordinates of the fifth and sixth carbons to the four shown.



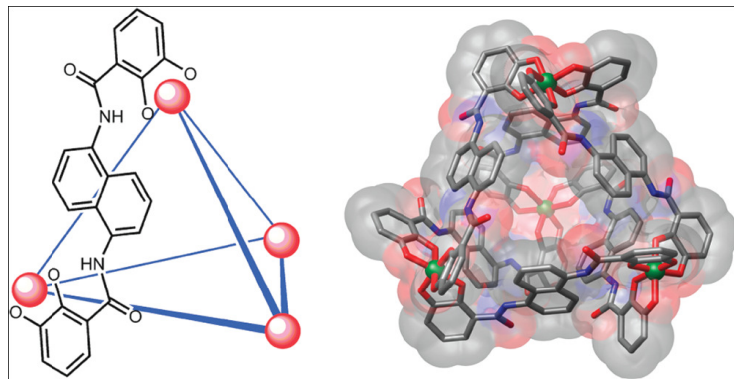
proposed structure



your partial structure

3. The compound $K_8(Cp^*_2Co)_3[Cp^*_2Co \subset Ga_4L_6]$ (here the \subset sign indicates host/guest encapsulation) [M. Pluth et al. *Inorg. Chem.* **2009**, *48*, 111-120] crystallizes in the space group $Fd\bar{3}c$ with $Z = 16$, $a = 50.0040(21)$ Å. [Parentheses indicate e.s.d.]

The ligand L (with a -4 charge) is defined in the upper left of the diagram. It spans the edges of the Ga_4L_6 cluster shown. The organometallic cation $Cp^*_2Co^+$ is a cobalt sandwich complex ($Cp^* = \eta^5$ -pentamethylcyclopentadienyl). [The sandwich complex is disordered within the cavity of the assembly and is not the focus of this question.]



Schematic representation of the M_4L_6 assembly with only one ligand shown for clarity. (Right) A space-filling model of the assembly looking toward the aperture coincident with the 3-fold axis.

- What Wyckoff position would you suggest for the Ga atoms? Why do you make this choice?
 - To what extent does this assignment limit the placement of the Ga atoms and their point symmetry?
 - The measured value of x for the Ga atom is 0.08909(3). What is the Ga-Ga distance for this structure, including the e.s.d.? (Hint: Keep in mind that you want the Ga-Ga distance within the same instance of the assembly. Other Ga-Ga distances aren't so meaningful.)
 - What restrictions are placed on the thermal parameters for the Ga centers? Show all work used to determine these restrictions.
4. Without looking at the space group tables, generate the symmetry operations found in the space groups below. Provide short justifications for any elements you claim.

- Pbam
- Pbcm

5. Evaluate the following statements for accuracy, providing the corrected statement if appropriate.

a) All centrosymmetric space groups are achiral.

b) All non-centrosymmetric space groups are chiral.

c) Anomalous scattering can be used to determine the absolute configuration of a chiral molecule and its enantiomer in Pbc_a.

d) The parameter n in the expression $f_0^{anom} = f_0 + \Delta f' + i\eta\Delta f''$ is refined to a value between 0 (racemic) and 1 (enantiopure), allowing crystallographic determination of the enantiomeric excess in a chiral crystal.