

CEM 913 SPRING 2002
Course in X-ray crystallography

Homework 3, 100 points
Due by February 7th

1. Determine whether the following group-subgroup relations are *translationseigliche* or *klassengleiche* or isomorphic. If the unit cell of the subgroup is enlarged this is stated on top of the arrow

$$\begin{array}{l} Cmcn \longrightarrow Pmcn \\ P2_1/c \longrightarrow P-1 \end{array}$$

$$\begin{array}{l} 2a, b, c \\ Pbcm \longrightarrow Pbcn \end{array}$$

$$\begin{array}{l} a, 3b, c \\ C 1 2/m 1 \longrightarrow C 1 2/m 1 \end{array}$$

$$\begin{array}{l} P 6_3/mcn \longrightarrow P 6_3 22 \\ P mnn \longrightarrow P mm2 \\ Pmmn \longrightarrow P 1 2_1/m 1 \end{array}$$

2. Derive the space group $P 2_1/m$. Draw two projections. One down the a- axis and one down b-axis. Given a point on a general position x,y,z derive all other equivalent positions. What is the plane-group when this space group is project down the a-, b- and c-axes?
3. Sodium bicarbonate NaHCO_3 is monoclinic and it was originally described with lattice parameters:

$$\begin{array}{l} a=7.51 \text{ \AA} \\ b=9.70 \text{ \AA} \\ c=3.53 \text{ \AA} \\ \beta=93.3 \end{array} \quad \text{space group } P 2_1/n$$

The positional parameters were:

	x	y	z
Na	0.286	0.004	0.713
C	0.077	0.237	0.287
O1	0.071	0.367	0.261
O2	0.205	0.163	0.193
O3	0.940	0.171	0.436

$$\begin{array}{l} \text{Later workers however later chose a unit cell with} \\ a=3.53 \text{ \AA} \\ b=9.70 \text{ \AA} \\ c=8.11 \text{ \AA} \\ \beta =112.25 \end{array} \quad \text{space group } P 2_1/c$$

Show graphically that these two cells (and space groups) are equivalent. Give the transformation matrix by which the original position parameters can be obtained in the $P 2_1/c$ space group and list the new coordinates.

4. Derive the general positions for space groups $P mc2_1$. Obtain the special positions by considering the coordinates of points lying on the mirror plane.