Estimating the Pearson Symbol Code given the composition, unit cell, d/I list and hkl's

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Introduction

Notes: For an introduction to Pearson Symbols, please see **Classifying materials using prototype structures and Pearson Symbols** (reference 5). Note that the only difference between Pearson Symbol Codes (PSC) and Pearson Symbols (PS) is that in a PSC, the numeric portion reflects the actual number of atoms in the unit cell, while in a PS, the numeric portion counts the number of crystallographic sites (occupied or not) in the unit cell.

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When an experimenter has a limited amount of data on a new material and is unlikely to get a single crystal solution to the structure, estimating the PSC can provide a key to an indirect solution.

Two reference tables are used to estimate the PSC: (1) general reflection conditions for crystal systems (**reference table 2**) and

(2) atomic volumes useful for estimating unit cell contents for metallic compounds with close packing of atom for close-packed structures (**reference table 1**).

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The following discussion assumes that the experimenter

- Knows the unknown material's composition,
- Has determined the unit cell size, and
- Has a d/I list along with the correct hkl for each d.

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Discussion

A PSC has three components:

1) a lower case letter for the crystal system,
2) an upper case letter for the centering or lack thereof, and
3) a number representing the number of atoms in the unit cell.

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Discussion

In this tutorial, we discuss a simple hexagonal unknown, but the experimenter should be aware that the following steps may be used for any unknown in any crystal system.

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Discussion
continued

1. The unknown's crystal system provides the first portion of the PSC. For this example, a hexagonal cell has been observed, and the lower case letter is h.

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Discussion
continued

2. Next we examine the observed hkl's to determine what general reflection conditions, if any, are present using reference table 2. In this example, our hypothetical hkl's show that the material is primitive hexagonal (hPn) and not hexagonal rhombohedral (hRn) where - h + k + l equals 3n. Thus the second element of the PSC is P (for primitive), and the PSC is hPn where n is a number yet to be determined.

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Discussion *continued*

3. The numeric, n, may be determined by:
   - Multiplying the atom fraction for each element by the atomic volume given in reference table 1,
   - Summing the products formed, and
   - Dividing the result into the unit cell volume.

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The estimated PSC may then be used as an entry into the Powder Diffraction File and compared to entries having a similar PSC and c/a.

Worked examples of this type are in the Metals and Alloys tutorials on *Constructing and Using Pearson Symbol Codes – Example 1 – hP7*, *Example 2 – hP20 to hP22*, and *Example 3 – mC16 to mC20*.

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