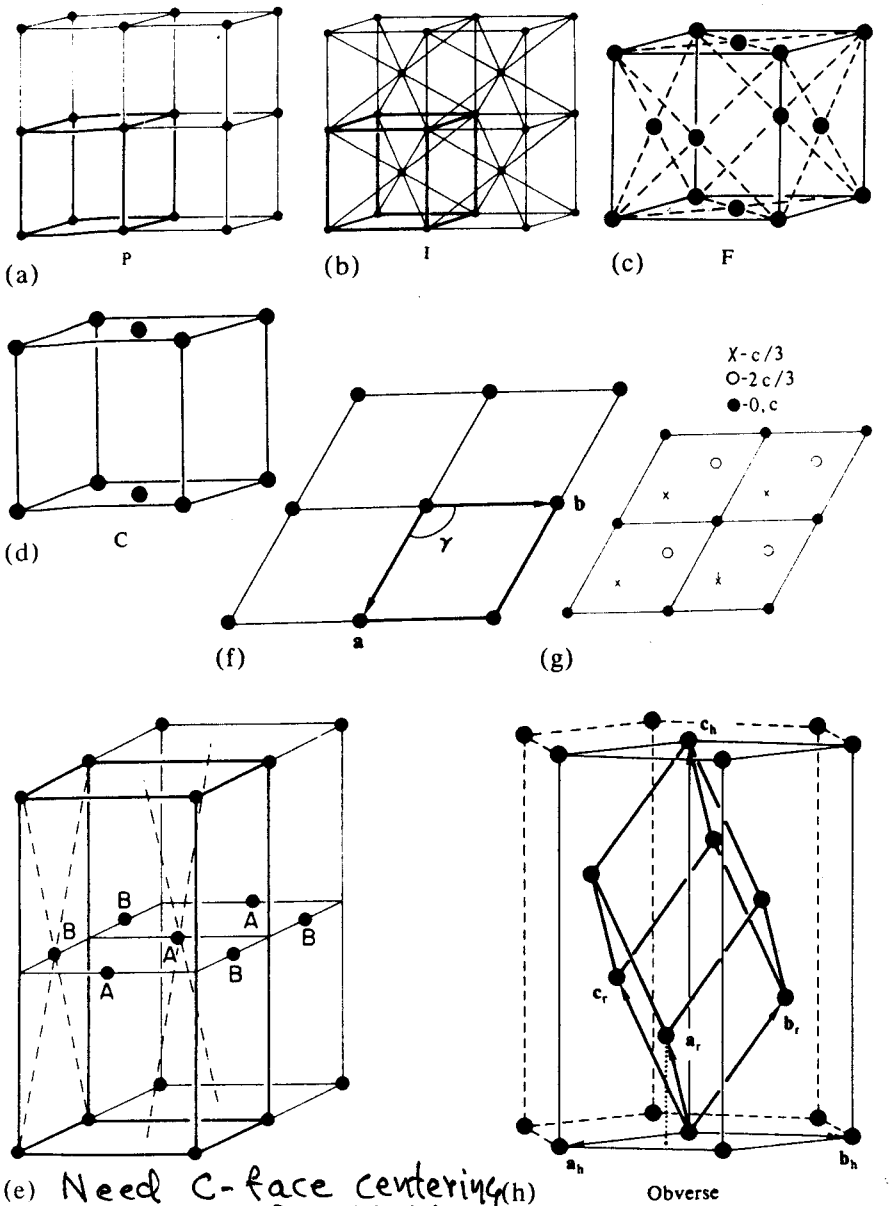
February 1, 2007

Lecture #06

Centering of a Crystal Lattice



Need C-face centering As well To Be Viable

Fig. 2-5 Types of centering of lattices. (a) Four-unit cells (not necessarily cubic). (b) Body centering, showing all four unit cells. (c) All-face centering, showing only one unit cell for clarity. (d) One-face centering, showing one unit cell. (e) An impossible way to center a lattice. (f) A projection of four trigonal unit cells. (g) Rhombohedral centering of these cells. (h) A rhombohedral unit cell in a rhombohedral lattice. The corresponding hexagonal cell, which is three times larger, is also shown.

(5b)

REFERENCE: BURNS

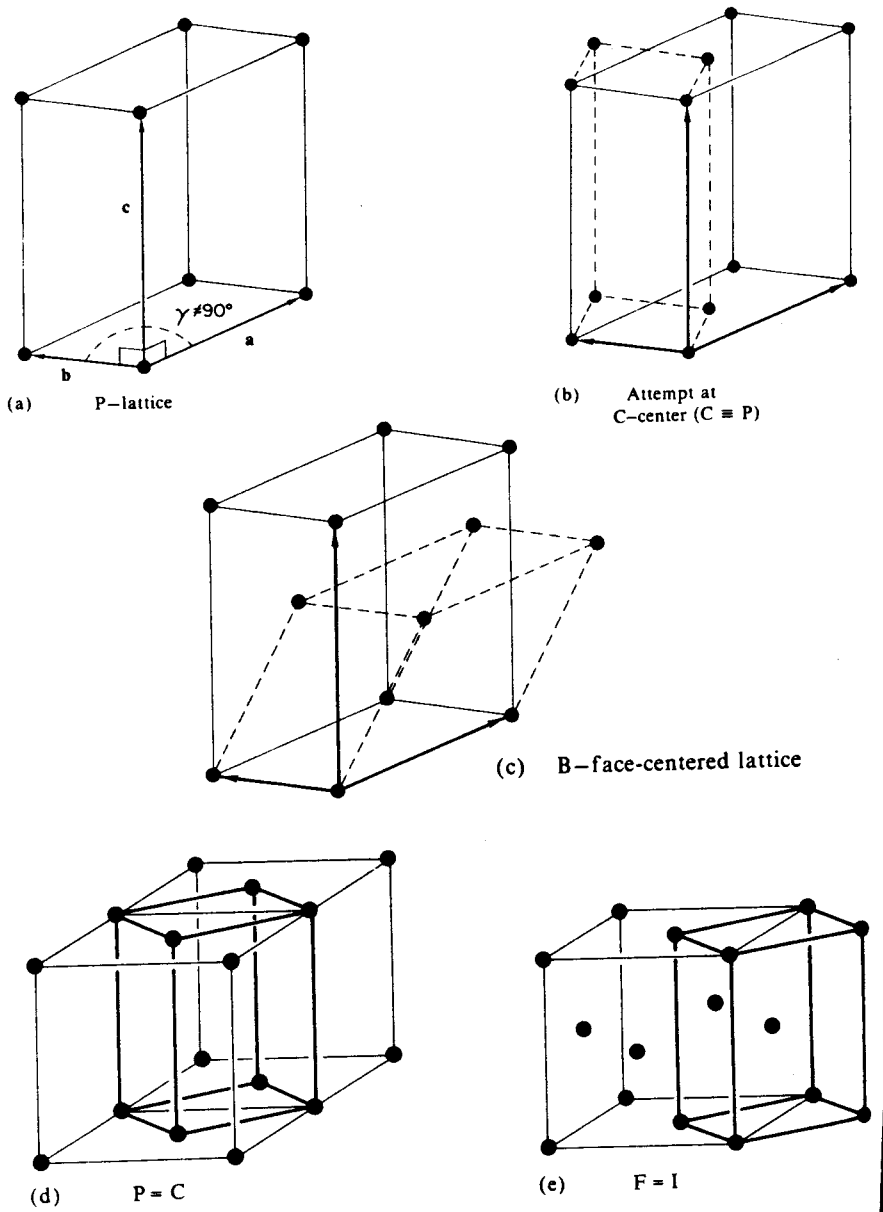
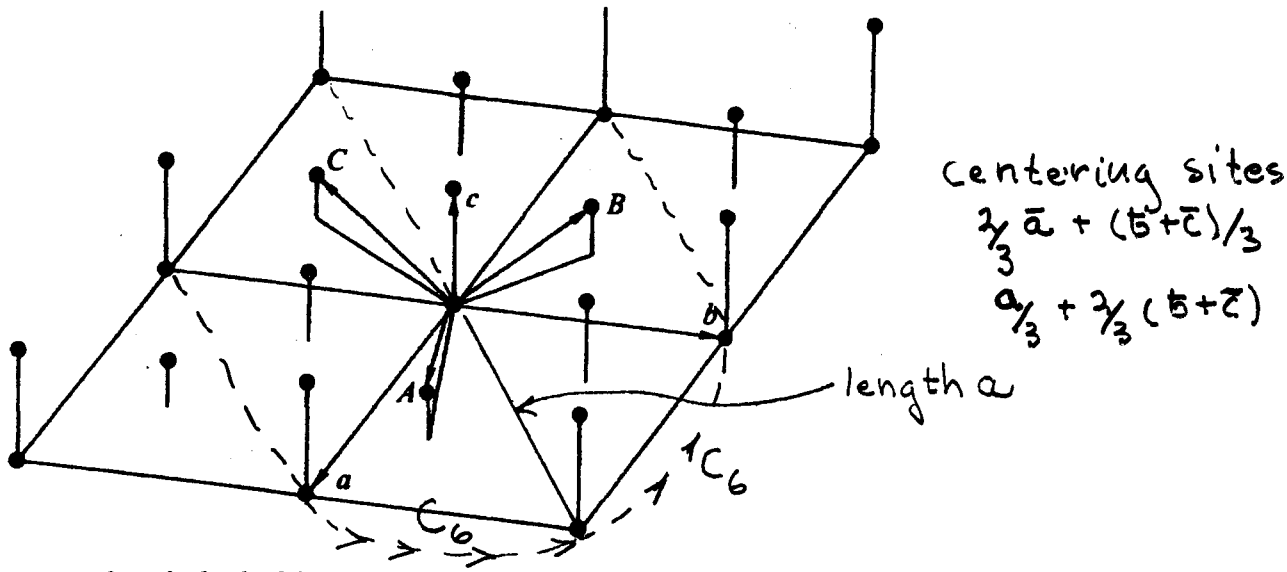


Fig. 2-6 (a) through (c) Several aspects of centering a monoclinic lattice. (d) and (e) Several aspects of centering a tetragonal lattice.

Rhobohedral Centering



centering sites
$\frac{2}{3}\bar{a} + (\bar{b}+\bar{c})/3$
$a/3 + \frac{2}{3}(\bar{b}+\bar{c})$

FIG. 3-7 *Rhombohedral lattice. The triply primitive hexagonal cell has axes a, b, c and lattice points added at $0,0,0$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$. Vectors from $0,0,0$ to $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$; and $-\frac{1}{3},-\frac{2}{3},\frac{1}{3}$ define the primitive rhombohedral cell.* Note that this destroys the 6_6 symmetry of the hexhagonal cell. However if it is considered to be trigonal the symmetry (which is C_3) is retained

~~In these cases,~~ It is possible to choose a primitive cell satisfying $a = b = c$, (i.e A, B, C) $\alpha = \beta = \gamma$. This lattice is called rhombohedral (symbol R). There are three equal axes inclined at equal angles with each other (Fig. 3-7). The trigonal threefold (or $\bar{3}$) axis in this case is along the body diagonal of the Lattice

Note that $\bar{3} = C_6^5$.

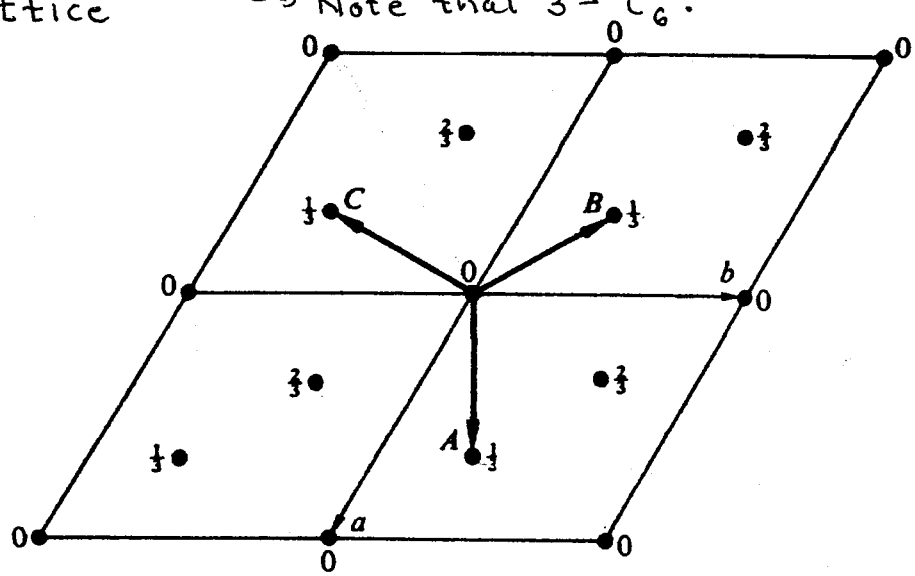


FIG. 3-8 *Rhombohedral lattice projected parallel to the threefold axis. Numbers next to points indicate z coordinates referred to hexagonal axes.*