

LATTICE

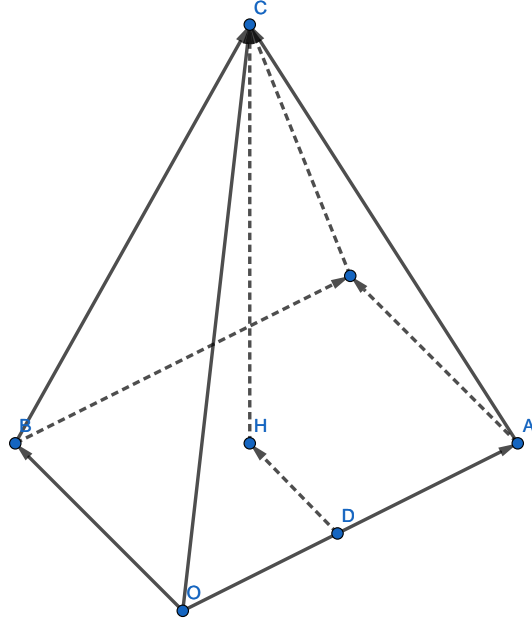


Figure 1: Periodic Boundary Box

$$\begin{cases} |OA| = a, |OB| = b, |OC| = c \\ \angle bc = \alpha, \angle ca = \beta, \angle ab = \gamma \\ OA = a i + 0 j + 0 k \\ OB = b \cos \gamma i + b \sin \gamma j + 0 k \\ OC = OD i + DH j + HC k \end{cases}$$

Monoclinic: $\alpha = \gamma = \pi/2$.

Orthogonal: $\alpha = \beta = \gamma = \pi/2$.

With $OA \cdot OC = ca \cos \beta$,

$$OD = c \cos \beta.$$

With $OB \cdot OC = bc \cos \alpha$,

$$DH = \frac{c}{\sin \gamma} (\cos \alpha - \cos \beta \cos \gamma).$$

With $HC^2 = OC^2 - OD^2 - DH^2$,

$$HC = \frac{c}{\sin \gamma} \sqrt{\sin^2 \gamma - \cos^2 \alpha - \cos^2 \beta + 2 \cos \alpha \cos \beta \cos \gamma}.$$

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Apr. 5, 2020.