Physics 745 - Group Theory

Homework Set 12 Due Monday, February 16

1. Diamond is a version of carbon. The position of the carbon atoms takes the form

$$\mathbf{r} = d\left(n_1 + x\right)\hat{\mathbf{x}} + d\left(n_2 + y\right)\hat{\mathbf{y}} + d\left(n_3 + z\right)\hat{\mathbf{z}}$$

where d = 356.683 pm, $\left(n_1, n_2, n_3\right)$ are arbitrary integers, and $\left(x, y, z\right)$ takes on the following eight values:

$$\left(x,y,z\right) \in \left\{\left(0,0,0\right), \left(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}\right), \left(0,\tfrac{1}{2},\tfrac{1}{2}\right), \left(\tfrac{1}{2},\tfrac{1}{2},0\right), \left(\tfrac{1}{2},0,\tfrac{1}{2}\right), \left(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}\right), \left(\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}\right), \left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}\right)\right\}$$

Thus there are eight carbon atoms per cell of size d^3.

(a) For what values of $\left(x, y, z\right)$ will $\mathbf{T} = dx\hat{\mathbf{x}} + dy\hat{\mathbf{y}} + dz\hat{\mathbf{z}}$ be a translation vector; *i.e.*, if there is a carbon atom at **r**, there will always be a carbon atom at $\mathbf{r} + \mathbf{T}$? To make your answer finite, only include values with $0 \le x, y, z < 1$.

(b) Find primitive vectors **a**, **b** and **c** such that *all* translation vectors take the form $\mathbf{T} = m_1\mathbf{a} + m_2\mathbf{b} + m_3\mathbf{c}$, where $\left(m_1, m_2, m_3\right)$ are integers. Demonstrate it explicitly for those vectors you found in part (a) (which will probably be trivial), and also for the three vectors $d\hat{\mathbf{x}}$, $d\hat{\mathbf{y}}$ and $d\hat{\mathbf{z}}$.

(c) What are the lengths of these vectors a, b, c and the angles between them, α, β, γ?