The lattice basis *LB* and the reciprocal lattice basis *RLB* given were:

$$LB = \left\{ a\begin{bmatrix} \sqrt{3}/2 \\ -1/2 \\ 0 \end{bmatrix}, a\begin{bmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{bmatrix}, c\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

$$RLB = \left\{ \frac{2\pi}{a}\begin{bmatrix} 1/\sqrt{3} \\ -1 \\ 0 \end{bmatrix}, \frac{2\pi}{a}\begin{bmatrix} 1/\sqrt{3} \\ 1 \\ 0 \end{bmatrix}, \frac{2\pi}{c}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

where $a = 2.46\ \text{Å}$ and $c = 6.71\ \text{Å}$.

The change of basis matrices to transform the relative coordinates to standard coordinates in $\mathbb{R}^3$ are as follows:

$$\underset{\mathbb{R}^3 \leftarrow LB}{P} = \begin{bmatrix} a\sqrt{3}/2 & a\sqrt{3}/2 & 0 \\ -a/2 & a/2 & 0 \\ 0 & 0 & c \end{bmatrix}$$

$$\underset{\mathbb{R}^3 \leftarrow RLB}{P} = \begin{bmatrix} 2\pi/a\sqrt{3} & 2\pi/a\sqrt{3} & 0 \\ -2\pi/a & 2\pi/a & 0 \\ 0 & 0 & 2\pi/c \end{bmatrix}$$

To find the $\mathbb{R}^3$ coordinates $[\boldsymbol{v}]_{\mathbb{R}^3}$ of the chosen vector (which exists in RLB coordinates), we must multiply by $\underset{\mathbb{R}^3 \leftarrow RLB}{P}$. I have chosen

$$[\boldsymbol{v}]_{RLB} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}.$$

$$[\boldsymbol{v}]_{\mathbb{R}^3} = \underset{\mathbb{R}^3 \leftarrow RLB}{P} [\boldsymbol{v}]_{RLB} = \begin{bmatrix} 2\pi/a\sqrt{3} & 2\pi/a\sqrt{3} & 0 \\ -2\pi/a & 2\pi/a & 0 \\ 0 & 0 & 2\pi/\end{bmatrix}$$

and we solve to obtain:

$$\boxed{[\boldsymbol{v}]_{\mathbb{R}^3} = \begin{bmatrix} 6\pi/a\sqrt{3} \\ 2\pi/a \\ 6\pi/c \end{bmatrix}}$$

We have found the $\mathbb{R}^3$-coordinates of **v**. We will use these $\mathbb{R}^3$-coordinates to find **v** in LB-coordinates. To convert $\mathbb{R}^3$-coordinates into LB-coordinates, we will use $\underset{LB \leftarrow \mathbb{R}^3}{P}$, which is simply the inverse of $\underset{\mathbb{R}^3 \leftarrow LB}{P}$. We will use the [A I] method to find the inverse:

$$\left[\begin{array}{ccc|ccc} \frac{a\sqrt{3}}{2} & \frac{a\sqrt{3}}{2} & 0 & 1 & 0 & 0 \\ -\frac{a}{2} & \frac{a}{2} & 0 & 0 & 1 & 0 \\ 0 & 0 & c & 0 & 0 & 1 \end{array}\right]$$

$$\begin{bmatrix} 1 & 1 & 0 & \frac{2}{a\sqrt{3}} & 0 & 0 \\ -1 & 1 & 0 & 0 & \frac{2}{a} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{c} \end{bmatrix} \qquad \textit{Scale rows} \ldots \textit{on th} \ldots$$

$$\begin{bmatrix} 1 & 1 & 0 & \frac{2}{a\sqrt{3}} & 0 & 0 \\ 0 & 2 & 0 & \frac{2}{a\sqrt{3}} & \frac{2}{a} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{c} \end{bmatrix} \qquad \textit{row}\, 2 =$$

$$\begin{bmatrix} 1 & 1 & 0 & \frac{2}{a\sqrt{3}} & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{a\sqrt{3}} & \frac{1}{a} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{c} \end{bmatrix} \qquad \text{Scale}$$

$$\begin{bmatrix} 1 & 0 & 0 & \frac{1}{a\sqrt{3}} & -\frac{1}{a} & 0 \\ 0 & 1 & 0 & \frac{1}{a\sqrt{3}} & \frac{1}{a} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{c} \end{bmatrix} \qquad row\,1 =$$

and we end up with:

$$\underset{LB\leftarrow\mathbb{R}^3}{P} = \underset{\mathbb{R}^3\leftarrow LB}{P}^{-1} = \begin{bmatrix} \frac{1}{a\sqrt{3}} & -\frac{1}{a} & 0 \\ \frac{1}{a\sqrt{3}} & \frac{1}{a} & 0 \\ 0 & 0 & \frac{1}{c} \end{bmatrix}$$

Now, to solve for $[\boldsymbol{v}]_{LB}$, we can multiply $[\boldsymbol{v}]_{\mathbb{R}^3}$ by this matrix.

$$[\boldsymbol{v}]_{LB} = \underset{LB\leftarrow\mathbb{R}^3}{P}[\boldsymbol{v}]_{\mathbb{R}^3} = \underset{\mathbb{R}^3\leftarrow LB}{P}^{-1}[\boldsymbol{v}]_{\mathbb{R}^3}$$

$$= \begin{bmatrix} \frac{1}{a\sqrt{3}} & -\frac{1}{a} & 0 \\ \frac{1}{a\sqrt{3}} & \frac{1}{a} & 0 \\ 0 & 0 & \frac{1}{c} \end{bmatrix} \begin{bmatrix} \frac{6\pi}{a\sqrt{3}} \\ \frac{2\pi}{a} \\ \frac{6\pi}{c} \end{bmatrix}$$

which we solve to obtain

$$\boxed{[\boldsymbol{v}]_{LB} = \begin{bmatrix} 0 \\ \frac{4\pi}{a^2} \\ \frac{6\pi}{c^2} \end{bmatrix}}.$$

The relative coordinate vectors are checked by multiplying by $\underset{\mathbb{R}^3 \leftarrow RLB}{P}^{-1}$ and $\underset{\mathbb{R}^3 \leftarrow LB}{P}$ for $[\boldsymbol{v}]_{\mathbb{R}^3}$ and $[\boldsymbol{v}]_{LB}$ respectively, which demonstrates them to be correct.

The question also asks which coordinates are most natural for the point. Each set of coordinates has benefits. Because the point was chosen with integer coordinates point using RLB-coordinates, these coordinates appear most natural; they're the only set of coordinates which are integers. The $\mathbb{R}^3$-coordinates are also a good choice because many applications use the standard $\mathbb{R}^3$ basis vectors, so it is useful to convert to them. The LB-coordinates represent the coordinates relative to lattice structure on the crystal, so they may be useful to analyze properties of the crystal relative to itself.