Electronic Supplementary Material (ESI) for RSC Advances.

# Supplementary Information for "Infrared and Raman spectra of $Bi_2O_2X$ and $Bi_2OX_2$ (X=S, Se, and Te) studied from first principles calculations"

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TABLE S1: The right angle scattering polarized configurations for the Raman active modes of orthorhombic $Bi_2O_2S$.

| Configuration | $A_g$ | $B_{1g}$ | $B_{2g}$ | $B_{3g}$ |
|---|---|---|---|---|
| X(YY)Z | $\surd$ | | | |
| X(ZZ)Y | $\surd$ | | | |
| Y(XX)Z | $\surd$ | | | |
| Y(ZZ)X | $\surd$ | | | |
| Z(XX)Y | $\surd$ | | | |
| Z(YY)X | $\surd$ | | | |
| Y(XY)X | | $\surd$ | | |
| Y(XY)Z | | $\surd$ | | |
| Z(XY)X | | $\surd$ | | |
| Z(XZ)X | | | $\surd$ | |
| Z(XZ)Y | | | $\surd$ | |
| Y(XZ)X | | | $\surd$ | |
| X(YZ)Y | | | | $\surd$ |
| Z(YZ)X | | | | $\surd$ |
| Z(YZ)Y | | | | $\surd$ |

TABLE S2: The back scattering polarized configurations for the Raman active modes of orthorhombic $Bi_2O_2S$.

| Configuration | $A_g$ | $B_{1g}$ | $B_{2g}$ | $B_{3g}$ |
|---|---|---|---|---|
| -X(YY)X | $\surd$ | | | |
| -X(ZZ)X | $\surd$ | | | |
| -Y(XX)Y | $\surd$ | | | |
| -Y(ZZ)Y | $\surd$ | | | |
| -Z(XX)Z | $\surd$ | | | |
| -Z(YY)Z | $\surd$ | | | |
| -Z(XY)Z | | $\surd$ | | |
| -Y(XZ)Y | | | $\surd$ | |
| -X(YZ)X | | | | $\surd$ |

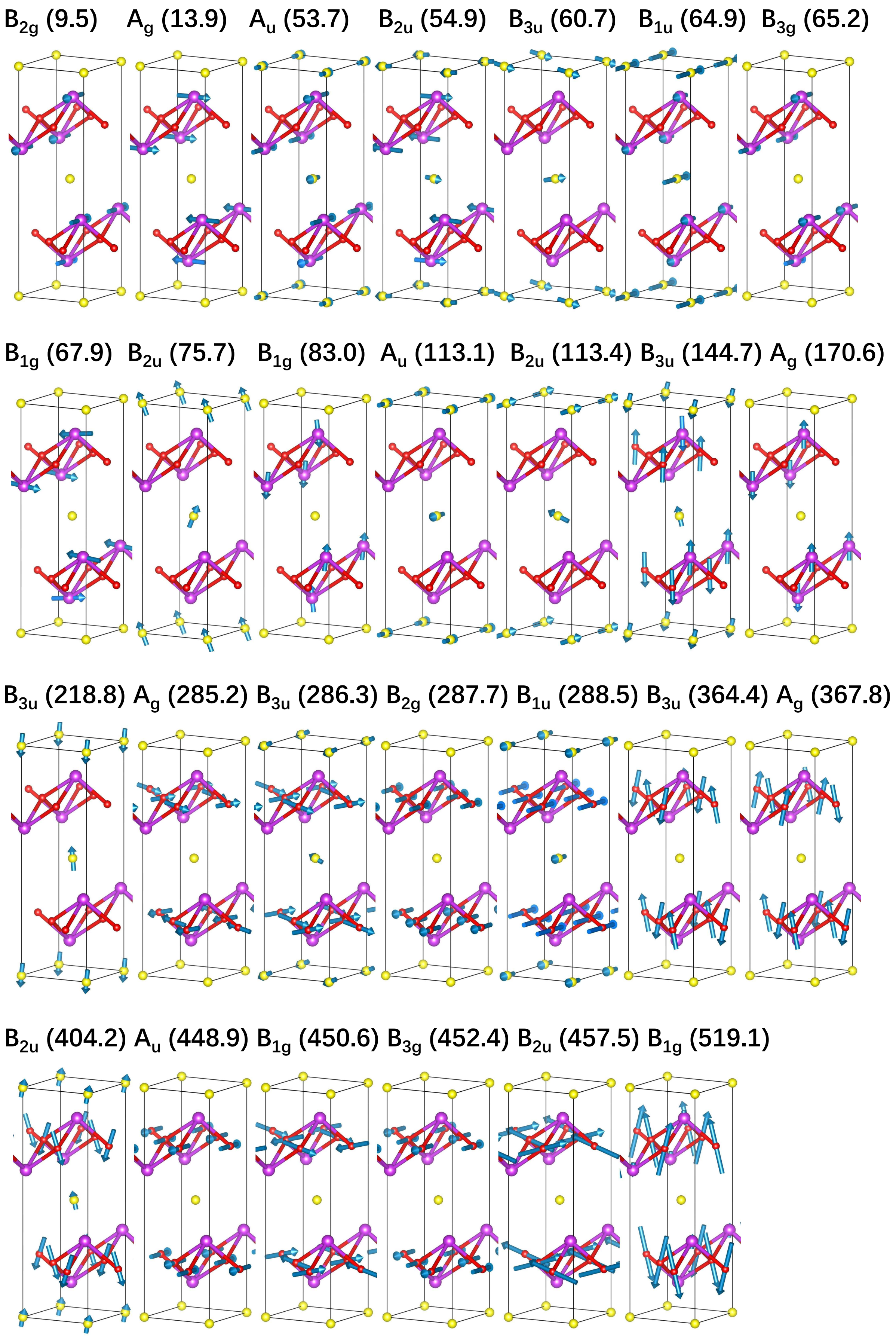

FIG. S1: Vibrational eigenvectors and Mulliken symbols of the zone-centered optical phonon modes shown in an orthorhombic $Bi_2O_2S$ (Pnnm). The purple, red, and yellow balls represent Bi, O, and S atoms respectively.

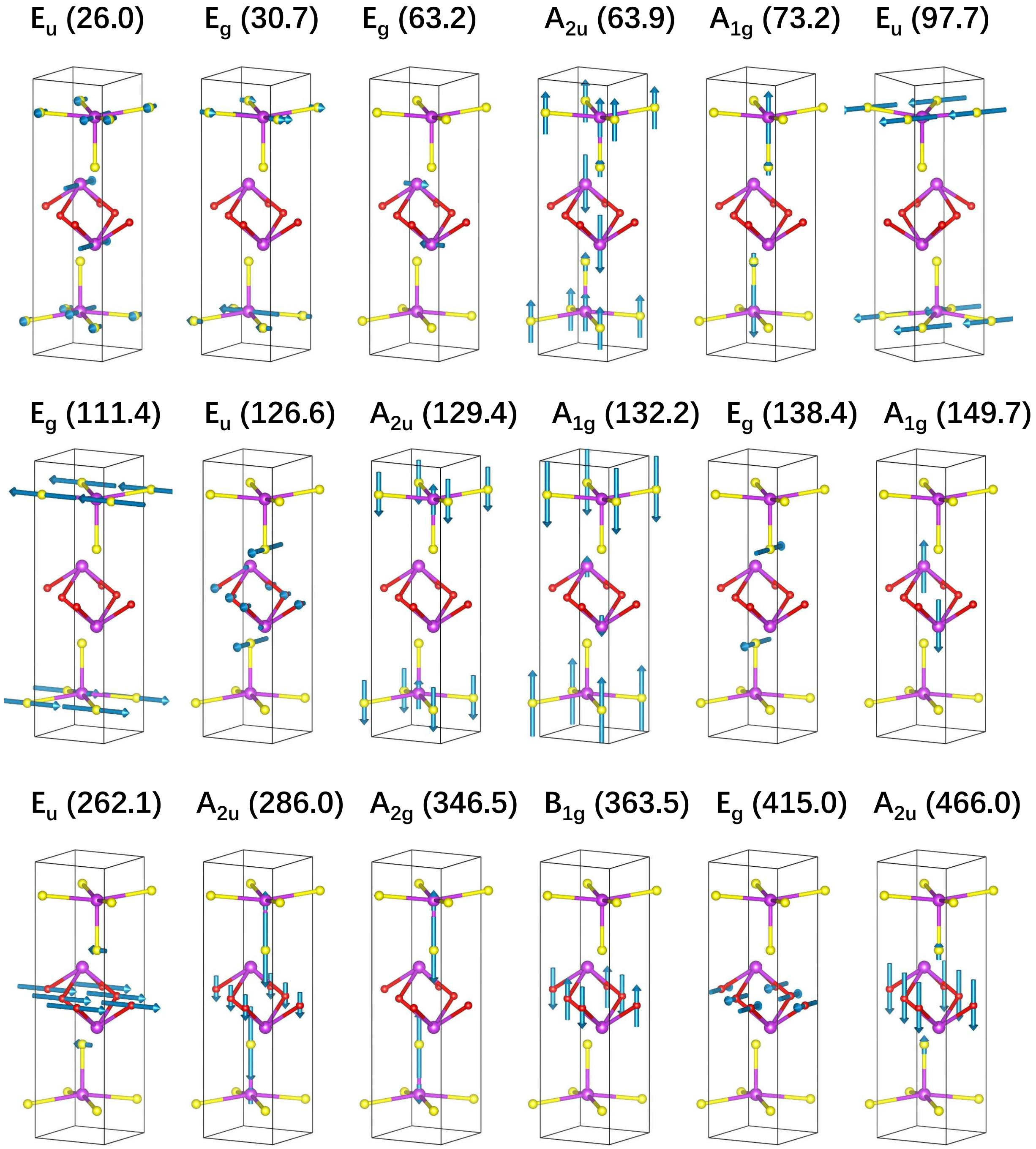

FIG. S2: Vibrational eigenvectors and Mulliken symbols of the zone-centered optical phonon modes shown in a tetragonal $Bi_2OS_2$ (P4/nmm). The purple, red, and yellow balls represent Bi, O, and S atoms respectively.