agonal components of Mn as the Mn-O bonding is almost uniform over a wide range of energy whereas a significant Co-O hybridization about 0.5 below the Fermi energy increases the diagonal component of Co BEC's. The BEC's of O are almost identical in both structures. Among all the species, Bi has the largest BEC, demonstrating a strong Bi-O covalancy. From all these observations we can conclude a significant magnetism dependent electrostructural coupling in the system very similar to what has been observed by Das et. al[16] for La_2NiMnO_6. However unlike the study in Ref. 16, we did not observe an anomalously large off-diagonal BEC for either of the magnetic specie.

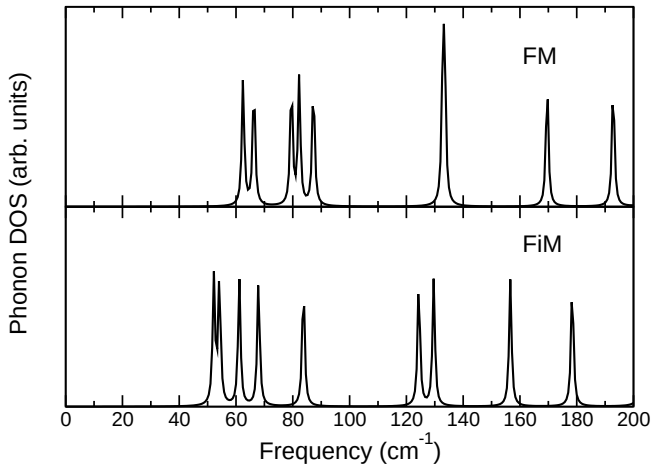

FIG. 3: Phonon DOS of IR-active modes for FM and FiM configurations.

Finally, we analyze the zone center phonon modes for FM and FiM structures. The eight lowest infra-red (IR) active modes are shown in Fig. 3. One can observe that the typical softening of IR-active modes could be as large as 10 cm^{-1}. The frequencies at 62, 66, 79, 82, 87, 133,133 and 169 cm^{-1} in the FM phase are shifted to 52, 54, 61, 67, 83, 124, 129 and 156 cm^{-1} in the FiM phase. The least shifted mode is at 133 cm^{-1} where the softening is associated with the further lifting of degeneracy of this mode. Subsequently there is an increase in the static dielectric constant in FiM phase. To understand the spin-phonon coupling better, we analyzed the softest mode (at 52 cm^{-1}) in the FiM state more carefully. By adding the atomic displacement due to this mode to the equilibrium atomic positions we find that the atomic displacements are such that the increase in Mn-O-Co angle with respect to FM state is very small. We find an average increase of about 2° of Mn-O-Co angle. This fact may contribute to the observation that the spin-phonon coupling though present, is small. Moreover, the contribution of Mn to the change in mode effective charges of the IR-active modes of two magnetic states as well as to dielectric constant is smaller compared to Co.

In summary, our GGA+U calculations reveal that Co and Mn are in high and intermediate spin states respectively in the double perovskite Bi_2CoMnO_6 with a calculated band gap of 0.3 eV. The computed dynamical charge matrices are highly anisotropic due to the low symmetry structure. Magnetic structure dependent phonon frequencies indicate a spin-phonon coupling in this compound. Our theoretically estimated spontaneous polarization of 5.88 $\mu C/cm^2$ is close to the experimental value observed for the thin film of a similar compound, Bi_2NiMnO_6.

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