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Raman scattering of filled and unfilled skutterudite compounds

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Raman scattering spectra of the filled skutterudite RT_4X_{12} (R=La, Ce, Pr and Nd, T=Fe, Os, X=P, Sb) and the unfilled CoP₃ have been measured. In the skutterudite family with cubic symmetry of $Im\bar{3}$ (T_h^5), Raman active mode is 2Ag + 2Eg + 4Tg. All Raman active modes are the vibrations of pnictogens; P or Sb.

Figure 1 shows the representative phonon Raman spectra of $CeFe_4P_{12}$ and CoP_3 . We can directly compare both spectra, because the lattice parameter and inter-atomic distances between $CeFe_4P_{12}$ and CoP_3 are close. In spite of the imperfect polarization dependence for CoP_3 , the phonon assignment has been obtained as shown in Fig. 1. The clear energy-increase are observed in CoP_3 for the Ag and Eg phonons, which correspond to the breathing and deforming vibration of P at the icosahedra. Since the higher energy peaks are stretching vibration between rare-earth and pnictogen, the *R-P* interaction in the filled skutterudite decreases the phonon energy. This result clearly shows the importance of the *R-P* interaction in the filled skutterudites.

In order to understand the microscopic difference, the normal mode analysis is performed and the detailed atomic interactions will be presented in our poster presentation.

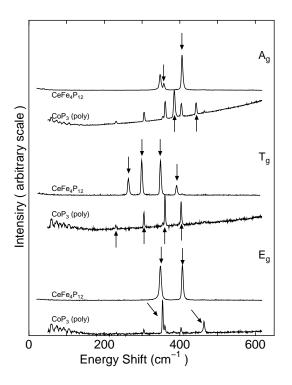


Figure 1: Raman spectra of $CeFe_4P_{12}(single)$ and $CoP_3(poly)$ measured at room temperature.