

## Figure 2

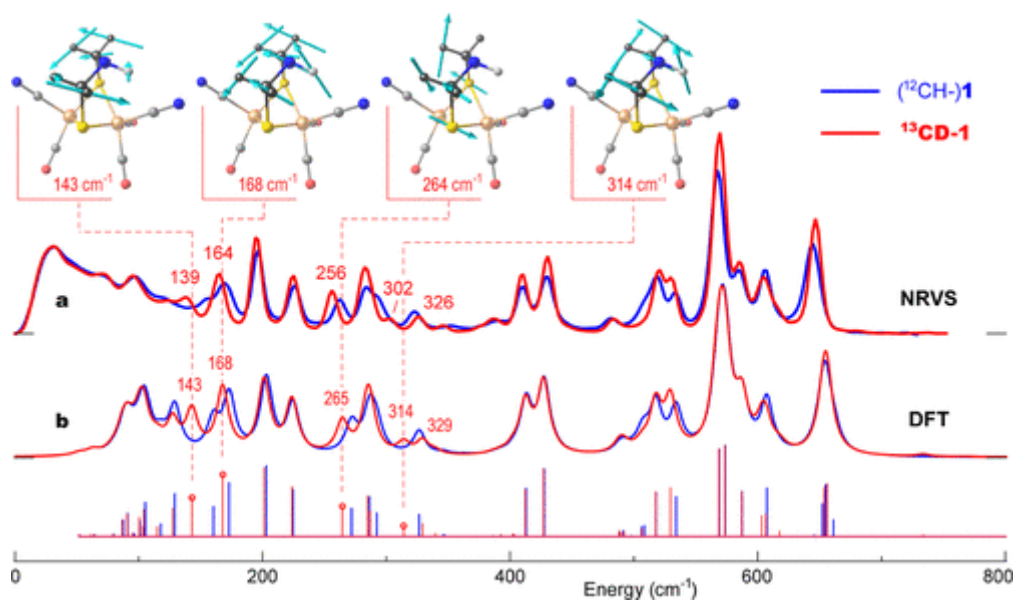


Figure 2.  $^{57}\text{Fe}$ -PVDOS for the  $[2\text{Fe}]_n$  precursor isotopologues **1** (blue) vs  $^{13}\text{CD-1}$  (red) from (a) NRVS experiments and (b) DFT calculations. Sticks correspond to individual DFT normal mode energies and intensities before lineshape convolution. For  $^{13}\text{CD-1}$ , important band positions are labeled, and atomic motions in selected normal modes are shown.