

Figure 3

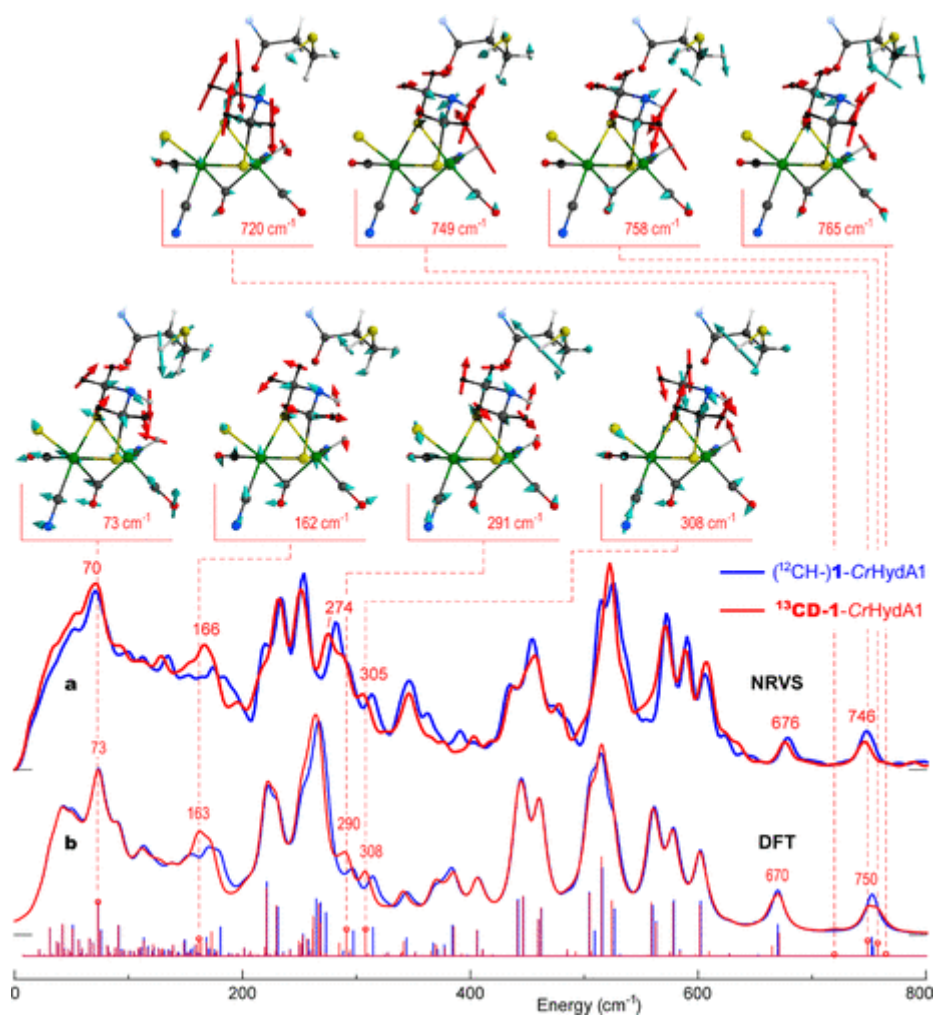


Figure 3. ^{57}Fe -PVDOS for the H_{hyd} state isotopologues **1-CrHydA1** (blue) vs $^{13}\text{CD-1-CrHydA1}$ (red) from (a) an NRVS experiment and (b) DFT calculations. Sticks correspond to individual DFT normal mode energies and intensities before broadening. For $^{13}\text{CD-1-CrHydA1}$, important band positions are labeled, and atomic motions in selected normal modes are shown. Only the $[\text{2Fe}]_{\text{H}}$ and C169 fragments of the DFT model are shown with the methylene, H_{h} , and H_{ADT} hydrogen nuclei displacements indicated by red arrows.