## Figure 1

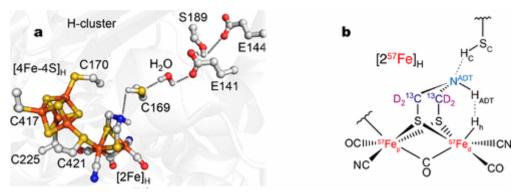


Figure 1. (a) [FeFe] hydrogenase active site including key amino acids in the proton transfer pathway (based on the PDB <u>4XDC(10)</u> structure of the *Cp*I enzyme from *Clostridium pasteurianum*, but using *Cr*HydA1 sequence numbering). (b) Schematic structure of the [2Fe]<sub>H</sub> subcluster in the H<sub>hyd</sub> state, showing the isotopically labeled nuclei <sup>57</sup>Fe, <sup>13</sup>C, and D (i.e. <sup>2</sup>H). The important hydrogens, H<sub>h</sub> (catalytic hydride at the distal Fe<sub>d</sub> iron), H<sub>ADT</sub> (at the ADT N<sub>ADT</sub> nitrogen), and H<sub>c</sub> (at the S<sub>c</sub> C169 sulfur), are shown.