Figure 1

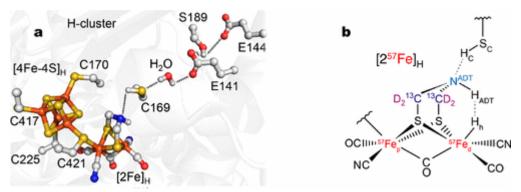


Figure 1. (a) [FeFe] hydrogenase active site including key amino acids in the proton transfer pathway (based on the PDB <u>4XDC(10)</u> structure of the *Cp*I enzyme from *Clostridium pasteurianum*, but using *Cr*HydA1 sequence numbering). (b) Schematic structure of the [2Fe]_H subcluster in the H_{hyd}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