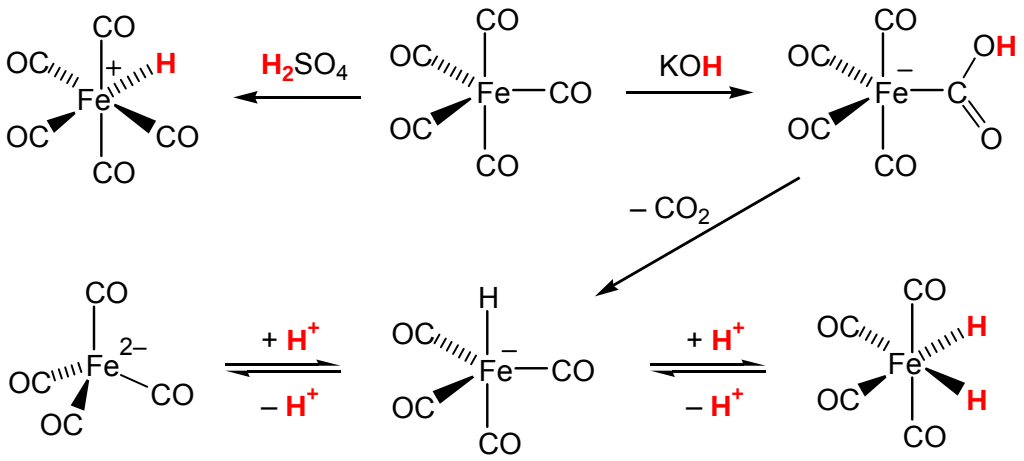
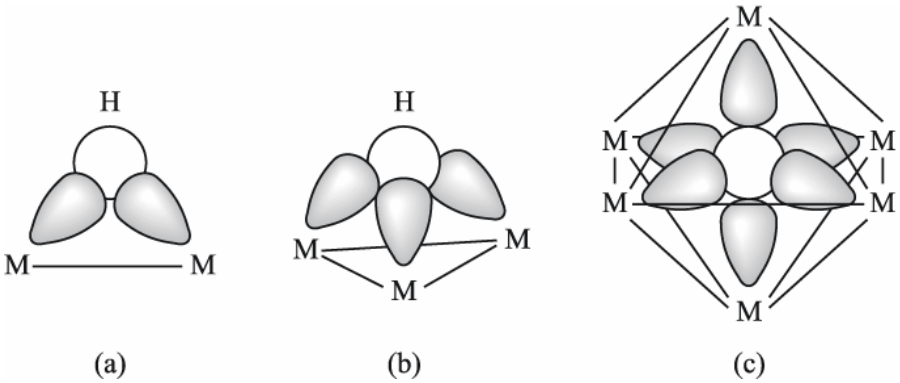
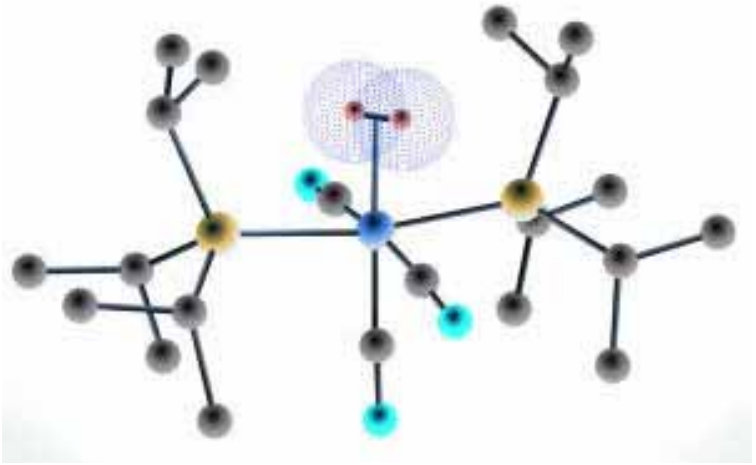


Synthesis of iron carbonyl hydride complexes



Overlap of the H 1*s* orbital with (a) two or (b) three appropriate metal hybrid orbitals to form μ-H and μ_3-H bridges. Interstitial hydride ligands (c) are also possible, forming a 7c-2e bond.



The first **dihydrogen** complex: Kubas' $W(CO)_3(P^iPr_3)_2(\eta\text{-}H_2)$

d_{HH} = 84 pm (in free H_2, 74 pm); d_{WH} = 175 pm; ν(HH) = 2690 cm^{-1}

δ_{HH} = -4.21 (24 Hz wide), δ_{HD} = -4.21 (8 Hz wide, 1:1:1 triplet, J_{HD} = 33 Hz) cf. J_{HD} = 43 Hz for HD gas

^{31}P NMR shows singlet (with W satellites) - J_{HD} is small