

Around central atom bond geometry symmetrisation, which forms the symmetry of the crystal .

X-ray crystallography is used to determine the structure of large biomolecules .
Crystal face is plotted on a stereographic net such as a Wulff net or Lambert net.
Point of atom in structure is labeled with its Miller index.

X-ray crystallography of proteins, DNA, RNA, carbohydrates, lipids

Symmetrisation geometry

Geometric symmetry	Formula	Structure	Geometry
linear stick 180°	C ₂ H ₂	H-C≡C-H	
trigonal planar 120°	CaCO ₃ ²⁻	 crystal	
bent angle 109.47°	ice H ₂ O	 109.47°	
0° C ρ=0.9167 g/mL; density -100° C ρ=0.9257 g/mL; density	water H ₂ O	 105°	
0° C ρ=0.9998425 g/mL; density +3.89° C ρ=0.9999999 g/mL; density +25° C ρ=0.9970479 g/mL; density			
trigonal pyramidal	:NH ₃		
tetrahedral, tetragonal	CH ₄		
octahedral, hexagonal bipyramidal	[Al(OH) ₆] ³⁻		

Geometric symmetry of central atom in coordinative compounds

$\text{K}_4[\text{Fe}(\text{CN})_6]$
Potassium hexa ciano ferrate(II)

Octahedral or Hexagonal object figure geometry :
 Bipyramidal

Donor-acceptor covalent bond
 Atoms of unshared electron pair : owners are donors : \rightarrow \square acceptor central atom

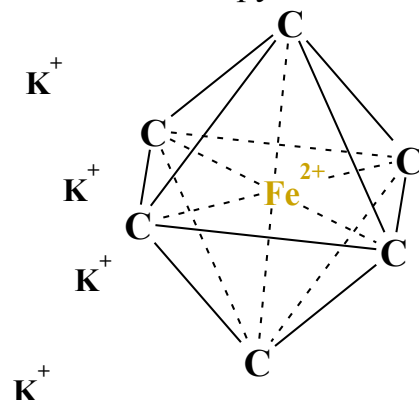
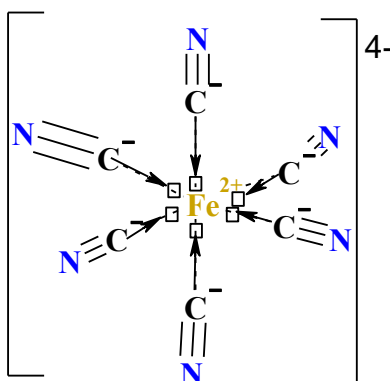
has 6 empty orbitals as acceptors \square of pair :

acceptor $\square\square\square\text{Fe}^{2+}\square\square\square$

acceptor and

donor $\text{N}\equiv\text{C}^- : \rightarrow \square\text{Fe}^{2+}\square \leftarrow : \text{C}\equiv\text{N}$

donor ;



$[\text{Cu}(\text{NH}_3)_4](\text{OH})_2$
tetra amino cooper(II) hydroxide

Tetrahedral or Tetragonal object figure geometry :

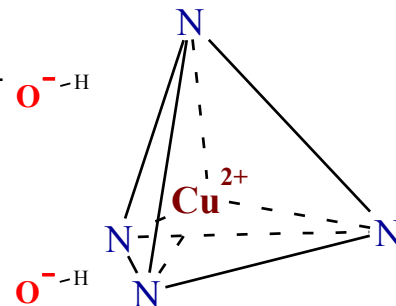
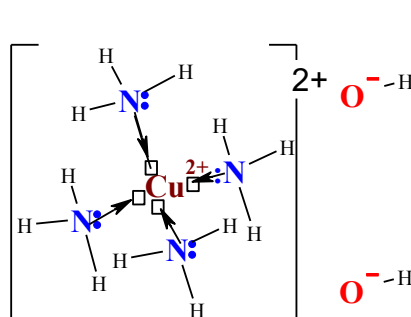
Donor-acceptor covalent bond

Atoms of unshared electron pair : owners are donors : \rightarrow \square acceptor central atom

has 4 empty orbitals as acceptors \square of pair :

acceptor $\square\square\text{Cu}^{2+}\square\square$ acceptor and

donor $\text{H}_3\text{N} : \rightarrow \square\text{Cu}^{2+}\square \leftarrow : \text{NH}_3$ donor ;



$[\text{Ag}(\text{NH}_3)_2]\text{Cl}$

Linear or Stick geometry :

di amino silver(I) chloride

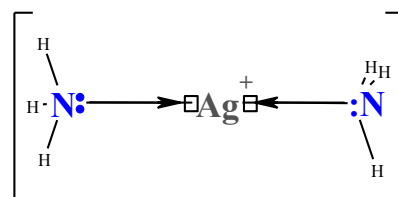
Donor-acceptor covalent bond

Atoms $\text{N} :$ of unshared electron pair : owners are donors $\text{N} : \rightarrow \square$ acceptor central atom $\square\text{Ag}^+\square$

has 2 empty orbitals as acceptors \square of pair :

acceptor $\square\text{Ag}^+\square$ acceptor and

donor $\text{H}_3\text{N} : \rightarrow \square\text{Ag}^+\square \leftarrow : \text{NH}_3$ donor ;



Cl^-

Linear or Stick geometry

$\text{N} : \text{---} \text{Ag}^+ \text{---} : \text{N}$

Main electron pair donor atoms are $\text{N} :$ and $: \text{O} :$ two unshared electron pairs owner oxygen

Geometric symmetry of metal ions Mg^{2+} , Ca^{2+} , Na^+ , K^+ , , , , , in human



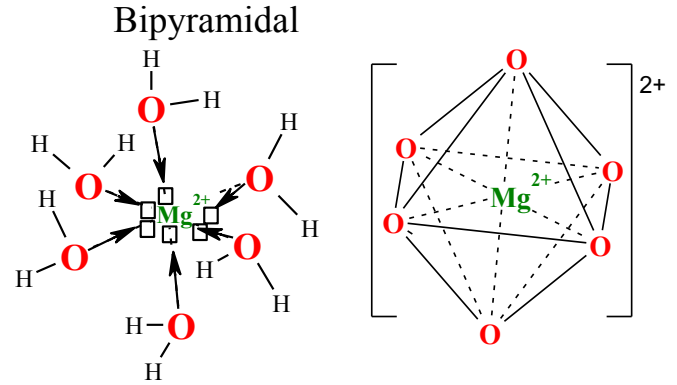
Octahedral or Hexagonal object figure geometry :

hexa aqua magnesium(II) cation

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners are donors **O:** → □ acceptor central atom Mg^{2+} has 6 empty orbitals as acceptors □ of pair :

acceptor □□□ Mg^{2+} □□□ acceptor and donor $H_2O:$ → □ Mg^{2+} □ ← **:OH₂** donor ;



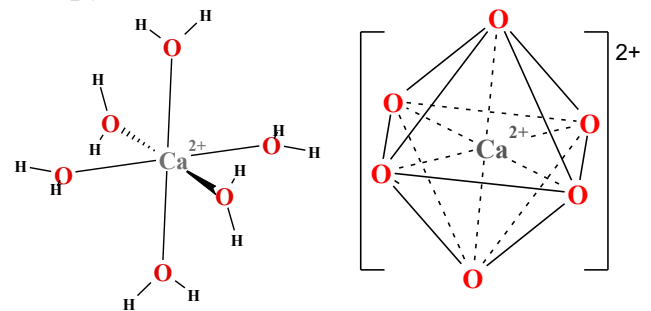
hexa aqua calcium(II) cation

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners are donors **O:** → □ acceptor central atom Ca^{2+} has 6 empty orbitals as acceptors □ of pair :

acceptor □□□ Ca^{2+} □□□ acceptor and donor $H_2O:$ → □ Ca^{2+} □ ← **:OH₂** donor ;

Octahedral or Hexagonal object figure geometry :



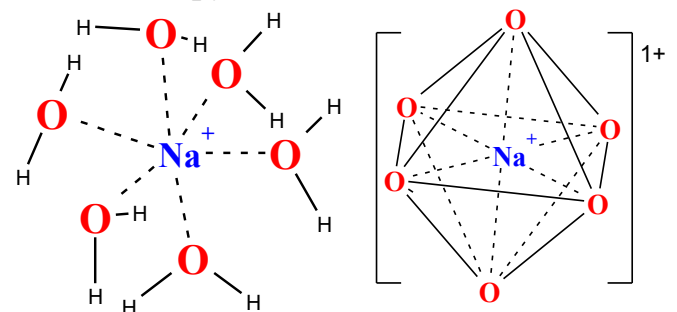
hexa aqua sodium(I)natrium cation

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners are donors **O:** → □ acceptor central atom Na^+ has 6 empty orbitals as acceptors □ of pair :

acceptor □□□ Na^+ □□□ acceptor and donor $H_2O:$ → □ Na^+ □ ← **:OH₂** donor ;

Octahedral or Hexagonal object figure geometry :



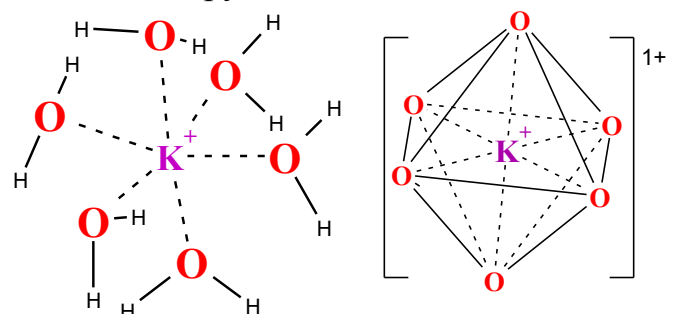
hexa aqua potassium(I)kalium cation

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners are donors **O:** → □ acceptor central atom K^+ has 6 empty orbitals as acceptors □ of pair :

acceptor □□□ K^+ □□□ acceptor and donor $H_2O:$ → □ K^+ □ ← **:OH₂** donor ;

Octahedral or Hexagonal object figure geometry :



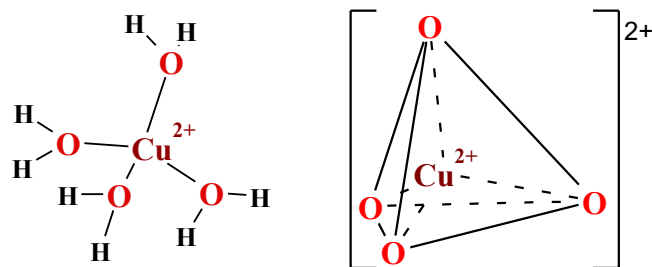
$[\text{Cu}^{2+}(\text{H}_2\text{O})_4]^{2+}$
tetra aqua cooper(II) cation

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners
 are donors **O:→□** acceptor central atom **Cu^{2+}**
 has 4 empty orbitals as acceptors □ of pair :

acceptor □□ **Cu^{2+}** □□ acceptor and
 donor **H_2O :→□ Cu^{2+} □←: **O** H_2** donor ;

Tetrahedral or Tetragonal object figure geometry :



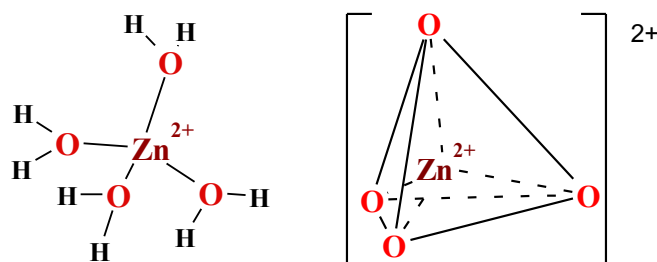
$[\text{Zn}^{2+}(\text{H}_2\text{O})_4]^{2+}$
tetra aqua zink(II) cation

Donor-acceptor covalent bond

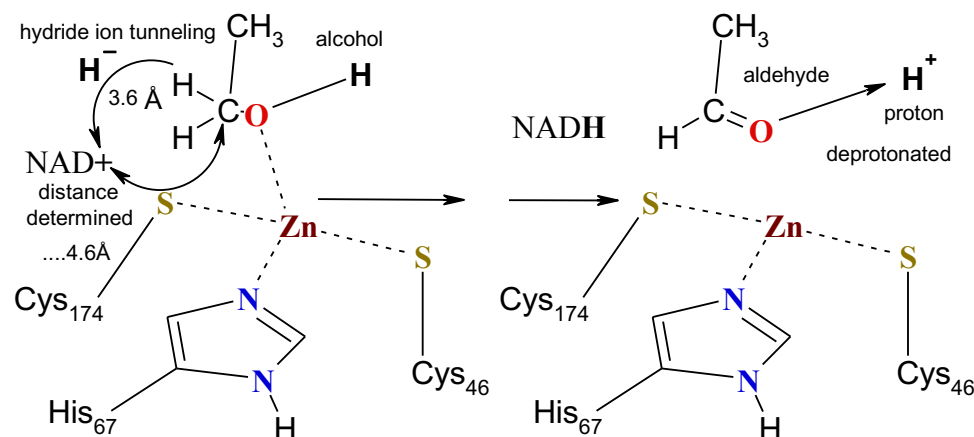
Atoms **:O:** of unshared electron pair : owners
 are donors **O:→□** acceptor central atom **Zn^{2+}**
 has 4 empty orbitals as acceptors □ of pair :

acceptor □□ **Zn^{2+}** □□ acceptor and
 donor **H_2O :→□ Zn^{2+} □←: **O** H_2** donor ;

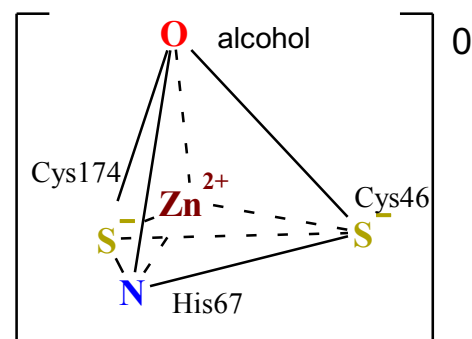
Tetrahedral or Tetragonal object figure geometry :



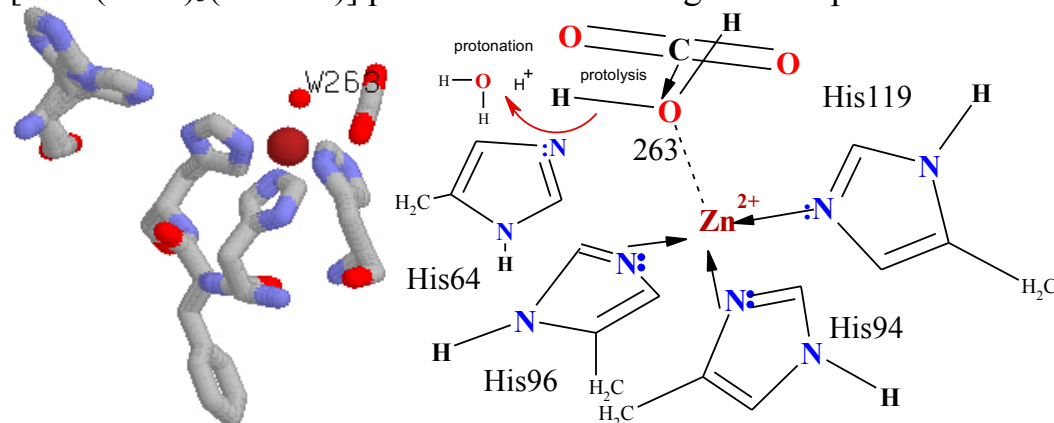
Alcohol dehydrogenase E.1 class1HLD.pdb **Zn^{2+}** coordinates Cys46-Cys174-His67-*alcohol*:
 $[\text{Zn}^{2+}(\text{S}^-\text{Cys})_2(\text{O}^-\text{alcohol})(\text{N}^-\text{His})]$ no charge of complex .



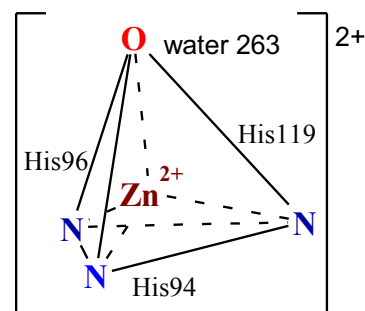
Tetrahedral, Tetragonal
 geometry



Carbonic Anhydrase E.2 class 2VVA.pdb **Zn^{2+}** coordinates His96-His94-HisHis119-*water*
 $[\text{Zn}^{2+}(\text{N}^-\text{His})_3(\text{O}^-\text{water})]$ positive +2 total charge of complex.



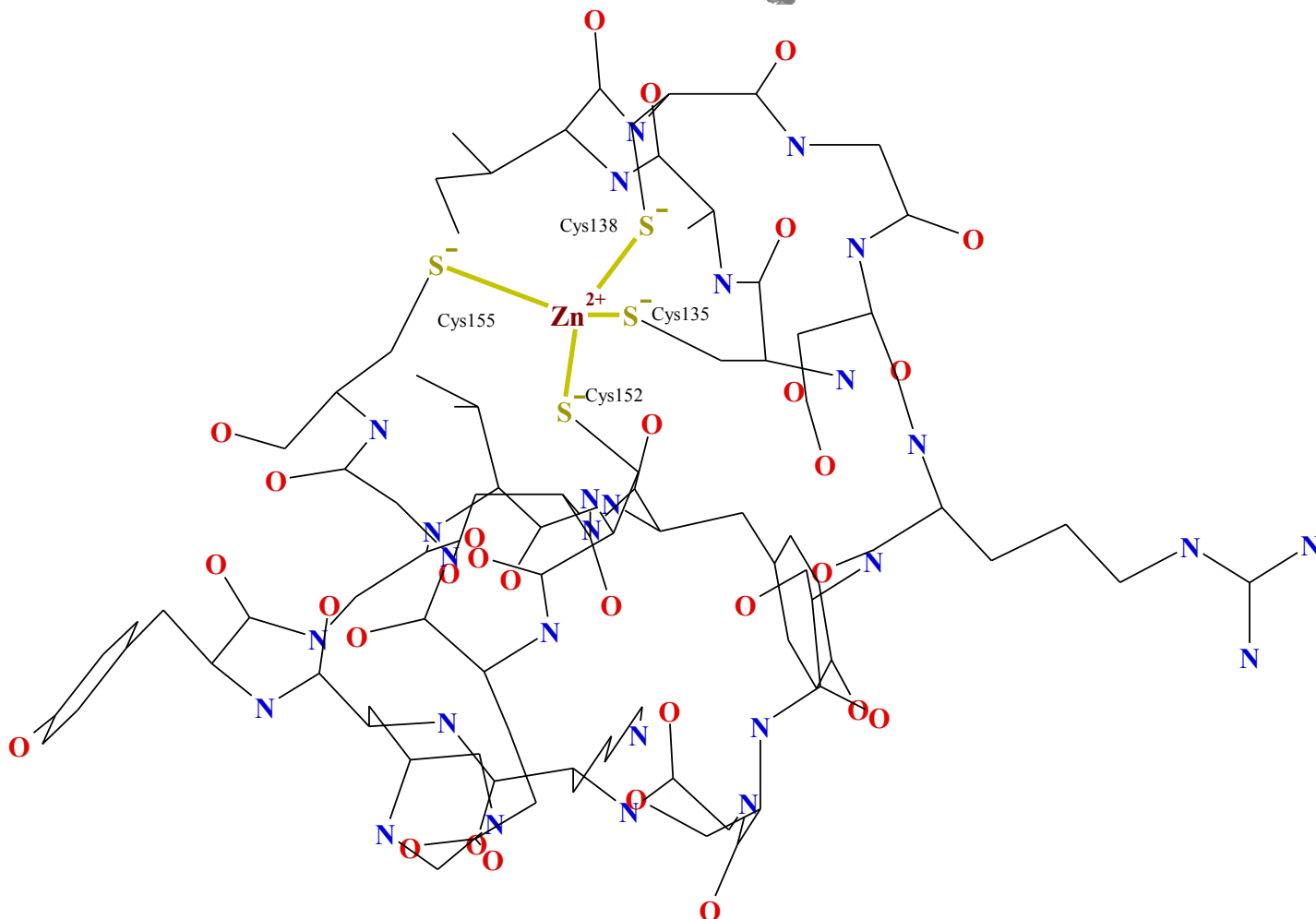
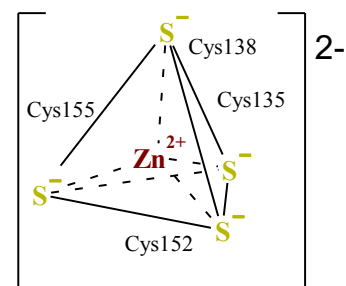
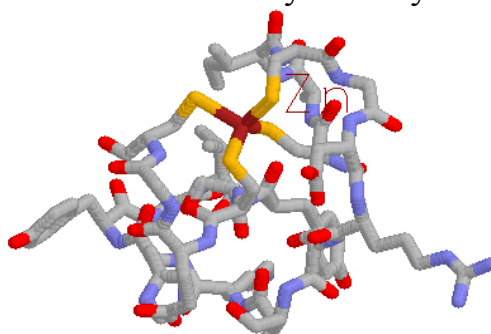
Tetrahedral, Tetragonal
 geometry



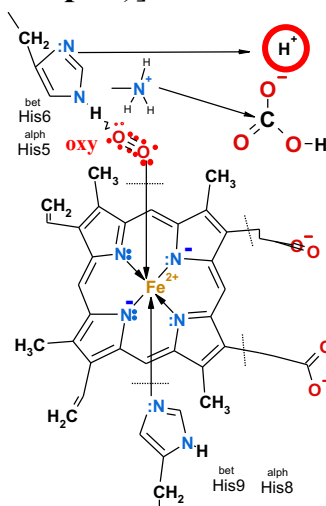
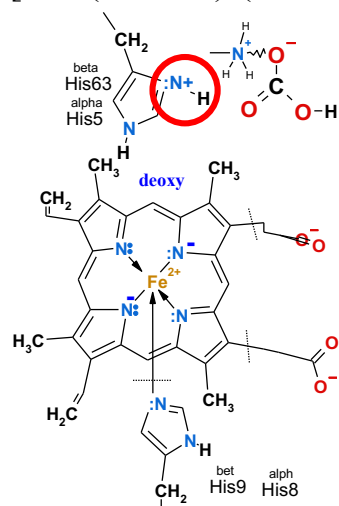
DNA binding Zn finger motifs 3DZY.pdb Zn^{2+} coordinates Cys138-Cys135-Cys152-Cys155

$[Zn^{2+}(S^-Cys)_4]^{2-}$ negative -2 total charge of complex.

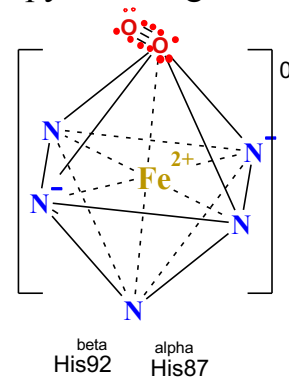
Tetrahedral, Tetragonal geometry



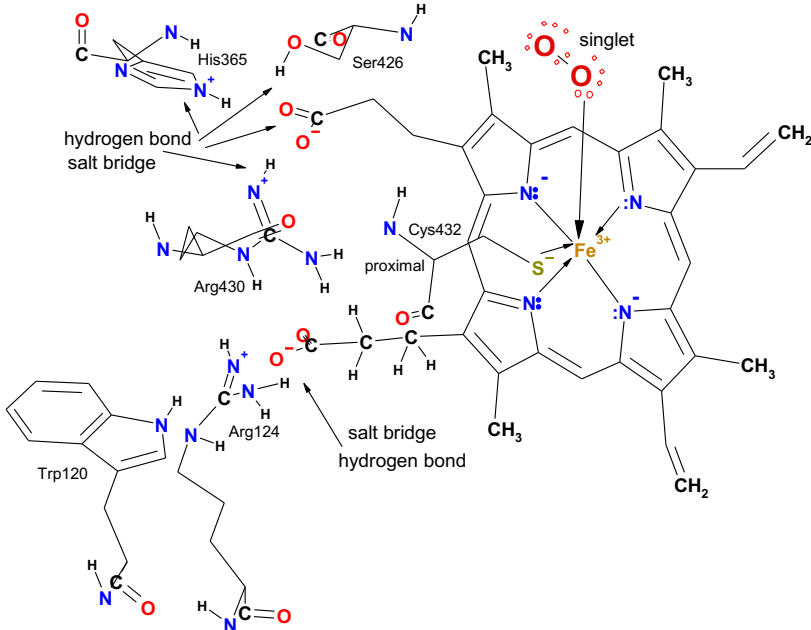
Shuttle hemoglobin deoxy-oxy Fe^{2+} coordinates Heme $N-N-N-N-N$ His63,58- $O\equiv O$ oxygen triplet $[Fe^{2+}(NHeme)_4(N_{His63,58})(O\equiv O \text{ oxygen triplet})]$ neutral zero 0 net charge of complex.



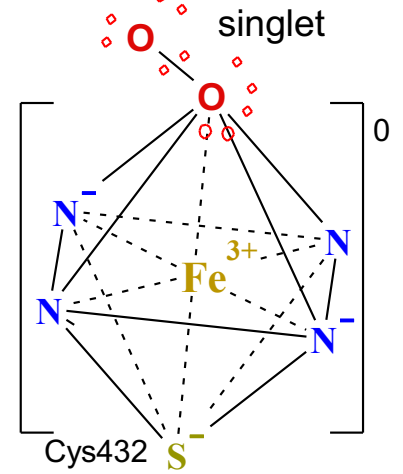
Octahedral or Hexagonal Bipyramidal geometry



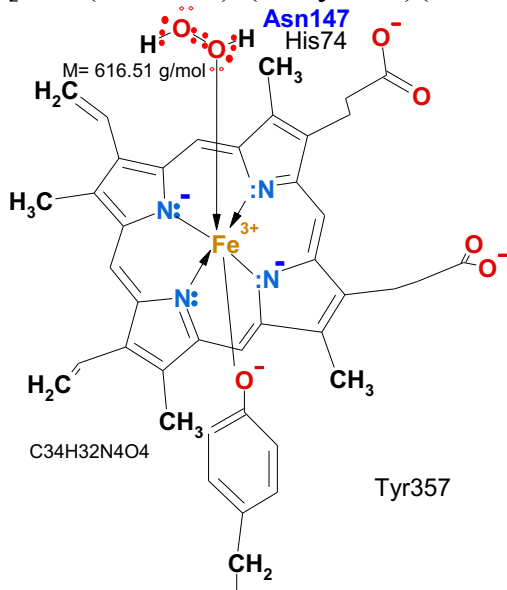
Cytochrom P450s Fe^{3+} coordinates Heme $\text{N-N-N-N-S-Cys432-O-O}$ oxygen singlet
 $[\text{Fe}^{3+}(\text{N Heme})_4(\text{S-Cys432})(\text{O-O oxygen singlet})]$ neutral zero 0 net charge of complex.



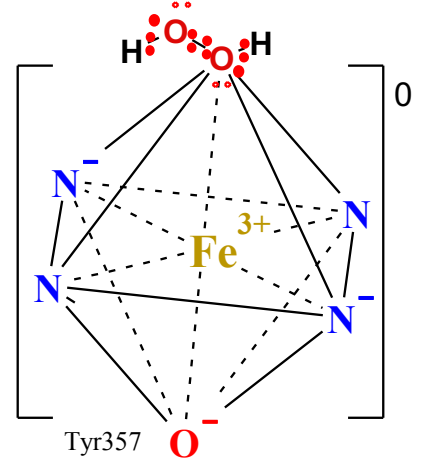
Octahedral or Hexagonal
Bipyramidal geometry



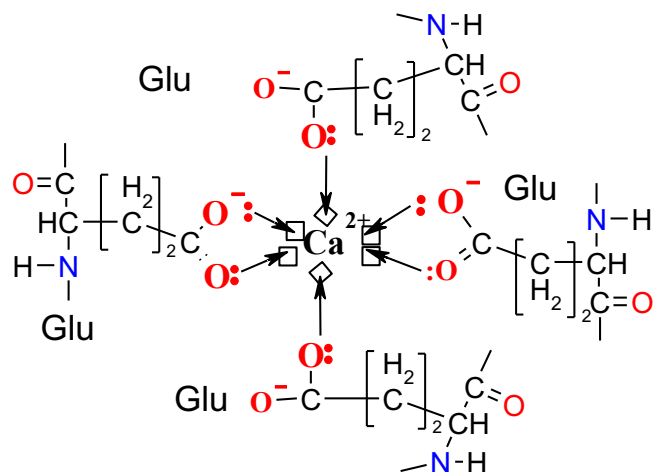
Catalase (EC 1.11.1.6) Fe^{3+} coordinates Heme $\text{N-N-N-N-O-Tyr357-HO-OH}$ peroxide
 $[\text{Fe}^{3+}(\text{N Heme})_4(\text{O-Tyr357})(\text{HO-OH peroxide})]$ neutral zero 0 net charge of complex.



Octahedral or Hexagonal
Bipyramidal geometry



Myosin contraction Ca^{2+} coordinates four Glutamate $-\text{COO}^-$ carboxylate six oxygen atoms
 $[\text{Ca}^{2+}(\text{Glu-COO}^-)_4 \text{ with } 4(\text{Glu-O}^-)_4 \text{ and two Glu-C=O}]$ having 2- total charge of complex.



Octahedral or Hexagonal
Bipyramidal geometry

