

Around central atom bond geometry symetrysation, 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

Symetrysation geometry

Geometric symmetry	Formula	Structure	Geometry
linear stick 180°	C_2H_2	$H-C\equiv C-H$	
trigonal planar 120°	CO_3^{2-}		
bent angle 109.47° 0° C -100° C	ice H_2O $\rho=0.9167 \text{ g/mL; density}$ $\rho=0.9257 \text{ g/mL; density}$		
bent angle 105° 0° C +3.89° C +25° C	water H_2O $\rho=0.9998425 \text{ g/mL; density}$ $\rho=0.9999999 \text{ g/mL; density}$ $\rho=0.9970479 \text{ g/mL; density}$		
trigonal pyramidal	$:NH_3$		
tetrahedral, tetragonal	CH_4		
octahedral, hexagonal bipyramidal	$[Al(OH)_6]^{3-}$		

Geometric symmetry of central atom in coordinative compounds

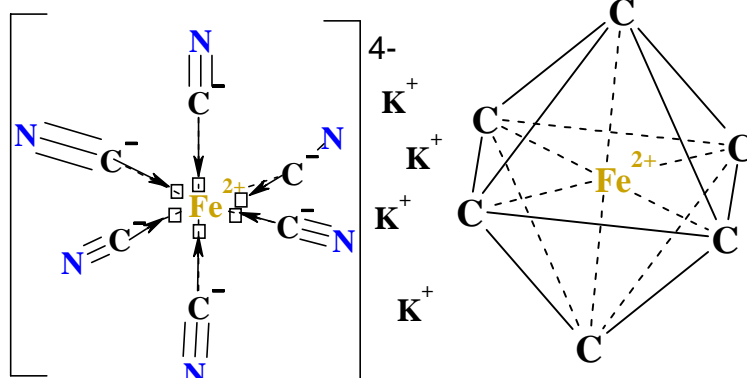
$\text{K}_4[\text{Fe}(\text{CN})_6]$
Potassium hexa ciano ferrate(II)

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 ;

Octahedral or Hexagonal object figure geometry :
 Bipyramid



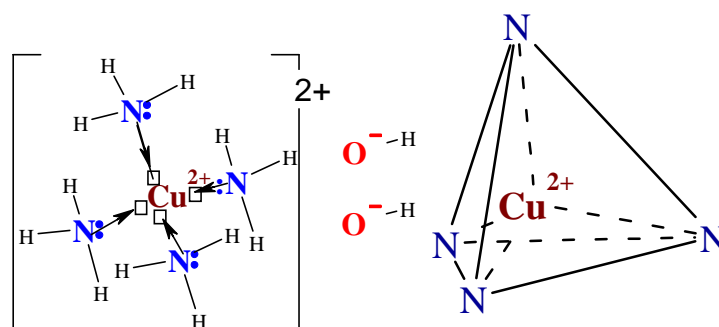
$[\text{Cu}(\text{NH}_3)_4](\text{OH})_2$
tetra amino cooper(II) hydroxide

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 ;

Tetrahedral or Tetragonal object figure geometry :



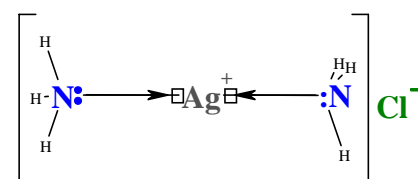
$[\text{Ag}(\text{NH}_3)_2]\text{Cl}$
di amino silver(I) chloride

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 ;

Linear or Stick geometry :



Linear or Stick geometry



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



hexa aqua magnesium(II) cation

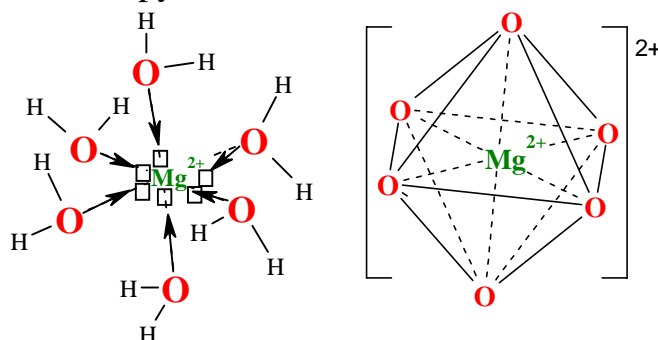
Donor-acceptor covalent bond

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 ;

Octahedral or Hexagonal object figure geometry :

Bipyramid



hexa aqua calcium(II) cation

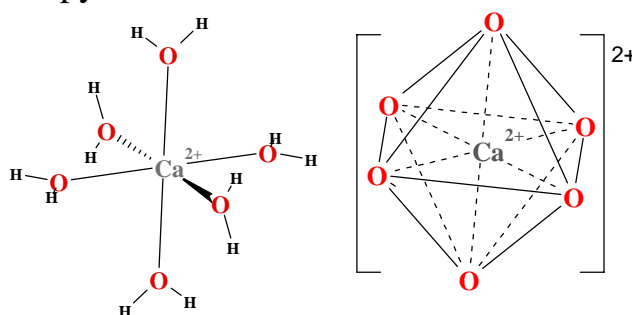
Donor-acceptor covalent bond

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 :

Bipyramid



hexa aqua sodium(I) natrium cation

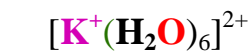
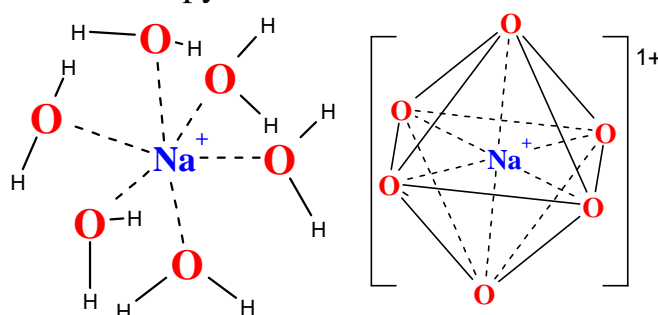
Donor-acceptor covalent bond

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 :

Bipyramid



hexa aqua potassium(I) kalium cation

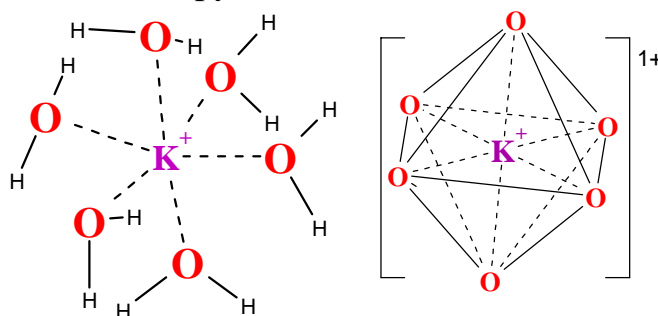
Donor-acceptor covalent bond

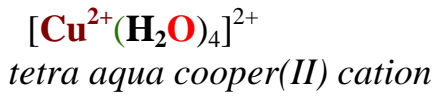
Atoms **:O:** of unshared electron pair : owners are donors **O:** → □ acceptor central atom K^+ has 6 empty orbitals as acceptors □ of pair :

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

Octahedral or Hexagonal object figure geometry :

Bipyramid



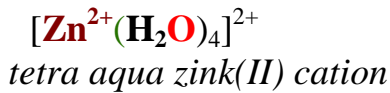
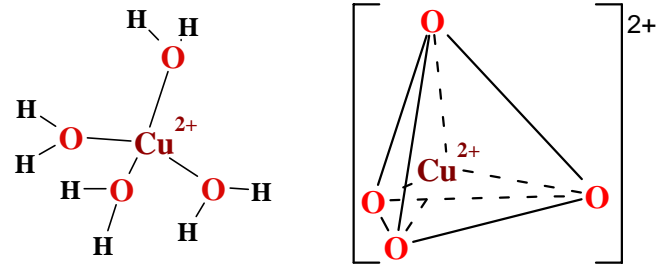


Tetrahedral or Tetragonal object figure geometry :

Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners
 are donors **O:→□** acceptor central atom **Cu²⁺**
 has 4 empty orbitals as acceptors □ of pair :

acceptor □□**Cu²⁺**□□ acceptor and
 donor **H₂O:→□Cu²⁺□←:OH₂** donor ;

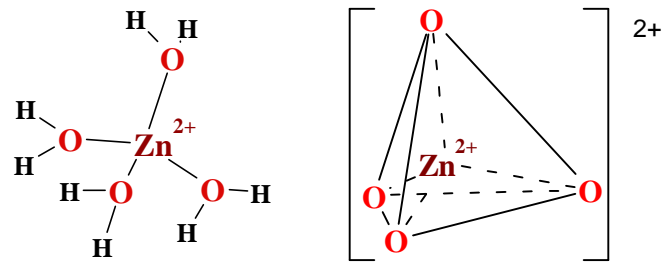


Tetrahedral or Tetragonal object figure geometry :

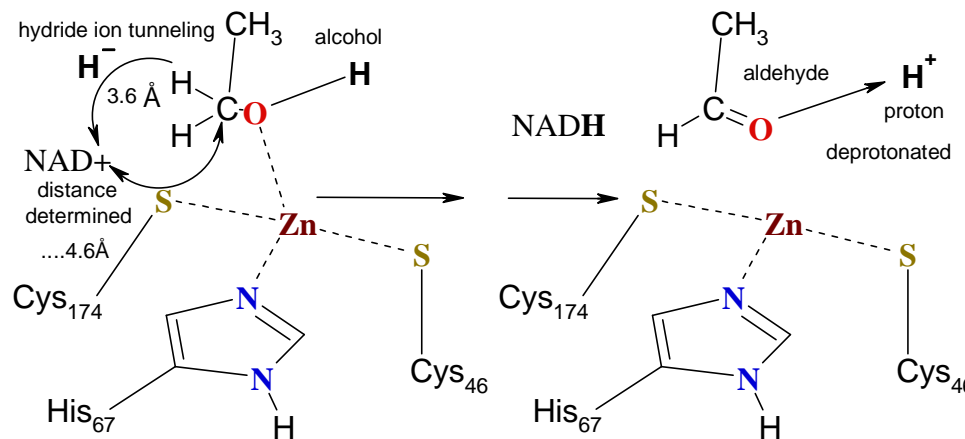
Donor-acceptor covalent bond

Atoms **:O:** of unshared electron pair : owners
 are donors **O:→□** acceptor central atom **Zn²⁺**
 has 4 empty orbitals as acceptors □ of pair :

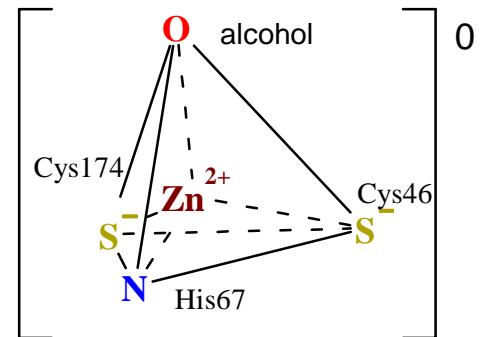
acceptor □□**Zn²⁺**□□ acceptor and
 donor **H₂O:→□Zn²⁺□←:OH₂** donor ;



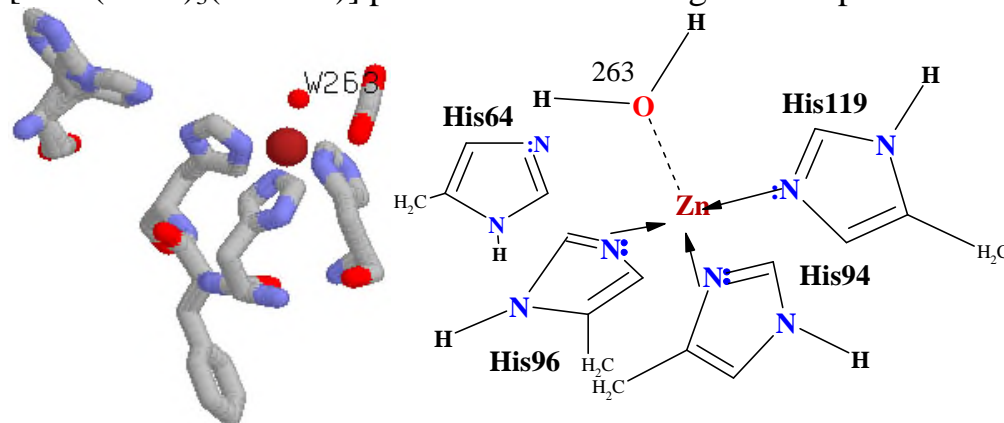
Alcohol dehydrogenase E.1 class1HLD.pdb **Zn²⁺** coordinates Cys46-Cys174-His67-alcohol:
 $[\text{Zn}^{2+}(\text{S}^-\text{Cys})_2(\text{Oalcohol})(\text{NHis})]$ no charge of complex .



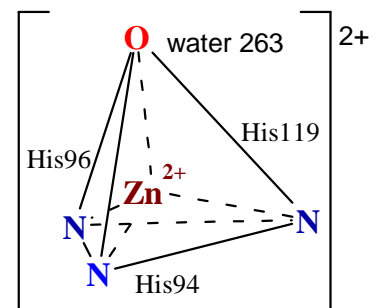
Tetrahedral, Tetragonal
 geometry



Carbonic Anhydrase E.2 class 2VVA.pdb **Zn²⁺** coordinates His96-His94-HisHis119-water
 $[\text{Zn}^{2+}(\text{NHis})_3(\text{Owater})]$ positive +2 total charge of complex.



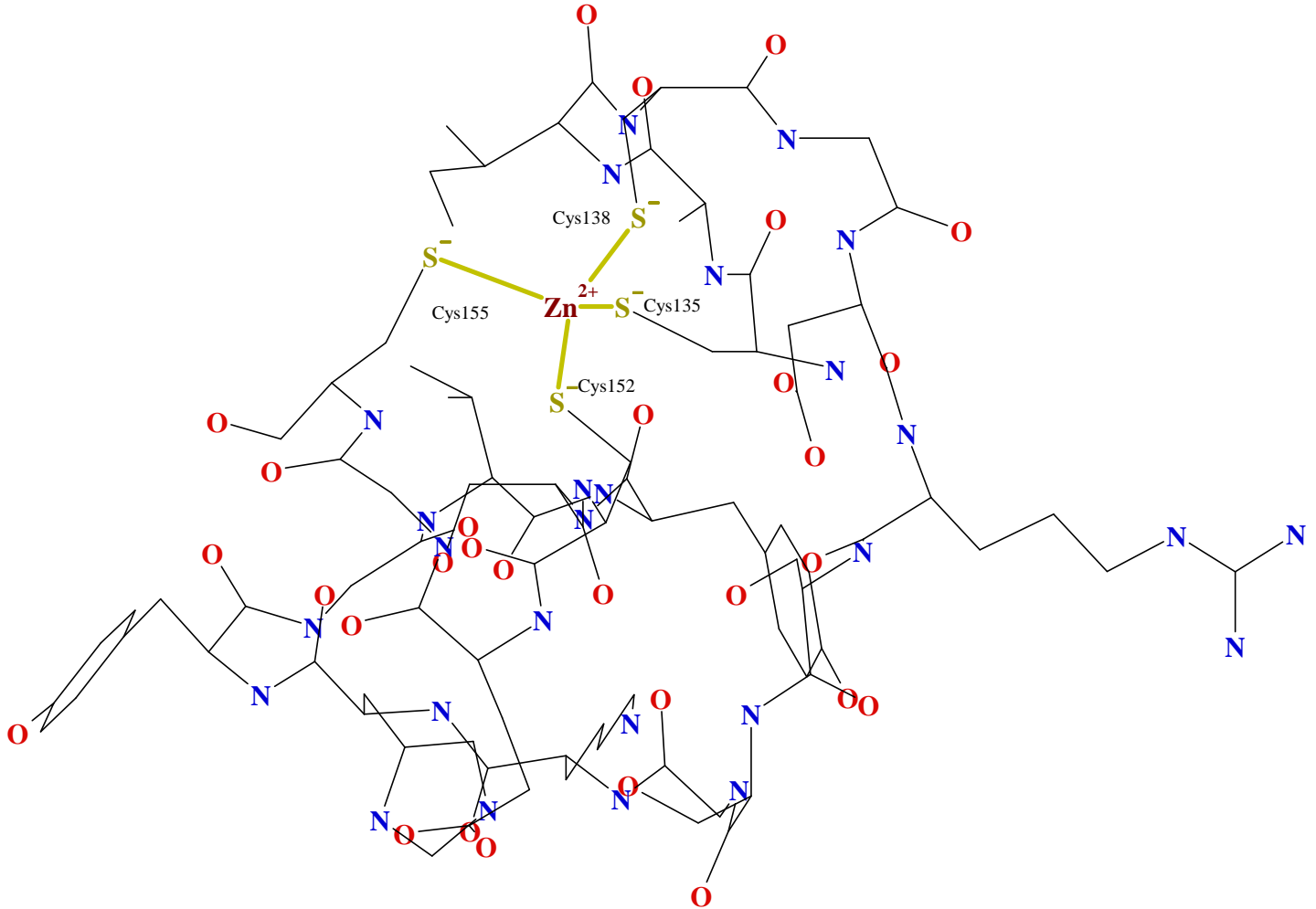
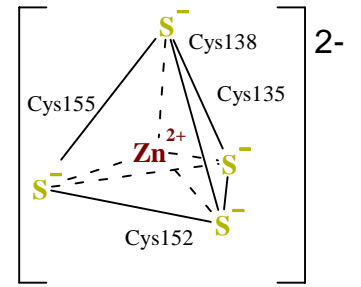
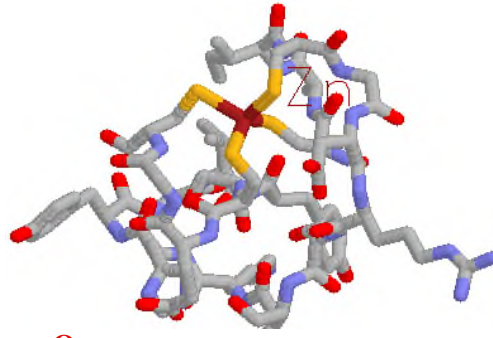
Tetrahedral, Tetragonal
 geometry



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

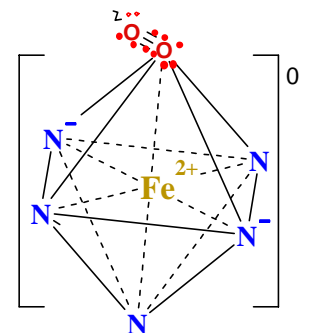
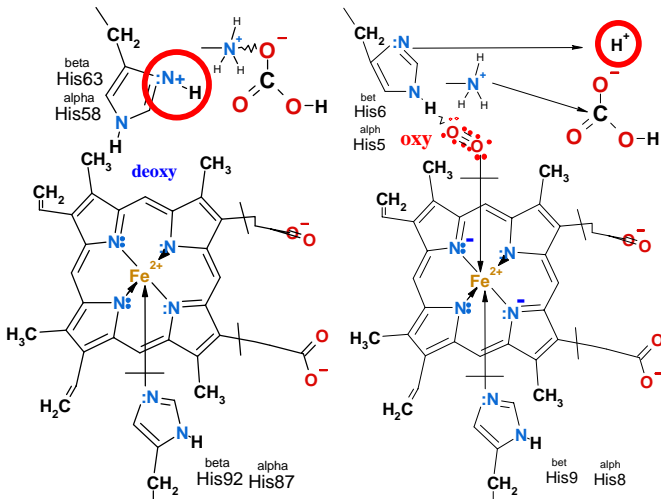
$[Zn^{2+}(S^-Cys)_4]^{2-}$ negative -2 total charge of complex.

Tetrahedral, Tetragonal geometry

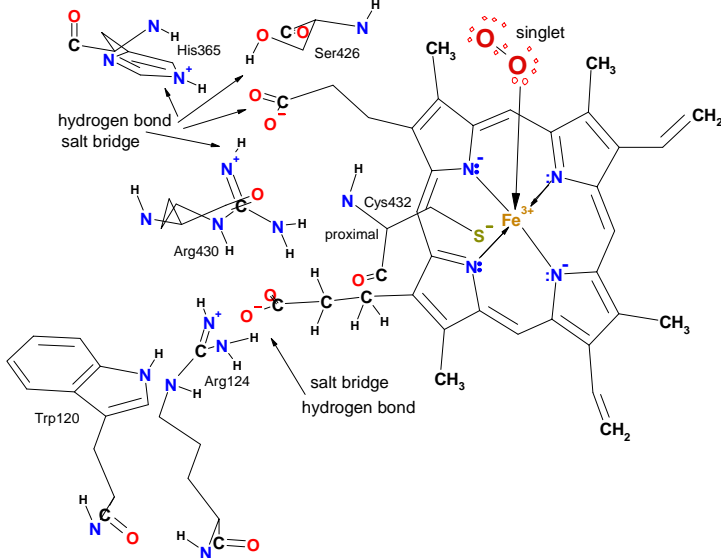


Shuttle hemoglobin deoxy-oxy Fe^{2+} coordinates Heme $N^- - N^- - N^- - N^-$ His63,58- $O \equiv O$ oxygene triplet $[Fe^{2+}(NHeme)_4(N_{His63,58})(O \equiv O \text{ oxygen triplet})]$ neutral zero 0 total charge of complex.

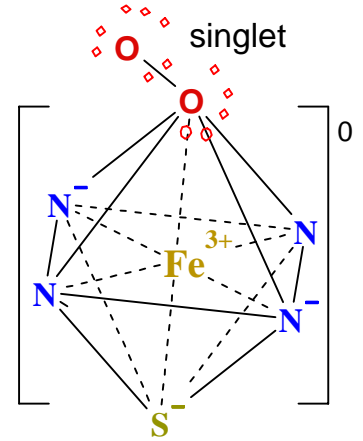
Octahedral or Hexagonal Bipyramid geometry



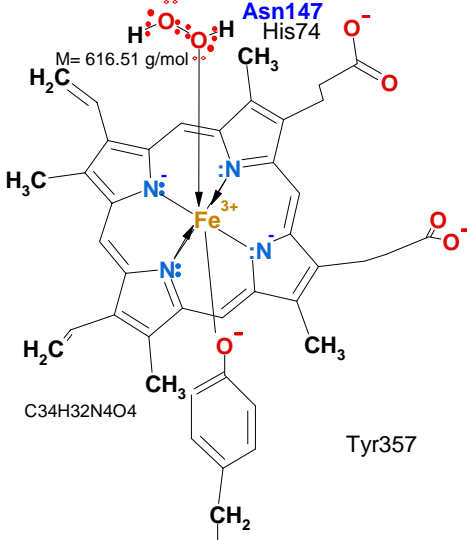
Cytochrome P450s Fe^{3+} coordinates HemeN-N-N-N-S⁻Cys432-O-O oxygen singlet
 $[Fe^{3+}(NHeme)_4(S^-Cys432)(O-O\ oxygen\ singlet)]$ neutral zero 0 total charge of complex.



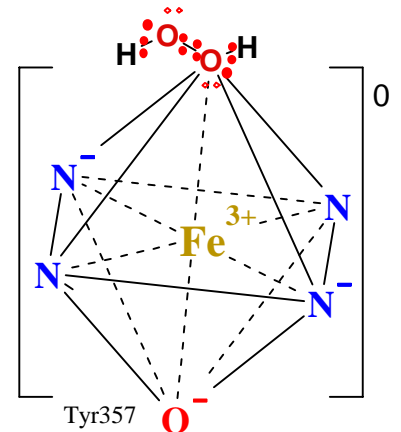
Octahedral or Hexagonal
Bipyramid geometry



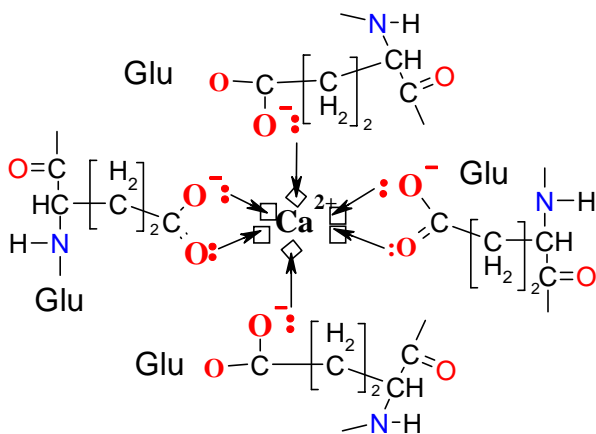
Catalase (EC 1.11.1.6) Fe^{3+} coordinates HemeN-N-N-N-O⁻Tyr357-HO-OH peroxide
 $[Fe^{3+}(NHeme)_4(O^-Tyr357)(HO-OH\ peroxide)]$ neutral zero 0 total charge of complex.



Octahedral or Hexagonal
Bipyramid geometry



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



Octahedral or Hexagonal
Bipyramid geometry

