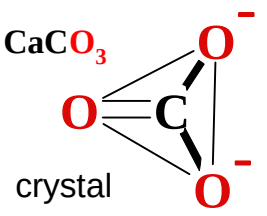
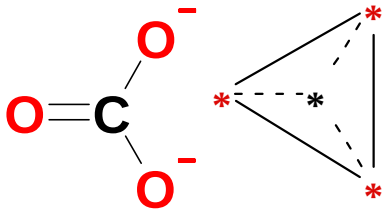
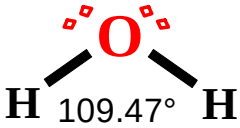
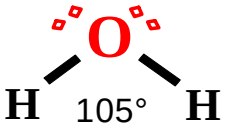
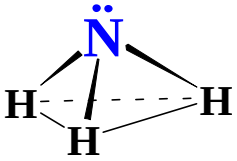
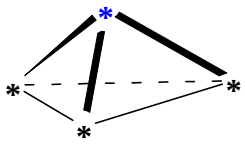
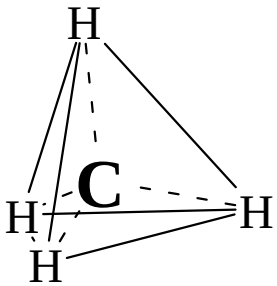
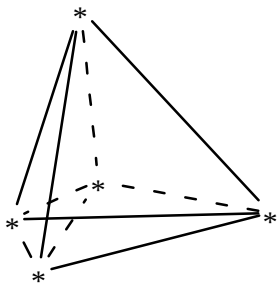
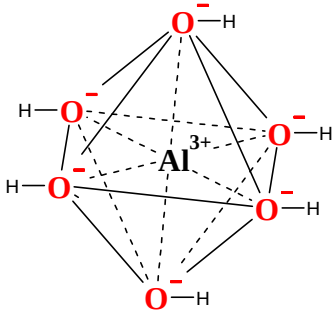
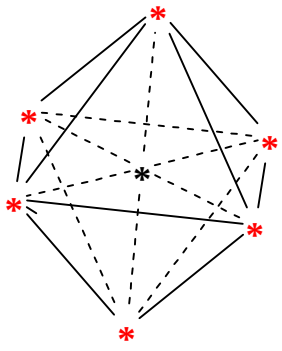
Around central atom bond geometry symmetrysation, which forms the symmetry of the crystal .

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

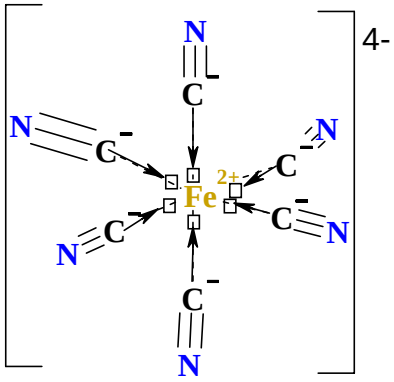
Symmetrysation geometry

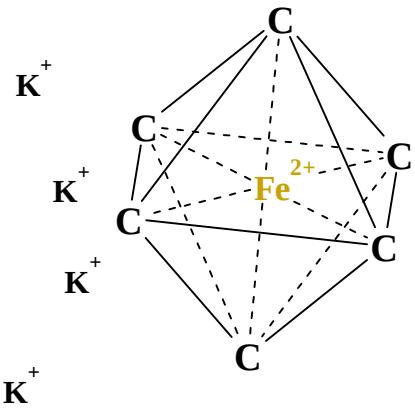
Geometric symmetry	Formula	Structure	Geometry
linear stick 180°	C_2H_2	H-C≡C-H	
trigonal planar 120°	CO_3^{2-}		
bent angle 109.47°	ice H_2O		
0° C	ρ=0.9167 $^{g}/_{mL}$; density		
-100° C	ρ=0.9257 $^{g}/_{mL}$; density		
bent angle 105°	water H_2O		
0° C	ρ=0.9998425 $^{g}/_{mL}$; density		
+3.89° C	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

$K_4[Fe(CN)_6]$
Potassium hexa ciano ferrate(II)

Octahedral or Hexagonal object figure geometry :
Bipyramidal

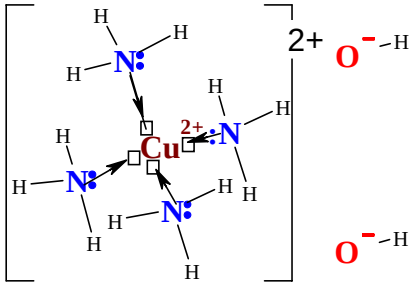


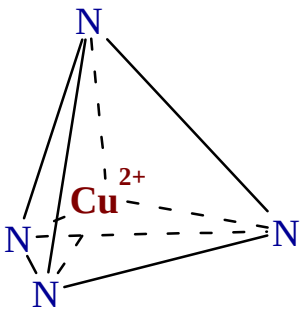


Donor-acceptor covalent bond
Atoms of unshared electron pair **:** owners are donors **:** → □ acceptor central atom
has 6 empty orbitals as acceptors □ of pair **:**
acceptor □□□**Fe^{2+}**□□□
acceptor and
donor **N≡C⁻:** →□**Fe^{2+}**□←**:⁻C ≡N**
donor ;

$[Cu(NH_3)_4](OH)_2$
tetra amino cooper(II) hydroxide

Tetrahedral or Tetragonal object figure geometry :





Donor-acceptor covalent bond

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

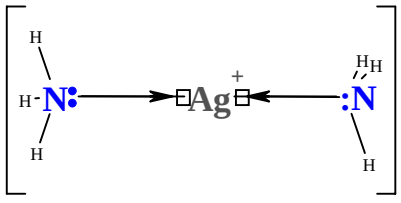
acceptor □□**Cu^{2+}**□□ acceptor and
donor **H_3N:** →□**Cu^{2+}**□←**:NH_3** donor ;

$[Ag(NH_3)_2]Cl$
di amino silver(I) chloride

Linear or Stick geometry :

Donor-acceptor covalent bond

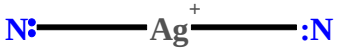
Atoms **N:** of unshared electron pair **:** owners are donors **N:** → □ acceptor central atom □**Ag^+**□
has 2 empty orbitals as acceptors □ of pair **:**



Cl^-

acceptor □**Ag^+**□ acceptor and
donor **H_3N:** →□ **Ag^+**□←**:NH_3** donor ;

Linear or Stick geometry



Main electron pair donor atoms are **N:** and **:O:** two unshared electron pairs owner oxygen

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

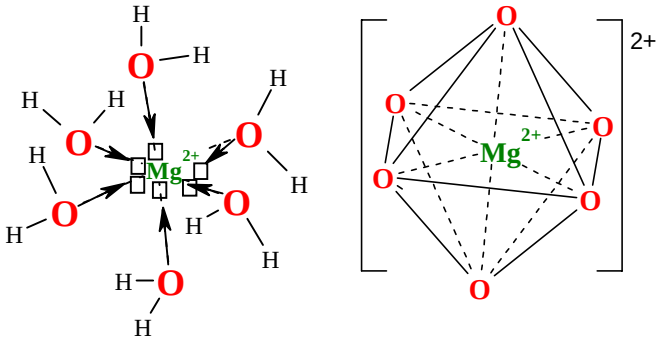
$[Mg^{2+}(H_2O)_6]^{2+}$
hexa aqua magnesium(II) cation

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+}□←:OH_2 donor ;

Octahedral or Hexagonal object figure geometry : Bipyramidal



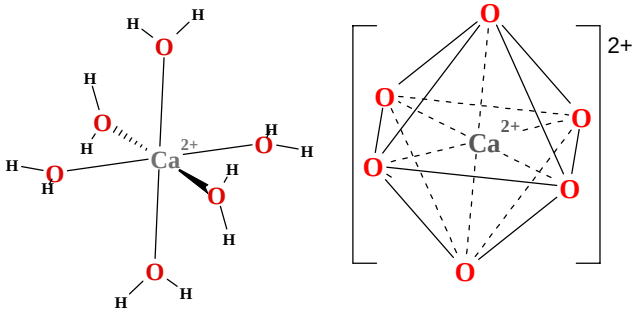
$[Ca^{2+}(H_2O)_6]^{2+}$
hexa aqua calcium(II) cation

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+}□←:OH_2 donor ;

Octahedral or Hexagonal object figure geometry : Bipyramidal



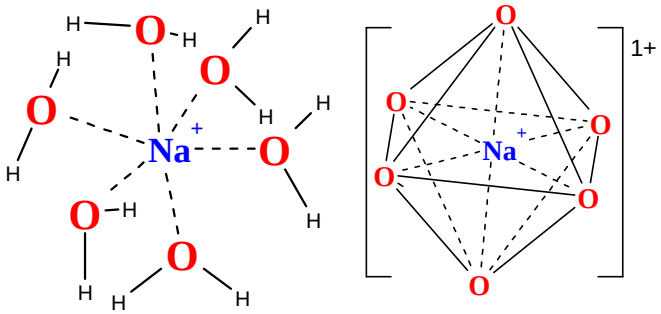
$[Na^{+}(H_2O)_6]^{2+}$
hexa aqua sodium(I)natrium cation

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^{+}□←:OH_2 donor ;

Octahedral or Hexagonal object figure geometry : Bipyramidal



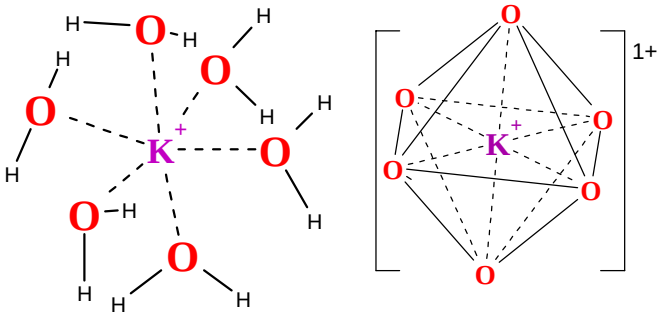
$[K^{+}(H_2O)_6]^{2+}$
hexa aqua potasium(I)kalium cation

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^{+}□←:OH_2 donor ;

Octahedral or Hexagonal object figure geometry : Bipyramidal



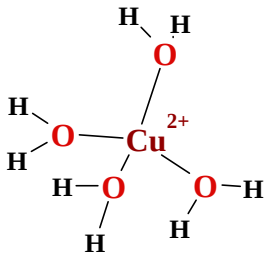
$[Cu^{2+}(H_2O)_4]^{2+}$ Tetrahedral or Tetragonal object figure geometry :

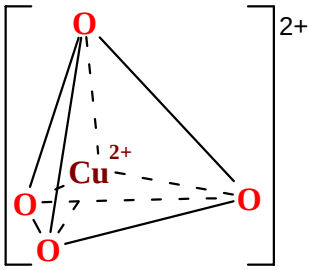
tetra aqua cooper(II) cation

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+}□←:OH_2 donor ;





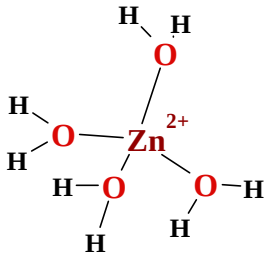
$[Zn^{2+}(H_2O)_4]^{2+}$ Tetrahedral or Tetragonal object figure geometry :

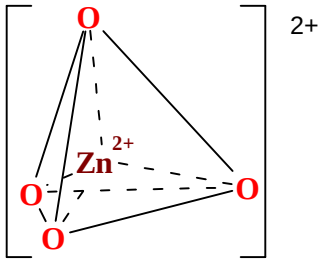
tetra aqua zink(II) cation

Donor-acceptor covalent bond

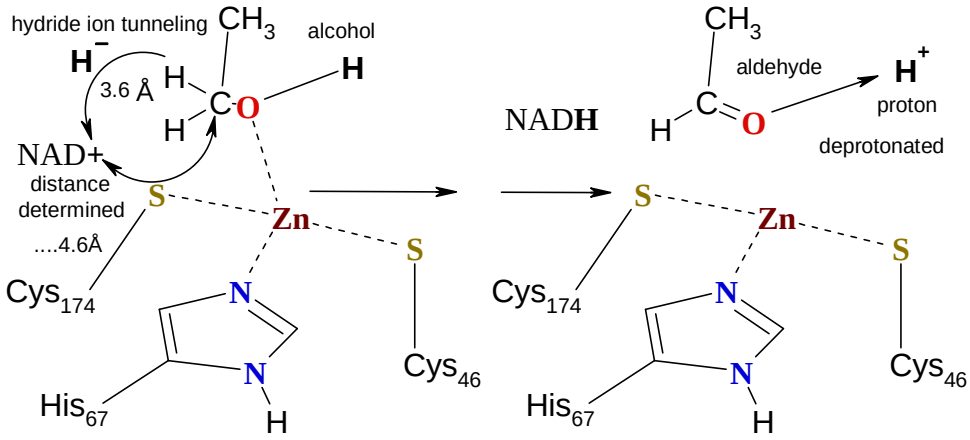
Atoms :O: of unshared electron pair : owners are donors O:→□ acceptor central atom Zn^{2+} has 4 empty orbitals as acceptors □ of pair :

acceptor □□Zn^{2+}□□ acceptor and donor H_2O:→□Zn^{2+}□←:OH_2 donor ;

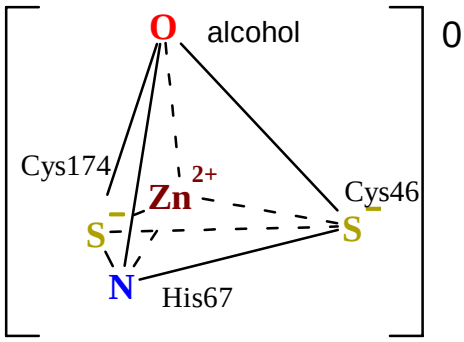




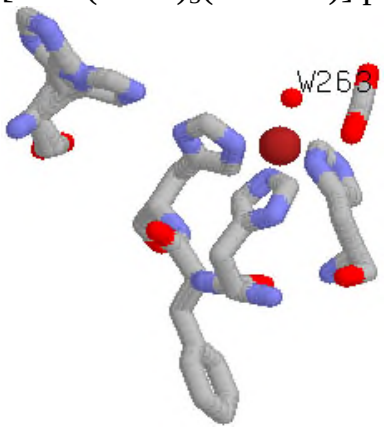
Alcohol dehydrogenase E.1 class1HLD.pdb Zn^{2+} coordinates Cys46-Cys174-His67-*alcohol*: [Zn^{2+}(S^-Cys)$_2$(O*alcohol*)(NHis)] no charge of complex .

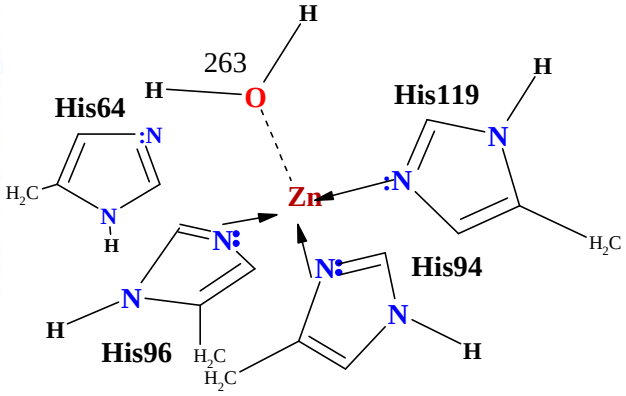


Tetrahedral, Tetragonal geometry

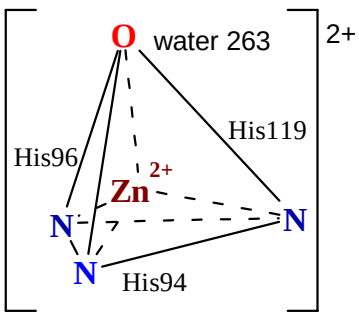


Carbonic Anhydrase E.2 class 2VVA.pdb Zn^{2+} coordinates His96-His94-HisHis119-*water* [Zn^{2+}(NHis)$_3$(O*water*)] positive +2 total charge of complex.





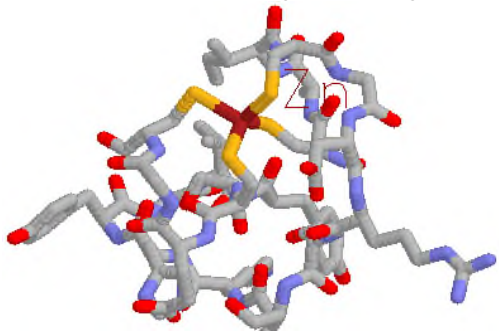
Tetrahedral, Tetragonal geometry

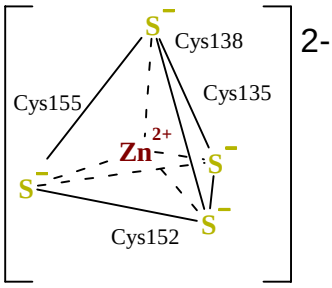


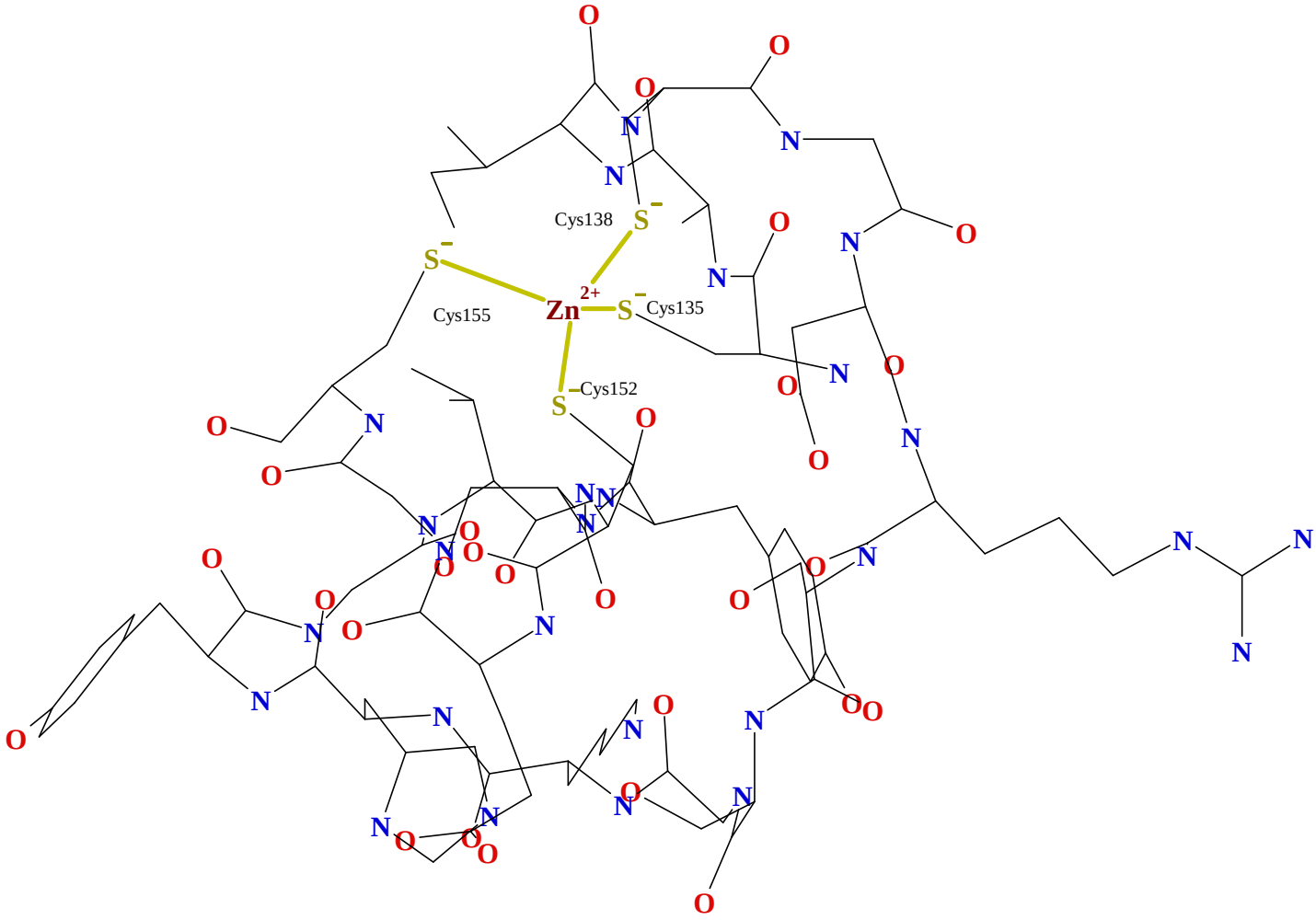
DNA binding Zn finger motifs 3DZY.pdb **Zn**$^{2+}$ coordinates Cys138-Cys135-Cys152-Cys155

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

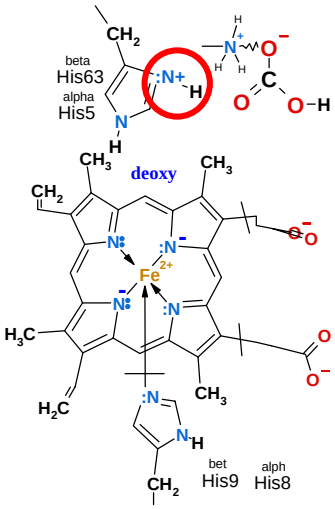
Tetrahedral, Tetragonal geometry

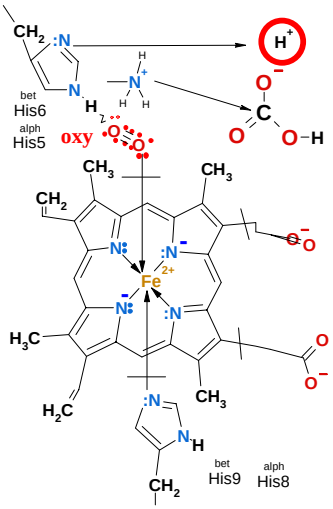




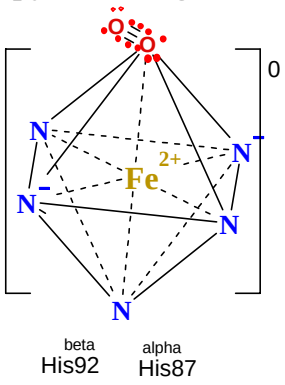


Shuttle hemoglobin **deoxy**-**oxy** **Fe**$^{2+}$ coordinates Heme**N**$^{-}$-**N**-**N**$^{-}$-**N**-**N**His63,58-**O≡O** *oxygen* **triplet** $[Fe^{2+}(NHeme)_4(N$ His63,58$)(O{\equiv}O$ *oxygen* **triplet**$)]$ neutral zero 0 net charge of complex.

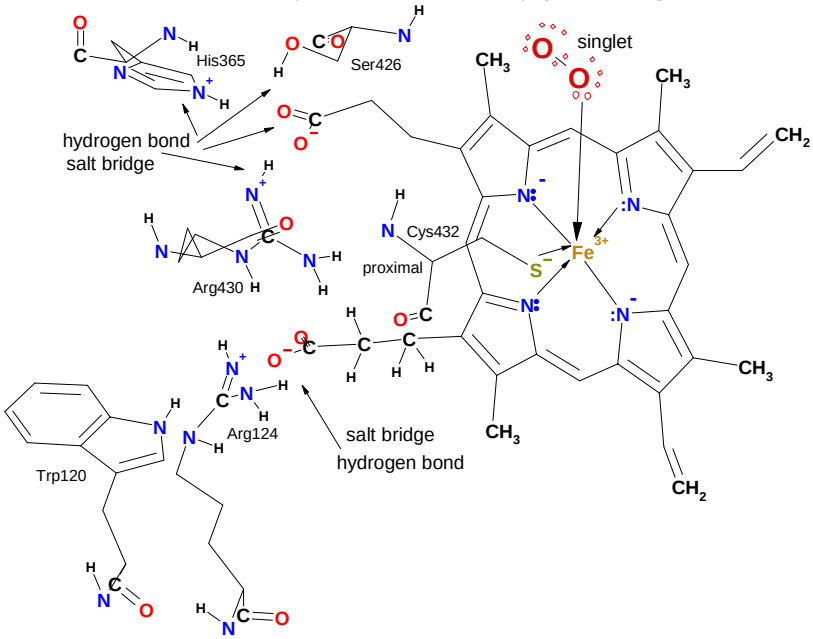




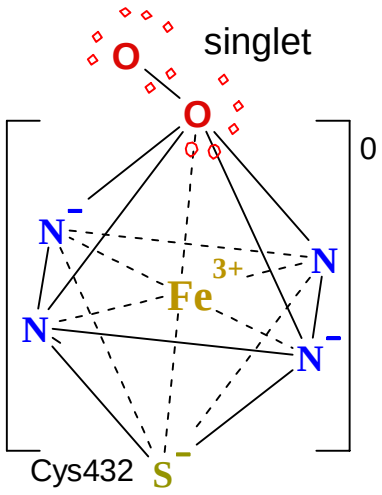
Octahedral or Hexagonal Bipyramidal geometry



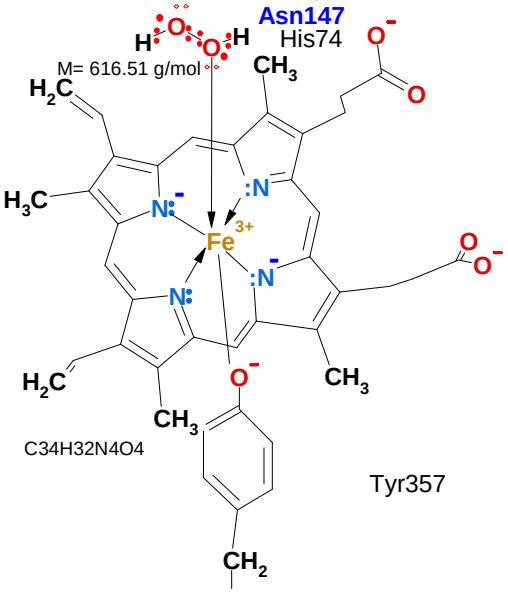
Cytochrom P450s **Fe**$^{3+}$ coordinates Hem **N**-**N**$^{-}$-**N**-**N**$^{-}$-**S**$^{-}$Cys432-**O**-**O** *oxygen* **singlet**
[**Fe**$^{3+}$(**N** Hem)$_4$(**S**$^{-}$Cys432)(**O**-**O** *oxygen* **singlet**)] neutral zero 0 net charge of complex.



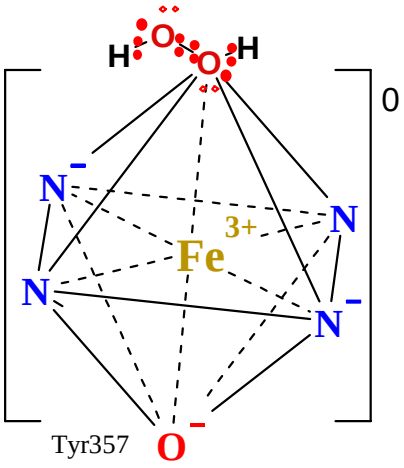
Octahedral or Hexagonal Bipyramidal geometry



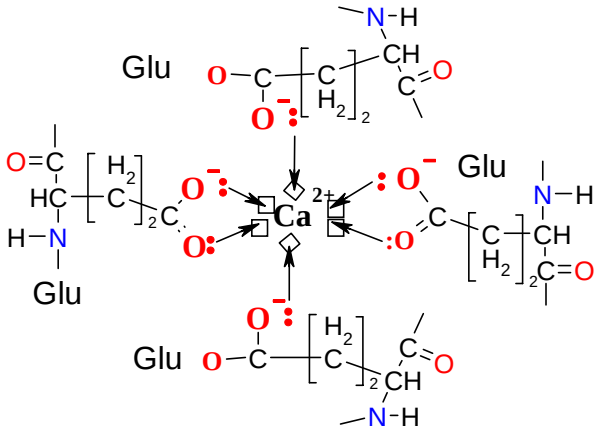
Catalase (EC 1.11.1.6) **Fe**$^{3+}$ coordinates Heme **N**-**N**$^{-}$-**N**-**N**$^{-}$-**O**$^{-}$-Tyr357-H**O**-O**H** *peroxide*
[**Fe**$^{3+}$(**N** Heme)$_4$(**O**$^{-}$Tyr357)(H**O**-O**H** *peroxide*)] neutral zero 0 net charge of complex.



Octahedral or Hexagonal Bipyramidal 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 Bipyramidal geometry