IUPAC Advancing Worldwide Chemistry

What's in a Name?
Possibly DEATH and TAXES!

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Possibly Death and Taxes

- Historical allusion

Possibly Death and Taxes

- “In this world nothing can be said to be certain, except death and taxes.” *– Benjamin Franklin, 13 November 1789*

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What’s in a Name?

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What’s in a Name?

- Nomenclature!

Possibly Death and Taxes

- Could Franklin have been thinking about nomenclature when he wrote this famous line to Jean Baptiste Le Roy?

Possibly Death and Taxes

- Link to nomenclature?

Possibly Death and Taxes

- Link to nomenclature?
- In the event of a spill/clean-up, clear communication is vital.
- Taxation and duties, and their related regulations, rely on nomenclature.

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Nomenclature is the Blood of Chemistry

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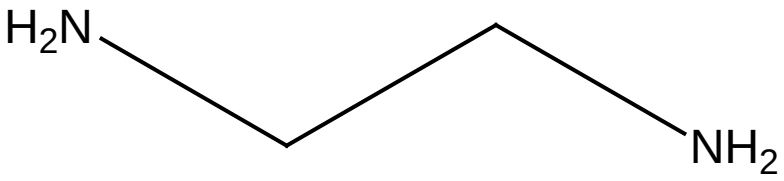
- Makes some people a bit squeamish
- Mixing different types can cause trouble
- It can get messy

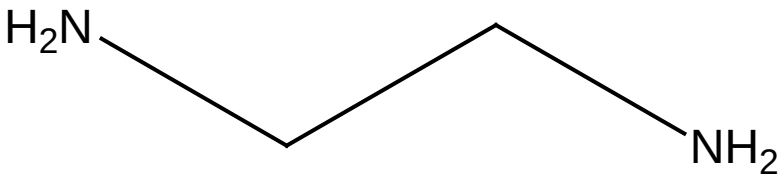
What are some of the dangers associated with DHMO?

Each year, Dihydrogen Monoxide is a known causative component in many thousands of deaths and is a major contributor to millions upon millions of dollars in damage to property and the environment. Some of the known perils of Dihydrogen Monoxide are:

- Death due to accidental inhalation of DHMO, even in small quantities.
- Prolonged exposure to solid DHMO causes severe tissue damage.
- Excessive ingestion produces a number of unpleasant though not typically life-threatening side-effects.
- DHMO is a major component of acid rain.
- Gaseous DHMO can cause severe burns.
- Found in biopsies of pre-cancerous tumors and lesions.
- Given to vicious dogs involved in recent deadly attacks.



- A molecule with a venerable history…



- A molecule with a venerable history…

  …that was dropped and made a big mess

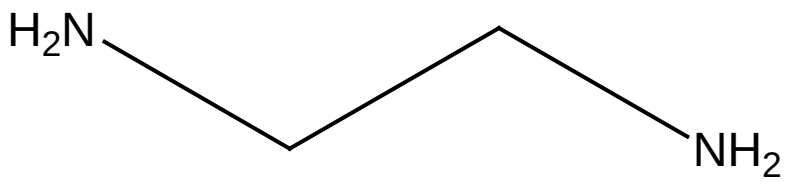
Hazardous Substances and New Organisms Act

- Regulates all use of chemicals and micro-organisms in the work place.
- Only chemicals that have been approved by ERMA may be used.

Hazardous Substances and New Organisms Act

- Section 33 exemption for Research and Education
- ERMA Code of Practice
- 30 s access time for MSDS Sheets

- But how reasonable is this?



An Inorganic Example

- copper(II) acetate monohydrate

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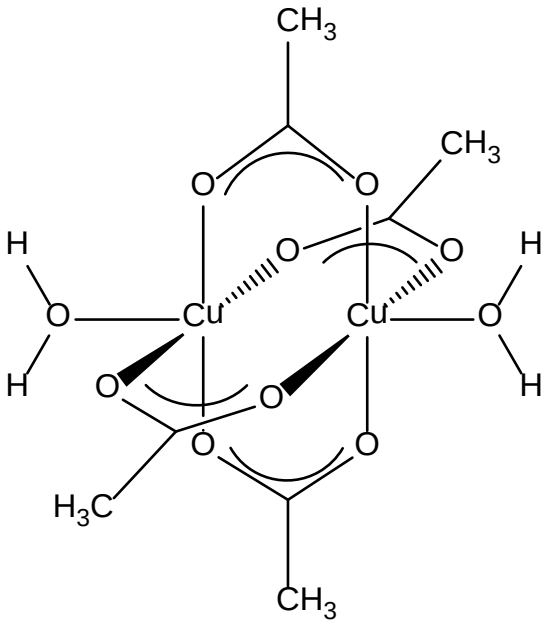
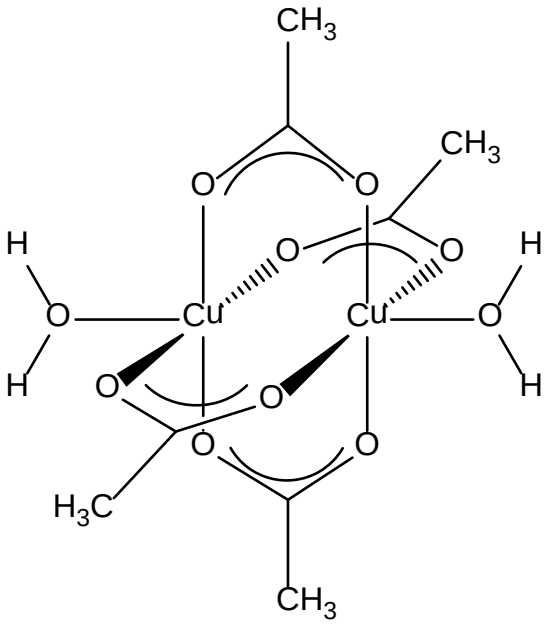


An Inorganic Example

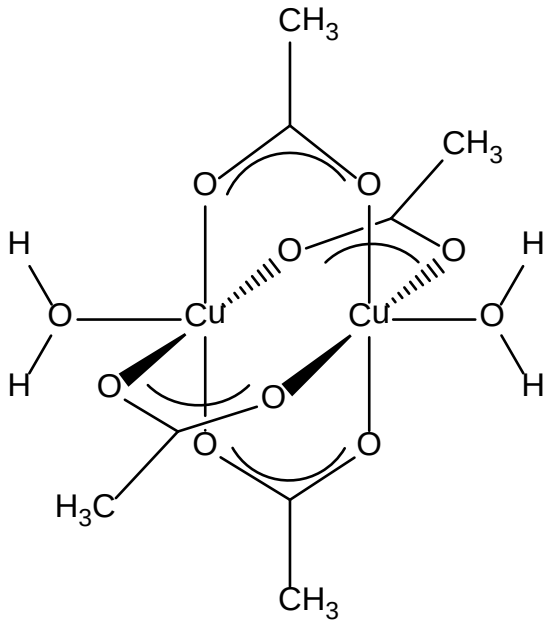
- copper(II) acetate monohydrate



- dicopper(II) tetraacetate dihydrate

An Inorganic Example

- copper(II) acetate monohydrate



- dicopper(II) tetraacetate dihydrate
- tetrakis(μ-acetato-κ^2*O*,*O*′)bis[(aqua)copper(II)]

There are Multiple Names for any given Compound

This a problem:

- Health and Safety
- Patents and Commercial Activity
- Taxation
- Government/International Regulations
- Computer Applications

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- PINs and InChIs

PINs and InChIs

- Preferred IUPAC Names
  - All nomenclatures are still allowed for general users
  - One preferred for legal and regulatory purposes

- International Chemical Identifier
  - Formula, connectivity, configuration, tautomers, isotopes etc
  - Coded into character string
  - Can be decoded
  - Bar codeable

Other Outputs

- Blue Book
- Principles of Chemical Nomenclature

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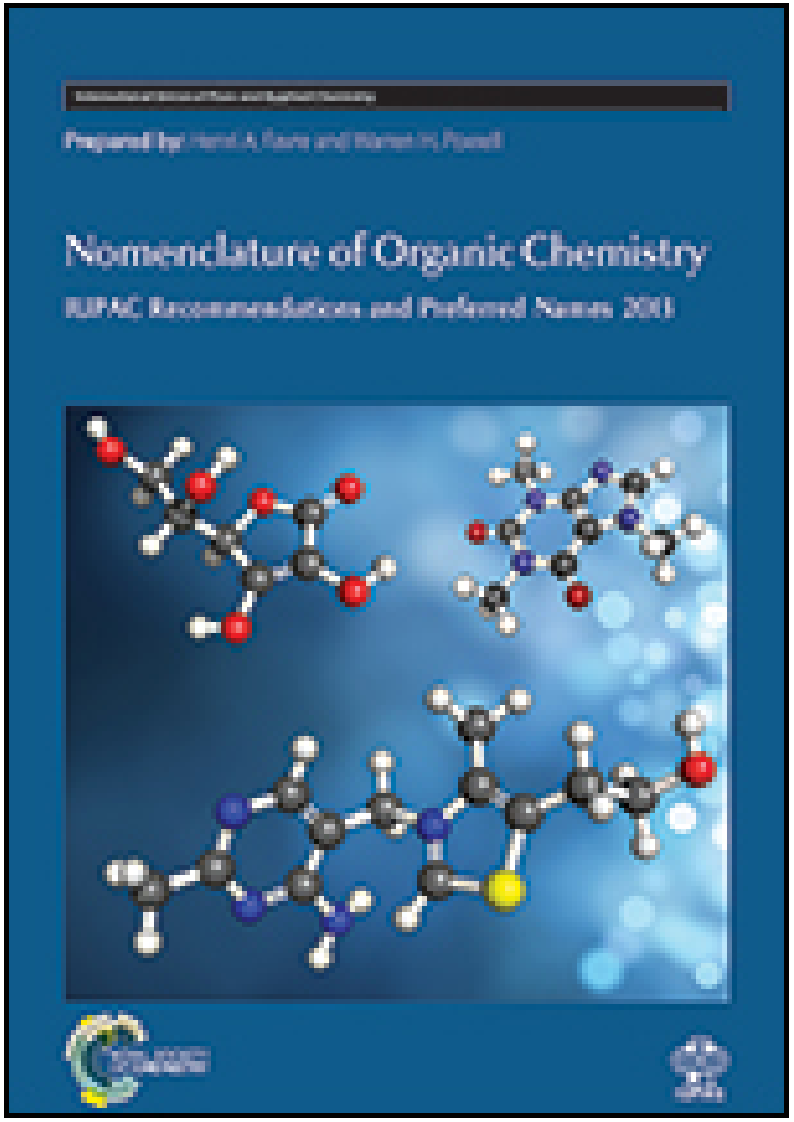
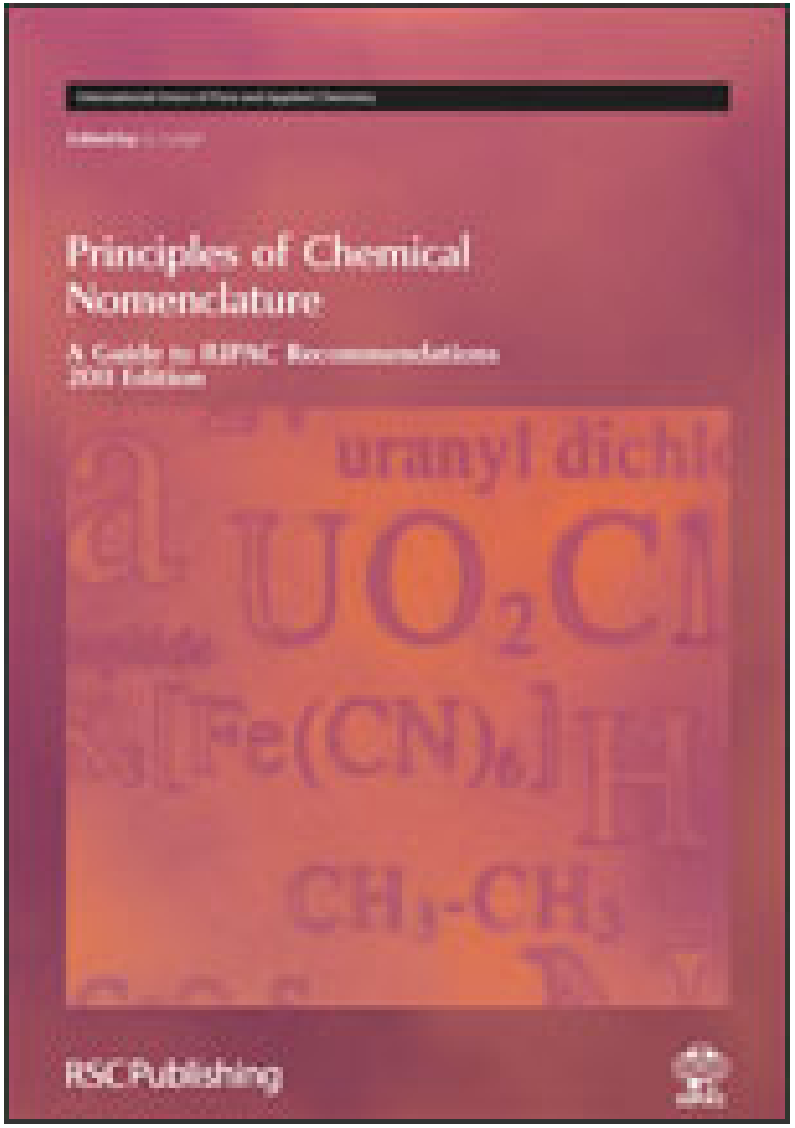
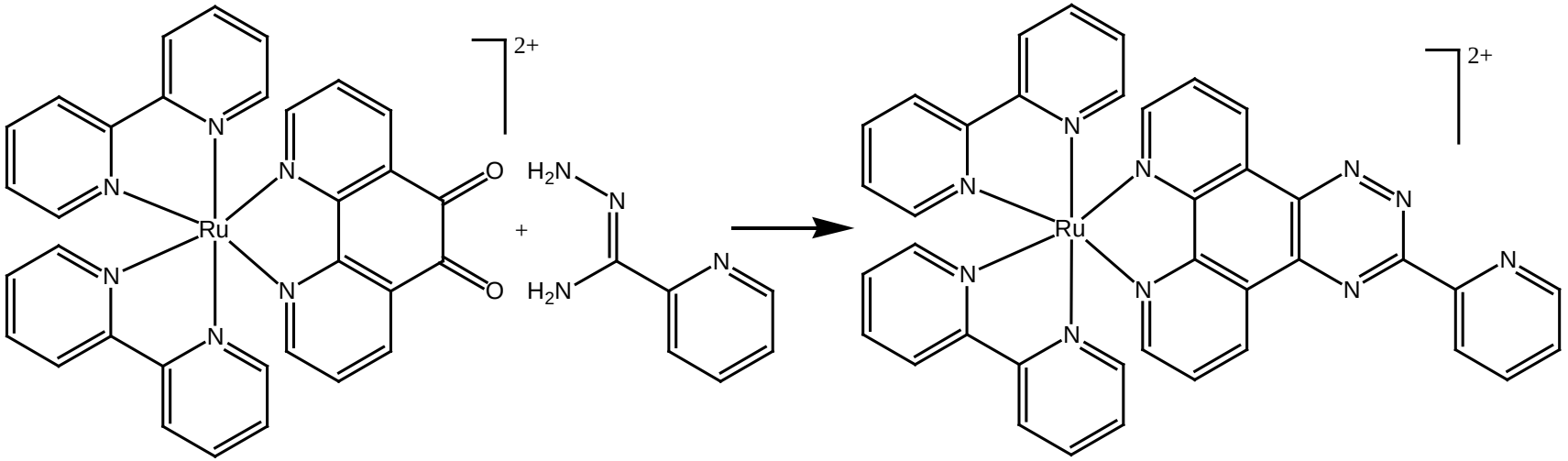


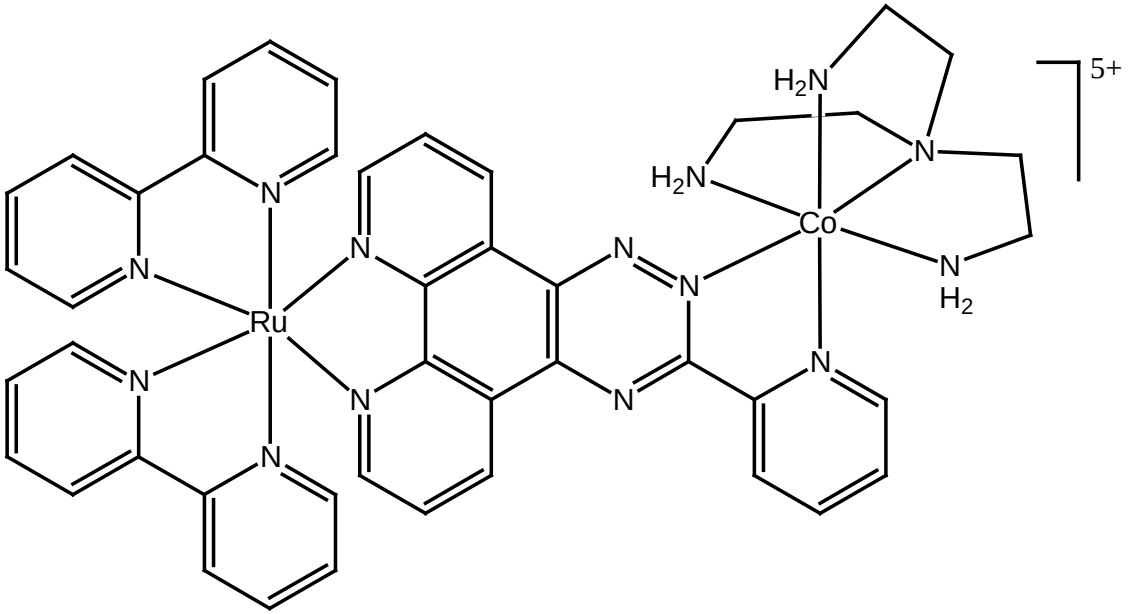


Other Outputs

- Blue Book
- Principles of Chemical Nomenclature
- Essentials documents
  - Inorganic nomenclature and organic nomenclature each condensed to four sides…
- Kappa grammar

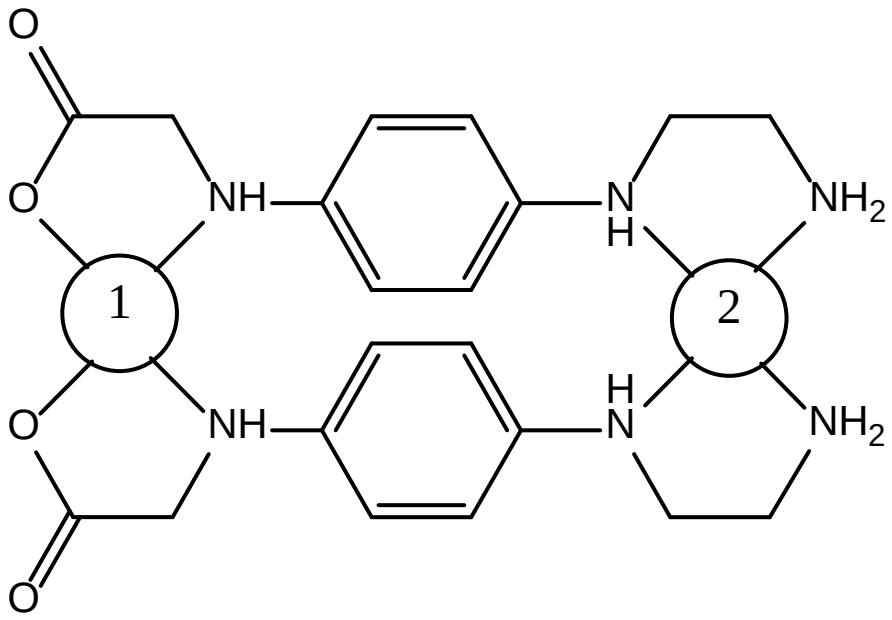


(*OC*-6)-bis(2,2’-bipyridine-κ^2*N*){3-(pyridin-2-yl)[1,2,4]triazino[6,5-*f*][1,10]phenanthroline-κ^2*N*}ruthenium(II)



(*OC*-6)-(*OC*-6-34)-bis(2,2'-bipyridine-1κ²*N*)[*N*,*N*-bis(2-amino-2κ*N*-ethyl)ethane-1,2-diamine-2κ²*N*]{μ-3-(pyridin-2-yl-2κ*N*)[1,2,4]triazino-2κ*N*²-[6,5-*f*][1,10]phenanthroline-1κ²*N*}ruthenium**cobalt**(5+)

Polynuclear Isomers



[bis{μ-([4-{(2-amino-2κ*N*-ethyl)amino-2κ*N*}phenyl] glycinato-1κ*N*,1κ*O*)}

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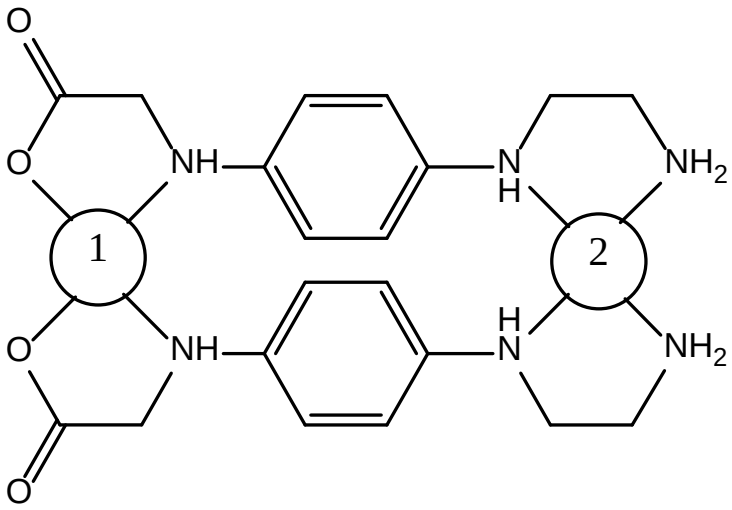
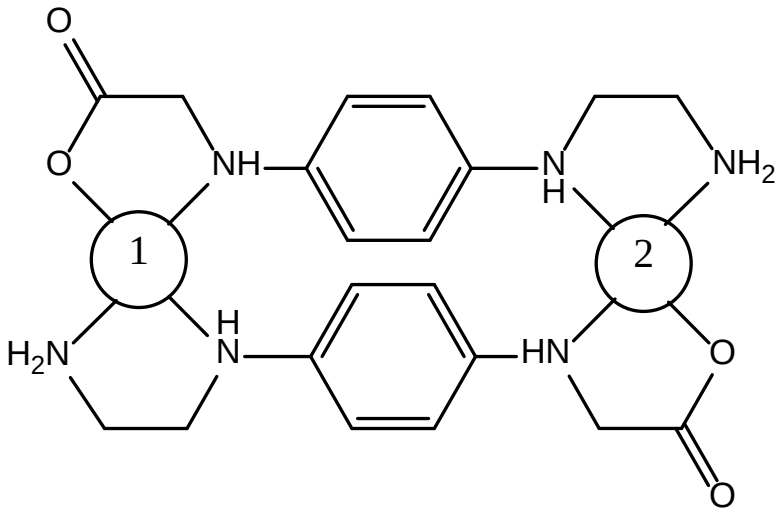
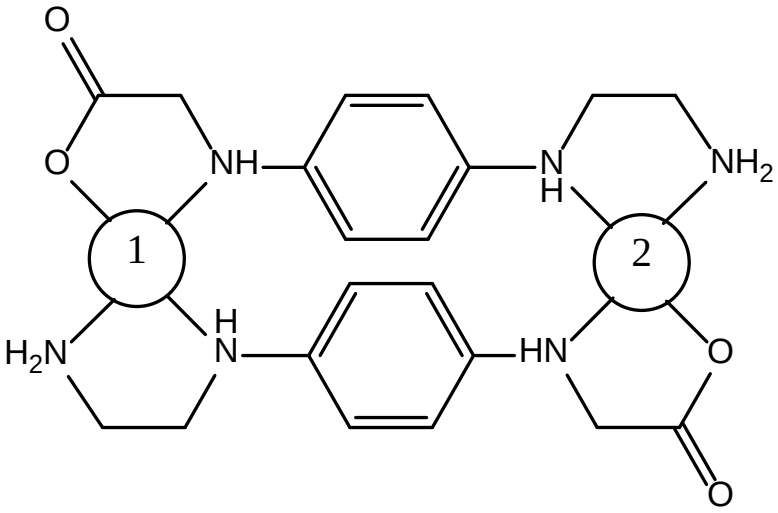


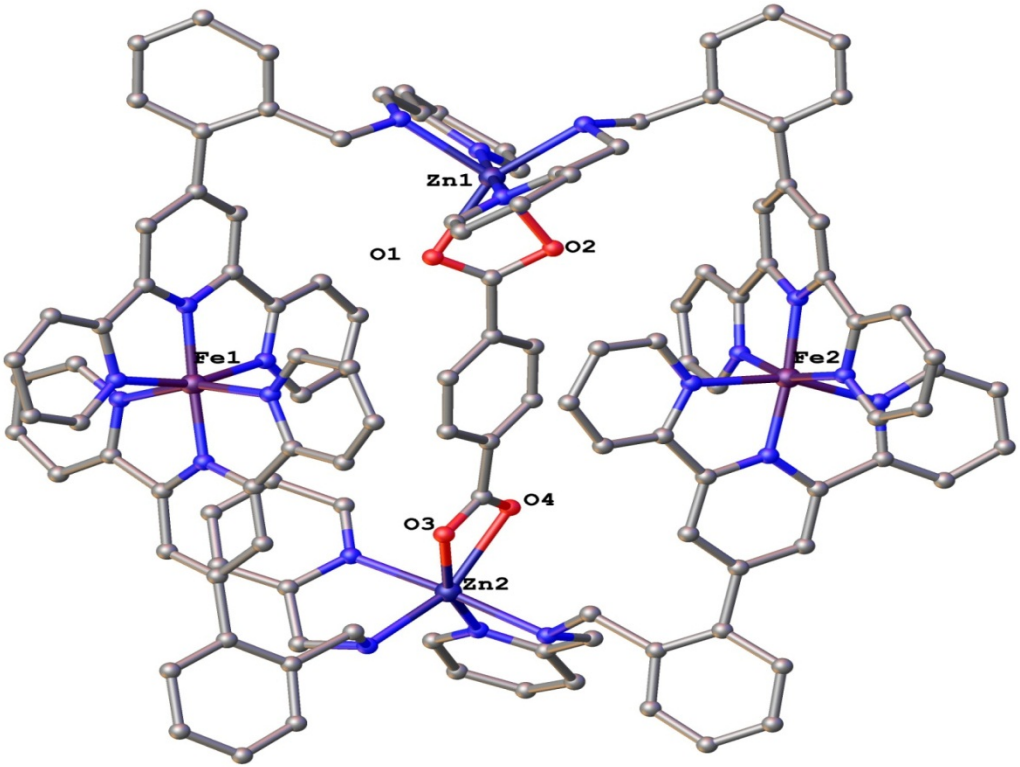


[bis{μ-([4-{(2-amino-2κ*N*-ethyl) amino-2κ*N*}phenyl]glycinato-1κ*N*,1κ*O*)}

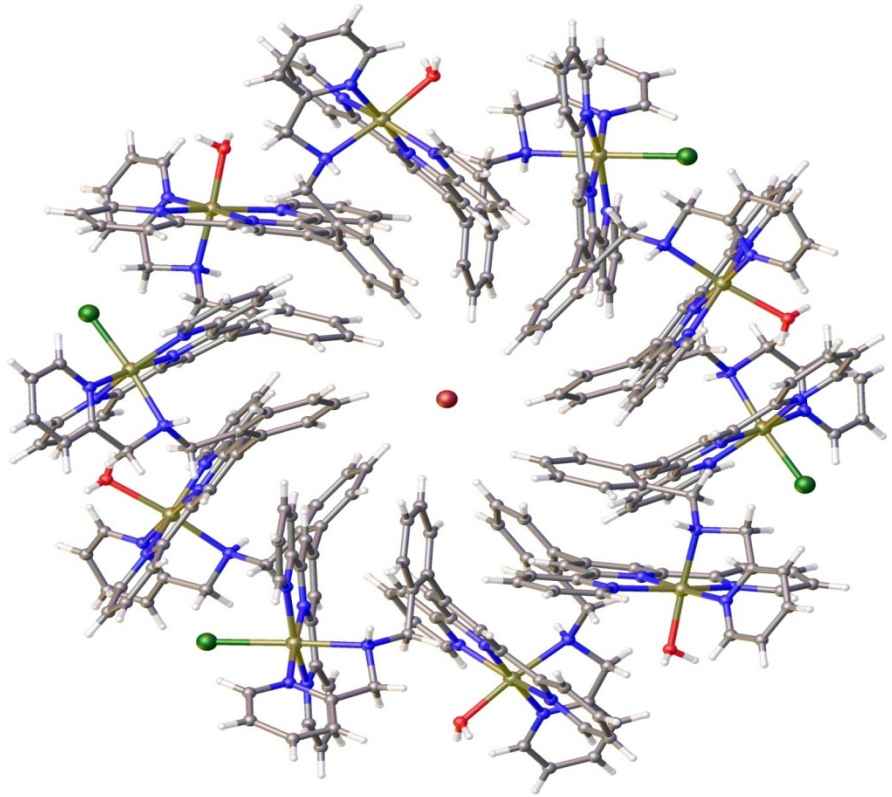


[{μ-([4-{(2-amino-1κ*N*-ethyl)amino-1κ*N*-}phenyl]glycinato-2κ*N*,2κ*O*)}{μ-([4-{(2-amino-2κ*N*-ethyl)amino-2κ*N*}phenyl]glycinato-1κ*N*,1κ*O*)}]]

[bis{μ-([4-{(2-amino-[1κ1*N*,2κ2*N*]-ethyl)amino-[1κ1*N*,2κ2*N*]}phenyl]glycinato-[1κ2*N*,2κ1*N*,1κ2*O*,2κ1*O*])}]



μ-benzene-1,4-dicarboxylato-3κ^2*O*^{1,1a}:4κ^2*O*^{4,4a}-tetrakis-μ-4′-{2-(2-pyridyl-[3κ1*N*,3κ2*N*,4κ3*N*,4κ4*N*]-methylamino-[3κ1*N*,3κ2*N*,4κ3*N*,4κ4*N*]-methyl) phenyl}-2,2’:6’,2”-terpyridine-[1κ^{3}1*N*,1κ^{3}3*N*,2κ^{3}2*N*,2κ^{3}4*N*]-diirondizinc(6+)



hexaaqua-1κ*O*,2κ*O*,3κ*O*,4κ*O*,5κ*O*,6κ*O*-tetrachlorido-7κ*Cl*,8κ*Cl*,9κ*Cl*,10κ*Cl*-decakis-μ-4′-{2-(2-pyridyl-[1κ1*N*,2κ2*N*,3κ3*N*,4κ4*N*,5κ5*N*,6κ6*N*,7κ7*N*,8κ8*N*,9κ9*N*,10κ10*N*]-methylamino-[1κ1*N*,2κ2*N*,3κ3*N*,4κ4*N*,5κ5*N*,6κ6*N*,7κ7*N*,8κ8*N*,9κ9*N*,10κ10*N*]-methyl) phenyl}-2,2’:6’,2”-terpyridine-[1κ^{3}2*N*,2κ^{3}10*N*,3κ^{3}4*N*,4κ^{3}9*N*,5κ^{3}7*N*,6κ^{3}8*N*,7κ^{3}1*N*,8κ^{3}3*N*,9κ^{3}5*N*,10κ^{3}6*N*]-decanickel(16+)