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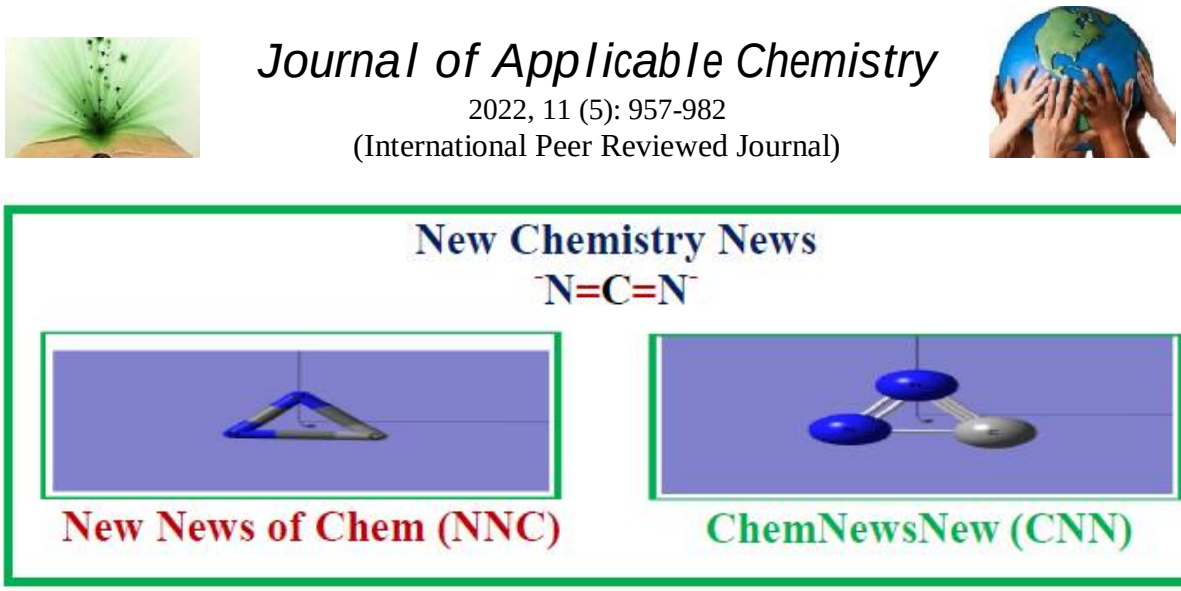

CNN – 48

Regiunbonds

Information Source	ACS.org ; sciencedirect.com
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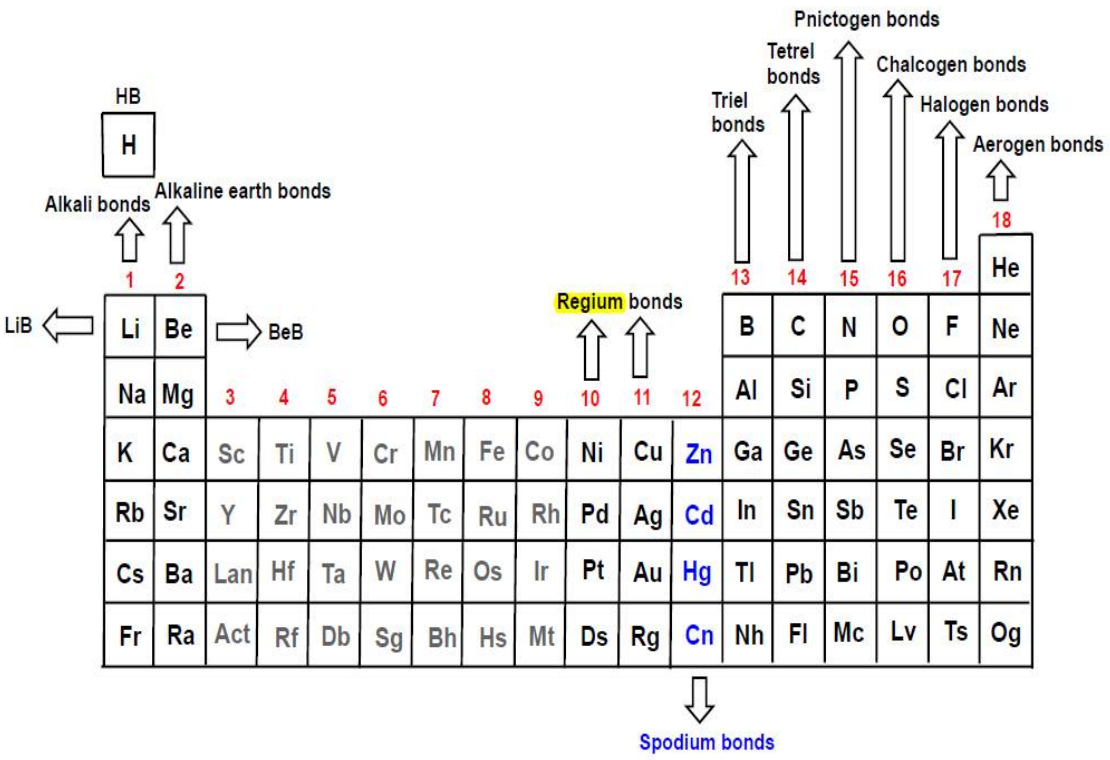
Conspectus: Regium atoms (RiA: [Cu; Ag; Au;Rg] ; [Ni; Pd; Pt; Ds]) belong to 11th and 10thgroup of 18 column chemical-elements-periodic-table. RiA exhibits Lewis's acid (LA) behaviour. RiAs forms complexes or adducts with Lewis bases (LB) including molecules or species with π electron systems. The regium (like triel, tetrel, pnic(t)ogen, chalcogen, halogen, aerogen, hydrogen, spodium, alkali, alkaline-earth) bond is also understood in terms of the σ-hole concept proposed by Politzer and Murray.

Knowledge based intelligent-pipe-line (with imbedded XI [:Artificial, eXplainable, Natural, Super Intelligence] of machine learning, deep learning, deep-NNs and preliminary-consciousness tools/work flows have been target/focus of our investigations of speciation in different phases and environments evolving into better and better approaches in trans-disciplinary chemical sciences. The multi-way flow/fusion with Physics, Biology based state-of-knowledge intervention-stunts will take the man-made scientific approaches towards greatest-benefit-to-human-kind.

Keywords: Interactions; Energy; Physics; Chemistry-Biology; Bonds; No-Bonds; Chemical bonds (CB); Electrovalent-B; Covalent Bond (CovB); Non-Covalent Chemical bonds (NCCB): [Nobel gas (Regiun), Halogen,Chalcogen, Pnicogen (or Pnictogen), Tetrel, Triel , Spodium, Regium (or Coinage), alkali, alkaline earth, Hydrogen [{strong, weak}, dihydrogen, hydride]], Synthesis, spectroscopy, computational quantum chemistry, Molecular dynamics

Layout		
I	Regiun bonds in chemical systems	K(nowledge)Lab
II	Select Research Titles	rsr.chem1979
III	SupInf Fig (Sif)	

I. Regiun bonds in chemical systems



Column# Periodic table	Abbrev	Abbrev	$$ bonds
	$$Bond	$$Atom	
1G	HyB	HyA	Hydrogen

Column#	Abbrev	Abbrev	$$ bonds
18G	NgB	NgA	Nobel gas
	AeB	AeA	Aerogen
17G@	HaB	HaA	Halogen
16G@	ChB	ChA	Chalcogen
15G	PnB	PnA	Pnicogen or Pnictogen
14G	TtB	TtA	Tetrel
13G	TrB	TrA	Triel
12G	SpB	SpA	Spodium

11G	CiB or RiB	CiA or RiA	Coinage or Regium
10G	RiB	RiA	Regium

Regiun bond is defined as non-covalent interaction between any electron donating moiety (Lewis base) and an chemical element of group 11 or 10 (RiA) acting as Lewis acid

2G	AEB AlkEarB	AEB AlkEarA	Alkaline-Earth
1G	AkB AlkB	AkA AlkA	Alkali

II. *Select Research Titles*

Dibismuthates as linking units for bis-zwitterions and coordination polymers	Inorganic chemistry 59.18 (2020): 13270-13280. https://doi.org/10.1021/acs.inorgchem.0c01619
Fekete, Csilla, Jamie Barrett, Zoltán Benkő, and Dominikus Heift.	
	RiB. 01

Alkyl methyl imidazolium-based ionic liquids at the Au (111) surface: anions and alkyl chain cations induced interfacial effects	The Journal of Physical Chemistry C 123.24 (2019): 15087-15098. https://doi.org/10.1021/acs.jpcc.9b03242
Kamalakannan, Shanmugasundaram, Muthuramalingam Prakash, Muneerah Mogren Al-Mogren, Gilberte Chambaud, and Majdi Hochlaf	
	RiB. 02

Adsorption of hydrophobic and hydrophilic ionic liquids at the Au (111) surface	ACS omega 3.12 (2018): 18039-18051. https://doi.org/10.1021/acsomega.8b02163
Shanmugasundaram Kamalakannan, Muthuramalingam Prakash, Gilberte Chambaud, and Majdi Hochla	
	RiB. 03

Regium− π Bonds Are Involved in Protein–Gold Binding	The Journal of Physical Chemistry Letters 11.19 (2020): 8259-8263. https://doi.org/10.1021/acs.jpclett.0c02295
Piña, María de las Nieves, Antonio Frontera, and Antonio Bauzá	
	RiB. 04

Regium–π bonds: An unexplored link between noble metal nanoparticles and aromatic surfaces	Chemistry–A European Journal 24.28 (2018): 7228-7234. https://doi.org/10.1002/chem.201800820
Frontera, Antonio, and Antonio Bauzá	
	RiB. 05

Alkorta, Ibon, et al. "Regium bonds between Silver (I) pyrazolates dinuclear complexes and Lewis bases (N2, OH2, NCH, SH2, NH3, PH3, CO and CNH)."	Crystals 10.2 (2020): 137. https://doi.org/10.3390/cryst10020137
Alkorta, Ibon, Cristina Trujillo, Goar Sánchez-Sanz, and José Elguero	
	RiB. 06

What's in a name?‘Coinage-metal’non-covalent bonds and their definition	Physical Chemistry Chemical Physics 20.29 (2018): 19332-19338. https://doi.org/10.1039/C8CP03432J
Legon, Anthony C., and Nicholas R. Walker	
	RiB. 07

Rivalry between regium and hydrogen bonds established within diatomic coinage molecules and Lewis acids/bases	ChemPhysChem 21.22 (2020): 2557-2563. https://doi.org/10.1002/cphc.202000704
Sánchez-Sanz, Goar, Cristina Trujillo, Ibon Alkorta, and José Elguero	
	RiB. 08

Interaction between trinuclear regium complexes of pyrazolate and anions, a computational study	International journal of molecular sciences 21.21 (2020): 8036. https://doi.org/10.3390/ijms21218036
Alkorta, Ibon, José Elguero, Cristina Trujillo, and Goar Sánchez-Sanz	
	RiB. 09

Detection and Properties of H2O··· Ag-- Cl and H2S··· Ag--Cl by Rotational Spectroscopy	Angewandte Chemie 122.1 (2010): 185-187. https://doi.org/10.1002/ange.200905799
Harris, Stephanie J., Anthony C. Legon, Nicholas R. Walker, and David E. Wheatley	
	RiB. 10

A Computational Study of the Interaction of Trinuclear Regium Complexes of Pyrazolate with Anions	International journal of molecular sciences 21.21 (2020): 8036. https://doi.org/10.3390/ijms21218036
Ibon Alkorta , José Elguero, Cristina Trujillo and Goar Sánchez-Sanz	
	RiB. 11

Cooperativity effects between regium-bonding and pnicogen-bonding interactions in ternary MF··· PH3O··· MF (M= Cu, Ag, Au): An ab initio study	Molecular Physics 118.24 (2020): e1784478. https://doi.org/10.1080/00268976.2020.1784478
Zhang, Zan, Tian Lu, Luyang Ding, Guanyu Wang, Zhaoxu Wang, Baishu Zheng, Yuan Liu, and Xun Lei Ding	
	RiB. 12

Unconventional π-hole and Semi-coordination regium bonding interactions directed supramolecular assemblies in pyridinedicarboxylato bridged polymeric Cu (II) Compounds: Antiproliferative evaluation and theoretical studies	Inorganica Chimica Acta 525 (2021): 120461. https://doi.org/10.1016/j.ica.2021.120461
Sarma, Pinku, Pranay Sharma, Antonio Frontera, Miquel Barcelo-Oliver, Akalesh K. Verma, Trinayan Barthakur, and Manjit K. Bhattacharyya	
	RiB. 13

Probing Au··· O and Au··· P regium bonding interaction in AuX (X= F, Cl, Br)··· RPHOH (R= CH3, F, CF3, NH2, CN) complexes	Computational and Theoretical Chemistry 1179 (2020): 112800. https://doi.org/10.1016/j.comptc.2020.112800
Zhou, Fengxiang, Yuan Liu, Zhaoxu Wang, Qingyuan Yang, and Baishu Zheng	
	RiB. 14

Computational chemistry methods for modelling non-covalent interactions and chemical reactivity—An overview	Journal of the Indian Chemical Society 98.11 (2021): 100208. https://doi.org/10.1016/j.jics.2021.100208
Hajji, Melek, Nadeem Abad, Mohamed A. Habib, Salima Moftah H. Elmgirhi, and Taha Guerfel	
	RiB. 15

Theoretical study of cooperativity between hydrogen bond–hydrogen bond, halogen bond–halogen bond and hydrogen bond–halogen bond in ternary FX… diazine … XF (X= H and Cl) complexes	Molecular Physics 114.23 (2016): 3464-3474. https://doi.org/10.1080/00268976.2016.1236992
Masoodi, Hamid Reza, Sotoodeh Bagheri, and Mahdiyeh Ranjbar.	
	RiB. 16

Comparison of hydrogen and halogen bonds between dimethyl sulfoxide and hypohalous acid: Competition and cooperativity	Molecular Physics 115.14 (2017): 1614-1623. https://doi.org/10.1080/00268976.2017.1308030
An, Xiulin, Xin Yang, Bo Xiao, Jianbo Cheng, and Qingzhong Li.	
	RiB. 17

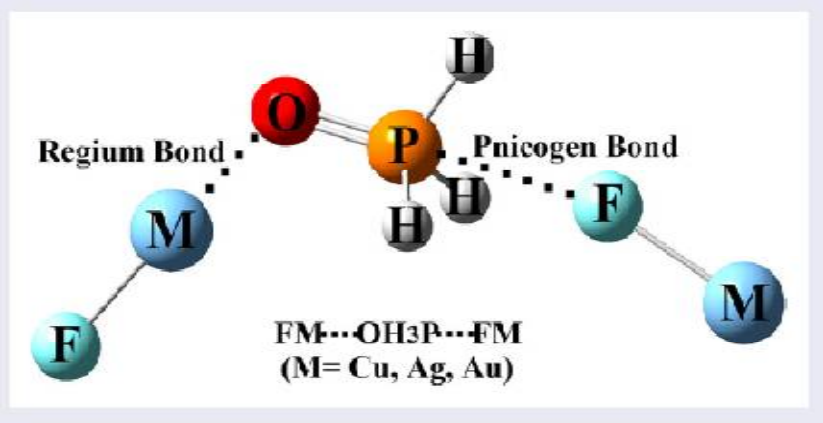
"Cooperative effects of hydrogen, halogen and beryllium bonds on model halogen-bonded FCl… YZ (YZ= BF, CO, N2) complexes in FX′… FCl… YZ trimers (FX′= FH, FCl, F2Be)	Molecular Physics 113.13-14 (2015): 1991-1997. https://doi.org/10.1080/00268976.2015.1027755
McDowell, Sean AC, and Dania S. Hamilton.	
	RiB. 18

III. Sup Inf Fig (Sif)

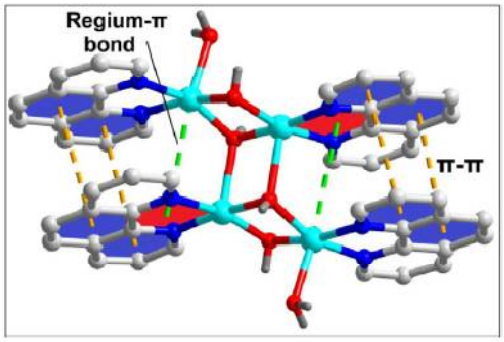
Regiun [Cu; Ag; Au;Rg] Bond (RiB, 11G)

[Ni; Pd; Pt; Ds] Bond (RiB, 10G)

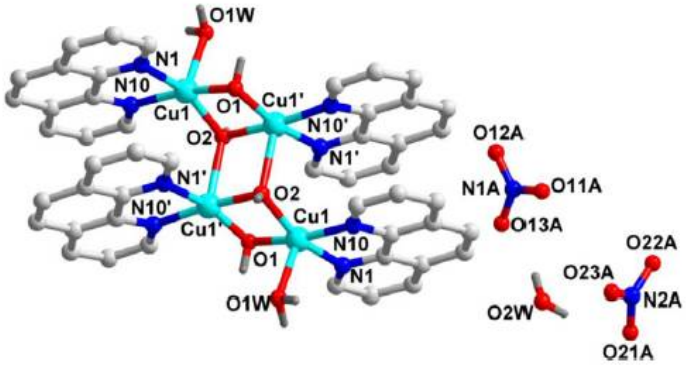
Regium Bond *[Cu Ag Au]*	*Pnicogen Bond*	RiB.	02



Regium- π(chelate) and π- πstacking
Cationic unit of compound 2

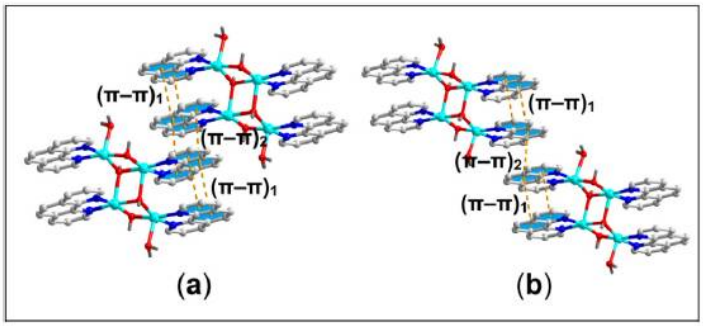


Molecular structure



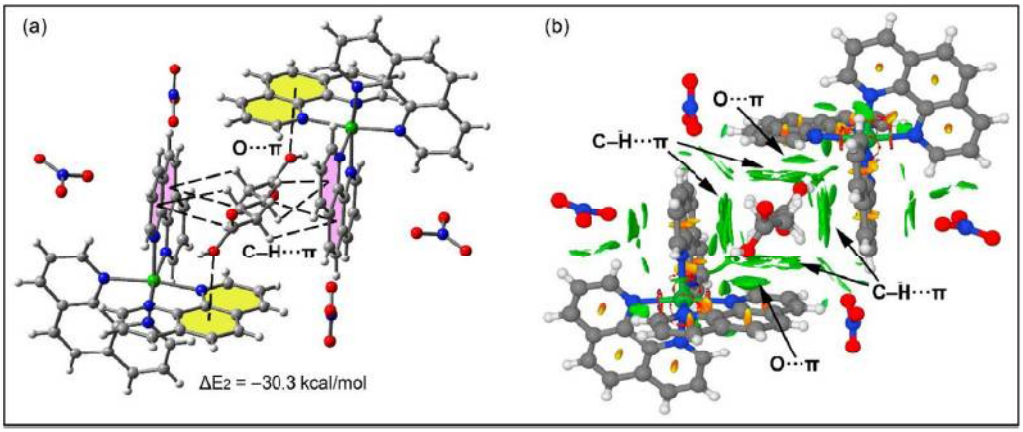
$[Cu_4 (phen)_4 (H_2O)_2 (OH)_4]4NO_3•2H2O_{(2)}]$

Crystal structure of compound 2



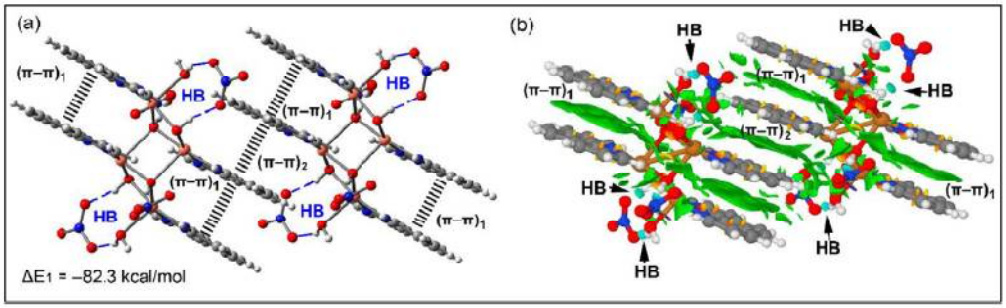
Cooperative (π–π) $_1$ /(π–π) $_2$ /(π–π) $_1$ ternary π-stacked assembly

Interaction of adp moiety with two [Ni(phen) 3] 2 +



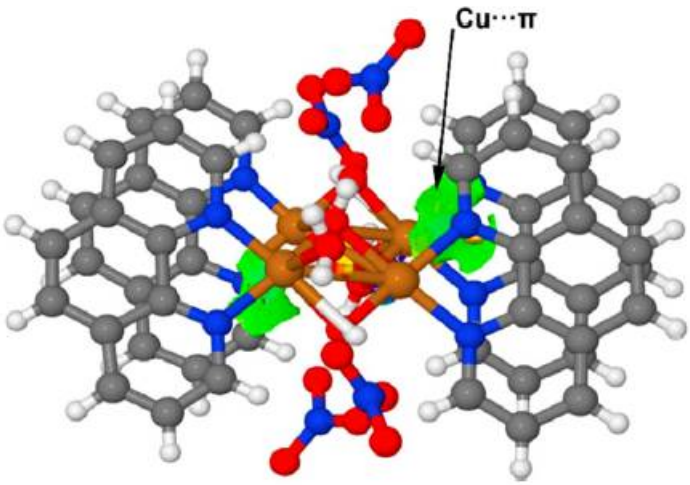
(a) O •••πand C–H •••πinteractions indicated as black dashed lines
(b) NCI surface

Dimer of compound 2

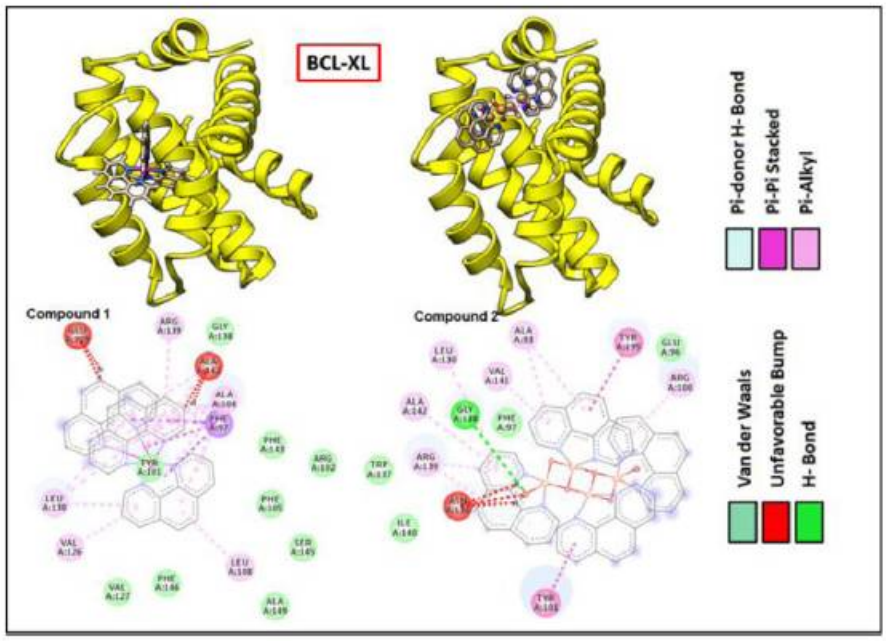


(a) black dashed lines: π-stacking interactions
(b) NCI surface of the (π–π) 1 /(π–π) 2 /(π–π) 1 π-stacked assembly compound 2

NCI surface of the compound 2

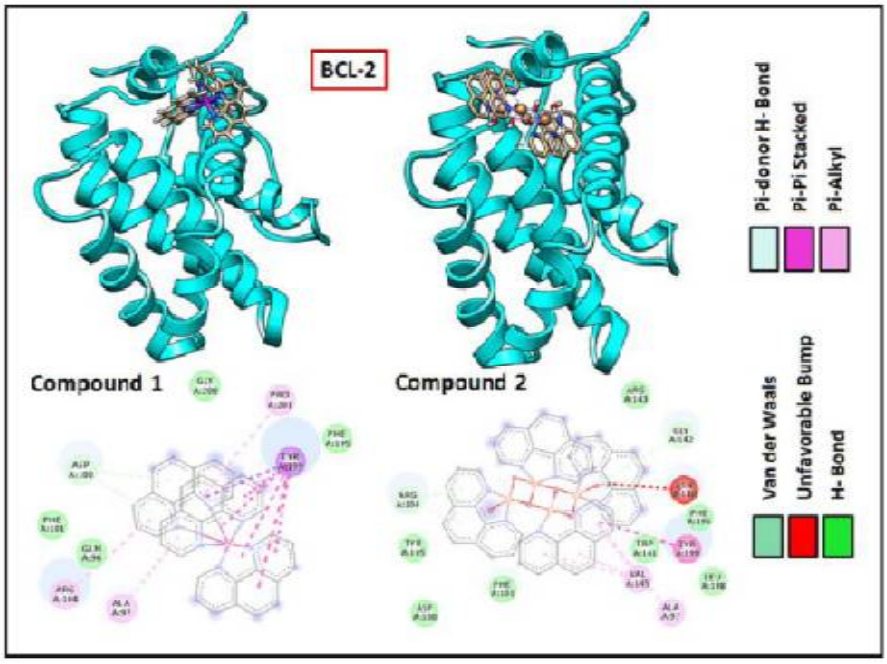


Docking structures of the compounds 1 and 2 with BCL-XL receptor



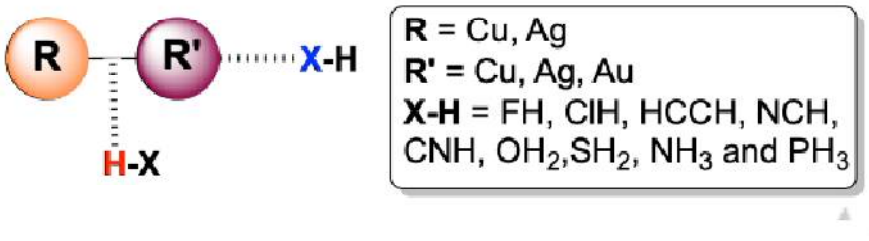
- Chemical interactions are shown along with ligand atoms and interacting amino acids in the inhibitor binding sites of receptors

Docking structures of the compounds 1 and 2 with BCL-2 receptor

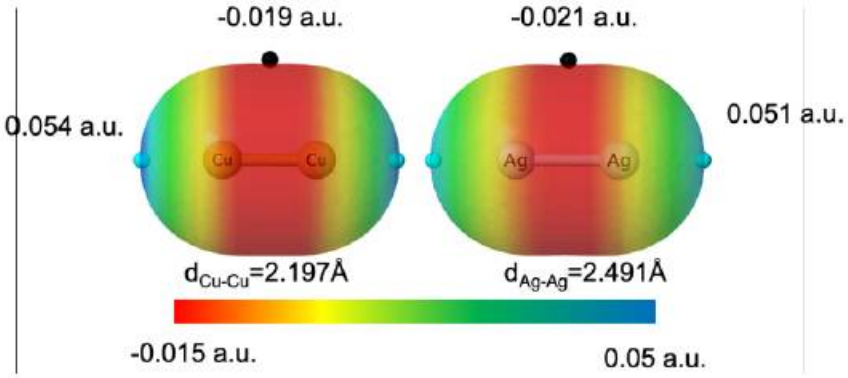


- Chemical interactions are shown along with ligand atoms and interacting amino acids in the inhibitor binding sites of receptors

Systems under study

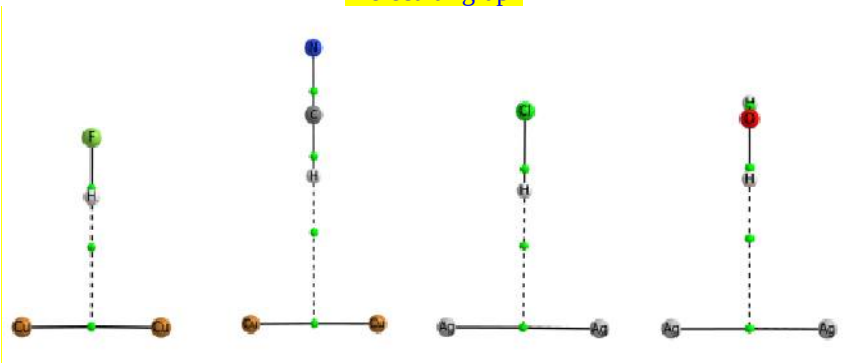


MESP



Ag2 and Cu2 monomers

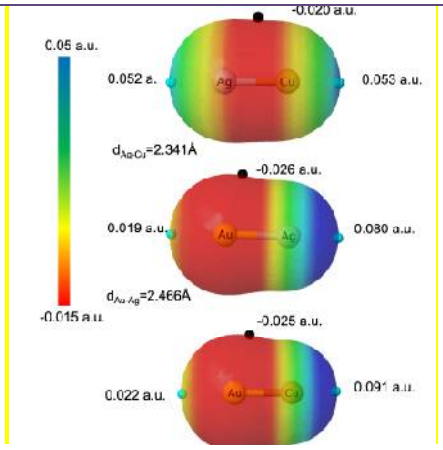
Molecular graph



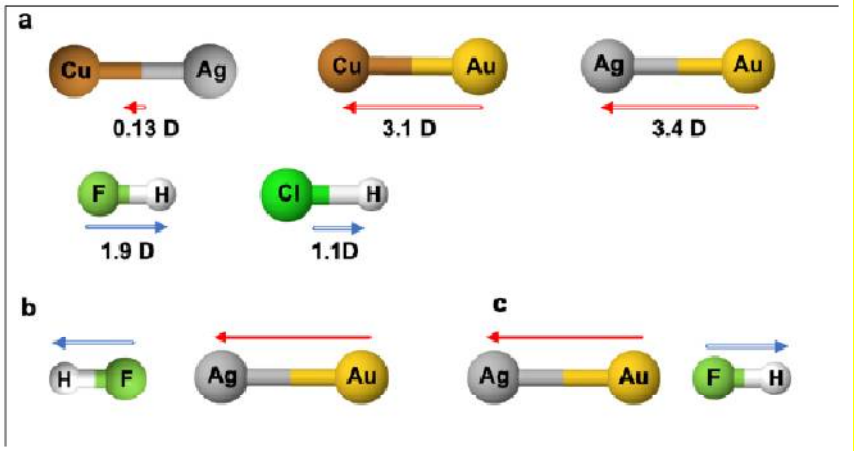
Cu2:HF Cu2:HCN Ag2:HCl Ag2:HOH

ESPRR' molecules

MP2/jul-cc-pVTZ



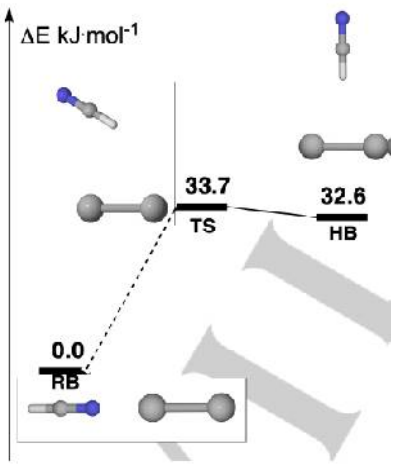
Dipole moments (D)



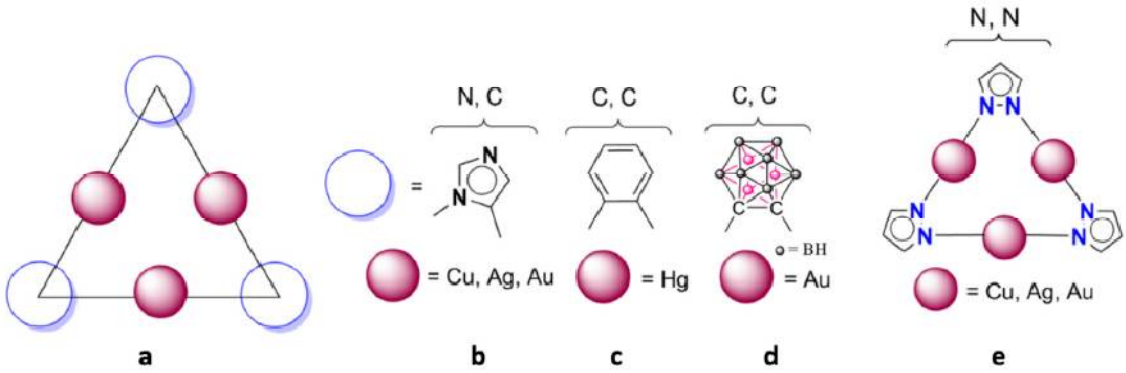
Regium bonds B) H-F…AgAu (C) AgAu…F-H

F…Ag **Au…F**

Potential energy surface
Ag2:HCN complex

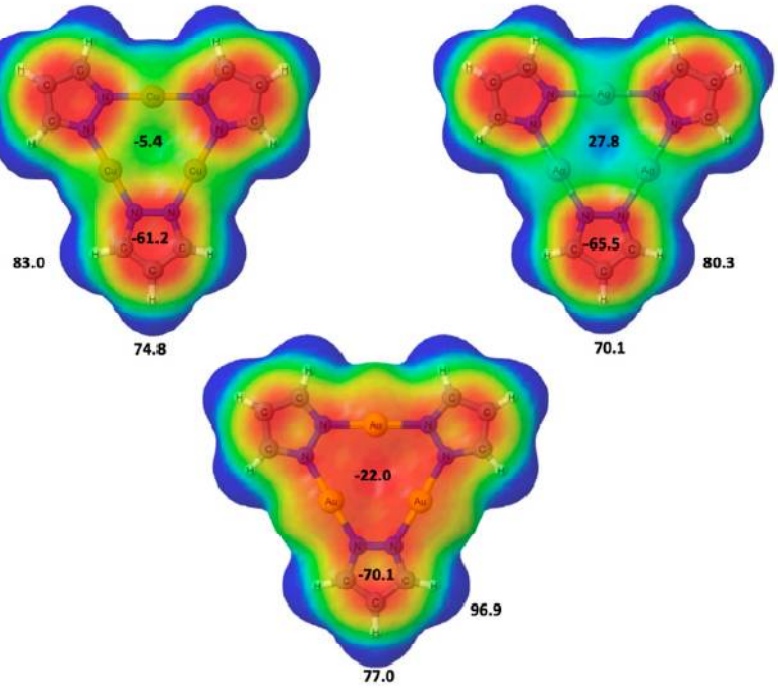


Structures

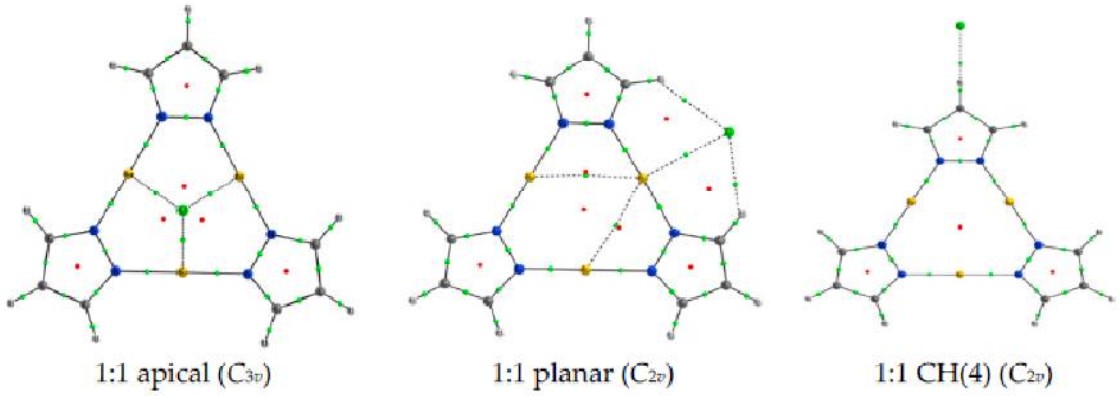


Full red circles : metal;
(a) Emptyblue circles the ligand
(b) Imidazolate ligands linked by N and C atoms
(c) Phenylene ligands linkedby C atoms
(d) 1,2-Dicarba-closo-dodecaborane ligands linked by C atoms
(e) Pyrazolate ligands linked by N atoms

MESP (Pz-M)3

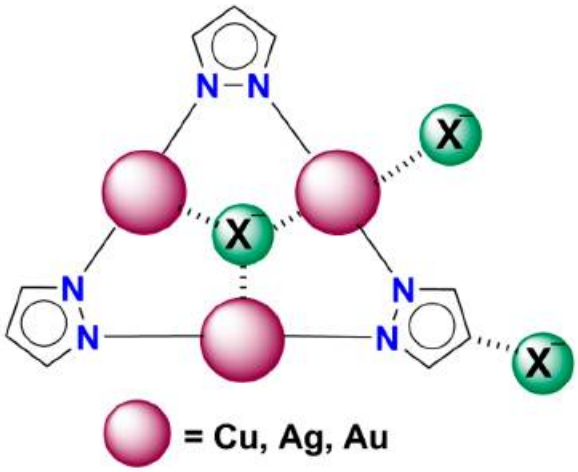


Molecular graph

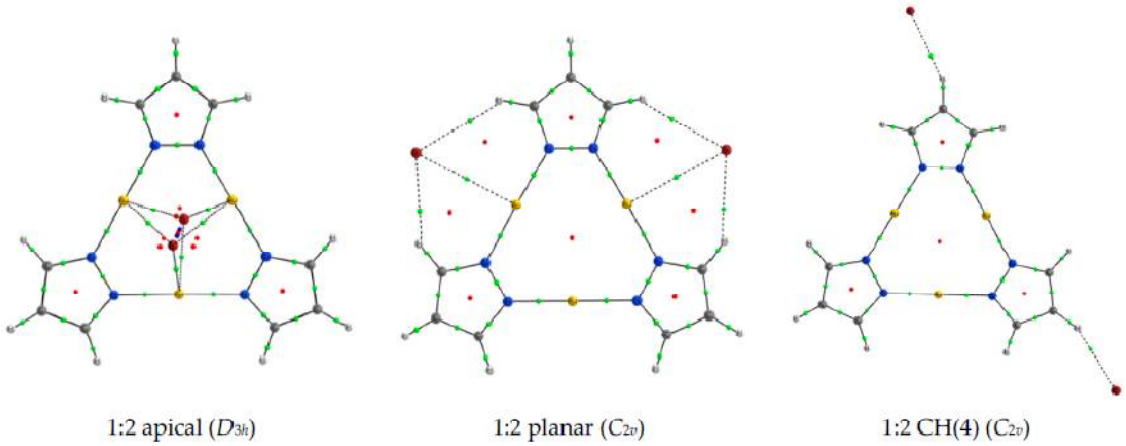


- ✓ Three minima located for the 1:1 (Pz-Au)3: Cl–
- ✓ Small green and red dots : position of the bond and ring critical points

Complexes with X- (X = F, Cl and Br)

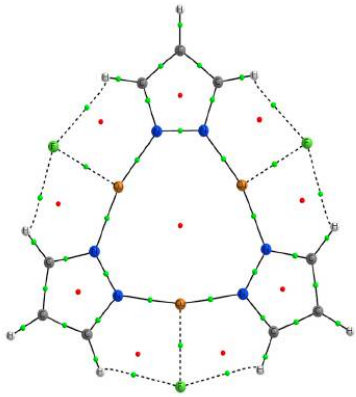


Molecular graph

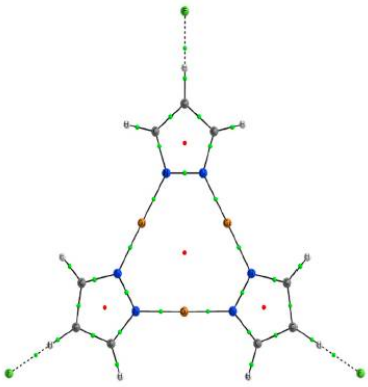


- ✓ Three minima located for the 1:2 (Pz-Au)3 and Br–
- ✓ Small green and red dots : position of the bond and ring critical points

Molecular graph



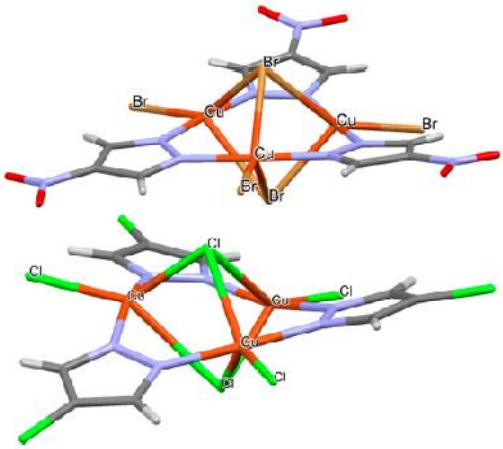
1:3 planar (D_{3h})



1:3 CH(4) (D_{3h})

- ✓ Three minima located for the 1:3 (Pz-Au)3:F−.
- ✓ Small green and red dots : position of the bond and ring critical points

Refcodes ELODOY (up) and OBOQAY (down)



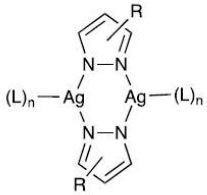
(Pz-M)3: anions

Regium Bond

[Ag]

RiB. 06

Structure of the complexes

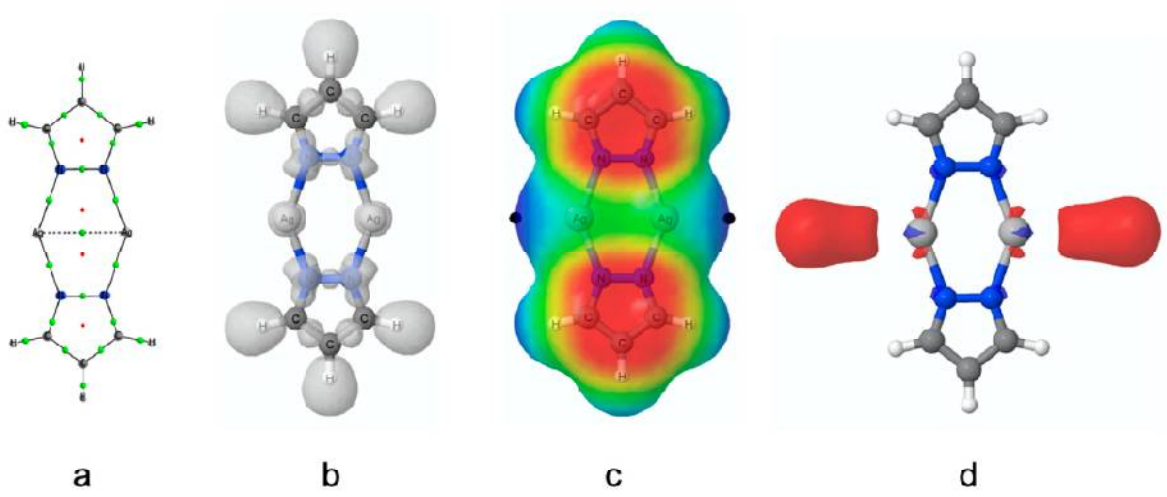


R = H, 4-NO_2, 3,5-diMe, 4-Cl,

L = N_2, OH_2, NCH, SH_2, NH_3, PH_3, CNH

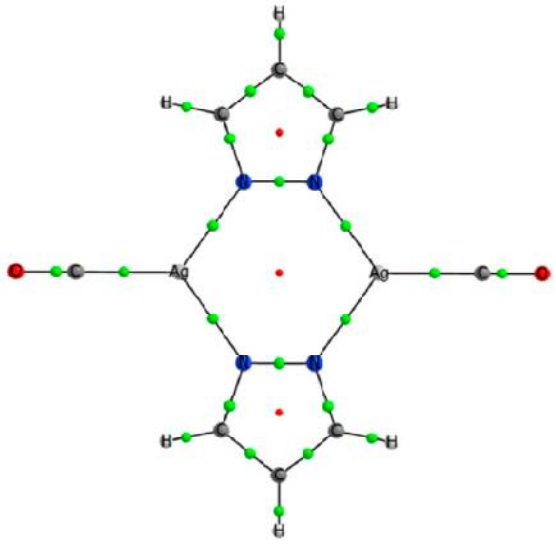
n = 0, 1, 2, 4

$(PzAg)_2$	$(PzAg)_2(PH_3)_2$	$(4NO_2pzAg)_2(PH_3)$
$(PzAg)_2(N_2)_2$	$(PzAg)_2(CO)_2$	$(4NO_2pzAg)_2(PH_3)_2$
$(PzAg)_2(OH_2)_2$	$(PzAg)_2(CNH)_2$	$(4NO_2pzAg)_2(PH_3)_4$
$(PzAg)_2(NCH)_2$	$(PzAg)_2(PH_3)$	$(DMepzAg)_2$
$(PzAg)_2(SH_2)_2$	$(PzAg)_2(PH_3)_4$	$(4ClpzAg)_2$
$(PzAg)_2(NH_3)_2$	$(4NO_2pzAg)_2$	$(DMepzAg)_2(PH_3)_2$
		$(4ClpzAg)_2(PH_3)_2$

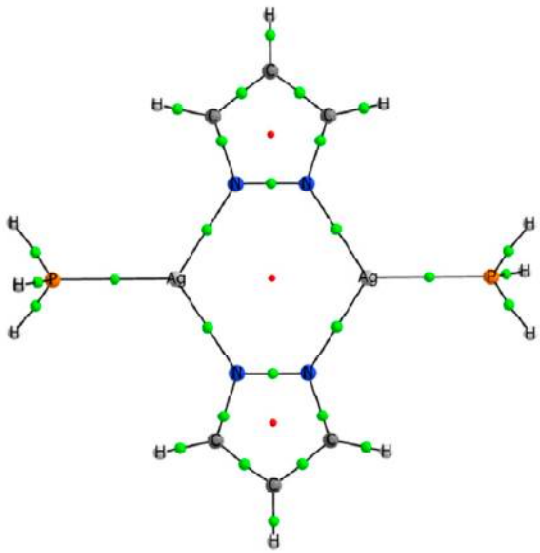


(a) Molecular graph
Green and red dots : location of bond and ring critical points
(b) Electron localization function (ELF)
(c) MESP
(d) LUMOorbital of the (PzAg)2 system

Bond crit points (BCP)
Ring crit points (RCP)

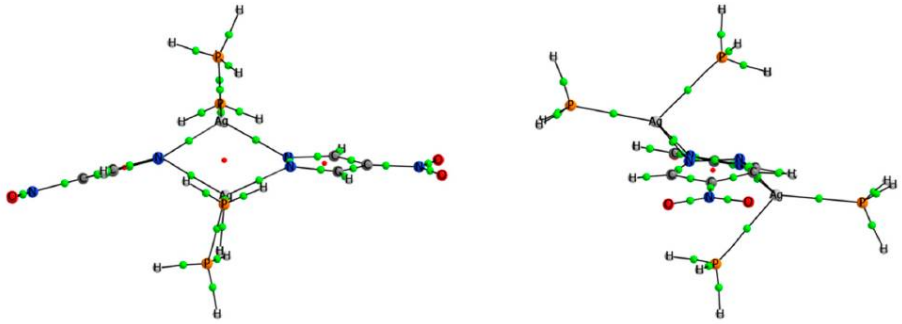


(PzAg)2(CO)2



(PzAg)2(PH3)2

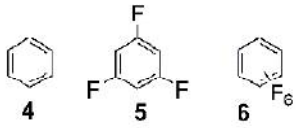
Two orthogonal views
(4NO2pzAg)2(PH3)4 complex



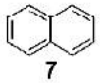
Regium Bond [ ]		RiB.	05

Species

1, M = Cu
2, M = Ag
3, M = Au



4 **5** **6**



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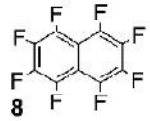

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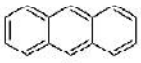

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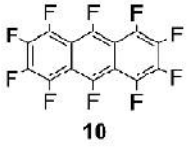

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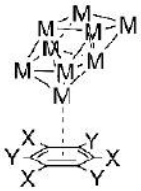
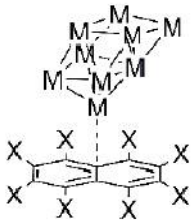
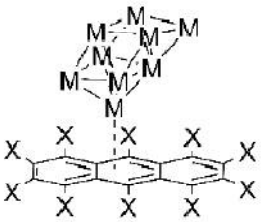


11, M = Cu, X = Y = H
12, M = Ag, X = Y = H
13, M = Au, X = Y = H
14a, M = Cu, X = F, Y = H
14b, M = Cu, X = F, Y = H
15a, M = Ag, X = F, Y = H
15b, M = Ag, X = F, Y = H
16a, M = Au, X = F, Y = H
16b, M = Au, X = F, Y = H
17, M = Cu, X = Y = F
18, M = Ag, X = Y = F
19, M = Au, X = Y = F

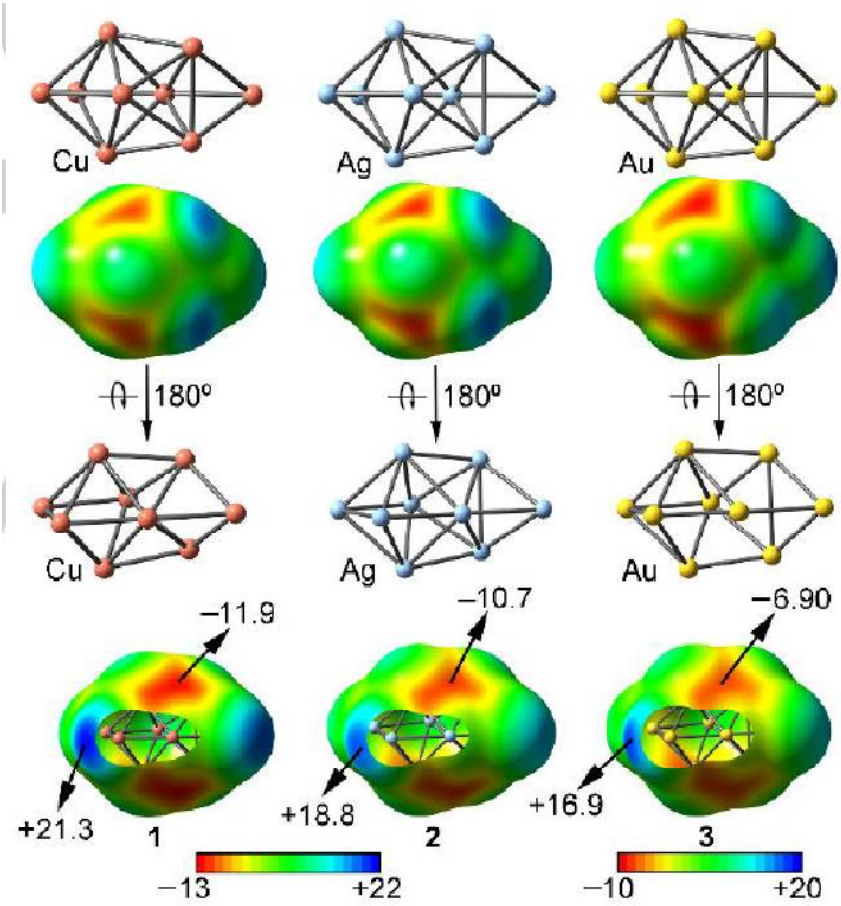


20, M = Cu, X = H
21, M = Ag, X = H
22, M = Au, X = H
23, M = Cu, X = F
24, M = Ag, X = F
25, M = Au, X = F

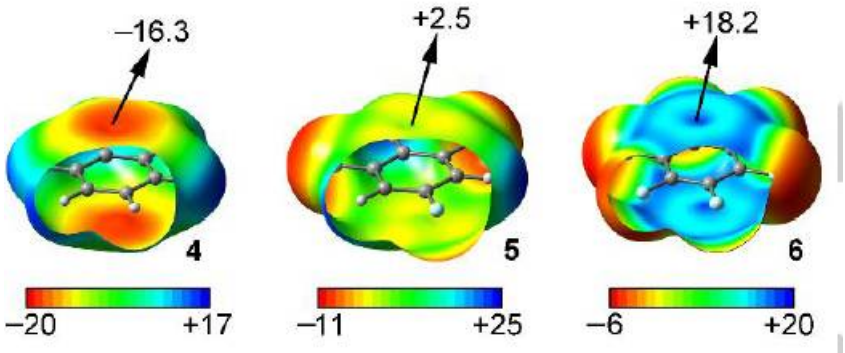


26, M = Cu, X = H
27, M = Ag, X = H
28, M = Au, X = H
29, M = Cu, X = F
30, M = Ag, X = F
31, M = Au, X = F

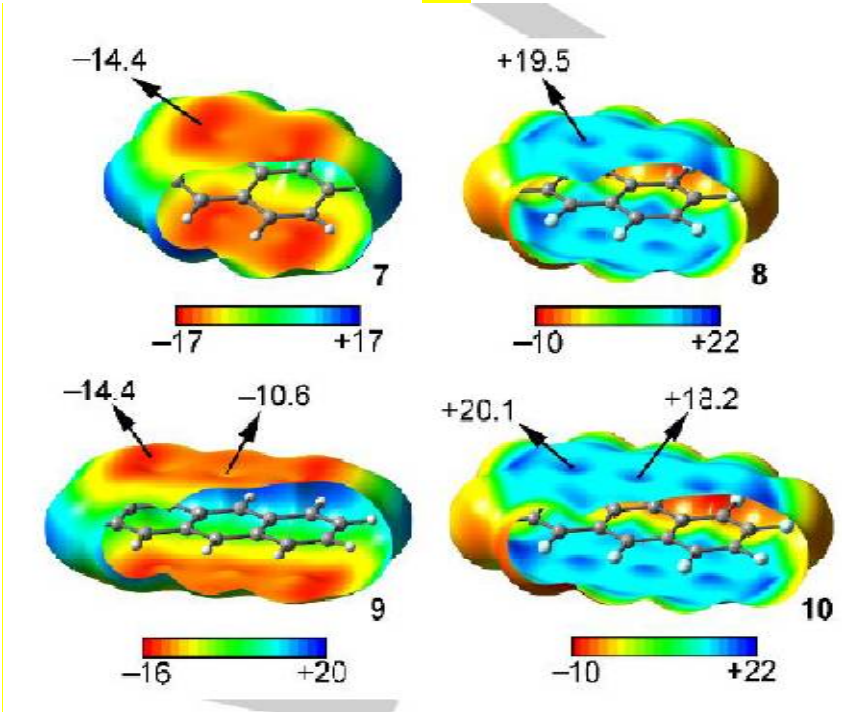
MESP


Cu
Ag
Au
180°
180°
180°
Cu
Ag
Au
−11.9
+21.3
1
−13
+22
−10.7
+18.8
2
−6.90
+16.9
3
−10
+20

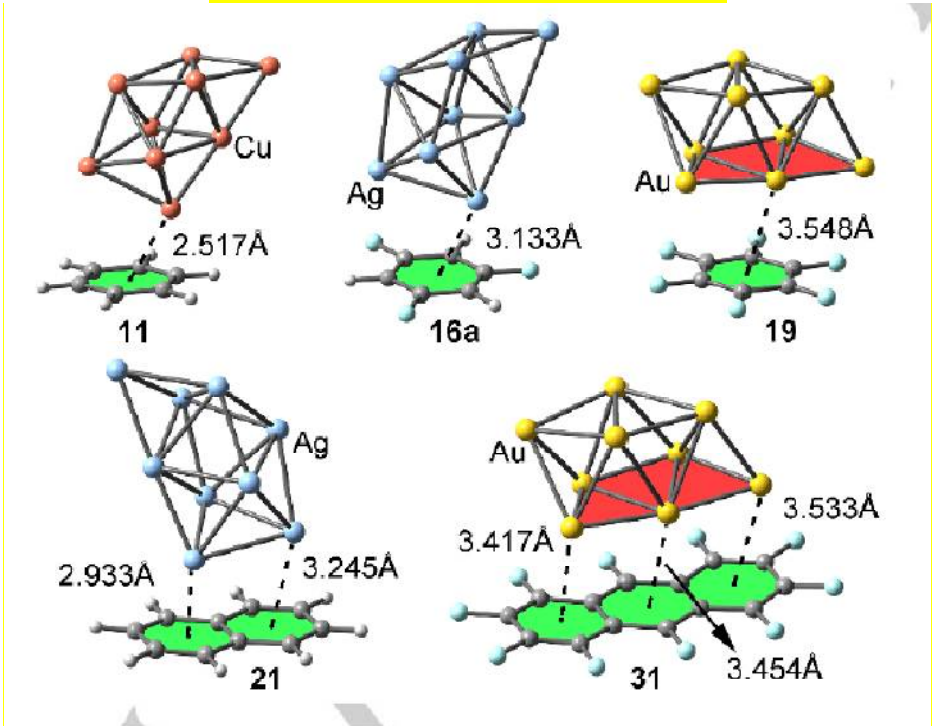
ESP


−16.3
4
−20
+17
+2.5
5
−11
+25
+18.2
6
−6
+20

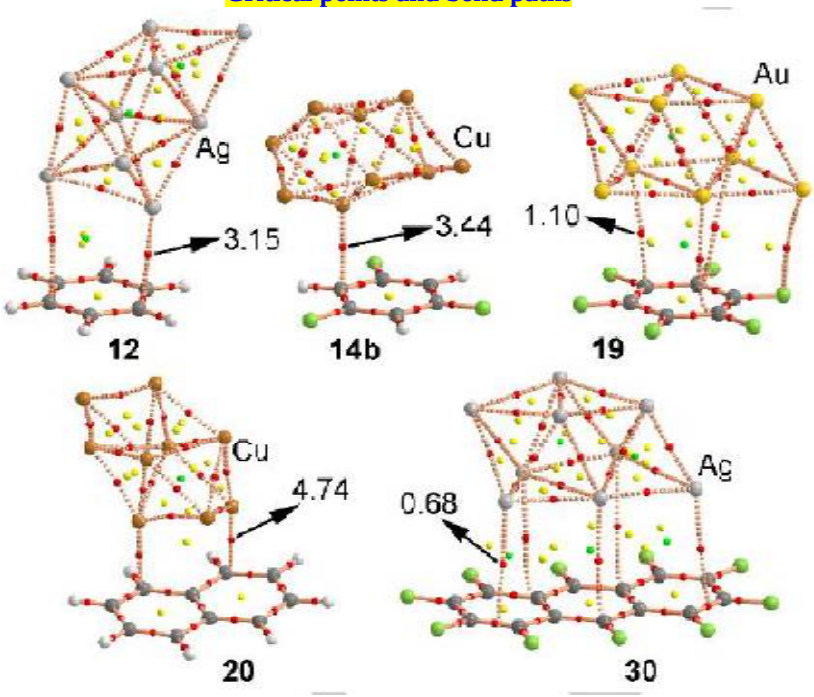
ESP



Optimized geometries
PBE0-D3/def2-TZVPP//PBE0-D3/def2-TZVP



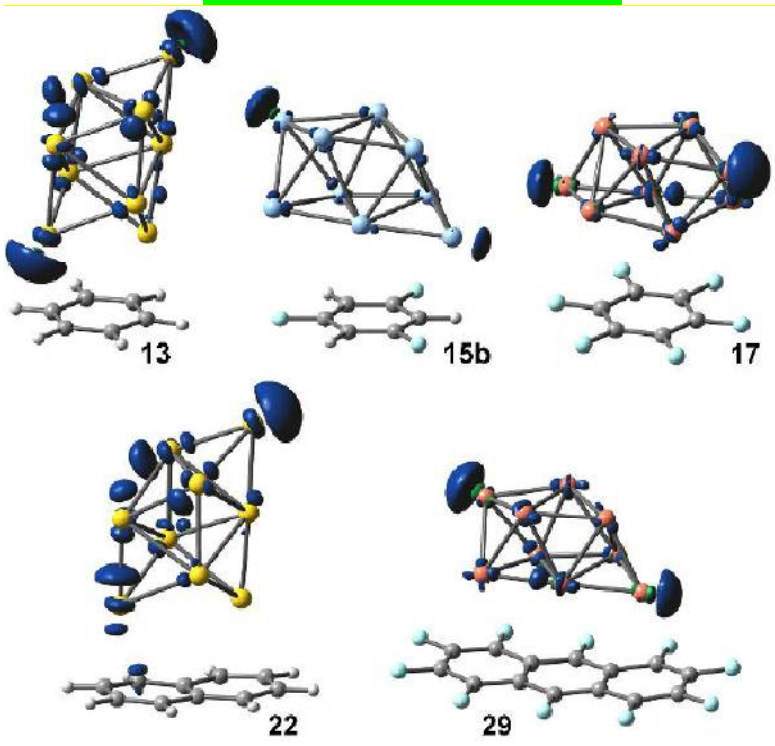
Critical points and bond paths



Bond, ring, cage critical points: red, yellow, green spheres

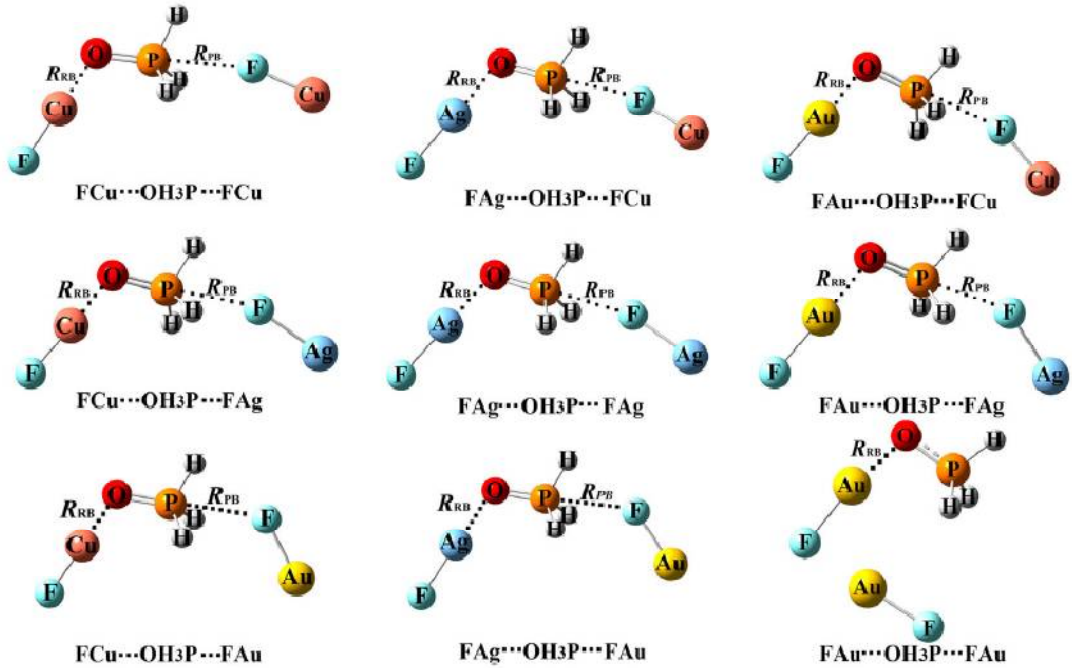
Spin Density plots

PBE0/def2-TZVP//PBE0/def2-TZVP

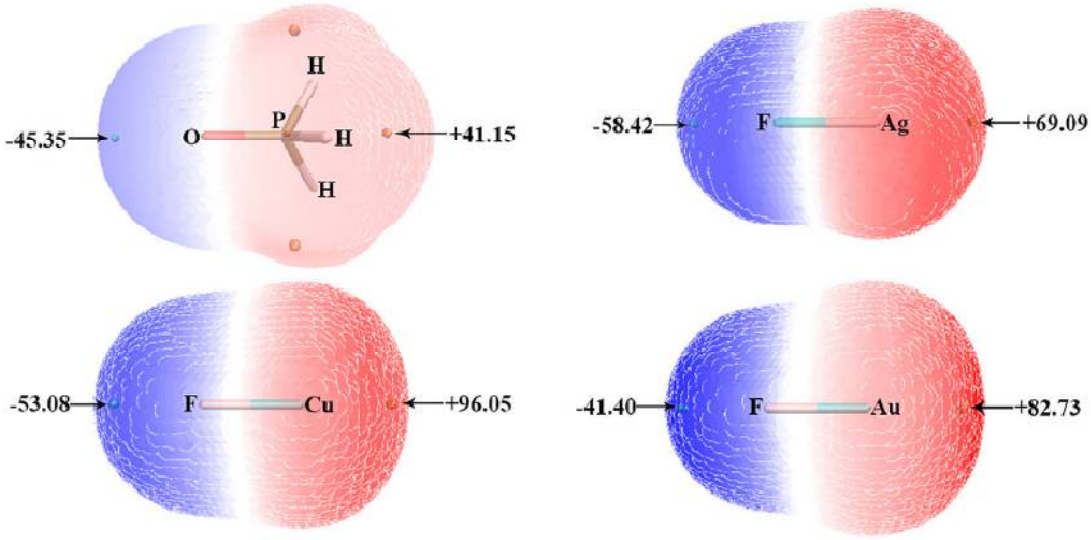


Optimised Geometry

MP2/aug-cc-pVTZ level

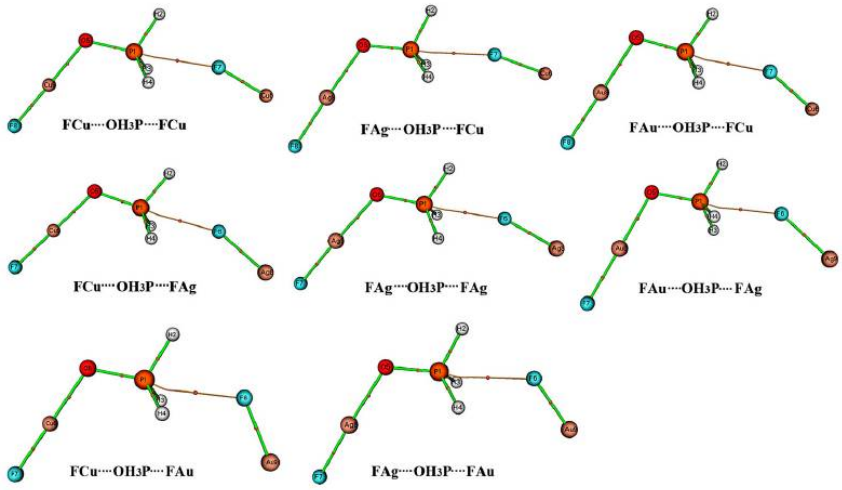


ESP



Molecular graphs of the ternary complexes

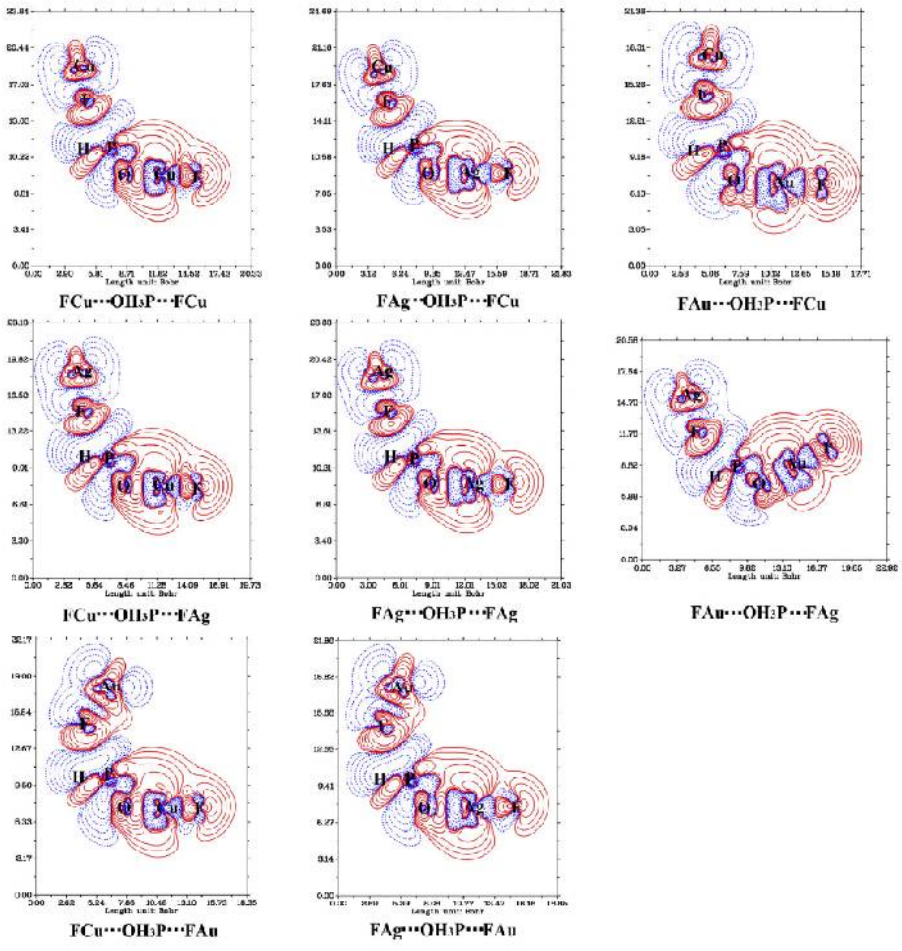
MF···PH3O···MF (M = Cu, Ag, Au)



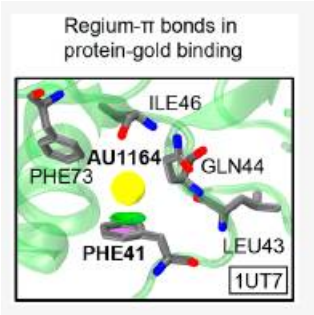
- Red dots : bond critical points

Computed density difference plots

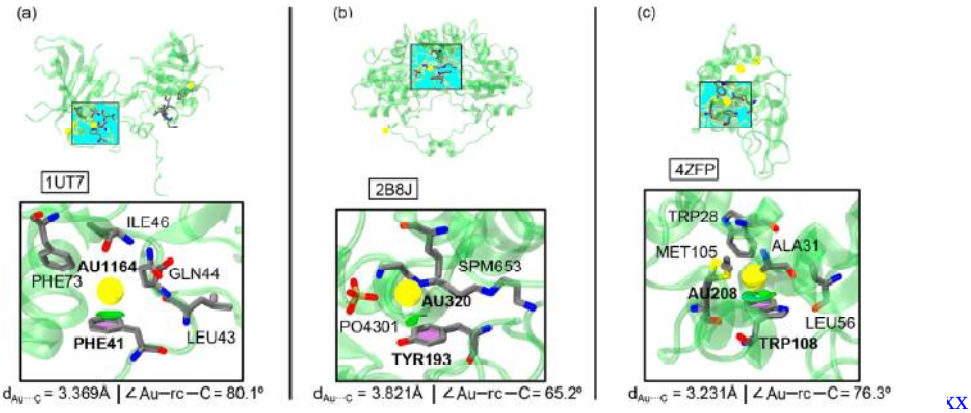
Ternary complexes
MF···PH3O···MF (M = Cu, Ag, Au)



Regium-π bond

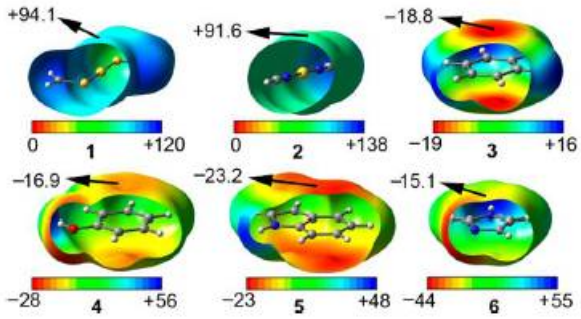


Partial views of the X-ray structures

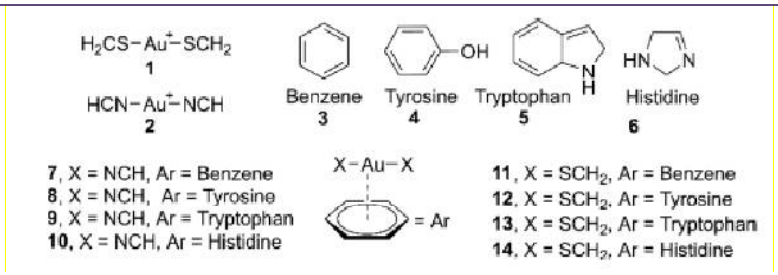


✓ Regium–π interaction is magnified in bottom part of figure
✓ NCIplot analyses are denoted by the green isosurfaces inside

ESP



Compounds 1–6
Complexes 7–14



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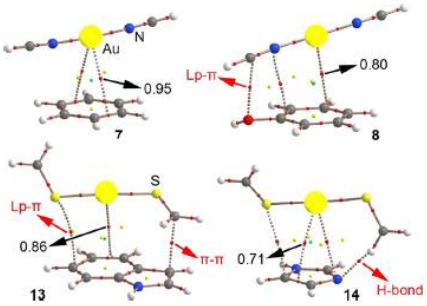
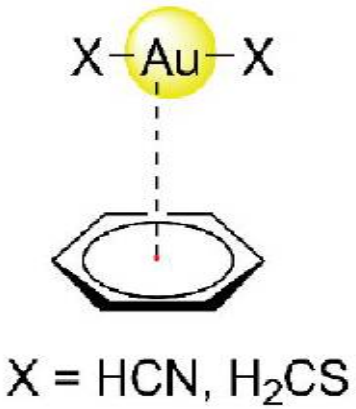
Bond, ring, and cage critical points are as red, yellow, and green dots



Regium Bond *[Au]*		RiB.	03SI

xx



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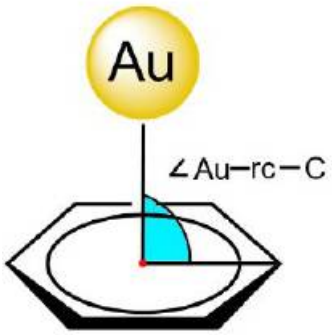
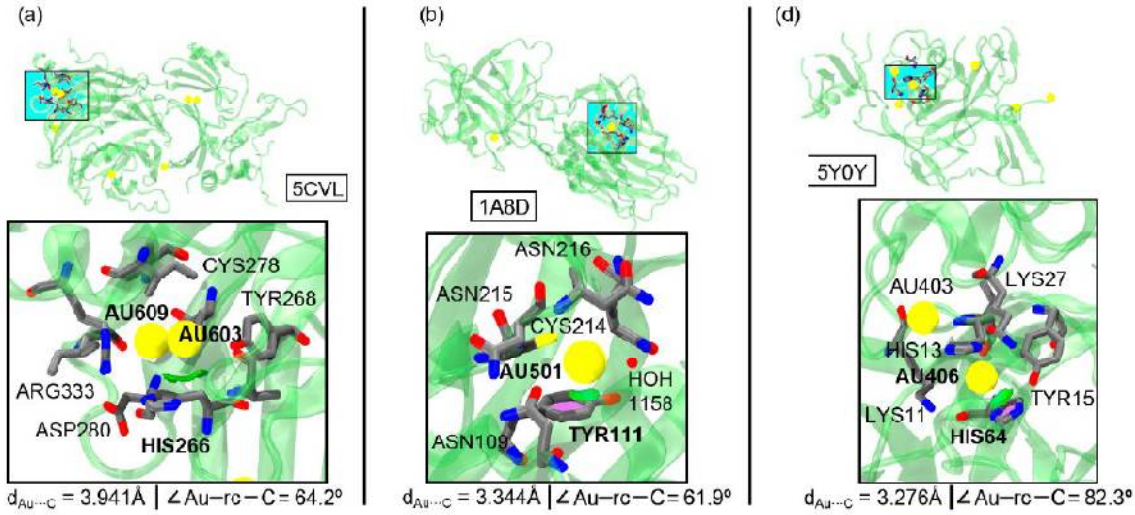


Regium-π interaction model

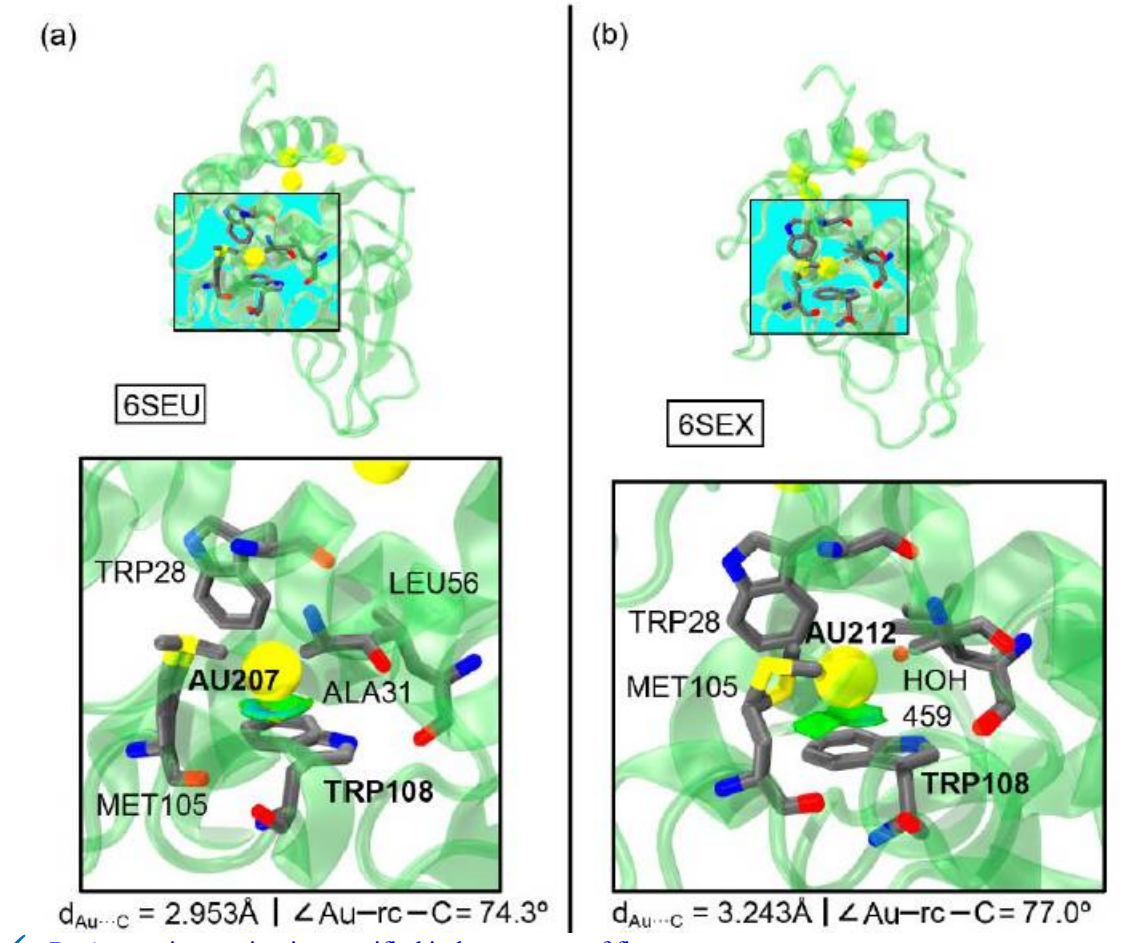
Partial views of the X-ray structures



✓ Regium–π interaction is magnified in bottom part of figure

✓ NCIplot analyses are denoted by the green isosurfaces inside

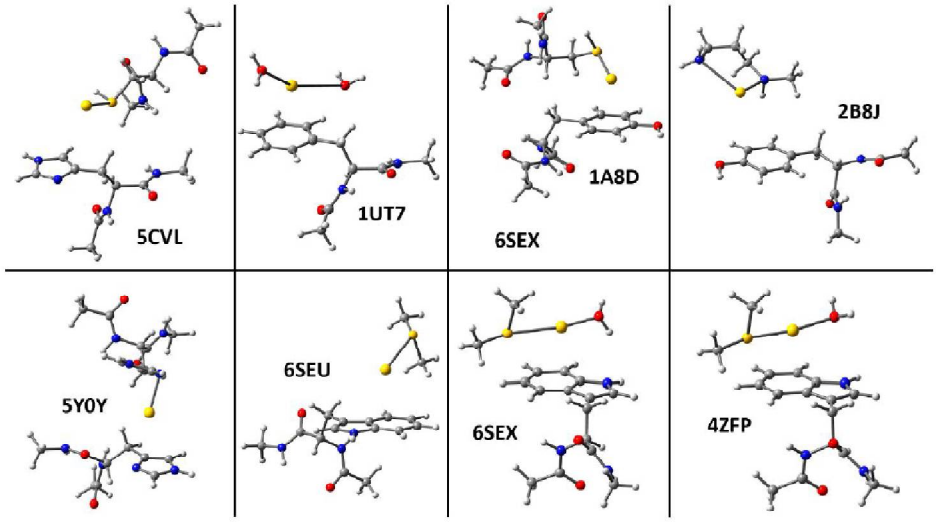
Partial views of the X-ray structures



✓ Regium–π interaction is magnified in bottom part of figure

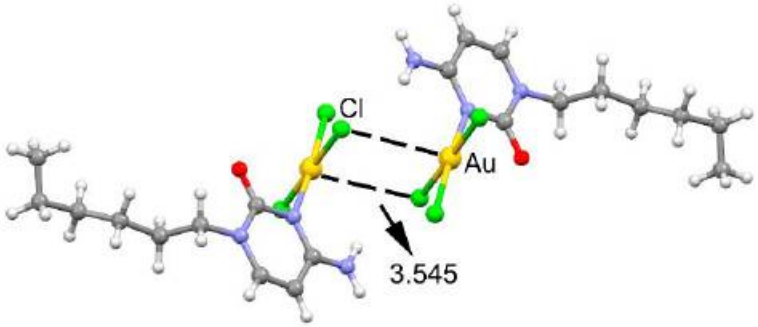
✓ NCIplot analyses are denoted by the green isosurfaces inside

Theoretical models
To compute regium-π binding energies in the PDB

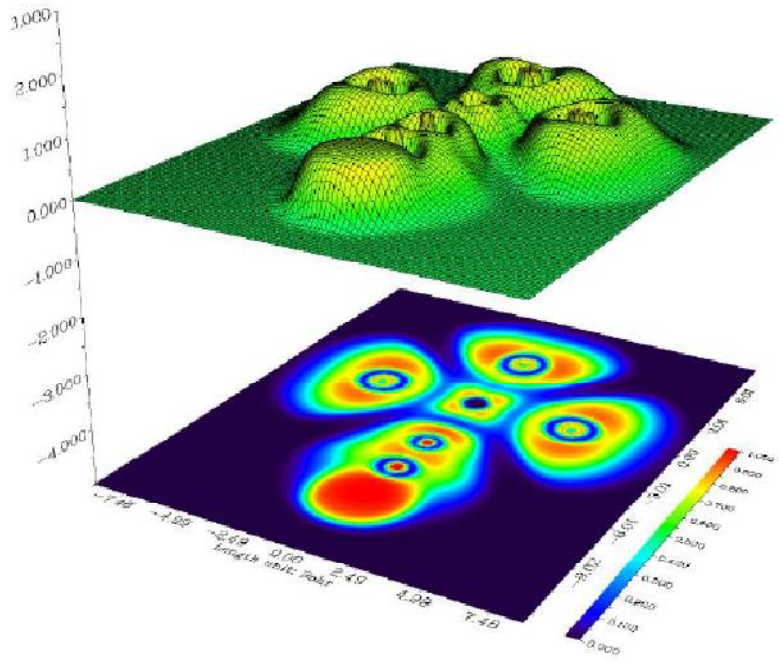


Regium Bond *[Au]*		SpB.	06

Trichlorido-(1-hexylcytosine)gold(III) complex dimer
solid state



Electron localization function (ELF) analysis



- Charge density of the Au–N bond is depleted along the bond path
- Au–N bond has higher electrostatic than covalent character