

Electronic Supplementary Information (ESI)

Structures, physicochemical properties, and applications of T–Hg^{II}–T, C–Ag^I–C, and other metallo-base-pairs†

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Metallo-base pairs in duplexes are compiled and classified according to several factors, metal ions, strand orientation, etc. (Same metallo-base pairs appear in several sections.)

Ag(I)	2-9
Cu(II)	10-14
Hg(II)	15-18
Other metal ions	18-20
Metallo-base-pairs in parallel duplexes	21-22

Electronic Supplementary Information (ESI)

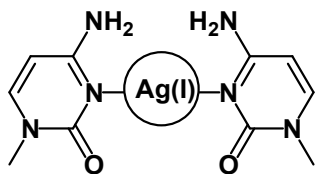
Metallo-base-pairs containing plural metal ions

22-24

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Ag(I)-----

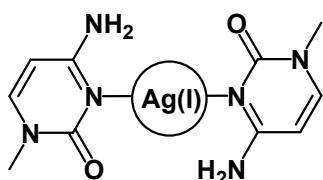
Pyrimidine bases



Akira Ono, Shiqi Cao, Humika Togashi, Mitsuru Tashiro, Takashi Fujimoto, Tomoya Machinami, Shuji Oda, Yoko Miyake, Itaru Okamoto, and Yoshiyuki Tanaka

“Specific interactions between Silver(I) Ions and Cytosine–Cytosine Pairs in DNA Duplexes”

Chem. Commun., **2008**, 4825-4827..



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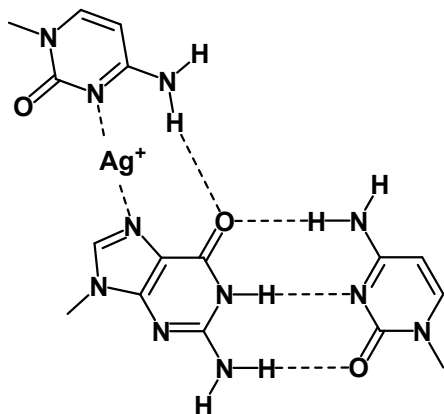
“Synthesis of covalently linked parallel and antiparallel DNA duplexes containing the metal-mediated base pairs T-Hg(II)-T and C-Ag(I)-C” *Chem. Commun.*, **2011**, 47, 1542-1544.

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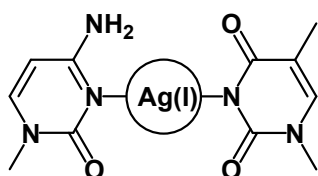
Silver(I)-Mediated Cytosine Self-Pairing is Preferred Over Hoogsteen-Type Base Pairs with the Artificial Nucleobase 1,3-Dideaza-6-Nitropurine

Nucleosides, Nucleotides Nucleic Acids, **2010**, 29, 27–38;

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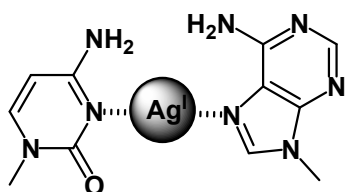
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Silver Ion Unusually Stabilizes the Structure of a Parallel-Motif DNA Triplex
J. Am. Chem. Soc., **2009**, *131*, 3826–3827



Hidehito Urata, Eriko Yamaguchi, Yasunari Nakamura and Shun-ichi Wada
Pyrimidine–pyrimidine base pairs stabilized by silver(I) ions
Chem. Commun., **2011**, *47*, 941–943

Tatsuya Funai, Junko Nakamura, Yuki Miyazaki, Risa Kiri, Osamu Nakagawa, Shun-ichi Wada, Akira Ono, and Hidehito Urata
“Regulated Incorporation of Two Different Metal Ions into Programmed Sites in a Duplex by DNA Polymerase Catalyzed Primer Extension”
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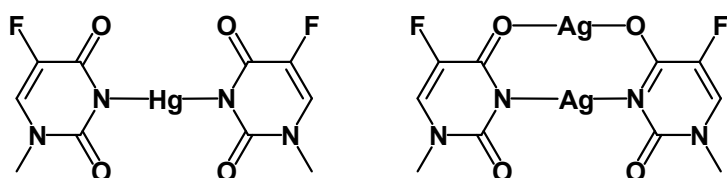
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Tatsuya Funai, Yuki Miyazaki, Megumi Aotani, Eriko Yamaguchi, Osamu Nakagawa, Shun-ichi, Wada, Hidetaka Torigoe, Akira Ono, and Hidehito Urata

Ag^I Ion Mediated Formation of a C–A Mismatch by DNA Polymerases

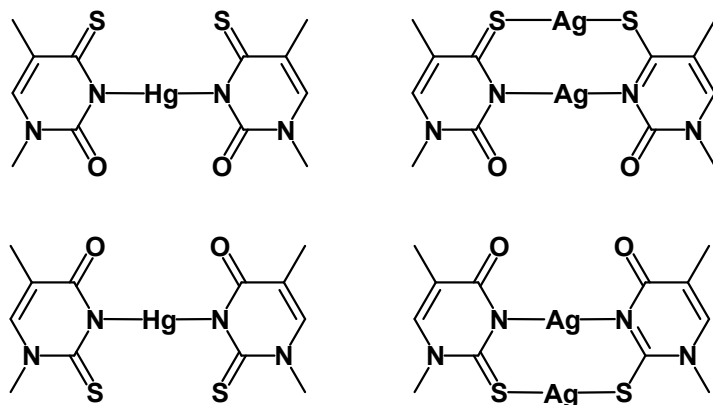
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“Switching Metal Ion Binding Selectivity of Chemically Modified Uracil Pairs in DNA Duplexes Triggered by pH Change”

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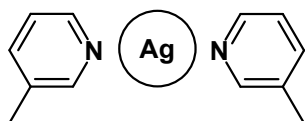
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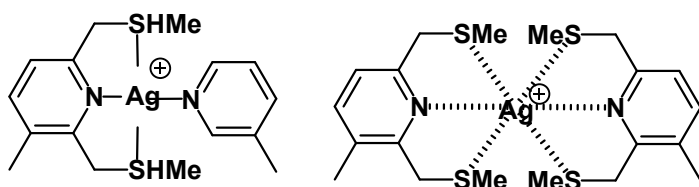
Synthetic bases



Tanaka, K.; Yamada, Y.; Shionoya, M.

Formation of silver(I)-mediated DNA duplex and triplex through an alternative base pair of pyridine nucleobases.

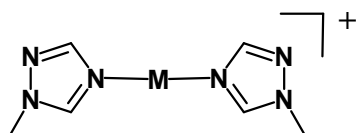
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Zimmermann, N.; Meggers, E.; Schultz, P. G.

A novel silver(I)-mediated DNA base pair.

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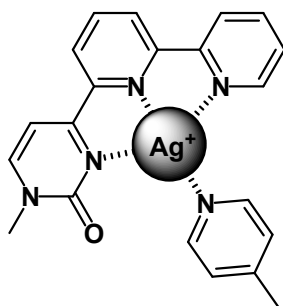


Dominik Böhme, Nicole Dupre, Dominik A. Megger, and Jens Müller

Conformational Change Induced by Metal-Ion-Binding to DNA Containing the Artificial 1,2,4-Triazole Nucleoside

Inorg. Chem., **2007**, *46*, 10114-10119.

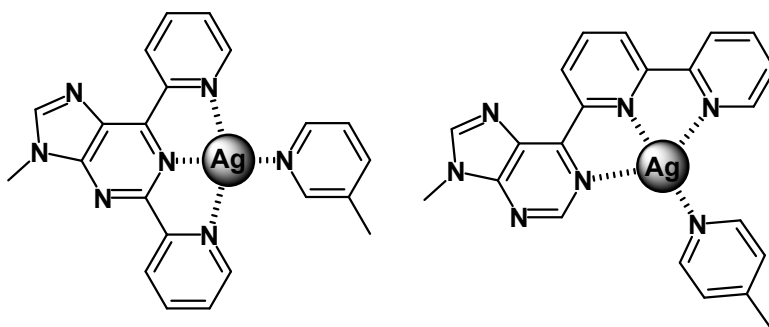
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Shin, D. W.; Switzer, C.

A metallo base-pair incorporating a terpyridyl-like motif: bipyridylpyrimidinone- Ag(I) 3 4-pyridine.

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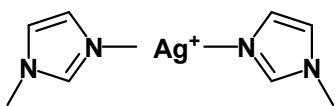


Heuberger, B. D.; Shin, D.; Switzer, C.

Two Watson_Crick-like metallo base-pairs.

Org. Lett. **2008**, *10*, 1091–1094.

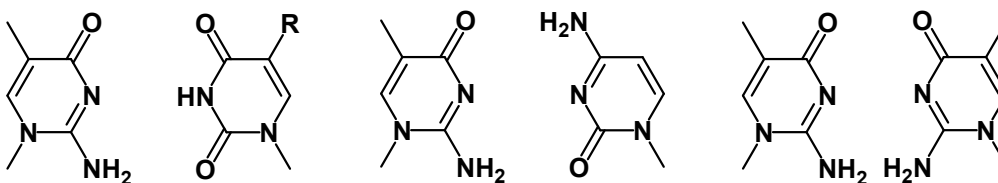
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Silke Johannsen, Nicole Megger, Dominik Böhme, Roland K. O. Sigel and Jens Müller
Solution structure of a DNA double helix with consecutive metal-mediated base pairs
NATURE CHEMISTRY **2010**, *2*, 229-234.

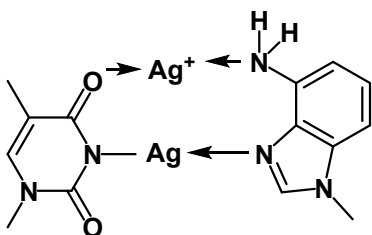
Kristina Petrovec, Bart Jan Ravoo and Jens Müller
Cooperative formation of silver(I)-mediated base pairs
Chem. Commun., **2012**, *48*, 11844-11846.

Sadhana Kumbhar, Silke Johannsen, Roland K.O. Sigel, Mark P. Waller, Jens Müller
A QM/MM refinement of an experimental DNA structure with metal-mediated base pairs
Journal of Inorganic Biochemistry, **2013**, *127*, 203–210.



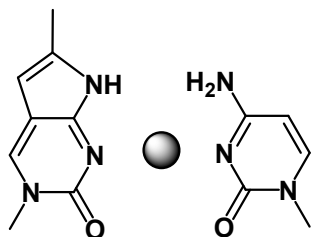
(No complex structure is indicated)

Hidehito Urata, Eriko Yamaguchi, Yasunari Nakamura and Shun-ichi Wada
Pyrimidine–pyrimidine base pairs stabilized by silver(I) ions
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Contiguous Metal-Mediated Base Pairs Comprising Two AgI Ions
Chem. Eur. J., **2011**, *17*, 6533 – 6544.

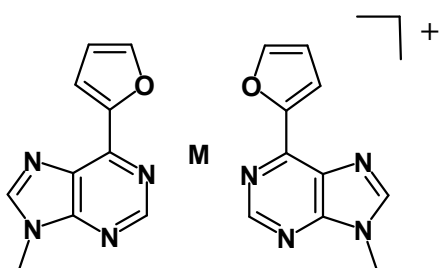
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Ki Soo Park, Joon Young Lee and Hyun Gyu Park

Mismatched pyrrolo-dC-modified duplex DNA as a novel probe for sensitive detection of silver ions

Chem. Commun., **2012**, 48, 4549–4551

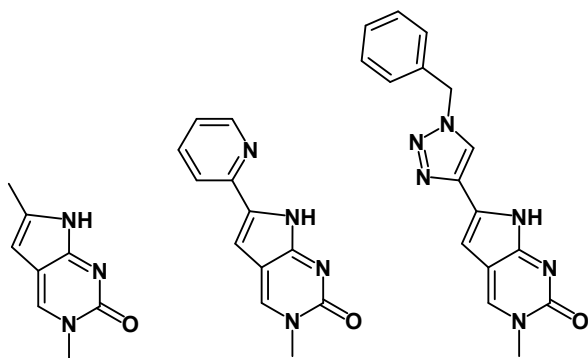


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Indranil Sinha, Jutta Kösters, Alexander Hepp and Jens Müller

6-Substituted purines containing thienyl or furyl substituents as artificial nucleobases for metal-mediated base pairing

Dalton Trans., **2013**, 42, 16080–16089

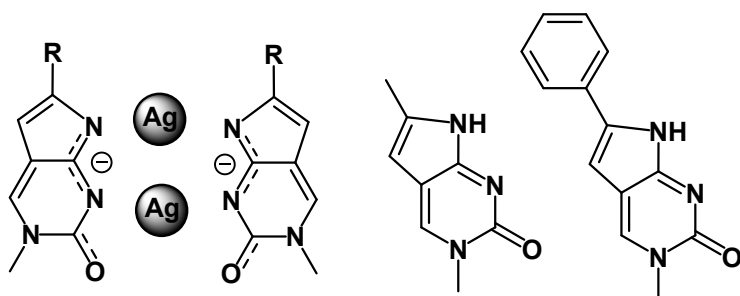


Hui Mei, Ingo Röhl, and Frank Seela

Ag⁺-Mediated DNA Base Pairing: Extraordinarily Stable Pyrrolo-dC–Pyrrolo-dC Pairs Binding Two Silver Ions

J. Org. Chem., **2013**, 78, 9457–9463

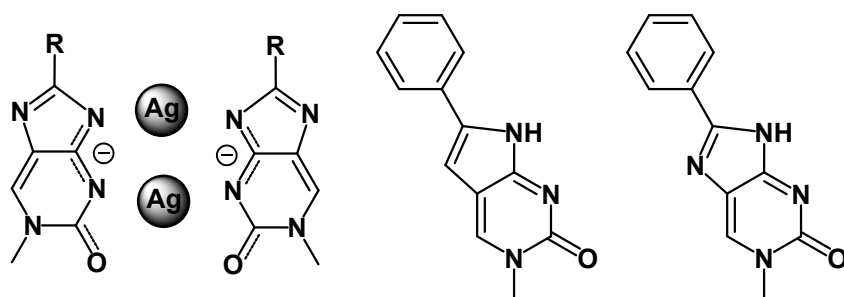
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Hui Mei, Haozhe Yang, Ingo Röhl, and Frank Seela

Silver Arrays Inside DNA Duplexes Constructed from Silver(I)-Mediated Pyrrolo-dC–Pyrrolo-dC Base Pairs

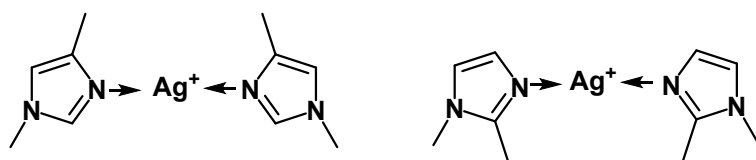
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Imidazo-dC Metal-Mediated Base Pairs: Purine Nucleosides Capture Two Ag⁺ Ions and Form a Duplex with the Stability of a Covalent DNA Cross-Link

Chem. Eur. J. **2014**, *20*, 16248 – 16257

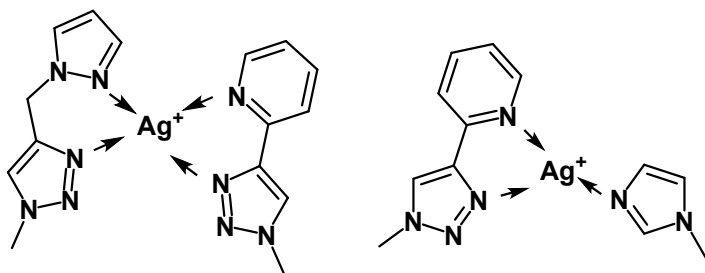


Susanne Hensel, Nicole Megger, Kristina Schweizer and Jens Müller

Second generation silver(I)-mediated imidazole base pairs

Beilstein J. Org. Chem. **2014**, *10*, 2139–2144

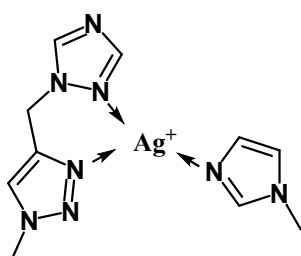
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Tim Richters, Olga Krug, Jutta Kcsters, Alexander Hepp, and Jens Müller

A Family of “Click” Nucleosides for Metal-Mediated Base Pairing: Unravelling the Principles of Highly Stabilizing Metal-Mediated Base Pairs

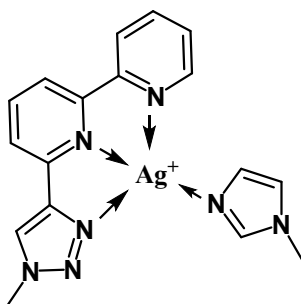
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A Metal-Mediated Base Pair with a [2+1] Coordination Environment

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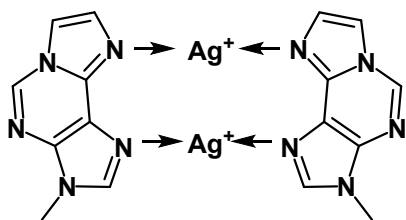


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"A tridentate "click" nucleoside for metal-mediated base pairing"

J. Inorg. Biochem. **2015**, *148*, 116-120.

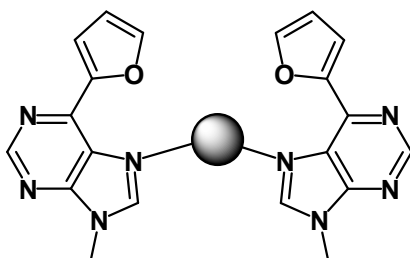
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S. Mandal, A. Hepp, J. Müller

"Unprecedented dinuclear silver(I)-mediated base pair involving the DNA lesion 1,*N*⁶-ethenoadenine"

Dalton Trans. **2015**, *44*, 3540-3543



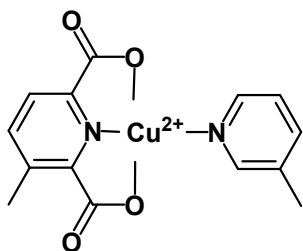
I. Sinha, C. Fonseca Guerra, J. Müller

"A Highly Stabilizing Silver(I)-Mediated Base Pair in Parallel-Stranded DNA"

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Cu(II)-----



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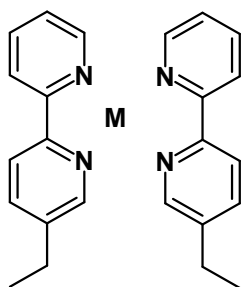
A novel copper-mediated DNA base pair.

J. Am. Chem. Soc. **2000**, *122*, 10714–10715.

Atwell, S.; Meggers, E.; Spraggon, G.; Schultz, P. G.

Structure of a copper-mediated base pair in DNA.

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(No complex structure is indicated in the manuscript)

Haim Weizman; Yitzhak Tor

2,2'-Bipyridine Ligand: A Novel Building Block for Modifying DNA with Intra-Duplex Metal Complexes

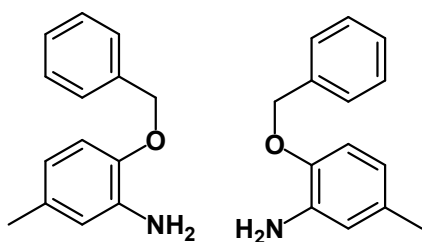
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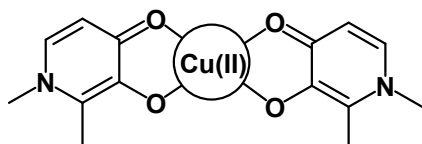
An approach to metal-assisted DNA base pairing: novel β -C-nucleosides with a 2-aminophenol or a catechol as the nucleobase

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Efficient incorporation of a copper hydroxypyridone base pair in DNA.
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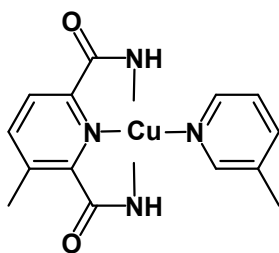
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A Discrete Self-Assembled Metal Array in Artificial DNA
Science, **2003**, *299*, 1212-1213.

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Programmable self-assembly of metal ions inside artificial DNA duplexes
Nat Nanotechnol. **2006**, *1*, 190-194

Mallajosyula, S. S.; Pati, S. K.
Conformational tuning of magnetic interactions in metal-DNA complexes.
Angew. Chem., Int. Ed. **2009**, *48*, 4977–4981.

Schlegel, M. K.; Essen, L.-O.; Meggers, E.
Duplex structure of a minimal nucleic acid.
J. Am. Chem. Soc. **2008**, *130*, 8158–8159.

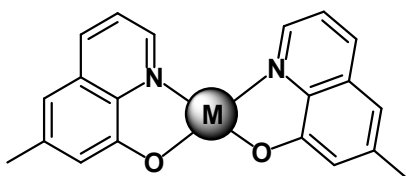
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Zimmermann, N.; Meggers, E.; Schultz, P. G.

A second-generation copper(II)-mediated metallo-DNA-base pair.

Bioorg. Chem., **2004**, *32*, 13–25.

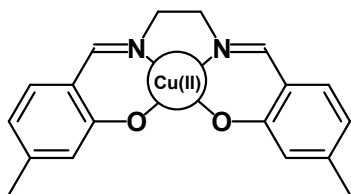


Zhang, L. L.; Meggers, E.

An extremely stable and orthogonal DNA base pair with a simplified three-carbon backbone.

J. Am. Chem. Soc. **2005**, *127*, 74–75.

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Guido H. Clever, Kurt Polborn, and Thomas Carell

A Highly DNA-Duplex-Stabilizing Metal–Salen Base Pair

Angew. Chem. Int. Ed., **2005**, *44*, 7204–7208

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Controlled Stacking of 10 Transition-Metal Ions inside a DNA Duplex

Angew Chem Int Ed. **2007**, *46*, 250-253.

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Antiferromagnetic Coupling of Stacked CuII–Salen Complexes in DNA

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Guido H. Clever, Yvonne Scrtl, Heather Burks, Werner Spahl, and Thomas Carell

Metal–Salen-Base-Pair Complexes Inside DNA: Complexation Overrides Sequence Information

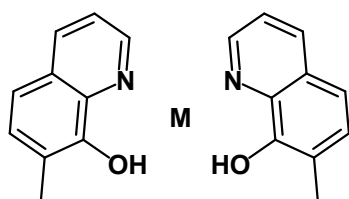
Chem. Eur. J., **2006**, *12*, 8708–8718

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Reversible bond formation enables replication and amplification of a crosslinking salen complex as an orthogonal base pair

Nat Chem. **2011**, *3*, 794-800.

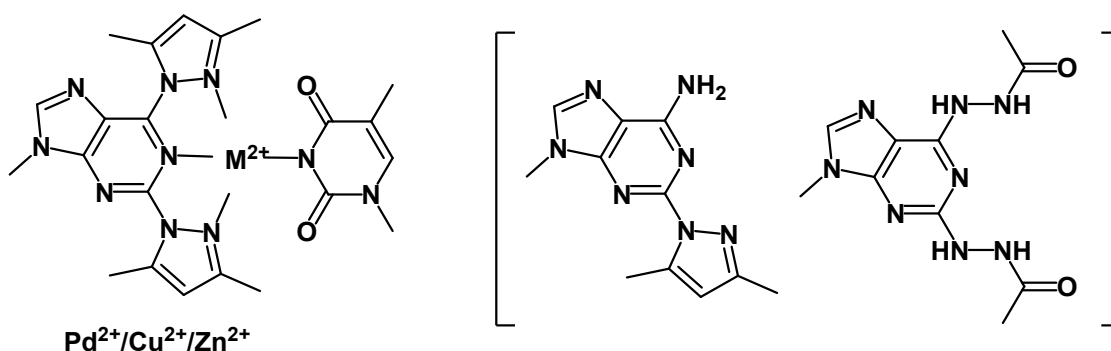
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Thomas Ehrenschwender, Wolfgang Schmucker, Christian Wellner, Timo Augenstein, Patrick Carl, Jeffrey Harmer, Frank Breher, and Hans-Achim Wagenknecht

“Development of a Metal-Ion-Mediated Base Pair for Electron Transfer in DNA”

Chem. Eur. J., **2013**, *19*, 12547 – 12552.



Sharmin Taherpour, Harri Lönnberg and Tuomas Lönnberg

“2,6-Bis(functionalized) purines as metal-ion-binding surrogate nucleobases that enhance hybridization with unmodified 2'-O-methyl oligoribonucleotides”

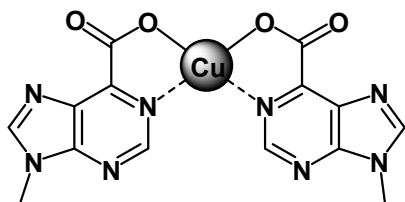
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S. Taherpour, O. Golubev and T. Lönnberg

“Metal-ion-mediated base pairing between natural nucleobases and bidentate 3,5-dimethylpyrazolyl-substituted purine ligands”

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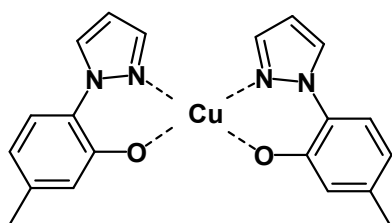
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Eun-Kyong Kim and Christopher Switzer*

Bis(6-carboxypurine)-Cu²⁺: A Possibly Primitive Metal-Mediated Nucleobase Pair

Org. Lett., **2014**, 16, 4059–4061.



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DNA based multi-copper ions assembly using combined pyrazole and salen ligandosides

Chem. Sci., **2015**, 6, 632–638



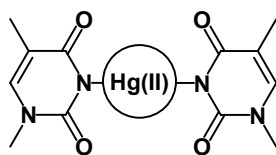
Wei Li, Xuyin Zhao, Jinli Zhang, Yan Fu

“Cu(II)-coordinated GpG-duplex DNA as peroxidase mimetics and its application for label-free detection of Cu²⁺ ions”

Biosensors and Bioelectronics, **2014**, 60, 252–258.

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Hg(II)-----



Sidney Katz

“The reversible reaction of Hg(II) and double-stranded polynucleotides. A step-function theory and its significance”

Biocimica et Biophysica Acta, **1963**, 68, 240-253.

Linda D. Kosturko, Cynthia Folzer, Robert F. Stewart

“The crystal and molecular structure of a 2:1 complex of 1-methylthymine-mercury(II)”

Biochemistry, **1974**, 19, 3949-3951.

Zsuzsanna Kuklenyik & Luigi G. Marzilli

“Mercury(II) site-selective binding to a DNA hairpin. Relationship of sequence-dependent intra- and interstrand cross-linking to the hairpin-duplex conformational transition”

Inorg. Chem., **1996**, 35, 5654-5662.

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“Novel Highly Selective Mercury Sensing in Aqueous Solutions: Fluorescence Resonance Energy Transfer associated with Hairpin Structure Formation of Oligonucleotide Derivatives derived by Mercury-Mediated Thymine-Hg-Thymine Pair Formation”

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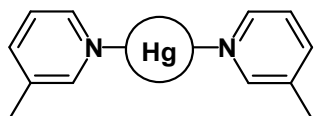
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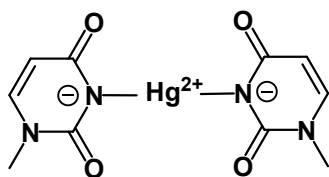
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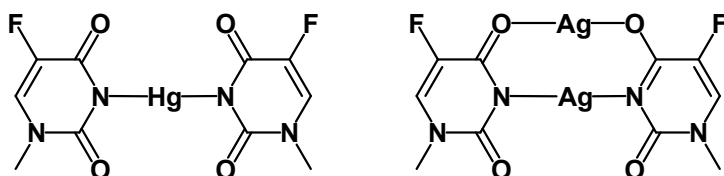
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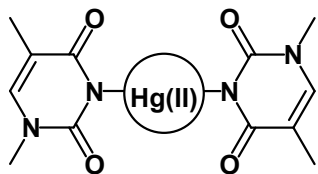


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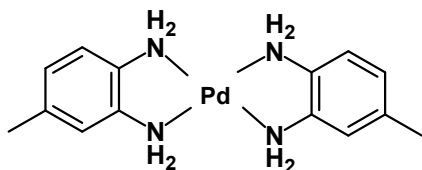
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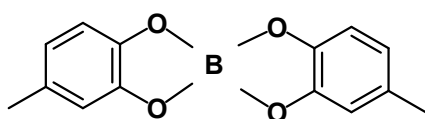
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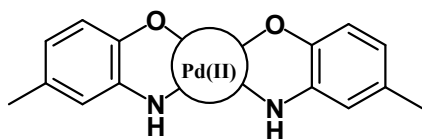
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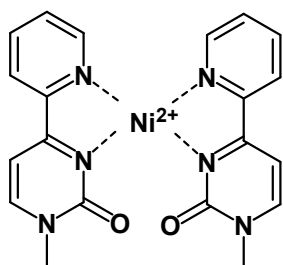
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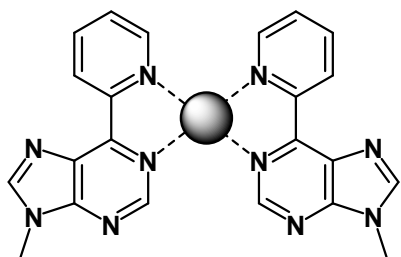


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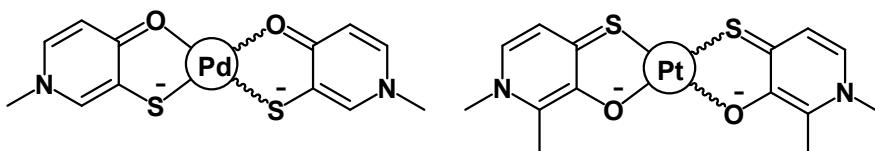
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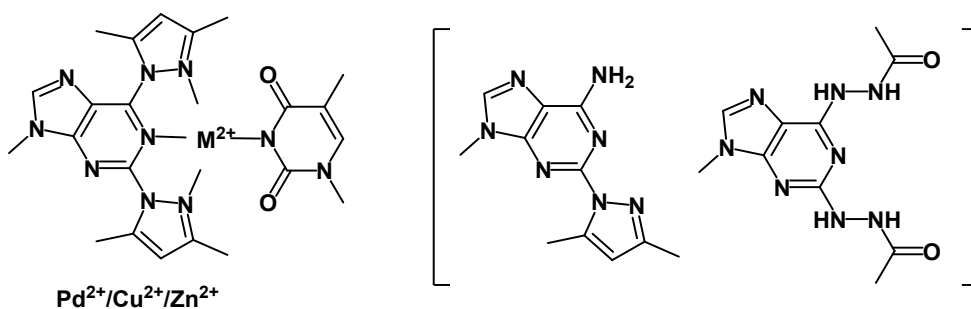
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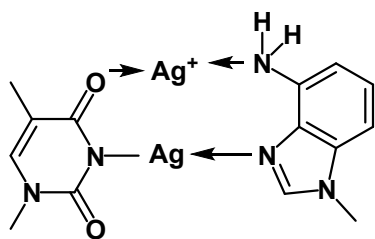
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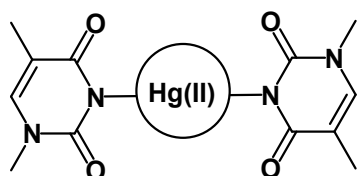
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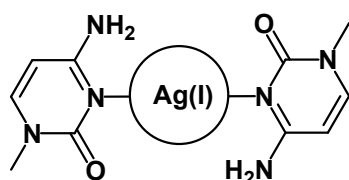
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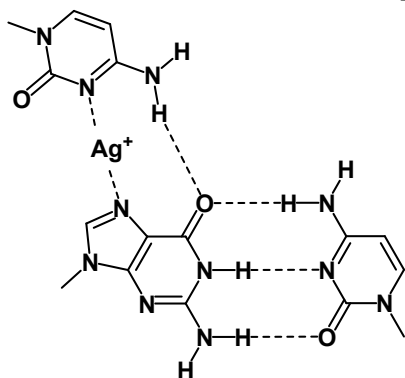
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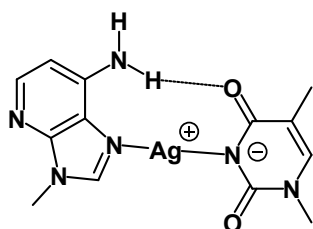
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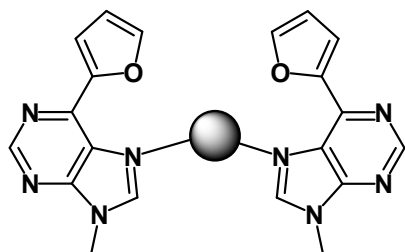


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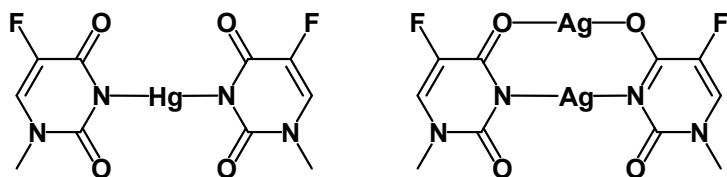
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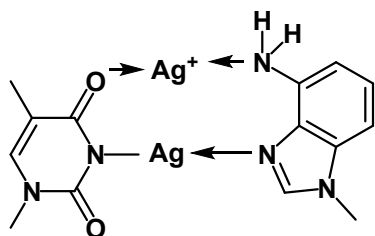
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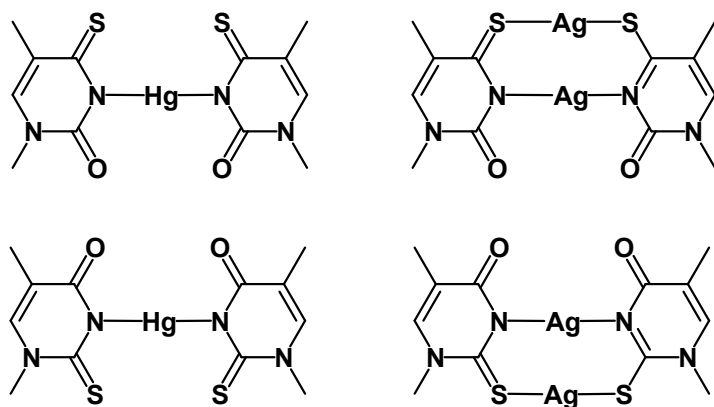
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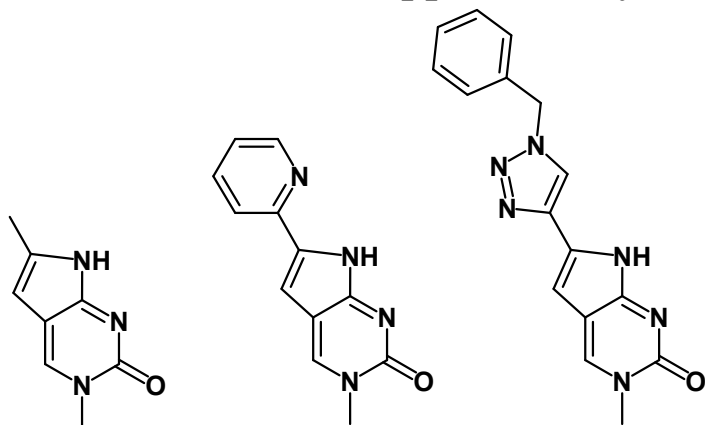


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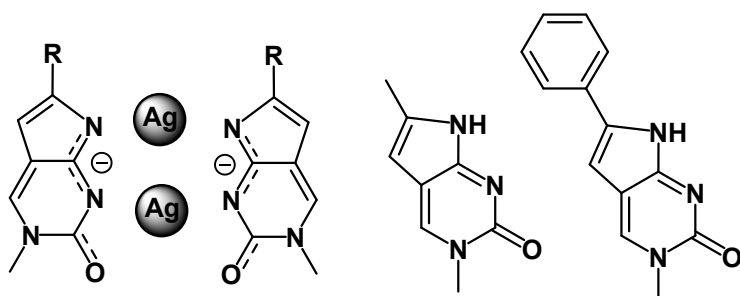
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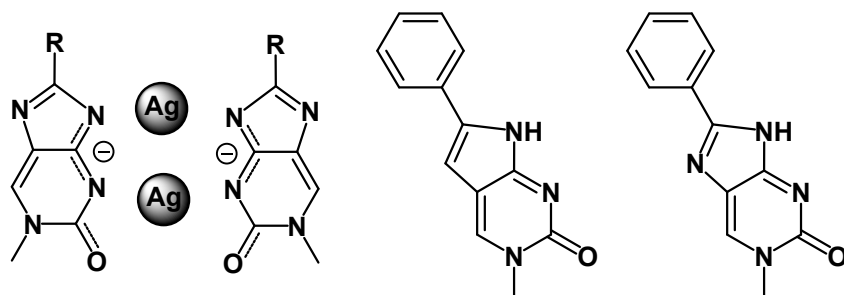
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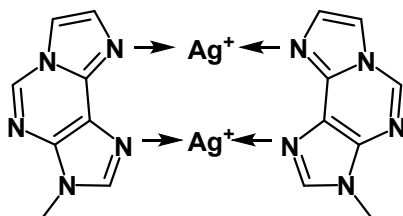
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