



IV INTERNATIONAL SYMPOSIUM

«NONCOVALENT INTERACTIONS IN SYNTHESIS,
CATALYSIS, AND CRYSTAL ENGINEERING»

SAINT PETERSBURG, JUNE 29TH - JULY 3RD 2026

BOOK OF ABSTRACTS

The Book of Abstracts is composed of materials provided by the authors, who are fully responsible for their content. The organizers made only minor editorial corrections.

Saint Petersburg 2026

Compiled by Anton V. Rozhkov

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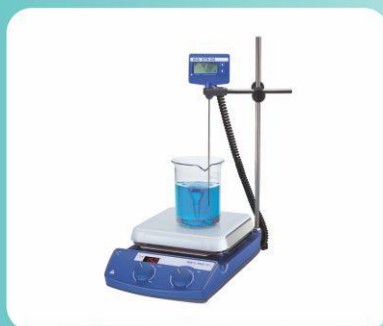
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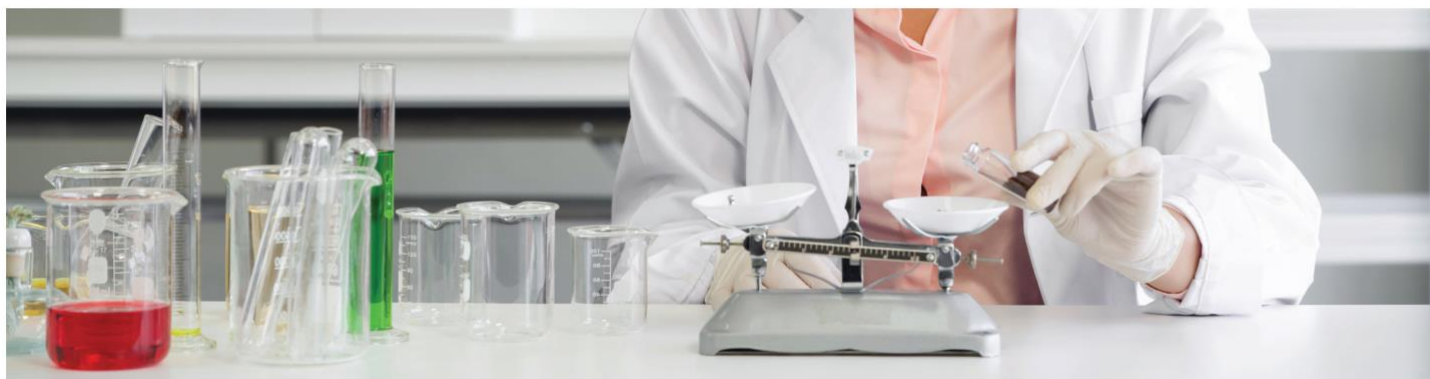
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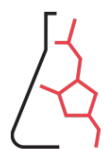
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Schedule for the IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

June 29th

Assembly Hall of the main building of SPbU, Universitetskaya emb. 7-9
(Актuый зал Главного здания СПбГУ, Университетская наб., д. 7-9)

08:30 REGISTRATION

09:30 OPENING

Session chair: Peter Tolstoy (Петр Михайлович Толстой)

09:40 Valentine Ananikov (Валентин Павлович Анаников)
N.D. Zelinsky Institute of Organic Chemistry RAS, Russia
Making Chemistry an Exact Science

10:15 Elena Bagryanskaya (Елена Григорьевна Багрянская)
N.N. Vorozhtsov Institute of Organic Chemistry SB RAS, Russia
Application of pulsed EPR spectroscopy to study non-covalent interactions in biopolymers

10:40 Oksana Kholdeeva (Оксана Анатольевна Холдеева)
Boreskov Institute of Catalysis SB RAS, Russia
The role of protonation and charge density in oxidation catalysis with polyoxometalates

11:05 Giuseppe Resnati
Dept. Chemistry, Materials, Chemical Engineering “Giulio Natta” Politecnico di Milano, Italy
The Expanding set of σ -Hole Adducts

11:20 COFFEE BREAK

Session chair: Elena Bagryanskaya (Елена Григорьевна Багрянская)

11:50 Igor Fedyushkin (Игорь Леонидович Федюшкин)
G.A. Razuvaev Institute of Organometallic Chemistry, Russian Academy of Sciences, Russia
1,3-Diaza-2-metalloles (DAMs): A New Generation of Catalysts for Polymerization Reactions

12:25 Guo-Hong Ning
College of Chemistry and Materials Science, Guangdong Provincial Key Laboratory of Supramolecular Coordination Chemistry, Jinan University, Guangzhou, Guangdong
Covalent Metal-Organic Frameworks: Fusion of the COFs and MOFs

12:50 Snežana Zarić
University of Belgrade, Serbia
Hydrogen bonds in the second coordination sphere of metal complexes: Key role of metal oxidation state and coordination number

13:05 Natalia Belkova (Наталья Викторовна Белкова)
A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia
Photo-enhanced reactivity of nickel hydride complexes

13:20 CONFERENCE PHOTO

13:30 LUNCH

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

Session chair: Natalia Belkova (Наталья Викторовна Белкова)

- 15:10** Valentine Nenajdenko (Валентин Георгиевич Ненайденко)
Lomonosov Moscow State University, Russia
Design and Synthesis of Phenanthroline Diamides for f-Element Separation
- 15:45** Nikolay Semenov (Николай Андреевич Семенов)
Novosibirsk Institute of Organic Chemistry RAS, Russia
Chalcogenadiazole based chalcogen bond donors: supramolecular architectures, optical properties and cationic activation
- 16:10** Igor Antipin (Игорь Сергеевич Антипин)
A.E. Arbuzov Institute of Organic and Physical Chemistry, Russia
Absolute Asymmetric Supramolecular Synthesis — Engineering of Enantiomorphic Crystals
- 16:35** Vladislav Blatov (Владислав Анатольевич Блатов)
Samara State Technical University, Russia
Topological analysis of noncovalent interactions in crystals: methods and tools
- 16:50** COFFEE BREAK

Session chair: Nikolay Semenov (Николай Андреевич Семенов)

- 17:20** Ekaterina Gulyaeva (Екатерина Сергеевна Гуляева)
A.N. Nesmeyanov Institute of Organoelement Compounds of RAS, Russia
A role of amine/ammonia interconversion in high productive hydrogen evolution from amine-boranes
- 17:35** Yulia Budnikova (Юлия Германовна Будникова)
A.E. Arbuzov Institute of Organic and Physical Chemistry, Russia
Noncovalent and Covalent Interactions in Metal-Catalyzed Selective C-H Functionalizations
- 17:50** Ilya Taydakov (Илья Викторович Тайдаков)
P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Russia
Coordination compounds of lanthanides with aromatic, heterocyclic and heteroatomic 1,3-diketones, – the relationship between molecular structure and luminescent properties
- 18:05** Zufar Gafurov (Зуфар Нафигуллович Гафуров)
A.E. Arbuzov Institute of Organic and Physical Chemistry, Russia
Unsymmetrical PCN Pincer Nickel Complexes: From Non-Covalent Interactions to Catalytic Oligomerization of Ethylene
- 18:20** Yana Safinskaya (Яна Валерьевна Сафинская)
St. Petersburg State University, Russia
Controlling Regioselectivity and Reaction Rates of Arylation through Anion Coordination to σ -Hole Donors
- 18:30** Alexandr Khudozhitkov (Александр Эдуардович Художитков)
Novosibirsk State University, Russia
Hydrogen Bonding and Ion Dynamics in Protic Ionic Liquid Probed with ^2H NMR
- 18:40** Paulina Kalle (Паулина Калле)
Kurnakov Institute of General and Inorganic Chemistry, Russia
From Chain Rotation to Ferroelasticity: Potassium Alkanoates C3–C6
- 18:50** Konstantin Belov (Константин Васильевич Белов)
G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Russia
Solvation and Noncovalent Interaction Effects in Stabilizing the Molecular Structure of Etoricoxib

19:30 WELCOME PARTY (River Palace Hotel, Maly prospect V.O., 1)

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Session chair: Igor Antipin (Игорь Сергеевич Антипин)

- 17:20** Lev Zelenkov (Лев Евгеньевич Зеленков)
School of Physics, Harbin Institute of Technology, Harbin, China
Stacked Organic–Inorganic Cocrystals of Group 10 Metal Dithiocarbamates with π -Acceptor Benzene Derivatives
- 17:35** Pavel Demakov (Павел Андреевич Демаков)
Nikolaev Institute of Inorganic Chemistry SB RAS, Russia
Non-covalent interactions in functional 1,10-phenanthroline-based REE(III) metal-organic frameworks
- 17:50** Pavel Abramov (Павел Александрович Абрамов)
Nikolaev Institute of Inorganic Chemistry, Russia
Argentophilic interactions in polymeric silver thiolates and related polynuclear complexes
- 18:05** Anton Shalygin (Антон Сергеевич Шалыгин)
Zelinsky Institute of Organic Chemistry RAS, Russia
Molecular states of hydrogen peroxide in ionic liquids according to FTIR spectroscopy and DFT calculations
- 18:20** Sergey Kovalenko (Сергей Александрович Коваленко)
A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia
Influence of NHC bonding mode on reactivity of Re(I) complexes
- 18:30** Klykova Angelina (Ангелина Петровна Клыкова)
Lomonosov Moscow State University, Russia
Bispidinium-directed supramolecular halometallates
- 18:40** Anastasia Kolbunova (Анастасия Викторовна Колбунова)
Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Russia
closo-B₁₂-fused carboxonium ions: synthesis and mechanistic insights
- 18:50** Daniil Sobenin (Даниил Валерьевич Собенин)
Moscow Aviation Institute (National Research University), Russia
Polymer-stabilized Fe(III) complexes with poly(vinylpyrrolidone): structure, molecular-weight effects, and application against iron-deficiency chlorosis
- 19:00** Roman Burlutsky (Роман Олегович Бурлуцкий)
Lomonosov Moscow State University, Russia
Bimetallic Sandwich Complexes Derived from Ferrocenyl Fulvenes and Cyclopentadienes

June 30th

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

Session chair: Elena Tupikina (Елена Юрьевна Тупикина)

09:30 Vladimir Fedin (Владимир Петрович Федин)
Nikolaev Institute of Inorganic Chemistry SB RAS, Russia
Guest@MOF: The Role of Non-Covalent Interactions

10:05 Evgeny Tretyakov (Евгений Викторович Третьяков)
N.D. Zelinsky Institute of Organic Chemistry, Russia
Non-covalent interactions in the design of molecular-based magnets

10:30 Maria Kalinina (Мария Александровна Калинина)
Frumkin Institute of Physical Chemistry and Electrochemistry, Russia
Configuration Complexity as a Predictor of Synergy in Hybrid Materials

10:55 Labconcept (ЛабКонцепт)
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11:10 COFFEE BREAK

Session chair: Eugene Tretyakov (Евгений Викторович Третьяков)

11:40 Baode Zhang
Liaoning Petrochemical University, People's Republic of China
Crystal structures of semicrystalline polyimides tailored by intramolecular and intermolecular interactions

11:55 Sergey Baykov (Сергей Валентинович Байков)
St. Petersburg State University, Russia
Supramolecular Approach to Upgrade NCI Donors

12:10 Leonid Kononov (Леонид Олегович Кононов)
N.D. Zelinsky Institute of Organic Chemistry, Russia
Noncovalent Interactions and Solution Structure: Concentration and Mixing Mode as Key Environmental Variables in Chemical Reactions

12:25 Tatyana Shestimerova (Татьяна Алексеевна Шестимерова)
Lomonosov Moscow State University, Russia
Halogen Bonding as a Tool for Tuning the Structure and Properties of Hybrid Halometallates

12:40 Vladimir Larionov (Владимир Анатольевич Ларионов)
A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Russia
Chiral-at-Cobalt(III) Complexes with Hydrogen Bond Donor Amino Groups and Their Applications

12:55 Anastasiya Eliseeva (Анастасия Александровна Елисеева)
St. Petersburg State University, Russia
Tuning Electrophilic-Nucleophilic Dualism of Pt(II) and Pd(II) Metal Centers

13:10 LUNCH

Main building of SPbU, Universitetskaya emb. 7-9, room 2053
(Главное здание СПбГУ, Университетская наб., д. 7-9, ауд. 2053)

Session chair: Maria Kalinina (Мария Александровна Калинина)

- 11:40** Ivan Ananyev (Иван Вячеславович Ананьев)
N.S. Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences, Russia
Descriptors of Noncovalent Interactions: From Spatial to Electronic Structure to Energy. And Back to Geometry?
- 11:55** Kamila Kydralieva (Камиля Асылбековна Кыдралиева)
Moscow Aviation Institute (National Research University), Russia
Versatility of Non-Covalent Humic Acids in Advanced Materials and Sustainable Technologies
- 12:10** Juliya Kostina (Юлия Вадимовна Костина)
Topchiev Institute of Petrochemical Synthesis RAS, Russia
Noncovalent Polymer–Small Molecule Interactions: From Structural–Molecular Plasticization to a Dynamic Conformational Theory of Adhesion
- 12:25** Vera Varfolomeeva (Вера Васильевна Варфоломеева)
Samara National Research University, Russia
The organizing role of hydrogen bonds in pre-reaction complexes of formyl chloride conjugation with glutathione
- 12:40** Olga Kataeva (Ольга Николаевна Катаева)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
The Interplay between Noncovalent Interactions, Polymorphism and Dynamic Properties of Crystals
- 12:55** Guldjan Dzhardimalieva (Гульжиан Искаковна Джардималиева)
Federal Research Centre of Problems of Chemical Physics and Medicinal Chemistry RAS, Russia
Noncovalent interactions as the basis of self-healing in metallopolymer systems: from general approaches to copolymers with embedded coordination nodes
- 13:10** LUNCH

University Center, Birzhevaya Liniya 6
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Session chair: Vladimir Larionov (Владимир Анатольевич Ларионов)

- 14:50** Andrey Karasik (Андрей Анатольевич Карасик)
Arbuzov Institute of Organic and Physical Chemistry of FRC Kazan Scientific Center of RAS, Russia
Design of Luminescent Materials: Balancing Intramolecular and Intermolecular Interactions
- 15:25** Sergey Tunik (Сергей Павлович Туник)
St. Petersburg State University, Russia
Effects of noncovalent interactions in photophysics of aggregated d⁸ square-planar and d¹⁰ complexes in solid state and in soft matter nanomaterials
- 15:50** Oleg Filippov (Олег Андреевич Филиппов)
A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Russia
The Art of Structural Instability: Living Life Through Non-Covalent Bonds
- 16:15** Mikhail Kiskin (Михаил Александрович Кискин)
N.S. Kurnakov Institute of General and Inorganic Chemistry, Russia
Selection of photoresists based on zinc carboxylate complexes
- 16:30** COFFEE BREAK

Session chair: Segrey Tunik (Сергей Павлович Туник)

- 17:00** Olga Shiryayeva (Ольга Андреевна Ширяева)
Lomonosov Moscow State University, Russia
Hybrid biomimetic catalyst based on layered Tb(III) hydroxide nanosheets and zinc porphyrinate: a first step toward abiotic glycolysis
- 17:10** Konstantin Tumbinskiy (Константин Алексеевич Тумбинский)
Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Russia
Synergistic effect in hybrid photocatalytic material based on quasi-two-dimensional MoS₂ particles and layered Tb³⁺ hydroxide integrated with zinc porphyrinate
- 17:20** Arina Olbrykh (Арина Павловна Ольбрых)
Nesmeyanov Institute Of Organoelement Compounds, Russian Academy Of Sciences, Russia
Coinage bonding between Group 11 and Group 10 Metals
- 17:30** Alexander Buravlev (Александр Андреевич Буравлев)
Novosibirsk Institute of Organic Chemistry SB RAS, Russia
Secondary bonding interactions for molecular magnetism: rare double hysteretic magnetic bistability in π -complex of fluorocarbon 1,3,2-benzodithiazolyl with naphthalene
- 17:40** Angelina Iova (Ангелина Анатольевна Иова)
Arbuzov Institute of Organic and Physical Chemistry of FRC Kazan Scientific Center of RAS, Russia
Rational design of functional complexes with 3d-/4f-metal ions based on 1,3-disubstituted derivatives of (thia)calix[4]arenes
- 17:50** Pavel Petunin (Павел Васильевич Петунин)
Tomsk Polytechnic University, Russia
Linear Dichroism in Crystals of Nitronyl Nitroxide Radicals
- 18:00** Artur Dzeranov (Артур Альбертович Дзеранов)
Moscow Aviation Institute, Russia
Role of Non-Covalent Interactions in the Mechanism of Ciprofloxacin Degradation by Mesoporous Magnetite-Based Catalysts Modified with Humic Acids
- 18:10** Nikita Mayorov (Никита Сергеевич Майоров)
Institute of General and Inorganic Chemistry, Russia
Hydrogen bond activated hydrogen peroxide coordination to In(III)

Main building of SPbU, Universitetskaya emb. 7-9, room 2053
(Главное здание СПбГУ, Университетская наб., д. 7-9, ауд. 2053)

Session chair: Oleg Filippov (Олег Андреевич Филиппов)

- | | |
|-----------------------------|--|
| P 1
17:00 | Omar Alkhuder
<i>St. Petersburg State University, Russia</i>
Phosphine Oxides as a Probe of Total Hydrogen Bond Strength |
| P 2
17:05 | Ivan Arteeв (Иван Сергеевич Артеев)
<i>Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</i>
A family of copper silsesquioxane cages with pyrazolate and diimine ligands: synthesis, structure, supramolecular organization and catalytic properties |
| P 3
17:10 | Gleb Borisov (Глеб Николаевич Борисов)
<i>Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</i>
Directed synthesis of Re(i) complexes with different nhc bonding modes |
| P 4
17:15 | Stepan Galiakhmetov (Степан Андреевич Галиахметов)
<i>St. Petersburg State University, Russia</i>
Alkylation of Phosphine Chalcogenides: σ-Hole Enhancement |
| P 5
17:20 | Varvara Gomonyuk (Варвара Алексеевна Гомонюк)
<i>MIREA – Russian Technological University, Russia</i>
The nature of non-covalent interactions of norbornene and norbornadiene with a palladium surface |
| P 6
17:25 | Nataliya Zolotareva (Наталья Вадимовна Золотарева)
<i>G.A. Razuvaev Institute of Organometallic Chemistry of the Russian Academy of Sciences, Russia</i>
Non-Covalently Assembled Multidecker Diazadiphosphapentalenes |
| P 7
17:30 | Margarita Kostareva (Маргарита Борисовна Костырева)
<i>St. Petersburg State University, Russia</i>
Inverted Halogen Bonds in Square-Planar Pt(II) and Pd(II) Iodide Isocyanide Complexes |
| P 8
17:35 | Taisiya Kuzina (Таисия Дмитриевна Кузина)
<i>Murmansk Arctic University, Russia</i>
Electrostatic interactions – an in-depth study in gelatin–agar coacervates |
| P 9
17:40 | Alsu Nugmanova (Алсу Галимовна Нугманова)
<i>Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Russia</i>
Synergy Effect in GO-Based Hybrid Photocatalysts under Electric Field Activation |
| P 10
17:45 | Ilya Prolov (Илья Викторович Проломов)
<i>N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Russia</i>
A quantum-chemical study of the electronic structure and reactivity of non-innocent transition-metal complexes with peroxide-derived ligands |
| P 11
17:50 | Andrey Sabanin (Андрей Русланович Сабанин)
<i>A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Russia</i>
Synthesis of Re(I) and Mn(I) complexes containing 1,5-diaza-3,7-diphosphocyclooctane ligand |
| P 12
17:55 | Marina Stozharova (Марина Андреевна Стожарова)
<i>St. Petersburg State University, Russia</i>
Halogen bonding in diaryliodonium dichromates |
| P 13
18:00 | Arina Stroeва (Арина Сергеевна Строева)
<i>St. Petersburg State University, Russia</i>
Aggregation-Induced Emission in Au(III) CNC-Pincer Complexes: The Role of Isonitrile vs. Alkynyl Coligands |

- P 14**
18:05 Maria Subbotina (Мария Романовна Субботина)
St. Petersburg State University, Russia
Bismuthophilic interactions in dimers of homoleptic Bi^{III} dithiocarbamates
- P 15**
18:10 Alexey Terentev (Алексей Владимирович Терентьев)
Samara National Research University, Russia
A quantum chemical approach to the study of reactions involving hydrogen bonds in a neutral environment
- P 16**
18:15 Semen Tsybulin (Семен Валерьевич Цыбулин)
St. Petersburg State University, Russia
H-bond-assisted and sterically facilitated reactivity of *o*-dimethylaminoaryloximes and imines
- P 17**
18:20 Edem Chakalov (Эдем Рустемович Чакалов)
St. Petersburg State University, Russia
(De)coupled proton transfer in (HCO₃)₂⁽²⁻⁾ dimers in kalicinite, KHCO₃: a periodic DFT and LMP2 description
- P 18**
18:25 Vladimir Chernyshev (Владимир Владимирович Чернышев)
Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Russia
New chiral ionic HOF materials based on cationic octahedral Co(III) complexes

July 1st

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

- 09:30** Giuseppe Resnati
Dept. Chemistry, Materials, Chemical Engineering "Giulio Natta" Politecnico di Milano, Italy
Workshop opening
- 9:40** Antonio Frontera
Departament de Química, Universitat de les Illes Balears, Spain
The Matere Bond
- 10:10** Giancarlo Terraneo
Dept. Chemistry, Materials, Chemical Engineering "Giulio Natta" Politecnico di Milano, Italy
Programming Materials through σ - and π -Interactions: From Stability to Function
- 10:40** Jean-Pierre Djukic
Université de Strasbourg, France
Weak Electron Density Sharing: the missing link in the reactivity and cohesion of *d*-block transition metal complexes
- 11:10** COFFEE BREAK
- 11:40** Snežana Zarić
University of Belgrade, Faculty of Chemistry, Serbia
Interactions of square planar metal complexes
- 12:10** Ekaterina Bartashevich (Екатерина Владимировна Барташевич)
South Ural State University, Russia
The σ -hole and p-hole Tetrel Bonds: are the principles same?
- 12:40** Natalia Soldatova (Наталья Сергеевна Солдатова)
Tomsk Polytechnic University, Russia
Halonium Salts in the Design of Halogen-Bonded Supramolecular Architectures
- 13:10** LUNCH
- 14:50** Yanchuan Zhao
State Key Laboratory of Fluorine and Nitrogen Chemistry and Advanced Materials, Shanghai
Noncovalent Interactions for Chemosensing and Construction of Porous Molecular Crystals
- 15:20** Daniil Ivanov (Даниил Михайлович Иванов)
St. Petersburg State University, Russia
 σ -Hole Electrophilicity of Acido Ligands
- 15:50** Yao Wang
School of Chemistry and Chemical Engineering, Shandong University, China
Catalysis with Carbon-Bonding Interactions

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

POSTER SESSION (14:50-18:00)

- P 19** Jacob Abulkhaev (Якоб Умарович Абулхаев)
St. Petersburg State University, Russia
Palladium(II) complexes featuring 5-acetylmethyl-1,2,4-oxadiazoles as ditopic acceptors of halogen bonding
- P 20** Alexey Akulov (Алексей Александрович Акулов)
Ural Federal University, Russia
Azolo[*a*]pyrimidine-Based Iodonium Ylides: Synthesis and Properties
- P 21** Antonova Elina (Элина Вадимовна Антонова)
St. Petersburg State University, Russia
Design of Phosphorescent Platinum(II) Complexes via Noncovalent Interactions
- P 22** Konstantin Bolshakov (Константин Михайлович Большаков)
Zelinsky Institute of Organic Chemistry RAS, Russia
Intermolecular interactions in novel highly-energetic 3,3-dinitroazetidines: viewpoint from azetidine geometry
- P 23** Anastasiya Busygina (Анастасия Андреевна Бусыгина)
St. Petersburg State University, Russia
Halogen Bonding Involving Mixed Dithiocarbamate Platinum(II) Complexes
- P 24** Fyodor Verkhov (Фёдор Константинович Верхов)
Novosibirsk Institute of Organic Chemistry, Russia
Noncovalent Interactions in Crystals of Methanol Solvates of 1*H*-imidazo[4,5-*b*]phenazine
- P 25** Elena Vlasova (Елена Евгеньевна Власова)
St. Petersburg State University, Russia
Polyfluoroaromatic Bisselanes as Polytopic Donors of Noncovalent Interactions
- P 26** Dariya Gerasimova (Дарья Павловна Герасимова)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
Kryptoracemate and racemic crystal of chiral thiourea with 1,2,3,4-tetrahydro-1-naphthyl fragment
- P 27** Yulia Glushan (Юлия Игоревна Глушань)
Ural Federal University, Russia
The First Example of Iodonium Ylides Derived from 7-Hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one
- P 28** Anna Gorshkova (Анна Ильинична Горшкова)
Lomonosov Moscow State University, Russia
Pickering emulsions stabilized by g-C₃N₄ or GO/g-C₃N₄ for photocatalytic degradation of organic pollutants
- P 29** Aleksandra Gubanova (Александра Николаевна Губанова)
St. Petersburg State University, Russia
Azine-*N*-oxides: *N*-O-group as a tool for expanding the reactivity of azines
- P 30** Mikhail Zapesotskii (Михаил Янович Запесоцкий)
Lomonosov Moscow State University, Russia
Copper and silver iodides coordination polymers with bicyclic amines as linkers
- P 31** Dmitrii Zakharychev (Дмитрий Викторович Захарычев)
Institute of Organic and Physical Chemistry A.E. Arbuzov FIC Kazan Scientific Center of RAS, Russia
Chiral discrimination in solid solutions of timolol maleate enantiomers: energetic aspects

- P 32** Kamil Ivshin (Камиль Анатольевич Ившин)
Institute of Organic and Physical Chemistry A.E. Arbuzov FIC Kazan Scientific Center of RAS, Russia
Structure and properties of cocrystals based on benzofuroxanes with anthracene and its methyl derivatives
- P 33** Arina Istratii (Арина Денисовна Истратий)
N.S. Kurnakov Institute of General and Inorganic Chemistry, Russia
Crystals of Polymeric Complexes Containing a Triphenylphosphine Fragment
- P 34** Sergey Kartashov (Сергей Владиславович Карташов)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
From the Pauli Exclusion Principle to Electron Pairs: Exchange Charge Density as a Structural Descriptor
- P 35** Vsevolod Korchagov (Всеволод Дмитриевич Корчагов)
St. Petersburg State University, Russia
Synthesis of Polyfluoroaromatic Selenides with Triazole Fragments as Donors of Non-covalent Interactions
- P 36** Maxim Kruglov (Максим Леонидович Круглов)
St. Petersburg State University, Russia
Sterically promoted organometallic synthesis of benzo[g]indoles
- P 37** Danil Krutin (Данил Вячеславович Крутин)
St. Petersburg State University, Russia
Cooperative Effects of Noncovalent Interactions on I $\cdots$ N Halogen Bonds in C₆F₄I₂ $\cdots$ HMTA Complexes
- P 38** Vasilisa Kulikova (Василиса Андреевна Куликова)
A.N. Nesmeyanov Institute of Organoelement Compounds, Russia
Hydrogen and tetrel bonding in reactions of silanes with proton donors and CO₂
- P 39** Alfia Kurmanova (Альфия Фаридовна Курманова)
Buketov Karaganda National Research University, Kazakhstan
Molecular Docking Study of Non-Covalent Interactions in Nitroxoline Inclusion Complexes with Functionalized β -Cyclodextrins
- P 40** Evlaliia Levchuk (Еввалия Алексеевна Левчук)
St. Petersburg State University, Russia
Cocrystals of 4-nitro-5-chalcogenocyanatophthalonitriles with α -haloazines
- P 41** Dmitrii Lobanov (Дмитрий Сергеевич Лобанов)
St. Petersburg State University, Russia
Pyridine C–H arylation reaction: hydrogen-bonding makes the difference
- P 42** Olga Lodochnikova (Ольга Александровна Лодочникова)
Institute of Organic and Physical Chemistry A.E. Arbuzov FIC Kazan Scientific Center of RAS, Russia
«Racemic compound-like» crystallization of homochiral organic compounds: the role of prostereogenic groups in the formation of pseudosymmetry elements
- P 43** Kristina Lotsman (Кристина Александровна Лоцман)
St. Petersburg State University, Russia
Chalcogen Bond Donors Featuring the Ar^F–Ar Motif: Synthesis and Self-Assembly
- P 44** Vladimir Melnikov (Владимир Евгеньевич Мельников)
St. Petersburg State University, Russia
Role of π - π stacking in cyclization pathways of heterocycle-fused enediynes under Nicholas reaction conditions
- P 45** Alina Menshikova (Алина Валерьевна Меньшикова)
N.S. Kurnakov Institute of General and Inorganic Chemistry RAS, Russia
Crystals of 3-(4-bromobenzylidene)-2,5-dihydro-1H-pyrrolinium salts with benzoic acid: structure and non-covalent interactions

- P 46** Stepan Meshalkin (Степан Алексеевич Мешалкин)
St. Petersburg State University, Russia
A data-driven framework for classification of carbon–lithium bonding in organolithium aggregates using quantum chemical descriptors
- P 47** Ilya Mikheev (Илья Андреевич Михеев)
Kurnakov Institute of General and Inorganic Chemistry RAS, Russia
Self-organisation of porphyrines: a design of potential phototherapeutic agents
- P 48** Alena Mostovaya (Алёна Станиславовна Мостовая)
MIREA, Russia
Structural features and bonding variability in the design of polynuclear copper(II) complexes with benzimidazole derivatives
- P 49** Darina Nasyrova (Дарина Ильдаровна Насырова)
N.D. Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, Russia
Cluster approach to estimation of the noncovalent interactions' energy in a crystal
- P 50** Varvara Nikitina (Варвара Васильевна Никитина)
Samara State Technical University, Russia
A new method for determining $\pi - \pi$ interactions in crystal structures
- P 51** Mikhail Orlov (Михаил Сергеевич Орлов)
St. Petersburg State University, Russia
Computational Study of Intermolecular Interactions in Polycaprolactone-Based Drug–Polymer Systems
- P 52** Vasilisa Rudenko (Василиса Андреевна Руденко)
St. Petersburg State University, Russia
Development of QTAIM-based correlations for estimating C–H $\cdots$ X (X = O, N) hydrogen bond energies
- P 53** Alina Saifina (Алина Фәядовна Сайфина)
Institute of Organic and Physical Chemistry A.E. Arbuzov FIC Kazan Scientific Center of RAS, Russia
Optically active sulfones based on 4-aminothiophenol and 5-menthyloxy- and 5-bornyloxy-2(5H)-furanones: crystal structure and stereochemical features
- P 54** Aida Samigullina (Аида Ильдусовна Самигуллина)
N.D. Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, Russia
Polymorphism in the Crystal Structures of Symmetrical Ortho-Diiodoaromatic Compounds
- P 55** Dariya Sedlova (Дарья Вадимовна Седлова)
A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia
Hydricity and reactivity of nickel pincer complexes with naphthalene-based pincer ligands
- P 56** Valentina Sobornova (Валентина Владиславовна Соборнова)
G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Russia
Analysis of the Structural and Sorption Characteristics of NCC Aerogel-Based Composites Modified with Phenamates Using Nuclear Magnetic Resonance
- P 57** Robert Fayzullin (Роберт Рүстемович Файзуллин)
Institute of Organic and Physical Chemistry A.E. Arbuzov FIC Kazan Scientific Center of RAS, Russia
Interatomic Charge Transfer and Associated Phenomena in Covalent, Coordination, and Noncovalent Bonds
- P 58** Fedonin Anton (Антон Павлович Федонин)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
Supramolecular organization in ternary crystals based on coronene and tcnq derivatives
- P 59** Lubov Frantsuzova (Любовь Вадимовна Французова)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
Crystal structure features of cyclic thiazine sulfinamides: types of stereoisomeric recognition

- P 60** Khrustaleva Aleksandra (Александра Антоновна Хрусталева)
St. Petersburg State University, Russia
Isomorphism of para-substituted polyfluorobiphenyl sulphides
- P 61** Gleb Tsytsura (Глеб Евгеньевич Цыцюра)
St. Petersburg State University, Russia
H-bond-mediated isomer selection in Pd-complex with pyridone-type chelating ligand
- P 62** Anna Shurukhina (Анна Владимировна Шурухина)
St. Petersburg State University, Russia
Optical properties of graphite-like carbon nitride $g\text{-C}_3\text{N}_4$ of different morphologies
- P 63** Kirill Yudin (Кирилл Михайлович Юдин)
Lomonosov Moscow State University, Russia
Mixed-Valent Chloroantimonate of Diazabicyclo[2.2.2]octane
- P 64** Gleb Yakovlev (Глеб Борисович Яковлев)
A.N. Nesmeyanov Institute Of Organoelement Compounds RAS, Russia
Modulating photophysical properties of Group 11 Metal complexes with pyridine-pyrazole derivatives via noncovalent interactions

July 2nd

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

	<i>Session chair: Andrey Karasik (Андрей Анатольевич Карасик)</i>
09:30	Elena Shubina (Елена Соломоновна Шубина) <i>A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Russia</i> Multifarious World of Hydrogen Bonds: from discovery to involvement in catalysis
10:05	Andrey Voshkin (Андрей Алексеевич Вошкин) <i>Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Russia</i> Functional eutectic solvents: design and selectivity
10:30	Konstantin Zhizhin (Константин Юрьевич Жижин) <i>Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Russia</i> Non-covalent interactions in the chemistry of boron cluster compounds: from structural characteristics to materials with desired properties
10:55	Sergey Adonin (Сергей Александрович Адонин) <i>Favorsky Irkutsk Institute of Chemistry SB RAS, Russia</i> Supramolecular adducts of halometalates and di- or polyhalogens
11:10	COFFEE BREAK
	<i>Session chair: Andrey Voshkin (Андрей Алексеевич Вошкин)</i>
11:40	Ilya Khodov (Илья Анатольевич Ходов) <i>G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Russia</i> Impact of Non-Covalent Interactions on Conformational Dynamics of Pharmaceutical Molecules: NMR and Computational Insights
11:55	Ravshan Shamsiev (Равшан Сабитович Шамсиев) <i>MIREA, Russia</i> Non-covalent interactions in Pd-catalysed selective hydrogenation of norbornadiene
12:10	Ekaterina Titova (Екатерина Михайловна Титова) <i>A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Russia</i> Mn(I) and Re(I) complexes containing diphosphine ligands with pendant amines: synthesis, structure and reactivity
12:25	Aleksey Mikhaylov (Алексей Александрович Михайлов) <i>Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Russia</i> Ammonium peroxogermanate: a hydrogen-bond-stabilized precursor for germanium-based materials
12:40	Tatyana Koptseva (Татьяна Сергеевна Копцева) <i>G.A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences, Russia</i> Bimetallic Hydrides of Group 13 Metals: From σ-Complexes to Reductive Elimination
12:55	Sergey Tokarev (Сергей Дмитриевич Токарев) <i>A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Russia</i> Photoinduced processes in homo- and heterobimetallic ruthenium (II) complexes with imidazo[4,5-f][1,10]phenanthrolines for various purposes
13:10	LUNCH

Main building of SPbU, Universitetskaya emb. 7-9, room 2053
(Главное здание СПбГУ, Университетская наб., д. 7-9, ауд. 2053)

Session chair: Konstantin Zhizhin (Константин Юрьевич Жижин)

- 11:40** Ilya Klyukin (Илья Николаевич Ключин)
Kurnakov Institute of General and Inorganic Chemistry RAS, Russia
Quantum Chemical Study of Non-covalent Complexes of *Closo*-Dodecaborate Anions $[B_{12}H_{11}X]^Y-$ with Blocked Amino Acids
- 11:55** Nikolay Voron'ko (Николай Георгиевич Воронько)
Murmansk Arctic University, Russia
Noncovalent Interactions in Fish Gelatin–Sulfated Polysaccharide Complexes
- 12:10** Alexandra Timralieva (Александра Акбулатовна Тимралиева)
Infochemistry Scientific Center, ITMO University, Russia
Supramolecular Assembly of N-Heterocycles in Levitating Droplet Cluster and Water-in-Oil Droplets Flow
- 12:25** Aleksandr Rogachev (Александр Валерьевич Рогачев)
Kurnakov Institute of General and Inorganic Chemistry, Russia
Dinitrobenzoates of cadmium and 3d metals as structural analogues for penta- and tetrafluorobenzoates
- 12:40** Irina Pustolaikina (Ирина Анатольевна Пустолайкина)
Buketov Karaganda National Research University, Kazakhstan
In Silico Insight into Non-Covalent Interactions of Epoxybenzoxocine Derivatives as Potential Antiviral Agents
- 13:10** LUNCH

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

Session chair: Elena Grachova (Елена Валерьевна Грачева)

- 14:50** Igor Alabugin (Игорь Владимирович Алабугин)
Florida State University, USA
Electronic Origin of Supramolecular Control in Radical Cascades: Transient 2c,3e Interactions
- 15:25** Aleksandr Artem'ev (Александр Викторович Артемьев)
Nikolaev Institute of Inorganic Chemistry, Russia
New advances in the chemistry and photophysics of copper(I) diimine-diphosphine complexes
- 15:50** Ilya Gridnev (Илья Дмитриевич Гриднев)
N.D. Zelinsky Institute of Organic Chemistry RAS, Russia
Enantioselection in Asymmetric Hydrogenation: Approach of the Substrate towards a Catalyst Enabled by Noncovalent Interactions
- 16:15** Aleksei Titov (Алексей Александрович Титов)
A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Russia
Cyclic Metal Complexes as Lewis Acids or Bases for Supramolecular Host–Guest Chemistry

COFFEE BREAK

Session chair: Aleksandr Artem'ev (Александр Викторович Артемьев)

- 17:00** Julia Voronina (Юлия Константиновна Воронина)
N.S. Kurnakov Institute of General and Inorganic Chemistry RAS, Russia
Theoretical assessment of the effect of non-covalent interactions on biological activity
- 17:15** Maria Ustimova (Мария Алексеевна Устимова)
A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Russia
Small molecule non-covalent interactions with biomolecules
- 17:30** Vlad Travkin (Владислав Владимирович Травкин)
A.E. Arbuzov Institute of Organic and Physical Chemistry RAS, Russia
Assembling of petroporphyrins in vacuum-deposited layers
- 17:45** Nikita Kostin (Никита Андреевич Костин)
Federal State Budgetary Educational Institution of Higher Education Dmitry Mendeleev University of Chemical Technology, Russia
Thermodynamics and kinetics of co-crystallization of 2,4-dinitrodiazophenol and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane
- 18:00** Yuliya Sozinova (Юлия Игоревна Созинова)
G.A. Razuvaev Institute of Organometallic Chemistry of the Russian Academy of Sciences, Russia
Hydrogen-Bonded Adducts of dpp-bianH₂ with N-Heterocycles
- 18:10** Maxim Sokolov (Максим Римович Соколов)
Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Russia
Photocatalytic activity of nanocomposites based on two-dimensional nanoparticles of molybdenum disulfide and layered Tb³⁺ and Eu³⁺ hydroxides
- 18:20** Nikita Shimin (Никита Андреевич Шимин)
Samara National Research University, Russia
Geometric and quantum-chemical approaches to evaluating intermolecular interactions
- 18:30** Pavel Vololdin (Павел Андреевич Володин)
Kazan (Volga Region) Federal University, Russia
Key role of intermolecular π -stacking in formation of 3d-metal complexes based on o-xylylenediamine supported salen-type ligands
- 18:40** Sofya Marikovskaya (Софья Марковна Мариковская)
Boreskov Institute of Catalysis, Russia
Effect of cation nature on catalytic performance of Zr/Hf-substituted polyoxometalates in H₂O₂-based selective oxidation

Main building of SPbU, Universitetskaya emb. 7-9, room 2053
(Главное здание СПбГУ, Университетская наб., д. 7-9, ауд. 2053)

Session chair: Ilya Gridnev (Илья Дмитриевич Гриднев)

- 17:00** Anton Lobanov (Антон Валерьевич Лобанов)
Moscow Pedagogical State University, Russia
Noncovalent Complexes of Chlorophyll and Hemin with Biocompatible Polymers
- 17:15** Kirill Bulanin (Кирилл Михайлович Буланин)
St. Petersburg State University, Russia
Study of the dynamics of organic cations in hybrid perovskites using vibrational spectroscopy methods
- 17:30** Aleksandr Voronin (Александр Павлович Воронин)
G.A. Krestov Institute for Solution Chemistry of Russian Academy of Sciences, Russia
Complexation in Crystal, Solution and Vapor: Congruent Sublimation and Cocrystallization Thermodynamics of [Caffeine + 3-Hydroxybenzoic Acid] (1:1)
- 17:45** Dmitry Yakhvarov (Дмитрий Григорьевич Яхваров)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
Noncovalent interactions in synthesis and design of new catalytic systems based on black phosphorus and organonickel sigma-complexes
- 18:00** Aleksei Abdulmyanov (Алексей Рафикович Абдульмянов)
Samara National Research University, Russia
Noncovalent Interactions in the Crystal Structure of $\text{UO}_2(\text{BrCH}_2\text{CH}_2\text{COO})_2$
- 18:10** Viktoria Soloveva (Виктория Андреевна Соловьева)
Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russia
New di- and tripodal heterocyclic N-donor ligands based on bis- and tris(triazolyethyl)amines for 3d-metal complexes formation
- 18:20** Yuliya Toikka (Юлия Николаевна Тойкка)
St. Petersburg State University, Russia
Synthesis and structural studies of $\text{trans}[\text{CuX}_2(\text{NCNR}_2)_2] \cdot 2\text{HAB}$ complexes (X = Cl, Br; HB = 1,4- $\text{C}_6\text{I}_2\text{F}_4$, 1,3,5- $\text{C}_6\text{I}_3\text{F}_3$)
- 18:30** Matvey Shurikov (Матвей Константинович Шуриков)
National Research Tomsk Polytechnic University, Russia
Cage-like nucleophiles in supramolecular design of exchange coupled systems
- 18:40** Pavel Egorov (Павел Андреевич Егоров)
Institute of General and Inorganic Chemistry RAS, Russia
The role of hydrogen bonds in enhancing the coordination of hydrogen peroxide with tin(IV)

July 3rd

University Center, Birzhevaya Liniya 6
(Университетский центр СПбГУ, Биржевая линия, д. 6)

<i>Session chair: Sergey Konchenko (Сергей Николаевич Конченко)</i>	
09:30	Andrei Shevelkov (Андрей Владимирович Шевельков) <i>Lomonosov Moscow State University, Russia</i> Controlling optical properties of hybrid metal halide complexes using strong and weak interactions
10:05	Elena Grachova (Елена Валерьевна Грачева) <i>St. Petersburg State University, Russia</i> Noncovalent interactions in the design of luminophores based on Pt(II) complexes
10:30	Maxim Sokolov (Максим Наильевич Соколов) <i>Nikolaev Institute of Inorganic Chemistry SB RAS, Russia</i> Argentophilic interactions – rivals of hydrogen bonds?
10:55	Yuriy Tveryanovich (Юрий Станиславович Тверьянович) <i>St. Petersburg State University, Russia</i> Metallophilic interactions in inorganic semiconductors
11:10	COFFEE BREAK
<i>Session chair: Maxim Sokolov (Максим Наильевич Соколов)</i>	
11:40	Sergey Konchenko (Сергей Николаевич Конченко) <i>Nikolaev Institute of Inorganic Chemistry SB RAS, Russia</i> Design and Synthesis of Benzothiazole Derivatives and Their d-f Heterometallic Complexes: Harnessing Non-Covalent Interactions
12:05	Petr Prikhodchenko (Петр Валерьевич Приходченко) <i>Kurnakov Institute of General and Inorganic Chemistry RAS, Russia</i> The key role of hydrogen bonds in obtaining nanomaterials from peroxide systems
12:30	Alexandra Zvyagina (Александра Игоревна Звягина) <i>Frumkin Institute of physical chemistry and electrochemistry RAS, Russia</i> Ultrathin coatings based on graphene oxide and gold nanoparticles for surface-enhanced Raman spectroscopy
12:45	Andrey Marchenko (Андрей Владимирович Марченко) <i>Southern Federal University, Russia</i> Anion-cation interactions in protonated naphthalene “proton sponges” in crystals as a consequence of spatial congestion
13:00	Aleksey Bilyachenko (Алексей Николаевич Биляченко) <i>A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Russia</i> (Supra)molecular assembly in cage metallasilsesquioxanes
13:15	CLOSING



PLENARY LECTURES



IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Making Chemistry an Exact Science

Valentine P. Ananikov

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In recent years, it has become increasingly evident that chemistry, as a scientific discipline, has reached a critical juncture where further progress is unattainable without a transition toward precision, reproducibility, and digital data processing. Despite the inherent complexity of the systems under investigation, modern chemistry frequently continues to rely on qualitative methodological formulations, abstract schematics, and fragmented reaction descriptions. Consequently, the yields of chemical processes reported in the scientific literature are often inconsistent. Furthermore, the poor reproducibility of yields in published chemical reactions has been tacitly accepted by the scientific community as a "norm" [1], a standard that is fundamentally incompatible with the principles of the natural sciences. When scaling reactions to industrial production volumes, this lack of reproducibility presents significant challenges, frequently necessitating extensive supplementary experimentation. This not only impedes scientific progress but also diminishes the efficiency of industrial implementation in the development of novel materials and technologies.

Chemistry must evolve into a rigorously exact science, characterized by highly reproducible results, verifiable yields, and digital algorithms that can be seamlessly integrated into real-world technological processes. To achieve this, it is imperative to openly acknowledge existing methodological shortcomings, cultivate a more precise scientific infrastructure, and foster collaborative efforts across the entire scientific community. Only through such concerted action can the field transition toward truly effective laboratory and industrial solutions.

These issues are discussed in this report and illustrated with specific examples demonstrating the impact of impurities and contaminants, phantom catalysis, challenges in the spectral identification of compounds, and inaccuracies in experimental reporting [2–4]. Furthermore, this work provides an analysis of the factors influencing the reproducibility of chemical reactions and proposes strategic approaches to rectify the current situation.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

1,3-Diaza-2-metalloles (DAMs): A New Generation of Catalysts for Polymerization Reactions

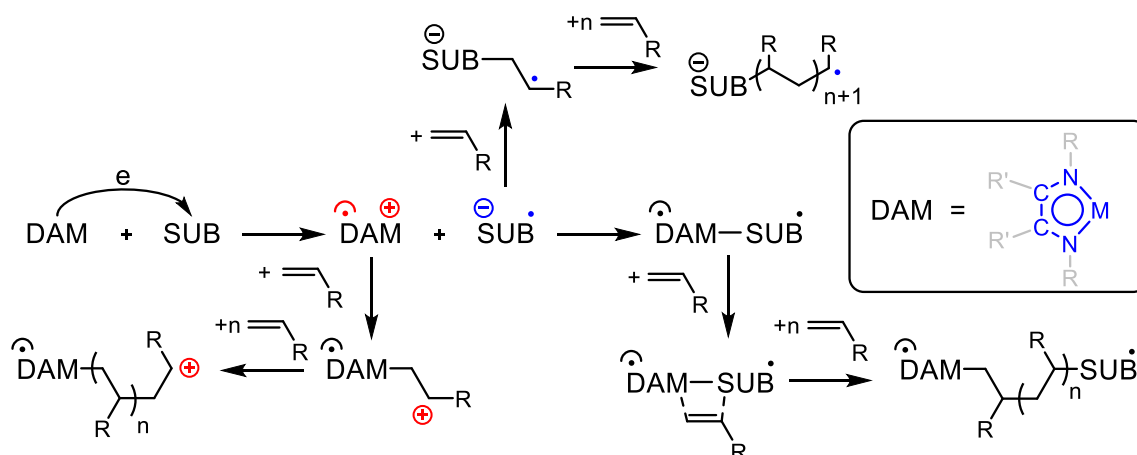
I.L. Fedyushkin^{1,2}, V.M. Makarov^{1,2}

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Single-electron transfer between 1,3-diaza-2-metalloles (DAMs) and organic substrates (SUB) is expected to yield ion-radical pairs, [DAM^{•+}SUB^{•-}], whose cationic, anionic, and radical centers are capable of initiating the polymerization of suitable monomers via cationic, anionic, and radical mechanisms. This presentation will provide current data on the polymerization of acrylic monomers and cyclic esters mediated by 1,3-diaza-2-metalloles.



Acknowledgements

This work was carried out using the equipment of the Shared Facility Center "Analytical Center of the IOMC RAS". The portion of this work concerning L-lactide polymerization was performed within the framework of State Assignment No. 073-00095-26-02 of the Ministry of Education of the Russian Federation for the year 2026, under the research topic "Development of Methods for the Preparation of Novel Polymeric Materials".



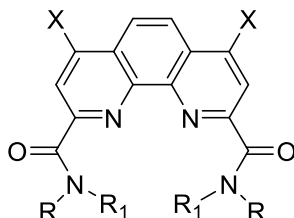
IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Design and Synthesis of Phenanthroline Diamides for f-Element Separation

Valentine G. Nenajdenko

Lomonosov Moscow State University, Leninskie Gory 1 Bld. 3, 119991 Moscow, Russia
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The development of highly selective ligands for f-element separation represents a pressing challenge. Such ligands are critically required for the production of high-purity rare earth elements (REEs), without which the existence and advancement of innovative technologies in energy, electronics, transportation, communication systems, and numerous other vital fields of modern engineering would be impossible. The application of these ligands underpins extraction-based technologies for spent nuclear fuel (SNF) reprocessing in the nuclear energy sector. Diamides of 1,10-phenanthroline-2,9-dicarboxylic acid constitute one of the most promising classes of ligands for addressing these challenges. This presentation discusses the synthesis, coordination chemistry, and extraction performance of such ligands.





IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Guest@MOF: The Role of Non-Covalent Interactions

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This report will examine the results of research on the synthesis, structure, and functional properties of metal–organic frameworks (MOF) and inclusion compounds based on them.^{1–3} Frameworks with permanent porosity are used for the separation of hydrocarbons, as well as for solving the complex problem of separating water isotopomers. Particular attention will be paid to the identification of host–guest structures. Studying such structures allows us to identify specific interactions that determine the selectivity of separation and luminescent detection of substances with similar physicochemical properties. Bifunctional MOFs, demonstrating both high selectivity for gas adsorption and luminescent detection of specific analytes, will also be discussed.

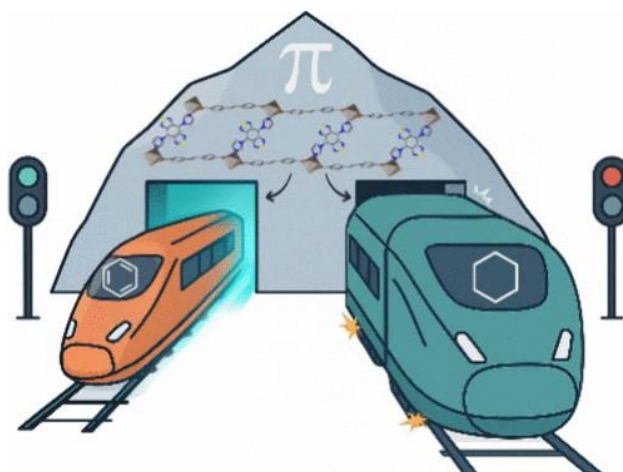


Figure 1. Host-guest non-covalent interactions for separation and sensing

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Design of Luminescent Materials: Balancing Intramolecular and Intermolecular Interactions

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During the last two decades one type of heterocyclic diphosphines, namely 1,5,-diaz-3,7-diphosphacyclooctanes (P_2N_2 -ligands), became privileged ligand system for constructing novel transition metal catalysts. However, the potential of P_2N_2 -ligands for creating luminescent systems based on copper group metals has been not demonstrated.¹

Cyclic structure of P_2N_2 -ligands forms predicted 3-dimensional first and second coordination spheres of complexes, as well as type and force of intra- and intermolecular noncovalent interactions. Balancing intra- and intermolecular interactions in the crystals or solutions of complexes of P_2N_2 -ligands with fluorophoric exocyclic substituents one could control the luminescence effectiveness and responding to external stimuli, which can be used for establishing temperature, pH and presence of some small organic molecules.²⁻³

Solvent-exchange and thin-film hydration procedures allow us to obtain biocompatible core-shell and micellar NPs based on complexes of cyclic P,N -ligands. The nanoparticles could be regarded as promising contrasting agents for confocal microscopy and anti-cancer drugs due to their ability to catalyze the formation of reactive oxygen species (ROS) in the tumor cells.⁴

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Multifarious World of Hydrogen Bonds: from discovery to involvement in catalysis

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Hydrogen bonding and other noncovalent interactions accompany the reactions, both stoichiometric and catalytic, that involve polar substrates and functionalized metallocomplexes^{1,2} (Figure 1).. In this lecture we conceptualize our knowledge of hydrogen bonding involving metal hydrides and attempted to illustrate the role of these interactions in metal-ligand cooperation catalysis. Although it might add complexity to the reaction mechanism, taking into account these noncovalent interactions might be an important tool to affect a reaction rate and selectivity^{3,4}.

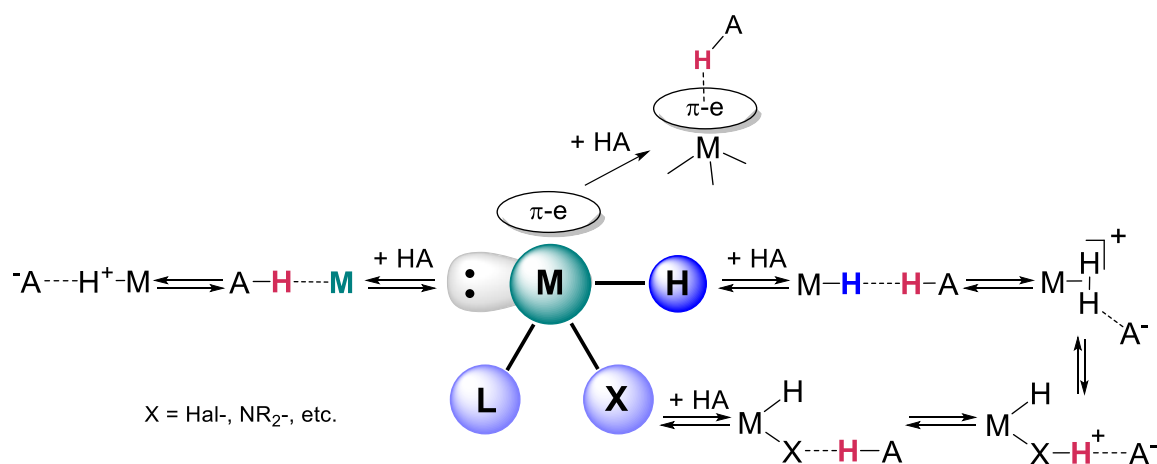


Figure 1. Potentially basic centers in a generic transition metal hydride complexes: hydrogen bonding and proton transfer reactions.

Acknowledgements

The financial support by RSF project № 24-13-00283 is gratefully acknowledged

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Electronic Origin of Supramolecular Control in Radical Cascades: Transient 2c,3e Interactions

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Designing intermolecular control for short-lived neutral intermediates such as radicals remains a fundamental challenge. Here, we show how propargylic alkoxy groups act as supramolecular “chaperones” that guide Bu_3Sn radicals to the correct alkyne site in multifunctional substrates.¹

We demonstrate that these directing effects originate from transient through-space two-center, three-electron (2c,3e) interactions between the radical and a lone pair of a propargylic heteroatom. Although such bonds have been less explored, largely because they involve radicals that are inherently transient and formally violate the octet rule, they represent a powerful and underutilized stabilizing force. In our parallel research, we have shown that these interactions can drive electron upconversion;² here, we establish their role in supramolecular control of radical reactivity.

These interactions selectively stabilize addition at the propargylic position over competing pathways, enabling efficient and selective radical cyclization/fragmentation cascades in oligoalkyne systems. Non-covalent acceleration further enables a traceless directing strategy via elimination during the final aromatization step.³

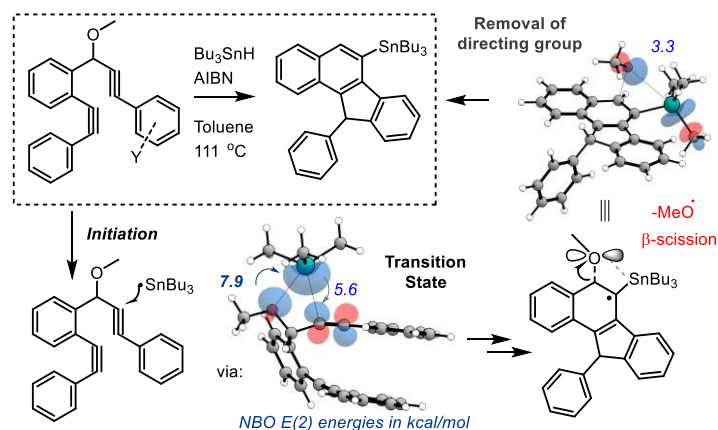


Figure 1. Non-covalent interactions with Sn- and O-centered radicals in alkyne cascade

Acknowledgements

We gratefully acknowledge support of the Russian Science Foundation (grant no. 25-73-31002).

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Controlling optical properties of hybrid metal halide complexes using strong and weak interactions

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The efficiency of light-absorbing haloplumbates has reached 27%, making them very attractive for modern photovoltaics. Their drawback is dangerous neurotoxicity of lead halide complexes, making the prospects of lead-based light-harvesting materials doubtful and motivating searching for analogs among halide complexes of other post-transition metals containing a lone ns^2 pair. No surprise that such a search has already resulted in hybrid compounds displaying very different properties, including thermochromism, vaporchromism, non-linear optical response, and bright wideband luminescence, aside from photovoltaic activity.

As long as various ns^2 cations have been utilized in new compounds, no common rules for their synthesis have so far been laid. However, our work has made it obvious that the overwhelming majority of new hybrid compounds can be prepared from a variety of solvents, where only simple complexes exist in solutions, whereas the process of crystallization regulates their oligo- or polymerization into more complex units.

In this paper, we show that the elaborated synthetic procedures under dynamic conditions lead to desired hybrid compounds. Specifically, we focus on hybrid halometallates that exhibit two important properties. One of them is light harvesting, which primarily relies on the proper width of the band gap, being near 1.4 eV. We have introduced new approaches to the optimization of the band gap. The first one employs an inclusion of additional I_2 molecules that bind iodobismuthate anions into extended structures with a concomitant decrease in the band gap to acceptable values of 1.5 eV and below. The second one relies on the formation of in-gap states in the band structure, which is achieved by combining empty and occupied p-states of bismuth and antimony, for which a combination of M^{3+} ($M = Sb, Bi$) and Sb^{5+} is required.

With respect to bright wideband luminescence, we show that combining advantages of light emitting antimony(III) halides and the established structure directing function of various cyclic amines, we have synthesized a number of hybrid compounds with extremely distorted 1D-polymeric anions that display remarkable long-lived bright luminescence previously observed only for diluted metal-based complexes.

Breaking the limits of ns^2 metal cations, we introduce in this paper various hybrid complexes bearing d-metal centers. These new compounds exhibit numerous new properties ranging from bright narrow-band luminescence to magnetic ordering. In all cases, we pay utmost attention to the role of weak and noncovalent interactions that ensure integrity and perfect crystallographic order in compounds in question.

Acknowledgements

This work is supported through the state assignment #AAAA-A21-121011590082-2.

KEYNOTE LECTURES



IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Application of pulsed EPR spectroscopy to study non-covalent interactions in biopolymers

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Non-covalent interactions play a crucial role in the formation of biopolymer complexes. EPR spectroscopy provides insights into molecular structure and dynamics, exchange and dipole–dipole interactions between electron spins, rate constants of radical reactions and their underlying mechanisms, as well as local parameters such as pH and oxygen concentration. The utility of EPR in biophysics expanded significantly with the introduction and development of pulsed EPR techniques, particularly the Pulse Electron DOuble Resonance (PELDOR) / Double Electron–Electron Resonance (DEER) method. These techniques employ specific pulse sequences to measure the dipole–dipole interaction between unpaired electrons, enabling distance measurements in the nanometer range.¹

This report overviews our recent results obtained using continuous-wave (CW)^{2,3} and pulsed^{4–7} dipolar EPR spectroscopy, and their applications to study the structure and dynamics of non-covalent complexes of DNA repair enzymes with DNA duplexes and inhibitors. CW-EPR using a ¹³C triarylmethyl radical (TAM) as an intracellular spin probe effectively reports on physiological properties, including intracellular pH and mobility³. This technology has potential applications in metabolic diseases (such as lysosomal storage disorders) as well as in studying tumor oxygenation. The redox-activated probe establishes a novel strategy for the non-invasive assessment of tumor acidosis, with significant implications for personalized diagnostics and therapy evaluation.

pH-sensitive spin labels hold great potential for exploring electrostatic interactions in non-covalent DNA–protein complexes, where fine-tuning of local charge is critical for function². A pH-sensitive label demonstrated excellent sensitivity in detecting DNA duplex formation and formamidopyrimidine–DNA glycosylase (Fpg) binding, allowing us to measure changes in the local electrostatic potential. DNA duplexes with the spin label placed near the active site were constructed and verified by EPR and molecular dynamics².

The final topic concerns a recently developed EPR approach based on TAM-¹⁹F ENDOR for measuring distances in biomolecules and DNA duplexes⁷.

Acknowledgements

This work was supported by the Russian Science Foundation (No. 25-13-00327).

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

The role of protonation and charge density in oxidation catalysis with polyoxometalates

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Transition-metal-substituted polyoxometalates (M-POM) are anionic metal-oxygen clusters that possess thermodynamic stability to oxidation and are widely used as catalysts for liquid-phase selective oxidations.¹ In this lecture, we discuss how non-covalent interactions affect catalytic performance of M-POM (M = Ti^{IV}, Zr^{IV}) in the oxidation of thioethers, alkenes, and alcohols with environmentally benign oxidants, aqueous hydrogen peroxide and *tert*-butyl hydroperoxide (TBHP).²⁻⁵ In particular, we address the key role of protonation and polyanion charge density (q/M), which depends on the POM structural type (Fig. 1), for different stages of the catalytic oxidation process.

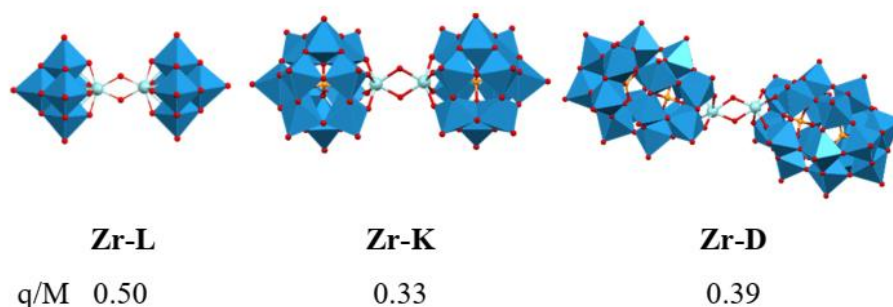


Figure 1. Zr-POMs of the Lindqvist (L), Keggin (K) and Dawson (D) structures and corresponding polyanion charge density (q/M).

Protons reduce the high negative charge of POM, making it and related peroxo species more electrophilic and thereby favoring oxygen atom transfer to nucleophiles. Our recent studies implicated that the structural effect in oxidation catalysis with M-POM can often be rationalized in terms of the polyanion charge density, which decreases in the order $L > D > K$. The rate of alkene, thioether and alcohol oxidation inversely correlates with q/M , provided that side reactions (e.g. H_2O_2 dismutation over Zr-POM producing $^1O_2$ and/or $HO_2^{\cdot}$)⁶ do not contribute significantly to the oxidation process. Correlations with charge density are even more evident for oxidations with TBHP, which is not decomposed by Zr-POM.

Acknowledgements

This work was supported by the Russian Science Foundation (grants No. 23-13-00156 and 23-13-00156-II).

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Covalent Metal-Organic Frameworks: Fusion of the COFs and MOFs

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Metal–organic frameworks (MOFs) and covalent organic frameworks (COFs), as emerging porous crystalline materials, have attracted remarkable attentions in chemistry, physics and materials science. MOFs are constructed by metal clusters (or ions) and organic linkers through coordination bonds, while COFs are prepared by pure organic building block via covalent bonds. Owing to the nature of linkage, MOFs and COFs have their own shortcomings. Typically, the relatively weak bond strengths of coordination bonds lead to poor chemical stability of MOFs, which limit their practical implementations. On the other hand, due to the strong covalent bonds, although COFs exhibits rather higher stability under harsh conditions compared to MOFs, the lack of open metal sites restricts their functionalization and application. Therefore, it is hypothesized that “cream-skimming” of MOF and COF would address these drawbacks and produce a new class of crystalline porous material, namely covalent metal–organic frameworks (CMOFs), with unprecedented structural complexity and advanced functionality.

In the past few years, our group have specifically focus on the development of coinage metal (Cu, Ag and Au) cyclic trinuclear units (CTUs) based CMOFs by networking CTUs with dynamic covalent chemistry (DCC). CTUs exhibits trigonal planar structures with high chemical stability and functionated groups of amines or aldehyde can be easily introduced on the skeleton. Notably, CTUs also features interesting properties including metallophilic attraction, π -acidity/basicity, luminescence and catalytic activity.¹ Therefore, we envisioned that the CTUs-based CMOFs would be a promising platform not only for development of novel synthetic strategies, but also for potential applications in many research fields including gas absorption/separation, sensor, full-color display, and catalysis.²⁻⁸

In this presentation, we summarize the recent progress on CTU-based CMOFs, starting with linkage and topological design, structural transformation, morphological control, and potential applications in various fields. We also discuss the future opportunities of these interesting CMOFs as a promising platform to explore the challenges in this rapidly developed research field of crystalline porous materials by combining the advantages of MOFs and COFs.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Chalcogenadiazole based chalcogen bond donors: supramolecular architectures, optical properties and cationic activation

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1,2,5-chalcogenadiazoles – a class of heterocyclic compounds with an interesting set of inherent properties, most notably the π -acceptor properties due to the electron deficiency of the heterocyclic π -system and therefore high electron affinity. As π -acceptors these compounds are used for the preparation of radical-anion salts, charge transfer complexes and building blocks for polyconjugated organic semiconductor materials. At the same time these compounds display σ -acceptor properties through the formation of chalcogen bonding (*ChB*) – a secondary bonding interaction between a LB and a region of depleted electron density with a local positive electrostatic potential – a σ -hole.^[1]

Values of the local maxima of electrostatic potential in σ -holes of chalcogenadiayoles – $V_{S,max}$, characterizing the ability to form *ChBs*, can be tuned via adding electron withdrawing groups to the molecule. Yet, for neutral chalcogenadiazoles these values are moderate compared to many other σ -hole donors. However, one of the potential strategies to activate σ -hole interactions is to turn neutral molecules into cations via N-alkylation of chalcogenadiazole ring. Chalcogen bonding is a major factor affecting the supramolecular architectures of chalcogenadiazoles and their supramolecular complexes. Typical to chalcogenadiazoles are double *ChB* $[E \cdots N]_2$ ($E = S, Se, Te$) supramolecular synthons, however, certain other architectures are also possible if other competing interactions take place. Notably upon complexation with anions a new long wave-length charge transfer band appears in the electronic absorption spectra. This spectral change is used for spectrophotometric determination of complex formation constants, and possibly as an analytical signal for the colorimetric sensing of certain LBs, while fluorescent response remains elusive.

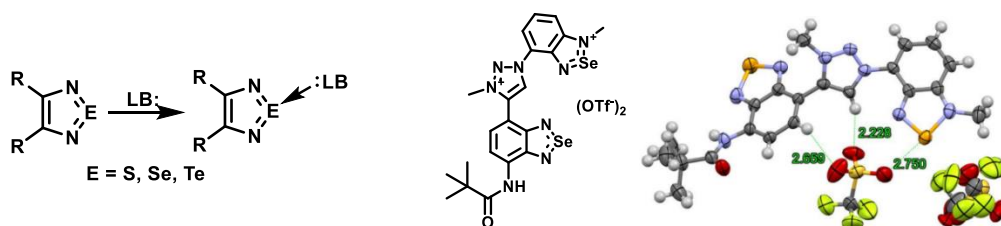


Figure 1. Left: ChB formation scheme. Right: XRD structure of novel cationic chalcogenadiazole based anion receptor.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Absolute Asymmetric Supramolecular Synthesis — Engineering of Enantiomorphic Crystals

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Homochirality is one of the signatures of life. The spontaneous generation of homochirality in an achiral environment is very important to understand the origin of life in the universe.¹⁻³ In this report an absolute asymmetric supramolecular synthesis by analogy with absolute asymmetric organic synthesis is introduced.

On the examples of metacyclophane and thiazolo[3,2-a]pyrimidine derivatives, a hierarchical approach to the implementation of absolute asymmetric supramolecular synthesis in the crystalline phase by tuning non-covalent intermolecular interactions leading to the formation of optically active products from achiral or racemic precursors is demonstrated.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Non-covalent interactions in the design of molecular-based magnets

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Among stable organic radicals, nitroxide radicals stand out for their exceptional stability, synthetic accessibility, and structural versatility. These compounds have gained recognition as key building blocks in the development of molecule-based magnets. In this area of research, scientists have primarily focused on assembling functionalized nitroxides into exchange-coupled clusters or bulk magnets via solid-state arrangements [1].

We demonstrate that chloro-, bromo-, and iodo-substituted nitronyl nitroxides (Hal–NN) undergo self-assembly in the crystalline state through the combined action of halogen bonds (XB) and hydrogen bonds (HB). Theoretical calculations reveal that XBs play a dominant role in mediating the association of these nitroxides – specifically via atoms carrying spin densities of opposite signs (Figure 1). This interaction promotes ferromagnetic intermolecular exchange interactions. Notably, this research provides the first evidence that XBs can create pathways that facilitate ferromagnetic intermolecular exchange between paramagnetic centers in nitronyl nitroxide organic radicals [2].

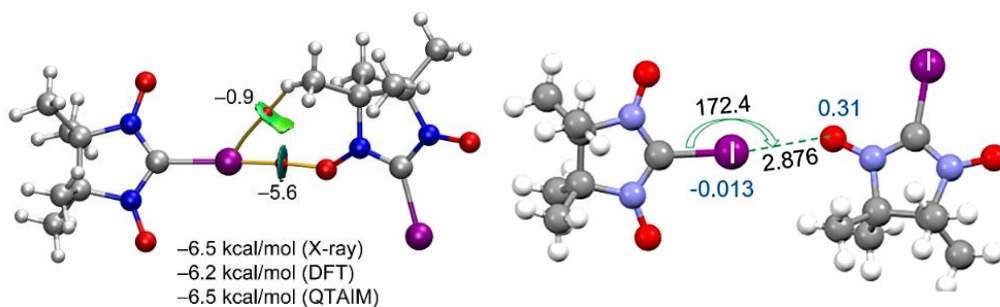


Figure 1. QTAIM and NCIplot analysis of XB and HB interactions in I–NN (left panel). A representative pair of I–NN radicals (right panel) with their geometric parameters (black labels, in Å and deg.) and Mulliken atomic spin populations (blue labels).

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Configuration Complexity as a Predictor of Synergy in Hybrid Materials

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Hybrid materials combine organic and inorganic components at the nanoscale. They are promising for chemical sensing, organic electronics, catalysis, and photocatalysis. Their defining feature is functional synergy, the ability to show non-additive properties not found in the individual components. Many synergistic materials appear in the literature, but the nature of the phenomenon remains unclear. Most studies state synergy without connecting it to structure. A unified framework is missing. Synergy cannot be predicted, only observed.

This work examines hybrid photocatalysts assembled from zinc porphyrinates and two-dimensional inorganic particles (graphene oxide, molybdenum sulfide, terbium and europium hydroxides). All use a common supramolecular motif, the paddlewheel coordination of zinc acetate clusters. Binary and ternary hybrids were studied in the photodegradation of organic compounds. The transition from additive to non-additive functional behavior follows from increasing structural complexity.

We propose a new framework to describe synergy in hybrid photocatalysts. The synergistic potential of a hybrid can be represented as a graph. Vertices correspond to structural motifs where charge and energy separate and transfer. Edges correspond to possible pathways for converting light into chemical work. This graph is analogous to a control flow graph in software engineering, which maps all possible execution paths in a program. In that field, cyclomatic complexity measures the number of independent paths and predicts the likelihood of unexpected behavior. In our framework, configuration complexity serves a similar but inverted purpose. Higher complexity means more pathways for an absorbed photon to sample multiple components before relaxing. It therefore predicts the likelihood of non-additive, synergistic behavior.

This approach offers a foundation for machine learning and neural networks to discover, design, and predict functional synergy in hybrid materials.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

EFFECTS OF NONCOVALENT INTERACTIONS IN PHOTOPHYSICS OF AGGREGATED d^8 SQUARE-PLANAR and d^{10} COMPLEXES IN SOLID STATE AND IN SOFT MATTER NANOMATERIALS.

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Aggregation of organic and organometallic chromophores significantly affects their photophysical properties, leading either to emission quenching or, conversely, to emission enhancement, while also altering the energy of emissive transitions in organometallic compounds. Non-covalent interactions as the driving force of aggregation (van der Waals forces, hydrogen bonds, π -stacking, metallophilic and hydrophobic interactions) are generally nearly an order of magnitude weaker than intramolecular covalent bonds. However, they are numerous and can be further supported by aggregate packing within a crystalline unit cell or amorphous matrices, as well as through external covalent linkages.

Among the aforementioned non-covalent interactions, **π -stacking of aromatic ligand systems** and **metallophilic interactions** exert the greatest influence on the spectral and photophysical properties of organometallic chromophores. This is because virtually all typical excited states (MLCT, LC, LLCT) are localized on the metal ion orbitals and/or the aromatic systems of the ligands, and any perturbation of these orbitals affects the energy and dynamics of the transitions responsible for absorption and emission. Among luminescent transition metal complexes, **square-planar d^8 complexes of Pd(II), Pt(II), and Au(III)** and **d^{10} complexes of Au(I)** exhibit a particular propensity for aggregation due to the absence of steric hindrance to aggregate formation. For these emitters, in addition to an increase in emission quantum yield via suppression of non-radiative vibrational and rotational relaxation of excited states, a substantial lowering of the emission transition energy is observed – even shifting into the near-infrared region (the so-called biological tissue transparency window). This feature is of great importance for biomedical research.

This presentation will cover: (i) the main structural types of aggregates formed by the aforementioned complexes in different aggregation states; (ii) the influence of various non-covalent interactions on specific photophysical parameters of aggregated luminophores; (iii) key strategies for the directed manipulation of these parameters; and (iv) experimental approaches for stabilizing the resulting aggregates both in the solid phase and in "soft" nanomaterials – such as micelles based on amphiphilic block copolymers – with the aim of applying these luminescent aggregates in practical areas such as luminescent bioimaging and biosensing.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

The Art of Structural Instability: Living Life Through Non-Covalent Bonds

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Noncovalent interactions are ubiquitous in nature and play a fundamental role in the bonding of chemical systems. In contrast to covalent bonds, intra- and intermolecular noncovalent interactions are typically weak, exhibiting much lower energy - a characteristic directly reflected in the term "noncovalent". Due to the active development of these topics during recent years, most achievements in chemistry in the 21st century already is and will continue to be largely determined by noncovalent interactions.

Our own contributions in this area encompass diverse acid–base interactions involving transition-metal and main-group element hydrides. These interactions ultimately determine the reactivity of hydrides in both stoichiometric and catalytic processes, including (de)hydrogenation, dehydrocoupling, and alkene isomerization. Furthermore, they offer a versatile tool for the fine-tuning of metal complex properties¹⁻⁵.

Among various noncovalent interactions, this lecture will focus on those involving the CO group of metal carbonyl complexes. The metal-bound CO ligand has traditionally been viewed as a standard "lone pair base" through the oxygen atom, or as a π -base via the electron density of the triple bond. We demonstrate that an alternative mode can be effectively triggered by applying a suitable partner - specifically, the N-lone pair of a 1,5-diaza-3,7-diphosphacyclooctane ligand, which turns the CO group into a π -acid. This interaction not only governs the ligand conformation but also leads to dramatic changes in the CO stretching vibration frequency. Since $\nu(\text{CO})$ is widely used as a characteristic parameter for determining ligand donor properties (the Tolman Electronic Parameter), neglecting this type of noncovalent interaction can - and indeed has - led to significant misinterpretations.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Functional eutectic solvents: design and selectivity

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The development of extraction technologies requires the creation of new, efficient, and safe extractants to address complex technological challenges such as the recycling of spent batteries, magnets, and other materials. One of the most promising directions is the development of extractants based on eutectic solvents due to their environmental safety and low flammability¹. Among the wide variety of eutectic solvents, functional eutectic solvents occupy a special place because of their unique properties for solving specific applied problems. The emergence of this subclass reflects the transition from initial fundamental research to the creation of advanced scientific developments and the formation of new competitive technologies.

The presentation will discuss methodological approaches to the design of functional eutectic solvents with tailored physicochemical properties and to controlling their extraction capacity. Specific examples will demonstrate that increases in the efficiency² and selectivity³ of extraction systems are achieved through targeted modeling of extractant properties and the rational selection of functional components.

Thus, the broad potential of functional eutectic solvents in solving hydrometallurgical problems will be demonstrated, which is a necessary condition for ensuring sustainable economic growth and achieving technological leadership for the Russian Federation.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Non-covalent interactions in the chemistry of boron cluster compounds: from structural characteristics to materials with desired properties

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Non-covalent interactions play a significant role in the chemistry of boron cluster compounds^{1,2}. Present report will focus on the features of non-covalent interactions in the case of *closo*-borate anions $[B_nH_n]^{2-}$ ($n = 10, 12$) and their derivatives. A distinctive feature of these systems is the ability to form non-covalent interactions both through *exo*-polyhedral hydrogen atoms and through B-B-B edges. In the case of substituted cluster anions, the atoms of the *exo*-polyhedral substituent make a significant contribution to the formation of molecular associates. Dihydrogen contacts $BH \cdots HX$ ($X = C, N, O$) are the most studied. This type of interaction determines the stereoselectivity of nucleophilic addition processes in borylated nitriles of the general form $[B_nH_{n-1}NCR]^-$ ($n = 10, 12$; $R = Alk, Ar$)³.

Closo-borate anions and their derivatives are considered as promising platforms for medicine (BNCT, drugs with antiviral/antibacterial activity). For effectiveness of a drug, it must bind with target biomolecules, such as proteins. Non-covalent interactions play a key role in the binding between small molecules and biomolecules. Present report will analyze the main types of interactions between clusters and biopolymers. In addition to biopolymers, cluster compounds can form non-covalent interactions with various organic and inorganic systems. Derivatives of boron cluster anions can serve as one of the components for creating hybrid aerogels based on silica. $BH \cdots HOSi$ contacts play a significant role in the structural motif of the resulting aerogels. Derivatives of boron cluster anions are capable of non-covalently binding to polymer matrices based on polylactide and polycaprolactone. A series of materials based on substituted *closo*-borates and corresponding polymeric filaments for 3D printing have been obtained. These materials showed good strength characteristics, as well as controlled release.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

New advances in the chemistry and photophysics of copper(I) diimine-diphosphine complexes

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Copper(I) diimine–(di)phosphine complexes of the general formula $[\text{Cu}(\text{NN})\text{PP}]^+$ constitute one of the largest and most extensively studied classes of thermally activated delayed fluorescence (TADF) materials. These compounds continue to attract significant attention as emitters for OLEDs and LEECs, as well as photocatalysts for a variety of organic transformations [1].

The presentation will highlight original approaches to the design of $[\text{Cu}(\text{NN})\text{PP}]^+$ complexes with targeted properties, including:

- the introduction of chiral substituents into the diimine ligand as a novel strategy for the development of low-cost materials exhibiting highly efficient circularly polarized thermally activated delayed fluorescence (CP-TADF) [2];
- perchlorination of the diimine ligand as a new route toward deep-red TADF emitters displaying negative thermal quenching of emission [3];
- variation of the counterion as an innovative strategy for improving the performance of TADF-active $[\text{Cu}(\text{NN})\text{PP}]^+$ complexes [4].

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Enantioselection in Asymmetric Hydrogenation: Approach of the Substrate towards a Catalyst Enabled by Noncovalent Interactions

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Numerous experimental and computational data accumulated in the field of transition metals catalyzed asymmetric hydrogenation testify for the approach of the substrate to a catalyst enabled by weak non-covalent interactions being the stereoselective stage of the catalytic cycle. It is followed by practically barrierless and strongly exergonic migratory insertion that fixes the results of stereoselection.

Activity and selectivity of an effective chiral catalyst can be governed solely by Noncovalent Interactions.

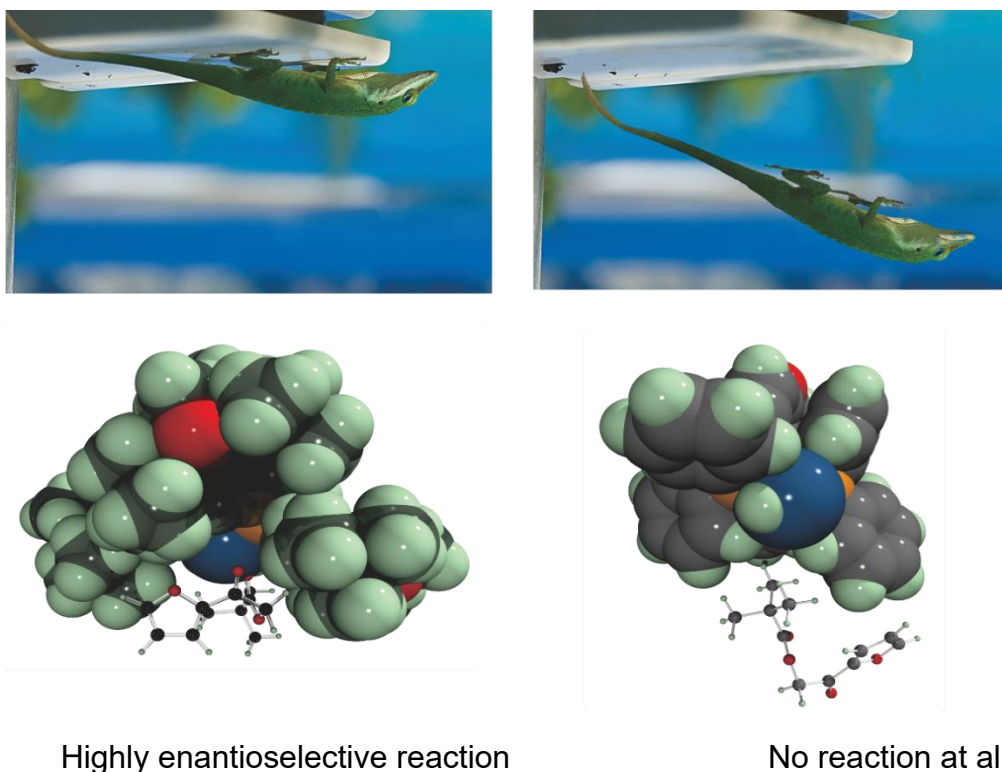


Figure 1. Lack of sufficiently extended network of weak non-covalent interactions can prevent the substrate binding.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent interactions in the design of luminophores based on Pt(II) complexes

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Mononuclear alkynyl complexes of Pt(II) represent an important class of functional compounds, namely, highly efficient luminophores, which are used in many practical areas related to light generation.

A feature of Pt(II) complexes is a tendency toward highly organized aggregation, both in the solid state and in solution, involving a variety of noncovalent interactions. This ability of Pt(II) complexes supports the development of *stimuli-responsive* materials based on them, designed to demonstrate changes in photophysical properties under external influences such as changes in pressure or temperature, the presence of some compounds, etc.

On the other hand, the photophysical properties of Pt(II) complexes are relatively easy to tune using the electronic properties of the ligands. Moreover, the enhancement of the luminescent response to external influences can be achieved by introducing specific groups to the periphery of the ligand environment.

This talk discusses the design, synthesis, and photophysical properties and their dependence on noncovalent interactions for Pt(II) complexes with electron-withdrawing groups in ligand environment.^{1–6}

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Argentophilic interactions – rivals of hydrogen bonds?

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Silver ions Ag^+ have a unique ability to "attract" one another and form short contacts, indicating a bonding interaction. The silver-silver distance is much shorter than the sum of van der Waals bonds, and the energy is estimated at 5–15 kcal/mol level, which almost reaches the values that are characteristic of hydrogen bonds. Argentophilic interactions are of interest in materials science due to their potential to influence macroscopic properties, such as negative thermal expansion or compressibility coefficients, as well as photophysical properties (emission)¹ This presentation will focus on the chemistry of perfluorinated metal aryl thiolates $[\text{MSAr}^f]$ ($\text{M} = \text{Ag}, \text{Au}$; Ar^f is a fluorinated aryl moiety such as C_6F_5 or $\text{C}_6\text{F}_4\text{-C}_6\text{F}_5$). Reactions of $[\text{AgSAr}^f]$ with pyridines ($\text{L} = \text{py}$, 2-Mepy, 3-Mepy, 4-Mepy etc.) yield 1D coordination polymers $[\text{AgSAr}^f(\text{L})]$, which are characterized by argentophilic interactions ($\text{Ag}\cdots\text{Ag}$ 3.0–3.2 Å) and luminescent behavior (temperature-sensitive emission at 450 – 550 nm).

Other examples include some silver carboxylates, such as malate $[\text{Ag}_2(4\text{-Me-py})_4(\text{mal})]$ ($\text{Ag}\cdots\text{Ag}$ 3.06 Å) [2] or malonate $[\text{Ag}_2(3\text{-Me-py})_{2.9}\{\text{CH}_2(\text{COO})_2\}]$ ($\text{Ag}\cdots\text{Ag}$ 2.87 Å) [3], and polynuclear cationic complexes, such as $[\text{Ag}_4(\text{DMF})_{12}]^{4+}$ found in $[\text{Ag}_4(\text{DMF})_{12}][\text{PW}_{11}\text{NbO}_{40}]$ ($\text{Ag}\cdots\text{Ag}$ 3.22 Å).

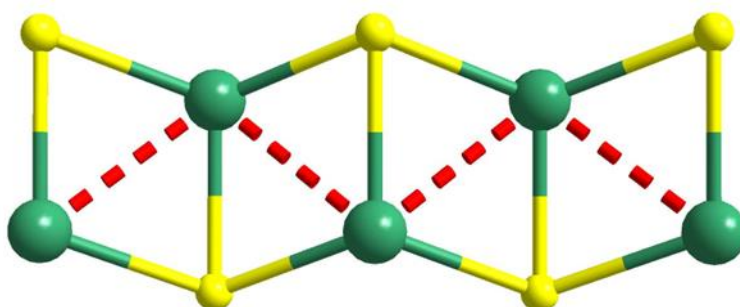


Figure 1. Argentophilic interactions in the structure of $[\text{Ag}(\text{SAr}^f)(\text{L})]$. $\text{Ag}(\text{I})$ shown in green, S in yellow. Organic substituents at S and pyridine ligands at Ag are omitted for clarity.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Design and Synthesis of Benzothiazole Derivatives and Their *d-f* Heterometallic Complexes: Harnessing Non-Covalent Interactions

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The work focuses on the design and synthesis of organic benzothiazole derivatives and their corresponding *d-f* heterometallic complexes¹, leveraging non-covalent interactions along two directions. First, we exploit intra- or intermolecular hydrogen bonding to design compounds with “mobile” protons (Fig. 1a) capable of Excited-State Intra/Intermolecular Proton Transfer (ESIPT). This dynamic process modulates luminescence properties, enabling a way toward new photoresponsive materials². Second, we design ligands featuring distinct donor centers (N and P atoms, Fig. 1b) to selectively coordinate *d*- and *f*-ions, including Cr/Ln, Ni/Ln, Pt/Ln, W/Ln, and Au/Ln combinations, with these complexes promising as luminescent or magnetic scaffolds. Varying the bridge length between the N and P donors allows precise tuning of the metal–metal distance. Thus, non-covalent interactions through ligand design govern the spatial arrangement between *d*- and *f*-ions, enabling controlled assembly of heterometallic systems with tunable properties.

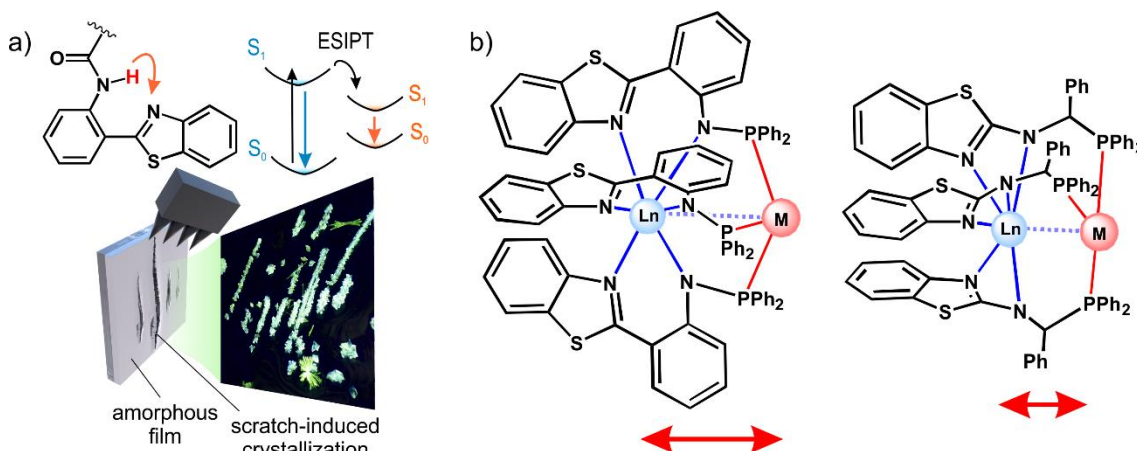


Figure 1. (a) Compounds with “mobile” protons capable of ESIPT and their potential as photoresponsive materials. (b) General structure of heterometallic complexes with N,P-donor ligands featuring a varied metal-metal distance.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

The key role of hydrogen bonds in obtaining nanomaterials from peroxide systems

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Hydrogen peroxide possesses a unique combination of properties, including environmental friendliness, acidic properties, the ability to form peroxy and hydroperoxy complexes, the ability to form hydrogen bonds, redox properties, and the ability to undergo exothermic decomposition. These properties offer broad potential for the application of hydrogen peroxide-based systems in the production of nanomaterials. This report discusses various methods for producing nanomaterials from peroxide systems and the key role of non-covalent interactions, particularly hydrogen bonds, in these processes.¹⁻³

The talk examines the specific features of the sol-gel process in peroxide systems, determined by the properties of hydrogen peroxide. Hydrogen peroxide, on the one hand, initiates the polycondensation of the initial hydroxy complexes due to its acidic properties, and, on the other, limits the polycondensation process and stabilizes the sol, forming hydroperoxy complexes. Examples of self-assembly of thin films based on peroxide-containing sols are discussed, where hydrogen bonds involving hydroperoxy ligands also play a key role in ensuring the affinity of peroxide-containing particles for the surfaces of materials of various compositions and morphologies.⁴

The effectiveness of approaches to the synthesis of nanomaterials using controlled thermal decomposition of hydrogen-bond-stabilized crystalline peroxy complexes is demonstrated. This approach enables the production of films based on highly dispersed oxides, as well as oxide materials with unique chemical properties (e.g., high solubility in water), which can be used not only as target products but also as intermediate systems for further chemical modification.⁵⁻⁶

Acknowledgements

This work was supported by the Russian Science Foundation (grant no. 22-13-00426-П, <https://rscf.ru/en/project/22-13-00426/>).

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IUPAC WORKSHOP



IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”



The Matere Bond

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The expansion of the σ -hole concept has revolutionized our understanding of noncovalent interactions, extending beyond classical halogen bonding to include Group 7 elements like manganese, technetium, and rhenium.¹ This presentation explores the physical nature and structural influence of the matere bond, a directional noncovalent interaction where these metals act as electrophilic sites to accept electron density from nucleophiles. Characterized by electron-deficient regions opposite covalent bonds, matere bonds are identified through molecular electrostatic potential surfaces and computational tools like QTAIM and NCIPLOT, which confirm their attractive donor-acceptor nature. Recent breakthroughs demonstrate that X-ray photoelectron spectroscopy serves as a robust tool for identifying these interactions in non-crystalline materials, as the Re 4f_{7/2} binding energy correlates strongly with interaction length and shifts to lower values upon bond formation. Beyond its role in crystal engineering for the self-assembly of anionic dimers and 1D polymers, the matere bond significantly influences the efficiency of organometallic catalysts and contributes to the structural integrity of manganese-containing proteins in biological systems. This overview underscores the matere bond as a versatile tool for the design of advanced functional materials and the understanding of complex bioinorganic architectures.²

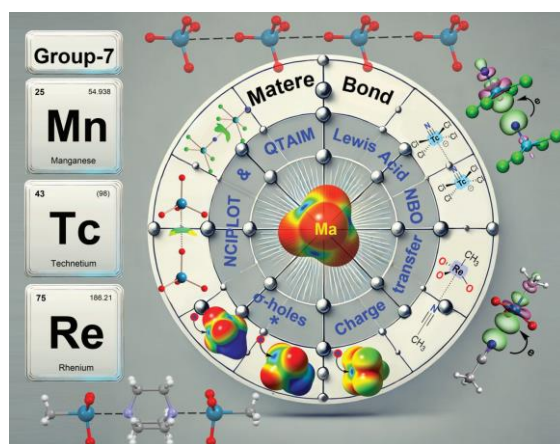


Figure 1. Caption. Please use graphics with reasonable resolution

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Programming Materials through σ - and π -Interactions: From Stability to Function

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Noncovalent interactions are increasingly recognized as key tools for programming structure and function in advanced materials. σ and π interactions¹ offer complementary features — directionality, tunability, and electronic modulation — that can be synergistically exploited across different material platforms.

In hybrid organic–inorganic perovskites, halogen bonding enables reversible control over crystal structure, acting as a supramolecular switch that drives thermally induced phase transitions.² This molecular-level modulation translates into macroscopic optical responses, including thermochromism and birefringence, demonstrating how σ -interactions can govern dynamic functionality in solid-state materials. Conversely, in fluorinated azido-functionalized systems, intramolecular pnictogen bonding plays a crucial role in enhancing molecular stability. Directional N $\cdots$ F interactions enforce conformational control and significantly mitigate decomposition and explosive behavior. These examples highlight a unifying perspective in which σ - and π -interactions operate cooperatively to control both reactivity and functionality. Their integration provides a powerful strategy for designing adaptive, stable, and multifunctional materials, paving the way toward programmable matter in materials science.

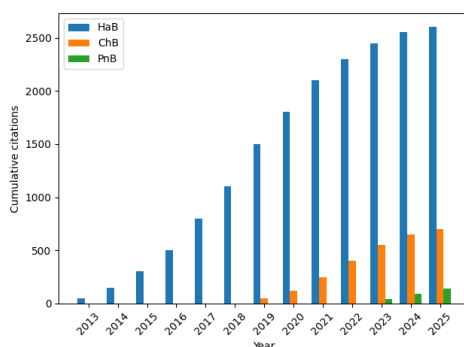


Figure 1. Histogram showing the annual citations for the IUPAC recommendations defining halogen bonding (HaB), chalcogen bonding (ChB), and pnictogen bonding (PnB), starting from 2014 (Source Google Scholar)

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Weak Electron Density Sharing: the missing link in the reactivity and cohesion of *d*-block transition metal complexes

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Noncovalent interactions play a significant role in the chemistry of *d*-block transition metals.

Noncovalent interactions are primarily categorized into van der Waals forces and local weak electron density sharing (WEDS) interactions.¹ The latter play a crucial role in influencing the reactivity of reactions involving transition metals. The presence of attractive WEDS in pre-reactive complexes signals a system's readiness to overcome the transition state during a concerted reaction.¹ The

Independent Gradient Model (IGM), which assesses the strength of WEDS interactions, offers a valuable analysis that was previously overlooked: it reveals significant electron density redistributions along a reaction pathway and shows how atomic centers near the reaction site contribute to these shifts.²

Additionally, IGM provides new insights into the stabilization of “coordinatively unsaturated” metal centers, offering a fresh perspective on their stability under typical conditions.³

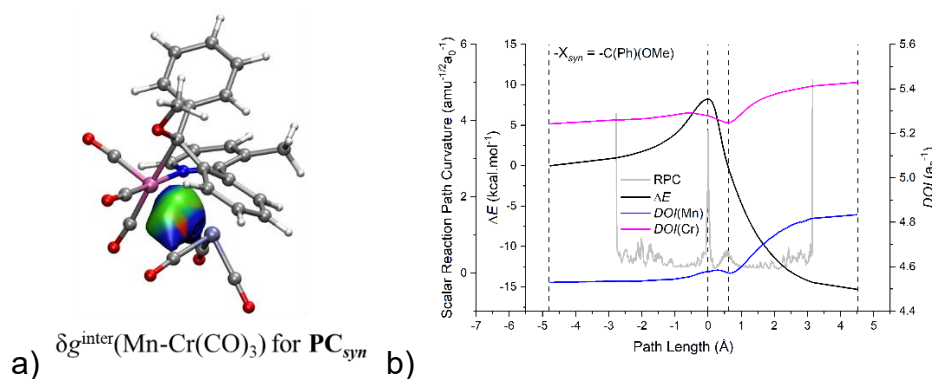


Figure 1. a) δg^{inter} isosurface of the interaction between the $\text{Cr}(\text{CO})_3$ moiety and the Mn centre of a spirylene (cutoff: $\delta g^{\text{inter}} = 0.003 \text{ a}_0^{-4}$, and blue-green-red color code in the range $-0.04 < \text{sign}(\lambda_2)\rho < 0.04 \text{ a}_0^{-3}$ with isosurface colored according to the signed density from blue = attractive interactions to red = repulsive interactions).³ b) Originally, the formation of Cr-Mn spirylene was thought to produce a valence electron-deficient binuclear complex where NCI were thought to provide stabilization; IGM's DOI descriptor shows that, for the most part, stabilization can be rooted in WEDS.³

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E. Hénon and Y. Cornaton are gratefully acknowledged for their contributions.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Interactions of square planar metal complexes

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In the square planar complexes electrostatic potential above d-element can be positive, making them electrophiles. However, d-elements in square planar complexes can be also nucleophiles, since the value of electrostatic potential above the d-element can significantly vary, depending on d-element atomic number and ligands bind to the d-element.

The data in the crystal structures from the Cambridge Structural Database revealed that benzene ring forms stacking interactions with square planar d-element complexes. The CCSD(T)/CBS and DFT calculations showed that the strongest point on potential curve is geometry with center of the benzene above metal atom. The calculated interaction energies of nickel(II), copper(II), zinc(II), palladium(II), and platinum(II) complexes with benzene are from -4.95 to -6.89 kcal/mol, significantly stronger than stacking between two benzene molecules, -2.73 kcal/mol.^{1,2}

The calculations showed increase of interaction energies with increase of positive potential above the central metal atom. Complex of platinum(II) has the least positive potential and interaction energy of -4.95 kcal/mol, while zinc(II) complex has the largest positive potential and interaction energy of -6.89 kcal/mol.²

In interaction between two square planar complexes with chelate rings, the interaction of d-element central atom with negative electrostatic potential can be also observed. The interaction energy of stacking interactions between two nickel(II) bis(dithiolene) complexes is -10.34 kcal/mol.³

Acknowledgements

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The σ -hole and p-hole Tetrel Bonds: are the principles same?

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We are interested in the types of intramolecular noncovalent bonds formed by boron or carbon atoms in the fragments $O...T...O/O-T...O$ ($T = B$ or C atoms) of substituted 9-anthracenyl derivatives¹ with penta-coordinated carbon or boron atoms. In the isoelectronic states for the Tr and Tt atoms, when the number of valence electrons of B atom is equal to that on C^+ , the atoms B deliver their p-hole regions to participate in the TrB ($O...B$). Meanwhile, the atoms C^+ share their p-hole region to participate in the TtB ($O...C^+$) bonds, correspondently.

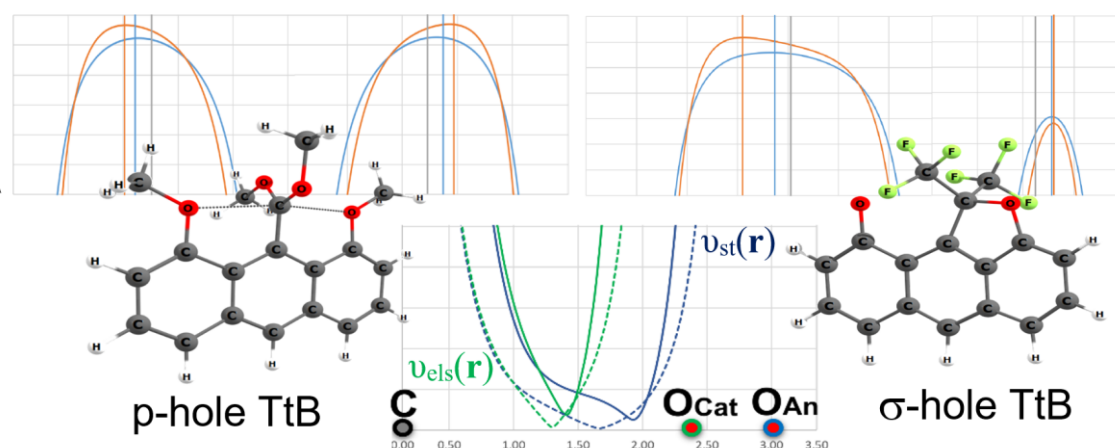


Figure 1. Superposition of the total static and electrostatic potentials and their gradients along $O...C^+...O$ and $O...C-O$ bond lines in HOYWAT and AKIKIO crystals. Calculations were made in WinXPRO program²

We compared the electronic features of the typical “ σ -hole TtB” formed by C atom (TtB) in its tetrahedral configuration with the analogical case for the penta-coordinated C^+ in the “p-hole TtB bond”. The gradient of electrostatic potential has fallen identically for the p-hole and σ -hole starting from C nuclei and until 1.2 Å along the bond line. The gradient of total static potential behaves similarly for both cases until 1.0 Å; then some difference between the weaker and stronger $C...O$ bonds is observed.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Halonium Salts in the Design of Halogen-Bonded Supramolecular Architectures

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Design of organic supramolecular architectures inevitably meets with the issue of low predictability of supramolecular arrangement of organic molecules due to the large number of noncovalent interactions affecting to assembly of organic molecules and sometimes the low stability of the supramolecular assembly.

Halogen bonding can be considered as one of the most promising tools for the design of organic supramolecular architectures, while use of halonium salts as halogen bonding donors give more stable charge-supporting halogen bonds.

A deep analysis of the structural database shows that monocationic halonium salts bearing monoanionic counterions tend to form 0D heterotetrameric supramolecular architectures.¹ We studied how to use this fact for the design of more complex supramolecular architectures by increasing of charged sites in the cationic and anionic parts of the molecules.^{2–4}

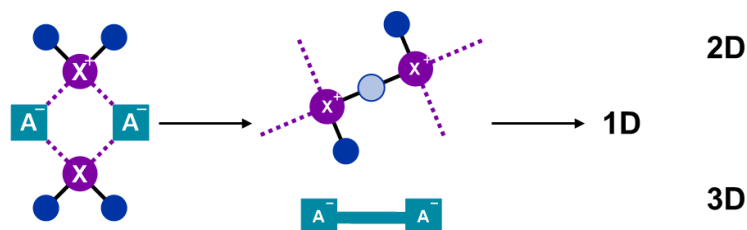


Figure 1. Rational design of complex supramolecular architectures with halonium salts.

Acknowledgements

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Noncovalent Interactions for Chemosensing and Construction of Porous Molecular Crystals

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Non-covalent interactions are fundamental to the development of sophisticated analytical tools and advanced functional materials. In this study, we harness diverse non-covalent interactions for two distinct applications: dynamic chemosensing and gas separation. First, for chemosensing, we developed a class of fluorine-containing probes based on non-covalent dynamic recognition to establish a ^{19}F NMR dynamic labeling detection strategy. By utilizing instantaneous and reversible non-covalent interactions between the probes and target components, this strategy enables the in situ dynamic labeling of multiple components within complex systems without physical separation or prior covalent labeling. Through this process, chemical information is converted into real-time, chromatography-like ^{19}F NMR signals. By exploiting subtle differences in non-covalent binding affinities, this platform facilitates the multi-component monitoring of biological metabolic processes and the enantioselective imaging of small molecules via non-covalent chiral recognition. Furthermore, extending the power of non-covalent assembly to material design, we successfully constructed organic porous molecular crystals. By rationally engineering halogen bonding within these crystalline frameworks, we achieved the highly efficient separation of SF_6/N_2 gas mixtures. Together, this work demonstrates the remarkable versatility of non-covalent interactions, providing powerful tools for deciphering complex biological systems and addressing critical industrial separation challenges.

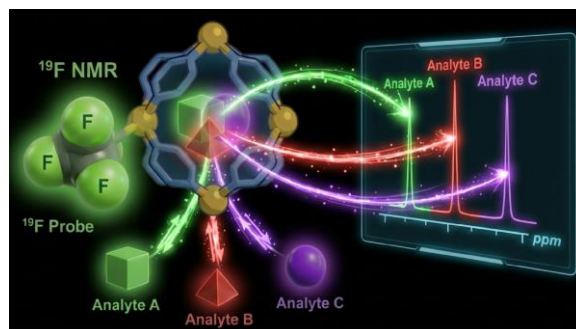


Figure 1. ^{19}F NMR sensing platform based dynamic interactions

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

σ -Hole Electrophilicity of Acido Ligands

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σ -Hole interactions are actively studied as tools for supramolecular chemistry, crystal engineering, and catalysis.^{1–3} Most of studies of σ -hole interactions involve organic species, where electrophile sites are located on p-elements, bound to other p-elements, for example, in the C–I and C–S bonds.

In this work, we presented three types of systems, where anionic acido ligands can also be σ -hole electrophiles (Figure 1). In the first type of systems, iodide ligands were activated by coordination to electronegative, highly charges Pt^{IV} centers,⁴ which lead to the formation of $\text{Pt}-\text{I}\cdots\text{Nu}$ interactions the solid state. In the systems of second type, iodide ligands in the coordination spheres of Pd^{II} and Pt^{II} centers were co-activated by additional $\text{C}-\text{X}\cdots\text{I}$ halogen bonds. Finally, we found sulfur-centered σ -hole interactions, where electrophilicity of S atoms in dithiocarbamate ligands R_2NCS_2^- in square planar Cu^{II} , Ni^{II} , Pd^{II} , and Pt^{II} complexes was provided by external π -holes of neighboring molecules. Formation of the σ -hole interactions were confirmed by X-ray diffraction experiments and further computational studies.

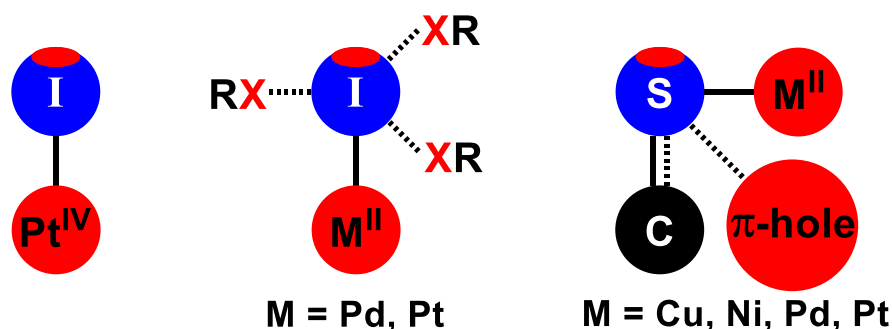


Figure 1. Activation of σ -holes on iodide ligands by Pt^{IV} (left) or $\text{Pd}^{\text{II}}/\text{Pt}^{\text{II}}$ with alkyl halides (central) or on dithiocarbamate sulfur atoms by metal centers and π -holes

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Catalysis with Carbon-Bonding Interactions

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Carbon bonding refers to the noncovalent interactions between electrophilic carbon atoms and electron donors, which can be viewed as nucleophilic addition or substitution processes frozen at the noncovalent contact stage.^[1] Given that carbon-bonding interactions are ubiquitous, research into carbon-bonding catalysis carries dual significance: it not only provides a new platform for catalyzing organic reactions, but also introduces fresh perspectives for understanding reaction mechanisms.

Enabled by the discovery of highly active catalysts, Wang and coworkers introduced the concept of carbon-bonding catalysis by achieving several representative benchmark reactions.^[2] Subsequently, the strategy of carbon-bonding metal catalysis was established, highlighting the role of carbon bonding in modulating reactivity and selectivity in metal-catalyzed reactions.^[3] More recently, chiral carbon-bonding donors have been developed, and experimental results indicate that these donors can induce asymmetric induction.^[4] Although carbon-bonding catalysis is still in its infancy, these findings unequivocally demonstrate that carbon bonding is a viable strategy for catalyzing chemical reactions, paving the way for its future application in more efficient synthesis.

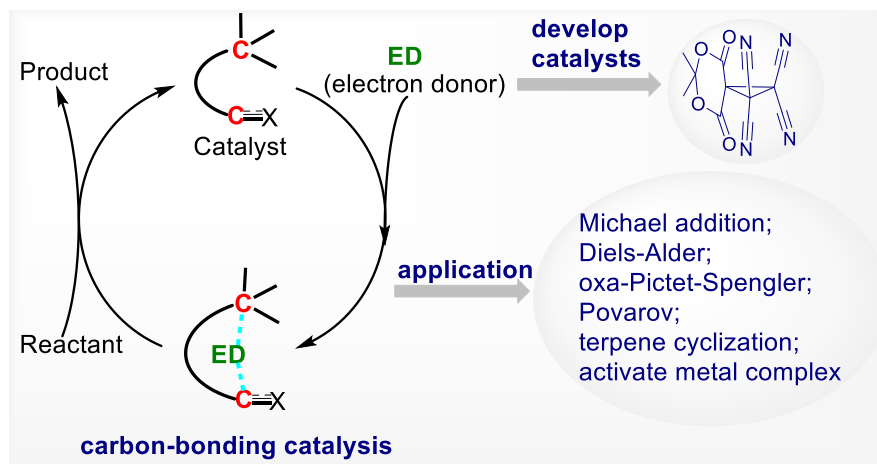


Figure 1. Carbon-bonding catalysis.

Acknowledgements

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ORAL PRESENTATIONS



IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

The Expanding set of σ -Hole Adducts

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The distribution of the electron density in bonded atoms is typically anisotropic. For instance, the accumulation of electron density in the regions of the σ -covalent bonds is compensated by a depletion of electron density opposite to these bonds. As a result, these depletion regions, named σ -holes, frequently have a positive electrostatic potential and an electrophilic character and are the zones of preferential approach of nucleophiles (e.g., lone pair possessing atoms). σ -Holes and nucleophiles thus form attractive interactions, named σ -hole bonds, and this is the case also when the σ -hole electrostatic potential in the isolated molecular entity is negative as it can be changed to positive by polarization phenomena induced by the solvent, when in solution, or by surrounding molecular entities, when in the solid. We have reported how σ -holes bonds can assemble various anions, e.g., periodate, perhenate, and bromate anion, into anion $\cdots$ anion supramolecular adducts.¹ Here we will extend the casuistry of this unconventional self-assembly to other anions and we will discuss also cases wherein the electrophilic element forming the σ -hole bonds is a new entry in the palette of the σ -hole bond donors (e.g., chromium and platinum, Figure 1).²

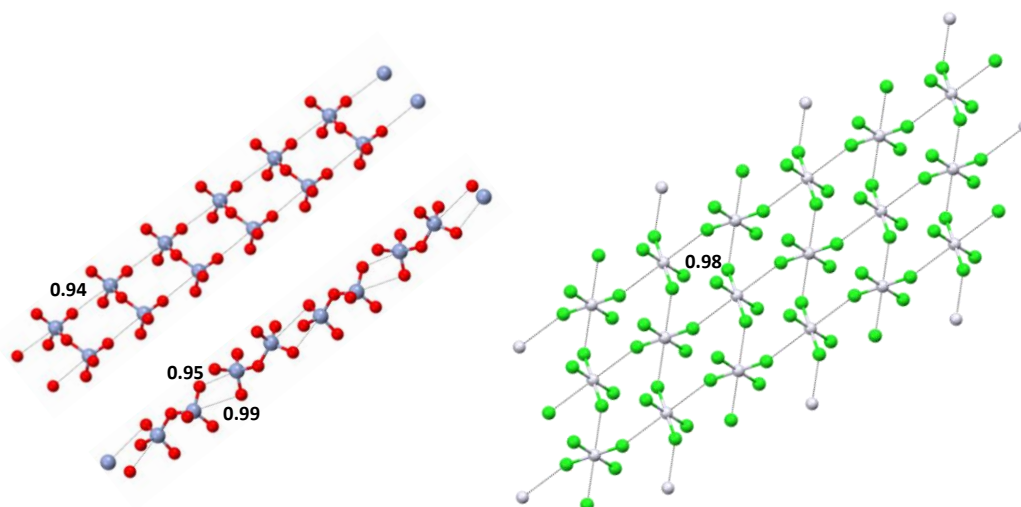


Figure 1. Left: anionic ribbon (top) and infinite chain (bottom) present in crystalline [4,4'-bipyridine]-1,1'-diium dichromate and quinolinium dichromate, respectively; right: (4,4)-network present in cyclohexylammonium tetrachloridoplatinate; color code: sly blue, Cr; red, O; whitish, Pt; green Cl; Cr $\cdots$ O and Pt $\cdots$ Cl σ -hole bonds are black dotted lines; Nc values are reported.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hydrogen bonds in the second coordination sphere of metal complexes: Key role of metal oxidation state and coordination number

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Hydrogen bonds in the second coordination sphere of metal complexes are important in numerous areas such as catalysis, biochemistry, molecular recognition, materials, separation of metals, medicine, synthesis, and environmental science.

This study focuses on hydrogen bonding involving coordinated ligands, which can act as hydrogen bond donors or acceptors.¹⁻³ The results are based on analysis of data from crystal structures from the Cambridge Structural Database and on high-level quantum chemical calculations. The data show that coordination to a metal ion strongly affects hydrogen-bonding behavior of ligand molecules since electron density is changed. Coordinated ligands become stronger hydrogen-bond donors and weaker hydrogen-bond acceptors.

The data show the influence of various factors in metal complexes: ligand type, atomic number of metal, charge of complex, oxidation state of metal and coordination number. The most important is influence of the charge of the complex, charged complexes form significantly stronger interactions. Ligand type also has important influence, while atomic number of metal has the smallest influence.

The results show that hydrogen bond strength significantly depends on the oxidation state and coordination number of the metal center, actually on (OS/CN) ratio. A higher OS/CN ratio strengthens hydrogen bonds when coordinated ligands act as donors, but weakens their acceptor ability. Quantum-chemical calculations reveal a clear relationship between hydrogen-bond energies and electrostatic potentials. SAPT analysis further shows that electrostatic interactions are the dominant stabilizing contribution in these systems.¹ The calculated trends agree well with the data observed in crystal structures.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

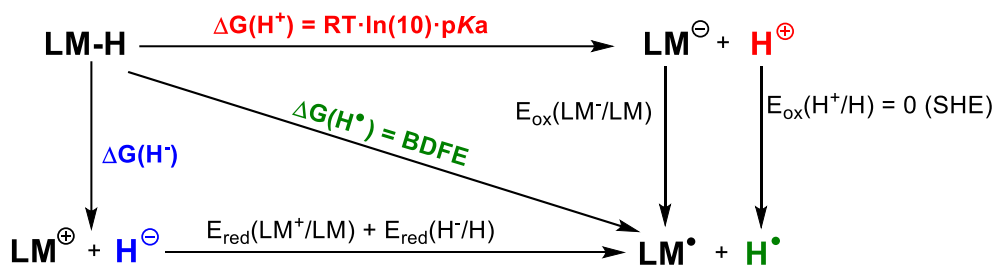
Photo-enhanced reactivity of nickel hydride complexes

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The reactivity of transition metal hydride complexes is determined by three possible pathways for M–H bond cleavage: homolytic cleavage with the formation of a hydrogen radical (H[•]) and heterolytic cleavage with the formation of a proton (H⁺) or hydride ion (H[−]) (Scheme 1).¹ The transfer of a hydride ion (H[−]) to/from an organic substrate is the turnover-limiting step in many catalytic and stoichiometric transformations including (de)hydrogenation, hydrofunctionalization, olefin isomerization, hydroformylation, electrochemical formation of H₂, CO₂ reduction etc. These processes are mediated by transition metal hydrides and nowadays a considerable attention is devoted to the use of 3d metals complexes as an alternative to noble metals.² However despite some advantages they come with a distinct set of limitations and key challenges, originating from different electronic structure and reactivity. In this report we discuss the role of NCI in M-H bond cleavage³ and the effect of photoexcitation on the M-H reactivity in the nickel hydrides supported by naphthalene-based POCOP-pincer ligands.



Scheme 1. Thermodynamic cycle connecting proton/hydride donating abilities, redox potentials, and M-H bond energy

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Topological analysis of noncovalent interactions in crystals: methods and tools

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Modern world-wide crystallographic databases contain huge amount of information on crystal substances, which could be used for discovering correlations between chemical composition of a substance and its local or overall periodic structure. As a result, knowledge bases and artificial intelligence systems can be developed as important tools for designing new materials. To automatically process the crystallographic data, we need universal algorithms and software, which can be applied to the analysis of crystal structures of any composition and complexity.

We present a general workflow for determining, discriminating and classifying noncovalent interactions and their patterns in crystals of any chemical nature. The workflow includes the following steps: (i) extracting the initial crystallographic information from databases or CIF files; (ii) determining covalent bonds and noncovalent interactions based on the Voronoi partition of a crystal space; (iii) discriminating the noncovalent interactions between hydrogen bonds, specific halogen interactions, π -stacking interactions and van der Waals interactions using sets of geometrical and topological criteria; (iv) calculating geometrical parameters of the noncovalent interactions; (v) calculating topological invariants for patterns of the noncovalent interactions and (vi) topological classification of the patterns by comparing their topological invariants with the invariants of reference patterns. All the steps are algorithmized and implemented into our program package *ToposPro* (<https://topospro.com>).¹ Typical topological motifs of noncovalent interactions are stored in our *TopCryst* databases (<https://topcryst.com>).²

Using this workflow we have processed all (more than 1.4 million) crystal structures of organic and coordination compounds, which are deposited in the Cambridge Structural Database (release of October 2025). We have characterized the most abundant topological motifs for hydrogen bonds, halogen-halogen and π -stacking interactions, computed geometrical parameters of the interactions and refined the criteria for their determination. We discuss the possible routes for implementation of the developed methods and tools as well as the obtained new data into chemical information systems. Applications of the workflow to the analysis of particular crystal structures of organic and coordination compounds are also presented.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

A role of amine/ammonia interconversion in high productive hydrogen evolution from amine-boranes

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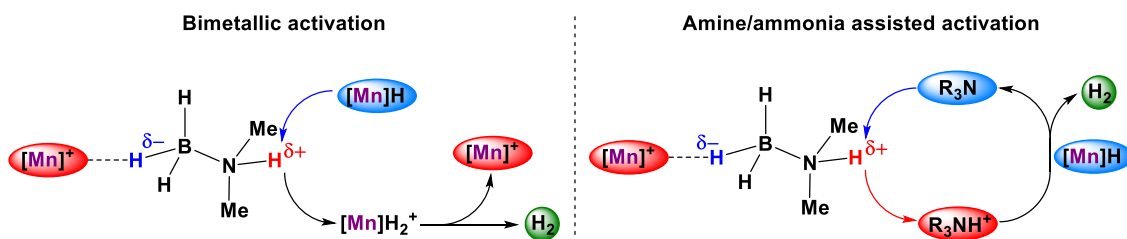
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The conventional approach to developing catalytic systems involves variation of the metal complex structure and the reaction conditions over a wide range. We chose an alternative strategy, aiming to develop highly efficient catalysts by investigating the key steps of catalytic reactions and identifying the factors that govern them. Previously, we demonstrated that Mn(I) complex with bis-*N*-heterocyclic carbene ligand is highly active in dehydrogenation of dimethylamine-borane (Me_2NHBH_3), affording TOF $>1200 \text{ h}^{-1}$ at 0.005 mol% loading.¹ The combined action of cation ($[\text{Mn}]^+$) and hydride ($[\text{Mn}]\text{H}$) derivatives allows the formation of non-covalently bonded complex with Me_2NHBH_3 , enabling the subsequent activation of N–H and B–H bonds (Scheme 1, left).

In the present study we tuned this unconventional mechanism by introducing trialkylamines (R_3N , $\text{R} = \text{Et}$, $n\text{Bu}$) and their corresponding ammonium salts (Scheme 1, right). The interconversion of amine and ammonia supplements the basic and acidic centers of the catalytic species, facilitating the rate-determining step and consequently enhancing the activity of the catalytic system. In a result, we reduced the catalyst loading to 0.001 mol% and achieved TOF $>450000 \text{ h}^{-1}$ under optimized conditions. The obtained TOF value is not only two orders of magnitude higher than that of the original system but also surpasses the activity of all known transition metal systems for dehydrogenation of dimethylamine-borane. Furthermore, Mn(I) system with amine/ammonia co-catalyst operates effectively on a gram scale, achieving full conversion for 2.0 g of Me_2NHBH_3 and producing approximately 0.8 L of H_2 in less than one hour even with non-purified solvent and substrate. The exceptional activity of this relatively inexpensive and robust catalytic system suggests its potential application in fuel cell technology, where amine-boranes serve as hydrogen storage material.



Scheme 1. Activation of Me_2NHBH_3 by bisNHC Mn(I) complexes.

Acknowledgements

This work was supported by RSF grant (№ 24-13-00283).

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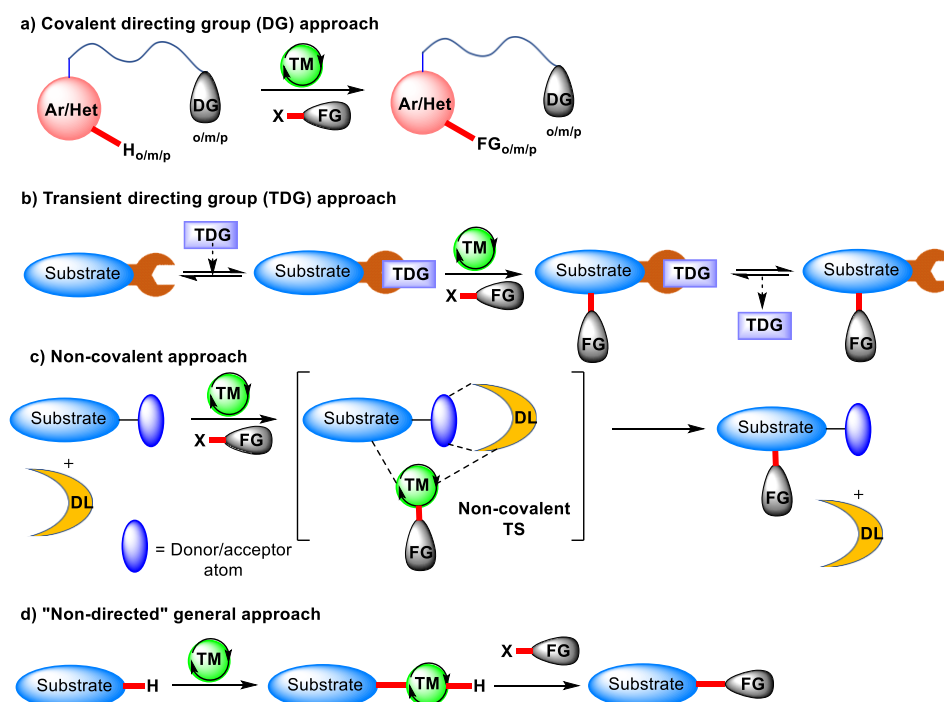
IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent and Covalent Interactions in Metal-Catalyzed Selective C-H Functionalizations

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C—H bond being the fundamental backbone of organic compounds, the potential of a C—H functionalization to amend a molecule overrides traditional routes on grounds of step and atom economy. This has triggered the development of various strategies with the aim to alter the physicochemical properties of specific compounds or add on molecular complexity. Irrespective of aliphatic or aromatic setup, the C—H bonds, vicinal to a functional group, are relatively easier to functionalize either by exploiting its acidity or by taking the advantage of its coordinating ability to the metal. Moving further toward distal positions, C—H functionalization is engrossed with several issues including the intrinsic inertness as well as regioselectivity due to the overabundance of multiple C—H bonds with subtle reactivity differences. This report focuses on discussing various approaches for proximal vs distal arene C—H functionalization based on directing group assisted protocols. Remote arene functionalization harnessing the non-covalent interactions is especially interesting. Although non-covalent interactions are prevalent in enzymatic reactions but translating such interaction in regioselective functionalization of small molecule in synthetic scale is rarer. A “non-covalent approach” is being actively developed, in which templates for C-H functionalization are designed to exploit various non-covalent interactions, sometimes involving additional ligands (DL).



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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Coordination compounds of lanthanides with aromatic, heterocyclic and heteroatomic 1,3-diketones, – the relationship between molecular structure and luminescent properties

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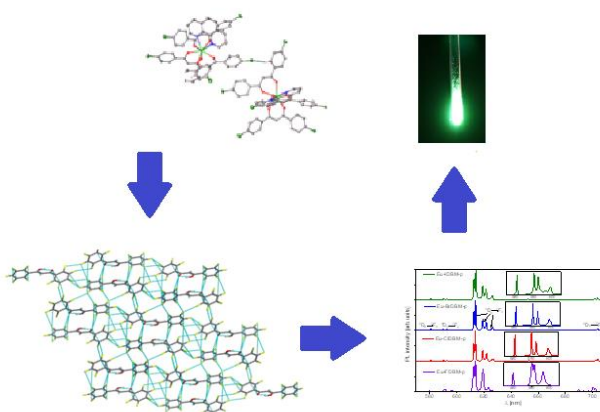
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The design of effective luminescent materials is a key challenge in modern engineering and technology. Lanthanide coordination compounds offer great potential for the synthesis of luminescent materials that emit in the visible and near-infrared region of the spectrum.

Unfortunately, to date, the development of effective materials has been more a result of chance than of a deliberate selection of ligands. This presentation will outline a new approach to the development of such materials, based on a detailed study of energy transfer mechanisms in complexes and the investigation of their relationship with the molecular and supramolecular structure of these compounds.

Examples of various complexes with aromatic ligands containing heteroatoms will be examined, and the influence of the ligand structure and the complex as a whole on the individual stages of electronic excitation energy transfer within them will be discussed.



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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Unsymmetrical PCN Pincer Nickel Complexes: From Non-Covalent Interactions to Catalytic Oligomerization of Ethylene

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Nickel(II) pincer complexes are highly efficient catalysts for olefin oligomerization due to the tunable steric and electronic properties of their ligands.¹ Herein we report a comparative study of two families of unsymmetrical PCN pincer nickel(II) halides bearing pyrazole (^{Pyr}PCN)NiX and benzothiazole (^{BzTz}PCN)NiX (X = F, Cl, Br, I) side-arms.^{2,3} The fluoride complex (^{Pyr}PCN)NiF exhibits unique behavior among halides in terms of halogen-bonding capability toward the halogen-bond donor, iodopentafluorobenzene. Cyclic voltammetry combined with EPR reveals that oxidation of (^{Pyr}PCN)NiF and (^{BzTz}PCN)NiF leads to halide decooordination, generating vacant coordination sites — essential for catalysis. The high nucleophilicity of the fluoride ligand is at the origin of the observed phenomena.

Furthermore, we have tested the catalytic activity of these complexes in ethylene oligomerization. The (^{BzTz}PCN)NiX systems achieve TOF up to 200×10^3 mol C₂H₄·mol Ni⁻¹·h⁻¹ — an order of magnitude higher than pyrazole analogues. DFT calculations attribute this to ligand hemilability: the flexible benzothiazole arm dissociates more readily, generating a vacant coordination site essential for catalysis. This work highlights two complementary strategies for tuning nickel pincer complexes: exploiting non-covalent interactions and enhancing ligand flexibility through rational side-arm modification.

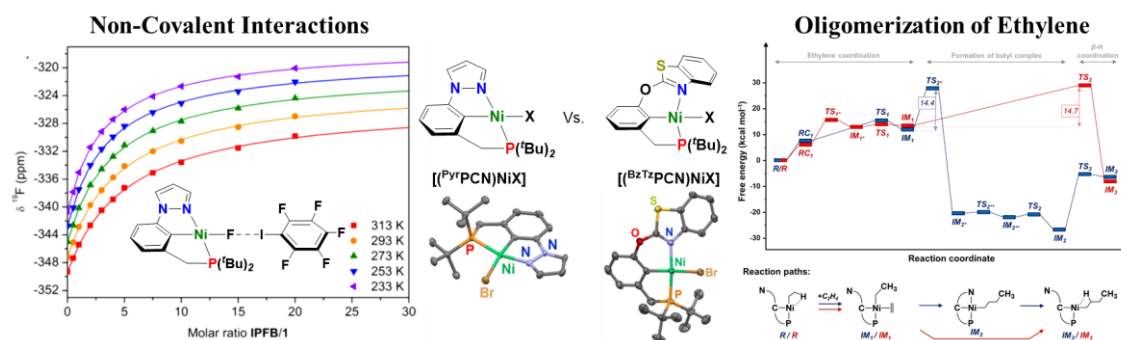


Figure 1. Unsymmetrical PCN pincer nickel(II) complexes.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Stacked Organic–Inorganic Cococrystals of Group 10 Metal Dithiocarbamates with π -Acceptor Benzene Derivatives

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Planar electron-deficient benzene derivatives can act as efficient supramolecular partners for square-planar group 10 metal dithiocarbamates, generating hybrid organic–inorganic cococrystals with distinct stacking motifs. Based on two related systems, we show that π -acceptor arenes such as halogenated dihaloperfluorobenzenes (1,2-dibromoperfluorobenzene FBrB and 1,2-diiodoperfluorobenzene FIB) and 1,2,4,5-tetracyanobenzene (TCB) direct the assembly of Ni, Pd, and Pt dithiocarbamates into either reverse sandwich architectures or parallel-displaced layered stacks. In cococrystals with FBrB/FIB, the key structure-directing motif is the $\{MS_4\} \cdots \pi$ -hole interaction, where the dithiocarbamate-based $\{MS_4\}$ fragment behaves as an integrated nucleophilic platform toward the electron-deficient arene, leading to reverse sandwich packing. Notably, this motif is realized across the whole Ni–Pd–Pt¹ triad, including Ni^{II}. TCB promotes extended alternating stacks with parallel-displaced layered organization. In this case, multiple $M \cdots C$ and $S \cdots C$ contacts operate cooperatively, and sulfur-centered interactions effectively compensate for intrinsic metal-dependent differences, resulting in closely similar packing for all three metals². These results demonstrate that π -acceptor benzene derivatives are versatile cocrystal formers for group 10 dithiocarbamates and provide a useful platform for controlling stacked architectures in crystal engineering, from localized reverse sandwich motifs to more extended layered assemblies.

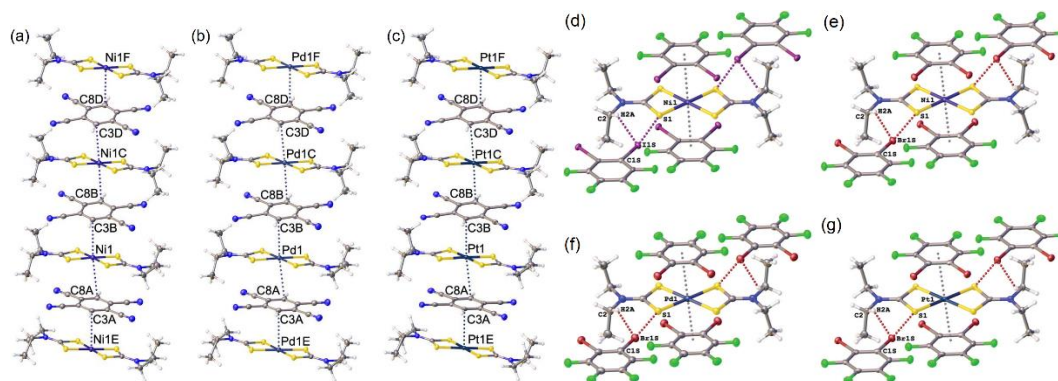


Figure 1. Crystal packing motifs in cocrystals of group 10 metal dithiocarbamates with π -acceptor benzene derivatives: layered stacking in $M(dtc)_2 \cdot TCB$ (a–c) and reverse sandwich assembly in $M(dtc)_2 \cdot 2(FBrB/FIB)$ (d–g).

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Non-covalent interactions in functional 1,10-phenanthroline-based REE(III) metal-organic frameworks

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1,10-phenanthroline is important in chemistry as N-donor chelator capable of coordination to the metal ions of diverse Pearson's hardnesses. It values in construction of chromophores and luminophores, including rare earth element(III) complexes. Owing to the fruitful emissive and sensor properties of such materials, their supramolecular features often remain silent in the relevant literature.

Our significant effort has been made for investigation of phen-based REE(III) metal-organic frameworks due to its ability to act both an antenna and a self-emitter, anticipating that interplay between these two emission pathways can strongly affect joint dual emission characteristics at only minor changes in phen supramolecular environment. Solvent-driven tuning of interlayer $\pi \dots \pi$ stacking distances, which accompanied reversible phase transitions, provided emission color tuning in layered $[\text{Sm}_2(\text{phen})_2(\text{NO}_3)_2(\text{chdc})_2] \cdot 2\text{Solv}$ systems.¹ Exfoliation of $[\text{Ln}_2(\text{phen})_2(\text{NO}_3)_2(\text{chdc})_2] \cdot 2\text{DMF}$ MOF nanosheets onto an optical fiber surface gave their robust binding by non-covalent interactions with the applications in bioimaging, color mixing and, notably, clear increase of phen phosphorescence mode for $\text{Y}(\text{d}^0)$ -based nanosheets compared to the powder.² A series of $[\text{Ln}_2(\text{phen})_2\text{Cl}_2(\text{chdc})_2] \cdot \text{phen}$ (**A**) gave excitation wavelength- and guest-dependent emission coloration applied in pyridine, C_6H_6 and thiophene sensing.

As well, other intermolecular interaction types can be added to the phen ligand by different substituents, retaining its emissive aromatic antenna core. A methylation of phen in 4,7-positions led to the pore *expansion* and PLQY increase in $[\text{Tb}_2(\text{dmphen})_2(\text{NO}_3)_2(\text{chdc})_2] \cdot 2\text{DMF}$ applied in nitroaromatics detection.³ Addition of N-morpholyl substituent gave water-stable $[\text{Tb}_2(\text{morphen})_2\text{Br}_2(\text{chdc})_2]$ MOF for metal ion sensing.⁴ Chiral networks $[\text{Tb}_2(\text{borphen})_2\text{Cl}_2(\text{chdc})_2] \cdot x\text{Solv}$ (**B**) have been designed using 4,7-di((+)-borneol)-functionalized phen ligand.

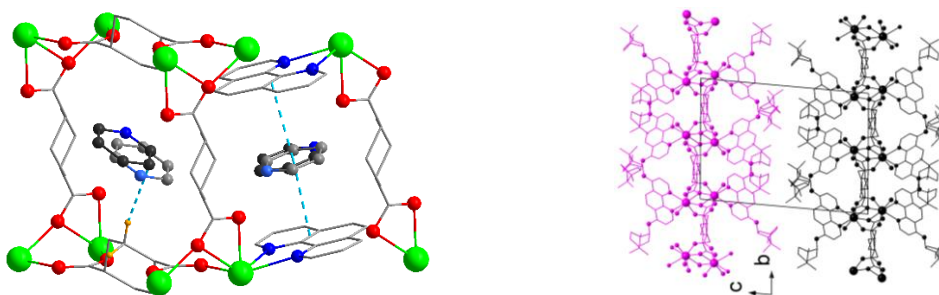


Figure 1. Guest pyridine positions in **A** (left) and coordination layer packing in **B** (right)

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Argentophilic interactions in polymeric silver thiolates and related polynuclear complexes

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In this contribution we use polymeric silver thiolates $[\text{Ag}(\text{S-R})]_n$ ($\text{R} = \text{tBu}$, or $\text{Ar}^f = \text{perfluorinated aryl group}$) as building blocks to construct various complexes of polymeric or molecular structure.¹⁻³ *E.g.* white amorphous solids of $[\text{Ag}(\text{S-R})]_n$ can be dissolved in pyridine or picolines (py-Me) producing “virtual libraries” of oligomeric structures. Such oligomers can associate into crystals of initial $[\text{Ag}(\text{S-R})]_n$ or produce new 1D coordination polymers based on $[(\text{py-R})\text{Ag}(\text{S-Ar}^f)]_n$ chains which can be fused to give ladder-like structures. In this way, we obtained 17 new complexes which were structurally characterized by SCXRD analysis; they represent four structure types. Most of the complexes (14 of the 17) demonstrate infinite ribbon-like structure formed by the fusion of two $[(\text{py-R})\text{Ag}(\text{S-Ar}^f)]_n$ chains. The majority of the structures feature argentophilic interactions ranging from infinite $\text{Ag}\cdots\text{Ag}$ chains to isolated dimers.

Transformation of $[\text{Ag}(\text{S-tBu})]_n$ oligomers can be directed by the presence of different agents in the reaction solution. Some examples will be presented focusing on $\text{Ag}\cdots\text{Ag}$ interactions.

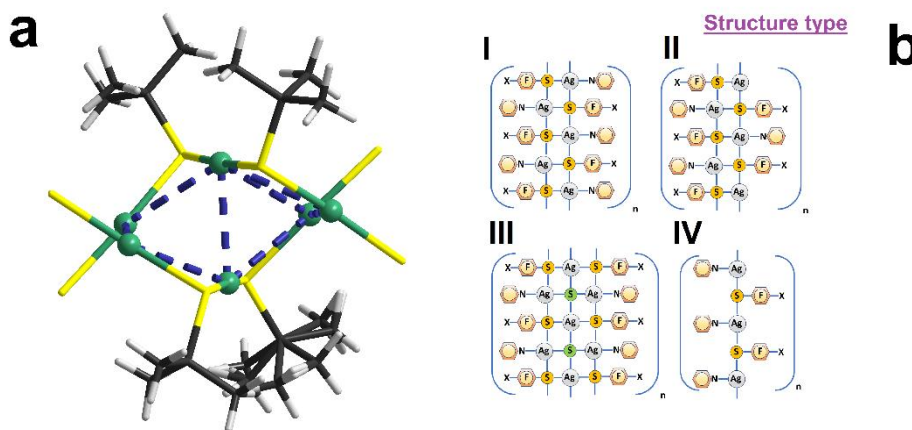


Figure 1. (a) Structure of $\{\text{Ag}_6(\text{S-tBu})_6\}$ monomeric unit in the structure of $[\text{Ag}(\text{S-tBu})]_n$; (b) four structure types of $[(\text{py-R})\text{Ag}(\text{S-Ar}^f)]_n$ coordination polymers

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Molecular states of hydrogen peroxide in ionic liquids according to FTIR spectroscopy and DFT calculations

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The search for and development of novel solvents, is of great practical importance for fine organic synthesis. In recent years, ionic liquids (ILs), combining high polarity with the ability to form supramolecular aggregates through extensive hydrogen bonding, have been increasingly studied as solvents for the selective catalytic oxidations of organic substrates. Most applications of ionic liquids in selective oxidation catalysis focus on the use of "green" oxidizing agents, such as H_2O_2 . Indeed, the hydrogen bond donating ability and Lewis acidity of ILs can assist in the activation of H_2O_2 for various oxidative transformations.¹ However, the molecular states of H_2O_2 dissolved in various ILs have not been scrutinized. Infrared spectroscopy is considered among the most powerful methods to probe the molecular state of water,² CO_2 ³ and other small molecules in ILs and also non-covalent interactions in ILs.⁴

This work presents an ATR (attenuated total reflectance) FTIR spectroscopic study of the molecular state of dissolved H_2O_2 in several ILs based on the 1-butyl-3-methylimidazolium cation ($[\text{bmim}]^+$) and $[\text{PF}_6]^-$, $[\text{BF}_4]^-$, $[\text{NTf}_2]^-$, $[\text{OTf}]^-$, $[\text{MeOSO}_3]^-$, $[\text{CF}_3\text{COO}]^-$, $[\text{CH}_3\text{COO}]^-$, $[\text{Br}]^-$ and $[\text{Cl}]^-$ anions. Furthermore, quantum-chemical (DFT) calculations combined with bonding analysis using an independent gradient model based on Hirshfeld partition (IGMH) provide insight into the atomic contributions to these non-covalent interactions.

It has been found that the positions of the O–H stretching modes depend on the basicity of the anion, but certain spectral features depend on the anion's structure. The shift in the symmetric stretching modes of the O–H bonds correlate with the strength of the hydrogen bonding of H_2O_2 with the anion, which increases in the following order: $[\text{PF}_6]^- < [\text{BF}_4]^- \leq [\text{NTf}_2]^- < [\text{OTf}]^- < [\text{MeOSO}_3]^- < [\text{CF}_3\text{COO}]^- < [\text{Br}]^- < [\text{CH}_3\text{COO}]^- \sim [\text{Cl}]^-$. DFT modelling with IGMH analysis allows explaining the observed bonding patterns based on the concept of ion pairing in ILs. Namely, wavenumber shift and the structure of the putative H_2O_2 -IL complexes with a demonstration contribution of H_2O_2 molecule atoms to the interaction with IL atoms. The results obtained allowed us to draw conclusions about the use of certain types of ILs as solvents in the selective oxidation of organic substances.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Crystal structures of semicrystalline polyimides tailored by intramolecular and intermolecular interactions

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Semi-crystalline polyimides display outstanding mechanical performance and thermal resistance. Great efforts have been made to synthesize polyimides with high crystallinity by molecular design^{1,2}. However, the mechanisms underlying the association between crystal structure and molecular chain still remain unclear. In this research, polyimide was synthesized by AAPB (5-amino-2-(p-aminophenyl) benzoxazole and ODPA (4, 4'-oxydi-phthalic anhydride, (AAPB and ODPA) by thermal imidization³. WXRd and molecular dynamic(MD) simulation are employed to investigate the insight of the crystalline structure. WXRd results indicate that two intense peaks at $2\theta = 13.9^\circ$ and 17.8° , corresponding to the interlayer spacings of $d = 6.35$ and 4.98 Å, respectively, and also the less intense peak at 26.2° corresponding to $d = 3.40$ Å. MD simulations suggest that the intermolecular interactions dictate the global formation of crystal structure while the intramolecular interactions tailor the local crystal structure, as shown is Figure1.

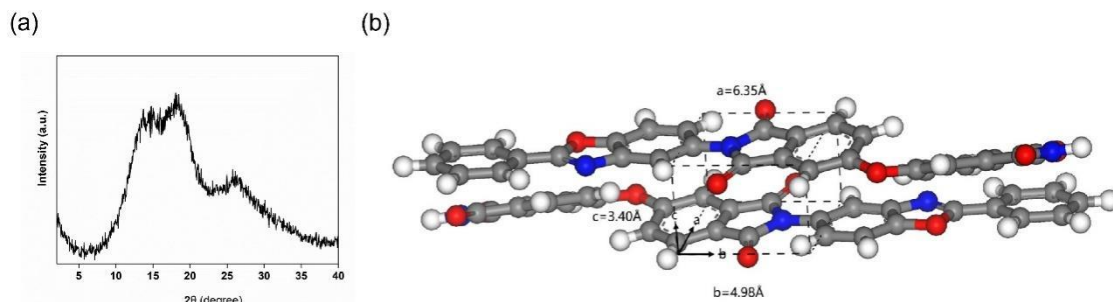


Figure 1. The WAXD patterns (a) and the MD simulation (b) crystal structure of PI (AAPB-ODPA)

(In models of molecules, gray spheres represent carbon atoms, white spheres represent hydrogen atoms, red spheres represent oxygen atoms, and blue spheres represent nitrogen atoms.)

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Supramolecular Approach to Upgrade NCI Donors

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Noncovalent interactions (NCIs) play a significant role in determining the properties of various functional materials and inhibitors of pharmaceutically relevant enzymes. The stability of such supramolecular ensembles is determined by the strengths of these interactions; therefore, not all compounds are suitable for the construction of stable multicomponent systems. A key concept in assessing the potential of a compound to act as a noncovalent donor is the presence of a σ -hole—a region of local electron density depletion characterized by a positive electrostatic potential. The strength of the resulting noncovalent interaction directly depends on the magnitude of the σ -hole on the atom involved, which in turn is determined by the atom's polarizability as well as the nature of the covalently bonded (via σ -bonds) substituents. In particular, electron-withdrawing groups increase the σ -hole potential and, consequently, the ability of the compound to form noncovalent interactions. We found that, the σ -hole potential can also be significantly enhanced through noncovalent interactions with a strong π -electron deficient planar species (Figure 1).^{1,2}

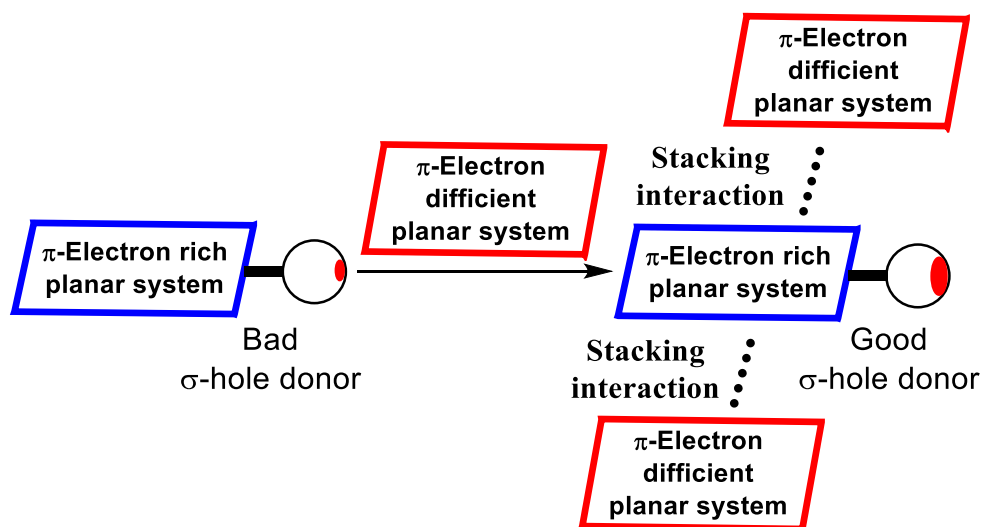


Figure 1. Activation of σ -hole donors with an electron-deficient species.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent Interactions and Solution Structure: Concentration and Mixing Mode as Key Environmental Variables in Chemical Reactions

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Among factors determining the pathway and the outcome of a chemical reaction performed in solution, only some depend on the structural and electronic features of the molecules of reactants, which are considered to be well understood. This is not the case for the “environmental variables”,¹ many of which can be traced back to the structure of reaction solutions (see the reviews²⁻⁴ on nano- and meso-scale structuring of solutions). The real reacting species in solutions seem to be not just individual molecules but more complex supramolecular entities (*supramers*²) that, generally, comprise both solute and solvent molecules brought together by noncovalent interactions.^{2,3}

Concentration of reactants and their mixing mode (the flow regime under microfluidic conditions) are key variables that can dramatically modulate both the reactivity and the stereochemical outcome of a chemical reaction.⁵⁻⁷ A study of unpromoted glycosylation of 4-alkoxyphenols under PTC conditions revealed unusual sensitivity of both yield (0–66%) and stereoselectivity ($\alpha:\beta = 1:5$ – $280:1$) not only to the nature of the electrophile and nucleophile, but also to the concentration of reagents (5–200 mmol/L) and the mixing mode, which under microfluidic conditions is governed by the flow rate and the type of mixer used. The reactivity of the glycosyl donor and the stereochemical course of this S_N1 -like reaction appear to be controlled by both the presentation of donor molecules on the *surface* of supramers and their *internal* structure, which becomes accessible to other reagents upon flow-induced disaggregation of the supramers.

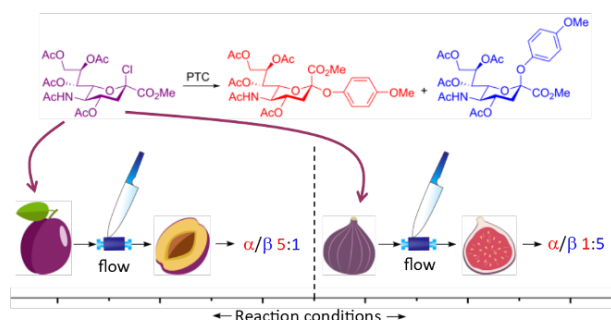


Figure 1. Dramatic dependence of stereoselectivity on “environmental variables”.

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Halogen Bonding as a Tool for Tuning the Structure and Properties of Hybrid Halometallates

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Polyhalides, particularly polyiodides, attract considerable interest due to their remarkable structural diversity and potential applications in the synthesis of light-absorbing materials for perovskite photovoltaics. Incorporation of polyhalide fragments such as I_2 or I_3^- into halometallate structures results in modifications of the electronic structure and band gap narrowing due to the emergence of additional weak intermolecular interactions.

In organic ammonium polyiodides, both covalent I–I bonds (2.75–2.95 Å) and secondary I...I interactions (3.1–3.5 Å), resulting in either discrete I_n^- anions or extended supramolecular assemblies. For example, thiazolinium and 3-hydroxypiperidinium pentaiodides formally contain I_5^- anions composed of I_3^- and I_2 fragments; however, their crystal structures exhibit extended chain motifs, which are uniquely branched in the former case and form a "comb-like" arrangement in the latter. Even simple triiodide anions are capable of forming both ordered and disordered linear chains as well as more complex ribbon-like motifs depending on the nature of the organic cation. To analyze the nature of interactions within the polyiodide fragments, topological analysis of the electron localization function (ELF) and non-covalent interaction (NCI) analysis were employed. It was demonstrated that Hal_2 molecules can act as supramolecular linkers, forming halogen bonds with halometallate anions and thereby increasing the dimensionality of the anionic substructure. Using compounds based on p-phenylenediammonium, $(A1H_2)_2M_2I_{10}$, and homopiperazinium, $(A2H_2)_2M_2I_{10}(I_2)$ ($M = Sb, Bi$), as examples, it was shown that the incorporation of I_2 molecules linking biotetrahedral $M_2I_{10}^{4-}$ anions into chains through I...I contacts of 3.42–3.43 Å results in a decrease in the band gap by approximately 0.6 eV. Similarly, linking the chain-like BiI_4^- anions into layers by I_2 molecules through I...I contacts of 3.53 Å in $(A1H_2)(BiI_4)_2(I_2)$ also leads to band gap narrowing.

In general, the formation of polyiodometallate anions strongly depends on the nature of the organic counterion. For one of the cations studied, association of I_2 molecules to preformed $Bi_2I_{10}^{4-}$ or $Cu_3I_6^{3-}$ anions was observed, resulting in the formation of $Bi_2I_8(I_3)_2^{4-}$ or $Cu_3I_4(I_3)_2^{3-}$ species, respectively. Strong halogen bonding also enhances the stability of polyhalide compounds. For instance, $(A2H_2)_2Sb_2I_{10}(I_2)$ remains stable up to 130°C, while the addition of Br_2 allows the preparation of an isomorphous and relatively stable polybromoantimonate, $(A2H_2)_2Sb_2Br_{10}(Br_2)$.

The obtained results demonstrate that both the nature of the organic cation and the system of secondary Hal...Hal interactions are key factors governing the topology of polyanionic fragments and the electronic structure of polyhalide materials.

Acknowledgements

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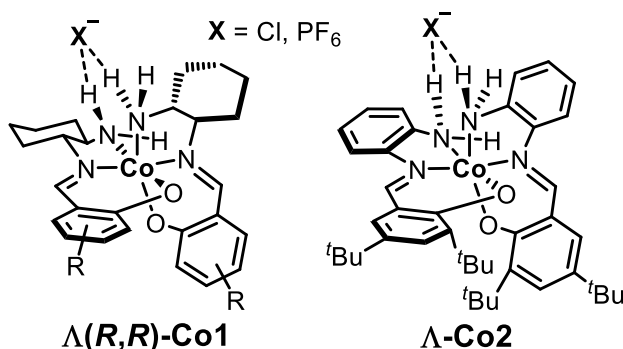
Chiral-at-Cobalt(III) Complexes with Hydrogen Bond Donor Amino Groups and Their Applications

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Chiral metal-templated systems are widely used in various fields, such as catalysis, biochemistry, and material chemistry.¹ We have developed a prospective class of chiral octahedral Co(III) complexes **1** based on commercially available chiral diamines and various salicylic aldehydes (Figure).²⁻⁴ These complexes can activate substrates through the ligand sphere via well-orchestrated hydrogen bonding non-covalent interactions, rather than the coordination metal centre.¹ In these complexes, the amino groups act as effective hydrogen bond donors due to their coordination with the metal ion. We have demonstrated that they efficiently catalyze asymmetric reactions²⁻⁴ and can be applied as efficient selectors in chiral sensors for the recognition of enantiomers of bioactive compounds in real systems.^{5,6} In addition, we prepared the chiral Co(III) complex **2** with exclusive metal-centered chirality and its resolution on enantiomers (Λ and Δ isomers).⁷



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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Tuning Electrophilic-Nucleophilic Dualism of Pt(II) and Pd(II) Metal Centers

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In square-planar d^8 metal complexes, the metal centers can engage in two opposing types of noncovalent interactions. Their filled d_{z^2} -orbitals allow them to function as nucleophiles toward σ/π -hole donors, whereas their vacant p_z -orbitals enable them to act as electrophiles toward electron-rich atoms. Using the Pt(II) xanthate complex $[\text{Pt}(\text{S}_2\text{COEt})_2]$ and I-substituted perfluoroarenes, we demonstrated that the donor's geometry alone can control which of the two metal-involving bonding modes occurs.¹ A 120° σ -hole donor promotes nucleophilic $\text{I}\cdots\text{Pt}$ halogen bonding, whereas linear 180° donors favor electrophilic $\text{Pt}\cdots\text{S}$ semicoordination. For $[\text{M}(\text{S}_2\text{CO}^i\text{Pr})_2]$ complexes, varying the metal across the Ni–Pd–Pt triad within the same $[\text{MS}_4]$ core systematically shifts the balance from electrophilic $\text{M}\cdots\text{S}$ contacts (Ni) to pure nucleophilic π -hole $\cdots\text{M}$ bonding (Pt), with Pd(II) exhibiting ambiphilic behavior (Figure 1).² The $[\text{MS}_4]$ core thus serves as a versatile platform for tuning metal-involving contacts via two independent pathways: (i) metal substitution down the triad and (ii) geometric control of the σ -hole donor. This dual tunability provides a predictive basis for designing supramolecular systems with tailored electrophilic/nucleophilic behavior at the metal centers.

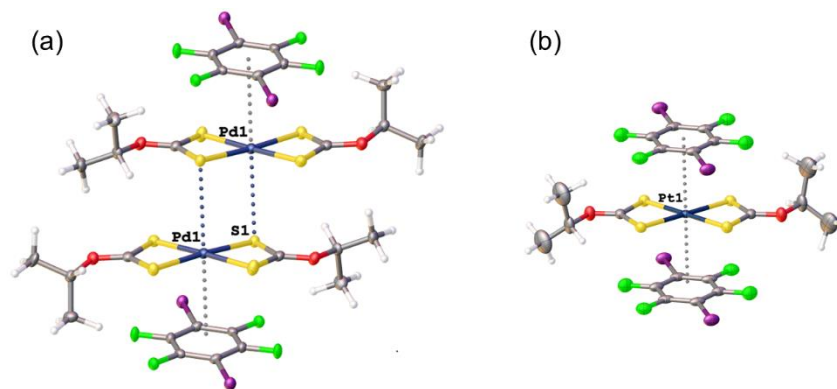


Figure 1. Metal-involving noncovalent interactions in the cocrystals of $[\text{Pd}(\text{S}_2\text{CO}^i\text{Pr})_2]$ (a) and $[\text{Pt}(\text{S}_2\text{CO}^i\text{Pr})_2]$ (b) with 1,4-diiodotetrafluorobenzene. Short contacts are given by dotted lines, and thermal ellipsoids are shown with 50% probability.

Acknowledgements

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Descriptors of Noncovalent Interactions: From Spatial to Electronic Structure to Energy. And Back to Geometry?

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Since its emergence, the concept ‘noncovalent interactions’ is intimately linked to the description of chemical structures in real space, which is directly accessible only from crystallographic data or theoretical computations. Geometric descriptors such as van der Waals radii or molecular volume are now routinely applied in a number of instances, spanning from the identification of structure-directing interactions to explaining the relative stability of polymorphs.

At the same time, geometrical descriptors have repeatedly criticized when one turns out to the electronic structure in real space: a shortened interatomic contact does not guarantee a bonding interaction; a thermodynamically less stable polymorph can be denser; geometry alone cannot reveal the nature of the interaction, whereas electronic structure analysis supposedly can, etc. But what is ‘bonding’? Why must a more stable polymorph be denser? Does electronic structure analysis really shed unambiguous light on the ‘interaction’s nature’?

The purpose of this contribution is not to answer these questions (as it basically provokes a senseless terminology dispute) but to demonstrate that a well-posed question can unify all descriptors, no matter what level of chemical matter (geometry, electronic structure, energy) they are invoked to understand.

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Versatility of Non-Covalent Humic Acids in Advanced Materials and Sustainable Technologies

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Non-covalent interactions of humic acids (HA), which are natural supramolecular systems, are fundamental to their diverse functions and environmental roles. Our recent innovative research has focused on harnessing these interactions - including electrostatic attraction, hydrophobic forces, hydrogen bonding, and π - π stacking - to develop advanced materials and solutions across various fields.¹ Our studies have demonstrated HA utility in enhancing electrostatic and steric stabilization of iron oxides nanoparticles (NPs) shifting the isoelectric point and sorption capacity towards heavy metals.² Furthermore, the tunable nature of these interactions is being exploited in the design of magnetite-silica NPs³ for development of pH-responsive drug delivery systems, particularly for ciprofloxacin (CIP).⁴ The development of antibacterial surfaces leveraging precise control over HA-silica-CIP surface interactions, utilizing electrostatic and other interactions, has demonstrated potential to inhibit *Escherichia coli*. Our group also explores the role of non-covalent HA complexes in the sorption and bioavailability of pharmaceuticals, offering environmental remediation potential.⁴ For the first time, novel nonstoichiometric interpolyelectrolyte complexes (NIPEC) of HA with polycations (PEI, PDADMAC) have been developed to protect soil from erosion by forming stable protective layers.⁵ Beyond remediation, our research extends to agricultural applications, including the development of nanofertilizers based on goethite intercalated coal complexed with HA for enhanced plant growth.⁶ These innovative research underscores the versatility of non-covalent HA complexes, paving the way for their application in sustainable environmental technologies, advanced material science, and pharmaceutical development.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent Polymer–Small Molecule Interactions: From Structural–Molecular Plasticization to a Dynamic Conformational Theory of Adhesion

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Structural–molecular plasticization is a term introduced by the authors¹ to describe a thermodynamically compatible polymer–solvent system in which hydrogen bonding between the solvent and energetically less favorable conformers of the polymer repeat unit induces their transition into more energetically favorable conformations². This process promotes conformational ordering within the polymer repeat unit, while the residual solvent associated with the polymer matrix may act either as a plasticizer or as an antiplasticizer³.

An increase in the fraction of conformers with a specific orientation in the polymer repeat unit (conformational ordering) is reflected not only in the values of structural parameters derived from ATR-FTIR spectra, but also in the values of the energy characteristics of the surface of the films of this polymer, which correlate with the value of the thermodynamic work of adhesion^{4,5}.

Taken together, these observations support the development not only the theory of polymer plasticization but also of a new approach to the description of adhesion. Specifically, controlling the content of specifically oriented functional groups in the polymer repeat unit enables variation of the number of adhesion-active segments at the interface.

Using films obtained from chloroform and tetrahydrofuran solutions of an amphiphilic polymer based on cyclooctene with oxalate side groups, we demonstrate the influence of conformational transitions in the polymer repeating unit through the formation of non-covalent interactions between the polymer and the solvent (structural-molecular plasticizer) on the surface energy and thermodynamic work of adhesion.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

The organizing role of hydrogen bonds in pre-reaction complexes of formyl chloride conjugation with glutathione

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Interest in reactions involving the formyl chloride (CHClO) intermediate from dichloromethane (CH₂Cl₂) in the condensed phase and *in vivo* is due to the ambiguity in the identification of the end products and the contradictory nature of the transformation schemes proposed to date. It is known that CHClO, like other acyl halides, can react with various nucleophiles¹, including glutathione (GSH). The mechanism by which cells protect themselves during detoxification of strong toxins, such as CH₂Cl₂, which accounts for up to 71% of CHClO formation, remains unclear. In this work, various schemes of conjugation of CHClO with GSH were investigated. The choice between competing reaction pathways is determined by the reaction barrier $\Delta G^\ddagger$.^{2,3} Therefore, we combined quantum chemical calculations performed using the CCSD(T)/def2-TZVPPD// ω -B97M-D4/def2-TZVPPD method with published *in vivo* data. The organizing role of hydrogen bonds in the pre-reaction complexes of CHClO conjugation with GSH was established. This is due to the participation of the CHClO hydrogen atom and the formation of an additional hydrogen bond in the reaction center. The $\Delta G^\ddagger$ values were shown to depend on the number of water molecules, the size of the reaction center, and the number of functional groups involved in the proton transfer². The obtained data on the reactivity of GSH functional groups (NH₂, NH, OH, COOH, SH) with respect to CHClO allowed us to establish the detoxification pathways of CH₂Cl₂. For the first time, the pathway of the interaction of CHClO with GSH to form N-formyl GSH, rather than S-formyl GSH, as previously assumed, was established



N-formyl GSH is thermodynamically more stable than S-formyl GSH, with a G_{relative} value of 46.9 kJ/mol. **For N-formylation to occur, both the stability of the product and the nucleophilicity of GSH are important.** Hydrogen-bonded catalysis by water alters the reaction profiles, shifting the balance toward N-formylation. Water molecules not only compete as nucleophiles but also participate in the organization of the transition state, facilitating the reaction with GSH at the NH₂ group. The existence of a stable end product, N-formyl GSH, explains the discrepancy in pharmacokinetic models of approximately 20-30% of the deficit in CH₂Cl₂/CO balance observed *in vivo* in rats. The proposed CH₂Cl₂ metabolism scheme opens new prospects for the development of more accurate pharmacokinetic models and a scientifically based revision of approaches to hygienic standardization and hazard classification of CH₂Cl₂.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

The Interplay between Noncovalent Interactions, Polymorphism and Dynamic Properties of Crystals

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Noncovalent interactions account for different important aspects associated with crystals beyond three-dimensional structure, including physical properties, polymorphism and polymorphic phase transitions, as well as microscopic and macroscopic dynamic properties.

The research involves the studies of the nature of noncovalent interactions, their directionality and energy characteristics, as determined by X-ray single crystal diffraction and quantum chemistry calculations, and demonstrates their impact on structural transformations upon phase transitions and physical properties of polymorphs.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent interactions as the basis of self-healing in metallopolymer systems: from general approaches to copolymers with embedded coordination nodes

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Self-healing polymers are capable of restoring their original properties and functions after damage. The possibility of extending the service life of functional coatings and structural components makes such materials attractive from both fundamental and applied perspectives. Metallopolymers constitute a particularly interesting class in this context, as the healing process and the ultimate material characteristics can be tuned by varying the nature of the metal center and the ligand environment. The recovery ability of these systems is governed by a combination of reversible, dynamic noncovalent interactions, including metal-ligand coordination, hydrogen bonding, electrostatic effects, local solvation, and interfacial interactions, which collectively control chain mobility and the reconstruction of the damaged interface.

Contemporary approaches to the design of autonomously self-healing metallopolymer systems are considered, with particular emphasis on how the nature of the metal center and its ligand environment govern both the healing process and the resulting material properties.¹ At the same time, it is important to recognize that a dynamic coordination bond is not the sole driving factor of the healing process, which is governed by several types of labile interactions operating across multiple length scales, from the local environment of the metal center to the interfacial boundary of the damaged region.

Against this background, results on the development of high-strength self-healing metallopolymers are presented. In the systems under consideration, embedded coordination nodes are formed in situ during polymerization through the use of metal acrylate complexes.² This strategy makes it possible to regard the coordination node as an integral element of the polymer architecture and to link the general principles of noncovalent interaction chemistry with the rational design of functional polymeric materials. It is shown that the introduction of the phenylterpyridine ligand not only alters the local coordination environment of the metal center, but also affects the interfacial polarity, the hydration of the damaged region, and the ability of the material to reconstruct coordination contacts across the crack interface.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Selection of photoresists based on zinc carboxylate complexes

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Modern microelectronics relies on nanotechnological processes that can be achieved using EUV lithography ($\lambda \sim 10 \text{ \AA}$).¹ Since EUV photons (92 eV) initiate uncontrolled processes, including the generation of photoelectrons and secondary electrons in photoresists, a pressing challenge is finding compounds with high photoadsorption, which can be achieved by incorporating metal ions such as platinum, silver, indium, tin, zinc, and others.² This has driven interest in molecular metal complexes as promising photoresists whose physicochemical properties can be chemically modified. Varying the nature of substituents in carboxylate groups and neutral donor ligands that inhibit polymerization in the metal coordination environment provides a convenient tool for adjusting the solubility of complexes and the possibility of forming amorphous films, for example, by spin-coating.

As part of the ongoing research on expanding components for nanolithography, results on the design of new zinc metal complexes with carboxylate ligands, the study of their structure, and the production of thin films will be presented.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Supramolecular adducts of halometalates and di- or polyhalogens

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Anionic homoleptic halide complexes, or halometalates (HM), represent an extensive class of compounds characterized by a rich diversity of structural types. For example, Bi(III) can form discrete anions with nuclearity ranging from 1 to 8, as well as one- and two-dimensional coordination polymers (in totaling more than 40 types differing in structure and composition)

One of the common features of HM is their ability to form supramolecular associates with di- and polyhalides in the solid state via halogen bonding (HB). This phenomenon was first described over 50 years ago, but it was not systematically studied until the mid-2010s.

This report will present the results obtained by our research group in this area over recent years (a total of about 100 complexes have been synthesized, predominantly of Bi, Sb, Te, Sn, and Pb).



IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Impact of Non-Covalent Interactions on Conformational Dynamics of Pharmaceutical Molecules: NMR and Computational Insights

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Non-covalent interactions are key factors governing the conformational equilibria of small molecules and significantly influence their physicochemical and pharmaceutical properties. This work summarizes recent studies combining NMR spectroscopy, particularly NOESY, with quantum-chemical calculations to investigate conformational behavior in solution and confined systems. Using bicalutamide and etoricoxib as model compounds, a strong dependence of conformer populations on solvent polarity was demonstrated, with shifts between “closed” and “open” structures driven by hydrogen bonding and solvation effects. Quantitative NOESY analysis enabled reliable determination of conformer ratios and their correlation with energetic preferences. In addition, studies of flufenamic and mefenamic acids in aerogel-based matrices revealed that intermolecular interactions with porous materials can significantly modify conformational distributions and stabilize metastable states. Solid-state and high-pressure NMR further highlighted the role of weak interactions in sorption and phase behavior. Overall, the results confirm that NMR spectroscopy is a powerful tool for elucidating the role of non-covalent interactions in conformational analysis, providing valuable insights for drug development and materials design.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Non-covalent interactions in Pd-catalysed selective hydrogenation of norbornadiene

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Derivatives of norbornadiene (NBD) and norbornene (NBE) are promising intermediates for organic synthesis¹. Despite the absence of conjugation between double bonds in NBD molecule, kinetic studies² have demonstrated the ability of selective hydrogenation of NBD to NBE on heterogeneous Pd catalysts. To understand the mechanism of the NBD hydrogenation reaction, in this study modelling of possible options of interactions of NBD and NBE molecules with Pd(111) and Pd(100) surfaces, as well as the various pathways for the formation of NBE from NBD, norbornane from NBD, and the by-product nortricyclane from NBD was carried out.

The DFT study was performed using the PBE functional. The Pd(111) and Pd(100) surfaces were modelled using the cluster approximation. According to calculations³ the type of adsorption structure NBD and NBE molecules depends primarily on their endo/exo-orientation upon approach to the surface. In this case, the double bonds of NBD and NBE are coordinated via di- σ - or π - bonds. For NBD molecule the endo-tetra- σ - is most energetically preferable ($E_{\text{ads}} = 43.7\text{--}48.5$ kcal/mol). For the NBE molecule, due to non-covalent interactions between H atoms and Pd surface, the most energetically preferable is exo-di- σ -structure ($E_{\text{ads}} = 25.8\text{--}27.4$ kcal/mol).

Analysis of the energy profiles suggests that the Pd surface type and the differences in the adsorption mechanisms of NBE and NBD molecules play a decisive role in the selective hydrogenation of NBD. Thus, the Pd(100) surface is highly selective in NBD adsorption, but inactive for its hydrogenation.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Mn(I) and Re(I) complexes containing diphosphine ligands with pendant amines: synthesis, structure and reactivity

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Monocarbonyl Mn(I) complexes with 1,5-diaza-3,7-diphosphacyclooctane (P_2,N_2) ligand were investigated as H_2 oxidation electrocatalysts.¹ The pendant amine was found to function as a hemilabile ligand: nitrogen atom is capable of reversibly coordination to the metal center.² At the same time the only example of tricarbonyl Mn(I) complex type $Mn(P^{Ph}_2,N^{R}_2)(CO)_3Br$ has been synthesized by R. M. Bullock et al.³ and no studies on its reactivity have been conducted. The only example of this type complex. Despite an extensive exploration of manganese complexes, the chemistry of rhenium complexes is almost unexplored.

In this contribution we present the synthesis of neutral Mn(I) and Re(I) bromide complexes $M(P^{Ph}_2,N^{R}_2)(CO)_3Br$ ($M = Mn, Re$; $R = pTol, CH_2pTol, CH(Ph)_2$) with different P_2,N_2 -ligands and cationic complexes, which were obtained from previous ones. Structures of all complexes were established on the basis of XRD analysis and NMR and IR spectroscopy data.

The possibility of protonation of Mn(I) and Re(I) complexes by Bronsted acids (CF_3COOH , CF_3SO_3H) and influence of the nature of the metal atom and P_2,N_2 -ligand on this process has been studied.

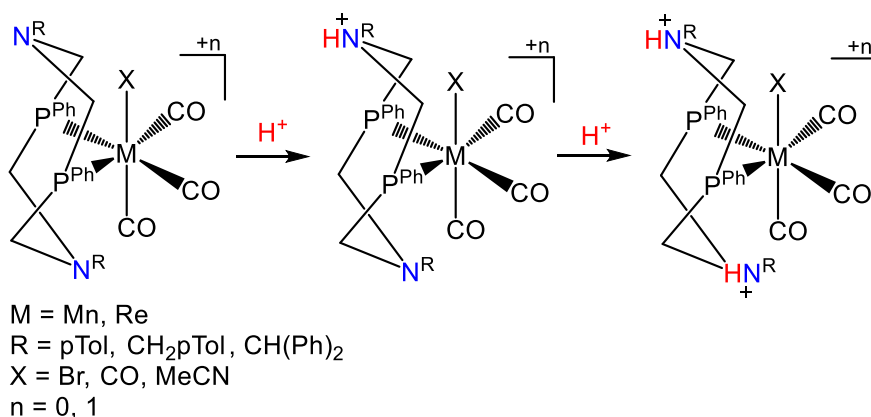


Figure 1. Protonation of Mn(I) and Re(I) complexes

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Ammonium peroxogermanate: a hydrogen-bond-stabilized precursor for germanium-based materials

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Germanium compounds are widely used in microelectronics, optics, solar cells, and sensing technologies. However, their high cost necessitates the development of synthetic methodologies that provide high, near-quantitative yields of germanium-containing products. This requires the design of new, convenient germanium precursors with enhanced reactivity and improved aqueous solubility compared to conventional compounds.

Crystalline ammonium peroxogermanate, $(\text{NH}_4)_6[\text{Ge}_6(\mu\text{-OO})_6(\mu\text{-O})_6(\text{OH})_6]\cdot 6\text{H}_2\text{O}$, has been proposed as a precursor for the synthesis of a highly water-soluble form of germanium oxide. It comprises centrosymmetric hexanuclear peroxogermanate anions $[\text{Ge}_6(\mu\text{-OO})_6(\mu\text{-O})_6(\text{OH})_6]^{6-}$ with six μ -oxo- and six μ -peroxo groups forming negatively charged layers. The space between these layers is filled by ammonium cations and water molecules, forming a highly stable structure due to hydrogen bonding. Thermal decomposition of this compound at 300 °C for 10 min yields amorphous GeO_2 with a water solubility of up to 100 g L⁻¹, which is more than twenty times higher than that of conventional amorphous GeO_2 . Such a solution can be employed in reactions with both basic and acidic reagents, affording a wide range of germanium-containing salts, including germanium sulfide, germanium hydrogen phosphate, and potassium germanate. In the absence of acid or base, hexagonal germanium oxide precipitates from the aqueous GeO_2 solution.¹

This approach enables precise control over the amount of germanium introduced into the system, thereby allowing the synthesis of composite materials with tailored compositions based on germanium compounds. In particular, materials based on germanium oxide, sulfide, nitride, phosphide, and reduced graphene oxide with varying active-phase contents have been prepared. The applicability of these materials as anode components in lithium-ion batteries has been demonstrated.^{2,3}

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Bimetallic Hydrides of Group 13 Metals: From σ -Complexes to Reductive Elimination

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In recent years main group metal hydrides have garnered a significant attention, mainly due to their potential in hydrogen storage and organic synthesis. An enhancement of efficiency of main group metal hydrides in these applications can be achieved by their combination with transition metals. In the context of dehydrogenation transition metals provide for a lower activation energy and improve hydrogen release efficiency. Regarding reducing abilities, the activation of M–H bonds at transition metal centers is expected to lead to a new generation of dehydrogenating systems due to their cooperative behavior.

In this study, we have demonstrated the reactivity of the sterically hindered hydrides of Group 13 metals bearing a redox-active Ar-bian ligands toward transition metal carbonyl and cyclopentadienyl derivatives. We obtained a new family of heterobimetallic complexes of aluminum, whose stability arises from a unique synergy between covalent bonding in the $\text{Al}(\mu^2\text{-H})_2\text{TM}$ hydride bridges, the direct TM–Al interactions and intramolecular electrostatic interactions of atomic charges.¹ In contrast to aluminum, the interaction of paramagnetic gallium hydrides with transition metal carbonyls leads to spontaneous release of molecular hydrogen or hydrogen chloride, resulting in the formation of a low-valent imidazole species $(\text{Ar-bian})\text{Ga}\cdot$, which subsequently acts as a ligand for the transition metal, displacing one CO molecule from the carbonyl derivative. This represents a classical reductive elimination process.

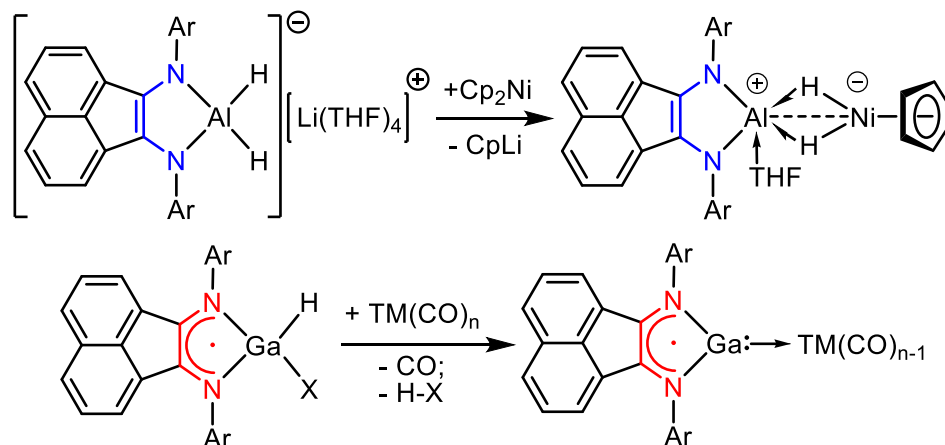


Figure 1. The reactions of aluminum and gallium hydrides with transition metal derivatives.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Photoinduced processes in homo- and heterobimetallic ruthenium (II) complexes with imidazo[4,5-f][1,10]phenanthrolines for various purposes

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In this work, a series of new monoruthenium(II) and heterobimetallic complexes were synthesized and studied. These complexes are capable of photoinduced electron transfer to the conduction band of some semiconductor materials (Fig. 1) and other recipients. In first case, such photosensitization process will reduce the operating temperature of semiconductor gas sensors and thus reduce their energy consumption.

We have shown that studied complexes were suitable for electron transfer from excited state to the conduction band of SnO₂ and In₂O₃. Modification of the surface of nanoparticles of SnO₂ and In₂O₃ with Ru(II) complexes gave hybrid organic-inorganic materials. Hybrid sensors appeared to have reproducible sensory signal in the presence of analyte gases NH₃, NO₂ and NO at room temperature in air under periodic illumination with visible light. Some materials were able to determine NO₂ and NO within 0.25–2 ppm at room temperature under illumination with red LED. The MPC of the daily dose of NO is 2.6 ppm.

The introduction of the second metal cation into the complex allows the properties of the complex to be tuned by changing the electron density, while the metal itself can function as a receptor center, ensuring selective interaction of sensor with analyte molecules.¹ For instance, it is known that iron-containing complexes have a high affinity for oxygen, carbon monoxide; organometallic copper complexes are prone to adsorption of hydrogen sulfide, nitrogen oxides and sulfur-containing organic molecules. So, we introduced a second cation into ruthenium (II) complexes. The resulted heterobimetallic complexes showed various photophysical behavior depending on the donor or acceptor nature of the second coordination site. Bimetallic complexes also helped to control the affinity of the surface towards one or another gas, which resulted in improved selectivity of gas analysis while maintaining room temperature operation.

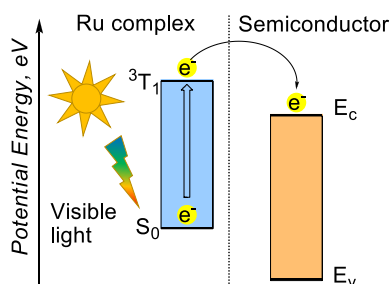


Figure 1. Photoinduced sensitization in a hybrid semiconductor-dye material

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Quantum Chemical Study of Non-covalent Complexes of *Closo*-Dodecaborate Anions $[B_{12}H_{11}X]^{y-}$ with Blocked Amino Acids

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Non-covalent interactions (NCIs) are one of the cornerstones of modern chemistry and associated sciences¹. In previous work² non-covalent complexes of *closo*-borate anions $[B_nH_{n-1}X]^{y-}$ with glycine were investigated. In water, glycine exists in a zwitterionic form and contains two polar groups: COO^- , NH_3^+ . Protein molecules can also contain similar groups, but their most important structural motif is the peptide bond. To understand how boron anions bind to proteins, it was necessary to model clusters with molecules containing a peptide bond. Thus, in present work theoretical elucidation of molecular complexes of *closo*-borate anions $[B_nH_{n-1}X]^{y-}$ ($X = H, NH_3, OH, SH, F$) with N-acetyl-A-methylamide aminoacids ($A =$ glycine, alanine, phenylalanine, serine and asparatic acid) was performed.

Based on the results obtained, it can be concluded that the introducing of a substituent to the boron cage leads to a more stable noncovalent complex between the blocked amino acid and the cluster species. The most energetically stable complexes were formed in the case of hydroxy $[B_{12}H_{11}OH]^{2-}$ and ammonium $[B_{12}H_{11}NH_3]^-$ derivatives. Hydroxy derivatives $[B_{12}H_{11}OH]^{2-}$ generally formed two hydrogen bonds between the *exo*-polyhedral oxygen atom and two hydrogen atoms of amide groups. In contrast, in the case of $[B_{12}H_{11}NH_3]^-$, hydrogen bonds were formed between only one *exo*-polyhedral hydrogen atom and oxygen atom of an amide group or in case of serine hydroxy group.

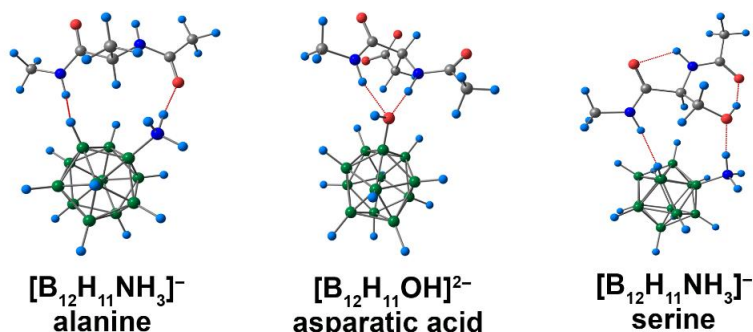


Figure 1. Optimised structures of molecular complexes of $[B_{12}H_{11}X]^{y-}$ with blocked alanine, asparatic acid and serine.

Acknowledgements

This work was supported by the Russian Science Foundation (project no. 25-23-00530).

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Noncovalent Interactions

in Fish Gelatin–Sulfated Polysaccharide Complexes

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Biopolymer hydrogels possess a unique set of properties (rheomorphic structure, biocompatibility, biodegradability, environmental friendliness, and raw material availability) and are widely used in areas related to human life safety, health, and nutrition. Among biopolymer gelling agents in the food industry, gelatin, traditionally industrially obtained from bovine and porcine connective tissue, occupies one of the leading positions. For economic, epidemiological, and religious-cultural reasons, the need to replace gelatin from these raw materials with gelatin from alternative sources, in particular, fish gelatin, has become urgent. However, due to its amino acid composition, fish gelatin has unsatisfactory thermal, rheological, and functional properties.¹ We set out to solve this problem by modifying fish gelatin with sulfated polysaccharides from red seaweeds (in particular, agar or κ-carrageenan).

Spectroscopy (¹H NMR, Fourier transform IR, and UV) revealed that gelatin and polysaccharides in the aqueous phase engage in intermolecular noncovalent interactions (electrostatic and hydrophobic interactions, hydrogen bonds). The dominant role of these interactions depends on the ambient temperature.² As a result of noncovalent binding, biopolymers form large supramolecular complexes, which are particles of a new dispersed phase. Using the dynamic quasi-elastic laser light scattering method, it was shown that the size and ζ-potential of the complexes depend on the mass ratio of biopolymers, pH, and ionic strength of the aqueous phase. The regions of stable dispersions of the gelatin–polysaccharide complexes were determined using phase diagrams of aqueous mixtures of biopolymers.³

Fish gelatin–sulfated polysaccharide hydrogels formed upon cooling of the initial dispersions were studied by differential scanning calorimetry and shear rheometry. Hydrogels are characterized by increased gelation rates and temperatures, heats of fusion, and rheological properties comparable to those of porcine skin gelatin. SEM revealed that the microstructure of the complex hydrogel consists of a cellular fish gelatin network reinforced with sulfated polysaccharide fiber mesh. The prospects for the practical use of hydrogels based on fish gelatin–polysaccharide complexes in the industry of food and biologically active additives are considered.

Acknowledgements

The work was supported by the Russian Science Foundation, project No. 23-64-10020.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Supramolecular Assembly of N-Heterocycles in Levitating Droplet Cluster and Water-in-Oil Droplets Flow

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Supramolecular assembly of small N-heterocycles is mostly interesting as a key process for pre-RNA research, but some attempts are made to achieve functional materials based on it.^{1,2} The spontaneous assembly is characterized by a wide range of morphology differences and corresponding functions changes due to the slight perturbation of the synthetic medium.³

To control the medium parameters, droplet microfluidic approach was adapted to canonical assembly process of melamine cyanurate and more complex melamine barbiturate. The configuration of microfluidics system was developed to enable fast micro-crystallization in droplets flow also as in situ monitoring of crystallization rate for the first time. The effect of concentration control in microvolumes was investigated in detail.

A containerless approach to supramolecular crystallization was also provided in levitating droplet cluster to perform basics of logic gates. Two-signal positive processes were performed in levitating droplets such as color change and crystals formation.

Classic hydrogen bonding formation between cyanuric acid/melamine with complementary nucleobases of single-stranded DNA was also studied in levitating microdroplets and the formation of condensed complexes was performed. Density functional theory calculations also as molecular docking simulations were provided to explain the difference in N-heterocycle-nucleobase assembly and its further condensation in levitating droplets.

The obtained results can be considered as a basics for further investigation of microvolume highly controlled synthesis of supramolecular materials both for fundamental and practice-orientated research.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Dinitrobenzoates of cadmium and 3d metals as structural analogues for penta- and tetrafluorobenzoates

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The ability of 2,4- and 3,5-dinitrobenzoates to form coordination compounds with structures similar to those of pentafluorobenzoates and tetrafluorobenzoates allowed us to obtain new types of complexes with benzoic acid derivative anions bearing strong electron-withdrawing substituents. Previously, the structures of several pentafluorobenzoate and tetrafluorobenzoate complexes were determined based on quantum chemical calculations; however, actual compounds were not obtained for every structural type.

The synthesis of cadmium 2,4- and 3,5-dinitrobenzoates with 2,2'-dipyridyl and 1,10-phenanthroline derivatives yielded a complete set of structures discussed in the quantum chemical modeling of the formation of pentafluorobenzoate and tetrafluorobenzoate polymeric and binuclear structures. The synthesis of the 3,5-dinitrobenzoate coordination polymer $[\text{Mn}_2(\text{phen})_2(3,5\text{dnb})_4]_n$ confirmed our hypothesis that cadmium cannot form analogs of manganese coordination polymers due to the higher stability of binuclear complexes.

Unlike chelating N-donor proligands, monodentate pyridine derivatives do not disrupt polynuclear structures. This allowed us to use an excess of them in reactions and obtain complexes in which they act simultaneously as ligands and solvate molecules. Among the 3,5-dinitrobenzoate complexes, the most interesting compound turned out to be a 1D coordination polymer of a previously unknown type, $[\text{Cd}_2(\text{quin})_2(\text{H}_2\text{O})_2(3,5\text{dnb})_4]_n \cdot 2n(\text{quin})$, in which double-bridging bonding by carboxylate anions alternates with double-bridging bonding by water molecules. Not only all aromatic fragments of the ligands but also the quinoline solvate molecules participate in the formation of two intramolecular stacks.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

In Silico Insight into Non-Covalent Interactions of Epoxybenzooxocine Derivatives as Potential Antiviral Agents

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Non-covalent interactions play a crucial role in molecular recognition processes between small-molecule drugs and target proteins, fundamentally determining the stability and specificity of the resulting complexes. Since 2021, Professor I.V. Kulakov's research group has been systematically synthesizing epoxybenzooxocine derivatives as structural analogs of natural integrastatins, demonstrating a broad spectrum of antiviral activity, specifically against HIV-1 and SARS-CoV-2.^{1,2} The evaluation of their antiviral potential is complemented by *in silico* studies, incorporating binding affinity estimation and detailed mapping of non-covalent interactions via AutoDock Vina and Discovery Studio. This report provides an *in silico* assessment of the inhibitory potential of several compounds toward HIV-1 RT (PDB ID: **3V81**) and SARS-CoV-2 RdRp (PDB ID: **7AAP**), focusing on the contributions of distinct non-covalent interactions between the ligands and target protein residues.

Table 1 Non-covalent interactions between studied ligands and target protein receptors

Ligand	Receptor	Conventional Hydrogen Bond	Pi-Alkyl	Pi-Pi T-shaped	Pi-Anion
13a	7AAP	ILE37, ASP36	VAL204	PHE35	ASP218
16b	3V81	DG720	DG719	TYR501	ILE505, PRO420, ALA508

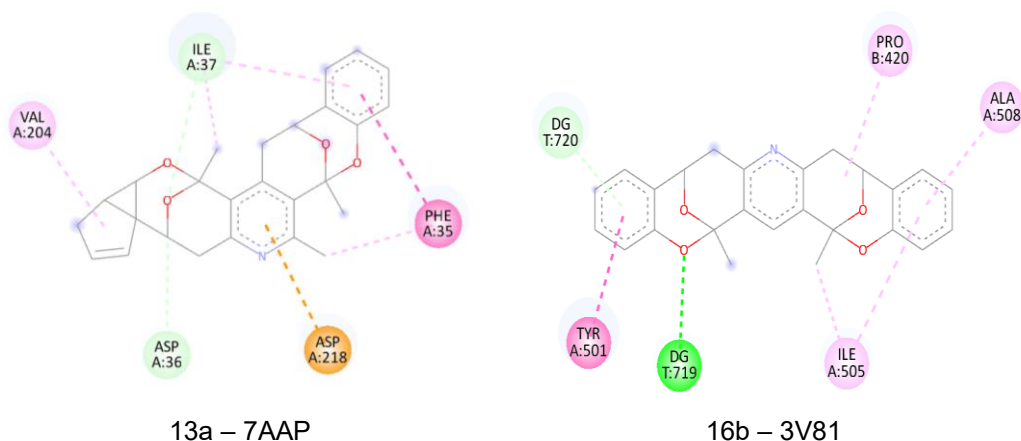


Figure 1. 2D visualization of interactions between the ligand and target protein residues

Acknowledgements

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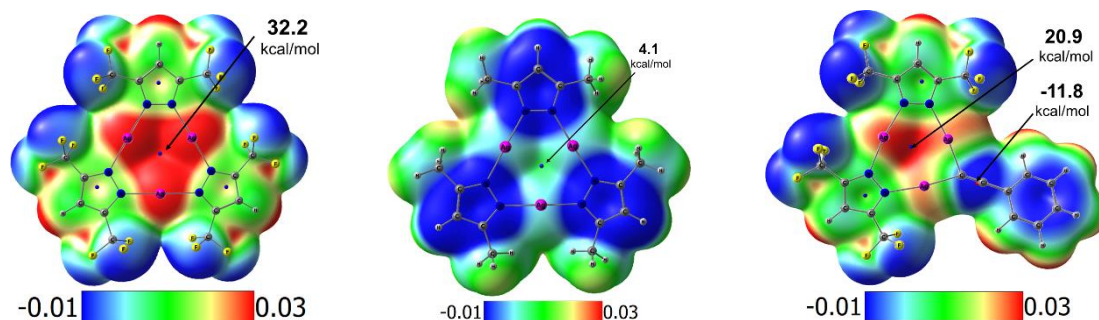
Cyclic Metal Complexes as Lewis Acids or Bases for Supramolecular Host–Guest Chemistry

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This lecture explores two types of cyclic metal complexes that can act as Lewis acids or bases depending on the ligand. Among the most studied examples are the cyclic trinuclear coinage metal pyrazolate complexes with the general formula $[MPz]_3$ ($M = Cu, Ag, \text{ or } Au$; $Pz =$ substituted pyrazolate ligand).¹ Metal-directed self-assembly of these metallamacrocycles yields preorganized cyclic platforms bearing multiple convergent binding sites, thereby enhancing both the affinity and selectivity of guest recognition through cooperative Lewis acidic/basic interactions.¹ The planar geometry of these complexes facilitates metallophilic interactions in the solid state, leading to the formation of excimeric excited states and determining their distinctive photophysical properties. As Lewis acids, these compounds form noncovalent intermolecular complexes with various bases, including carbonyl compounds, π -electronic systems, and even halide ligands. This opens up opportunities for the design of new supramolecular assemblies with predictable structures and properties. By simply varying the substituents in pyrazolate ligands, one can tune the properties of metal centers from acidic to basic.² Particular attention is paid to mercury-containing systems, which have been intensively investigated as efficient and selective anion receptors. The potential applications of these metal-containing cyclic complexes include molecular recognition, ion transport, sensing, the development of tunable luminescent materials, and other areas. These compounds complement the functionality of conventional organic hosts while offering unique properties not available in other hosts.



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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Theoretical assessment of the effect of non-covalent interactions on biological activity

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The development of modern materials science and industry, primarily the pharmaceutical industry, requires constant improvement of methods for obtaining new compounds with specified properties. This is due, among other things, to the problem of rapidly increasing resistance to commonly used medications and the difficulties of managing pharmacokinetics. One of the simplest and most convenient ways to design new materials is to use multi-component organic crystals or coordination compounds, which are complex mixtures of organic and/or inorganic blocks, opening up a wide range of possibilities for customizing the composition and structure of new compounds. The creation of organic multicomponent crystals and coordination compounds with a similar set of organic molecules as ligands will allow us to evaluate the influence of metal ions on the structure of organic fragments and the system of non-covalent interactions, which in turn determines the properties of the compounds, including their biological properties.

This work focuses on the relationship between non-covalent interactions in organic and related coordination compounds and their activity towards various proteins. As part of the study, derivatives of pyrroline, pyrrolidine, and thiouracil have been studied using X-ray crystallography, quantum chemistry, and molecular docking modelling, both as individual compounds and as complexes and multicomponent crystals of various compositions. It has been shown that coordination compounds have higher biological activity than individual organic compounds, which is due to a significant change in the types and amounts of non-covalent interactions. In particular, in most cases, the affinity of a ligand for a protein is primarily influenced by a combination of weak non-covalent interactions rather than strong hydrogen bonding.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Small molecule non-covalent interactions with biomolecules

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Biomolecules are the keys to life. The importance of the biomolecules, such as nucleic acids, proteins, carbohydrates and lipids, is well known. In parallel, there are a number of categories of small molecules which are very common in our practices, including drugs, dyes, natural products, surfactants, etc. Thus, the interactions of the larger biomolecules with smaller substances are of great importance.

Fluorescent dyes play a crucial role in various bioimaging applications, offering valuable insights into cellular processes and molecular interactions. These dyes have been widely explored as probes for visualizing cellular organelles and biomolecules, including nucleic acids. As an example, the noncovalent recognition of DNA by small fluorescent molecules primarily relies on dominant binding modes, such as intercalation, groove binding, or electrostatic interactions with the sugar–phosphate backbone. Herein, we demonstrated the study of styryl dyes as fluorescent probes for biomolecules and organelles (e.g., mitochondria, cytoplasm and membrane). Styryl dyes exhibit a unique “light-switch” behavior, remaining nonfluorescent until they interact with biomolecules (such as DNA), resulting in a strong fluorescence signal. This property, combined with their high affinity for nucleic acids, provides an advantage in detecting and visualizing specific DNA sequences without background interference.

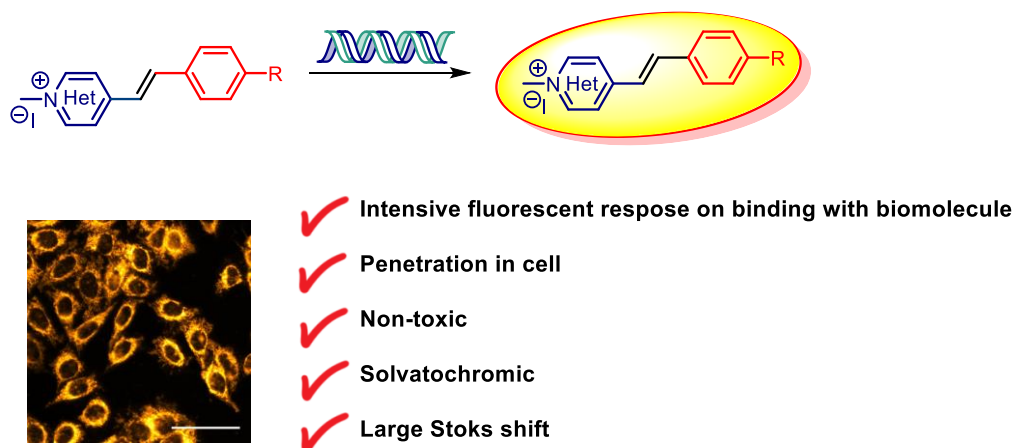


Figure 1. Representation of fluorescent dyes for non-covalent binding with biomolecules

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Assembling of petroporphyrins in vacuum-deposited layers

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The presence of tetrapyrrolic metal complexes (petroporphyrins) in fossil fuels is a well-known fact used in both discussions of the organic matter evolution and in determining the origin of production. Despite this, the question of their own solid-state organization remains open. One of the reasons is that the proper isolation of petroporphyrins from the crude poses certain difficulties, after overcoming which the researchers obtain a mixture of etioporphyrin-type ligands with the same metal (here – vanadium),¹ but different peripheral structure – Fig. 1. This mixture can either be used as an end-product with certain practically interesting properties (e.g., photoelectrical, catalytic),² or separated into individual components. The latter remains a challenging task for organic chemists.

In this work, we investigate the formation of thin solid petroporphyrin (VO-PPs) films using the high-vacuum evaporation technique.^{1,2} Our previous results revealed a dependence of the sublimate composition on the process conditions.¹ The substrate temperature T_g was varied from 25 to 180°C in order to stimulate the self-ordering of porphyrin molecules during deposition. At $T_g=150^\circ\text{C}$, the root-mean-square surface roughness of the 80 nm VO-PPs films measured by AFM reaches its maximum of 11.6 nm in the series, while the X-ray diffraction signal in the low 2θ range becomes close to that of the pure VO-EtioP-III phase, corresponding to the (100) plane – Fig. 1. The lateral specific conductivity σ of these films is $2.5 \cdot 10^{-9}$ S/cm, but it increases 160-fold under 1sun illumination. In VO-PPs films with $T_g=25^\circ\text{C}$ the σ value is about an order of magnitude less; the photocurrent correlates with the full width at half-maximum of the Soret-band in the absorption spectrum.

The approaches to tuning the phase composition of mixed molecular films by adjusting the substrate and source temperatures are discussed.

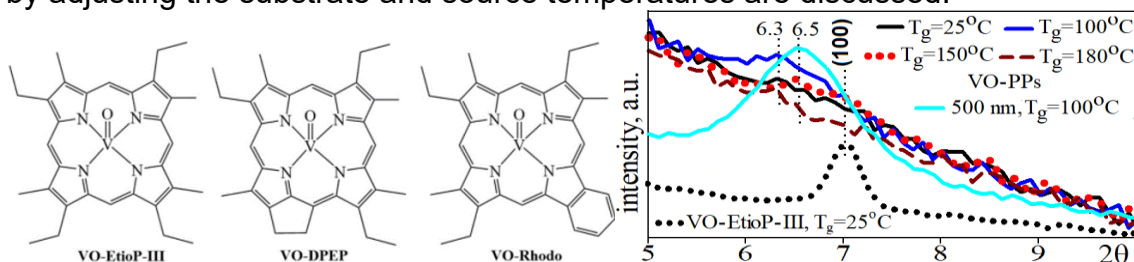


Figure 1. Molecular structures of three basic vanadyl petroporphyrins: Etio-, DPEP-, and Rhodo-type (left). Fragments of X-ray patterns of VO-PPs films deposited in vacuum on Si(111) at different T_g compared to the signal from the VO-EtioP-III film after annealing (right).

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Thermodynamics and kinetics of co-crystallization of 2,4-dinitrodiazophenol and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane

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Co-crystallization of energetic compounds is a new and promising method for creating materials with improved detonation and performance characteristics, exhibiting high thermal stability and low sensitivity to mechanical stimuli¹.

In our work, we investigated the homogeneous nucleation kinetics of a new energetic co-crystal of 2,4-dinitrodiazophenol and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane in a binary solvent system CH₃CN/CCl₄ under anti-solvent crystallization conditions (solvent/anti-solvent) at two temperatures, 25 and 50 °C, and two solvent ratios, 5 and 10 % CH₃CN/CCl₄.

It was shown that the nucleation kinetics of the co-crystal increase relative to the nucleation kinetics of its coformers with decreasing temperature and increasing supersaturation.

The thermodynamic functions of co-crystal formation were also determined by the solubility method² in the individual solvent's isopropanol and dichloroethane.

Analysis of the thermodynamic functions shows that the co-crystal is entropy-driven, its thermal stability relative to the coformers increases with rising temperature (Table 1), and the Gibbs free energy becomes negative at temperatures above 40 °C.

Table 1. Thermodynamic functions of a co-crystal

Solvent	$\Delta G_{cf}^{o,298}$, кДж/моль	$\Delta H_{cf}^{o,298}$, кДж/моль	$T\Delta S_{cf}^{o,298}$, кДж/моль
Isopropanol	1.2	29.4	-28.2
Dichloroethane	1.1	29.9	-28.8

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Noncovalent Complexes of Chlorophyll and Hemin with Biocompatible Polymers

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A serious obstacle to the development of biocidal agents based on tetrapyrroles (TP) is their insolubility in water.^{1, 2} This report provides an possibility of forming complexes of hemin (Hem) and chlorophyll (Chl) with natural (carboxymethylcellulose, chitosan, sodium alginate, pectin, dextran, and inulin) and artificial polymers (polyethyleneimine, polyallylamine, polyvinyl alcohol, polyvinylpyrrolidone, polyethyleneglycol, etc.) was studied.

To determine the stability of the complexes in water, the Benesi-Hildebrand graphical method was used, which uses an equation relating the optical absorption of TP and the concentration of the polymer:

$$\lg \frac{A_f - A_0}{A - A_0} = n \lg[C] + \lg K_B ,$$

where A_0 , A_f , A are the initial, final and intermediate values of the optical density of TP solutions with polymers, C is the polymer concentration (mol/l), K_B is the binding constant of TP with the polymer (l/mol), n is the number of polymer molecules per one TP molecule. Data on the stoichiometry and stability ($K_B = 10^5$ - 10^6 l/mol) of the complexes, as well as the results of a study of their biocidal properties were obtained.

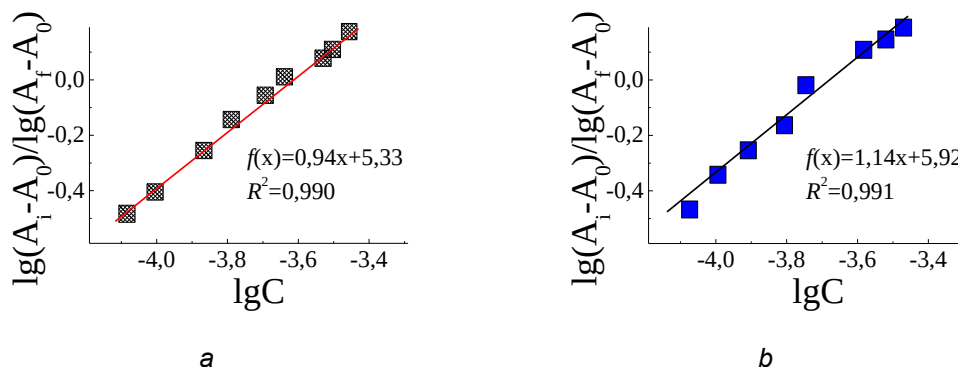


Figure 1. Benesi-Hildebrand dependence for the complexation of Hem with polyethyleneimine (a) and Chl with inulin (b) as an example.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Study of the dynamics of organic cations in hybrid perovskites using vibrational spectroscopy methods

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Currently, there is considerable interest in organic-inorganic halide perovskites, which possess unique properties that make them suitable for use in the manufacture of photonic, optoelectronic, and photoelectric devices.

At present, vibrational spectroscopy has been increasingly used to study perovskite materials.^{1, 2} The combination of Raman and IR spectroscopy data allows better understanding the structure and dynamics of organic-inorganic compounds, namely, the interaction of "soft" organic cations with an inorganic framework, as well as the behavior of this structure under temperature changes, including phase transitions.

In this work, vibrational spectroscopy and density functional theory (DFT) calculations were employed. Analysis of the dynamics of organic MA ($\text{CH}_3\text{-NH}_3^+$) and Py ($\text{C}_5\text{H}_5\text{NH}^+$) cations in the hybrid perovskite MAPbBr_3 (3D) and perovskitoid PyPbBr_3 (1D) over a 90-300K temperature range was performed.

The effect of broadening of IR bands at different temperatures was analyzed by estimating the vibrational correlation time τ_c , which depends on the full half-widths of the IR bands.³ Figures 1 and 2 show dependences of full half-widths of the IR bands and tau values from the MAPbBr_3 sample temperature.

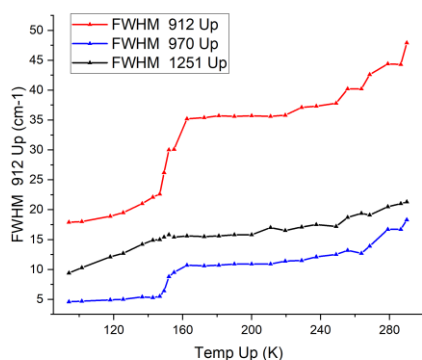


Figure 1

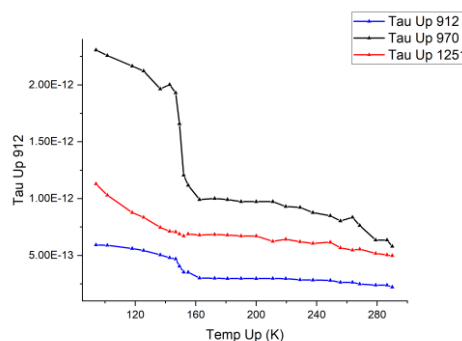


Figure 2

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Complexation in Crystal, Solution and Vapor: Congruent Sublimation and Cocrystallization Thermodynamics of [Caffeine + 3-Hydroxybenzoic Acid] (1:1)

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We report a combined experimental and computational thermodynamic study of cocrystal sublimation and formation, using the [caffeine + 3-hydroxybenzoic acid] (1:1) cocrystal as a model. Predictive models for cocrystal formation commonly rely on lattice energy (E_{latt}) or related quantities (H_{latt} , G_{latt}). While E_{latt} parameterization for single-component crystals is well established, experimental sublimation enthalpies for multicomponent molecular crystals are scarce and limited to incongruently sublimating solids.¹ Guided by the hypothesis that cocrystals whose components have comparable vapor pressures favor congruent sublimation, we selected the caffeine/3OHBA pair from a sublimation database and proved the phase stability of their cocrystal during resublimation. Temperature dependencies of the vapor pressures of caffeine and 3-hydroxybenzoic acid above the cocrystal were obtained by the transpiration method. The pressures of components were found to differ by less than 5%. A mathematical framework is developed to derive the thermodynamic functions of cocrystal sublimation, and thermal corrections to enthalpy and vapor pressure are calculated from molar heat capacities of solids obtained from DSC experiments with Al_2O_3 reference and molar heat capacities of gas-phase species computed at CBS-QB3 level of theory. The sublimation enthalpy $\Delta_{\text{sub}}H$ was found to be $222.1 \text{ kJ}\cdot\text{mol}^{-1}$, the Gibbs energy $\Delta_{\text{sub}}G = 106.1 \text{ kJ}\cdot\text{mol}^{-1}$ and derived cocrystallization enthalpy $\Delta_{\text{cc}}H = -1.8 \text{ kJ}\cdot\text{mol}^{-1}$. Solution thermodynamics in acetonitrile (293.2–313.2 K) accounting for 1:1 complexation ($K_{11} = 1149$ at 298 K) gave a corrected $\Delta_{\text{cc}}H$ of $-50.2 \text{ kJ}\cdot\text{mol}^{-1}$. CBS-QB3 calculations indicate a thermodynamically favorable heterodimer in the gas phase ($\Delta_{\text{dim}}G = -7.4 \text{ kJ}\cdot\text{mol}^{-1}$, $\Delta_{\text{dim}}H = -51.0 \text{ kJ}\cdot\text{mol}^{-1}$ at 298 K), supporting a two-stage sublimation mechanism with heterodimers in the vapor. Incorporating gas-phase complexation into the sublimation cycle yields the cocrystallization enthalpy $\Delta_{\text{cc}}H = -52.8 \text{ kJ}\cdot\text{mol}^{-1}$, consistent with solution data. The study highlights that solution and vapor-phase complexation must be considered in cocrystal thermodynamics.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Noncovalent interactions in synthesis and design of new catalytic systems based on black phosphorus and organonickel sigma-complexes

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Organometallic complexes and phosphorus compounds are important components of industrial catalysts and have been used for obtaining various types of practically important organic and inorganic derivatives and polymeric materials.^{1,2}

Relatively recently discovered black phosphorus³ consisting of 2D polyphosphorus layers bonded by noncovalent interactions represents a very promising material for application in catalysis,^{4,5} biology and medicine.⁶ In the same time, organonickel complexes bearing sigma-bonded organic fragment at nickel centre can be successfully used for *in situ* generation of active catalysts by combination with some other materials and noncovalent interactions between the components.

In this lecture an application of black phosphorus and organonickel sigma-complexes of type [NiBr(Aryl)(bpy)], where Aryl – *ortho*-substituted phenyl, bpy – 2,2'-bipyridine, for creation and design of new catalysts for hydrogen evolution reaction (HER) and carbon dioxide reduction reaction (CO₂RR) will be discussed.^{7,8}

Acknowledgements

This work is financially supported by the Russian Science Foundation (project 23-13-00427-P)

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Metallophilic interactions in inorganic semiconductors

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It is known that semiconductor inorganic crystals are brittle due to the directionality and short-range nature of the covalent bonds that form them. However, in recent years it has been discovered that a number of Ag chalcogenide based semiconductors exhibit plasticity (δ). Their δ is so great that it allows these crystals to be cold rolled into flexible wire and foil. This opens up numerous possibilities for the practical application of such materials. For further development of such materials, a key question is the fundamental cause of the phenomenon of anomalous plasticity (PAP) of inorganic semiconductors. In papers devoted to the study of PAP, the main attention is paid to the features of the crystal structure and the possibility of interlayer slip. The authors of the report argue that the fundamental reason for the PAP of these materials is a specific chemical interaction. We are talking about non-directional metallophilic Ag-Ag bonds that exist in addition to covalent metal-chalcogen bonds. The following facts serve as evidence. The double van der Waals radius for Ag is 3.44 Å. In the monoclinic lattice of Ag₂S, each Ag atom is surrounded by n=6 other Ag atoms, with an average distance of $\bar{R}=3.14\pm0.05$ Å. For the orthorhombic lattice of Ag₂Se n=4; $\bar{R}=3.14\pm0.17$ Å. Quantum chemical studies¹ have confirmed the existence of metallophilic interactions in Ag₂S and Ag₂Se not only for crystals but also for molecular complexes that imitate the amorphous structure. Measurements have shown that the δ of glassy chalcogenides semiconductors increases with increasing silver chalcogenide content². Furthermore, the δ of Ag₂Se in the amorphous state is higher than in the crystalline state. Thus, the fundamental cause of PAP is the peculiarities of the chemical bonds in the materials under discussion, and not their crystal structure. This opens up the possibility of creating glassy materials for infrared optics that have an increased ability to relax mechanical stresses.

A study of chalcogenide glassy semiconductors revealed that the energy of a single Ag-Ag metallophilic bond in the Ag₂Se semiconductor is 0.3 eV. It was also demonstrated that metallophilic interactions affect more than just the mechanical properties of inorganic semiconductors. For example, it was found that the formation of these interactions leads to an increase in the glass transition temperature of chalcogenide glassy semiconductors.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Ultrathin coatings based on graphene oxide and gold nanoparticles for surface-enhanced Raman spectroscopy

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Hybrid coatings based on reduced graphene oxide (rGO) and gold nanoparticles (AuNPs) offer a promising platform for surface-enhanced Raman scattering (SERS), combining electromagnetic enhancement from AuNP plasmons with chemical enhancement via analyte adsorption on rGO. We report a facile approach to fabricate uniform SERS substrates by immobilizing AuNPs onto GO sheets through citrate-mediated reduction of HAuCl_4 , followed by interfacial assembly at the aqueous/hexane boundary and vertical transfer onto silicon supports. GO was reduced via microwave irradiation under an argon atmosphere. Atomic force microscopy (AFM) analysis confirmed that the proposed method yields homogeneous GO monolayers decorated with immobilized AuNPs up to 15 nm in diameter. Notably, nanoparticle growth occurred predominantly at the sheet edges, indicating that structural defects in GO serve as nucleation sites for gold crystallization.

The suitability of the coatings for SERS applications was validated using rhodamine 6G (R6G) as a probe molecule. The analyte was deposited from solution to form a sub-monolayer with approximately 50% surface coverage. Well-resolved SERS spectra were successfully acquired for this system. In contrast, isolated 18 nm AuNPs exhibited no enhancing effect on the analyte, as the Raman signal was completely obscured by R6G fluorescence. While standalone rGO effectively quenched analyte fluorescence, the enhancement remained insufficient for the detection of Raman bands.

The synergistic integration of rGO and AuNPs thus provides ultrathin, uniform coatings that simultaneously suppress background fluorescence and amplify Raman signals, highlighting their potential for sensitive, label-free analytical applications.

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ANION-CATION INTERACTIONS IN PROTONATED NAPHTHALENE "PROTON SPONGES" IN CRYSTALS AS A CONSEQUENCE OF SPATIAL CONGESTION

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Until recently, the vast majority of XRD studies of many dozens of cations of both the parent "proton sponge" (DMAN) and its derivatives focused on the energy, dynamics of the NHN hydrogen bond, and especially on the geometric parameters of the [NHN]⁺ bridge, such as its length (N...N), linearity (angle NHN), degree of asymmetries (ratio N-H/H...N), which is more influenced by the spatial effects of substituents in the naphthalene system.¹⁻³

Much less attention was paid to the issue of anion-cation interactions, which are quite complex in nature and are most pronounced in the solid phase. In this case, several factors have a great influence on the anion-cationic interactions: in addition to the already mentioned length and symmetry of the NHN hydrogen bond, both the size and shape of the anion X⁻ and its nucleophilicity make a significant contribution. The dispersion of the positive charge of the DMAN·H⁺ cation with the participation of NMe₂ groups also leads to increased interaction with the anion due to short intermolecular CH...X⁻ contacts. An extraneous particle (for example, water, a solvent used to grow crystals) often interferes with the anion-cation interaction, the reasons for which are also discussed in this report.

We have made the first attempt to systematize all the information available on this subject. This can be useful from the point of view of modeling such fundamental biochemical processes as proton transfer (catalysis) and molecular recognition.

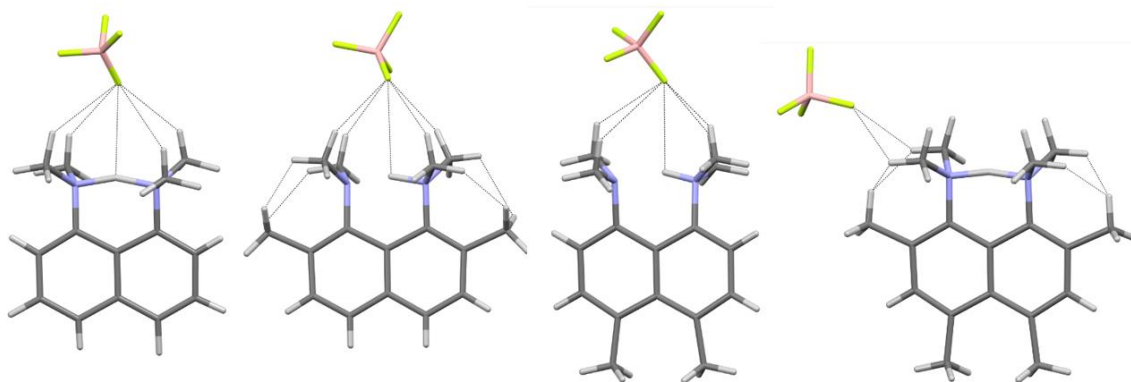


Figure 1. Crystal structures of tetrafluoroborates of parent "proton sponge" (DMAN·HBF₄) and its methyl derivatives with short contacts highlighted

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

(Supra)molecular assembly in cage metallasilsesquioxanes

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Cagelike metallasilsesquioxanes is a growing class of metallacomplexes with impressive (supra)molecular architectures and wide list of applications.^{1, 2} Lecture will present recent results of our group in molecular design of metallasilsesquioxanes, including varying of steric factors in silsesquioxane ligands. Catalytic properties of resulted complexes will also be discussed.

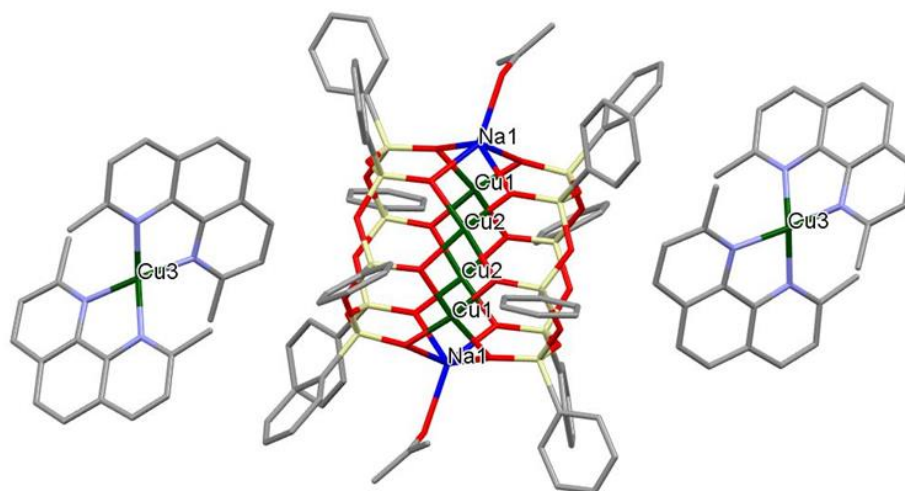


Figure 1. Molecular structure of ionic coppersodiumsilsesquioxane complex with neocuproine $[(\text{Ph}_6\text{Si}_6\text{O}_{12})_2\text{Cu}_4\text{Na}_2(\text{acetone})_2][\text{Cu}(\text{neo})_2]_2$ ³

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Second coordination sphere hydrogen bonds in rational design of metal-based drugs

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Non-covalent interactions, specifically hydrogen bonds, in the second coordination sphere (SCS) of metal ions play a fundamental role in the structural organization, transformations, and reactivity of biomolecules — including RNA, DNA, and proteins.¹ A growing body of experimental evidence highlights the enormous significance of SCS hydrogen bonds across diverse fields, including biomimetic and enantioselective catalysis, molecular recognition, supramolecular self-assembly, and even the origins of life.²⁻⁴ As early as development of the first generation of platinum-based anticancer agents, the deliberate formation of SCS hydrogen bonds between a metallodrug and its biological target was recognized as an important factor influencing structure-activity relationships of metal-based therapeutics.

In this report, a retrospective overview of the key strategies employed in the rational design of bioactive coordination and organometallic compounds will be provided focusing on the role of SCS hydrogen bonds in their interaction and binding with relevant biological targets, including nucleic acids, proteoglycans, ion channels, and lipids. Additionally, the recent efforts in the development of pH-responsive organometallics based on palladium(II) complexes bearing protic acyclic diaminocarbenes (ADC) are discussed as an illustration of a rational approach to design selective mitochondria-targeted antiproliferative agents.⁵

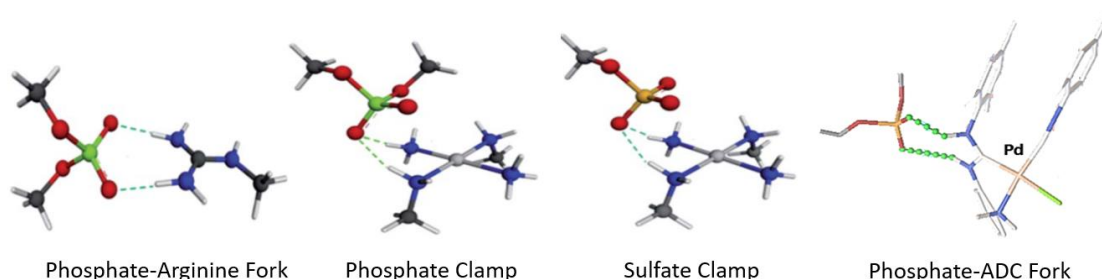


Figure 1. Hydrogen bonding motifs in the second coordination sphere of bioactive metal complexes.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Controlling Regioselectivity and Reaction Rates of Arylation through Anion Coordination to σ -Hole Donors

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Halonium salts have found widespread application in supramolecular chemistry as halogen bond donors. Furthermore, these compounds have proven themselves to be versatile arylating agents. In this work, we combined the consideration of these applications of σ -hole donors and established the effect of charged nucleophile coordination to the σ -holes of onium salts on the regioselectivity and rate of arylation reactions.¹ The interaction of chloronium and bromonium salts with morpholine leads to the predominant formation of the *ortho*-substituted biphenyl (**Figure 1**). The addition of tetrabutylammonium fluoride to the reaction mixture alters the regioselectivity of the reaction with the chloronium salt, making the *meta*-isomer the major product. We also performed ¹H NMR monitoring of the reactions and established that fluoride significantly accelerates the reaction of morpholine with onium salts. The effect of the chloride anion on the reaction rate with the chloronium salt proved to be complex, whereas for the bromonium salt, a decrease in the reaction rate was observed in the presence of chloride. Other halides, due to high charge delocalization, bound less tightly to the σ -holes of the onium salts and did not alter the reaction rate or regioselectivity.

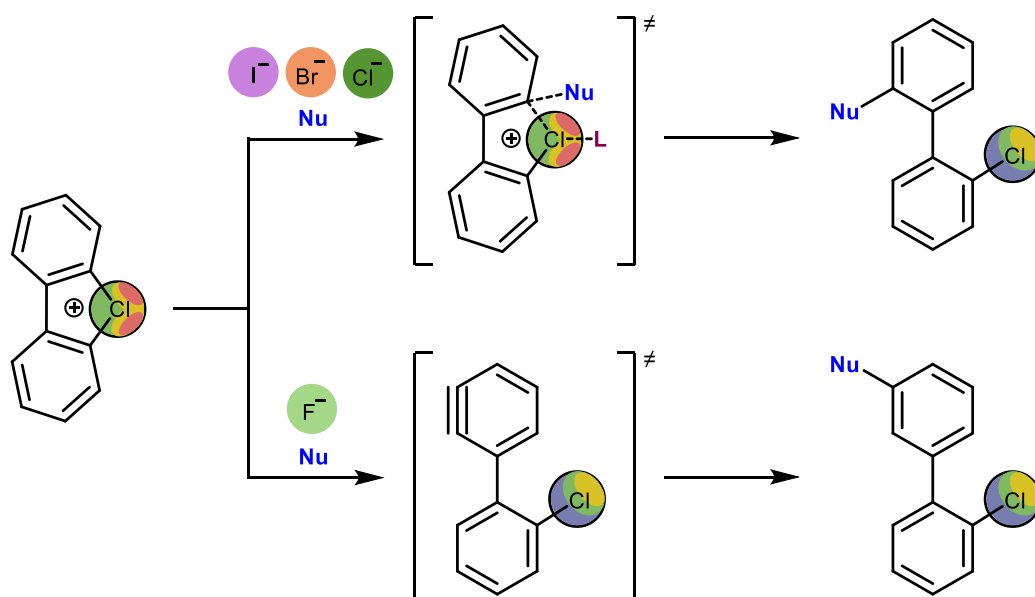


Figure 1. Regioselectivity of the arylation reaction involving chloronium salt.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Hydrogen Bonding and Ion Dynamics in Protic Ionic Liquid Probed with ^2H NMR

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Protic ionic liquids (PILs) – formed by proton transfer from a Brønsted acid to a base – are attractive for their easy synthesis and tunable properties. Hydrogen bonding between the cation and anion plays a key role in determining macroscopic properties such as viscosity and polarity, yet its influence on microscopic ion dynamics remains poorly understood.

In this work, we use variable-temperature ^2H NMR spectroscopy (113–453 K) to investigate the phase behavior and ion dynamics in a series of trialkylammonium- and trialkylphosphonium-based PILs with anions of varying basicity ($[\text{NTf}_2]^-$, $[\text{OTf}]^-$, $[\text{OMs}]^-$). The measurements are made in a broad temperature region 113–453 K that covers both solid and liquid phase. In the solid state we determine quadrupole coupling constant for deuterium located in cation and characterize melting phase transition. The cation dynamics is derived from the spin relaxation times of deuterium.

We find that anion basicity has a markedly stronger influence on ammonium ionic liquids than on their phosphonium counterparts, where hydrogen bonding is systematically weaker. The coexistence of ionic and neutral forms dramatically affects both the ^2H NMR line shape and relaxation behavior, providing new insights into the interplay between proton transfer equilibria and ion mobility. It is demonstrated that mobility in neutral form is slower by 3 orders of magnitude than in ionic state due to the clustering.

Our results demonstrate that ^2H NMR is a powerful probe of both hydrogen bonding and dynamic heterogeneity in protic ionic liquids, with direct implications for understanding structure–property relationships in this important class of ionic materials.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

From Chain Rotation to Ferroelasticity: Potassium Alkanoates C3–C6

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Potassium alkanoates KC3–KC6 possess a layered structure formed by rigid ionic potassium-oxygen layers and mobile hydrocarbon chains. The homologous series allows a gradual increase of the van der Waals contribution while keeping the ionic framework unchanged. This makes the system an ideal model for studying how the balance of non-covalent interactions governs structural dynamics and functional properties.

Using temperature-dependent powder and single-crystal XRD, crystal structures and structural transitions of the polymorphs of KC3–KC6 have been studied for the first time. In all cases, phase transitions occur without disruption of the potassium-oxygen layer – only the organic subsystem rearranges.

The key finding is a qualitative change in the dynamic regime upon chain elongation. In KC3 and KC4, van der Waals contacts between chains are still relatively weak and isotropic. The chains retain the ability to undergo conformational changes. In KC5 and KC6, the increased van der Waals contribution makes interchain contacts sufficiently strong and anisotropic to forbid rotation. The chains are forced to move collectively, synchronously changing their tilt angle relative to the potassium-oxygen layer (Fig. 1). It is this collective regime that generates spontaneous lattice strain, which manifests as ferroelasticity – the presence of a domain structure switchable by mechanical stress. An additional effect observed is the increase of thermal expansion anisotropy with chain length. The highest value of the linear thermal expansion coefficient along the chains reaches 920 MK^{-1} for KC6, indicating extreme anisotropy.

Elongation of the hydrocarbon chain in the KC3–KC6 series leads not merely to a quantitative increase in the van der Waals contribution, but to a qualitative change in the structural dynamics mechanism: from chain rotation (KC3, KC4) to collective tilt change (KC5, KC6). This change is the direct cause of ferroelasticity in the longer-chain representatives. The combination of strong anisotropic thermal expansion and switchable domain structure opens perspectives for thermal actuators, mechanical sensors, and optical devices.

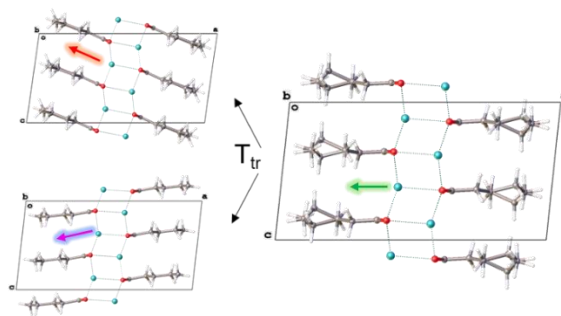


Figure 1. The ferroelastic phase transition in KC5: paraelastic phase (right) and two ferroelastic domains (left)



IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Solvation and Noncovalent Interaction Effects in Stabilizing the Molecular Structure of Etoricoxib

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The search for routes to obtain and modify solid forms of biologically active compounds requires a comprehensive understanding of the driving patterns behind the stabilization of molecular structures in various media. The relationship between the spatial structure of molecules in a saturated solution and in the crystalline phase provides opportunities for the targeted control of nucleation. In particular, during polymorphic and solvatomorphic screening, the recrystallization medium is a key factor in determining the formation of different solid forms. In this context, the study of intra- and intermolecular interactions that stabilize specific molecular structures is essential for a comprehensive understanding of solvation effects.

In the present work, a conformational screening of etoricoxib, a new-generation non-steroidal anti-inflammatory drug, has been carried out in solvents of varying polarity. Using modern quantum-chemical calculation methods and nuclear magnetic resonance spectroscopy, the influence of the solvent on the redistribution of conformer populations differing in the relative arrangement of three substituted rings- α , β , and γ (see Figure 1)-has been demonstrated. This type of conformational mobility determines etoricoxib's ability to form multiple solid forms. The obtained results are consistent with structural analyses from the Cambridge Crystallographic Data Centre database, confirming the potential of the proposed approach for the rapid assessment of the propensity to form conformation-driven solid forms.

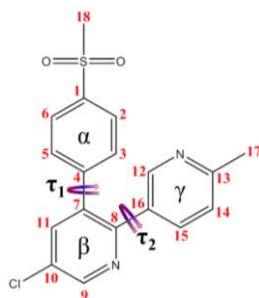


Figure 1. Molecular structure of etoricoxib with α , β , and γ ring fragments indicated.

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Influence of NHC bonding mode on reactivity of Re(I) complexes

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Previously, our laboratory developed a highly efficient catalytic system for the dehydrogenation of dimethylamine borane (DMAB) based on a Mn(I) complex containing a bidentate NHC ligand, demonstrating record-breaking performance metrics (TON = 18200, TOF = 1200 h⁻¹).¹ A detailed mechanistic study using other manganese complexes with phosphine and phosphine-carbene ligands established that the rate of this process increases with an increase in the kinetic hydricity ($\Delta G^\ddagger_{H-}$) of the hydride complexes formed *in situ*.^{1, 2} Thus, one strategy for enhancing the efficiency of the catalytic system is to increase the donor capacity of the complex's ligand environment. On the other hand, an alternative approach to increasing hydricity is the replacement of the 3d metal (manganese) with a heavier 5d metal (rhenium).³

Herein, we present the synthesis of two novel Re(I) complexes featuring a bidentate NHC ligand in both normal-normal and abnormal-normal binding modes, along with an evaluation of their catalytic performance in amine-borane dehydrogenation. Notably, the NHC coordination exerts a fundamental influence on the reactivity of the rhenium complexes in the hydride ion transfer reactions.

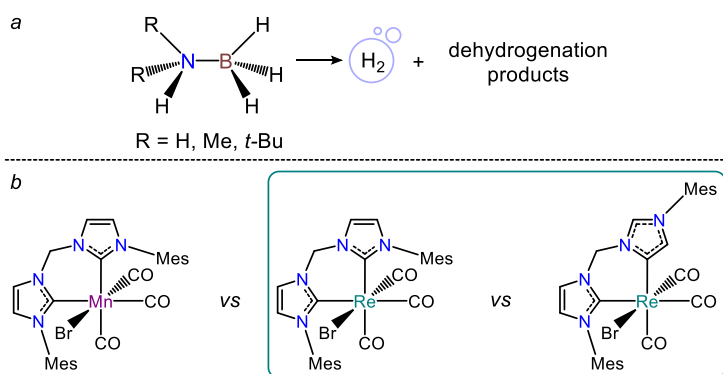


Figure 1. (a) Dehydrogenation of amine-borane; (b) objects of investigation.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Bispidinium-directed supramolecular halometallates

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This work is devoted to the study of halometallates, which are of considerable interest in modern supramolecular chemistry, with particular emphasis on compounds directed by organic cations, specifically bispidine derivatives (Fig. 1).

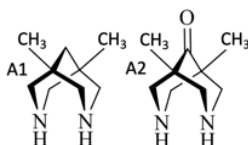


Fig.1. Structures of amines

Bispidine and its derivatives are amphiphilic amines in which a hydrophobic rigid polycyclic framework is combined with hydrophilic protonatable nitrogen atoms capable of forming directional hydrogen bonds. Owing to this dual nature, bispidinium cations efficiently organize the supramolecular environment in hybrid halometallates.

In this work, we reproducibly synthesized a series of air-stable crystalline compounds in which bispidine derivatives stabilize different types of halometallate anions: bioctahedral $[M_2X_{10}]^{4-}$ fragments ($M = Sb, Bi; X = Cl, Br$), isolated tetrahedral $[FeX_4]^-$ ($X = Cl, Br$) and $[MnBr_4]^{2-}$ anions, as well as mixed-valence bromoantimonate units. In all cases, the organic cations do not merely act as charge-compensating species but participate in the formation of hydrogen-bonded cationic substructures, including one-dimensional chains, ribbons, and more complex assemblies incorporating Br^- anions and water molecules. The network of $N-H\cdots X$, $N-H\cdots O$, and $O-H\cdots X$ interactions determines packing of the organic and inorganic substructures and stabilizes the resulting crystal architectures. The effect of introducing a keto group into the amine structure on the formation of the cationic substructure was also investigated. Antimony- and manganese-containing compounds exhibit luminescence, whereas iron-containing halometallates display antiferromagnetic ordering at low temperature; the corresponding photophysical and magnetic characteristics were investigated in this work.

The unusually low optical band gaps of the mixed-metal compounds $(A1H_2)_4[Sb^{III}_2Br_{10}(Sb^VBr_6)_2(Br)_2]$ (**1**) and $(A1H_2)[Bi^{III}Br_6Sb^VBr_6](H_2O)$ (**2**), equal to 1.27 and 1.58 eV, respectively, are attributed, according to quantum-chemical calculations, to the formation of in-gap states. The coexistence of Sb(III) and Sb(V) in compound **1** was confirmed by ^{121}Sb Mössbauer spectroscopy.

Thus, bispidinium cations act as efficient structure-directing agents, generating diverse supramolecular motifs through a system of hydrogen bonds and thereby stabilizing the crystal structures of the resulting halometallates.

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closo-B₁₂-fused carboxonium ions: synthesis and mechanistic insights

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Boron cluster compounds (*closo*-borates, carboranes, metallocarboranes) exhibit pronounced electron-donating properties, enabling them to effectively stabilize highly reactive species, including onium ions. In particular, nitrilium and oxonium derivatives of boron clusters are widely used as convenient starting platforms for constructing boron-containing functional molecules.

This work focuses on borylated carboxonium ions based on [B₁₂H₁₂]²⁻. While our earlier electrophile-induced nucleophilic substitution (EINS) approach using BF₃/AlCl₃ and carboxylic acids/esters proved limited in substrate scope,¹ we discovered that *closo*-dodecaboranyl esters [B₁₂H₁₁OC(O)R]²⁻ undergo clean intramolecular cyclization in the presence of (diacetoxyiodo)benzene (PIDA).² DFT calculations revealed that the cyclization mechanism consists globally of two steps: (1) electrophilic concerted iodination-deprotonation of the boron cage, where the *exo*-polyhedral substituent acts as an acceptor of the cluster hydrogen, followed by (2) nucleophilic attack of the carbonyl oxygen on the B–I bond to release iodobenzene and form the cyclic product. Structural features, including noncovalent intra-/intermolecular interactions, of intermediates and transition states were investigated using the QTAIM approach.

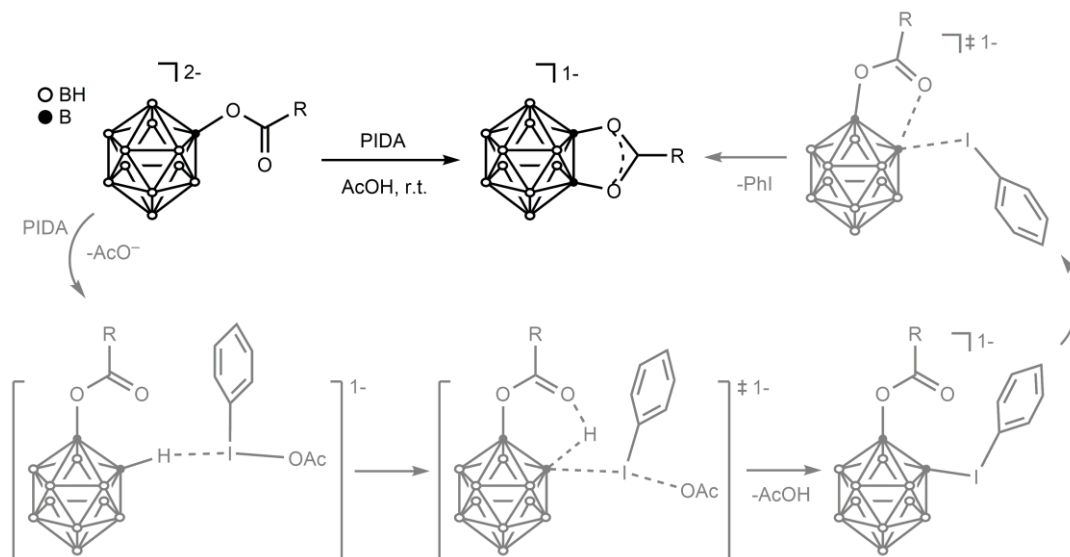


Figure 1. The formation pathway of *closo*-dodecaborate-fused carboxonium ions

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Polymer-stabilized Fe(III) complexes with poly(vinylpyrrolidone): structure, molecular-weight effects, and application against iron-deficiency chlorosis

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Fe(III) complexes with poly(vinylpyrrolidone) (PVP) and the model ligand N-methylpyrrolidone (NMP) were synthesized in anhydrous isopropanol. It was shown that NMP forms a discrete ionic pair, $[\text{Fe}(\text{NMP})_2\text{Cl}_2]^+[\text{FeCl}_4]^-$, whereas in the PVP system a polymer-stabilized structure, $[\text{Fe}(\text{PVP})_2\text{Cl}_2]^+[\text{FeCl}_4]^-$, is formed. The cationic Fe(III) center is coordinated by the carbonyl groups of PVP through the oxygen atom, while $[\text{FeCl}_4]^-$ anions are retained within the polymer matrix.

The structure of the complex was confirmed by UV-Vis, infrared, Raman, and Mössbauer spectroscopy, as well as by DFT modeling with solvent effects. The key markers of complex formation are the $\text{O}(\text{C}=\text{O}) \rightarrow \text{Fe}(\text{III})$ LMCT band, the low-frequency shift of $\nu(\text{C}=\text{O})$, Fe-O/Fe-Cl vibrations, and the presence of several types of Fe(III) centers. The iron content in $[\text{FePVP}]$ reaches a plateau of approximately 11.9 wt.%, which is consistent with the formation of a unified polymer-ionic structure.

Fe(III) complexes with PVP of different molecular weights, namely 10, 30, 40, 90, and 360 kDa, were also obtained. They were studied as agents for correcting iron-deficiency chlorosis in cucumber plants, with the $[\text{FePVP}30\text{kDa}]$ complex showing the best performance.

Using the $[\text{FePVP}]$ complex, truly zero-valent iron nanoparticles, nZVI, were obtained in solution for the first time, and their Fe(0) state was confirmed by a chemical methyl viologen assay. It was established that nZVI formation proceeds through the $\text{Fe}(\text{III}) \rightarrow \text{Fe}(\text{II}) \rightarrow \text{Fe}(\text{0})$ sequence and is described by the Erofeev-Kolmogorov topochemical model, while water and oxygen switch the system toward the formation of mixed oxide/oxyhydroxide particles $\text{Fe}^{\text{II}}_x\text{Fe}^{\text{III}}_y\text{O}_z$.

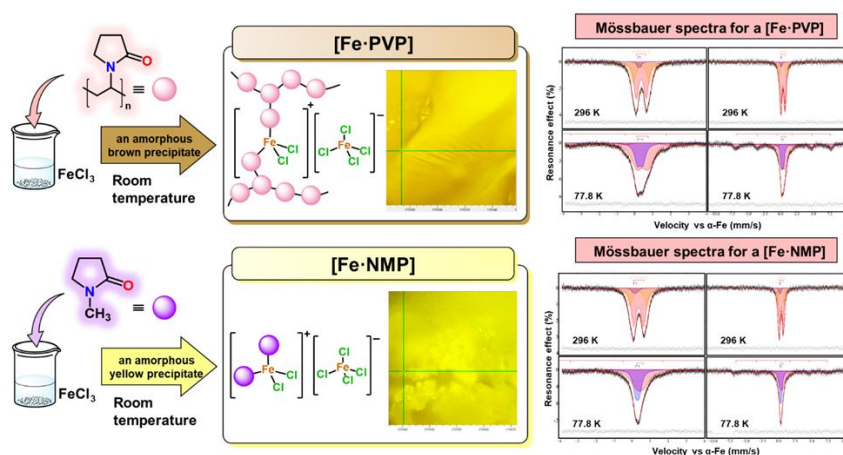


Figure 1. Structure and Mössbauer Spectra of $[\text{FePVP}]$ and $[\text{FeNMP}]$ Complexes.

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Bimetallic Sandwich Complexes Derived from Ferrocenyl Fulvenes and Cyclopentadienes

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Bimetallic catalysis, which exploits cooperative interactions between metal centers¹, represents an attractive strategy for the development of catalysts with enhanced activity and selectivity. This drives the demand for rationally designed bimetallic architectures, particularly as analogues of highly efficient monometallic systems. In this context, metallocene-based bimetallic compounds are of considerable interest as potential catalysts; however, their development remains largely limited to structures featuring multiple active sites connected by short bridging units². Current synthetic approaches are primarily focused on the design of metal-containing ligands capable of generating the target architectures upon coordination of a second metal center.

Herein, we report the synthesis of new cyclopentadienyl-type Fe/Au and Fe/Cr complexes obtained via a synthetic strategy based on ferrocenyl-substituted fulvenes. Fulvene- and cyclopentadienyl-derived ligands were coordinated to gold- and chromium-containing fragments through organolithium and organosodium intermediates. The reactivity of the resulting complexes was further investigated and, in several cases, enabled incorporation of a third metal center (Figure 1). Both covalent and noncovalent M–M interactions in these compounds, either directly observed or generated through redox processes, are currently under investigation.

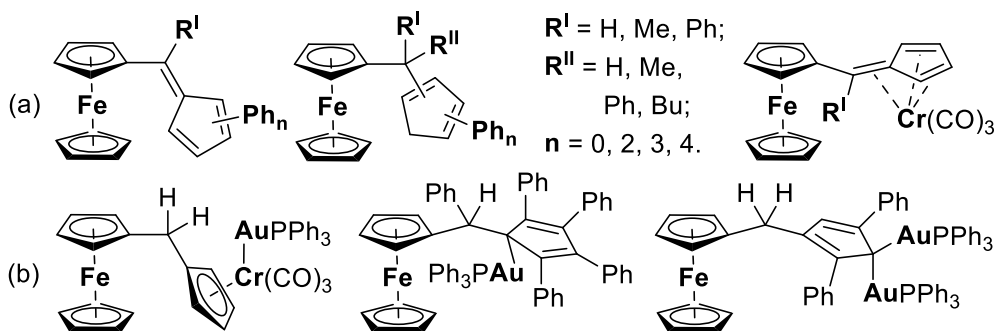


Figure 1. Ferrocenyl ligands for bimetallic complex assembly (a) and representative examples of the synthesized compounds (b).

Acknowledgements

This work was supported by the Russian Science Foundation under Project №25-73-00040, <https://rscf.ru/project/25-73-00040/>.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hybrid biomimetic catalyst based on layered Tb(III) hydroxide nanosheets and zinc porphyrinate: a first step toward abiotic glycolysis

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Biomimetic catalysis is one of the fields undergoing the most intensive development in the sphere of catalytic processes. The main advantage of this approach is the combination of the high catalytic activity of natural enzymes with the stability and availability of synthetic materials. The use of biomimetic catalysts ensures environmental friendliness and high efficiency and selectivity under normal or near-physiological conditions. These factors highlight the importance of developing strategies to produce materials capable of mimicking key biochemical transformations such as glycolysis, and of implementing cascade and cyclic catalytic and photocatalytic processes. Hybrid biomimetic systems are a promising solution because they combine the photocatalytic properties of an organic component with the catalytic properties of an inorganic matrix, offering potential synergy of these properties.

In this work, zinc tetracarboxyphenylporphyrinate (ZnTCPP), which is renowned for its photocatalytic activity and serves as a receptor analogue, was chosen as the basis for the metal-organic framework (MOF). Nanosheets of layered terbium(III) hydroxochloride (LTb(III)H), which exhibit catalytic and optical properties, were employed as the inorganic template. We obtained the hybrid material SURMOF/LTb(III)H using the non-covalent self-assembly method. The obtained material has the potential to exhibit the properties of both a heterogeneous photocatalyst and an artificial enzyme.

We demonstrated that two-dimensional LTb(III)H particles obtained via liquid-phase exfoliation in a 2-methylimidazole solution can act as an inorganic matrix for assembling ordered hybrid structures by integrating a SURMOF based on ZnTCPP and Zn(OAc)₂ onto their surface. The resulting SURMOF/LTb(III)H hybrid catalyst is highly effective in biomimetic dephosphorylation reactions, as demonstrated using the model substrates bis-nitrophenyl phosphate and ATP. The hybrid material also exhibits photocatalytic activity, generating singlet oxygen upon irradiation in the UV-visible range, as demonstrated in the photodegradation of rhodamine 6G. These findings confirm the promising potential of this hybrid material as a photo- and biomimetic catalyst in various processes, including the implementation of abiotic glycolysis under anaerobic conditions.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Synergistic effect in hybrid photocatalytic material based on quasi-two-dimensional MoS₂ particles and layered Tb³⁺ hydroxide integrated with zinc porphyrinate

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Increasing anthropogenic pollution of water and the atmosphere by persistent organic compounds is a pressing environmental issue of our time. This drives the need for powerful and versatile photocatalysts capable of degrading various classes of pollutants, especially under visible light, for which classical semiconductor materials are unsuitable.

The creation of hybrid materials that combine the mechanical and semiconducting properties of inorganic compounds with the optical properties of organic chromophores, leveraging the synergy of the components, represents a rational and actively explored approach for developing modern photocatalysts. Despite the popularity of this approach, most research focuses on the functional properties of the materials, often neglecting the search for the fundamental causes of the synergistic effect.

In this work, following a method previously developed by us¹, a new hybrid material was synthesized based on quasi-two-dimensional MoS₂ particles mechanically doped, using a previously described method², with layered Tb³⁺ hydroxide (LTbH), integrated with a surface metal-organic framework of zinc porphyrinate (SURMOF). The resulting material, MoS₂/LTbH/ZnTCPP SURMOF, was characterized by a wide range of complementary analytical techniques for structure and composition. Thanks to the integration of all components, the hybrid exhibited outstanding photocatalytic activity in the photodegradation reactions of several persistent compounds, including 2,6-dichlorophenol and the antibiotic levofloxacin. The key result of this work is a comprehensive explanation of the principles underlying the synergistic effect and the establishment of interaction mechanisms between the components of the hybrid system.

Acknowledgements

The work was supported by the Russian Science Foundation (grant No. 23-73-00095).

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Coinage bonding between Group 11 and Group 10 Metals

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Group 11 coinage metals engage in specific directional bonds with electron-rich partners such as π -electron systems. Here, we demonstrate an example of coinage bonding between Pt(II)/Pd(II), whose diffuse d_{z^2} orbitals are capable of acting as electron donors,¹ and Cu(I)/Ag(I) ions in cyclic pyrazolates [AgPz]₃. (Fig.1a) Owing to the electron-withdrawing -CF₃ groups on the pyrazolate ligands, these group 11 complexes function as π -hole donors at the linearly coordinated N–M–N metal centers.^{2,3} A series of bimetallic assemblies was synthesized and fully characterized. X-ray diffraction analysis reveals intermolecular M...M distances that are substantially shorter than the sum of the van der Waals radii, yet longer than typical covalent bonds. NMR spectroscopy confirms that the intermolecular interactions persist in the solution. A comprehensive theoretical analysis confirms the electron-accepting role of the group 11 metal centers. (Fig.1b) Collectively, these data demonstrate that the coinage bond constitutes a real, measurable, and structurally directive noncovalent interaction.

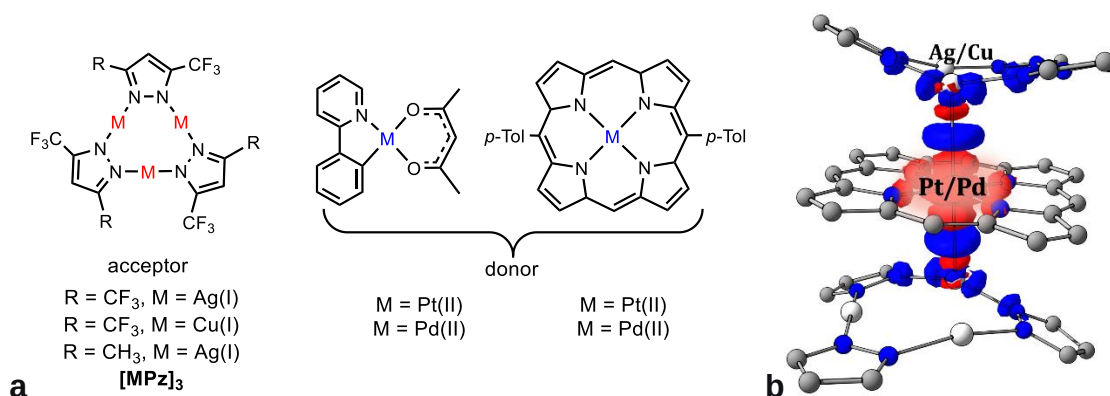


Figure 1. Schematic representation (a) and NOCV-based deformation density channels for adduct of Pt(II) or Pd(II) with [MPz]₃ (b).

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Secondary bonding interactions for molecular magnetism: rare double hysteretic magnetic bistability in π -complex of fluorocarbon 1,3,2-benzodithiazolyl with naphthalene

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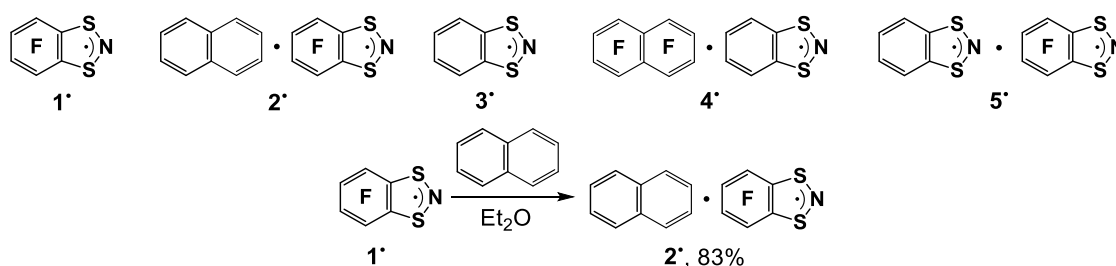
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Solid 1,3,2-benzodithiazolyl radicals exhibit magnetic bistability, which can be tuned by secondary bonding interactions (SBIs).¹ Cocrystallization of radicals **1**[•] and **3**[•], and that of the radicals and C₁₀R₈ (R = H, F), was studied. π -Complex **2**[•] was prepared, whereas preparations of complexes **4**[•] and **5**[•] failed (Scheme 1).



Scheme 1. Radicals **1**[•] and **3**[•] together with complexes **2**[•], **4**[•] and **5**[•].

Crystalline **2**[•] displayed three temperature-dependent polymorphs, two of which were structurally defined by XRD to disclose arene-polyfluoroarene π -stacking, together with interstack F $\cdots$ H and N $\cdots$ N SBIs. In the 256–266 and 140–182 K ranges, two hysteretic magnetic transitions were observed involving in the last case partial dimerization of **1**[•] radicals via N $\cdots$ N SBIs (Figure 1).

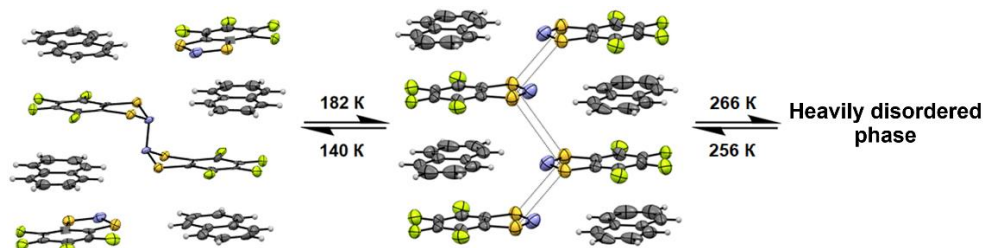


Figure 1. Hysteretic magneto-structural transitions in complex **2**[•].

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Rational design of functional complexes with 3d-/4f-metal ions based on 1,3-disubstituted derivatives of (thia)calix[4]arenes

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Coordination compounds based on 3d- and 4f-metal cations are of interest due to the combination of their diverse functional properties, such as single molecular magnetism (SMM)¹ and luminescence², and have potential applications in quantum spintronics, the development of new luminescent materials, and catalysis³.

(Thia)calix[4]arenes are an attractive macrocyclic platform for the creation of coordination compounds whose functional properties can be tuned by varying the nature and conformation of the macrocycle⁴, functionalization of the lower rim, including the introduction of Schiff bases^{5,6}, and spacers of varying lengths⁷.

This paper presents the synthesis and structure of new Co^{II,III}, Fe^{III}, Cu^{II}, Ln^{III} (Ln = Dy, Tb, Er) complexes based on 1,3-disubstituted derivatives of (thia)calix[4]arenes functionalized with salicylideneamine coordinating centers⁸.

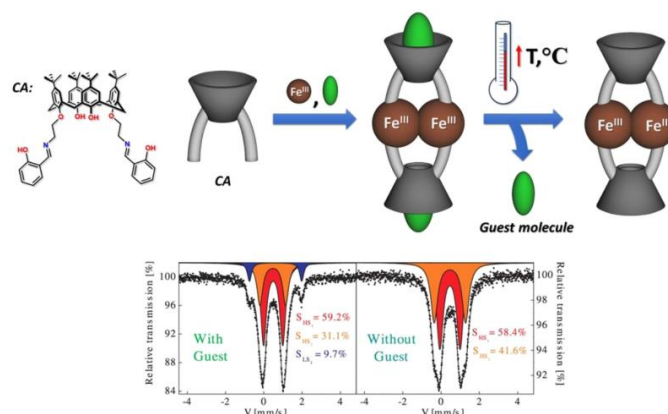


Figure 1. First evidence of a guest-induced spin transition for a binuclear Fe(III) complex based on calix[4]arene functionalized with Schiff bases.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Linear Dichroism in Crystals of Nitronyl Nitroxide Radicals

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Linear dichroism is a fundamental optical phenomenon characterized by the anisotropic absorption of linearly polarized light, which manifests as orientation-dependent color variations. This intrinsic property supports a wide range of technological implementations, including nanophotonic components, high-performance polarizing filters, and environmentally responsive materials. Recent advances have further extended its utility to precision analytical platforms and biomedical imaging modalities.

Despite considerable progress in the development of dichroic media, studies on organic compounds have largely been restricted to closed-shell molecular architectures. By contrast, nitronyl nitroxide radicals have emerged as highly promising candidates for photonic applications, owing to their exceptional chemical stability and well-defined crystallization behavior. The synergistic combination of spin-mediated magnetism, reversible redox activity, and intense visible-region absorption establishes a versatile framework for transducing external stimuli into coupled optical, electronic, and magnetic responses. Such multifunctionality offers considerable potential for advancing next-generation smart materials.

Herein, we report the first systematic investigation of linear dichroism in crystalline nitronyl nitroxide derivatives. Six radical compounds were synthesized and thoroughly, followed by a combined structural and optical analysis utilizing single-crystal X-ray diffraction (XRD) and polarization-dependent absorption spectroscopy. By clarifying the structural origins of this anisotropic behavior, we anticipate that our findings will guide the rational design of advanced functional materials engineered for multi-stimuli responsiveness.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Role of Non-Covalent Interactions in the Mechanism of Ciprofloxacin Degradation by Mesoporous Magnetite-Based Catalysts Modified with Humic Acids

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The development of heterogeneous Fenton-type catalysts based on magnetite (Fe₃O₄) for the oxidative degradation of recalcitrant pharmaceutical pollutants, such as ciprofloxacin (CIP), requires not only a high density of active sites but also optimized sorption driven by directional non-covalent interactions. In this study, pristine magnetite nanoparticles (M), humic acids-modified magnetite (HAM), and magnetite formed in statu nascendi on a mesoporous aminosiloxane matrix without/with HA (TAM and TAHA-M)¹ were investigated to elucidate the contribution of various types of forces to sorption and catalytic efficiency.

According to FTIR spectroscopy data, the immobilization of HA onto the M and TA matrix surfaces occurs through Fe–O–Si bonds and multiple bonds involving –COOH, –OH, and –NH₂ groups. Analysis of low-temperature N₂ adsorption isotherms within the Dubinin–Radushkevich and Frenkel–Halsey–Hill models revealed that the characteristic adsorption energy is consistently below 8 kJ/mol (ranging from 3.67 to 4.87 kJ/mol), unequivocally indicating a physical, non-covalent nature of the primary binding. The surface fractal dimension (D_f) increases from 2.48 (M) to 2.60 (TAHA-M), reflecting enhanced geometric irregularity and a greater number of accessible sites for weak interactions.

Maximum sorption (54 mg/g at pH 9) occurred on HAM despite its low surface area, due to combined electrostatic, π - π , hydrophobic, and H-bonding interactions.² TAM exhibited weak sorption (<12%), maximizing Fe²⁺/Fe³⁺ site accessibility. Catalytic CIP degradation (100 mM H₂O₂) revealed competition between sorption and oxidation. TAM removed 84% at pH 5 and 67% at pH 9, up to 8-fold over sorption alone. Kinetics followed a two-stage process. HA-modified systems retained CIP near the surface via strong non-covalent interactions but partially blocked iron sites, reducing •OH generation. HA chelation suppressed Fe leaching (<3 wt.%).

These results indicate that the sorption and catalytic behavior of the composites is largely governed by the balance between non-covalent interactions and active site accessibility. While the minimally modified TAM exhibits the highest catalytic performance due to unrestricted access to iron centers, the incorporation of HA effectively suppresses iron leaching through chelate formation, albeit with some trade-off in activity.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hydrogen bond activated hydrogen peroxide coordination to In(III)

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Hydrogen peroxide is a weak ligand that typically does not form stable complexes with metal ions in polar solvents, including water. The investigation of complexation between indium trichloride and anhydrous H₂O₂, used both as a reagent and solvent in the presence of 18-crown-6, as well as in a diethyl ether solution, resulted in the isolation of several new indium(III) hydrogen peroxide complexes [InCl₃(H₂O)₂(H₂O₂)]·18-crown-6, [InCl₂(18-crown-6)][(H₂O₂)InCl₄] and [fac-InCl₃(H₂O₂)_{0.5}(H₂O)_{0.5}(18-crown-6)]. Despite being a weaker ligand than 18-crown-6 or diethyl ether, H₂O₂ displaces both from the coordination sphere of In(III). To investigate this phenomenon, we performed ¹H NMR experiments at different temperatures and DFT calculations, assuming that hydrogen bonding between H₂O₂ and diethyl ether modifies the properties of H₂O₂.

The ¹H NMR signal of H₂O₂ in 0.03 M solution in Et₂O (Fig. 1A) is broadened and asymmetric at 25–0 °C and becomes more complex upon cooling to –40 °C, accompanied by a downfield shift (9.73 to 10.04 ppm). This is probably a result of H₂O₂ self-association and/or its hydrogen bonding with diethyl ether.

DFT calculations performed using dimethyl ether (Me₂O) and diethyl ether (Et₂O) as model ethers for H-bonded H₂O₂·ether adducts demonstrated that H-bonding through an OH group proton increases the basicity of the participating oxygen atom in H₂O₂. For example, molecular electrostatic potential (MEP) minimum for O₂H₂···2(OMe₂) adduct on H₂O₂ oxygen atom is –56.1 kcal/mol, whereas MEP minimum for isolated H₂O₂ and Me₂O is –33.4 and –35.5 kcal/mol respectively. Thus, hydrogen bonding activates H₂O₂, making it a stronger Lewis base and enabling competitive coordination to In(III).

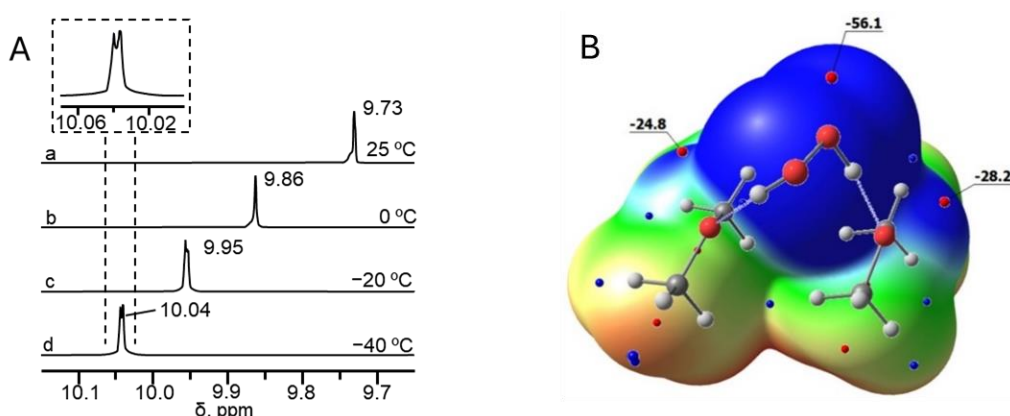


Figure 1. (A) Fragments of ¹H NMR spectra of H₂O₂ in Et₂O (0.03 M) at different temperatures and (B) the molecular electrostatic potential (MEP) surface at 0.001 a.u. for hydrogen bonded complex of H₂O₂ with two Me₂O molecules.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hydrogen-Bonded Adducts of dpp-bianH₂ with N-Heterocycles

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The design of hydrogen-bonded organic frameworks (HOFs) requires organic donor–acceptor blocks with preorganized hydrogen-bonding geometry. Among promising platforms, derivatives of the redox-active ligand dpp-bian have been considered, yet the metal-free reduced form — N,N'-bis(2,6-diisopropylphenyl)acenaphthylene-1,2-diamine (dpp-bianH₂) — remained the least explored in this context. We have previously shown that enediamine is an effective reductant, capable of reducing molecular oxygen to H₂O₂,¹ but its ability to form directional non-covalent interactions has not been systematically investigated.

In this work, we obtained a series of monomeric adducts of dpp-bianH₂ with nitrogen-containing heterocycles (DBU, 2,2'-bipyridine, pyridine, and pyrazine), in which the components are held together by intermolecular N–H···N hydrogen bonds. All compounds were characterized by elemental analysis, NMR and IR spectroscopy, and their molecular structures were determined by single-crystal X-ray diffraction. These results expand the set of organic building blocks for HOFs and demonstrate the potential of redox-active ene-1,2-diamines in supramolecular design.

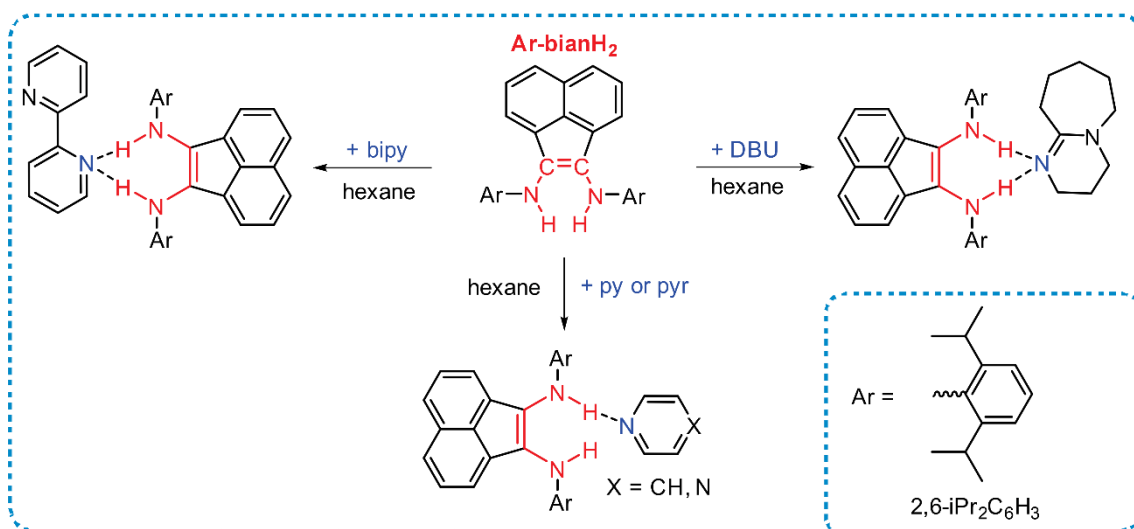


Figure 1. Formation of hydrogen-bonded adducts of dpp-bianH₂ with N-containing heterocycles.

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The research was conducted within the framework of a Russian state assignment, with experimental measurements performed at the «Analytical Center of the IOMC RAS».

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Photocatalytic activity of nanocomposites based on two-dimensional nanoparticles of molybdenum disulfide and layered Tb³⁺ and Eu³⁺ hydroxides

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This work introduces a new approach to fabricating semiconductor nanocomposite photocatalysts that are active in the visible spectrum, using a mechanochemical doping method.¹ Chemically pure monolayer nanoparticles of layered Tb³⁺ and Eu³⁺ hydroxides (LTbH and LEuH), as well as molybdenum disulfide (MoS₂), were obtained via liquid-phase exfoliation in a 2-methylimidazole solution. The LTbH and LEuH nanoparticles act as doping agents, enabling the introduction of Tb³⁺ and Eu³⁺ ions as single-atom centres on the surface of molybdenum disulfide (MoS₂) nanosheets through ultrasonic or mechanical treatment. The defective structure of the hydroxide nanosheets ensures efficient ion transfer, thereby preventing the formation of a Tb- and Eu-rich bulk phase, as would occur with soluble Tb and Eu salts. The resulting LTbH/MoS₂ and LEuH/MoS₂ nanocomposites exhibit tenfold greater photocatalytic activity in the Rhodamine 6G photodegradation model reaction than pristine MoS₂ upon UV excitation. In contrast to the LEuH/MoS₂ nanocomposite, which is only active upon UV excitation, the LTbH/MoS₂ nanocomposite exhibits activity in both the UV and visible light spectral regions. This is consistent with time-resolved photoluminescence spectroscopy data indicating a longer excited-state lifetime in the visible region compared to LEuH/MoS₂. Doping several other semiconductors (TiO₂, BN and graphene oxide) also yielded nanocomposites with photocatalytic activity in the visible range, confirming the versatility of the proposed method. Therefore, these results reveal the potential for using Tb³⁺ as a universal dopant in the preparation of a wide range of semiconductor nanocomposite photocatalysts active in the visible spectrum.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Geometric and quantum-chemical approaches to evaluating intermolecular interactions

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The widespread use of ionic liquids in the extraction of U(VI) and the lack of knowledge of the possibilities of interaction in aqueous systems containing quaternary ammonium base cations, uranyl cations, and carboxylate ions as ligands has become a determining factor in the synthesis and study of new uranyl methacrylate complexes with trimethylbenzylammonium and triethylbenzylammonium cations of the composition $R[UO_2(C_4H_5O_2)_3]$, where $R = (CH_3)_3BzN^+$ (I) or $(C_2H_5)_3BzN^+$ ($Bz = C_6H_5CH_2$) (II).

The calculation of all possible non-valent interactions that play a crucial role in the formation of a three-dimensional framework was carried out using the molecular Voronoi-Dirichlet polyhedra (MVDP) method. According to the data obtained, 6 (I) and 4 (II) out of 15 theoretically possible types of intermolecular contacts are realized in crystals I and II containing atoms of five chemical elements. The main binding of molecular fragments into a three-dimensional network occurs due to H/O dipole-dipole interactions with a partial contribution over the area of the MVDP faces corresponding to all intermolecular contacts in 29.4% (I) and 32.1% (II), and dispersion interactions (H/H and H/C contacts) with a contribution of 68.7% (I) and 67.0% (II).

A comparison of the MVDP method with the Hirschfeld surface method is shown in Table 1. As in our previous work¹, both methods demonstrate similar qualitative and quantitative characteristics of intermolecular contacts.

Table 1. Comparison of MVDP methods and Hirschfeld surfaces in structures I and II

Contact type A/Z	I		II	
	Δ_{AZ} , % MVDP	Δ_{AZ} , % HS	Δ_{AZ} , % MVDP	Δ_{AZ} , % HS
O/O	1.4	0.8	-	-
C/O	0.3	0.6	-	-
H/O	29.4	28.4	32.1	35.2
C/C	0.2	-	0.9	-
H/C	10.8	8.8	15.1	11.5
H/H	57.9	61.3	51.9	53.2
Sum	100	99.9	100	99.9

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

KEY ROLE OF INTERMOLECULAR π -STACKING IN FORMATION OF 3d-METAL COMPLEXES BASED ON *o*-XYLYLENEDIAMINE SUPPORTED SALEN-TYPE LIGANDS

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Nowadays, there is a still growing interest in design of new molecular catalysts, sensors, magnetic switches with controlled structure and functions^{1–3}. One of the feasible approaches is based on the usage of the metal organic complexes, based on salen-type ligands. These fascinating compounds display a wide range application, due to high synthetic availability and modulation ability. In general, by varying the spacer group flexibility, the nature of the grafted substituents and the metal ion, one can adjust the molecular structure, crystal packing of corresponding M-salen complexes.

In this work, we firstly report on the formation of the M-salen like complexes which coordination motif was controlled using the noncovalent intermolecular π -stacking in the crystalline phase. For this purpose, a new salen-type ligand, obtained using the *o*-xylylene spacer group between two salicylideneamine moieties, was specially designed. As a result, the complexes with unprecedented M/L stoichiometries 2/1 were generated for this class of compounds^{4–5}.

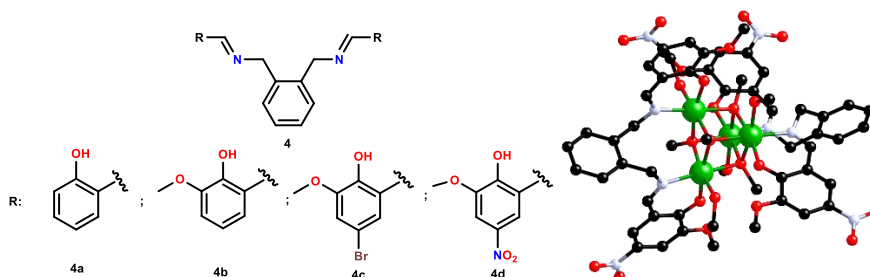


Figure 1. Structure of target Schiff bases **4a-d** and the structure of the complex based on the Ni^{II} cation and ligand **4d**

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Effect of cation nature on catalytic performance of Zr/Hf-substituted polyoxometalates in H₂O₂-based selective oxidation

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Polyoxometalates (POMs) substituted with zirconium(IV) or hafnium(IV) ions are promising catalysts for the selective oxidation of organic substrates using the green oxidant – aqueous hydrogen peroxide. Such metal-oxide-like anionic metal-oxygen clusters exhibit high resistance to oxidation and hydrolysis and can serve as molecular models for studying oxidation mechanisms [1]. The aim of this work was to investigate the influence of cation nature (tetrabutylammonium, TBA, or tetrahexylammonium, THA) on the catalytic properties of Zr- and Hf-monosubstituted Keggin-type polyoxotungstates $Q_{8-x}H_x[PW_{11}O_{39}M(OH)]_2$ ($Q = TBA$ or THA , $M = Zr$ or Hf) in the oxidation of alkenes of various structures with aqueous H₂O₂.

A series of TBA and THA salts of Zr(Hf)-POM was synthesized, namely $TBA_8[PW_{11}O_{39}Zr(OH)]_2$ (TBA-Zr), $TBA_{7.5}H_{0.5}[PW_{11}O_{39}Hf(OH)]_2$ (TBA-Hf), $THA_8[PW_{11}O_{39}Zr(OH)]_2$ (THA-Zr), and $THA_{7.5}H_{0.5}[PW_{11}O_{39}Hf(OH)]_2$ (THA-Hf), following a literature procedure [2] and characterized by IR spectroscopy, ³¹P and ¹⁸³W NMR, elemental and thermal analysis, and potentiometric titration.

The interaction of the TBA and THA salts of Zr(Hf)-POM with H₂O and H₂O₂ was studied by FT-IR-ATR and HR-ESI-MS, respectively. It was found that replacing the TBA cation with THA promotes monomerization of the initial dimeric polyanion in CH₃CN solution and favors the formation of hydroperoxo species. THA salts exhibit higher activity as compared to their TBA analogues in the non-productive decomposition of H₂O₂, which is consistent with the assumption that THA cations promote the transformation of the POM dimer to the more active monomeric form.

Studies on the catalytic oxidation of cyclohexene, limonene and 1-octene with H₂O₂ revealed that the effect of the cation (as well as heterometal) nature depends on the specific alkene substrate. For cyclohexene, higher epoxide selectivity (76% at 36% conversion) was achieved in the presence of THA-Hf while, for epoxidation of octene-1, TBA-Zr and TBA-Hf showed clear advantages over THA-salts. The obtained data indicate an increase in the electrophilicity of the active peroxo species upon switching from TBA to THA cation. The results acquired can serve as a basis for the rational design of efficient homogeneous oxidation catalysts based on POMs.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Noncovalent Interactions in the Crystal Structure of $\text{UO}_2(\text{BrCH}_2\text{CH}_2\text{COO})_2$

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A structural study of the new anhydrous complex $\text{UO}_2(\text{BrCH}_2\text{CH}_2\text{COO})_2$ was carried out. The compound is built from infinite polymeric chains in which the U atom has a coordination number of 7, including the two axial O atoms of the uranyl group. Half of the bromopropionate ions act as bidentate bridging ligands, while the other half function as monodentate bridging ligands. To establish the nature of the interchain interactions governing the packing of the polymeric chains, three approaches were applied: the method of molecular Voronoi–Dirichlet polyhedra¹ (**MVDP**), non-covalent interaction analysis² (**NCI**), and **QTAIM** analysis³.

The **MVDP** approach made it possible to quantitatively estimate the contributions of different intermolecular contacts to the total Voronoi–Dirichlet surface. The dominant contribution arises from dispersive H/C contacts (24.3%) and H/Br interactions (10.9%), whereas direct Br/Br contacts make only a negligible contribution (1.3%). The **NCI** analysis indicated the predominance of weak van der Waals, mainly dispersive, interactions involving the methylene groups, while the geometry of the C–Br $\cdots$ Br contacts ($\angle 145^\circ$) is unfavorable for the formation of classical σ -hole halogen bonds. The **QTAIM** topological analysis of the electron density revealed a pronounced charge asymmetry between the two crystallographically independent bromine atoms. Regions of negative Laplacian of the electron density in the valence shell of Br(1) indicate localization of electron density associated with lone pairs, making this atom capable of forming directional weak electrostatic contacts with H atoms of neighboring chains.

Thus, it was shown that the introduction of a Br atom into the carboxylate ligand does not lead to the predominance of halogen bonding, but rather redistributes the balance of intermolecular forces toward dispersive and weak electrostatic H/Br contacts, which determine the supramolecular architecture of the complex.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

New di- and tripodal heterocyclic *N*-donor ligands based on *bis*- and *tris*(triazolylethyl)amines for 3*d*-metal complexes formation

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Complexes of 3*d*-element cations with *N*-donor ligands based on 1*H*-1,2,3-triazoles offer significant potential for the development of functional materials¹. The synthesis of such novel coordination compounds enables the production of various crystalline materials with tunable catalytic, magnetic, luminescent, and adsorption properties². Therefore, developing rational approaches to ligand design — specifically those that influence the structural motif, coordination geometry, and resulting properties of the complexes — is of crucial importance.

This work focused on a rational design of new *N*-donor ligands featuring 1*H*-1,2,3-triazole groups as coordinating centers, which are linked by a bis- or tris(ethanediyl)amine platform, which displaying a particular coordination ability with the used 3*d* metal cations. The corresponding *bis*- and *tris*-1*H*-1,2,3-triazole derivatives bearing –Ph, α-Py, β-Py, or pyrazolyl substituents at the C4 position of the triazolyl ring were successfully synthesized (Fig. 1a). Novel 0*D*–3*D* coordination assemblies were formed, when they were involved in interaction with Co(II), Fe(II), Cu(II) ions (Fig. 1b). Their structures were established using single-crystal X-ray diffraction analysis. General factors influencing on the formation of coordination compounds were thorough studied.

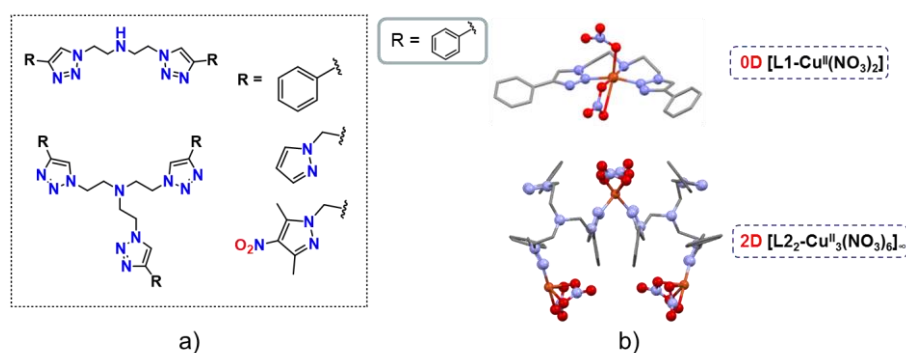


Figure 1. a) target *N*-donor ligands are derivatives of *bis*- and *tris*-1*H*-1,2,3-triazoles b) 0*D* and 2*D* coordination compounds based on L1 and L2 with Cu(II) cations

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Synthesis and structural studies of *trans*-[CuX₂(NCNR₂)₂]·2HaB complexes (X = Cl, Br; HB = 1,4-C₆I₂F₄, 1,3,5-C₆I₃F₃)

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The work is devoted to the study of new cocrystal structures derived from copper(II) halides, dialkylcyanamides (NCNR₂, R₂ = Me₂, Et₂, C₅H₁₀) and halogen bond (HaB) donors. In this context, new cocrystals bearing square-planar copper(II) *trans*-[CuX₂(NCNMe₂)₂]·2HaB (HaB = 1,4-C₆I₂F₄, 1,3,5-C₆I₃F₃) were obtained, the structural features of these compounds were determined, and structure-determining non-covalent interactions were identified on geometric criteria and quantum-chemical calculations. The influence of the solvent and the nature of the R substituent in the NCNR₂ ligand on the feasibility of cocrystal formation were systematically investigated. The potential for forming bifurcate contacts, as well as σ - and π -hole bonds involving HaB donors was evaluated. The possibility of the metal center acting as a nucleophile in p-hole interactions with perfluoroarenes were also assessed. Such interactions may contribute to the stabilization of less common square-planar copper(II) complexes – similarly to what is observed in cocrystals of palladium(II) or platinum(II) complexes with dialkylcyanamides and HaB donors.^{1,2}

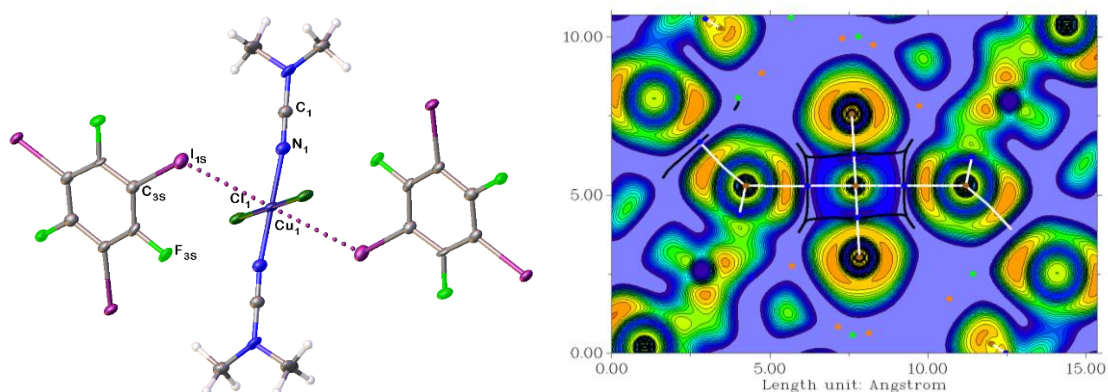


Figure 1. The structure of [Cu(II)*trans*-Cl₂(NCNMe₂)₂]·2(1,3,5-C₆I₃F₃) and calculated Cu-I interactions by Hirshfeld surface analysis

Acknowledgements

This work was supported by the Russian Science Foundation (project № 25-13-00035)

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Cage-like nucleophiles in supramolecular design of exchange coupled systems

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Molecular magnets are promising building blocks for next-generation computing and storage materials, however, the precise control of their magnetic properties remains a challenge that could be addressed by direct intermolecular interactions like halogen bonding (XB).^{1–3}

Cage-like nucleophiles could provide structural diversity to supramolecular assemblies as well as intriguing physical properties. This observation was previously established in our work where a substantial enhancement of the exchange interaction was observed upon incorporating 1,4-diazabicyclo[2.2.2]octane molecule into supramolecular architecture.³

In the present work we have investigated 1,3,5,7-tetraazaadamantane and 1,3,5-triaza-7-phosphaadamantane as Lewis bases in supramolecular systems with a spin-labeled XB donor. Variation of solvents and the component ratio allowed us to conduct crystal screening, revealing a cocrystal with sufficient exchange interaction strength (Figure 1).

While the resulting magnetic properties require further tuning and study, the investigation identifies nucleophiles with exposed lone pairs as promising XB acceptors for supramolecular design of exchange-coupled systems.

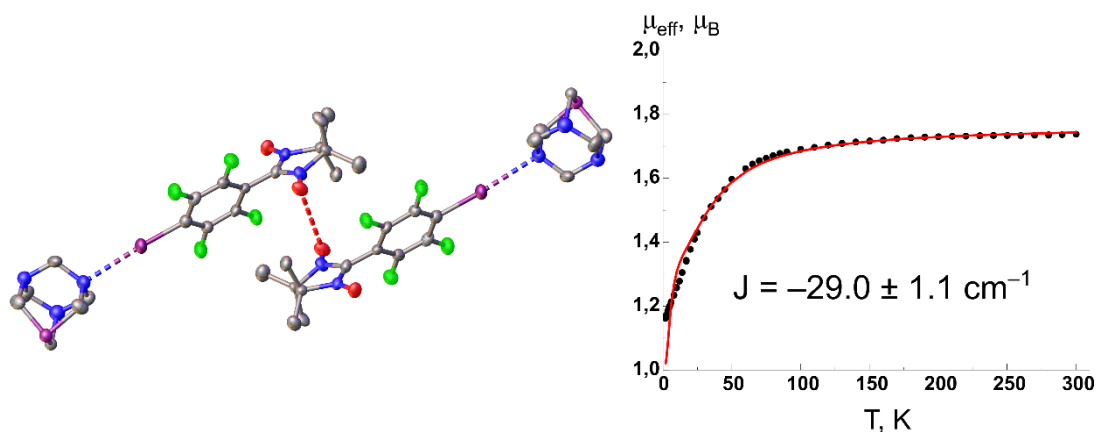


Figure 1. Crystal structure and experimental temperature dependence of the effective magnetic moment μ_{eff} of the new cocrystal. Fitting curve is shown as red solid line.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

The role of hydrogen bonds in enhancing the coordination of hydrogen peroxide with tin(IV)

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Interaction between tin tetrachloride and H₂O₂ has previously been studied using ¹¹⁹Sn and ¹⁷O NMR spectroscopy, and new complexes formed upon the addition of 18-crown-6 ether to SnCl₄–H₂O₂ and H₂O₂ with H₂O systems were structurally characterized.¹

In the present work, we synthesized hydrogen peroxide complexes with organotin chlorides to investigate the relationship between the Lewis acidity of the coordination center and the strength of the coordination bond. In these complexes, we tuned the Lewis acidity of the Sn(IV) center by varying the number of electron-accepting chloride ligands and the nature of the organic fragment. A direct correlation was established between the total energy of two hydrogen bonds formed by the H₂O₂ ligand and the length of the Sn–O coordination bond: a higher total hydrogen-bond energy corresponds to a shorter Sn–O distance. In the series of aryl organotin chlorides, a shortening of the Sn–O distance was observed when moving from [Ph₃SnCl(H₂O₂)] to [*p*-Tol₃SnCl(H₂O₂)], contrary to expectations that decreasing the acidity of the metal center would lead to an increase in the Sn–O distance in the hydrogen peroxide complex. This behavior can be explained by a synergistic effect of hydrogen bonding involving both the solvated and the Sn(IV)-coordinated hydrogen peroxide molecules, as well as the crown ether present in the compound.

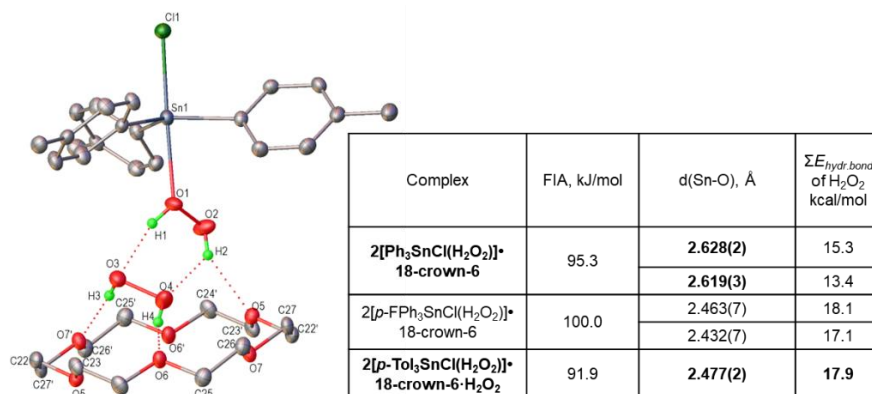


Figure 1. The asymmetric unit in the crystal structure of [*p*-Tol₃SnCl(H₂O₂)]·18-crown-6·H₂O₂. The inset on the right shows a table with the data obtained for the synthesized H₂O₂ complexes with aryl organotin chlorides.

Acknowledgements

This work was supported by the Russian Science Foundation (grant no. 22-13-00426-Π).

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FLASH PRESENTATIONS



Phosphine Oxides as a Probe of Total Hydrogen Bond Strength

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Phosphine oxides are known for their exceptional sensitivity to hydrogen bonding, making them valuable molecular probes for characterizing these interactions. The P=O group exhibits a highly sensitive spectroscopic response that enables measurable NMR parameters to be directly correlated with the underlying geometries of hydrogen bonds, thereby allowing a detailed assessment of hydrogen bond strength.¹

The distinctive response of the P=O group arises from the high sensitivity of the ³¹P nucleus,² whose chemical shift undergoes substantial changes upon the formation of non-covalent interactions.^{3,4} Historically, phosphine oxides have been employed in ³¹P NMR spectroscopy as probes to characterize the electron-withdrawing properties of solvents and other compounds with Lewis acidity,⁵ as well as the proton donating ability of compounds with Brønsted acidity.³ Predicted ³¹P chemical shifts of phosphine oxides have also been used to theoretically estimate the strength of noncovalent interactions.^{6,7}

In this work, experimental ³¹P NMR chemical shifts of triphenylphosphine oxide are used to evaluate the strength of P=O...H-O hydrogen bonds. Complexes containing one or two hydrogen bonds formed between Ph₃P=O and 24 substituted phenols were investigated by liquid-state NMR spectroscopy in a polar aprotic solvent (liquefied freonic mixture, CDF₃/CDF₂Cl) at low temperature (100 K). We show that the change in the ³¹P chemical shift upon complexation, ΔδP, correlates strongly with the overall strength of all hydrogen bonds formed at the P=O group. Thus, ΔδP serves as a reliable spectroscopic indicator for estimating total binding energies in phosphine oxide systems.

Furthermore, using DFT calculations with implicit solvation (PCM) and explicit solvation (2–3 solvent molecules), we reached a semi-quantitative agreement between calculated and experimental ΔδP values. It was evident that progressing from the gas phase to PCM, followed by the addition of two or three explicit solvent molecules, brings the computed data points increasingly closer to the experimental values.

Finally, we conclude that in solution Ph₃P=O tends to form three hydrogen bonds, where solvent molecules form CH...O hydrogen bonds, occupying all vacant spots, left around the P=O moiety after its complexation with phenols.

Acknowledgements

This work is supported by the RSF grant 23-13-00095.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

A family of copper silsesquioxane cages with pyrazolate and diimine ligands: synthesis, structure, supramolecular organization and catalytic properties

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Cagelike metallasilsesquioxanes is a large class of coordination compounds with wide structural diversity and different functional properties.¹ The silanolate cages' ability to react with additional organic ligands opens the way to new heteroleptic metal complexes with unique catalytic and supramolecular properties. In this work, we report about synthesis of new family of copper methylsilsesquioxanes decorated with both pyrazolate and diimine (1,10-phenanthroline and 2,2'-bipyridine) ligands. All this compounds have Cu₆-nuclearity with copper centers sandwiched by two Si₅ cyclic silanolates and organic molecules acting as bridging or chelate ligands for external copper ions. When bromine-substituted pyrazole is used in the self-assembly reaction of silsesquioxane cage, the supramolecular structure changes drastically (Fig. 1). Bromine atom forms halogen bond with ethanol solvent. Chain of hydrogen bonds with molecules of solvent (ethanol) connects the neighbouring cages to form 1D supramolecular formation.

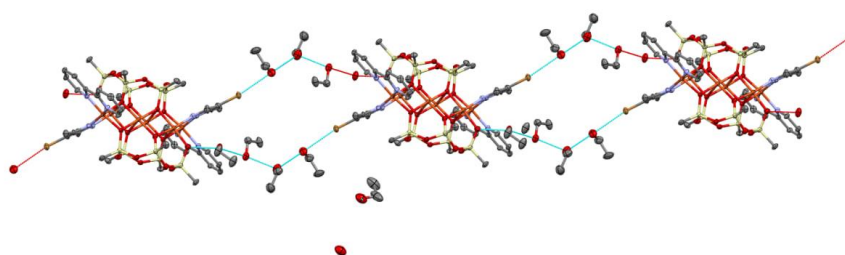


Figure 1. Net of halogen/hydrogen bonds in crystal structure of compound **5**.

We have also investigated catalytic activity of newly synthesized compounds in CuAAC reaction. To the best of our knowledge, copper silsesquioxanes' activity in this reaction has not been studied yet. Various triazoles have been synthesized in high (up to 99%) yields.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

DIRECTED SYNTHESIS OF RE(I) COMPLEXES WITH DIFFERENT NHC BONDING MODES

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In recent years, bisNHC (NHC = N-heterocyclic carbene) have attracted considerable attention as efficient bidentate σ -donor ligands¹. Due to the high strength of the metal–carbene bond and the pronounced donor properties of bisNHCs, rhenium(I) carbonyl complexes containing these ligands are considered promising catalytic, photoactive, and radiopharmaceutical systems². It is known that the formation of abnormal N-heterocyclic carbenes coordinated through the C4/C5 carbon atom of the imidazole ring is generally realized either by blocking the C2 position (commonly by Me or Ph substituent) or in complexes of late transition metals (Rh, Ir, Pd). C4/C5-bound carbenes exhibit higher σ -donor ability compared to classical C2-bound NHCs, which leads to a significant change in the reactivity of metal complexes³. However, despite extensive progress in carbene chemistry, examples of rhenium(I) biscarbene complexes with a mixed bonding mode (aNHC–NHC) have not been described.

In the present work, the conditions for the directed syntheses of rhenium(I) complexes with different bonding modes of bisNHC ligands are presented (Fig. 1). It was established that the use of the labile *fac*-Re(CO)₃(MeCN)₂Br precursor in the presence of a bisimidazolium salt and Et₃N selectively affords a rhenium(I) complex with a mixed coordination mode (aNHC–NHC) without prior protection of the C2 position of the imidazole ring. It is assumed that the formation of *fac*-(aNHC–NHC)Re(CO)₃Br proceeds via a base-assisted concerted metalation–deprotonation (bCMD) pathway involving the weak base Et₃N. These findings are of interest for the further design of functional Re(I) complexes.

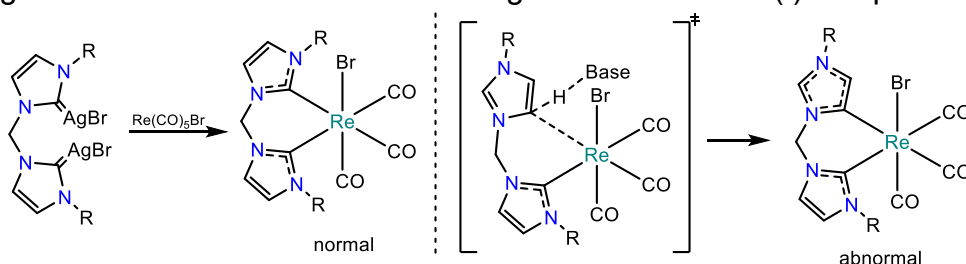


Figure 1. Objects of investigation

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Alkylation of Phosphine Chalcogenides: σ -Hole Enhancement

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Phosphine chalcogenides R_3PCh exhibit a distinctive electronic structure at the chalcogen atom. There is a region of negative electrostatic potential, enabling it to act as an electron donor. Conversely, a positive electrostatic potential region (located along the extension of the covalent bond, known as the σ -hole) allows these molecules to form chalcogen bonds.¹ This dual nature enables their use in various fields, such as catalysis, crystalline and molecular design.^{2,3} Moreover, the presence of ^{31}P allows them to be used as NMR probes for studying non-covalent interactions.⁴ However, even phosphine tellurides often form only weak chalcogen-bonded complexes in solution due to the limited magnitude of the σ -hole. To enhance chalcogen-donating properties, various synthetic strategies based on functionalization of the chalcogen atom have been explored. Among them, alkylation represents an effective approach for tuning the electronic structure and increasing the σ -hole magnitude.

In this study, we investigate the alkylation reactions of phosphine chalcogenides, focusing on how substituents and the nature of the chalcogen atom affect the reaction kinetics and nucleophilicity of the chalcogen center. To assess the nucleophilicity of phosphine chalcogenides, we conducted a kinetic study using $^{31}P\{^1H\}$ NMR spectroscopy. Such structural modifications increase the σ -hole, enhancing chalcogen-donor properties and opening prospects for practical applications.

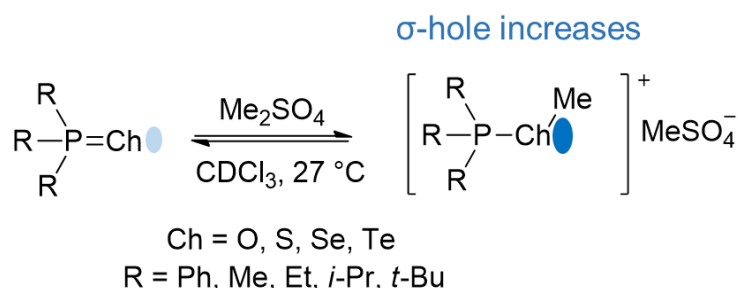


Figure 1. Scheme of the alkylation reaction of phosphine chalcogenides.

Acknowledgements

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All NMR spectra were recorded at the Center for Magnetic Resonance at the St. Petersburg State University Research Park.

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

The nature of non-covalent interactions of norbornene and norbornadiene with a palladium surface

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Norbornadiene (NBD), norbornene (NBE) and their derivatives are promising intermediates for organic synthesis. Heterogeneous catalytic processes are promising for the synthesis of norbornene derivatives. Recent studies¹ showed that it is possible to partially (selectively) hydrogenate NBD to NBE on heterogeneous Pd catalysts, despite the absence of conjugation between the double bonds in the NBD molecule.

Due to their structure, compounds with norbornene frame exhibit certain characteristic interactions with metals. Experimental studies of the adsorption of NBD and NBE on Ni and Pt surfaces² showed that their interaction with metals is primarily determined by the orientation of methylene bridge in the NBD and NBE molecules. In case of exo-adsorption methylene group is turned towards the metal surface (Fig. 1).

In this work a DFT investigation of the adsorption of NBE and NBD on Pd(111) and Pd(100) surfaces under periodic boundary conditions was carried out. The PBE-D3 functional was employed. A topological analysis of electron density distribution was carried out using QTAIM. It was found that during exo-adsorption of NBD and NBE molecules a non-covalent interaction occurs between the H atom of methylene bridge and the Pd atoms. The H—Pd distance during adsorption on Pd(111) and Pd(100) increases in the following sequence: NBD → NBE → norbornane. Despite the low H—Pd interaction energy, which can be estimated at 4.8-6.4 kcal/mol and 6.8-7.5 kcal/mol for NBD and NBE molecules respectively, it plays an important role in mechanism of selective hydrogenation of NBD.

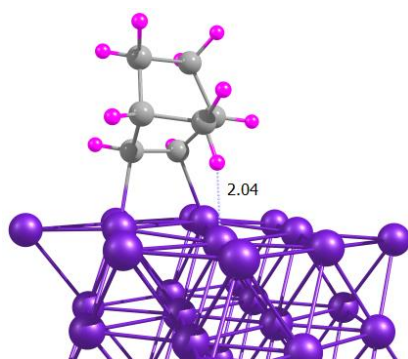


Figure 1. Exo-di- σ adsorption structure of NBE molecule on Pd(111)

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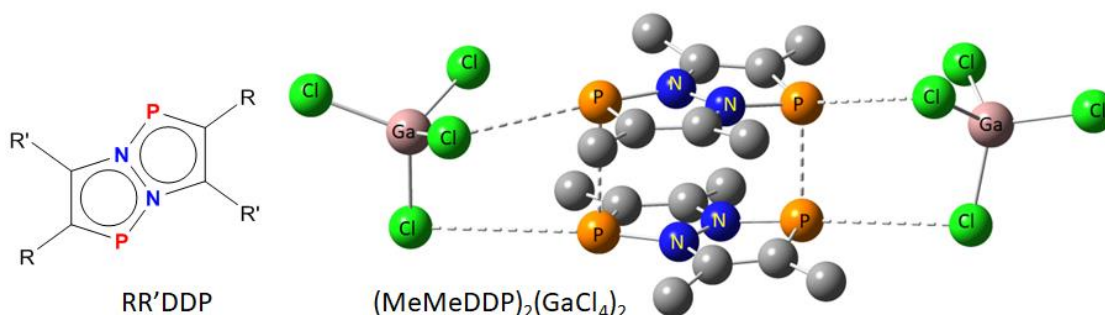
IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Non-Covalently Assembled Multidecker Diazadiphosphapentalenes

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As 10π -aromatic heterocycles, 3a,6a-diaza-1,4-diphosphapentalenes (RR'DDP) exhibit high polarizability and a tendency toward π -association. Double-decker dicationic RR'DDPs of the type $[(RR'DDP)_2]^{2+}[X^-]_2$ form a stable 18π -aromatic system through non-covalent $P\cdots P$ interactions, which range from 2.4 to 2.9 Å in the crystal.¹ According to ^{31}P NMR data, the phosphorus atoms are equivalent in solution.



The optoelectronic characteristics of $[(RR'DDP)_2]^{2+}[X^-]_2$ are determined by both the nature of the peripheral substituents (R,R') and the type of the counterion (X). For instance, the electronic absorption spectrum of ditriflate $[(\text{MeMeDDP})_2]^{2+}[\text{OTf}^-]_2$ exhibits a λ_{max} of 320 nm, whereas replacing the anion with $[\text{GaCl}_4^-]$ leads to a bathochromic shift to 347 nm. Double-decker RR'DDPs are prone to further π -association. Interaction with an additional donor molecule yields triple-decker molecules $[(RR'DDP)_3]^{2+}[X^-]_2$ and 1D-stacks $[(RR'DDP)_2(\text{D})]^{2+}[X^-]_2$, where D is an organic π -donor molecule (carbazole, dibenzothiophene). Diazadiphosphapentalenes and their double-decker derivatives exhibit temperature-dependent solid-state photoluminescence.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Inverted Halogen Bonds in Square-Planar Pt(II) and Pd(II) Iodide Isocyanide Complexes

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Organic and metal-bound iodine species with electron-withdrawing substituents are well-established as σ -hole donors in halogen bonding (XB).^{1,2} However, recent studies have shown that coordination to high-valent metals can polarize iodide ligands, induce positive σ -holes and enable them to act as XB donors.³ We now demonstrate that this activation extends to square-planar d^8 Pt(II) and Pd(II) iodide isocyanide complexes upon adduct formation with iodoform (CHI_3) and bromoform (CHBr_3).

DFT calculations reveal that adduct formation between $[\text{Ml}_2(\text{CNCy})_2]$ ($\text{M} = \text{Pd}$, left; $\text{M} = \text{Pd}, \text{Pt}$) and iodoform (CHI_3) generates significant positive electrostatic potential on the coordinated iodides. This σ -hole activation drives inverted $\text{M}-\text{I}\cdots\text{I}-\text{C}$ halogen bonds. QTAIM, MEP surfaces (**Fig. 1**) and ELF (**Fig. 2**) analyses confirm these noncovalent interactions and reveal the electronic structure of both conventional and inverted XBs.

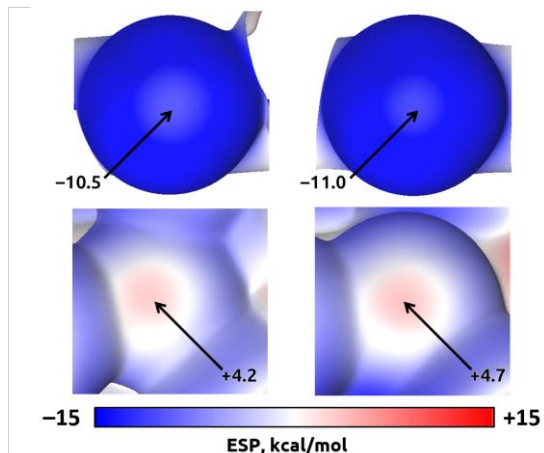


Figure 1. Molecular electrostatic potential surfaces for $[\text{Ml}_2(\text{CNCy})_2]$ ($\text{M} = \text{Pd}$, left; $\text{M} = \text{Pt}$, right) and their CHI_3 adducts, illustrating σ -hole activation on I ligands upon XBs formation.

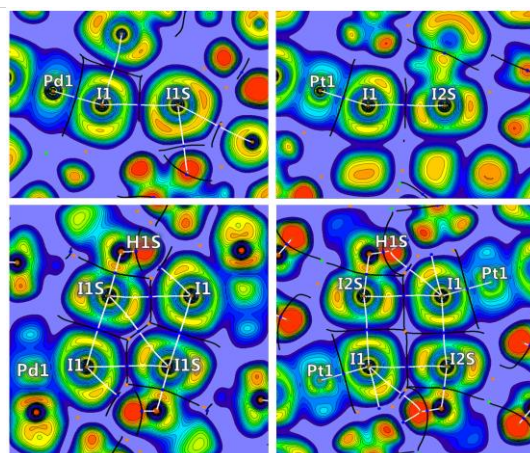


Figure 2. ELF projections for the conventional and inverted XBs $\text{I}\cdots\text{I}$ in the CHI_3 adducts of $[\text{Ml}_2(\text{CNCy})_2]$ ($\text{M} = \text{Pd}$, left; $\text{M} = \text{Pt}$, right).

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Electrostatic interactions – an in-depth study in gelatin–agar coacervates

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Among all protein–polysaccharide supramolecular structures possibly forming upon associative noncovalent interactions, coacervates are the most poorly surveyed yet appealing state. The exploration of coacervation phenomena is of benefit for both fundamental principles of organized matter composition understanding and novel biomaterials fabrication.

Since the driving force of coacervation are electrostatic interactions, the prominence should be given to systems containing polyelectrolytes with low degree of substitution due to increscent thermodynamic incompatibility. One is agar, a polysaccharide with relatively low content of ionic (sulfate) groups. To accompany it, gelatin from cold water fish species was selected, with respect to rational Russian Arctic bioresources treatment. In this study, we elucidate a framework of fish gelatin–agar coacervates formation and their properties in terms of electrostatic binding.

Two types of each biopolymer were used, varying in sulfate content (agar) and amino acid composition (fish gelatin), as well as in their molecular weight.

To examine gelatin–agar noncovalent aggregation in bulk of aqueous phase, methods of FTIR and UV spectroscopy, turbidimetry, and quasi-elastic laser light scattering were performed. Under certain *external* conditions: mass ratio, pH and ionic strength ranges, sulfo groups of agar and amino groups of gelatin get involved in electrostatic interactions, onwards giving a rise to supramolecular structures – inter(bio)polymeric complexes and coacervates formation. The influence on characteristics of gelatin–agar interaction (intermolecular distance, potential energy), as well as properties of aggregates in supernatant themselves (particle size, zeta potential) is also *internal* factors variation, *i.e.* biopolymers net charge and molecular weight. Thus, driving gelatin–agar system through different states, phase diagrams were built with a regions of biopolymer different compatibility.¹

The mechanical performance of isolated coacervate phase studied by 3D-rheometry appeared to be gel-like, revealing a structure of a two interpenetrating 3D-networks with contacts stabilized by electrostatic interactions, which is evident from strong pH and ionic strength dependence of rheological characteristics.² The composition of agar used determine the mesh-size of network and hardness, whereas gelatin component is in charge of elasticity and brittleness of coacervate phase.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Synergy Effect in GO-Based Hybrid Photocatalysts under Electric Field Activation

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Heterogeneous photocatalysis is key to solar-driven environmental remediation and green chemical synthesis. However, semiconductor-based photocatalysts are inefficient because of rapid recombination of photogenerated charge carriers. Strategies to mitigate this include hybrid material engineering and external stimuli application, but conventional electric field assistance requires catalyst immobilization on electrodes, leading to surface passivation and process complexity.

This study introduces an innovative, contactless strategy in which graphene oxide (GO)-based hybrid photocatalysts sensitised by chromophores from the phthalocyanine, porphyrin and perylene families are activated by an external electric field applied between insulated electrodes positioned outside the reaction medium. The photodegradation of 1,5-dihydroxynaphthalene (DHN), a model organic pollutant, was used as the test reaction.¹

The experimental findings demonstrate that the application of an external electric field (up to 4 kV) significantly enhances the photocatalytic decomposition rate of DHN by a factor of 1.5 to 2.3 in comparison with field-free conditions. In order to elucidate the underlying mechanism of this synergy effect, a comprehensive suite of physicochemical analyses was employed. This included UV-Vis and fluorescence spectrophotometry, time-resolved photoluminescence spectroscopy, fluorescence microscopy, and GC-mass spectrometry. The investigation reveals that the external field promotes a more efficient spatial separation of photoinduced charges and facilitates enhanced electron transfer from the GO matrix to the surrounding reaction environment.¹

Consequently, this contactless approach effectively overcomes the inherent limitations of conventional electrochemical photocatalysis by eliminating electrode degradation. The findings establish a promising pathway for the design of highly efficient, externally tunable, and cost-effective photocatalytic systems for sustainable "green" chemistry applications.

Acknowledgements

The authors are grateful to A.E. Alexandrov, D.A. Bunin, A.A. Averin, M.A. Kniazeva, M.Yu. Eremchev, A.V. Naumov, D.W. Boukhvalov, and B. König for their valuable contributions to this work. This work was supported by the Russian Science Foundation (project No 20-13-00279).

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

A quantum-chemical study of the electronic structure and reactivity of non-innocent transition-metal complexes with peroxide-derived ligands

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Non-innocent complexes can serve as a powerful tool for imparting reactivity to transition metals comparable to that of noble metal systems [1]. However, the instability of these complexes remains a serious obstacle, especially in the case of organic frameworks containing multiple heteroatoms. In our previous study, we investigated the reactivity of bi- and tricyclic aminoperoxides in the presence of iron(II) salts [2]. In this work, we present a comprehensive computational study of complexes formed by the formal insertion of an iron salt via the O–O bond of the organic (amino)peroxide scaffold, revealing new mechanisms underlying the stability of such complexes. Our study revealed the phenomenon of single-electron transfer (SET) from the bridging nitrogen in non-innocent ligands derived from amino peroxides, which effectively stabilizes the radical system (Figure. 1). In contrast, similar complexes derived from peroxides (without nitrogen) exhibit pronounced localization of an unpaired electron on the oxygen atoms coordinated to the iron atom, which confers significant oxidizing power upon them. Using quantum-chemical methods, including DLPNO-CCSD(T), density functional theory (ω B97X-D4), and multi-reference approaches (CASSCF/NEVPT2), we elucidate the electronic structures of the complexes and quantitatively assess trends in their stability, demonstrating that intramolecular SET significantly reduces the reactivity of complexes with a bridging nitrogen atom.

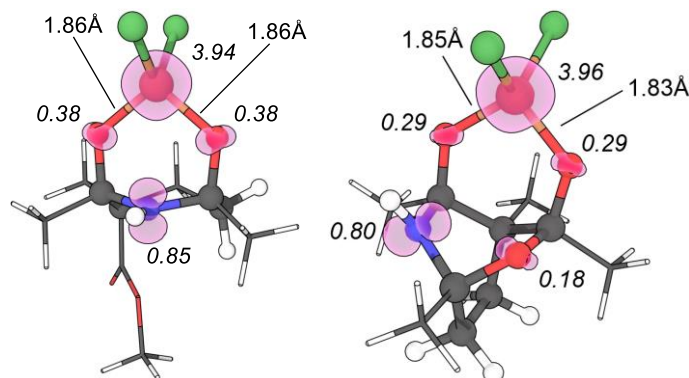


Figure 1. Spin density distribution in the bicyclic (left) and tricyclic (right) complexes

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Synthesis of Re(I) and Mn(I) complexes containing 1,5-diaza-3,7-diphosphocyclooctane ligand

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Homogeneous catalysis using organometallic manganese complexes continues to attract considerable attention during last decade,¹ since manganese abundance, relatively low cost and toxicity, and a wide variety of observed oxidation states. At the same time rhenium complexes have several advantages such as higher thermal stability, improved reactivity in specific catalytic processes, better stability of 19-electron radicals in electrochemical studies and photophysical properties.²

Manganese and rhenium complexes containing a 1,5-diaza-3,7-diphosphocyclooctane ligand deserve special attention due to the presence of two nitrogen atoms in the ligand, which can not only facilitate inter- and intramolecular proton transfer but also stabilize binding with H₂ or CO ligands, thereby lowering the barrier for heterolytic cleavage of H₂.³ Complexes containing this ligand are of interest as bifunctional catalysts with a basic center at the nitrogen atom and an acidic center at the metal atom.

Therefore, the aim of this work was to synthesize neutral and cationic complexes of Mn and Re containing a 1,5-diaza-3,7-diphosphocyclooctane ligand with various substituents on the nitrogen atom (R = pTol, CH₂pTol, CHPh₂). The influence of the nature of the metal atom and P₂N₂-ligand on the synthetic procedure and the yield of reaction has been studied.

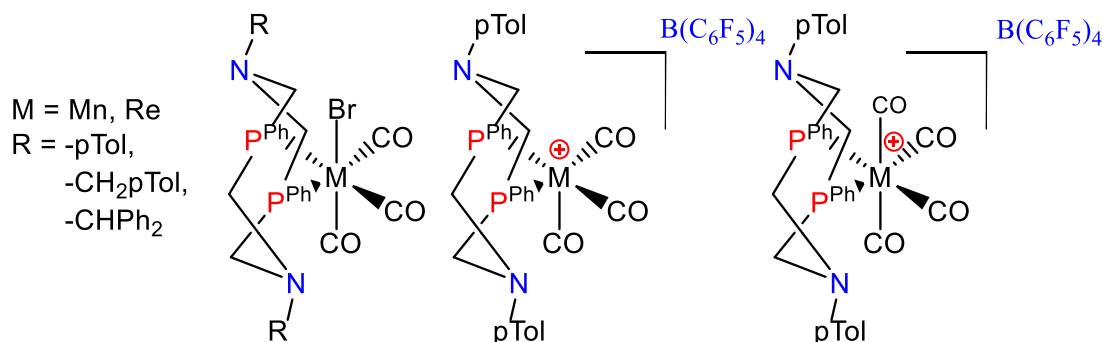


Figure 1. Neutral and cationic carbonyl Re(I) and Mn(I) complexes containing 1,5-diaza-3,7-diphosphocyclooctane ligand

Acknowledgements

The work was supported by the Russian Science Foundation (grant № № 24-13-00283).

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Halogen bonding in diaryliodonium dichromates

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Halogen bonding (XB), along with other noncovalent interactions, has become a key concept in supramolecular chemistry, polymer science, and crystal engineering. Conventional XB-based crystal design primarily relies on monovalent halogen compounds that provide a single σ -hole at the halogen(I) center, typically forming two-center interactions. As an alternative, diaryliodonium salts containing an iodine(III) center can act as double σ -hole donors. To complement such donors, acceptors with multiple nucleophilic sites are required. In this research, the dichromate anion was selected as a suitable XB-accepting building block.

Diaryliodonium dichromates, $[\text{Ar}_2\text{I}]_2[\text{Cr}_2\text{O}_7]$ (Ar = Ph, Mes), were obtained as a result of ion exchange reactions between aqueous solutions of potassium dichromate and diaryliodonium triflate. The single crystals of the complexes, suitable for X-ray diffraction (XRD), were obtained from water or a mixture of water and acetonitrile by slow evaporation of the solvent at room temperature. In addition, single crystals were grown from pyridine, and a solvent molecule was detected in their structure. XRD analysis of the crystals revealed different types of supramolecular assembly depending on the structure of the cation. In each case, $[\text{Cr}_2\text{O}_7]^{2-}$ acts as an XB acceptor, forming interionic XBs through two, four, or even five O-centers (Figure 1). These include diverse modes of "chelation" by the dichromate anion, as well as structures where cations or anions form polymer chains via XBs.

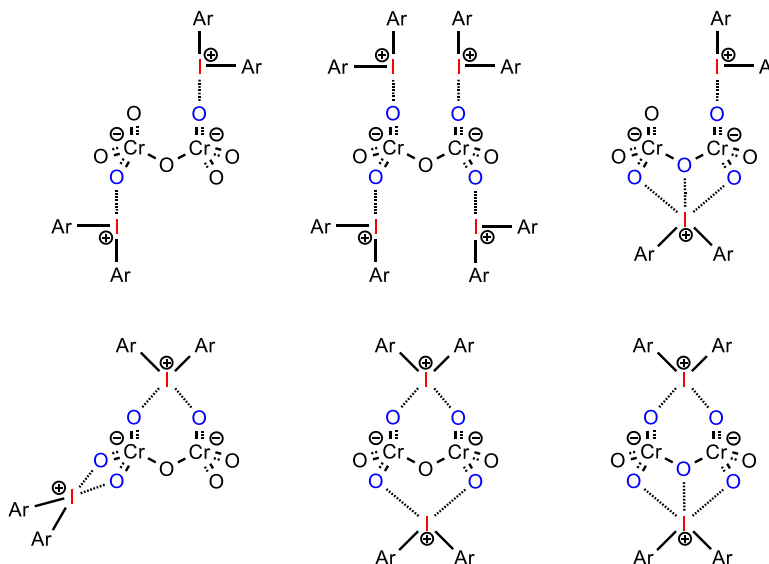


Figure 1. Dichromate as a multiple XB acceptor.

Acknowledgements

X-ray diffraction studies were carried out at the Research Centre for X-ray Diffraction Studies, St. Petersburg State University.



IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Aggregation-Induced Emission in Au(III) CNC-Pincer Complexes: The Role of Isonitrile vs. Alkynyl Coligands

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A series of six gold(III) complexes bearing the same tridentate CNC-pincer ligand (2,6-diphenylpyridine) was synthesized and characterized (Figure 1). The complexes differ in the fourth coligand: three cationic isonitrile derivatives and three neutral alkynyl derivatives. All compounds were fully characterized by NMR spectroscopy, ESI-MS, and XRD. Their photophysical properties were investigated in dichloromethane (DCM) solutions, DCM/toluene mixtures and in the solid state.

It was found that the isonitrile-containing complexes exhibit concentration-dependent aggregation even in pure DCM at elevated concentrations, forming supramolecular aggregates.¹ In contrast, the alkynyl analogues remain molecularly dissolved under identical conditions. In DCM/toluene mixtures, the cationic isonitrile complexes display typical aggregation-induced emission (AIE) behavior: weak emission in pure DCM, but intense luminescence upon increasing the toluene fraction, which promotes aggregate formation. In the solid state, the isonitrile complexes also exhibit strong AIE-type emission.

Importantly, no AIE effect was observed for the neutral alkynyl complexes either in concentrated solutions, DCM/toluene mixtures or in the solid state, highlighting the crucial role of the charge state and the nature of the coligand in enabling aggregation-induced emission.²

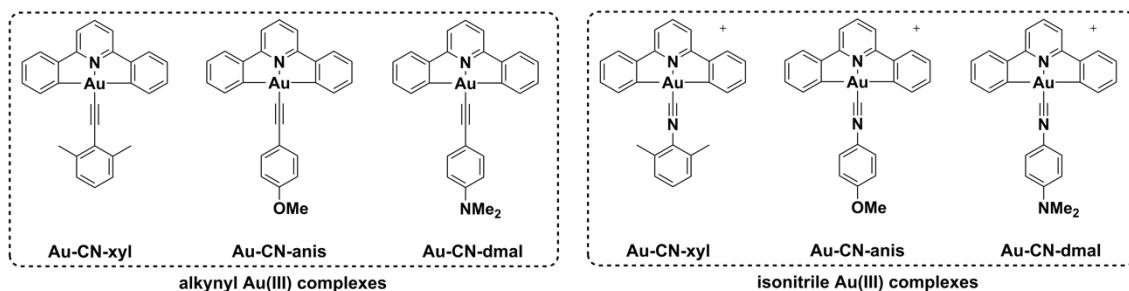


Figure 1. Investigated Au(III) complexes.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Bismuthophilic interactions in dimers of homoleptic Bi^{III} dithiocarbamates

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Many homoleptic dithiocarbamates exhibit rich supramolecular chemistry and often tend to dimerize through two additional M–S coordination bonds. Some of them also contain metallophilic interactions which can give rise to distinctive structural, electronic, or photophysical properties¹. Numerous homoleptic dithiocarbamate complexes of bismuth(III), as well as homoleptic dithiocarbamates of other metals, have been investigated as biologically active compounds, single-source precursors for sulfide and oxide nanoparticles and starting material for the preparation of sulfide thin layers².

Complex dimers were found in structures of [Bi(S₂CNR₂)₃] (NR₂ = NEt₂, N(CH₂)₄), bonded by noncovalent interaction Bi...S, which can be named pnictogen bonds according to IUPAC.

The nature of dimerization depends on the form of the substituent, crystal composition. In many structures of homoleptic dithiocarbamates pnictogen bonds are following by Bi...Bi interactions, which contribute dimerization of [Bi(S₂CNR₂)₃] molecules in solid state. In that dimers Bi...Bi distances less than two vdW Bi radii (4.17 Å), and even shorter than 4 Å. It was discovered that presence of Bi...Bi contact stand possible, when dimer contain two Bi...S bonds. Further theoretical calculations showed that Bi...Bi short contacts are formed by overlapping Bi-centered 6s- and 6p-orbitals mainly.

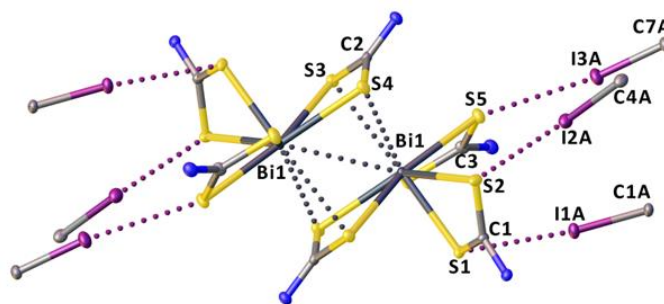


Figure 1. Structure of [Bi(S₂CNEt₂)₃]·1.5FIB with Bi...Bi contact and Bi...S pnictogen bonds. Substituents were removed for simplicity. 1,4-FIB = 1,4-diiodoperfluorobenzene.

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This work was supported by the Russian Science Foundation (grant no. 25-73-10092). X-ray diffraction data were obtained using equipment from the Research Center for X-ray Diffraction Research Methods (SPbSU).

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

A quantum chemical approach to the study of reactions involving hydrogen bonds in a neutral environment

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The present study is based on the task of searching for reaction pathways and selecting conditions that ensure control over the multistep mechanism of reactions of acyl chlorides with carboxylic acids in a neutral medium. Using the B3LYP/aug-cc-pVDZ method, 22 R₁COCl – R₂COOH systems were studied with R₁ = H, Me, *n*-Pr, *n*-Pen, CCl₃, Ar and R₂ = H, Me, *n*-Pr, *n*-Pen, CCl₃, Ar, MeAr with different orientations of the reacting molecules relative to each other.¹ It was shown that the reaction of benzoyl chloride with aliphatic and aromatic acids occurs as a direct one-step process. For trichloroacetyl chloride, the formation of anhydride is possible only through an intermediate. Trichloroacetyl chloride acts as an effective activating agent in a neutral medium. This key finding is directly related to another important result: proof of the decisive role of hydrogen-bonded pre-reaction complexes, the stability and structure of which are controlled by subtle electronic effects of substituents. The reaction outcome is determined by the competition between kinetic barriers and thermodynamic favorability, which allows us to move from acknowledging the process's complexity to controlling it.

When determining the structure and reactivity of flexible molecules, weak intra- and intermolecular hydrogen bonds must be taken into account. In the hydrogen-bonded acyl chloride–carboxylic acid system, which has competing reaction pathways, it is the prereaction complex that determines the geometric coordinates for subsequent attack by the nucleophile. It has been shown that the formation of this complex determines the discovery of a new, energetically efficient pathway, and the observed selectivity directly correlates with the decrease in the activation free energy $\Delta G^\ddagger$. In this case, the choice of calculation method and basis set is important. Experiments provide only a general understanding of the reaction and do not allow one to determine the influence of each specific stage. Quantum chemical calculations allow for a more nuanced assessment of the significance of each energetic component of a complex reaction and expand the ability to control its rate and direction.

The work also considered other modern quantum chemical methods and basis sets, such as ω -B97M-D4/def2-TZVPPD and CCSD(T)/def2-TZVPPD// ω -B97M-D4/def2-TZVPPD. The applicability of a method is typically verified by comparing results obtained using standard test sets, which primarily calculate rigid molecules, with a reference standard.^{2,3} It is important that the method also yield reliable results for flexible systems, where hydrogen bonds in pre-reaction complexes and transition states may have suboptimal orientations. Such bonds can significantly influence the course of a reaction.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

H-bond-assisted and sterically facilitated reactivity of *o*-dimethylaminoaryloximes and imines

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Non-covalent interactions, such as hydrogen bonding, are a promising tool for the activation of chemospecific transformations.¹ We have developed a synthetic toolbox, allowing for the controlled transformation of *o*-NMe₂-aryloximes and imines into nitriles and hard-to-reach N-heterocycles, activated via H-bonding with acids and facilitated by steric repulsion.²

It was shown, that oximes **1** in non-nucleophilic acidic media undergo Beckmann rearrangement giving nitriles **2**. Performing the reaction in nucleophilic media provides the selective preparation of pyrazoles **3**. Utilization of acetic acid as a reaction medium allows the preparation of isoxazoles **4**, facilitated by the substituents in position 8. A strong fixation of the NMe₂ group conformation and the source of radicals provide the transformation into benzo[*g*]indoles **5**. Imines **6** in acidic medium undergo cyclization to tetrahydroquinazolines **7** via hydride shift, facilitated by the *peri*-substituents.

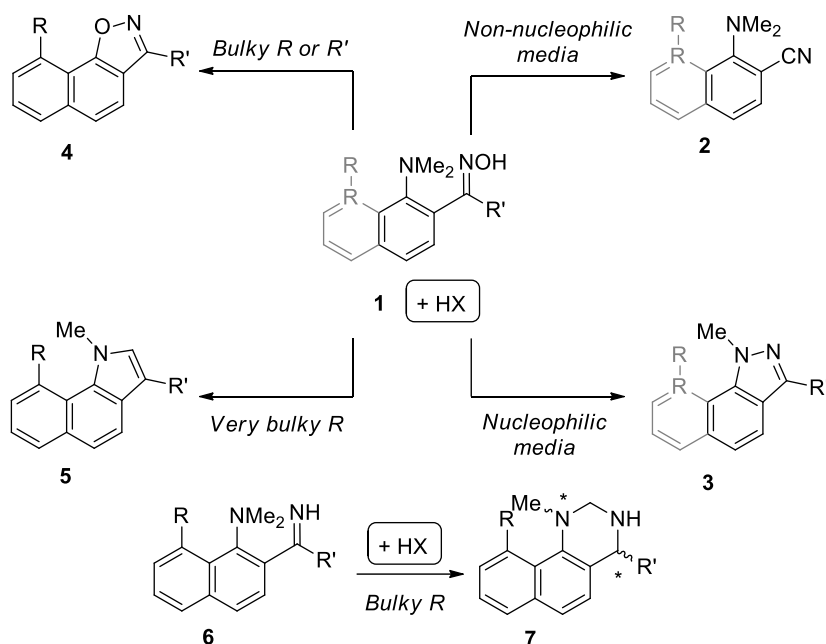


Figure 1. Transformations of *o*-dimethylaminoaryloximes and imines in acidic media

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

(De)coupled proton transfer in $(\text{HCO}_3)_2^{(2-)}$ dimers in kalicinite, KHCO_3 : a periodic DFT and LMP2 description

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Kalicinite is composed of the centrosymmetric H-bonded anion dimers, in which the pairs of $\text{HCO}_3^{(-)}$ ions are linked by two adjacent moderately strong H-bonds of ca. 2.58 Å (Fig. 1).¹ It has attracted significant attention in solid-state chemistry and physics on account of its unusually strong for hydrous minerals H-bonding observed at ambient pressure.² The issue of coupling of the collective intradimer double proton transfers along the H-bonds to the phonon vibrations of heavy atoms had been the subject of keen interest and debate for many years.

We have studied the anharmonic coupling between the high-frequency $\nu(\text{OH})$ and low-frequency $\nu_\sigma(\text{OO})$ modes by calculating the double-well potentials of the aforementioned transfers at fixed and relaxed O...O interatomic distances using five different Hamiltonians, viz. Hartree–Fock, PW91, PBE, B3LYP and Möller–Plesset with the second-order contribution to the correlation energy based on the localized orbitals (LMP2). The strongly anharmonic shape of the resulting double-well potential, governing the energy spacing between vibrational levels, is shown to be very sensitive to the chosen combination of the electronic and vibrational Hamiltonians. Numerical solution of the vibrational problem for the OH oscillators allowed us to evaluate transitions between the tunnel-split doublets of the ground and first excited vibrational levels. The best agreement with the latest experimental low-temperature inelastic neutron scattering data³ for KHCO_3 is achieved by using the B3LYP Hamiltonian for the collective proton transfer pathway which is decoupled from the crystal lattice.

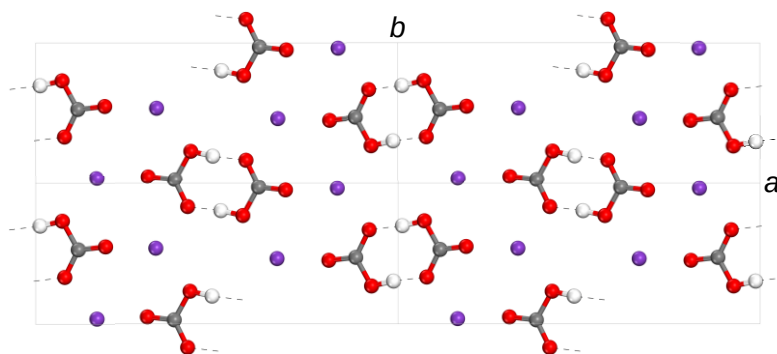


Figure 1. Projection of the ordered $P2_1/a$ structure of KHCO_3 on the (a,b) plane. H-bonds formed between the $\text{HCO}_3^{(-)}$ ions are indicated as black dashed lines.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

New chiral ionic HOF materials based on cationic octahedral Co(III) complexes

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One of the most promising areas of functional materials design is the creation of chiral porous metal organic (MOF) and covalent organic frameworks (COF). In addition to MOFs and COFs, hydrogen-bonded organic frameworks (HOFs) are self-assembled from pre-designed organic linkers through intermolecular hydrogen bonds, van der Waals forces, and π - π stacking interactions.¹ Due to the reversible and flexible nature of non-covalent bonds, HOFs display environmentally friendly preparation strategies under relatively mild conditions, easy regeneration and purification, fine biocompatibility, self-adaptive structure transformation, solution processability, and recyclability.²

Our previous work demonstrated that chiral octahedral Co(III) complex can form a homochiral porous assembly *via* H-bonding.³ We proposed that such Co(III) complexes could associate with polycarboxylic acids to form highly crystalline assemblies due to their H-donating ability through coordinated amino groups. In this work, we present two new promising materials: ionic HOFs based on chiral $\Lambda(R,R)$ -Co(III) **1** with terephthalic acid and complex **2** with 4,4'-biphenyldicarboxylic acid.

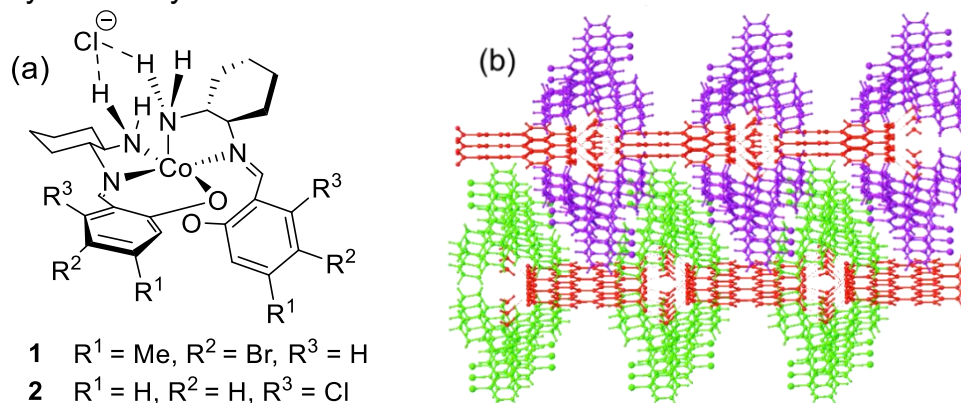


Figure 1. a) Structure of complexes **1**, **2**;

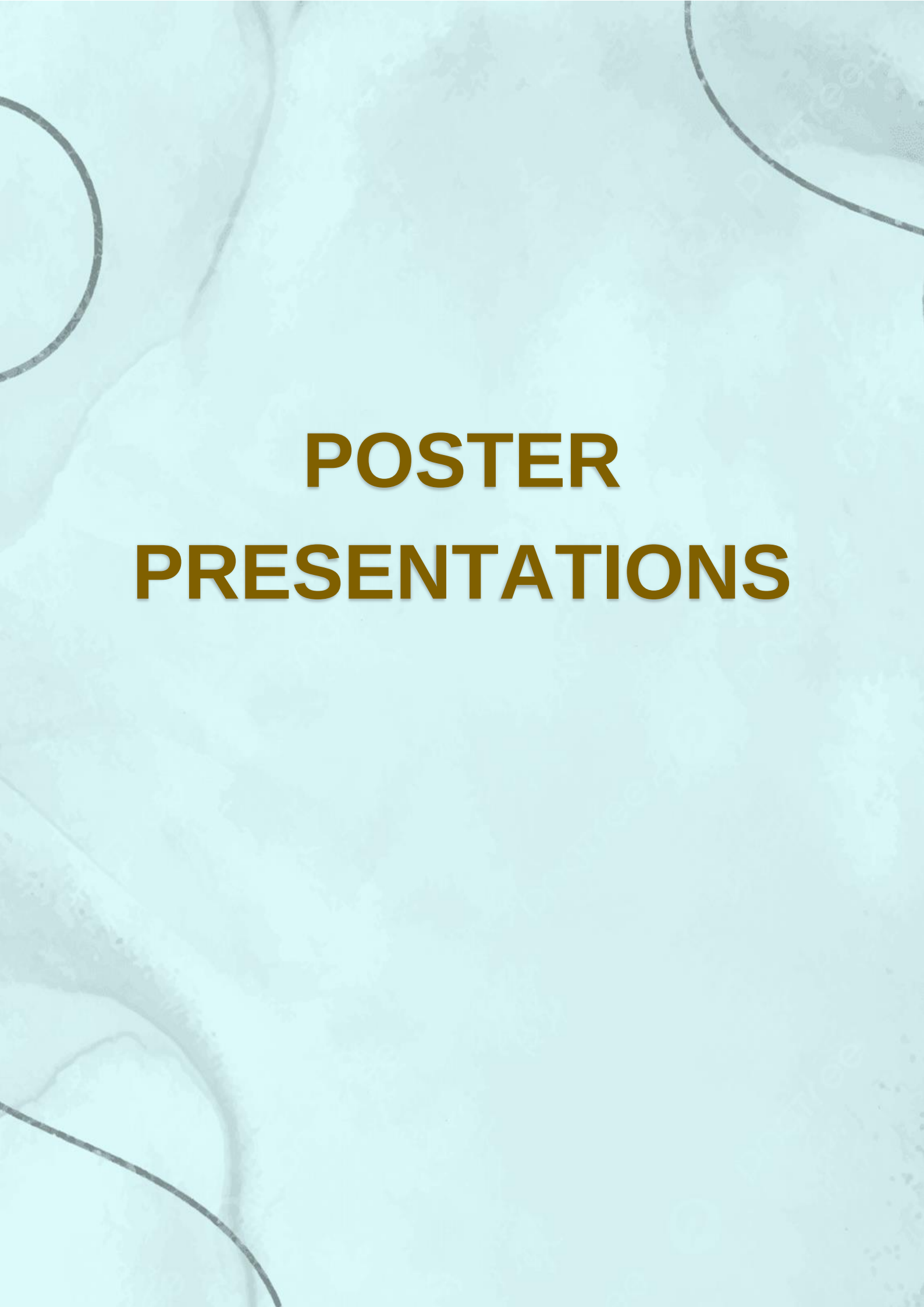
b) X-ray structure of HOF based on $\Lambda(R,R)$ -Co **2** (purple and green colors) and 4,4'-biphenyldicarboxylic acid (red color)

Acknowledgements

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POSTER PRESENTATIONS



IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Palladium(II) complexes featuring 5-acetylmethyl-1,2,4-oxadiazoles as ditopic acceptors of halogen bonding

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The development of supramolecular chemistry enables the creation of new functional materials based on metal complexes with tailored properties. Such complexes and their cocrystals find applications in various fields: the development of new materials for sensing applications, the design of catalytic systems, the advancement of luminescence diagnostic techniques, and the construction of functional materials with predefined properties. In this work, we present the results of a study on supramolecular structures based on palladium(II) complexes with 5-acetylmethyl-1,2,4-oxadiazole ligands, which form halogen bonds (HaB) with iodo-containing perfluoroaromatic compounds (Figure 1).

Cocrystals of three palladium(II) complexes **1–3** with HaB donors 1,4-FIB and 1,3,5-FIB were obtained and characterized: **1**·1,3,5-FIB, **2**·1,4-FIB, and **3**·1,4-FIB. The cocrystals were studied by single-crystal XRD. The formation of noncovalent contacts was investigated using quantum-chemical calculations. As a result, the formation of I···N HaBs was established, involving nitrogen atoms of the 1,2,4-oxadiazole ligand fragment and iodine atoms of 1,4-FIB and 1,3,5-FIB. These HaBs drive the formation of one-dimensional chain structures of different types (linear and zigzag), where palladium(II) complexes act as ditopic acceptors for halogen bonding. The systems exhibit multiple noncovalent interactions, including π -stacking contacts and palladium-involved contacts. The electrophilic-nucleophilic duality of the palladium center in intermolecular interactions was observed. These results expand the possibilities for designing supramolecular systems with controlled properties.

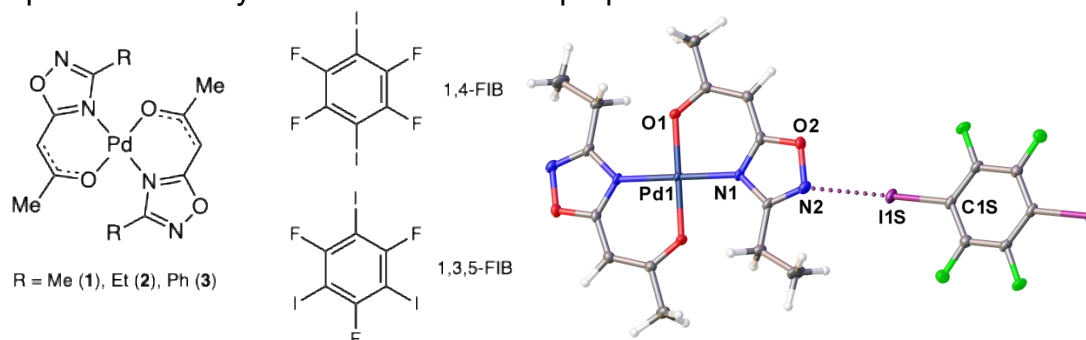


Figure 1. Complexes and HaB donors used (left); molecular structure fragment of cocrystal **2**·1,4-FIB demonstrating HaB formation (right).

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Azolo[a]pyrimidine-Based Iodonium Ylides: Synthesis and Properties

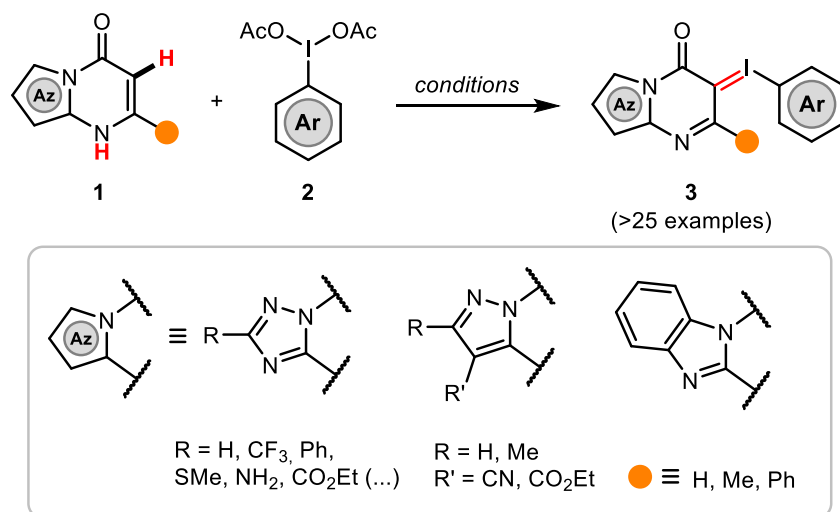
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In recent years, a serious attention has been drawn to organic compounds containing a hypervalent iodine (HVI) atom in their structure.¹ Among these, a special place is occupied by arylodonium ylides, characterized by their distinguishing halogen bonding properties and diverse reactivity.² Stability of such ylides strongly depends on the electron-withdrawing environment of the HVI center, with most of the known compounds of this class being derived from β -dicarbonyl species.

In this work, a rare example of stable monocarbonyl iodonium ylides is reported. In particular, it has been found that azolo[a]pyrimidones **1** can be readily transformed into ylides **3** via the reaction with (diacetoxy)iodoarenes **2**. As a result of this interaction, more than 25 previously undescribed HVI-containing azoloazine derivatives **3** have been isolated, with their structures being confirmed by NMR spectroscopy and mass spectrometry. Crystalline arrangement of some of these compounds has additionally been studied by X-ray diffraction analysis to demonstrate that the molecular packing of **3** is rendered by noncovalent interactions between its HVI atom and nucleophilic N-/O-centers of an adjacent molecule. Most of the obtained monocarbonyl iodonium ylides **3** can be stored for months in the freezer without any significant decomposition, which makes them convenient to handle for any further modifications. The ongoing research in our group is devoted to discovering the reactivity of **3** en route to novel azolo[a]pyrimidine derivatives with potential pharmacological activity.



Scheme 1. Synthesis of azolo[a]pyrimidine-based iodonium ylides **3**

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Design of Phosphorescent Platinum(II) Complexes via Noncovalent Interactions

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Organoplatinum(II) complexes are promising phosphorescent luminophores for optoelectronic, biosensing, and photocatalytic applications, including PHOLEDs. Their photophysical properties are strongly governed by the electronic and steric features of the ligand environment [1-3]; therefore, controlled ligand modification is an efficient strategy for tuning their optical behavior.

This work presents a systematic study of cyclometalated platinum(II) isocyanide complexes [Pt(ppy)L(CNR)] (**1–18**), where L = Cl or SCN. The introduction of halogenated aromatic isocyanides bearing Br or I substituents with positive σ -holes enables directional intermolecular interactions. In the crystals of [Pt(ppy)Cl(CNR)] complexes **1–4** (R = C₆H₄-2-I **1**, C₆H₄-4-I **2**, C₆H₃-2-F-4-I **3**, C₆H₃-2,4-I₂ **4**), the supramolecular organization is governed by I...Cl halogen bonds between the isocyanide substituent and the chloride ligand.

Changing the crystallization conditions for complex **2**, from CH₂Cl₂ to hot EtCN affords another polymorph, **2^{II}**, which contains metallophilic Pt...Pt contacts absent in **2^I**. As a result, **2^{II}** exhibits a red-shifted emission and a 24-fold higher photoluminescence quantum yield compared with **2^I**, 12% versus 0.5%. A similar enhancement is observed upon cocrystallization of complex **14** with 1,4-DITFB, giving the adduct **14**·½(1,4-DITFB), which shows a higher quantum yield while retaining the spectral profile of the parent complex. Thus, directional intermolecular contacts, including Pt...Pt, C–I...Cl–Pt, and isocyanide π -hole...d_z²[Pt^{II}] interactions, increase structural rigidity, suppress vibrational relaxation, and enhance photoluminescence.

Halogen bonding also controls the crystallization of thiocyanate complexes by stabilizing a specific linkage isomer in the solid state. Although complexes **15–18** (R = C₆H₃-2-F-4-I **15**, C₆H₃-2,4-I₂ **16**, C₆H₃-2-I-4-Br **17**, C₆H₃-2,4-Br₂ **18**) exist in CDCl₃ solution as equilibrium mixtures of S- and N-bound isomers, crystallization yields only one form: either N-coordinated **15^N**·CHCl₃/**15^N**·CH₂Cl₂ or S-coordinated **16^S**·CHCl₃, **17^S**·CHCl₃ and **18^S**·MeNO₂. The presence of X...S or X...N halogen bonds (X = Br, I) in all crystals confirms the decisive role of noncovalent interactions in determining the final isomeric form.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Intermolecular interactions in novel highly-energetic 3,3-dinitroazetidines: viewpoint from azetidine geometry

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Azetidine-containing compounds, apart from β -lactam antibiotics, are uncommon in modern organic chemistry, but they have found special application as moieties in high-energy density materials (HEDM)¹. The comprehensive effect of the azetidine cycle and its strain on the properties of energetic materials has not been studied yet.

We report preparation of several novel 3,3-dinitroazetidine compounds – their structures were determined by X-ray crystallography. We compared fold angles, bond lengths and intermolecular interactions of investigated compounds with literature-known azetidines and found that presence of numerous hydrogen-bond forming functional groups attached to 1 and 3 atoms of azetidine cycle lead to significant deviations from classical azetidine geometry ².

Molecule **1** has two fragments: zwitterionic triazolofurazan and 3,3-dinitroazetidine, which are coupled by N-N bond. The azetidine's fragment has a "puckered" conformation with 17.11(12)° and 16.50(12)° fold angles for two combinations of azetidine planes (unsubstituted azetidine has "puckering" angles of about 34°).

Molecule **2** has also two fragments: 3-(trinitromethyl)-1,2,4-triazole and 3,3-dinitroazetidine, which are coupled by N-N bond. The azetidine's fragment has 2.4(3)° and 9.6(4)° fold angles, which corresponds to almost planar structure

Crystal packings, azetidine geometries and sensitivity data were also analyzed for 3-((3,3-dinitroazetidin-1-yl)diazenyl)-5-(trifluoromethyl)-4H-1,2,4-triazole **3**, 3,3-dinitroazetidine bromide **4** and (1-(tert-butyl)-3-nitroazetidin-3-yl)methanol **5**.

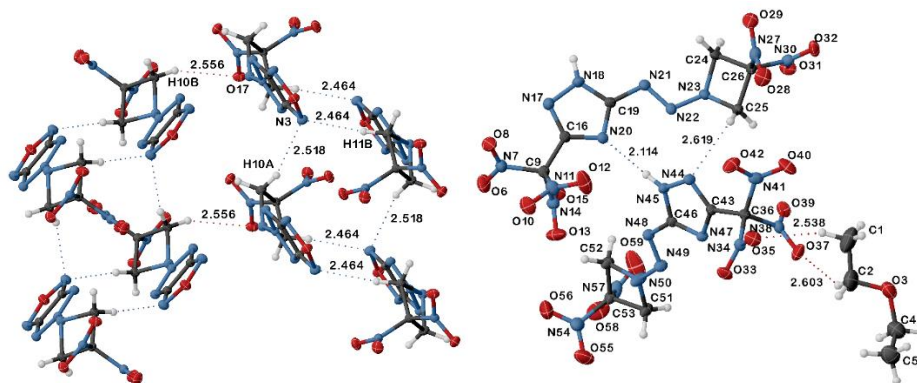


Figure 1. The intermolecular interactions of **1** and **2** in crystals

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Halogen Bonding Involving Mixed Dithiocarbamate Platinum(II) Complexes

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Due to their unique properties, noncovalent interactions have been attracting greater scientific interest for recent decades. They have already found their applications in various fields, from synthesis and catalysis to pharmaceuticals and crystal engineering. Hydrogen bonding is the most explored, whereas unconventional types of contacts, such as halogen (HaB) and chalcogen bonding, semicoordination, π -hole interactions, still remain poorly studied¹.

Square-planar transition metal complexes can be used as suitable objects for studying metal-based supramolecular systems². In this work, a chelate platinum(II) complex, [Pt(PPy)(S₂CN(CH₂)₆)] (PPyH – 2-phenylpyridine), was cocrystallized with several polyfunctional σ -hole donors, namely 1,3,5-triiodotrifluorobenzene, 1,4-diiodotetrafluorobenzene, octafluoro-4,4'-diiodo-1,1'-biphenyl, nonafluoro-4'-iodo-1,1'-biphenyl. The obtained cocrystals were studied by single crystal X-ray diffraction.

Upon analysis of the crystal structures, we observed two-center I $\cdots$ S HaBs involving ligands (fig. 1a) and rare metal-involving bifurcated (μ_2 -I) $\cdots$ [Pt^{II},S] HaBs (fig. 1c,d). Moreover, unusual (μ_2 -I) $\cdots$ [Pt^{II},C] contacts (fig. 1b), as well as trifurcated (μ_3 -I) $\cdots$ [Pt^{II},C,S] HaB (fig. 1c) have been discovered. The noncovalent nature of the revealed interactions was confirmed by DFT calculations.

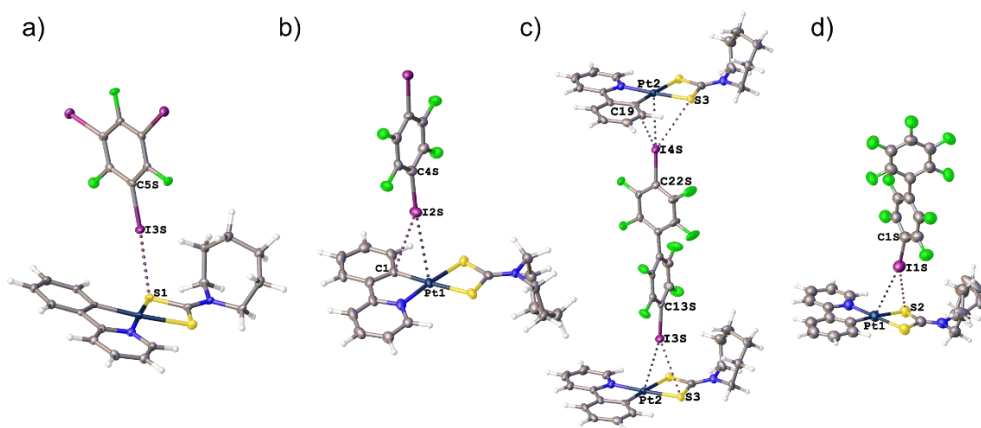


Figure 1. Halogen bonding in the cocrystals: a) two-center I $\cdots$ S HaB; b) bifurcated (μ_2 -I) $\cdots$ [Pt^{II},C] HaB; c) trifurcated (μ_3 -I) $\cdots$ [Pt^{II},C,S] and bifurcated (μ_2 -I) $\cdots$ [Pt^{II},S] HaBs; d) bifurcated (μ_2 -I) $\cdots$ [Pt^{II},S] HaB.

Acknowledgements

X-ray diffraction studies were performed at Saint Petersburg State University Research Centre for X-ray Diffraction Studies. This work was supported by the Russian Science Foundation (project 25-13-00035).

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Noncovalent Interactions in Crystals of Methanol Solvates of 1*H*-imidazo[4,5-*b*]phenazine

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Understanding the mechanisms of crystallization and molecular self-assembly provides insight into the dynamics of weak intermolecular interactions, thereby advancing crystallography and materials science. Noncovalent interactions such as hydrogen bonds, halogen bonds, and π -stacking play a key role in the formation of supramolecular ensembles and the fine-tuning of crystal properties. Typically, the acceptors of halogen bonds are lone-pair donors, a category that includes 1*H*-imidazo[4,5-*b*]phenazine (**IPh**). **IPh** is a promising scaffold for creating new functional materials. However, the crystal structure of **IPh** and its solvates remain unknown to date. The methanol solvate of **IPh** (**1**) and its co-crystal with 1,4-diiodotetrafluorobenzene (**2**), obtained by us and studied by SC-XRD, demonstrate that solvent molecules are not simply included in the cavities of the crystal structure but play a decisive role in its formation. **IPh** is shown to be a unique building block that allows for the construction of mixed hydrogen-/halogen-bonded frameworks due to the presence of multiple nitrogen atoms in its structure.

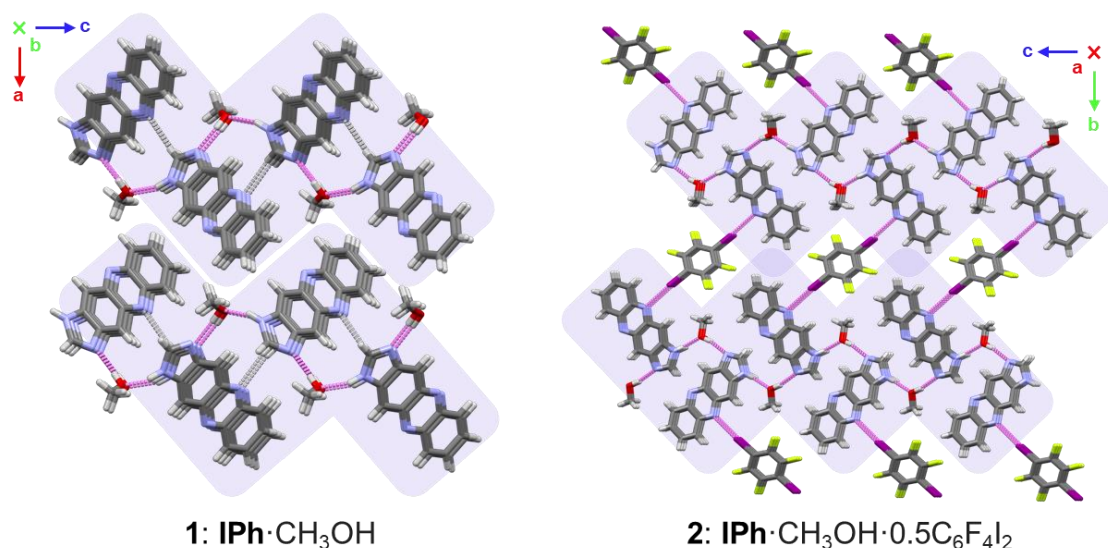


Figure 1. Views of the supramolecular layers along the *b* (left) and *a* (right) axes of **1** and **2**

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Polyfluoroaromatic Bisselanes as Polytopic Donors of Noncovalent Interactions

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Polytopic chalcogen bonding (ChB) donors – featuring several chalcogen atoms – have recently attracted immense scientific interest due to their ability to act as polyfunctional donors of noncovalent interactions. To induce σ -holes on the chalcogen atom, electron-withdrawing substituents such as acetylenes, cyanides, phosphines, and heterocycles are used; however, examples employing perfluoroaromatic substituents demonstrate that such bisselanes act as powerful donors of noncovalent interactions.¹ The presence of both fluorinated and non-fluorinated aromatic rings provides an additional tool for design via aryl–perfluoroaryl interactions.

In this work, a series of polyfluoroaromatic polytopic bisselanes (Figure 1) bearing various fluorinated and non-fluorinated substituents was obtained and theoretically studied. To assess the ability of the molecule to form noncovalent interactions, the molecular electrostatic potential (MEP) was calculated.

Our theoretical findings revealed that adding the non-fluorinating aryl fragment produced nonsymmetric (1-2 kcal/mol apart) sigma-holes on Se atom. The MEP values on Se atom are in range 14-23 kcal/mol.

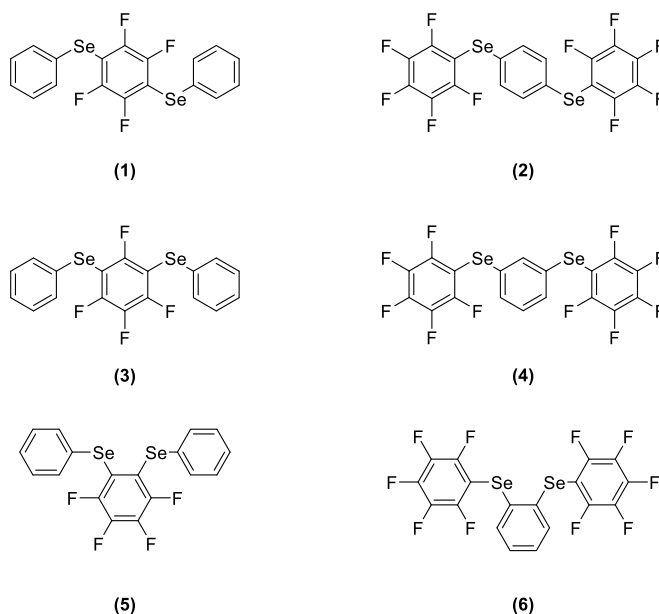


Figure 1. Polyfluoroaromatic bisselanes 1-6.

Acknowledgements

The support of the Russian Science Foundation (Project 25-13-00035) is gratefully acknowledged.

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KRYPTORACEMATE AND RACEMIC CRYSTAL OF CHIRAL THIOUREA WITH 1,2,3,4-TETRAHYDRO-1-NAPHTHYL FRAGMENT

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Kryptoracemates, or false conglomerates, are unique chemical compounds that crystallize in chiral space groups. These systems are the subject of active research due to their potential applications in materials science, including the creation of new functional materials such as one-dimensional conductors, photoconductors, and materials for nonlinear optics. Unlike traditional materials that utilize homochiral crystals, kryptoracemates can exhibit asymmetric properties while remaining within the confines of racemic systems.

A study of thiourea with a 1,2,3,4-tetrahydro-1-naphthyl moiety, containing a phenyl ring as an achiral substituent, led to the discovery of two polymorphic modifications of the racemic sample, one of which was found to be a kryptoracemate. The work presents a comparative analysis of homo- and heterochiral types of bonding, a detailed examination of the packing motifs of the racemic crystal and kryptoracemate, and also establishes differences in the thermodynamic stability of the crystalline forms.

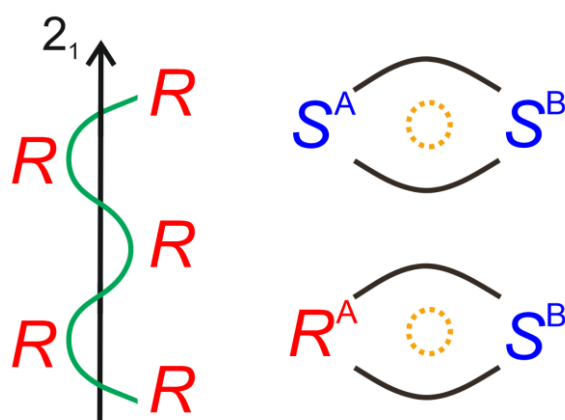


Figure 1. Schematic illustration of the crystallization types

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The First Example of Iodonium Ylides Derived from 7-Hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one

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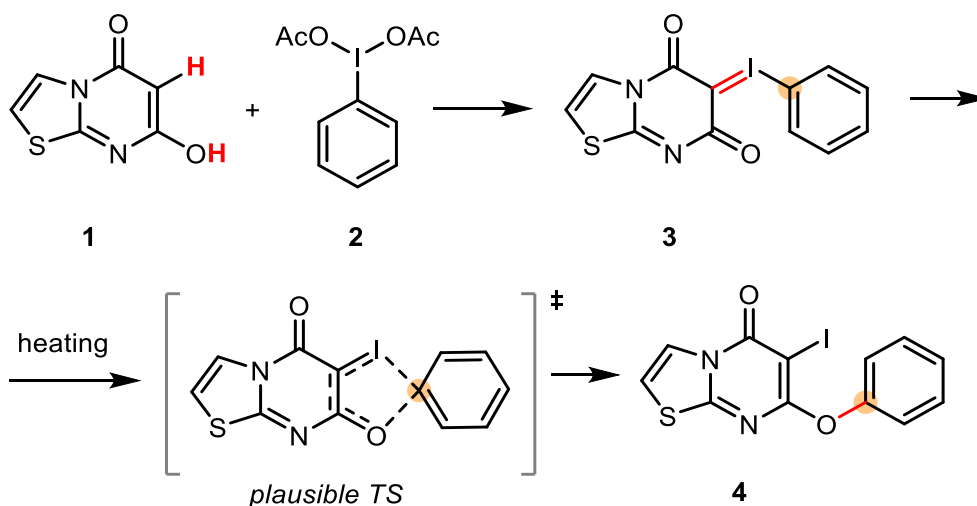
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Iodonium ylides occupy a valuable place among the compounds containing a hypervalent iodine atom in their structure.¹ This is due to their propensity to form relatively strong halogen bonds, which may account for their versatile reactivity in a multitude of synthetic transformations involving C–H insertion, cyclopropanation, transylation, and various rearrangements. In general, iodonium ylides can be considered as a useful instrument for the complex molecule construction.

In this study, we have utilized the iodonium activation strategy with regard to the azoloazine family, which is known for its pronounced pharmacological potential. In particular, it has been found that 7-hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one **1** can be transformed into the corresponding iodonium ylide **3** via the reaction with (diacetoxy)iodobenzene **2**. Further heating of **3** in DMF solution has led to regioselective thermal aryl migration, which is supposed to occur through the formation of the transition state² shown in Scheme 1. As a result, the aryl rearrangement product **4** has been obtained, with its structure being confirmed by X-ray diffraction analysis. Our current research is aimed at the synthesis of analogous azolo[*a*]pyrimidine-based iodonium ylides and further investigation of their reactivity.



Scheme 1. Synthesis of 7-hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one-based iodonium ylide **3** and its rearrangement to **4**

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Pickering emulsions stabilized by g-C₃N₄ or GO/g-C₃N₄ for photocatalytic degradation of organic pollutants

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Water contamination by toxic compounds, including industrial dyes and persistent oil-soluble organic contaminants, remains a critical global environmental challenge. Conventional remediation methods are frequently characterised by high costs and low efficiency in the presence of recalcitrant pollutants. Heterogeneous photocatalysis utilising visible-light-active semiconductors presents a promising alternative, but its application to hydrophobic substrates is limited by poor interfacial contact and low charge transfer efficiency of the photocatalyst.

The present study proposes an approach that integrates the photocatalytic properties of graphitic carbon nitride (g-C₃N₄) and its graphene oxide composite (GO/g-C₃N₄) with the Pickering emulsion platform. In such systems, the solid photocatalyst particles simultaneously act as a stabilizer of the oil-water interface, a sorbent, and a site for active radical generation. This architecture has been demonstrated to significantly intensify the contact between photogenerated active species and both water-soluble (hydrophilic) and oil-soluble (hydrophobic) substrates.

The sorption capacity and photocatalytic activity were analyzed using UV-visible spectrometry, fluorescence spectrometry, and microscopy. The high efficiency of the resulting Pickering emulsions in the photocatalytic degradation of different types of organic dyes has been confirmed by experimentation: hydrophilic (fluorescein, rhodamine 6G, and cresol red) and hydrophobic (Sudan IV). Introducing GO stabilizes the separation of photoinduced charges and accelerates electron transfer in the system, thereby increasing emulsion efficiency.

The findings obtained from this study provide substantial evidence that Pickering emulsions stabilized by g-C₃N₄ and its composites have considerable potential as a novel platform for solving applied problems, including wastewater treatment, the degradation of persistent organic pollutants, and the development of advanced photocatalysts.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Azine-*N*-oxides: *N*-O-group as a tool for expanding the reactivity of azines

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Azine-containing compounds readily participate in various non-covalent interactions, such as hydrogen and halogen bonding, π - π - and metal-ligand interactions¹. This property is actively used in the design of functional materials. To fine-tune the characteristics of these materials, the properties of azine moiety need to be precisely modulated. However, modification of the pyridine skeleton presents a significant synthetic challenge. One of the methods to expand the reactivity of azines is to introduce the *N*-oxide group². Here we present an approach to diversify the azine/azine-*N*-oxide chemistry expansion via steric strain release and electrophile promoted *N*-oxide activation.

It was found that alkene strain effectively activated quinoline-*N*-oxides towards 1,3-dipolar cycloaddition in catalyst-free conditions. Thus, a number of annelated non-planar heterocycles were obtained. Meanwhile, the electrophilic activation of the *N*-oxide group created the opportunity to direct the reaction pathway via solvent-substrate interaction. The *N*-deoxygenation was observed in polar solvents, while nonpolar solvents led to 2,2'-biazines formation under mild conditions allowing for the synthesis of compounds with sensitive functional groups.

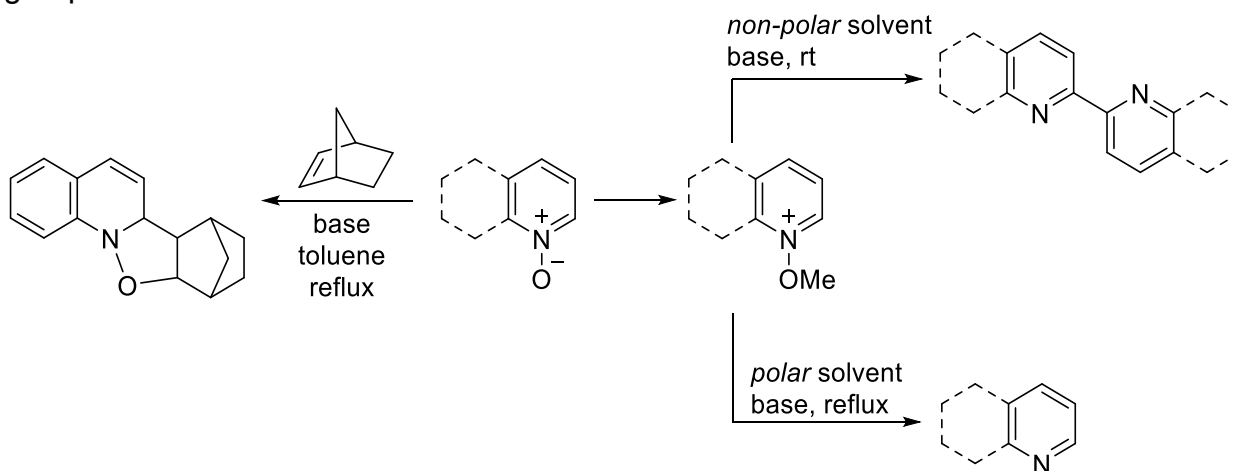


Figure 1. Azine/azine-*N*-oxide chemistry expansion via steric strain release and electrophile promoted *N*-oxide activation

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Copper and silver iodides coordination polymers with bicyclic amines as linkers

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Hybrid copper(I) and silver halide materials have attracted significant attention for applications in LEDs, OLEDs, scintillation detectors, and electro-optical devices. The main advantages of these materials are their structural flexibility and their ability to form crystals with different geometries depending on the synthesis conditions and the structure of the organic component.

In the present work, four new coordination polymers with the following compositions were synthesized and characterized: $[\text{Cu}_4\text{I}_4]\text{A}_2$ (**I**), $[\text{Cu}_6\text{I}_6]\text{A}_3$ (**II**), $[\text{Cu}_4\text{I}_4]\text{B}_2 \cdot \text{B}$ (**B** – tetramethylenediethylenetetramine) (**III**) and $[\text{Ag}_2\text{Cu}_6\text{I}_8][(\text{DABCO})_2\text{H}]_2$ (**DABCO** – diazabicyclo[2.2.2]octane) (**IV**).

Compound **I** was obtained as a single-phase powder from the solution. Single crystals of this compound, suitable for X-ray diffraction, were obtained by layer diffusion and structural analysis was performed ($\text{C}2/c$, $a = 26.9976(17) \text{ \AA}$, $b = 13.7560(10) \text{ \AA}$, $c = 16.4141(17) \text{ \AA}$, $\beta = 90.159(3)^\circ$, $R = 5.83\%$). As a by-product of crystallization, small crystals of compound **II** were also obtained ($R\bar{3}$, $a = 17.23652(10) \text{ \AA}$, $c = 25.69038(15) \text{ \AA}$, $R = 5.21\%$). Compound **III** was obtained after repeated recrystallization from acetonitrile as transparent single crystals ($I\bar{4}$, $a = 15.0335(2) \text{ \AA}$, $c = 15.4066(3) \text{ \AA}$, $R = 1.00\%$). In compounds **I** and **III** distorted cubic clusters $[\text{Cu}_4\text{I}_4]$ are connected into polymeric chains via organic ligands. In both cases, only two nitrogen atoms coordinate to each copper center. A notable structural feature of compound **III** is the presence of an amine solvate molecule.

Luminescence analysis of the compound **I** showed the absorption maximum at 365 nm and a broad emission band with a peak at 602 nm. The identification of compound **II** crystals among the mixture of crystals **I** and **II** was possible due to a significant shift of the luminescence peak to the green region (around 550 nm). Despite the structural similarities between compounds, **I** and **III**, the luminescence maxima differ slightly, being at 585 nm and 575 nm, respectively.

As an initial approach to the synthesis of mixed-metal clusters $[\text{Cu}_{4-x}\text{Ag}_x\text{I}_4]$, the readily-accessible ligand DABCO was selected. Related compounds, such as $[\text{Cu}_4\text{I}_4](\text{DABCO})_2$, have been previously reported. From aqueous solution, flat, square, transparent crystals of compound **IV** were obtained ($\text{P}2_1/\text{m}$, $a = 6.9837(2) \text{ \AA}$, $b = 21.0819(7) \text{ \AA}$, $c = 7.1664(3) \text{ \AA}$, $\beta = 94.482(3)^\circ$, $R = 2.44\%$). The structure consists of $\text{AgCu}_3\text{I}_4^-$ linear chain anions connected by $(\text{DABCO})_2\text{H}^+$ fragments into corrugated layers. Luminescence spectra were recorded and analyzed; the emission maximum is observed at 540 nm upon excitation at 340 nm.

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CHIRAL DISCRIMINATION IN SOLID SOLUTIONS OF TIMOLOL MALEATE ENANTIOMERES: ENERGETIC ASPECTS

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In most cases, chiral substances related to medicinal substances have stereospecific biological activity. This determines the tendency to use only optically pure compounds as a dosage form. In this regard, the effects of chiral discrimination in the solid phase are of particular importance, allowing for an increase in the optical purity of the substance during crystallization, including the production of individual enantiomers from the racemic phase.

Earlier, based on X-ray diffraction data for the corresponding phases and comparison with differential scanning calorimetry (DSC) data, we established [1] that timolol stereoisomers form a continuous series of solid solutions with a unique method of replacing stereoisomer molecules with each other at the nodes of the crystal lattice. The crystal packaging of such a system is based on a 1:1 racemic compound in which stereoisomers, moving along the axis of the composition, replace each other. At the same time, due to their conformational mobility, they adopt configurations as close as possible to those of their optical antipodes. The presented study attempts to provide a detailed thermodynamic description of this system.

Based on experimental data on the concentrations of individual enantiomers in the solvent used (THF), their activity coefficients were determined for saturated solutions of samples of varying enantiomeric compositions. These coefficients can be considered as a quantitative assessment of chiral discrimination in the crystalline phase. It was found that for a racemic crystal, the activity of the components is almost an order of magnitude lower than for an enantiopure crystal. This means that during crystallization, the racemic compound precipitates out of the solution first, and enantiomeric enrichment by the classical recrystallization method is impossible. However, if a sample enriched by more than 70% is placed in a limited amount of solvent, the solution will be enriched in the predominant component by almost an order of magnitude. This extraction option can be used for enantiomeric enrichment. Obviously, such significant effects of chiral discrimination should be taken into account when analyzing the biological activity of drugs.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Structure and properties of cocrystals based on benzofuroxanes with anthracene and its methyl derivatives

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A series of new charge-transfer cocrystals based on benzofuroxanes and anthracene, 9-methylanthracene, and 9,10-dimethylanthracene were synthesized and characterized by single-crystal X-ray diffraction, powder X-ray diffraction, solid-state electrochemistry, and UV-Vis spectroscopy. Single-crystal X-ray diffraction revealed that all cocrystals adopt a mixed-stack packing motif with alternating donor and acceptor molecules. Methyl substitution gradually increases the interplanar distance between the aromatic moieties within the stacks. Optical measurements and electrochemical data confirm that these materials are narrow-gap semiconductors. Remarkably, the optical band gap systematically narrows upon increasing the number of methyl substituents on the donor, demonstrating effective electronic structure tuning via simple chemical modification.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Crystals of Polymeric Complexes Containing a Triphenylphosphine Fragment

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The study of non-covalent interactions in polymers provides a deeper insight into the mechanisms of structure formation and enables targeted control over material properties. Understanding of these interactions coupled with the ability to directionally synthesize compounds with predetermined characteristics facilitates a more comprehensive investigation of the properties of the resulting materials and broadens the scope of their potential applications.

This work presents analysis of molecular and crystal structures of the reaction products of phosphorus-containing pyrrolidine derivatives with copper, zinc, and cobalt salts. It is shown that in some cases, metal complexes are formed with anions of monocarboxylic acids and pyrrolidine ligands, while in others, the ligand is decomposed into pyrrolidine and dioxodiphenylphosphinate parts, resulting in the formation of corresponding complexes. The pyrrolidine complexes have a molecular structure, while the phosphinate complexes have a polymeric one. Polymer complexes are formed presumably due to catalysis by the metal ions used (Fig. 1). Analysis of non-covalent interactions has shown that both in pyrrolidine and phosphinate complexes the crystals are formed mainly due to weak interactions – CH...O, CH...F, CH... π , as well as weak π ... π overlaps. In addition, in some complexes, interactions of the P...O and P...N type are formed. The presence of such non-covalent interactions is of particular interest for investigation.

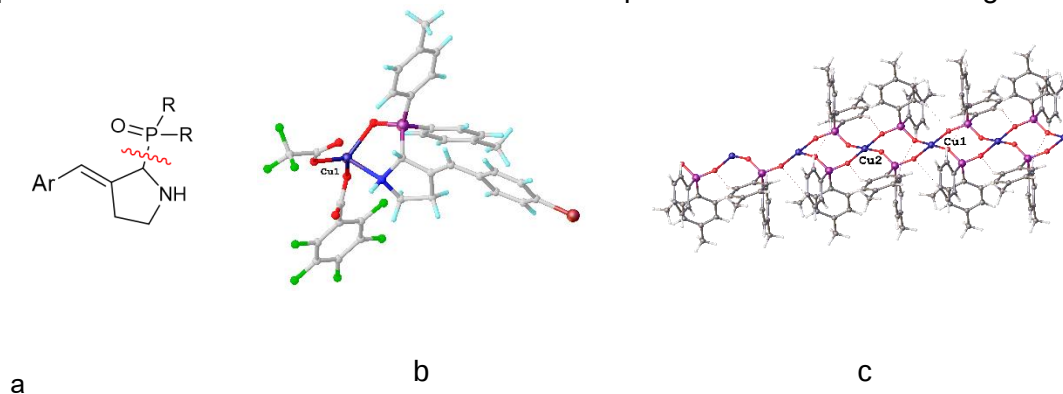


Fig.1 a) Scheme of bond breaking in ligand during the reaction; b) Molecular copper complex with phosphorus-containing pyrrolidine; c) Polymeric structure of the copper phosphinate complex

Acknowledgements

This work was supported by the Russian Science Foundation (project no. 23-13-00374-П)

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

From the Pauli Exclusion Principle to Electron Pairs: Exchange Charge Density as a Structural Descriptor

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The present work reports recent advances in the development of novel descriptors of chemical structure, which are based on the topology of the conservative exchange force field—a property whose distribution reflects the Pauli exclusion principle.^{1, 2}

In particular, the exchange charge density can be expressed in terms of a set of averaged characteristics of the exchange hole density: its local contribution, delocalization, and curvature.³ This, in turn, allows zones of negative values of this function to be interpreted as regions of the condensation of the density of electron pairs.⁴ Analysis of the exchange charge density distribution makes it possible to relate its structural features to chemically important concepts, such as lone and bonding electron pairs and core and valence electron shells.^{4, 5}

Within the local density approximation, the exchange charge density retains most of its structural features, which enables its use for the analysis of crystal structures derived from high-resolution, precision X-ray diffraction data.⁶

Acknowledgements

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Synthesis of Polyfluoroaromatic Selenides with Triazole Fragments as Donors of Non-covalent Interactions

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Chalcogen bonds have many useful applications, including construction of nanostructures, synthesis of organic conductors and usage in catalysis.¹ Based on the variety of applications of chalcogen bonds, it is essential to develop synthesis methods of compounds, which can potentially form strong chalcogen bonds, such as polyfluoroaromatic chalcogenides. The ability of forming chalcogen bonds can be described by the size of σ -hole on a chalcogen atom, which is commonly evaluated using ESP maps.² The usage of EWG is the simplest way to increase σ -hole on a chalcogen atom.

The key idea of this work is to increase σ -hole by adding a triazole fragment in polyfluorinated aryl substituents. The ESP was calculated for two similar compounds and the σ -hole on the Se atom turned out to be larger for the compound containing the triazole fragment (**Fig. 1**). Therefore, we developed the convenient method for the synthesis of previously unavailable selenides with a triazole fragment. These compounds are multifunctional donors of non-covalent interactions, including both stronger chalcogen bonds and stacking interactions and hydrogen bonds, including with the proton of the triazole fragment.

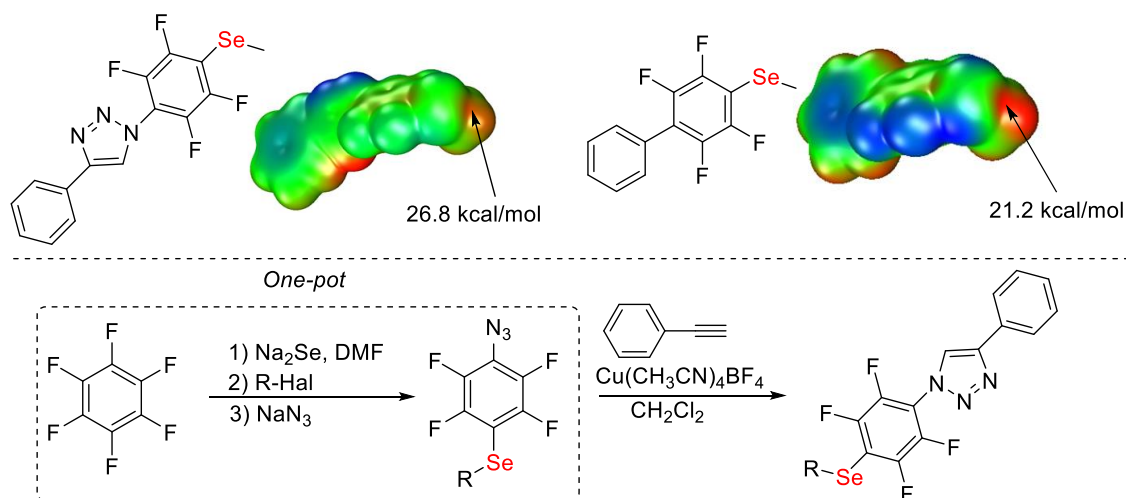


Figure 1. ESP maps: sizes of σ -holes comparison

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Sterically promoted organometallic synthesis of benzo[g]indoles

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Given the importance of indoles dozens of synthetic approaches were developed over the last decades. However, there is a lack of structurally simple methods, such as, for instance, intramolecular nucleophilic addition of α -aminomethyl lithium moiety to *ortho*-carbonyl group. The only implementations of such synthetic idea are two works of A. F. Pozharskii's research group^{1,2}. However, to this day the reaction scope is limited to a few examples of 1,8-bis(dimethylamino)naphthalene derivatives.

In this work we elucidate the influence of the buttressing effect on the cyclization of 2-methoxycarbonyl-1-dimethylamino-8-substituted naphthalenes **1** into benzo[g]indole derivatives **4** upon treatment with organolithium reagents. We demonstrate that 2-lithio-1-dimethylaminoarenes **2** bearing substituent in *ortho*- or *peri*-position exhibit highest efficiency for the indole formation (Fig. 1). This is due to the manifestation of buttressing effect, providing optimal balance between association, nucleophilicity and basicity of studied organolithiums. Buttressing effect plays key role in the activation of a substrate via steric pressure of substituent in position 8 on 1-NMe₂ group contributing to the formation of confined reaction center. Based on our experiments potential reaction intermediates indolone **5**, ketone **6** are excluded in favor of hemiketal complex **3**. The latter provides proximity of reacting centers via coordination of organolithium reagent to the initially formed hemiketal, allowing concerted deprotonation-substitution leading to the formation of dihydropyrrole ring.

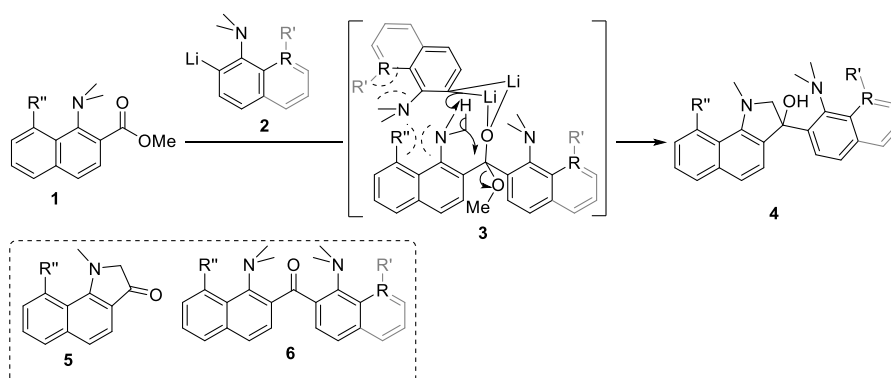


Figure 1. Sterically promoted organometallic synthesis of benzo[g]indoles

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Cooperative Effects of Noncovalent Interactions on I...N Halogen Bonds in C₆F₄I₂...HMTA Complexes

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Halogen bond (XB) is a directional noncovalent interaction between an electrophilic halogen atom and a nucleophilic site, widely used in supramolecular chemistry, catalysis, drug design, and materials science.¹ However, most theoretical studies of XBs rely on static calculations of isolated complexes in vacuum, neglecting additional interactions (NCIs) present in condensed phases and their dynamic nature. In real systems the interplay of multiple NCIs rather than isolated XBs drives complex assembly processes.²

In our work, we investigate how different types of additional NCIs modulate the strength and geometry of the I...N XBs in complexes of diiodotetrafluorobenzene (C₆F₄I₂) with hexamethylenetetramine (HMTA). These systems represent typical and widely used strong XB donors and acceptors and enable the analysis of multiple XBs formation. We combine static DFT/QTAIM/SAPT0 analysis of finite molecular clusters with *ab initio* molecular dynamics in explicit CHCl₃ solvent to quantify cooperativity effects. We show that additional NCIs can either strengthen and shorten the XB (cooperative effect), as observed for C–H...F hydrogen bonds and π ... π stacking, or elongate and weaken it (anti-cooperative effect), for example in the presence of a second I...N XB. The effects in solution are controlled by statistical occurrence of NCIs: cooperative C–H...I and C–H...F interactions are rare, short-lived contacts, whereas anti-cooperative C–H...N hydrogen bonds form a persistent contribution along the trajectories. These findings show how specific types of NCIs modulate XB strength and geometry, providing practical principles for rational design and application of XB-based catalysts and functional materials.

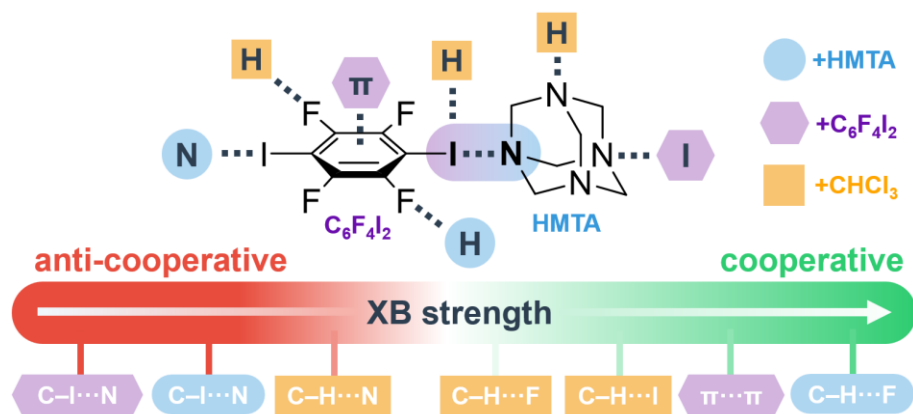


Figure 1. Examples of NCIs and their cooperativity effects on I...N XB considered in this work.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hydrogen and tetrel bonding in reactions of silanes with proton donors and CO₂

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Silanes are promising hydrogen carriers due to their low toxicity and ability to release hydrogen under mild conditions. Furthermore, silanes are widely used as reducing agents delivering hydride equivalents to unsaturated substrates such as carbonyls or CO₂, avoiding the direct use of molecular hydrogen. In this work, the solvent-free dehydrocoupling of phenylsilanes with alcohols in the presence of triethylamine was studied to produce molecular hydrogen and alkoxy silanes. Based on our previous works^{1, 2} and new kinetic investigations, we propose two distinct mechanisms depending on alcohol acidity: more acidic alcohols are deprotonated by the amine resulting in an alkoxide anion that coordinates to silane forming a tetrel bond, while less acidic alcohols (e.g., methanol) instead form a trimolecular hydrogen-bonded complex. Additionally, PNP-pincer complexes of group 10 metals were tested as catalysts in dehydrocoupling of phenylsilane with methanol. Despite relatively high basicity of the pincer ligand's nitrogen atom, these complexes, similarly to Et₃N, are unable to deprotonate methanol, forming instead a hydrogen bond. That leads to O–H bond activation and coordination to the silane before releasing H₂.³ The study also addressed the hydrosilylation of CO₂ and benzaldehyde with phenylsilanes, catalyzed by nickel complexes with naphthalene-based PCP-pincer ligands using thermal or UV activation. Adding B(C₆F₅)₃ as a Lewis acid co-catalyst enabled room-temperature reactions as well as improved silane conversions.

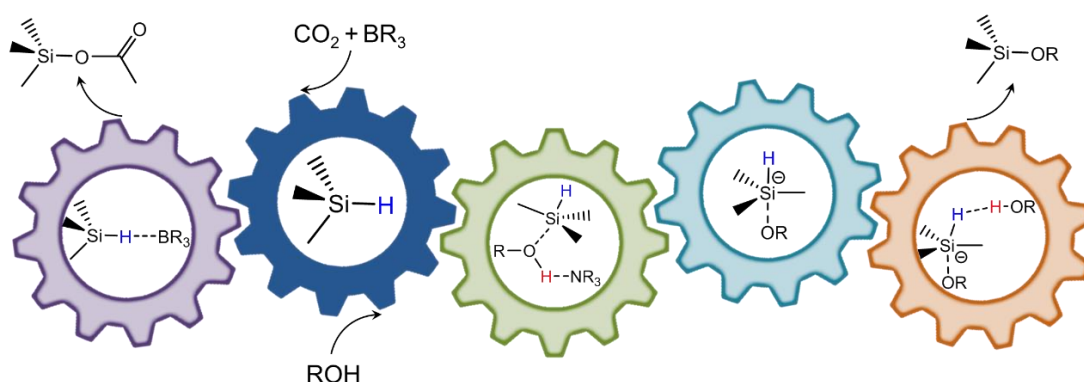


Figure 1.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Molecular Docking Study of Non-Covalent Interactions in Nitroxoline Inclusion Complexes with Functionalized β -Cyclodextrins

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Nitroxoline is a widely utilized antibiotic effective against various urinary tract infections.¹ However, its clinical application is significantly hindered by its poor aqueous solubility and low bioavailability. Encapsulation within functionalized β -cyclodextrin derivatives such as 2-Hydroxypropyl- β -cyclodextrin (HP- β -CD)², Methyl- β -cyclodextrin (Me- β -CD)³, and Sodium sulfobutyl ether β -cyclodextrin (SBE- β -CD), offers a promising strategy to substantially enhance the drug's aqueous solubility and overall bioavailability. The nature of host-guest complexation within these supramolecular assemblies is effectively elucidated through molecular docking using AutoDock Vina. According to the molecular docking results (Figure 1), the HP- β -CD complex exhibits the highest stability with a binding affinity of -5.7 kcal/mol, primarily driven by conventional hydrogen bonds (acceptor-acceptor type), whereas the Me- β -CD and SBE- β -CD complexes show slightly lower affinities of -5.1 and -5.0 kcal/mol, respectively. These *in silico* findings highlight the decisive role of specific non-covalent interactions in the formation of β -cyclodextrin supramolecular assemblies.

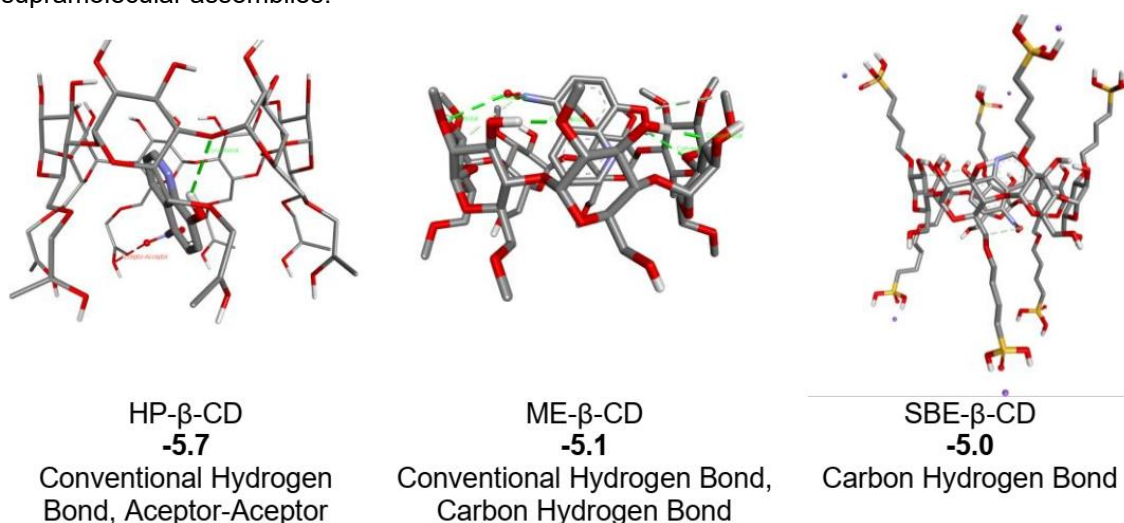


Figure 1. 3D molecular docking models, binding affinities (kcal/mol), and interaction profiles of nitroxoline inclusion complexes with HP- β -CD, ME- β -CD, and SBE- β -CD

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Cocrystals of 4-nitro-5-chalcogenocyanatophthalonitriles with α -haloazines

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It was shown earlier that 4-nitro-5-halophthalonitriles act as efficient halogen bond donors,¹ while their thio- and selenocyanato analogues (NPN-SCN and NPN-SeCN) can serve as supramolecular building blocks in cocrystallization with haloarenes.² In continuation of these studies, cocrystallization of NPN-SCN and NPN-SeCN with α -haloazines was performed. Four new cocrystals were obtained: NPN-SCN·(2-PyCl), NPN-SeCN·(2-PyCl), NPN-SeCN·(2-PyBr), and NPN-SeCN·(1-IsoqCl). The structures of all cocrystals were established by X-ray diffraction (Figure 1). It was found that NPN-SCN·(2-PyCl) and NPN-SeCN·(2-PyBr) are isostructural and exhibit identical packing patterns, whereas NPN-SeCN·(2-PyCl) and NPN-SeCN·(1-IsoqCl) demonstrate similar packing despite differences in their unit cell parameters. In all obtained structures, two types of noncovalent interactions responsible for supramolecular organization were identified: short Ch...N contacts and stacking interactions. Notably, halogen bonds X...N_{cyno}, characteristic of previously studied cocrystals with aryl halides,² were observed only in one pair of cocrystals: NPN-SCN·(2-PyCl) and NPN-SeCN·(2-PyBr). For NPN-SeCN·(2-PyCl) and NPN-SeCN·(1-IsoqCl), such contacts are not formed.

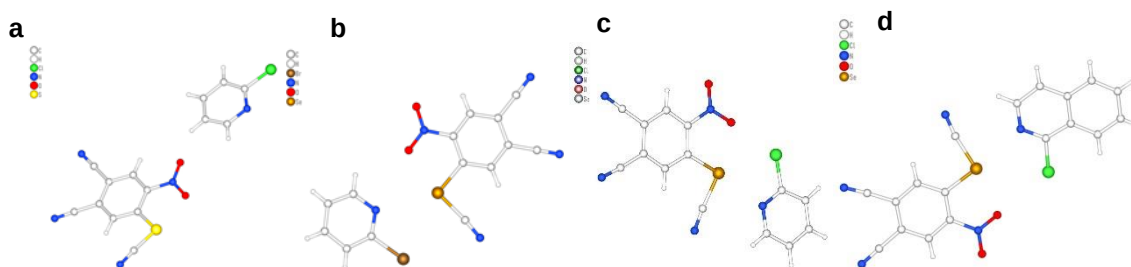


Figure 1. X-ray structures of cocrystals NPN-SCN·(2-PyCl) (a), NPN-SeCN·(2-PyBr) (b), NPN-SeCN·(2-PyCl) (c), and NPN-SeCN·(1-IsoqCl) (d)

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Pyridine C–H arylation reaction: hydrogen-bonding makes the difference

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Pyridine and its derivatives constitute an important class of N-heterocyclic compounds. Due to pyridine lone pair ability to engage in non-covalent interactions, these molecular motifs are widely used in supramolecular chemistry.¹ Yet, the precise control of N-donor strength depends on the one's synthetic ability to introduce functional groups at any needed molecular position. In this regard, the C–H pyridine activation seems appealing since it does not require pre-functionalization steps and relies on intrinsic molecular properties.

Here we present Pd-catalyzed C–H pyridine arylation approach based on C–H bond activation via hydrogen bond formation between ligand **L** and a substrate. Contrary to the literature precedent,² the pyridone-type ligand **L** was found to be effective in this transformation, allowing for the formation of arylated compounds. It was observed, that the reaction outcome strongly depended on the nature of substituents of both substrate and arylating agents. The electron-withdrawing groups promoted the transformation, while electron-donating groups suppressed the reaction.

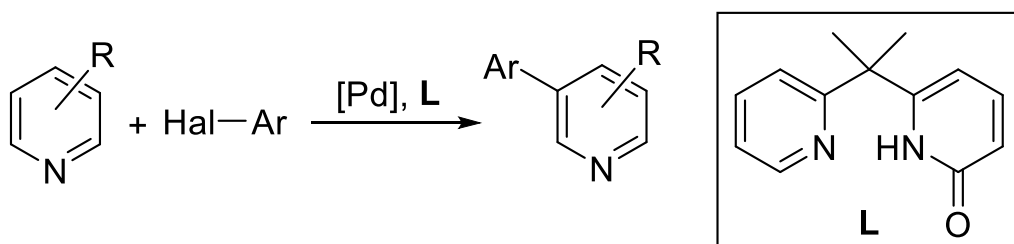


Figure 1. Arylation of pyridine and its derivatives

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«Racemic compound-like» crystallization of homochiral organic compounds: the role of prostereogenic groups in the formation of pseudosymmetry elements

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The crystallization options for homochiral samples of organic compounds are limited by the limited set of symmetry elements inherent in chiral space groups, which imposes certain conditions on the implementation of a particular homochiral associate in a crystal. Thus, a hydrogen-bonded homochiral chain in a crystal can be formed either by simple translation or by a helical axis – only these options are possible if there is a single independent molecule in the crystal. At the same time, the inclusion of an additional independent molecule in the cell makes it possible to implement a pseudosymmetric motif, similar to packages of truly racemic crystals. As a rule, pseudosymmetric crystallization of this kind is achieved due to significant conformational shifts of molecule B relative to molecule A. An interesting intrigue arises for systems containing a chiral hydrocarbon fragment in a natural configuration, carrying all the asymmetric centers of the molecule, and a prochiral substituent carrying functional groups capable of hydrogen bonding. What type is (pseudo)symmetry realized in a crystal? Which fragment will be the decisive influence? Of particular interest is the "work" of labile chiral centers (for example, the nitrogen atom) and prochiral groups: the sulfone group, the methylene group, the sides of the carbonyl group, and the LP on the formation of secondary interactions in a homochiral crystal. Namely, in the case of pseudosymmetric crystallization, the prochiral group is forced to participate by various atoms with opposite stereochemical descriptors in order to adjust to the emerging local non-crystallographic element of symmetry (center or plane). The report presents systems of this type: BODIPY derivatives with a myrtene fragment, mentanysulfone and fluoroquinolone derivatives with a pinene fragment.

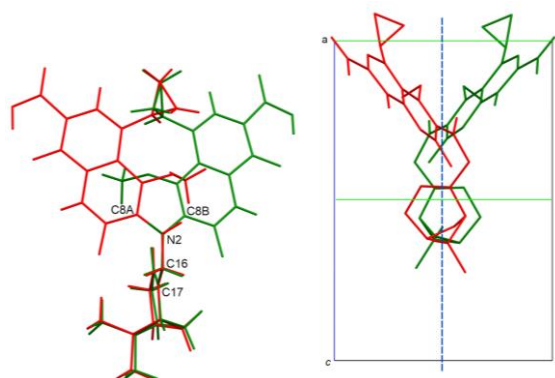


Figure 1. Pseudo-glide plane in a chiral crystal of a fluoroquinolone derivative

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Chalcogen Bond Donors Featuring the Ar^F–Ar Motif: Synthesis and Self-Assembly

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Polyfluoroaromatic chalcogenides have attracted considerable interest as versatile donors for noncovalent interactions, owing to the presence of both σ -holes on the chalcogen atom and π -holes on the polyfluoroaromatic rings.¹ In our recent work, we developed a synthetic route to selenides incorporating the Ar^F–Ar motif.² Many of the resulting compounds exhibit a remarkable tendency to form porous molecular crystals (PMCs) when crystallized from certain solvents.

This report explores the self-assembly of chalcogenides incorporating the Ar^F–Ar motif (**Fig. 1**, top). We will discuss: (i) the key noncovalent interactions between chalcogenide molecules that lead to different PMCs; (ii) the impact of substituents, chalcogen atoms, and solvent substitution on the type of PMC formed; and (iii) the structural changes accompanying solvent removal and replacement (**Fig. 1**, bottom).

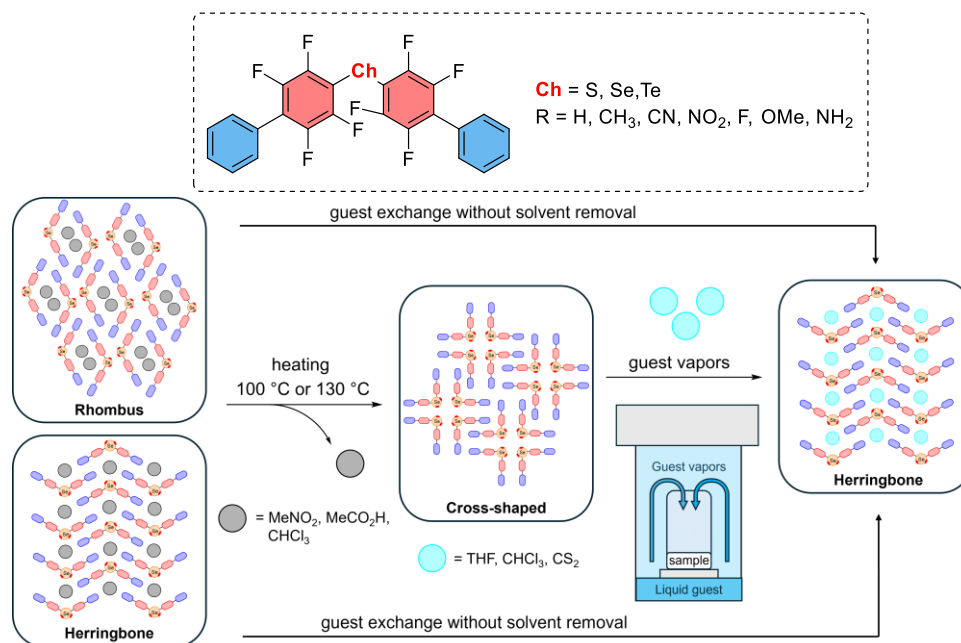


Figure 1. Structural type changes in PMCs upon guest removal and replacement

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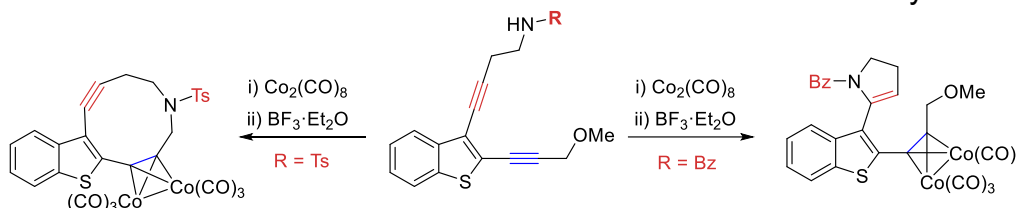
IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Role of π - π stacking in cyclization pathways of heterocycle-fused enediynes under Nicholas reaction conditions

Vladimir E. Melnikov, Elena Yu. Tupikina, Ekaterina A. Khmelevskaya, Natalia A. Danilkina, Irina A. Balova

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Electrophile-promoted cyclization is a powerful tool for the formation medium-sized heterocycles¹. However, it can sometimes become an undesirable process. For example, intramolecular hydroamination in benzothiophene-fused enediynes has been observed for the N-Bz derivative, instead of the expected Nicholas reaction observed for the N-Ts analogue (Scheme 1)². Recent studies indicate that the same trend is observed in N-Me indole-fused enediynes.



Scheme 1. Observed electrophilic cyclization of benzothiophene-fused enediynes

The aim of this work is to evaluate the role of noncovalent interactions, specifically π - π stacking, in the observed reaction pathways. Preliminary DFT calculations suggest that π - π stacking interactions are present in key structures along both reaction pathways (Figure 1).

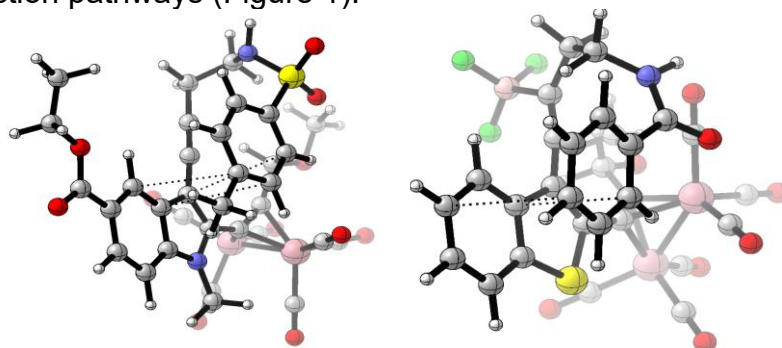


Figure 1. Observed structures with π - π stacking

DFT calculations will be performed to quantify the energetic contribution of π - π interactions to the stabilization of intermediates and/or transition states in competing pathways. The results are expected to provide a clearer understanding of how non-covalent interactions influence reaction selectivity in heterocycle-fused enediyne systems.

Acknowledgements

The study was supported by RSF (project № 25-73-20075), and carried out using the equipment of the SPbU Resource Center "Computer Centre"

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Crystals of 3-(4-bromobenzylidene)-2,5-dihydro-1*H*-pyrrolinium salts with benzoic acid: structure and non-covalent interactions

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At present it is evident that multicomponent crystals are suitable objects to combine the search for new molecular structures with the solution of specific practical tasks. In medicinal chemistry cocrystals allow for the targeted modification of properties of an active substance without altering its chemical structure. It is possible to increase the solubility of poorly soluble compounds through cocrystallization, enhance their bioavailability, improve powder flowability and compactibility, and achieve sustained drug release.¹ Beyond medicine, cocrystals are in demand for the creation of materials with specific optical and electronic characteristics. Multicomponent systems with conjugated π -systems and charge transfer are used in the creation of sensors, nonlinear optics, and as organic electronic components.²

This work presents a study of the molecular and crystal structures, as well as a detailed analysis of the crystal packing of polymorphic salts of arylidene-pyrrolidine with benzoic acid. It is evident that the main structural interaction in both crystals is hydrogen bonding, which forms an associate of two acid molecules and one pyrrolidine molecule in one case, and a classical ionic pair in the other. A wide range of interactions, including π - π interactions between aromatic rings and halogen contacts involving bromine atoms, contribute to the formation of the three-dimensional crystal structure. Analysis of their balance provides a key to the prediction of the properties of a crystal.

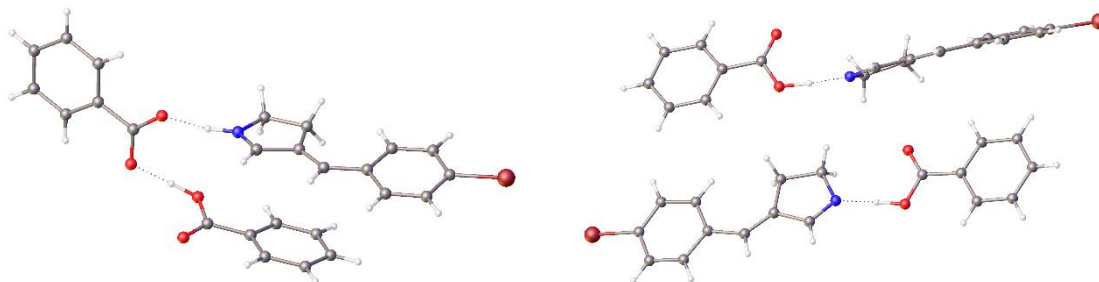


Figure 1 Cocrystals of benzoic acid and p-bromo-substituted 3-arylidene-pyrrolidine in different ratios

Acknowledgements

This work was supported by the Russian Science Foundation (project no. 23-13-00374-П)

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

A data-driven framework for classification of carbon–lithium bonding in organolithium aggregates using quantum chemical descriptors

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Organolithium compounds are key reagents in synthetic chemistry; however, their reactivity is governed by complex aggregation behavior and the nontrivial nature of the carbon–lithium (C–Li) bond. The latter cannot be unambiguously classified as purely covalent or purely ionic and spans a continuum from two-center to multicenter and nonclassical.

In this work, we present a data-driven framework for the classification of C–Li bonding motifs based on quantum chemical descriptors. A dataset of 81 *ab initio*-optimized aggregates (600 C–Li bonds) of methyllithium, *tert*-butyllithium, and phenyllithium was constructed to span a wide range of aggregation states and coordination environments.¹

A set of geometric, electronic, and topological descriptors derived from QTAIM and ELF analyses was evaluated and reduced to a minimal physically interpretable subset. The ELF basin electron population ($\langle \text{ELFpdr}^3 \rangle$) was identified as the key descriptor governing bonding classification.

Machine learning models, including a multitask neural network and a bootstrap-aggregated decision tree model, achieved high classification accuracy (up to 89%) for nucleophile type, aggregation state, and bond type.¹ Feature importance analysis revealed strong agreement between models and confirmed the dominant role of ELF-based descriptors.

Projection of the descriptor space demonstrates that C–Li bond types are well separated, whereas aggregation state and nucleophile identity show significant overlap, reflecting their continuous nature.

The proposed framework provides a scalable and interpretable approach for automated analysis of organolithium bonding and can serve as a basis for high-throughput studies of non-covalent and multi-center interactions in organometallic systems.

Acknowledgements

This work was financially supported by the RSF Grant No. 24-73-10155. Research was carried out using computational resources provided by the "Center for Computational Resources of National Research Center Kurchatov Institute" (<https://www.jscc.ru>) and the "Computer Center of SPbU" (<http://cc.spbu.ru>).

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Self-organisation of porphyrazines: a design of potential phototherapeutic agents

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Porphyrazines are an important class of tetrapyrrolic macrocycles, and their carboxylated forms attract ongoing researchers interest due to their potential applications in catalysis, sensing, photovoltaics and biomedicine.

In this work, we investigated the photochemical behavior of new octa-carboxyphenyl-substituted quinoxalinoporphyrazines (QPzR₈) in aqueous solutions and compared it with that of the corresponding pyrazinoporphyrazines (PyzPzR₈)^{1,2} (Fig. 1).

We observed patterns of change in the aggregation behavior of the synthesized macroheterocycles in solution, depending on the nature of the substituents and the solvent. This allows the photophysical properties of the complexes to be regulated.

We have found that aggregated forms of quinoxalinoporphyrazines can exhibit a photothermal effect. This ability, in combination with their absorption in the near-infrared therapeutic window and their higher stability compared to naphthalocyanines, establishes the potential of the obtained quinoxalinoporphyrazines as promising phototherapeutic agents.

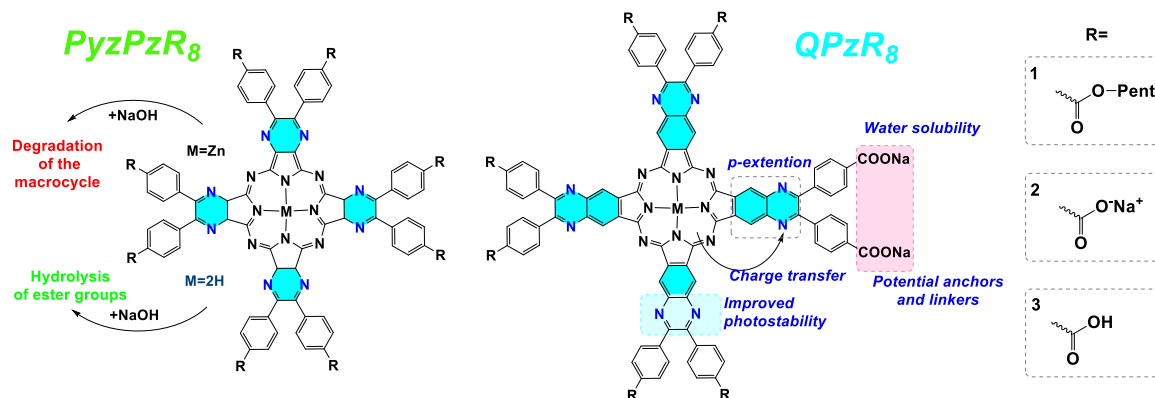


Figure 1. Structures of pyrazinoporphyrazines (PyzPzR₈) and quinoxalinoporphyrazines (QPzR₈)

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This work was supported by the grant of the Russian Science Foundation № 25-23-00419

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Structural features and bonding variability in the design of polynuclear copper(II) complexes with benzimidazole derivatives

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A systematic study of copper(II) complexation with benzimidazole derivatives bearing $-\text{CH}=\text{N}-$ (L^1) and $-\text{CH}_2-\text{NH}-$ (L^2) linkers revealed the influence of the solvent and the starting reagents on the product composition. New hexanuclear copper(II) complexes were obtained: $[\text{Cu}_6\text{Cl}_4(\text{BzCOO})_2\{(\text{BzCO})_2\text{O}\}_2]$ (**1**) ($\text{Bz} = 1\text{-methyl-1H-benzo[d]imidazol-2-yl}$) and $[\text{Cu}_6(\mu_2\text{-Cl})_6(\text{L}^{2'})_3]$ (**2**) ($\text{L}^{2'} = \text{N-(1-isopropyl-1H-benzo[d]imidazol-2-yl)-1-methyl-1H-benzo[d]imidazole-2-carboxamide}$). Complexes **1** and **2** were characterized by elemental analysis, IR and Raman spectroscopy and SC-XRD.

Complex **1** consists of tetranuclear and binuclear Cu-Cu chains with distances of 3.0561, 2.940, 2.995 Å, respectively, linked by a bridging BzCOO group formed *in situ*. The tetranuclear chain Cu centers are bridged by O atoms from $(\text{BzCO})_2\text{O}$; terminal Cu atoms are additionally coordinated by an imidazolium N atom and Cl^- . In the binuclear chain, Cu coordinates an O(BzCOO) and Cl^- . π - π stacking between aromatic rings is observed at 3.548 Å (Fig. 1a).

Complex **2** features nearly identical closed trinuclear Cu chains formed by bridging Cl atoms, linked by three $\text{L}^{2'}$ (formed *in situ*) ligands and a hydrogen atom delocalized between two bridging O atoms (Fig. 1b).

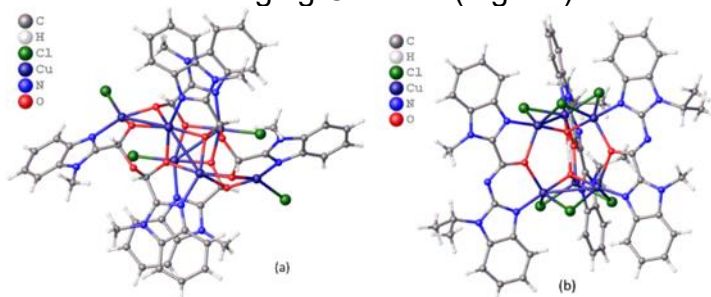


Figure 1. Molecular structures of complexes 1(a) and 2(b)

Thus, the high variability of chemical bonding in hexanuclear Cu(II) complexes **1-2** — including donor–acceptor interactions, metal–metal bonds, hydrogen bonds, and non-covalent aromatic interactions — serves as a tool for forming preorganized structures in single crystals. Magnetic exchange processes in clusters **1** and **2** were studied, and the results analyzed in the context of composition–structure–property relationships.

This work was performed within the framework of the state assignment of the Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, in the field of fundamental scientific research.



Cluster approach to estimation of the noncovalent interactions' energy in a crystal

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A wide variety of noncovalent interactions shapes and stabilizes the crystal structure. The most accurate tools for quantitatively estimating the energy of noncovalent interactions in crystals require quantum chemical calculations and, therefore, are often critically time-consuming. Optimizing the time and resource costs of determining the energy of noncovalent interactions in crystals remains a pressing issue.

The cluster approach involves calculating the energy of each dimer, consisting of the parent and adjacent molecules in the crystal structure. This conceptually simple approach allows for the automation of the calculation process and the estimation of the energy of noncovalent interactions without resorting to periodicity simulation. In this work, a machine-learned model was developed that can predict the energy of noncovalent interactions of a molecule in a crystal based on its set of crystalline dimers, and patterns in the formation of noncovalent interactions in crystals were also identified.

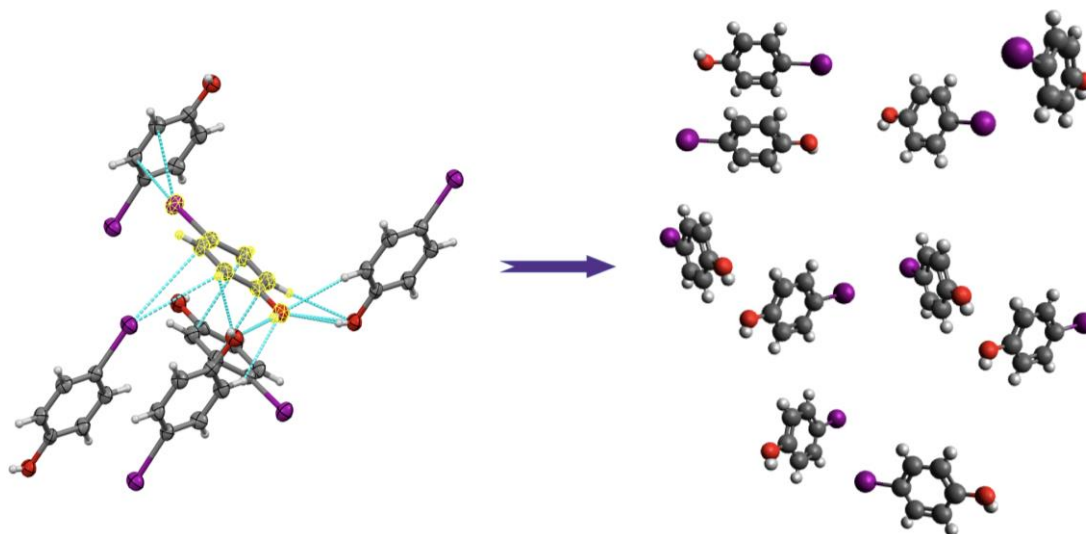


Figure 1. Visualization of the generation of a dimer set from a crystal structure cif-file



A new method for determining $\pi - \pi$ interactions in crystal structures

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The relevance of studying $\pi - \pi$ bonding in crystal structures is due to its key role in the formation of stable supramolecular assemblies, molecular crystals and sorbate-sorbent interactions in porous materials such as metal-organic frameworks. To determine and analyze $\pi - \pi$ interactions in a large number of crystal structures, one needs rigorous algorithms and robust criteria, which should be implemented into user-friendly software.

We have developed a new method for determining π -stacking interactions in crystal structures of any complexity and composition. Our approach based on the following geometric parameters: the distance d between the centroids of the aromatic rings (Fig. 1a), the angles α_1 and α_2 between the line connecting the centroids of two aromatic rings and the planes in which these rings lie (Fig. 1b), the tilt angle of one fragment relative to another, which is equal to the angle β between the normals to their planes (Fig. 1c), and the degrees of planarity of the interacting fragments, i.e. average deviation of atoms from the root-mean-square plane of the ring. We have computed these parameters for more than 90000 molecular coordination compounds and determined their limiting criteria, which characterize π -stacking interactions. The method is implemented in the AutoCN program, which is a part of the ToposPro program package¹. We have discussed how different types of π -stacking interactions can be determined based on the found criteria. The resulting π -stacking topological motifs are determined and classified.

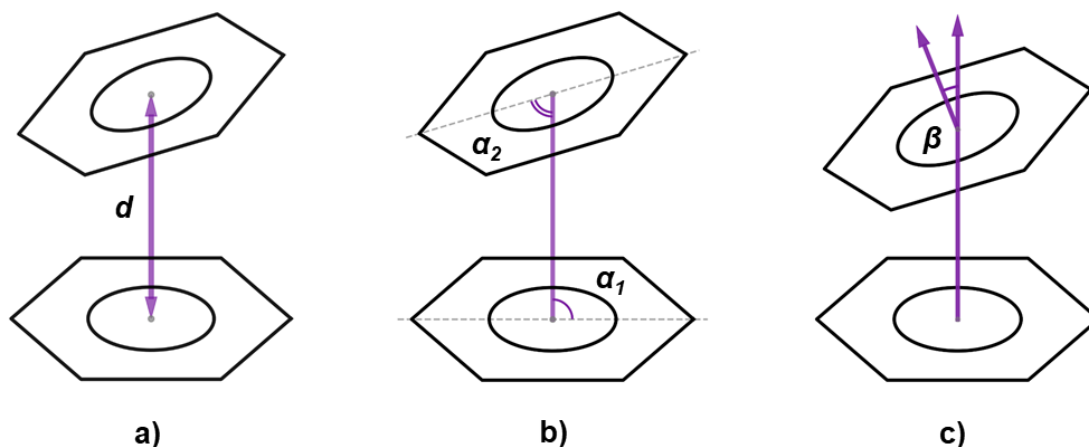


Figure 1. Geometric criteria for determining π -stacking interactions.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Computational Study of Intermolecular Interactions in Polycaprolactone-Based Drug–Polymer Systems

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Cytostatic agents are widely used in cancer therapy; however, their high toxicity and limited selectivity significantly restrict their clinical efficacy. Therefore, the development of nanoparticle-based drug delivery systems enabling controlled and predictable release of cytostatic agents remains an important challenge.

As a preliminary step, optimal computational approaches (functionals and basis sets) are being evaluated for two antituberculosis drugs, Dioxadet and Perclozone, which differ in their chemical nature: Perclozone is ionic, whereas Dioxadet is a neutral covalent molecule.

This work focuses on the nature and energetics of intermolecular interactions between Dioxadet (DXT) and PCL. Hartree-Fock and density functional theory (DFT) calculations with various basis sets were performed using Gaussian and ORCA packages; wavefunction analysis was carried out with Multiwfn. Conformational analysis and quantitative characterization of noncovalent interactions were performed. In particular, bond critical points corresponding to key hydrogen bonds were identified and analyzed within the QTAIM framework using the Lagrangian kinetic energy density, confirming the stabilizing character of the DXT–PCL interactions.

The results indicate that the B3LYP/6–31G(d) level provides a balanced and reliable description of the DXT–PCL system (Figure 1). Hydrogen bonding is the dominant stabilizing interaction, while dispersion contributions also play a significant role. The Perclozone–PCL system is currently under investigation. These findings contribute to the rational design of polycaprolactone-based drug delivery systems.

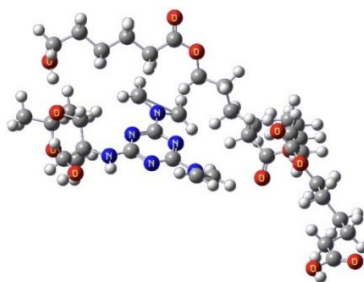


Figure 1. Optimized geometry of the DXT–PCL complex (four PCL chains) at the B3LYP/6–31G(d) level.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Development of QTAIM-based correlations for estimating C–H···X (X = O, N) hydrogen bond energies

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Hydrogen bonds play a key role in both the structure and properties of organic molecules, biomolecules, and supramolecular assemblies. For rational drug and material design, reliable estimation of hydrogen bond energy is crucial. However, there is no generally applicable and reliable approach to address this task. Therefore, the development of methods for quantitative assessment of hydrogen bond energy remains an important problem.¹ One approach to estimating hydrogen bond energy in complex systems is based on correlations with structural or QTAIM descriptors at the bond critical point (BCP).

In this work, we developed equations establishing quantitative relationships between hydrogen bond energy, geometric parameters and electron density properties. For this purpose DFT calculations were performed (PBE0-D3(BJ)/aug-cc-pVTZ) and QTAIM analysis for 49 C–H···O and 21 C–H···N model complexes with single C–H···X (X = O, N) hydrogen bond. Correlation equations were obtained using the least squares method (Figure 1). To our knowledge, this is the first set of correlations specifically developed for weak C–H···X (X = O, N) hydrogen bonds.

The obtained correlations can be used for quantitative estimation of C–H···X (X = O, N) hydrogen bond energy in biomolecular and supramolecular systems, though the applicability is currently limited to isolated complexes with a single hydrogen bond. The developed equations were applied to the rubredoxin protein which exists in oxidized and reduced forms. We showed that the strength of hydrogen bonds network significantly affects the properties of both redox forms, what is in a good agreement with available experimental data.²

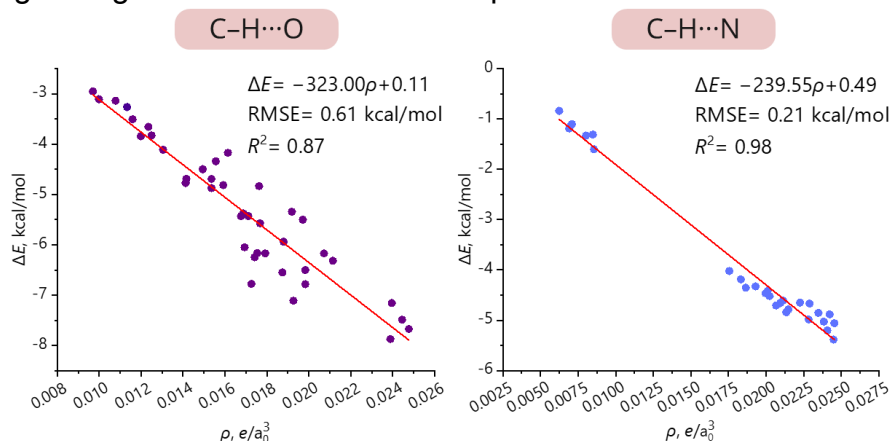


Figure 1. Developed in this work regression lines and correlation equations for C–H···X (X = O, N) hydrogen bonds

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

OPTICALLY ACTIVE SULFONES BASED ON 4-AMINOTHIOPHENOL AND 5-MENTHYLOXY- AND 5-BORNYLOXY-2(5H)-FURANONES: CRYSTAL STRUCTURE AND STEREOCHEMICAL FEATURES

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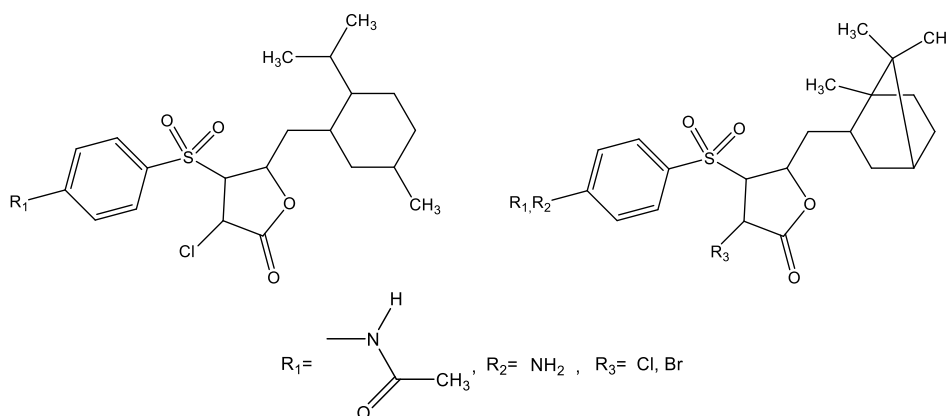
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The sulfones studied in this work are of particular interest as model systems, combining both chiral fragments (menthyl- and bornyloxy-2(5H)-furanones) bearing stereogenic centers of the molecule and achiral substituents: a donor amino group and a sulfonyl group acting as an acceptor and prochiral group. This raises the question of the nature of the supramolecular associates realized in the crystal, as well as their symmetry: do they possess true chirality or represent pseudoracemic forms.

The crystal structure of several chiral compounds of furanone series was studied. All studied compounds are characterized by the presence of two independent molecules in the unit cell, having significant differences both in configuration and in the hydrogen bonding system.



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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Polymorphism in the Crystal Structures of Symmetrical Ortho-Diiodoaromatic Compounds

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Obtaining and understanding the factors governing the formation of polymorphic forms of molecular crystals is an important and highly relevant task in crystallography. This is primarily because most functional materials based on molecular compounds are used in crystalline form, while the physicochemical properties of different polymorphs may vary significantly depending on the features of both the molecular and crystal structure.

The aim of this work was to investigate polymorphism in a series of symmetrically ortho-diiodo-substituted aromatic derivatives¹⁻² in order to identify general trends in intermolecular interactions and supramolecular organization. Using single-crystal X-ray diffraction analysis, the structures of four polymorphic pairs were determined, and a comparative study of their molecular and crystal structures was carried out, including a detailed examination of various non-covalent interactions ($X-H\cdots N$, $X-H\cdots I$, $I\cdots I$, $I\cdots N$, and $\pi\cdots\pi$ interactions).

It was shown that, in a number of derivatives, the nature of intermolecular interactions and the relative arrangement of the molecules influence the geometric parameters of the molecule itself, namely the deviation of the iodine atoms from the plane of the aromatic ring.

It was established that polymorphism in a series of nitrogen-substituted derivatives arises from competition between $I\cdots I$ and $I\cdots N$ non-covalent interactions. Even in the polymorphic pair of 1,2-diamino-4,5-diiodobenzene, where strong hydrogen bonds are present, polymorphism is governed by competition between secondary interactions involving iodine atoms.³

The paper will also present the results of empirical and semi-empirical approaches for visualizing similarities and differences in intermolecular interactions and for estimating their energies, as well as quantum-chemical calculations aimed at evaluating the stability of the polymorphic forms.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Hydricity and reactivity of nickel pincer complexes with naphthalene-based pincer ligands

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Transition metal hydrides are of interest for the development of efficient chemical hydrogen storage systems, as they participate as key intermediates in a range of reactions whose mechanistic steps involve proton transfer, hydride transfer, and H-H bond formation/cleavage^{1,2}. In this context, the hydricity of the M-H bond serves as a key quantitative parameter that enables prediction of the complex's reactivity. Pincer complexes are widely used in homogeneous catalysis due to their stability and the ability to fine-tune the metal center through ligand design^{3,4}. Moreover, considerable attention has recently been devoted to 3d metals, particularly nickel, owing to their lower cost and reduced environmental impact compared to noble metals, however, they are often limited by poor reactivity.

In this work, we propose a novel approach using a naphthalene-based pincer ligands, whose electronic system is capable of responding to external energy input and transmitting this effect directly to the M-H bond. The kinetic hydricity of the complexes was evaluated as a rate constant of the hydride ion abstraction, k_{H^-} , using trityl salts ($[\text{Ph}_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $[(p\text{-MeO-Ph})_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]$) as Lewis acids both in the dark and under UV irradiation ($\lambda = 365 \text{ nm}$). The trends in k_{H^-} obtained suggest for a change of the reaction mechanism from hydride (HT) to hydrogen atom transfer (HAT) upon irradiation. The possibility of HAT was explored also in the reaction of phenylsilane addition to olefins catalyzed by title nickel hydrides under UV irradiation.

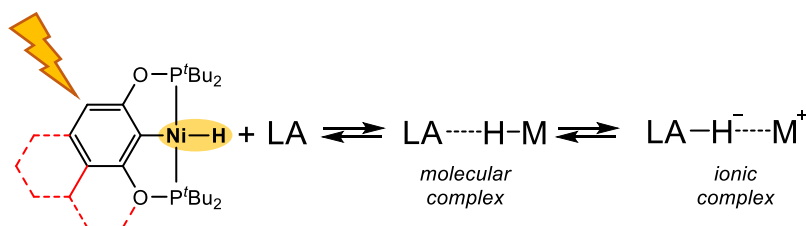


Figure 2. Hydride transfer from a metal hydride M-H to a Lewis acid (LA) accompanied by noncovalent interactions.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Analysis of the Structural and Sorption Characteristics of NCC Aerogel-Based Composites Modified with Phenamates Using Nuclear Magnetic Resonance

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Currently, microporous carrier matrices based on aerogels produced using supercritical fluid (SCF) technologies are widely used. The main strategy for modifying poorly soluble active pharmaceutical ingredients (APIs) involves their immobilization in amorphous form within the carrier pores. However, the mechanisms by which the microenvironment influences the properties of these composites remain insufficiently understood, underscoring the relevance of further research. In this study, we present the results of an investigation into composite materials based on nanocrystalline cellulose (NCC) aerogel impregnated with mefenamic acid (MA) and flufenamic acid (FA), using NMR spectroscopy in supercritical carbon dioxide (scCO₂).

Analysis of ¹³C NMR spectra recorded in scCO₂ for the pristine aerogel and the composite samples revealed an upfield shift of the CO₂ carbon signal (from 121.17 to 120.73 ppm for FA), indicating shielding of the carbon atoms due to sorption and incorporation of the dopant into the NCC pores. The characteristic sorption time for the pristine sample was 0.15 h, whereas for the composites with MA and FA it was 0.38 and 0.25 h, respectively, reflecting changes in the sorption properties of the matrix upon doping. Solid-state ¹³C magic-angle spinning (MAS) NMR confirmed that the matrix structure remains unchanged upon introduction of the dopants. In the spectrum of the FA composite, weak signals appeared in the 110–170 ppm region, corresponding to the carbon atoms of FA. A key result was obtained using ¹⁹F MAS NMR for the NCC_FA composite, which contains a trifluoromethyl group. Two signals were observed in the spectrum: one at –62.15 ppm, corresponding to amorphous FA within the pore volume, and another at –65.09 ppm, corresponding to a «liquid-like» state on the pore surface. This observation of two stable phase states of the same API within the porous structure is novel.

Thus, the application of a comprehensive NMR approach enabled a detailed investigation of the structural and sorption characteristics of NCC aerogel-based composites. The findings demonstrate the potential of aerogels as a platform for stabilizing amorphous forms of APIs and open up new opportunities for designing materials with tailored properties for targeted drug delivery.

Acknowledgements

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IV International Symposium “Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering”

Interatomic Charge Transfer and Associated Phenomena in Covalent, Coordination, and Noncovalent Bonds

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The report defines interatomic charge transfer in terms of the superposition of the conservative vector fields of the electrostatic force, the total static force, and the electron density gradient, and asserts a previously unreported response phenomenon induced by charge transfer that is intimately associated with the manifestation of exchange correlation. The proposed definition of interatomic charge transfer is compared with that formulated by Bader and Matta. On this basis, the report advances a critique of entrenched views regarding charge transfer upon complex formation between a Lewis acid and a Lewis base.

In conclusion, the report proposes a new approach for describing chemical structure and its evolution in terms of the superposition of the conservative vector fields of the electrostatic force, the exchange force, and the total static force. The principal types of interatomic interactions are classified according to the mutual spatial arrangement of the corresponding field elements.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

SUPRAMOLECULAR ORGANIZATION IN TERNARY CRYSTALS BASED ON CORONENE AND TCNQ DERIVATIVES

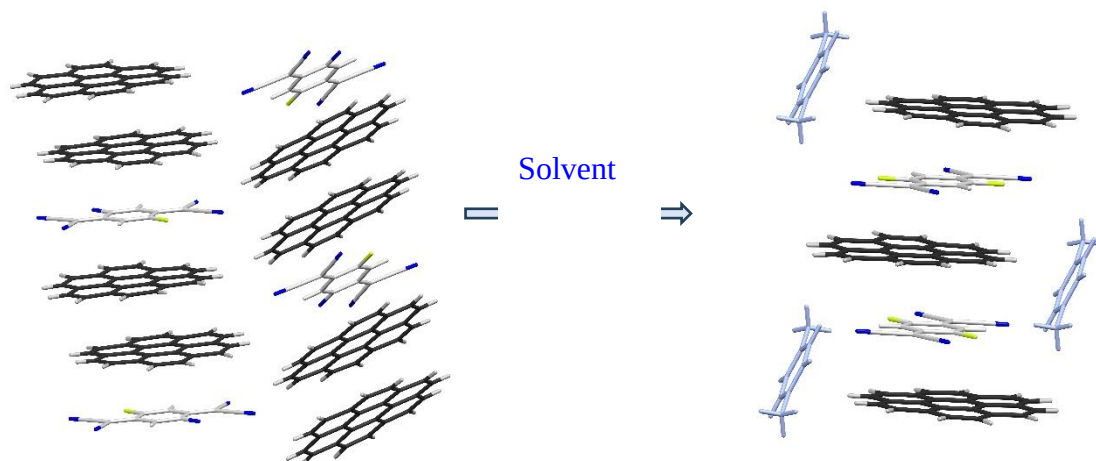
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A series of two- and three-component crystals based on coronene, mono- and difluoro-substituted TCNQ derivatives, and aromatic solvents (ethylbenzene, *para*- and *ortho*-xylene) as a third component has been grown. As it was shown by X-ray single crystal diffraction, the crystals are composed of mixed donor-acceptor stacks with different stoichiometry. The ratio of donor and acceptor molecules in crystals can be varied by the inclusion of aromatic solvents, which are located between the stacks being held by C-H $\cdots\pi$ interactions. They can also affect the disorder of coronene molecules and the tilt of the donor-acceptor stack in crystals.

Thus, solvate aromatic solvents proved to be an effective tool for controlling the ratio of components in donor-acceptor co-crystals and their supramolecular arrangement.



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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Crystal structure features of cyclic thiazine sulfinamides: types of stereoisomeric recognition

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Investigation of stereoisomer recognition processes during crystallization is a fundamental task of supramolecular chemistry and crystal engineering. In this work, using a series of cyclic sulfinamides of the thiazine series as an example, we analyze the evolution of supramolecular motifs from simple chains to complex three-dimensional packings, and also reveal the key role of secondary interactions in stabilizing homochiral associates.

Seven crystal structures of sulfinamides were studied by X-ray diffraction analysis and quantum chemical calculations. It was found that, despite the similar geometry of the molecules, different packing motifs are realized in the crystals. Furthermore, a transition from simple homochiral recognition at the level of 1D chains to complex combined associates and multilevel supramolecular organization governed by a set of non-covalent interactions is demonstrated ¹⁻³.

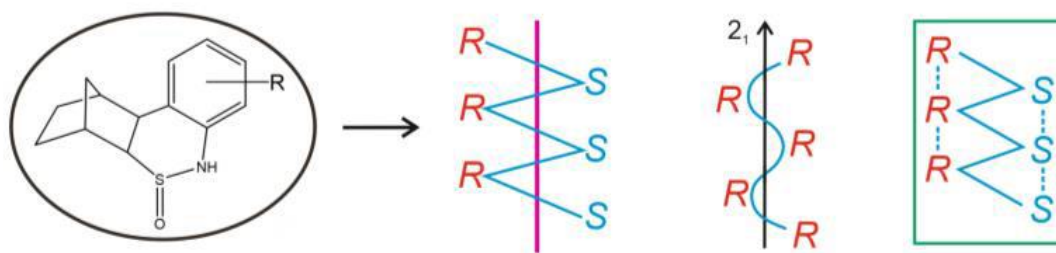


Figure 1. Types of packaging motifs

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Isomorphism of para-substituted polyfluorobiphenyl sulphides

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Porous organic frameworks represent a subject of significant interest in modern applied and fundamental chemistry. These materials can be assembled through weak non-covalent interactions, including hydrogen bonding (hydrogen-bonded organic frameworks, HOFs) and halogen bonding (halogen-bonded organic frameworks, XOFs).

In the present work, we synthesized the *para*-substituted polyfluorobiphenyl sulphides (Figure 1, left) according to a modified previously published method¹. X-ray diffraction (XRD) analysis of the obtained sulfides revealed that these compounds form adducts with solvent molecules. The main molecular framework is formed by complementary aryl-perfluoroaryl interactions between the fluorinated and non-fluorinated rings of the biphenyl substituent.

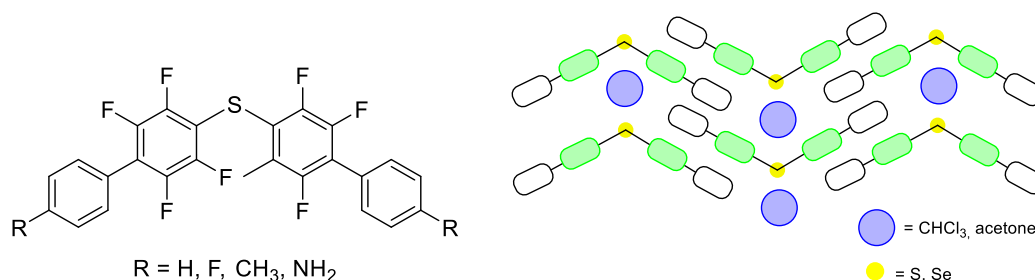


Figure 1. *Para*-substituted polyfluorobiphenyl sulfur derivatives (left) and their crystal packing pattern with a host solvent molecule (right)

Furthermore, their crystal structures were found to be isomorphic with those of the selenium-containing analogues, retaining the same overall structural framework (Figure 1, right). Due to these features, sulfur derivatives can be utilized instead of selenium ones, offering several advantages: non-toxicity, low cost of precursors, and milder reaction conditions for synthesis.

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

H-bond-mediated isomer selection in Pd-complex with pyridone-type chelating ligand

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Non-covalent interactions between ligands in transition metal complexes can stabilize the particular geometry and, as a result, affect the further reaction pathway. Therefore, synthesis and isolation of catalytic intermediates of metal-mediated reactions is an important instrument for mechanism elucidation.¹

Chelating pyridone-type ligands effectively assist the C–H cleavage step in palladium-catalyzed C–H functionalization reactions.² To study the pyridine C–H activation process, we have obtained the first example of Pd-complex **3** with pyridin-3-yl C-ligand and [2,2'-bipyridin]-6(1*H*)-one chelating ligand **2**.

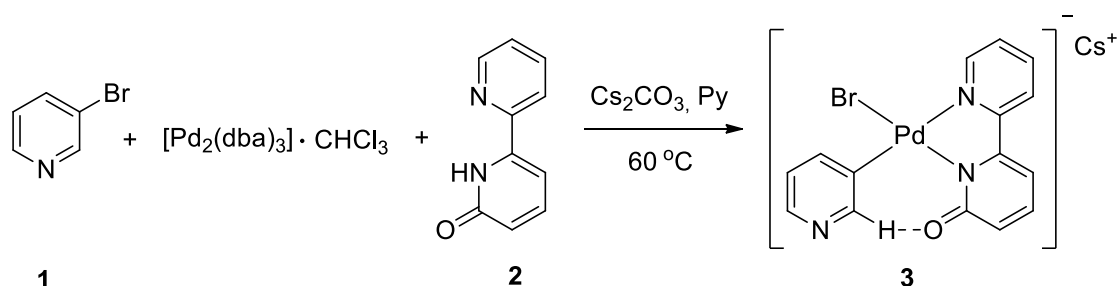


Figure 1. Synthesis of palladium(II) complex via oxidative addition process.

Using NMR spectroscopy, we found that the geometry of the Pd-complex **3** is determined by the H-bonding between the carbonyl group in the pyridone moiety of the ligand and the 2-hydrogen atom of the pyridine-3-yl fragment. Therefore, the oxidative addition of Pd(0) to Ar–Hal was governed by the hydrogen bonding, contrary to the literature examples.³

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Optical properties of graphite-like carbon nitride $g\text{-C}_3\text{N}_4$ of different morphologies

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The main methods of synthesis of graphite-like carbon nitride $g\text{-C}_3\text{N}_4$ samples¹ with different morphologies (spherical nanoparticles $g\text{-C}_3\text{N}_4$ (S1), nanotubes $g\text{-C}_3\text{N}_4$ (S2), nanosheets $g\text{-C}_3\text{N}_4$ (S3), nanotubes $g\text{-C}_3\text{N}_4$ (S4), nanospheres $g\text{-C}_3\text{N}_4$ (S5)) are considered. $g\text{-C}_3\text{N}_4$ layers are connected by non-covalent Van der Waals bonds, which can be easily broken by chemical or ultrasonic treatment. $g\text{-C}_3\text{N}_4$ samples are also used in catalysis for purifying water from organic impurities².

The developed options for the synthesis of such nanoparticles are discussed, in particular, samples of the same modification from different (melamine, dicyandiamide) precursors are obtained and samples are characterized using X-ray diffraction analysis and electron microscopy (Figure 1). Optical properties were determined using diffuse reflection spectroscopy (DDS) (Figure 2) and photoluminescence (PL) methods, which show changes in various optical parameters of $g\text{-C}_3\text{N}_4$ samples, such as the band gap, depending on the method of their preparation and the initial reagents. Using diffuse reflection spectroscopy, it was found that $g\text{-C}_3\text{N}_4$ samples absorb optical radiation in the wavelength range < 450 nm and have a bandgap of 2.87-3.45 eV.

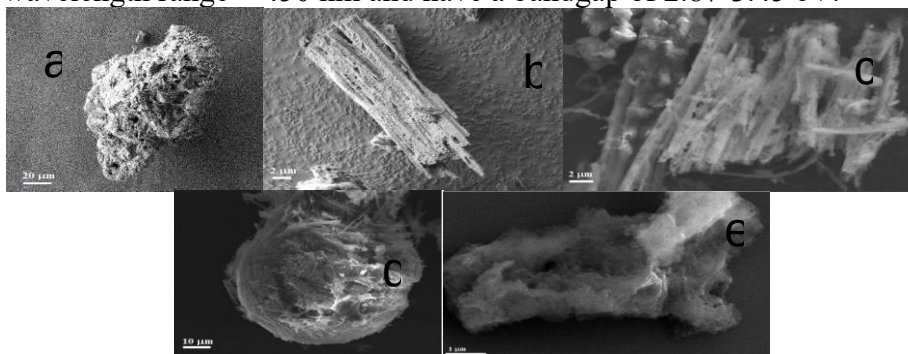


Figure 1. SEM images of synthesized $g\text{-C}_3\text{N}_4$ samples:

a) $g\text{-C}_3\text{N}_4/\text{S1}$; (b) $g\text{-C}_3\text{N}_4/\text{S3}$; (c) $g\text{-C}_3\text{N}_4/\text{S2}$; (d) $g\text{-C}_3\text{N}_4/\text{S4}$;
(e) $g\text{-C}_3\text{N}_4/\text{S5}$

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Mixed-Valent Chloroantimonate of Diazabicyclo[2.2.2]octane

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Mixed-valent compounds have attracted the attention of scientists since the discovery of the famous Fe(II, III) pigment – Prussian blue – in the 18th century. Subsequent studies have revealed a rich family of compounds containing transition or post-transition metals in two different oxidation states, which exhibit unusual physical properties, including superconductivity, magnetic phase transitions, and an intervalence charge-transfer absorption bands [1].

In this work, a new compound $(\text{dabcoH}_2)_7[\text{Sb}^{\text{V}}\text{Cl}_6][\text{Sb}_7^{\text{III}}\text{Cl}_{34}]\cdot 8\text{H}_2\text{O}$ was synthesized (dabco = 1,4-diazabicyclo[2.2.2]octane). Two chloroantimonates containing the dabcoH_2^{2+} cation have previously been reported: $(\text{dabcoH}_2)_2[\text{Sb}_2\text{Cl}_{10}]\cdot 2\text{H}_2\text{O}$ and $(\text{dabcoH}_2)[\text{SbCl}_5]\cdot \text{H}_2\text{O}$. In these compounds, the dabcoH_2^{2+} cation acts as a structure-directing agent, controlling the arrangement of the discrete binuclear $\text{Sb}_2\text{Cl}_{10}^{4-}$ anions in the first compound and the one-dimensional polymeric SbCl_5^{2-} chains in the second compound. In the new compound $(\text{dabcoH}_2)_7[\text{Sb}^{\text{V}}\text{Cl}_6][\text{Sb}_7^{\text{III}}\text{Cl}_{34}]\cdot 8\text{H}_2\text{O}$, a three-dimensional anionic framework $\text{Sb}_7^{\text{III}}\text{Cl}_{34}^{13-}$ is formed, whose cavities accommodate dabcoH_2^{2+} cations, $[\text{Sb}^{\text{V}}\text{Cl}_6]^-$ octahedra and water molecules. The compound exhibits a deep orange-red color, which is not typical for chloroantimonates(III) and can be attributed to the presence of antimony in two oxidation states. This compound crystallizes in the space group *Pbca* with the unit cell parameters $a = 27.1657(14)$ Å, $b = 27.2469(10)$ Å, $c = 27.2832(10)$ Å. The compound was obtained in pure form; thermogravimetric analysis indicates that it is air-stable and starts to lose water only above 160°C.

In conclusion, this work demonstrates for the first time the formation of mixed-valent hybrid chloroantimonates featuring unusually narrow band-gap of 2.12 eV and an uncommon crystal structure.

Acknowledgements

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IV International Symposium "Noncovalent Interactions in Synthesis, Catalysis, and Crystal Engineering"

Modulating photophysical properties of Group 11 Metal complexes with pyridine-pyrazole derivatives via noncovalent interactions

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Mononuclear Group 11 metal complexes with 2,2'-bipyridine derivatives (NN) and auxiliary bisphosphine (PP) ligands (Fig. 1a) are popular objects of photophysical studies due to their potential for use in optoelectronic materials. It has previously been shown that replacing the 2,2'-bipyridine ligand with 2-(pyrazol-5-yl)pyridine derivatives provides opportunities for fine-tuning the photophysical properties of the complexes by varying substituents on the NN ligand.^{1,2}

In this work, mixed-ligand copper(I) and silver(I) complexes based on pyridine-pyrazoles bearing phenyl and 9-anthracenyl substituents were obtained (Fig. 1b). The influence of noncovalent interactions on the photophysical properties of the obtained complexes is demonstrated. Specifically, the formation of π - π stacking interactions in the silver(I) complex with the pyrazole ligand L^{Ph} results in exciplex-type phosphorescence. Disruption of intermolecular interactions in the crystal leads to a change in the emission type to ligand-centered emission.³ Similar behavior is exhibited by complexes based on L^{Antr} , not only in the solid state but also in solution.

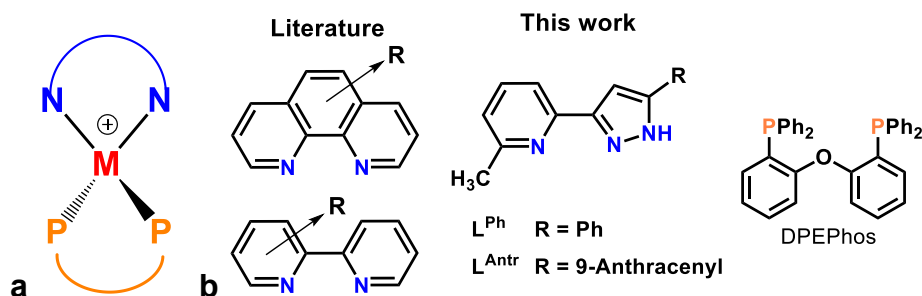


Figure 1. Schematic representation (a) and objects of research (b).

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