Praktični aspekti otvorene nauke -
- razmišljanja jednog hemičara

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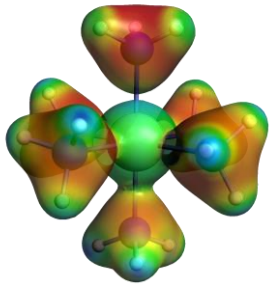
Zajednica otvorene nauke Srbije (OSCS)

08.02.2023

Predstavljanje

- Naučni savetnik (2022), IHTM
- Dr.rer.nat. (2010), Univerzitet u Friburu, Švajcarska
- Diplomirani hemičar (2005), Hemijski fakultet

- Računarska i teorijska hemija
- Molekulsko modelovanje
- Koordinaciona hemija



- Administrator repozitorijuma IHTM-a (CeR), 2019-
- Član NV IHTM
- Koordinator Transformcionog tima IHTM

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Otvorena nauka – kako je počelo (lična perspektiva)

Dani otvorene nauke
18-19.10.2018

---------- Forwarded message ---------
From: **Lynn Kamerlin** <lynn.kamerlin@kemi.uu.se>
Date: Tue, Oct 30, 2018 at 5:11 PM
Subject: Do you want to sign our Open Letter on Plan S
To: Lynn Kamerlin <lynn.kamerlin@kemi.uu.se>

Dear Colleagues,

You may have heard about 'Plan S', which was announce on September 4 2018.

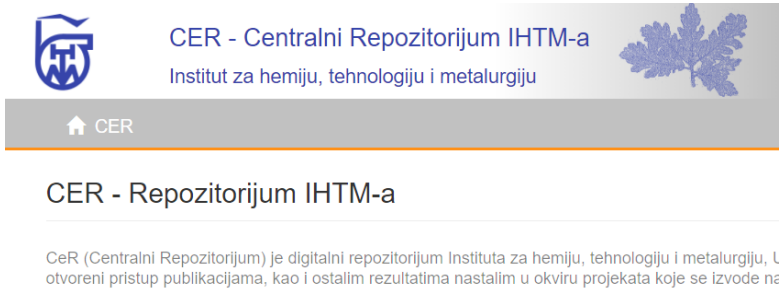
1.2.1. Data usage

- Elaborate on data usage in the proposed Project. Provide answers to all qu

TMMagCat will be entirely devoted to the principles of Open Science. All research dat
conform to the FAIR (findable, accessible, interoperable, and re-usable) principles.

  - What types of data will the Project generate/collect?

Poziv IDEJE Fonda za nauku
07.10.2020



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IHTM-a
05.02.2019

Article archivé
1 message

RAPPAZ Francois <francois.rappaz@unifr.ch> Wed, Sep 3, 2008 at 4:17 PM
To: ZLATAR Matija <matija.zlatar@unifr.ch>

Bonjour Monsieur,

J'ai pris la liberté d'archiver l'article ci-dessous sur rero doc.
Merci de me signaler tout problème.

Molecular mechanics study of nickel(ii) octaethylporphyrin adsorbed on graphite (0001)
url : http://doc.rero.ch/search.py?p=990__a:20080903155619-NA

Pour retrouver des travaux déposés sur les serveurs de documents académiques, utilisez par exemple BASE http://www.base-search.net/index.php?i=a (Ensemble des serveurs consultables par BASE: http://base.ub.uni-bielefeld.de/about_sources_en_date_up.html)

Bonne journée

François Rappaz

Centre de documentation de la Faculté des Sciences
Université de Fribourg
DokPe - Dokumentationszentrum der Naturwissenschaftlichen Fakultät Universität Freiburg
Pérolles CH-1700 Fribourg Switzerland

Otvorena nauka

- Otvoreni podaci
- Otvoreni pristup radovima
- Otvoreni softver (open source)
- Otvorene recenzije
- Otvoreni resursi za edukaciju
- Otvoreni materijali
- Otvorena infrastruktura
- Otvorene inovacije
- …

OTVORENO ZNANJE

- Transparentnost
- Reproducibilnost
- Odgovornost
- Politike otvorene nauke
- Diseminacija
- Saradnja
- Ponovna upotreba rezultata
- Povećanje kvaliteta
- …

- Intelektualna svojina
- Neko drugi dobija detaljne rezultate vašeg rada besplatno ?
- Vreme, plaćanje?

Nerazumevanje

Otvoreni pristup radovima

Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex †

Tina P. Andrejević, [a] Ivana Aleksic, [b] Jakob Kljun, [c] Marta Počkaj, [c] Matija Zlatar, [d] Sandra Vojnovic, [b] Jasmina Nikodinovic-Runic, [b] Iztok Turel, *[c] Miloš I. Djuran *[e] and Biljana Đ. Glišić *[a]

Author affiliations

Abstract

Dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz) was used as a ligand for the synthesis of new copper(II) and silver(I) complexes, $[CuCl_2(py\text{-}2pz)]_2$ (**1**), $[Cu(CF_3SO_3)(H_2O)(py\text{-}2pz)_2]CF_3SO_3{\cdot}2H_2O$ (**2**), $[Ag(py\text{-}2pz)_2]PF_6$ (**3**) and $\{[Ag(NO_3)(py\text{-}2pz)]{\cdot}0.5H_2O\}_n$ (**4**). The complexes were characterized by spectroscopic and electrochemical methods, while their structures were determined by single crystal X-ray diffraction analysis. The X-ray analysis revealed the bidentate coordination mode of py-2pz to the corresponding metal ion *via* its pyridine and pyrazine nitrogen atoms in all complexes, while in polynuclear complex **4**, the heterocyclic pyrazine ring of one py-2pz additionally behaves as a bridging ligand between two Ag(I) ions. DFT calculations were performed to elucidate the structures of the investigated complexes in solution. The antimicrobial potential of the complexes **1–4** was

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Article HTML

Supplementary files

Supplementary information
PDF (1187K)

Crystal structure data
CIF (385K)

Article information

https://doi.org/10.1039/D2RA07401J

Article type	Paper
Submitted	21 Nov 2022
Accepted	19 Jan 2023
First published	01 Feb 2023

Citation *RSC Adv.*, 2023, **13**, 4376-4393

- Zlatni (gold open-access)
- Zeleni (Green Open Access) – samostalno arhiviranje
- Platinski
- Hibridni

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- Istraživački podaci / Research data (bg.ac.rs): CCDC 2220150: Experimental Crystal Structure Determination. Crystallographic data for: "Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex" (bg.ac.rs)
- Supporting data for: "Deoxyribonuclease I Inhibitory Properties, Molecular Docking and Molecular Dynamics Simulations of 1-(Pyrrolidin-2-yl)propan-2-one Derivatives". Animation of molecular dynamics simulations II. (bg.ac.rs)
- Accepted version of articles Search (bg.ac.rs): What Is the Nature of Interactions of BF4–, NO3–, and ClO4– to Cu(II) Complexes with Girard’s T Hydrazine? When Can Binuclear Complexes Be Formed? (bg.ac.rs)

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Project supported by the Science Fund of the Republic of Serbia through the program IDEAS (#7750288). Principal investigator is Dr. Matija Zlatar

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Andrejević, Tina P.; Aleksić, Ivana; Kljun, Jakob; Počkaj, Marta; Zlatar, Matija; Vojnović, Sandra; Nikodinović-Runić, Jasmina; Turel, Iztok; Đuran, Miloš; Glišić, Biljana (Royal Society of Chemistry (RSC), 2023)

CCDC 2220150: Experimental Crystal Structure Determination. Crystallographic data for: "Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex"

Andrejević, Tina P.; Aleksić, Ivana; Kljun, Jakob; Počkaj, Marta; Zlatar, Matija; Vojnović, Sandra; Nikodinović-Runić, Jasmina; Turel, Iztok; Đuran, Miloš; Glišić, Biljana (The Cambridge Crystallographic Data Centre (CCDC), 2023)

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- CCDC 2220148: Experimental Crystal Structure Determination. Crystallographic data for: "Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex" (bg.ac.rs)
- Abstrakt sa konferencije: Magnetic anisotropy in pentagonal bipyramidal complexes of first-row transition metal ions (bg.ac.rs)
- Poster s konferencije: Magnetic anisotropy in pentagonal bipyramidal complexes of first-row transition metal ions (bg.ac.rs)
- Izveštaj: TMMagCat - D4.1 Report on the kick-off meeting (bg.ac.rs)
- Rad (open-access): Copper(II) and silver(I) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex (bg.ac.rs)
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- Rad (recenzirana verzija): Coordination preferences of NNO and NNS Schiff base ligands with Co(III) complexes: Synthesis, characterization and DFT calculation (bg.ac.rs)
- Prezentacija: Modeling metal-ligand bonds – from ground to excited states (bg.ac.rs)

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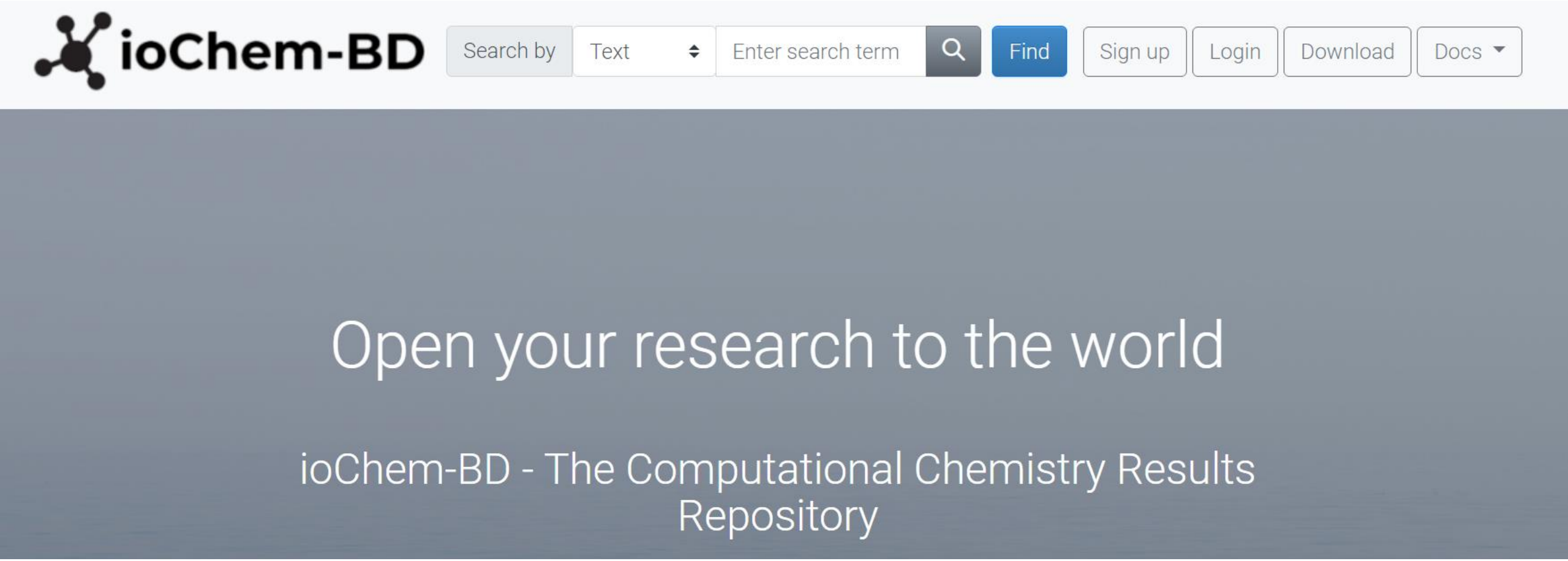

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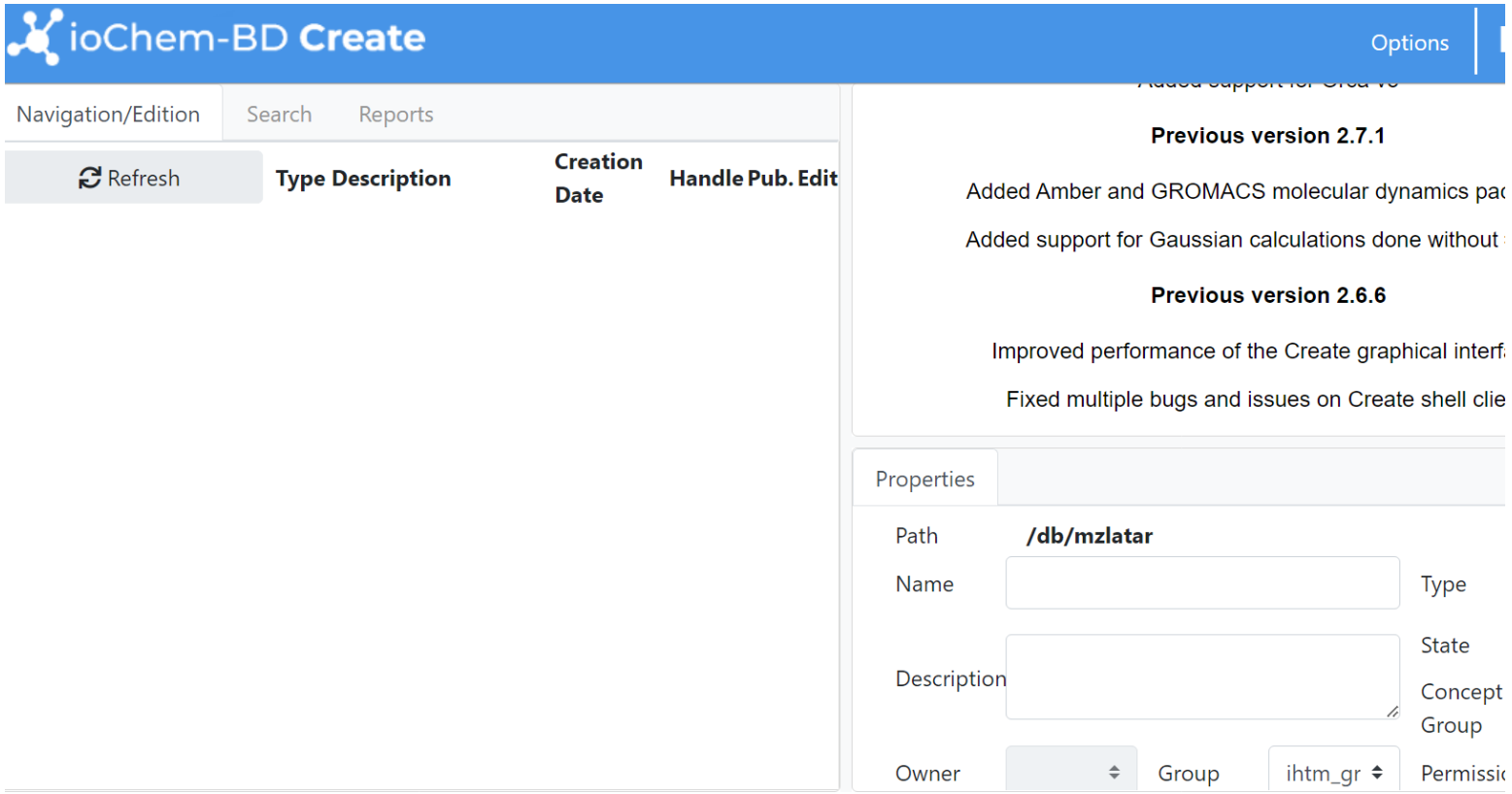

- Saradnja (unutar grupe, više grupa) – deljenje podataka
- Generisanje doi broja
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DATA ACCESSIBILITY

A data set collection of computational results is available at the iochem-bd platform, which can be accessed at www.dx.doi.org/10.19061/iochem-bd-4-10.

Istraživački podaci za računarsku hemiju

PBE, BP86, S12G, S12H and B3LYP level of theory.

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This dataset derived results are published in:
Manuscript title: Density functional approximations for consistent spin and oxidation states of oxoiron complexes
Journal: Int. J. Quantum Chem

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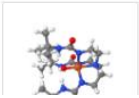
Preview	Title	Issue Date	Author(s)	Program	Method(s)	Basis Set	Energy	S
	Complex_10_HS_b3ly	11-Nov-2019	*Vlahovic, Filip; Universitat de*	*ADF; 2013; 01*	*DFT*	*TZ2P*		

- Saradnja (unutar grupe, više grupa) – deljenje podataka
- Generisanje doi broja
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Density functional approximations for consistent spin and oxidation states of oxoiron complexes - Vlahovic - 2020 - International Journal of Quantum Chemistry - Wiley Online Library

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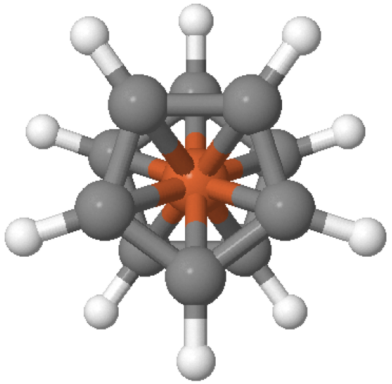

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output.cml	424.46 kB	Chemical Markup Language	Down

Metadata:

Title:	Fe_d5d_EDA
Authors:	Vlahovic, Filip Universitat de Girona
Issue Date:	18-Nov-2019
Publisher:	UdG
Description:	eda
URI:	https://www.iochem-bd.org//handle/10/216655
Appears in Collections:	Metallocenes__Rotating_iron_and_titanium_sandwich_complexes

GENERAL INFO

Title: Fe_d5d_EDA
Browse item: https://www.iochem-bd.org:443/handle/10/216655
Program: ADF 2013
Author: Vlahovic, Filip: Universitat de Girona
Formula: C 10 H 10 Fe 1
Calculation type: Single point (Phase gas)
Method(s): DFT (OPTX PBEc)
VWN
Core Treatment : Frozen Orbital(s)
Symmetry : D(5D)

ATOM INFO

Atomic coordinates [Å]

ATOM		x	y	z	TYPE	Core
1	Fe	0.0000	0.0000	0.0000		
2	C	0.0000	1.2157	-1.5963		
3	C	-1.1562	0.3757	-1.5963		
4	C	-0.7146	-0.9835	-1.5963		
5	C	0.7146	-0.9835	-1.5963		
6	C	1.1562	0.3757	-1.5963		
7	H	0.0000	2.3015	-1.5726		
8	H	-2.1889	0.7112	-1.5726		
9	H	-1.3528	-1.8620	-1.5726		
10	H	1.3528	-1.8620	-1.5726		
11	H	2.1889	0.7112	-1.5726		
12	C	0.0000	-1.2157	1.5963		
13	C	-1.1562	-0.3757	1.5963		
14	C	-0.7146	0.9835	1.5963		
15	C	0.7146	0.9835	1.5963		
16	C	1.1562	-0.3757	1.5963		
17	H	0.0000	-2.3015	1.5726		
18	H	-2.1889	-0.7112	1.5726		
19	H	-1.3528	1.8620	1.5726		
20	H	1.3528	1.8620	1.5726		
21	H	2.1889	-0.7112	1.5726		

MOLECULAR INFO

Charge 0
Multiplicity 1

JOB | SCF Converged

Bonding Energy (Summary)
Fit Test
MOs / SFO gross populations
MOs Energies
Mulliken Atomic Charges

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[ioChem-Find: Metallocenes__Rotating_iron_and_titanium_sandwich_complexes (iochem-bd.org)]

Hvala vam svima!

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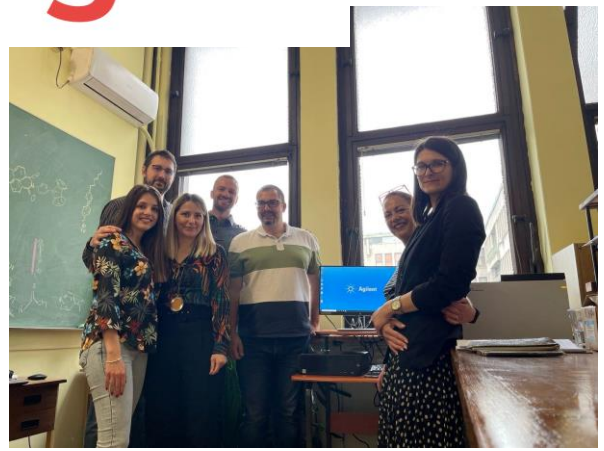

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