

DRUŠTVENE VESTI IN DRUGE AKTIVNOSTI

SOCIETY NEWS, ANNOUNCEMENTS, ACTIVITIES

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54. Mednarodna kemijska olimpijada

(Univerza Nankai, Tianjin, Kitajska)

Andrej Godec

UL, FKKT

Na Fakulteti za kemijo in Kemijsko tehnologijo v Ljubljani se je od 10. 7. do 18. 7. 2022 tednu odvijala 54. mednarodna kemijska olimpijada. To je tekmovanje srednješolcev v znanju kemije, vsako državo pa zastopa ekipa štirih najboljših. Priprave potekajo na Fakulteti za kemijo in kemijsko tehnologijo v Ljubljani, pri organizaciji dogodka pa sodelujemo z Zvezo za tehnično kulturo Slovenije. Mentorja ekipe sta dr. Berta Košmrlj in dr. Andrej Godec. V pripravi na to olimpijado so sodelovali tudi dr. Marta Počkaj, dr. Darko Dolenc, pomagali pa so še Martin Rihtaršič, Vid Kermelj in dr. Damjan Jan Pavlica.

Letošnjo olimpijado je organizirala Kitajska, zaradi epidemioloških razmer v tej državi pa je potekala na daljavo. Našo državo so zastopali dijaki **Dane Jemc** (Gimnazija Škofja Loka), **Matej Nastran** (Gimnazija Škofja Loka), **Nina Cankar** (Gimnazija Kranj) ter **Patrik Potočnik** (Gimnazija Škofja Loka).

Letošnje olimpijade se je sicer udeležilo 326 dijakov iz 84 držav. Naši dijaki so dosegli odličen rezultat: Dane, Matej, in Patrik so dobili bronasto medaljo, Nina pa častno omembo. ČESTITKE!

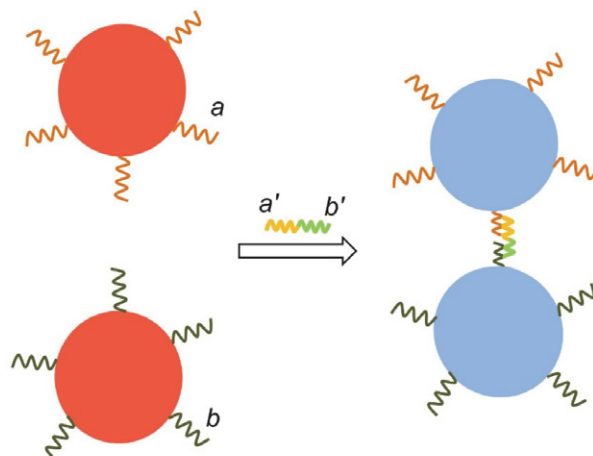


Slovenska ekipa na 54. Mednarodni kemijski olimpijadi: Dane, Patrik, Nina in Matej. Foto: Aljoša Seljak.

Na tekmovanju je bilo letos 9 teoretičnih nalog, za reševanje pa je sicer na voljo 5 ur časa. Naloge na olimpijadi so izjemno težke, tako da se dijaki udeležujejo priprav slovenske ekipe pa izberemo na treh nacionalnih izbirnih testih.

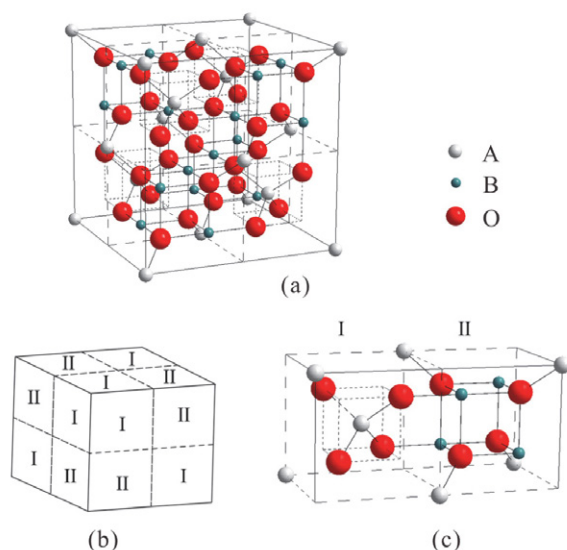
Seveda letošnje naloge niso mogle zaobiti epidemije, saj so hitre in enostavne metode za zgodnje odkrivanje

COVID-19 so nujno potrebne. Ena izmed obetavnih metod je detekcija s pomočjo nanodelcev zlata. Nanodelci zlata se zaradi njihovega visokega molskega ekstinkcijskega koeficienta (molske absorptivnosti) pogosto uporabljajo kot vidni odčitki na testnih lističih. Barvni izgled nanodelcev zlata je povezan z njihovo velikostjo in razpršenostjo. V splošnem velja, da večji kot so nanodelci zlata, bolj rdečkasta je njihova barva. Ko se nanodelci združijo, se barva spremeni iz rdeče v modro. Ko površino nanodelcev zlata modificiramo z dvema vrstama enoverzičnih fragmentov nukleinske kisline *a* in *b*, se nanodelci zlata v prisotnosti tarčne nukleinske kisline (*a'* *b'*) združijo. Pri tem se v nekaj minutah spremeni barva iz rdeče v modro (slika). Na osnovi tega bi lahko zaznavali prisotnost tarčnih nukleinskih kislin, značilnih za koronavirus, v vzorcih.



Tema prve naloge je bila opisana detekcija tarčnih nukleinskih kislin: dijaki so okarakterizirali spekter navedenih spojin, izračunali molarni ekstinkcijski koeficient raztopine nanodelcev zlata, ter na koncu še na osnovi podatkov izračunali koncentracijo virusne nukleinske kisline v originalnem vzorcu brisa žrela.

Druga naloga je bila povezana z glazuro. Črn glaziran porcelan je vrsta kitajskega porcelana, ki je bila še posebej priljubljena v času dinastij Tang in Song pred približno 1000 leti. Tovrstni keramični izdelki kot glavno barvilo vsebujejo železove okside, ki jih zmešajo z ostalimi prehodnimi kovinami, da dobijo različne temne odtenke, kot so kostanjeva, temno rjava ali črna barva. Črni glaziran porcelan je še danes na Kitajskem precej priljubljen. Tipična



črna glazura je sestavljena iz Fe-vsebujočih oksidov s spinelno strukturo. Spinelni oksidi imajo splošno formulo AB_2O_4 in njihova struktura je naslednja: O^{2-} ioni tvorijo kubični najgostejši sklad, v katerem kationi vrste A zasedajo eno osmino tetraedričnih praznin, kationi B pa eno polovico oktaedričnih praznin (slika).

Črno keramično glazuro, ki ima spinelno strukturo, lahko pripravimo s praženjem Fe_2O_3 in Cr_2O_3 v določenem razmerju v reduktivni atmosferi. Ko Fe_2O_3 in Cr_2O_3 reagirata v masnem razmerju 63.6 : 36.4, se popolnoma spremenita v čisto stehiometrično spojino.

Dijaki so morali okarakterizirati osnovno celico v takšnih spinelnih strukturah; del naloge pa je bil posvečen še vlogi kroma. Spremenljiva valenca kroma namreč ni pomembna samo za proizvodnjo pigmentov, ampak tudi za katalizo. Tipičen Philipsov katalizator za polimerizacijo etena je sestavljen iz kromovega oksida, nanesenega na porozen nosilec, kot je npr. amorfen silicijev dioksid. Dijaki so morali zapisati elektronsko konfiguracijo d elektronov $Cr(II)$ iona v takšnem katalizatorju, in izračunati energijo stabilizacije kristalnega polja CFSE) ter magnetni moment μ za $Cr(II)$ ion.

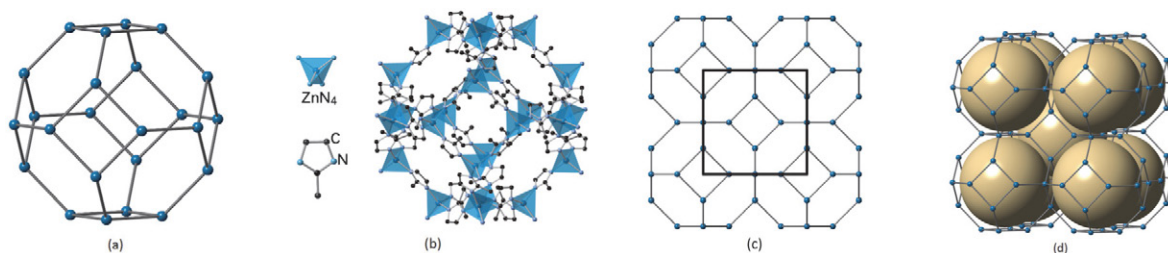
Tema tretje naloge je bilo zajemanje in pretvorba ogljikovega dioksida. Tehnologija direktnega zajema zraka

(DAC, ang. direct air capture), ki naj bi omogočila odstranitev CO_2 direktno iz zraka, je obetavna. Osnova metode DAC je mokro spiranje z alkalno raztopino hidroksida (običajno $NaOH$), v kateri se absorbira zračni CO_2 do vrednosti $pH \approx 10$. Porabljen sorbent se regenerira z dodatkom kalcijevega hidroksida. Bela oborina, ki nastane, razpade pri $700^\circ C$, pri čemer nastane CO_2 in še ena bela snov. Na koncu lahko pridobimo kalcijev hidroksid z hidracijo. Ta proces je energetsko zelo zahteven. ($H_2CO_3 : Ka_1 = 4.5 \times 10^{-7}$, $Ka_2 = 4.7 \times 10^{-11}$). Nedolgo nazaj pa so razvili elektrokemijski proces za regeneracijo alkalne raztopine, uporabljane v postopku mokrega spiranja za DAC. Čist plinast CO_2 bi lahko ponovno pridobili in shranili ali uporabili naprej. Proces je osnovan na elektrokemijskem sistemu za recikliranje H_2 (HRES; ang. H_2 -recycling electrochemical system), elektrokemijska celica pa vsebuje dve ionoselektivni membrani. Dijaki so morali zapisati in okarakterizirati vse navedene kemijske procese, mehanizme prenosa kationov v celici, ter izračunati hitrost nastajanja CO_2 .

Zeolitno-imidazolatna ogrodja ZIF so podskupina organskih ogrodij MOF in so tudi obetavni materiali za zajemanje in uporabo CO_2 . Strukture ZIF-ov so podobne strukturam zeolitov. Zanje so značilna 3D ogrodja s tetraedrično koordiniranimi kovinskimi ioni (npr. Zn^{2+} , Co^{2+}), ki so premoščeni z imidazolatnim ionom (Im^-) ali njegovimi derivati.

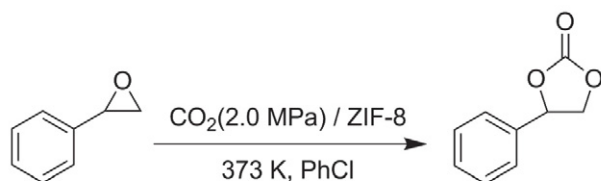
ZIF-8 je predstavnik ZIF-ov s sodalitim (SOD) ogrodjem, prikazanim na sliki. ZIF-8 je prvi pripravil kitajski znanstvenik Xiao-Ming Chen s sodelavci pri reakciji Zn^{2+} z 2-metilimidazolum ($CH_3(C_3N_2H_3)$, $HmIm$) (produkt so sprva poimenovali MAF-4). ZIF-8 kristalizira v kubičnem sistemu s parametrom osnovne celice $a = 1.632$ nm (faza brez topila). Efektivni premer pore, ki je prikazana s kroglo na sliki, znaša 1.16 nm. (slika 4)

Dijaki so morali okarakterizirati osnovno celico tega materiala, izračunati notranjo površino por ter poroznost materiala. ZIF-8 lahko igra tudi vlogo katalizatorja pri pretvorbi CO_2 v kemikalije z visoko dodano vrednostjo. Eden izmed najbolj obetavnih načinov za fiksiranje CO_2 je priprava cikličnih karbonatov s cikloadicijo. Spodaj je prikazan primer:



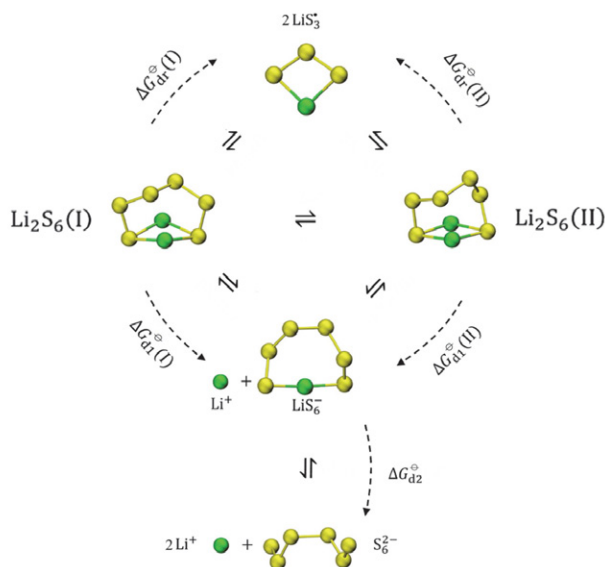
Slika 4:

(a) Topologija SOD kletke; (b) SOD kletka v ZIF-8, sestavljenem iz Zn^{2+} (v središčih tetraedrov) in imidazolnih ionov (H atomi so zaradi jasnosti prikaza izpuščeni); (c) Ogrodje SOD z označeno osnovno celico (kvadrat); (d) Nekaj por v ZIF-8 je poudarjenih z navideznimi krogli.



Dijaki so morali zapisati intermediate pri takšni reakciji, ter tudi urejeno enačbo za to reakcijo.

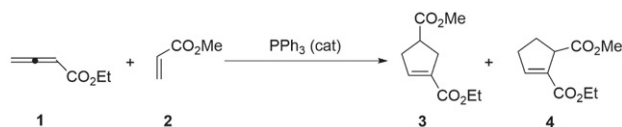
Četrta naloga je bila na temo žvepla, najprej elementarnim, in potem v obliki spojine pirit (FeS_2), ki je surovina pri industrijski proizvodnji elementarnega žvepla. S segrevanjem nastaja žveplo, pa tudi manjše količine plina SO_2 in še česa. Z merjenjem količin tega plina lahko zasledujemo potek reakcije; dijaki so morali izračunati izkoristek oziroma predvideti izgube žvepla v piritu v obliki stranskih produktov. Razen tega je naloga obravnavala tudi drugačno uporabo žvepla. Litij – žveplovna baterija ima visoko teoretično energijsko gostoto, ki presega konvencionalno Li-ion baterijo. Neto reakcijo v litij – žveplovni bateriji lahko poenostavljeno napišemo takole: $16 \text{ Li} + \text{S}_8 \rightarrow 8 \text{ Li}_2\text{S}$. Žveplo je katoda, kovinski litij pa je aktivni material anode pri praznjenju baterije. Dijaki so morali zapisati elektrodne reakcije v tej bateriji, izračunati mase aktivnih elektrodnih materialov, ter izračunati, koliko časa deluje in koliko bolje je to od litij-ionske baterije. V litij – žveplovih baterijah se med praznjenjem S_8 ne reducira direktno do Li_2S , ampak postopoma preko reakcij, pri katerih nastajajo različni topni litijevi polisulfidi (Li_2S_n , $n = 3-8$). Ti litijevi polisulfidi lahko difundirajo na anodo in tam povzročijo korozijo, kar pomeni izgubo aktivnega elektrodnega materiala. Ta pojav imenujemo »shuttle učinek«. Teoretične študije kažejo, da dva konformera s primerljivima energijama, $\text{Li}_2\text{S}_6(\text{I})$ in $\text{Li}_2\text{S}_6(\text{II})$ soobstajata v 1,2-dimetoksietanu (DME), ki je običajno topilo in elektrolit v litij-žveplovih baterijah. Disociacija Li_2S_6 v DME je prikazana spodaj:



Dijaki so morali okarakterizirati korozijo anode, predvideti s pomočjo termodinamskih podatkov, kje se nahaja ravnotežje, izračunati disociacijsko konstanto Li_2S_6 v DME (1,2-dimetoksietan (DME) je običajno topilo in elektrolit v litij-žveplovih baterijah), ter redoks potencial litija v tem topilu.

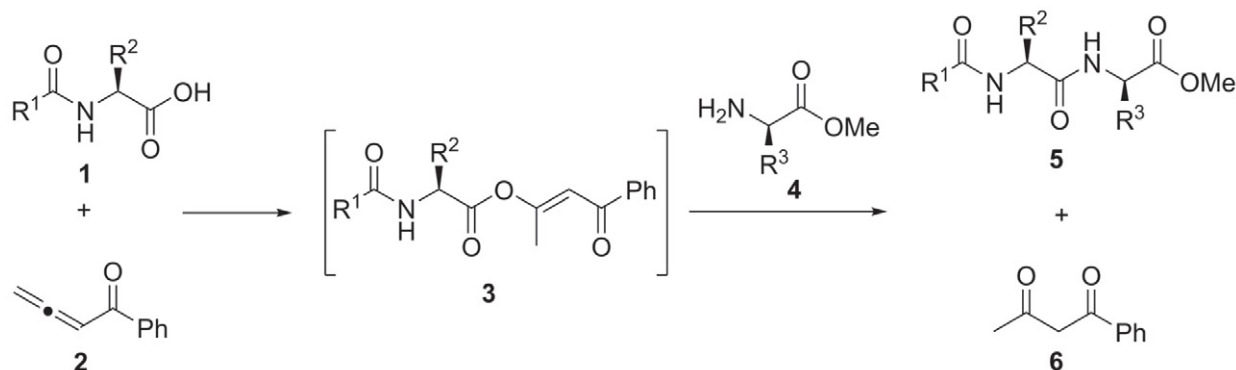
Peta naloga je bila povezana z onesnaževanjem ozračja. Dušikovi oksidi (vključno N_2O , NO , NO_2 , N_2O_4 in še drugi, kar skupaj napišemo kot NO_x) so eni od glavnih onesnaževalcev zraka. Povzročijo lahko probleme, kot so ozonska luknja, kisel dež, fotokemijski smog, in efekt tople grede. Zato moramo kontrolirati emisije in pretvorbe NO_x , da bi izboljšali kvaliteto zraka. Dijaki so raziskali oksidacijo NO v NO_2 preko reakcije $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$. Izračunali so hitrost te reakcije, ter s termodinamskimi podatki ovrednotili smer poteka reakcije ter položaj ravnotežja. V drugem delu naloge pa so preučevali načine za zmanjšanje emisij NO_x . En način za zmanjšanje emisij NO_x je oksidacija NO v NO_2 in nato absorpcija nastalega NO_2 z absorbenti. Vendar pa je zaradi nizkih koncentracij NO v izpuštih njegova spontana oksidacija v atmosferi prepočasna, da bi zadostila zahtevam industrije. Zato se za pospešitev te reakcije uporabljajo trdni katalizatorji. Oksidacija NO na površini specifičnega katalizatorja (**CatX**) poteka po zapletenem mehanizmu; predpostavili so, da se NO , NO_2 in O (iz disociacije O_2) adsorbirajo v eni plasti, in da so vsa adsorpcijska mesta za adsorpcijo teh vrst enakovredna. Deleži pokritosti površine katalizatorja θ so označeni kot θ_{NO} , θ_{NO_2} in θ_{O} . Dijaki so morali izpeljati zvezo med deležem pokritosti in konstanto reakcijskih hitrosti, ter izpeljati izraz za hitrost reakcije na začetku.

Šesta naloga je bila o fosfinih. Kiralne fosfine pogosto uporabljajo kot kiralne ligande pri katalizi s prehodnimi kovinami. V zadnjih dvajsetih letih se je močno razvilo področje organokatalize, med drugim so odkrili sintezne poti, kjer se uporablja nukleofilni fosfinski katalizator. Med temi je najbolj znana Lu-jeva (3+2) cikloadicija, ki jo je razvil kitajski znanstvenik Xiyan Lu. Naprimer etil aleoat **1** in metil akrilat **2** dajeta pri katalizi s trifenilfosfinom dva ciklopentenska derivata: **3** (večinski produkt) in **4** (manjšinski produkt).



Pri tej nalogi so morali dijaki dopolniti reakcijske sheme za to reakcijo in določiti stereokemijo vmesnih spojin.

Tema sedme naloge je bila sinteza kompleksnih peptidov in proteinov. Spajanje karboksilne in aminske skupine, da nastane peptidna vez, je osnovna reakcija pri sintezi peptidov in proteinov. Alenon **2** lahko uporabimo za aktivacijo karboksilne kisline **1** pod milimi reakcijskimi pogoji, pri čemer nastane intermediat **3**. Ta potem reagira z aminom **4** in daje amid **5** z dobrim izkoristkom. Pri tem nastane tudi stranski produkt **6**.



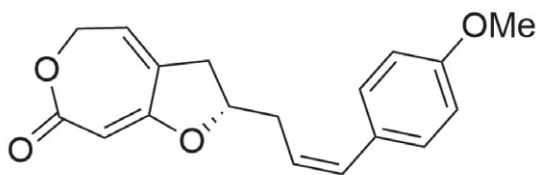
Na podoben način kot alenon lahko aktivira karboksilno kislino tudi *N*-etinil-*N*-metil-*p*-toluensulfonamid. Dijaki so morali najprej za oba primera narisati strukture spojin pri teh reakcijah in prikazati stereokemijo na vsakem od stereocentrov. S tem, ko peptidna veriga raste, postaja tvorba amidnih vezi vedno težja. Za sintezo proteinov zato klasične kondenzacijske metode niso uporabne. Pri prvi sintezi kristaliničnega govejega insulina so razvili metodo, temelječo na kemiji acilhidrazina. S tem so dosegli zahtevno spajanje dveh peptidov z nastankom amidne vezi med njima. Tudi za to reakcijo so morali dijaki narisati strukture spojin. Poleg sinteze iz aminokislin lahko znanstveniki uporabijo modifikacijo obstoječih proteinov. Na verigi proteina je več reaktivnih mest, kot so aminske, karboksilne in tiolne skupine. Najbolj nukleofilna je tiolna skupina in je zato najbolj reaktivna do elektrofilnih reagentov, kot je *N*-fenilmaleimid, na katerega se adira z Michaelovo adicijo. Tudi za ta primer so morali dijaki dopolniti reakcijsko shemo.

Osmo nalogo je imela naslov Čudežni kiralni spiro katalizator. Kiralne spojine so med drugim pomembne za človeško zdravje. Več kot 50 % zdravil, ki so trenutno v klinični uporabi, je čistih posamičnih enantiomerov kiralnih spojin. Sinteza kiralnih molekul v enantiomerno obogateni obliki je velik izziv. Skupina profesorja Qilin Zhou-ja na nankaiski univerzi je razvila vrsto visoko aktivnih kiralnih spiro-katalizatorjev. Ti so dvignili učinkovitost asimetrične sinteze na novo raven in se široko uporabljajo v farmacevtski proizvodnji. Ti katalizatorji dosegajo enantiomerni presežek do 99,9 % in se uporabljajo v zelo majhnih količinah, celo do 0,00002 mol%. Dijaki so v nalogi dopolnili reakcijsko shemo za sintezo teh spojin, in uporabo kiralnega spiro katalizatorja Ir-SpiroPAP za asimetrično totalno sintezo diterpena mulinanskega tipa.

Zadnja, deveta naloga, pa je bila totalna sinteza kapitlaktona. Rastlina *Curculigo capitulata*, ki raste na južnem Kitajskem, se že dolgo uporablja v tradicionalni kitajski medicini za zdravljenje mnogih bolezni. Iz korenin te rastline so izolirali spojino kapitlakton.



Mentorice in mentorji ter dijaki slovenske, madžarske in ukrajinske ekipe na letošnji olimpijadi. Naša ekipa: Andrej (glavni mentor, 1. z leve), Dane, Nina ter Matej (8., 9. ter 10. z leve), in Berta (mentorica, 11. z leve).



Capitulactone (**1**)

Njena struktura z absolutno konfiguracijo je bila določena z uporabo spektroskopskih podatkov in totalne sin-

teze. Sintezo **1** so začeli z jodiranjem kupilnega 4-bromoveratrola. Reakcija poteka preko več intermediatov, dijaki pa so morali tudi tukaj dopolniti reakcijsko shemo sinteze.

Letošnja olimpijada je bila posebna, saj smo v goste povabili še madžarsko in ukrajinsko ekipo. Obe sta prišli v soboto, 9.7.2022, in preživeli dneve do tekmovanja v druženju z našimi dijakinjami in dijaki ter na izletih. Na sliki so vse tri ekipe z mentoricami in mentorji, slika pa je bila narejena takoj po otvoritvi olimpijade v nedeljo, 10.7.

Takšno obliko dogodka so omogočile Fakulteta za kemijo in kemijsko tehnologijo, madžarsko ministrstvo za notranje zadeve, Zveza za tehnično kulturo Slovenije, Slovensko kemijsko društvo ter zavod Bunker. Vsem se iskreno zahvaljujemo za pomoč pri dogodku, ki je lep primer tega, da se da z meddržavnim sodelovanjem preseči trenutne politične in epidemiološke razmere, ter omogočiti sodelujočim izkušnjo »normalne« olimpijade.

Naslednje leto bo olimpijada v Švici, upajmo, da takrat v živo.

Tekst in foto: Andrej Godec

KOLEDAR VAŽNEJŠIH ZNANSTVENIH SREČANJ S PODROČJA KEMIJE IN KEMIJSKE TEHNOLOGIJE

SCIENTIFIC MEETINGS – CHEMISTRY AND CHEMICAL ENGINEERING

2022

October 2022

- 5 – 7 7 MS FOOD DAY
Florence, Italy
Information: <https://www.spettrometriadiamassa.it/Congressi/7MS-FoodDay/index.html>
- 14 CHEMISTRY AND CHEMICAL TECHNOLOGY 2022
Kaunas, Lithuania
Information: <https://cct-conference.ktu.edu/>
- 16 – 21 SCHOOL AND CONFERENCE ON ANALYSIS OF DIFFRACTION DATA IN REAL SPACE
Grenoble, France
Information: <https://workshops.ill.fr/event/306/>
- 12 – 14 CHEMICAL RESEARCH IN FLANDERS – CHEMISTRY CONFERENCE FOR YOUNG
SCIENTISTS 2022
Blankenberge, Belgium
Information: <https://crf-chemcys.be/>
- 21 – 22 XIV CONFERENCE OF CHEMISTS, TECHNOLOGISTS AND ECOLOGISTS OF THE
REPUBLIC OF SRPSKA
Banja Luka, Bosnia and Herzegovina
Information: <https://savjetovanje.tf.unibl.org/>
- 23 – 26 31ST INTERNATIONAL SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS
AND 11TH INTERNATIONAL CONGRESS ON BIODIVERSITY (ISCNP31 & ICOB11)
Naples, Italy
Information: <https://www.iscnp31-icob11.org/index.php>
- 23 – 26 ENERGY, ENVIRONMENT & DIGITAL TRANSITION
Milano, Italy
Information: <https://www.aidic.it/e2dt/>
- 23 – 25 5th CryoNET SYMPOSIUM
Copenhagen, Denmark
Information: <https://eventsignup.ku.dk/cryonet2022>

November 2022

- 8 – 11 SOLUTIONS IN CHEMISTRY 2022
Sveti Martin na Muri, Croatia
Information: <https://solutionsinchemistry.hkd.hr/>

- 6 – 11 EMBO PRACTICAL COURSE: VOLUME ELECTRON MICROSCOPY BY AUTOMATED SERIAL SEM
Lausanne, Switzerland
Information: <https://meetings.embo.org/event/21-serial-sem>

December 2022

- 5 4TH EUROPEAN FORUM ON NEW TECHNOLOGIES - CHEMICAL ENGINEERING AS APPLIED IN MEDICINE
Paris, France
<https://efce.info/4th+European+Forum+on+New+Technologies.htm>
- 5 – 8 ENVIRONMENTAL MEETING ON ENVIRONMENTAL CHEMISTRY 2022 – EMEC22
Ljubljana, Slovenia
Information: <https://www.emec22.com/>

2023**January 2023**

- 1 EUROPEAN FOOD CHEMISTRY CONGRESS XXI – EuroFoodChem XXI
Belgrade, Serbia
Information: <http://horizon2020foodentwin.rs/eurofoodchemxxi/>

March 2023

- 20 – 23 VIII INTERNATIONAL CONGRESS “ENGINEERING, ENVIRONMENT AND MATERIALS IN PROCESS INDUSTRY
Jahorina, Bosnia and Hercegovina
Information: <https://eem.tfv.ues.rs.ba/>

February 2023

- 8 – 11 EMBO WORKSHOP IN SITU STRUCTURAL BIOLOGY: FROM CRYO-EM TO MULTI-SCALE MODELLING
Heidelberg, Germany
Information: <https://www.embl.org/about/info/course-and-conference-office/events/iss23-01/>

July 2023

- 2 – 6 FEZA 2023 – 9TH CONFERENCE OF THE FEDERATION OF THE EUROPEAN ZEOLITE ASSOCIATIONS
Portorož-Portorose, Slovenia
Information: <https://feza2023.org/en/>
- 7 – 11 9TH EUCHEMS CHEMISTRY CONGRESS (ECC9)
Dublin, Ireland

Acta Chimica Slovenica

Author Guidelines

Submissions

Submission to ACSi is made with the implicit understanding that neither the manuscript nor the essence of its content has been published in whole or in part and that it is not being considered for publication elsewhere. All the listed authors should have agreed on the content and the corresponding (submitting) author is responsible for having ensured that this agreement has been reached. The acceptance of an article is based entirely on its scientific merit, as judged by peer review. There are no page charges for publishing articles in ACSi. The authors are asked to read the Author Guidelines carefully to gain an overview and assess if their manuscript is suitable for ACSi.

Additional information

- Citing spectral and analytical data
- Depositing X-ray data

Submission material

Typical submission consists of:

- full manuscript (PDF file, with title, authors, abstract, keywords, figures and tables embedded, and references)
- supplementary files
 - **Full manuscript** (original Word file)
 - **Statement of novelty** (Word file)
 - **List of suggested reviewers** (Word file)
 - **ZIP file containing graphics** (figures, illustrations, images, photographs)
 - **Graphical abstract** (single graphics file)
 - **Proposed cover picture** (optional, single graphics file)
 - **Appendices** (optional, Word files, graphics files)

Incomplete or not properly prepared submissions will be rejected.

Submission process

Before submission, authors should go through the checklist at the bottom of the page and prepare for submission.

Submission process consists of 5 steps.

Step 1: Starting the submission

- Choose one of the journal sections.
- Confirm all the requirements of the **checklist**.
- Additional plain text comments for the editor can be provided in the relevant text field.

Step 2: Upload submission

- Upload full manuscript in the form of a Word file (with title, authors, abstract, keywords, figures and tables embedded, and references).

Step 3: Enter metadata

- First name, last name, contact email and affiliation for all authors, in relevant order, must be provided. Corresponding author has to be selected. Full postal address and phone number of the corresponding author has to be provided.

- **Title and abstract** must be provided in plain text.
- Keywords must be provided (max. 6, separated by semicolons).
- Data about contributors and supporting agencies may be entered.
- **References** in plain text must be provided in the relevant text filed.

Step 4: Upload supplementary files

- Original Word file (original of the PDF uploaded in the step 2)
- **List of suggested reviewers** with at least five reviewers with two recent references from the field of submitted manuscript must be uploaded as a Word file. At the same time, authors should declare (i) that they have no conflict of interest with suggested reviewers and (ii) that suggested reviewers are experts in the field of the submitted manuscript.
- All **graphics** have to be uploaded in a single ZIP file. Graphics should be named Figure 1.jpg, Figure 2.eps, etc.
- **Graphical abstract image** must be uploaded separately
- **Proposed cover picture** (optional) should be uploaded separately.
- Any additional **appendices** (optional) to the paper may be uploaded. Appendices may be published as a supplementary material to the paper, if accepted.
- For each uploaded file the author is asked for additional metadata which may be provided. Depending of the type of the file please provide the relevant title (Statement of novelty, List of suggested reviewers, Figures, Graphical abstract, Proposed cover picture, Appendix).

Step 5: Confirmation

- Final confirmation is required.

Article Types

Feature Articles are contributions that are written on Editor's invitation. They should be clear and concise summaries of the author's most recent work written with the broad scope of ACSi in mind. They are intended to be general overviews of the authors' subfield of research but should be written in a way that engages and informs scientists in other areas. They should contain the following (see also general guidelines for article structure below): (1) an introduction that acquaints readers with the authors' research field and outlines the important questions for which answers are being sought; (2) interesting, novel, and recent contributions of the author(s) to the field; and (3) a summary that presents possible future directions. Manuscripts should normally not exceed 40 pages of one column format (font size 12, 33 lines per page). Generally, experts who have made an important contribution to a specific field in recent years will be invited by the Editor to contribute a **Feature Article**. Individuals may, however, send a proposal (of no more than one page) for a **Feature Article** to the Editor-in-Chief for consideration.

Scientific articles should report significant and innovative achievements in chemistry and related sciences and should exhibit a high level of originality. They should have the following structure:

1. Title (max. 150 characters),
2. Authors and affiliations,
3. Abstract (max. 1000 characters),
4. Keywords (max. 6),
5. Introduction,
6. Experimental,
7. Results and Discussion,
8. Conclusions,
9. Acknowledgements,
10. References.

The sections should be arranged in the sequence generally accepted for publications in the respective fields and should be successively numbered.

Short communications generally follow the same order of sections as Scientific articles, but should be short (max. 2500 words) and report a significant aspect of research work meriting separate publication. Editors may decide that a Scientific paper is categorized as a Short Communication if its length is short.

Technical articles report applications of an already described innovation. Typically, technical articles are not based on new experiments.

Preparation of Submissions

Text of the submitted articles must be prepared with Microsoft Word. Normal style set to single column, 1.5 line spacing, and 12 pt Times New Roman font is recommended. Line numbering (continuous, for the whole document) must be enabled to simplify the reviewing process. For any other format, please consult the editor. Articles should be written in English. Correct spelling and grammar are the sole responsibility of the author(s). Papers should be written in a concise and succinct manner. The authors shall respect the ISO 80000 standard [1], and IUPAC Green Book [2] rules on the names and symbols of quantities and units. The Système International d'Unités (SI) must be used for all dimensional quantities.

Graphics (figures, graphs, illustrations, digital images, photographs) should be inserted in the text where appropriate. The captions should be self-explanatory. Lettering should be readable (suggested 8 point Arial font) with equal size in all figures. Use common programs such as MS Excel or similar to prepare figures (graphs) and ChemDraw to prepare structures in their final size. Width of graphs in the manuscript should be 8 cm. Only in special cases (in case of numerous data, visibility issues) graphs can be 17 cm wide. All graphs in the manuscript should be inserted in relevant places and **aligned left**. The same graphs should be provided separately as images of appropriate resolution (see below) and submitted together in a ZIP file (Graphics ZIP). Please do not submit figures as a Word file. In **graphs**, only the graph area determined by both axes should be in the frame, while a frame around the whole graph should be omitted. The graph area should be white. The legend should be inside the graph area. The style of all graphs should be the same. **Figures and illustrations** should be of sufficient quality for the printed version, i.e. 300 dpi minimum. **Digital images and photographs** should be of high quality (minimum

250 dpi resolution). On submission, figures should be of good enough resolution to be assessed by the referees, ideally as JPEGs. High-resolution figures (in JPEG, TIFF, or EPS format) might be required if the paper is accepted for publication.

Tables should be prepared in the Word file of the paper as usual Word tables. The captions should appear above the table and should be self-explanatory.

References should be numbered and ordered sequentially as they appear in the text, likewise methods, tables, figure captions. When cited in the text, reference numbers should be superscripted, following punctuation marks. It is the sole responsibility of authors to cite articles that have been submitted to a journal or were in print at the time of submission to ACSi. Formatting of references to published work should follow the journal style; please also consult a recent issue:

1. J. W. Smith, A. G. White, *Acta Chim. Slov.* **2008**, *55*, 1055–1059.
2. M. F. Kemmere, T. F. Keurentjes, in: S. P. Nunes, K. V. Peinemann (Ed.): *Membrane Technology in the Chemical Industry*, Wiley-VCH, Weinheim, Germany, **2008**, pp. 229–255.
3. J. Levec, Arrangement and process for oxidizing an aqueous medium, US Patent Number 5,928,521, date of patent July 27, **1999**.
4. L. A. Bursill, J. M. Thomas, in: R. Sersale, C. Collola, R. Aiello (Eds.), *Recent Progress Report and Discussions: 5th International Zeolite Conference*, Naples, Italy, 1980, Gianini, Naples, **1981**, pp. 25–30.
5. J. Szegezdi, F. Csizmadia, Prediction of dissociation constant using microconstants, http://www.chemaxon.com/conf/Prediction_of_dissociation_constant_using_microconstants.pdf, (assessed: March 31, 2008)

Titles of journals should be abbreviated according to Chemical Abstracts Service Source Index (CASSI).

Special Notes

- Complete characterization, **including crystal structure**, should be given when the synthesis of new compounds in crystal form is reported.
- Numerical **data should be reported with the number of significant digits corresponding to the magnitude** of experimental uncertainty.
- **The SI system of units and IUPAC recommendations** for nomenclature, symbols and abbreviations should be followed closely. Additionally, the authors should follow the general guidelines when citing spectral and analytical data, and depositing crystallographic data.
- **Characters** should be correctly represented throughout the manuscript: for example, 1 (one) and l (ell), 0 (zero) and O (oh), x (ex), D7 (times sign), B0 (degree sign). Use Symbol font for all Greek letters and mathematical symbols.
- The rules and recommendations of the **IUBMB** and the **International Union of Pure and Applied Chemistry (IUPAC)** should be used for abbreviation of chemical names, nomenclature of chemical compounds, enzyme nomenclature, isotopic compounds, optically active isomers, and spectroscopic data.
- **A conflict of interest** occurs when an individual (author, reviewer, editor) or its organization is in-

volved in multiple interests, one of which could possibly corrupt the motivation for an act in the other. Financial relationships are the most easily identifiable conflicts of interest, while conflicts can occur also as personal relationships, academic competition, etc. **The Editors** will make effort to ensure that conflicts of interest will not compromise the evaluation process; potential editors and reviewers will be asked to exempt themselves from review process when such conflict of interest exists. When the manuscript is submitted for publication, **the authors** are expected to disclose any relationships that might pose potential conflict of interest with respect to results reported in that manuscript. In the Acknowledgement section the source of funding support should be mentioned. The statement of disclosure must be provided as Comments to Editor during the submission process.

- **Published statement of Informed Consent.** Research described in papers submitted to ACSi must adhere to the principles of the Declaration of Helsinki (<http://www.wma.net/e/policy/b3.htm>). These studies must be approved by an appropriate institutional review board or committee, and informed consent must be obtained from subjects. The Methods section of the paper must include: 1) a statement of protocol approval from an institutional review board or committee and 2), a statement that informed consent was obtained from the human subjects or their representatives.
- **Published Statement of Human and Animal Rights.** When reporting experiments on human subjects, authors should indicate whether the procedures followed were in accordance with the ethical standards of the responsible committee on human experimentation (institutional and national) and with the Helsinki Declaration of 1975, as revised in 2008. If doubt exists whether the research was conducted in accordance with the Helsinki Declaration, the authors must explain the rationale for their approach and demonstrate that the institutional review body explicitly approved the doubtful aspects of the study. When reporting experiments on animals, authors should indicate whether the institutional and national guide for the care and use of laboratory animals was followed.
- To avoid conflict of interest between authors and referees we expect that not more than one referee is from the same country as the corresponding author(s), however, not from the same institution.
- Contributions authored by **Slovenian scientists** are evaluated by non-Slovenian referees.
- Papers describing **microwave-assisted reactions** performed in domestic microwave ovens are not considered for publication in *Acta Chimica Slovenica*.
- *Manuscripts that are **not prepared and submitted** in accord with the instructions for authors are not considered for publication.*

Appendices

Authors are encouraged to make use of supporting information for publication, which is supplementary material (appendices) that is submitted at the same time as the manuscript. It is made available on the Journal's

web site and is linked to the article in the Journal's Web edition. The use of supporting information is particularly appropriate for presenting additional graphs, spectra, tables and discussion and is more likely to be of interest to specialists than to general readers. When preparing supporting information, authors should keep in mind that the supporting information files will not be edited by the editorial staff. In addition, the files should be not too large (upper limit 10 MB) and should be provided in common widely known file formats to be accessible to readers without difficulty. All files of supplementary materials are loaded separately during the submission process as supplementary files.

Proposed Cover Picture and Graphical Abstract Image

Graphical content: an ideally full-colour illustration of resolution 300 dpi from the manuscript must be proposed with the submission. Graphical abstract pictures are printed in size 6.5 x 4 cm (hence minimal resolution of 770 x 470 pixels). Cover picture is printed in size 11 x 9.5 cm (hence minimal resolution of 1300 x 1130 pixels)

Authors are encouraged to submit illustrations as candidates for the journal Cover Picture*. The illustration must be related to the subject matter of the paper. Usually both proposed cover picture and graphical abstract are the same, but authors may provide different pictures as well.

* The authors will be asked to contribute to the costs of the cover picture production.

Statement of novelty

Statement of novelty is provided in a Word file and submitted as a supplementary file in step 4 of submission process. Authors should in no more than 100 words emphasize the scientific novelty of the presented research. Do not repeat for this purpose the content of your abstract.

List of suggested reviewers

List of suggested reviewers is a Word file submitted as a supplementary file in step 4 of submission process. Authors should propose the names, full affiliation (department, institution, city and country) and e-mail addresses of five potential referees. Field of expertise and at least two references relevant to the scientific field of the submitted manuscript must be provided for each of the suggested reviewers. The referees should be knowledgeable about the subject but have no close connection with any of the authors. In addition, referees should be from institutions other than (and countries other than) those of any of the authors. Authors declare no conflict of interest with suggested reviewers. Authors declare that suggested reviewers are experts in the field of submitted manuscript.

How to Submit

Users registered in the role of author can start submission by choosing USER HOME link on the top of the page, then choosing the role of the Author and follow the relevant link for starting the submission process. Prior to submission we strongly recommend that you familiarize yourself with the ACSi style by browsing the journal, particularly if you have not submitted to the ACSi before or recently.

Correspondence

All correspondence with the ACSi editor regarding the paper goes through this web site and emails. Emails are sent and recorded in the web site database. In the correspondence with the editorial office please provide ID number of your manuscript. All emails you receive from the system contain relevant links. **Please do not answer the emails directly but use the embedded links in the emails for carrying out relevant actions.** Alternatively, you can carry out all the actions and correspondence through the online system by logging in and selecting relevant options.

Proofs

Proofs will be dispatched via e-mail and corrections should be returned to the editor by e-mail as quickly as possible, normally within 48 hours of receipt. Typing errors should be corrected; other changes of contents will be treated as new submissions.

Submission Preparation Checklist

As part of the submission process, authors are required to check off their submission's compliance with all of the following items, and submissions may be returned to authors that do not adhere to these guidelines.

1. The submission has not been previously published, nor is it under consideration for publication in any other journal (or an explanation has been provided in Comments to the Editor).
2. All the listed authors have agreed on the content and the corresponding (submitting) author is responsible for having ensured that this agreement has been reached.
3. The submission files are in the correct format: manuscript is created in MS Word but will be **submitted in PDF** (for reviewers) as well as in original MS Word format (as a supplementary file for technical editing); diagrams and graphs are created in Excel and saved in one of the file formats: TIFF, EPS or JPG; illustrations are also saved in one of these formats. The preferred position of graphic files in a document is to embed them close to the place where they are mentioned in the text (See **Author guidelines** for details).
4. The manuscript has been examined for spelling and grammar (spell checked).
5. The **title** (maximum 150 characters) briefly explains the contents of the manuscript.
6. Full names (first and last) of all authors together with the affiliation address are provided. Name of author(s) denoted as the corresponding author(s), together with their e-mail address, full postal address and telephone/fax numbers are given.
7. The **abstract** states the objective and conclusions of the research concisely in no more than 150 words.
8. Keywords (minimum three, maximum six) are provided.
9. **Statement of novelty** (maximum 100 words) clearly explaining new findings reported in the manuscript should be prepared as a separate Word file.
10. The text adheres to the stylistic and bibliographic requirements outlined in the **Author guidelines**.
11. Text in normal style is set to single column, 1.5 line spacing, and 12 pt. Times New Roman font is

recommended. All tables, figures and illustrations have appropriate captions and are placed within the text at the appropriate points.

12. Mathematical and chemical equations are provided in separate lines and numbered (Arabic numbers) consecutively in parenthesis at the end of the line. All equation numbers are (if necessary) appropriately included in the text. Corresponding numbers are checked.
13. Tables, Figures, illustrations, are prepared in correct format and resolution (see **Author guidelines**).
14. The lettering used in the figures and graphs do not vary greatly in size. The recommended lettering size is 8 point Arial.
15. Separate files for each figure and illustration are prepared. The names (numbers) of the separate files are the same as they appear in the text. All the figure files are packed for uploading in a single ZIP file.
16. Authors have read **special notes** and have accordingly prepared their manuscript (if necessary).
17. References in the text and in the References are correctly cited. (see **Author guidelines**). All references mentioned in the Reference list are cited in the text, and vice versa.
18. Permission has been obtained for use of copyrighted material from other sources (including the Web).
19. The names, full affiliation (department, institution, city and country), e-mail addresses and references of five potential referees from institutions other than (and countries other than) those of any of the authors are prepared in the word file. At least two relevant references (important recent papers with high impact factor, head positions of departments, labs, research groups, etc.) for each suggested reviewer must be provided. Authors declare no conflict of interest with suggested reviewers. Authors declare that suggested reviewers are experts in the field of submitted manuscript.
20. Full-colour illustration or graph from the manuscript is proposed for graphical abstract.
21. **Appendices** (if appropriate) as supplementary material are prepared and will be submitted at the same time as the manuscript.

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