Kratek opis usposabljanja mladega raziskovalca (*Short description of the Young Researcher's training)*

1. Raziskovalna organizacija (*Research organisation)*:

Univerza v Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo *University of Ljubljana, Faculty of Chemistry and Chemical Technology*

2. Ime, priimek in elektronski naslov mentorja (*Mentor's name, surname and email*):

Janez Cerkovnik (janez.cerkovnik@fkkt.uni-lj.si)

3. Šifra in naziv raziskovalnega področja (*Research field*):

1.04 Kemija *1.04 Chemical Sciences*

4. Kratek opis usposabljanja mladega raziskovalca (*Short description of the Young Researcher's training*):

Navedite tudi morebitne druge zahteve, vezane na usposabljanje mladega raziskovalca (npr. znanje tujih jezikov, izkušnje z laboratorijskim delom, potrebne licence za usposabljanje…).

Strukturna karakterizacija reaktivnih intermediatov iz družine verižnih trioksidov

V predlagani raziskavi nameravamo določiti strukture reaktivnih intermediatov iz družine verižnih trioksidov, trioksidana (HOOOH) in hidrotrioksidov (ROOOH), ki nastajajo pri nizko-temperaturni ozonaciji najrazličnejših organskih in organokovinskih substratov. Dosedanje raziskave so se večinoma osredotočale na izdatno teoretično raziskovanje kemije hidrotrioksidov in H_2O_3, še posebej mehanističnih aspektov njihovega nastanka in reaktivnosti [1]. Rentgenska strukturna karakterizacija takšnih intermediatov in/ali izolacija njihovih kovinskih kompleksov in kokristalov pa bi dala izjemno dragocene primere in geometrijske parametre v trdnem za te verižne triokside, in pripomogla k boljšemu razumevanju teh eksotičnih molekul, kakor tudi mnogih drugih procesov, v atmosferskih, bioloških in okoljskih sistemih, kjer nastopajo te kemijske zvrsti [2].

Predvidena je raziskava in strukturna karakterizacija treh tipov verižnih trioksidov:

a) trioksidan−kovinski kompleksi s "super" šibko koordinirajočimi anioni [3],
b) organski hidrotrioksidi (ROOOH) [4] in
c) organokovinski hidrotrioksidi (LMOOOH; L = ligand, M = kovina) [5].

Ker je za te kemijske zvrsti značilno, da so občutljive, reaktivne in nestabilne, bomo za delo z njimi uporabili specialne eksperimentalne tehnike. Slednje vključujejo nizkotemperaturne tehnike rokovanja in kristalizacije, nizkotemperaturno izolacijo in montiranje kristalov za nizkotemperaturno rentgensko difrakcijo na monokristalih, ter nizkotemperaturno ramansko, ATR-IR in NMR spektroskopijo. Po potrebi bomo poskuse izvajali v inertni atmosferi in v temeljito posušeni opremi in topilih. Poleg teh eksperimentalnih metod bomo na novo odkrite spojine in komplekse, za razumevanje njihovih kemijskih vezi, preučili tudi s kvantno-kemijskimi izračuni.

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Structural characterization of reactive intermediates of the straight-chain trioxide family

The aim of the proposed research is to obtain solid-state structural information for reactive intermediates of the straight-chain trioxide family, namely trioxidane (HOOOH) and hydrotrioxides (ROOOH), formed in the low-temperature ozonation reactions of various organic and organometallic substrates. The recent progress in this field has relied heavily on the theoretical exploration of hydrotrioxides and H_2O_3 chemistry, especially mechanistic aspects of their formation and reactivity [1]. The first X-ray structural characterizations of compounds having the −OOOH functional group or HOOOH, and/or the isolation of their metal complexes and co-crystals, would provide valuable and hitherto unknown examples of solid-state geometrical parameters for these straight-chain trioxides. This would enhance our understanding of these exotic molecules as well as the many important processes spanning atmospheric, biological, and environmental systems in which these species are implicated [2]. Research and structural characterization of three types of straight-chain trioxides are planned:

a) trioxidane−metal complexes of "super" weakly coordinating anions [3],
b) organic hydrotrioxides (ROOOH) [4], and
d) Organometallic hydrotrioxides (LMOOOH; L = ligand, M = kovina) [5].

Common features of ROOOH compounds are their sensitivity, reactivity, and instability. To overcome these drawbacks, specialized experimental techniques will be employed. These include low-temperature handling and crystallization techniques, low-temperature isolation and crystal mounting for low-temperature single-crystal X-ray diffraction, and low-temperature Raman, ATR-IR, and NMR spectroscopies. Where necessary, experiments will be carried out under inert atmosphere and in rigorously dried equipment and solvents. All of these experimental methods will be accompanied by quantum-chemical calculations in order to obtain a clear understanding of bonding in newly structurally-characterized compounds.

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