

## Copper(II) and sodium(I) complexes based on 3,7-diacetyl-1,3,7-triaza-5-phosphabicyclo[3.3.1]nonane-5-oxide : synthesis, characterization, and catalytic activity.

### Autorzy

Abdallah G. Mahmoud  
M. Fátima C. Guedes da  
Silva  
Ewelina I. Śliwa  
Piotr Smoleński  
Maxim L. Kuznetsov  
Armando J. L. Pombeiro

### Rok wydania

2018

### Czasopismo

Chemistry-An Asian Journal

### Numer woluminu

13

### Strony

2868-2880

### DOI

10.1002/asia.201800799

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

The reaction of 3,7-diacetyl-1,3,7-triaza-5-phosphabicyclo[3.3.1]nonane (DAPTA) with metal salts of Cu<sup>II</sup> or Na<sup>I</sup>/Ni<sup>II</sup> under mild conditions led to the oxidized phosphane derivative 3,7-diacetyl-1,3,7-triaza-5-phosphabicyclo[3.3.1]nonane-5-oxide (DAPTA=O) and to the first examples of metal complexes based on the DAPTA=O ligand, that is, [Cu<sup>II</sup>(μ-CH<sub>3</sub>COO)<sub>2</sub>(κO-DAPTA=O)]<sub>2</sub> (**1**) and [Na(κOO';2κO-DAPTA=O)(MeOH)]<sub>2</sub>(BPh<sub>4</sub>)<sub>2</sub> (**2**). The catalytic activity of **1** was tested in the Henry reaction and for the aerobic 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO)-mediated oxidation of benzyl alcohol. Compound **1** was also evaluated as a model system for the catechol oxidase enzyme by using 3,5-di-*tert*-butylcatechol as the substrate. The kinetic data fitted the Michaelis–Menten equation and enabled the obtainment of a rate constant for the catalytic reaction; this rate constant is among the highest obtained for this substrate with the use of dinuclear Cu<sup>II</sup> complexes. DFT calculations discarded a bridging mode binding type of the substrate and suggested a mixed-valence Cu<sup>II</sup>/Cu<sup>I</sup> complex intermediate, in which the spin electron density is mostly concentrated at one of the Cu atoms and at the organic ligand.

### Słowa kluczowe

copper, enzymes, homogeneous catalysis, oxidation, phosphane ligands

### Adres publiczny

<http://dx.doi.org/10.1002/asia.201800799>

### Strona internetowa wydawcy

[onlinelibrary.wiley.com](http://onlinelibrary.wiley.com)

Plik został wygenerowany dnia 2026-05-02 10:08:21

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/JbAS9ZH>.