

A synthetic manganese–calcium cluster similar to the catalyst of Photosystem II : challenges for biomimetic water oxidation.

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Rok wydania

2020

Czasopismo

Dalton Transactions

Numer woluminu

49

Strony

5597-5605

DOI

10.1039/d0dt00536c

Streszczenie

Herein, we report the synthesis, characterization, crystal structure, density functional theory calculations, and water-oxidizing activity of a pivalate Mn–Ca cluster. All of the manganese atoms in the cluster are Mn(IV) ions and have a distorted MnO₆ octahedral geometry. Three Mn(IV) ions together with a Ca(II) ion and four-oxido groups form a cubic Mn₃CaO₄ unit which is similar to the Mn₃CaO₄ cluster in the water-oxidizing complex of Photosystem II. Using scanning electron microscopy, transmission electron microscopy, energy dispersive spectrometry, extended X-ray absorption spectroscopy, chronoamperometry, and electrochemical methods, a conversion into nano-sized Mn-oxide is observed for the cluster in the water-oxidation reaction.

Adres publiczny

<http://dx.doi.org/10.1039/d0dt00536c>

Strona internetowa wydawcy

<https://www.rsc.org/>

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Plik został wygenerowany dnia 2026-06-15 09:09:17

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/WnyCW08>.