Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Can carbamates undergo radical oxidation in the soil environment? A case study on carbaryl and carbofuran.

Autorzy

Irmina Ćwieląg-Piasecka

Maciej Witwicki

Maria Jerzykiewicz

Julia Jezierska

Rok wydania

2017

Czasopismo

Environmental Science and Technology

Numer woluminu

51

Strony

14124-14134

DOI

10.1021/acs.est.7b03386

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Radical oxidation of carbamate insecticides, namely carbaryl and carbofuran, was investigated with spectroscopic (electron paramagnetic resonance [EPR] and UV–vis) and theoretical (density functional theory [DFT] and ab initio orbital-optimized spin-component scaled MP2 [OO-SCS-MP2]) methods. The two carbamates were subjected to reaction with $^{\bullet}$OH, persistent DPPH$^{\bullet}$ and galvinoxyl radical, as well as indigenous radicals of humic acids. The influence of fulvic acids on carbamate oxidation was also tested. The results obtained with EPR and UV–vis spectroscopy indicate that carbamates can undergo direct reactions with various radical species, oxidizing themselves into radicals in the process. Hence, they are prone to participate in the prolongation step of the radical chain reactions occurring in the soil environment. Theoretical calculations revealed that from the thermodynamic point of view hydrogen atom transfer is the preferred mechanism in the reactions of the two carbamates with the radicals. The activity of carbofuran was determined experimentally (using pseudo-first-order kinetics) and theoretically to be noticeably higher in comparison with carbaryl and comparable with gallic acid. The findings of this study suggest that the radicals present in soil can play an important role in natural remediation mechanisms of carbamates.

Adres publiczny

http://dx.doi.org/10.1021/acs.est.7b03386

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html

Plik został wygenerowany dnia 2026-11-11 07:06:53

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/DeiWgf7.