

Theoretical and experimental studies of the kinetics of the reaction of 1-chloropropane and fully deuterated 1-chloropropane with atomic chlorine.

Autorzy

Łukasz Fojcik

Dariusz S. Sarzyński

Andrzej Dryś

Zdzisław Latajka

Rok wydania

2021

Czasopismo

International Journal of
Chemical Kinetics

Numer woluminu

53

Strony

1157-1177

DOI

10.1002/kin.21522

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The overall rate constant for H-abstraction (k_H) from $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$ and D-abstraction (k_D) from $\text{CD}_3\text{CH}_2\text{CD}_2\text{Cl}$ by chlorine atoms is described by the formulas: and respectively. The results of the experiment show that the value of the kinetic isotope effect (k_H/k_D) for the overall rate constants is also temperature dependent in the temperature range of 298–550 K and can be expressed as . The titled reaction was also studied theoretically for the same range of temperatures and with both isotope substituents, just like in the experiment. The computations were made using the MP2 method and the aug-cc-pVDZ basis set. This paper presents detailed results relating to structural parameters of each of the compounds, complexes, and all energy stages important to the reaction mechanism analysis. It also describes all possible individual channels of the process and their feasibilities. In addition, a kinetic analysis of the process was carried out with branching ratio calculations. The results presented here have been compared with those discussed in a paper published earlier, in which the same process was investigated.

Słowa kluczowe

1-chloropropane reaction, chlorine atom reaction, fully deuterated 1-chloropropane, hydrogen abstraction, kinetic isotope effect

Adres publiczny

<http://dx.doi.org/10.1002/kin.21522>

Strona internetowa wydawcy

onlinelibrary.wiley.com