Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Three-level topology switching in a molecular Möbius band.

Autorzy

Marcin Stępień

Bartosz Szyszko

Lechosław Latos-Grażyński

Rok wydania

2010

Czasopismo

Journal of the American Chemical Society

Numer woluminu

132

Strony

3140-3152

DOI

10.1021/ja909913y

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Möbius π-conjugation in cyclic molecules leads to the reversal of Hückel aromaticity rules and affects the electronic and magnetic properties of these systems. We found the first example of a medium-sized macrocyclic structure that is sufficiently flexible to switch between three distinct π-conjugation topologies, planar (**T0**), Möbius (**T1**), and twisted Hückel (**T2**), without changing its oxidation level. The switching is under thermodynamic and kinetic control and can be realized in a three- or four-step cycle. On titration with trifluoroacetic acid (TFAH) or dichloroacetic acid (DCAH), the Möbius free base (**T1**-H_2), which is the preferred structure in dichlorofluoromethane at 150 K, undergoes a series of acid−base reactions involving changes of the π-conjugation topology. The forms observed in the course of titration involve a Möbius aromatic monocation ([**T1**-H_3]$^+$), an antiaromatic twisted Hückel species ([**T2**-H_4(A)]$^+$) containing a coordinated carboxylate anion (A = TFA, DCA), and two additional Möbius forms ([**T1**-H_4(A)$(HA)_n$]$^+$ (n = 1, 2)), containing complex carboxylate anions. The protonated forms undergo a thermally activated ring planarization to yield an antiaromatic quasi-planar dication [**T0**-H_4]$^{2+}$, characterized in the solid state as a TFA salt. The corresponding free base (**T0**-H_2) is metastable but can be trapped by addition of triethylamine at low temperatures.

Adres publiczny

https://doi.org/10.1021/ja909913y

Strona internetowa wydawcy

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

Plik został wygenerowany dnia 2026-11-01 23:17:43

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/EbcyS-P.