Issue 32, 2021

Previous Next

From the journal:
Physical Chemistry Chemical Physics

Anion states of halocamphor molecules: insights into chirally sensitive dissociative electron attachment†

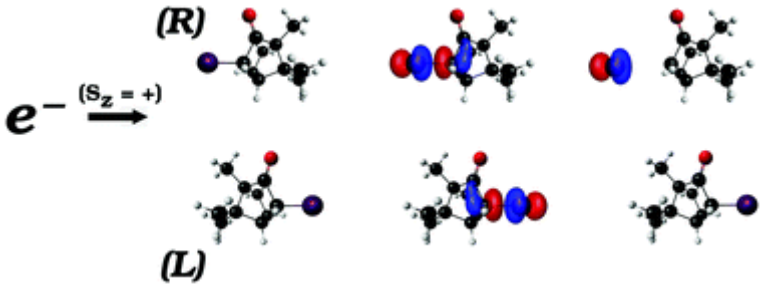
Julio Cesar Ruivo, [a] Fábris Kossoski [b] and Márcio T. do N. Varella [*a]

Author affiliations

Abstract

Recent measurements of spin-polarized electron collisions with halocamphor molecules have observed intriguing trends in their dissociative electron attachment (DEA) chiral asymmetries. While the differences between the DEA asymmetries of 3-bromocamphor (3BrC) and 3-iodocamphor (3IC) were consistent with the larger atomic number of iodine, the even higher chiral asymmetry reported for 10-iodocamphor (10IC) was unexpected. In fact, the helicity densities and the distances from the iodine atoms to the closest chiral centers would suggest smaller asymmetries for 10IC compared to 3IC. To better understand the observed trends, we performed electron scattering and bound state calculations, as well as Born–Oppenheimer molecular dynamics simulations for the three halocamphors. Our results indicate that the DEA signals stem exclusively from halide ions produced by the fast dissociation of low-lying σ* anion states. While we also found dipole bound states and higher-lying shape resonances, we do not expect those states to significantly contribute to the observed yields. Despite the fact that we do not account for the spin–orbit interactions or reaction dynamics, the energies and autoionization lifetimes of the σ* resonances strongly support larger DEA yields for 10IC than 3BrC. The more efficient dissociation could explain the fourfold difference between the maximum DEA chiral asymmetries, since the difference in the atomic numbers of iodine and bromine only accounts for a factor of two. Additionally, our calculations suggest that the twofold difference between

the DEA asymmetries of the iodocamphor isomers could be related to the partial suppression of the cross section for electron attachment to 3IC, compared to 10IC.



Supplementary files

Supplementary information
PDF (1502K)

Article information

https://doi.org/10.1039/D1CP02316K

Article type
Paper

Submitted
25 May 2021

Accepted
30 Jul 2021

First published
03 Aug 2021

Citation
Phys. Chem. Chem. Phys., 2021, **23**, 17616-17624

BibTex Go

Permissions
Request permissions

Social activity
Altmetric 1

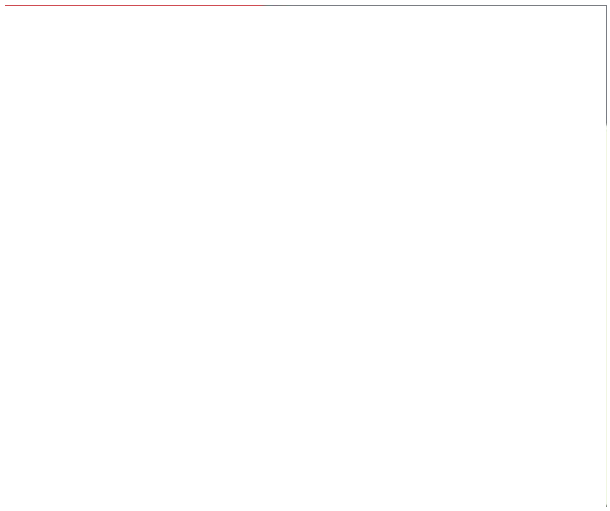
Tweet Share

Search articles by author

- Julio Cesar Ruivo
- Fábris Kossoski
- Márcio T. do N. Varella

Go

Spotlight



Registered charity number: 207890