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Protonated Ethylene Carbonate: A Highly Resonance-Stabilized Cation

Invited for this month's cover picture is the group of Prof. Andreas J. Kornath at the LMU in Munich (Germany). The cover picture shows the crystal structure of the salt of protonated ethylene carbonate $[C_3H_5O_3][Sb_2F_{11}]$. Protonated ethylene carbonate was synthesized by reacting the neutral compound in the superacidic system HF/SbF_5 at low temperature. Interestingly, the single-crystal X-ray structure analysis revealed a planar CO_3 moiety with nearly equal CO bond lengths. Further theoretical investigations of the cation led to the result, that it contains a remarkably delocalized 6π-electron system. On the cover this resonance stabilization is highlighted by p-orbitals on the CO_3 moiety. Read the full text of their Research Article at 10.1002/open.202100229.

What prompted you to investigate this topic/problem?

Since previous results from our group have shown that diprotonation of a simple cyclic ester such as γ-butyrolactone is not possible, we were interested to see if this could be achieved by expanding the potential basic centers. Therefore, we chose ethylene carbonate and expanded the basic centers from two to three, while maintaining the same ring size.

What was the biggest surprise (on the way to the results presented in this paper)?

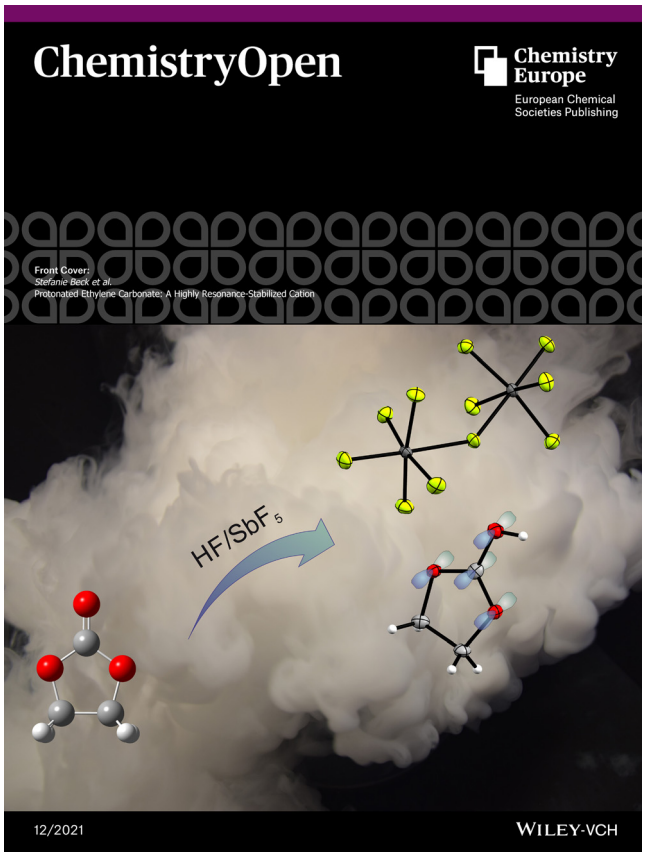
The biggest surprise was the analysis of the crystal structure, which revealed a planar CO_3 moiety with nearly equal CO bond lengths. This result led us to focus on and investigate the potential resonance stabilization.

What is the most significant result of this study?

The most significant result is that we were able to prepare a new compound with a highly remarkably delocalized 6π-electron system. Even if Y-aromaticity is controversially discussed in literature, the Y-shaped resonance stabilization of protonated ethylene carbonate is undeniable.

What are the main challenges in the broad area of your research?

The main challenges are safely handling and working with our basic but dangerous chemicals, like hydrogen fluoride or elemental fluorine. To ensure this, the preparation of each sample requires a lot of time and the absolute attention of each group member.



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