THE STRUCTURE OF STRAINED MOLECULES: THE EXAMPLE OF PARACYCLOPHANES.

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Cyclophanes are an interesting family of strained organic molecules that contain aromatic rings and aliphatic units that bridge the aromatic rings.[a] [2,2]-Paracyclophanes are an example of cyclophanes with two co-facially stacked benzene rings linked through ethylene chains.[b] The rigid connectivity and close positioning of the aromatic units in paracyclophane scaffolds makes them fundamentally important in supramolecular chemistry, while they find applications in material sciences due to their chiroptical and optoelectronic properties.[b,c] Structural homologues of [2,2]-paracyclophanes and different substitutions have features of chemical and industrial importance as they alter the photophysical and electrochemical properties of molecular scaffolds. Gas-phase studies of such molecular systems can provide the necessary isolated conditions to elucidate their structures and dynamics. One of the most powerful techniques to provide accurate gas-phase structures is high-resolution rotational spectroscopy.

We report an in-depth study of [2,2]-paracyclophanes using our broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer COMPACT in the 2-8 GHz frequency range.[d] We have explored the conformations and the intramolecular interactions of an alcohol-, an aldehyde- and, a ketone-substituted [2,2]-paracyclophane. The most stable conformations of all three derivatives obtained from quantum-chemical calculations and observed in experiments will be discussed along with the singly-substituted ^{13}C-isotopologues that facilitated the determination of the experimental structure of these molecules from the paracyclophane family.

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[b] Z. Hassan, E. Spuling, D. M. Knoll, J. Lahann, and S. Bräse, *Chemical Society Reviews*, **2018**, *47(18)*, 6947-6963.

[c] Y. Morisaki and Y. Chujo, *Bulletin of the Chemical Society of Japan*, **2019**, *92(2)*, 265–274.

[d] D. Schmitz, V. A. Shubert, T. Betz, and M. Schnell, *Journal of Molecular Spectroscopy*, **2012**, *280*, 77–84.