INFLUENCE OF HALOGEN VARIATION ON STRUCTURE AND INTERACTIONS IN VINYL HALIDE $(H_2C{=}CHX)\cdots CO_2$ (X = F, Cl, Br) COMPLEXES

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Chirped-pulse and resonant cavity Fourier-transform microwave spectroscopy have been used to investigate dimers of CO_2 with vinyl fluoride (VF), vinyl chloride (VCl) and vinyl bromide (VBr). For all three complexes, CO_2 is aligned adjacent to the X–C–H end (X = F, Cl, Br) of the ethylene subunit, with C–X$\cdots$C and C–H$\cdots$O contacts. For VF$\cdots CO_2$, a second isomer is also observed, with CO_2 roughly parallel to the H–C=C–F side of VF; however, there is no spectroscopic indication that similar structures are present for VCl$\cdots CO_2$ or VBr$\cdots CO_2$.

For vinyl fluoride$\cdots CO_2$, a full structural analysis has previously been published,[a] while for the Cl- and Br-containing species, insufficient data are presently available for complete structure determinations. However, structural information from ab initio calculations, ^{35}Cl/^{37}Cl and ^{79}Br/^{81}Br isotopic substitution, and analysis of chlorine and bromine nuclear quadrupole coupling constants will be presented. In addition, for this series of dimers containing C–H$\cdots$O contacts, further insight into the nature of the weak interactions may be obtained from Quantum Theory of Atoms in Molecules (QTAIM) and other *ab initio* analyses that are presently in progress.

[a] C. L. Christenholz, R. E. Dorris, R. A. Peebles, S. A. Peebles, *J. Phys. Chem. A*, **118**, (2014), 8765-8772.