CHARACTERIZATION OF WEAKLY BOUND HCF_3–OCS, H_2CF_2–OCS, H_3CF–OCS, AND HCF_3–CO_2 VAN DER WAALS COMPLEXES BY *AB INITIO* CALCULATIONS AND MICROWAVE SPECTROSCOPY.

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High resolution Fourier-transform microwave spectroscopy has been utilized in a systematic study of the structural and dynamic properties of a series of fluorinated methane molecules complexed to carbonyl sulfide and carbon dioxide. Theoretical data from *ab initio* calculations at the MP2/6-311++G(2d, 2p) level have provided good agreement with the observed experimental values. The structures of HCF_3–OCS and H_2CF_2–OCS have been determined from experimentally obtained rotational spectra fit to a Watson *A* reduction Hamiltonian to within 4 kHz. The *a*-type rotational spectrum of H_3CF–OCS has been assigned, however, *b*-type transitions still need to be located. The HCF_3–CO_2 spectrum showed a doubling of transitions into *A* and *E* states (by up to 1.5 MHz), and is currently fit to approximately 20 kHz using XIAM[a]. The ab initio structures of all the complexes within the series are very similar with O· · ·H distances consistently between 2.57-2.65 Å and O=C· · ·C bond angles of 61-64°, although with a wider range of H–C· · ·C angles (*ca.* 60° to 75°). Results for all members of the series will be presented and compared to theoretical data.

[a]XIAM v2.5e. H. Hartwig and H. Dreizler, *Z. Naturforsch* **51a**, (1996), 923.