CALCULATED SPECTROSCOPIC PROPERTIES FOR CLUSTER ANIONS OF TYPE $Hal^- \cdots HCCH$ (Hal: F, Cl, Br, and I)

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Large-scale coupled cluster calculations were carried out for the complexes formed by a halide anion and an acetylene molecule, all of which have linear equilibrium structures [a] [b]. The complex $[F \cdots H \cdots CCH]^-$ is most strongly bound and extremely anharmonic. A comparative discussion of various spectroscopic properties is given.

[a] P. Botschwina, T. Dutoi, M. Mladenović, Rainer Oswald, S. Schmatz and H. Stoll, Faraday Discuss., in press.
[b] P. Botschwina and H. Stoll, Phys. Chem. Chem. Phys., in press.