Amino acids form strongly bound anions when substituted with superhalogen ligands

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Abstract

The properties of AA-Y^- anions (where AA= cysteine, aspartic acid, lysine; Y=BF_3, PF_5) were investigated at the ab initio OVGF/6-311++G(3df,3pd)//MP2/6-311++G(d,p) level of theory. It is shown that introducing a superhalogen-like substituent to an amino acid (i.e., Cys, Asp and Lys) results in obtaining molecules that bind an excess electron relatively strongly. The electronic stabilities of such resulting daughter anions are predicted to be substantial (5.3-6.9 eV).