A Computational Exploration of Mechanisms for • -Bond Activation in the Reactions of Au^+ (^1S) with CF_3X (X=Cl, Br)

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The ability to activate sigma bonds is one of the most interesting characteristics of transition metals. Here, the reactions of Au^+(^1S) with several fluorinated methane analogs have been examined computationally using density functional methods. Optimized molecular geometries were located for intermediates and transition states which occur on reaction pathways resulting in both abstraction and elimination products. This level of theory predicts that with CF_3Br, product channels resulting in both Br^- abstraction and BrF elimination proceed via the expected activation of the C-Br bond; however, a stationary point resulting from C-F bond activation was also located with this neutral. C-F bond activation also leads to Br^- abstraction. Surprisingly, no stable intermediate was found as a result of C-Cl bond activation in CF_3Cl, but a transition state was established. All bimolecular products with this neutral proceed via activation of C-Cl bond, C-F bond, or in some cases both.