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Collision Induced Dissociation of Transition Metal Fluoride Complexes and the Multiply Charged Anions

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Abstract : Collision-induced dissociation (CID) can be used to study the intrinsic properties of ions in the gas phase.1 Decay pathways of transition metal difluoride complexes of titanium, zirconium, hafnium, and ruthenium were studied by CID in an ESI-Ion trap mass spectrometer. Furthermore, the decay pathways of multiply charged anions (MCAs) of titanium and zirconium were also studied. The CID results are illustrated by the behaviour of $(Cp^*)_2TiF_2$, which initially forms the ions $[M\text{-}F]^+$, $[M+Na]^+$, and $[M+K]^+$. The $[(Cp^*_2)TiF^+$ ion decays on resonant excitation to lose HF forming $[Cp^*(C_5Me_4CH_2)Ti]^+$ (Figure). The other major ion, $[(Cp^*)_2TiF_2+Na]^+$, decays on resonant excitation with production of $[(Cp^*)_2TiF_2]^+$ and $[C_5Me_4CH_2]^+$. We also report the behaviour of Cp_2MF_2 (M = Zr, Hf) and $Ru(PMe_3)_4F_2$. The decay pathway of the multiply charged anions (MCAs), notably TiF_6^{2-} and ZrF_6^{2-} was concluded to be ionic fragmentation with loss of F^- rather than electron detachment.

Keywords : collision induced dissociation, transition metal difluoride comolexes, multiply charged anions, mass spectrometry
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