

Consecutive fragmentations of the cubane-like zinc cluster $[\text{CH}_3\text{Zn}(\text{O-}i\text{-C}_3\text{H}_7)]_4$ upon electron ionization†

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The sequential dissociations of the tetranuclear zinc cluster-ion $[(\text{CH}_3)_3\text{Zn}_4(\text{O-}i\text{-C}_3\text{H}_7)_4]^+$ obtained by dissociative electron ionization of neutral $[(\text{CH}_3)_3\text{Zn}(\text{O-}i\text{-C}_3\text{H}_7)]_4$ are investigated by tandem mass spectrometry. After initial loss of a neutral $(\text{CH}_3)_3\text{Zn}(\text{O-}i\text{-C}_3\text{H}_7)$ unit to afford $[(\text{CH}_3)_2\text{Zn}_3(\text{O-}i\text{-C}_3\text{H}_7)_3]^+$, hydrogen migration leads to the expulsion of neutral acetone concomitant with $[(\text{CH}_3)_2\text{Zn}_3(\text{O-}i\text{-C}_3\text{H}_7)_2(\text{H})]^+$ as ionic fragment. Unimolecular dissociation of the latter gives rise to $[(\text{CH}_3)_2\text{Zn}_2(\text{O-}i\text{-C}_3\text{H}_7)]^+$ and neutral $\text{HZn}(\text{O-}i\text{-C}_3\text{H}_7)$. As demonstrated by collisional ionization of the neutral product, in the fragmentation of the dinuclear cluster $[(\text{CH}_3)_2\text{Zn}_2(\text{O-}i\text{-C}_3\text{H}_7)]^+$ neutral CH_3ZnH is formed, rather than the more stable fragments $\text{Zn} + \text{CH}_4$. From the resulting mononuclear species $\text{CH}_3\text{Zn}(\text{OC}(\text{CH}_3)_2)^+$ acetone is eliminated to afford CH_3Zn^+ as a quasi-terminal fragment ion.