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

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