

Calculations on $[\text{Be}_3\text{O}(\text{OCOR})_3]^+$ cations

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The fragmentation of the well-known $\text{Be}_4\text{O}(\text{OCOR})_6$ clusters ($\text{R} = \text{H}, \text{Me}, \text{Ph}, \text{Mes}$) through ionization in a mass spectrometer leads predominantly to $[\text{Be}_3\text{O}(\text{OCOR})_3]^+$ cations. Based on SCF calculations, these cations can be assigned a planar, highly symmetrical tricyclic core structure of D_{3h} symmetry. Our calculations confirm discrete energy minima for these cations and show that their stability is largely due to the favourable arrangement of alternating charges at neighbouring Be and O core atoms. The high polarity of Be-O bonds rules out any significant contributions from aromaticity. The aromatic stabilization was studied by performing Aromatic Ring-Current Shielding (ARCS) calculations on the $[\text{Be}_3\text{O}(\text{O}_2\text{CH})_3]^+$ cations. The obtained ring-current susceptibility for $\text{Be}_3\text{O}(\text{O}_2\text{CH})_3^+$ of 0.5 nA T^{-1} as compared to the ARCS values of 5.3, 2.2, and 1.5 nA T^{-1} for the isoelectronic $[\text{C}_{13}\text{H}_9]^-$, $\text{B}_3\text{N}(\text{N}_3\text{H})_3$, and $\text{B}_3\text{N}(\text{NOCH})_3$ molecules, respectively, shows that the $\text{Be}_3\text{O}(\text{O}_2\text{CH})_3^+$ cation is indeed nonaromatic.