

## A QUIRKY LITTLE FELLOW: Be<sub>3</sub> AND ITS ANION STUDIED BY PHOTOELECTRON SPECTROSCOPY

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Pure beryllium clusters have been the subject of a number of theoretical studies, but experimental validation for these studies has been lacking due to experimental hazards. The beryllium trimer has been predicted to be a closed shell  $D_{3h}$  neutral molecule, but limited computational studies have been carried out on the anion. In this study we present the first experimental data for the beryllium trimer and its anion. These data provide information on two transitions from the anion to the neutral, namely the  $Be_3^- X^2 A_2'' \rightarrow Be_3 X^1 A_1'$  and  $Be_3^- 1^2 A_1' \rightarrow Be_3 X^1 A_1'$  transitions. Ab initio electronic structure calculations have been validated against the experimental data, confirming the  $D_{3h}$  geometry of the neutral and anion ground states. Electronic transition energies computed at the EOM-CCSDT level of theory agree well with experimental measurements, but the spectra show little excited vibrational activity, in contrast to Franck-Condon simulations.