DISCOVERY OF DATIVE BONDING OF BERYLLIUM FLUORIDE ANION BY PHOTOELECTRON VELOCITY MAP IMAGING SPECTROSCOPY

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Beryllium can exhibit unusually strong attractive interactions under conditions where it is nominally a closed-shell atom. Two prominent examples are the Be_2 dimer and the He-BeO complex. Most recently, we examined the bonding of a similarly interesting molecule, the closed-shell Be-F^- anion. This molecule preserves the closed-shell character of the atoms as the electron affinity of F is high (328.16 kJ mol^{-1}) while that of Be is negative. Photoelectron velocity map imaging spectroscopy, in conjunction with coupled cluster electronic structure calculations, were used to determine the vibrational frequency for BeF^- and the electron affinity of BeF (approximately 8700 cm^{-1}). The latter has been used to determine a lower bound of 28480 cm^{-1}(343 kJ mol^{-1}) for the bond energy of BeF^-. The electronic structure calculations yielded predictions that were in good agreement with the observed data. A natural bond orbital analysis shows that BeF^- is primarily bound by a dative interaction.