

CLOSING THE (SINGLET-TRIPLET) GAP: BeOBe AND ITS ANION STUDIED USING PHOTOELECTRON SPECTROSCOPY

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Beryllium containing molecules often exhibit intense multi-reference character that can lead to large discrepancies in computational results depending on the treatment of electron correlation. Exemplary of this multi-reference character is the BeOBe molecule, which has long been a source of frustration for computational methods due to its very small singlet-triplet energy splitting. While the molecule has been studied experimentally before by laser induced fluorescence, this singlet-triplet gap had yet to be rigorously determined. Here we present the first experimental values for the BeOBe singlet triplet gap, obtained via Slow Electron Velocity Map Imaging (SEVI) spectroscopy on the BeOBe anion, as well as comparison to previous experiment and theoretical calculations. This new data links the singlet and triplet manifolds obtained in previous studies, providing new insight into this strange molecule.