MOLECULAR BEAM OPTICAL STUDY OF GOLD SULFIDE AND GOLD OXIDE[a]

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Gold-sulfur and gold-oxygen bonds are key components to numerous established and emerging technologies that have applications as far ranging as medical imaging, catalysis, electronics, and material science. A major theoretical challenge for describing this bonding is correctly accounting for the large relativistic and electron correlation effects. Such effects are best studied in diatomic, AuX, molecules. Recently, the observed AuS electronic state energy ordering was measured and compared to a simple molecular orbital diagram prediction[b]. Here we more thoroughly investigate the nature of the electronic states of both AuS and AuO from the analysis of high-resolution (FWHM$\cong$ 35MHz) optical Zeeman spectroscopy of the (0,0)$B^2\Sigma^- - X^2\Pi_{3/2}$ bands. The determined fine and hyperfine parameters for the $B^2\Sigma^-$ state of AuO differ from those extracted from the analysis of a hot, Doppler-limited, spectrum[c]. It is demonstrated that the nature of the $B^2\Sigma^-$ states of AuO and AuS are radically different. The magnetic tuning of AuO and AuS indicates that the $B^2\Sigma^-$ states are heavily contaminated.

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