Publications 2005-2009 of Friedrich Grein, Department of Chemistry, University of New Brunswick, Fredericton, NB, Canada.


201. F. Grein 2008. DFT and MRCI studies on ground and excited states of CrO₂. Chemical Physics 343, 231-240


199. S. Burrill and F. Grein 2007. MRCI studies on ground and excited states of CBr. Molecular Physics 105, 1891-1901


196. P. J. Bruna and F. Grein 2006. Theoretical studies on dications and trications of FH, ClH and BrH. Properties of the bound \( 1\tilde{1} \) states. Electron-spin g-factors and fine/hyperfine constants of the metastable \( X^3I^- \) states of ClH\(^2+\) and BrH\(^2+\). J. Phys. Chem. A 110, 4906-4917

195. P. J. Bruna and F. Grein 2006. The \( X^2A \) and \( A^2\tilde{1}^+ \) states of FH\(^+\), ClH\(^+\) and BrH\(^+\): a theoretical study of their g-factors and fine/hyperfine structures. Mol. Phys. 104, 429-446


192. S. Burrill and F. Grein 2005. Structure and Bonding of III/V compounds \( X_2Y_2 \), with \( X=\text{B, Al, Ga, and Y=N, P, As} \). J. Mol. Struct.: THEOCHEM 757, 137-142


189. P. J. Bruna and F. Grein 2005. Theoretical study on \( N_2^+ \), \( P_2^+ \), \( As_2^+ \), \( NP^+ \), \( NAs^+ \), and \( PAs^+ \): Hyperfine coupling constants for \( 1^2E_g^+ \), and electron-spin g-factors for \( 1^2E_g^+/1,2^2E_u^+(X_2^+) \) and \( 1,2^2E^+(XY^+) \) states. J. Mol. Spectrosc. 232, 125-138.