

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

213. Friedrich Grein **2009**. Theoretical studies on ground and excited states of the BrO₄ radical. Chem. Phys. Lett. **482**, 34-37.
212. Friedrich Grein **2009**. The ClO₄ radical: a theoretical study on ground and excited states. Mol. Phys. **107**, 2005-2013.
211. Pablo J. Bruna and Friedrich Grein **2009**. Theoretical study of electric moments, polarizabilities, and fine and hyperfine coupling constants of the B, C, A' and C'' states of N₂. Can. J. Phys. **87**, 589-600.
210. Friedrich Grein **2009**. Theoretical studies on the electronic spectrum of selenium dioxide. Comparison with ozone and sulphur dioxide. Chem. Phys. **360**, 1-6.
209. Friedrich Grein **2009**. Coupled cluster and density functional studies on geometries and energies of excited C_{2v} states of ozone. J. Chem. Phys. **130**, 124118 (1-9).
208. Pablo J. Bruna and Friedrich Grein **2009**. Axial Asymmetry of the Charge and Spin-Density Distributions in A States. Molecular Quadrupole Moments and Hyperfine Coupling Constants of CH, NH, OH, CF, LiO, NO, and FO. J. Phys. Chem. A **113**, 2615 - 2622.
207. Friedrich Grein **2009**. Ground and low-lying excited C_{2v} states of FeO₂ - A challenge to computational methods. International Journal of Quantum Chemistry **109**, 549-558.
206. Sonya Burrill and Friedrich Grein **2008**. Multireference configuration interaction studies on HCB_r. Can. J. Physics **86**, 1333-1343.
205. Konstantin V. Shuvaev, Andreas Decken, Friedrich Grein, Tareque S. M. Abedin, Laurence K. Thompson and Jack Passmore **2008**. NC-(CF₂)₄-CNSSN containing 1,2,3,5-dithiadiazolyl radical dimer exhibiting triplet excited states at low temperature and thermal hysteresis on melting-solidification: structural, spectroscopic, and magnetic characterization. Dalton Trans. **2008**, 4029 - 4037.
204. P. J. Bruna, F. Grein **2008**. The A²P_u state of N₂⁺: Electric properties, fine and hyperfine coupling constants, and magnetic moments (g-factors). A theoretical study. J. Mol. Spectroscopy **250**, 75-85.
203. J. M. Praetorius, D. P. Allen, R. Wang, J. D. Webb, F. Grein, P. Kennepohl, C. M. Crudden **2008**. N-Heterocyclic Carbene Complexes of Rh: Reaction with Dioxygen without Oxidation. J. Am. Chem. Soc. **130**, 3724-3725.
202. F. Grein **2008**. Hartree-Fock and standard density functional theory methods applied to excited states: The case of NO₂. Chem. Phys. Lett. **455**, 124-130

201. F. Grein **2008**. DFT and MRCI studies on ground and excited states of CrO₂. *Chemical Physics* **343**, 231-240
200. P. J. Bruna and F. Grein **2007**. Cylindrically Asymmetric Charge Density Distributions in Linear Molecules with Nonzero Electronic Angular Momentum. *J. Chem. Phys.* **127**, 074107, 1 - 12.
199. S. Burrill and F. Grein **2007**. MRCI studies on ground and excited states of CBr. *Molecular Physics* **105**, 1891-1901
198. F. Grein **2007**. Density functional and multireference configuration interaction studies on low-lying excited states of TiO₂. *J. Chem. Phys.* **126**, 034313-1 to 8
197. F. Grein, A. C. Chen, D. Edwards, C. M. Crudden **2006**. Theoretical and experimental studies on the Baeyer-Villiger oxidation of ketones and the effect of ν -halo substituents. *J. Org. Chem.* **71**, 861-872
196. P. J. Bruna and F. Grein **2006**. Theoretical studies on dications and trications of FH, ClH and BrH. Properties of the bound $1^5\Gamma^-$ states. Electron-spin g-factors and fine/hyperfine constants of the metastable $X^3\Gamma^-$ states of ClH²⁺ and BrH²⁺. *J. Phys. Chem. A* **110**, 4906-4917
195. P. J. Bruna and F. Grein **2006**. The X^2A and $A^2\Gamma^+$ states of FH⁺, ClH⁺ and BrH⁺: a theoretical study of their g-factors and fine/hyperfine structures. *Mol. Phys.* **104**, 429-446
194. F. Grein **2006**. Hyperfine coupling constants for N₂⁺, BO, AlO and GaO in rare-gas matrices, using the polarizable continuum model. *Chem. Phys. Lett.* **418**, 100-104
193. C. Clouthier, F. Grein and P. J. Bruna **2005**. Theoretical studies on singlet and triplet states of Ge₂. *Mol. Physics* **103**, 3253- 3261
192. S. Burrill and F. Grein **2005**. Structure and Bonding of III/V compounds X₂Y₂, with X=B, Al, Ga, and Y=N, P, As. *J. Mol. Struct.: THEOCHEM* **757**, 137-142
191. F. Grein **2005**. Rare Gas Effects on Hyperfine Coupling Constants of BO, AlO and GaO. *J. Phys. Chem. A* **109**, 9270-9278
190. C. M. Clouthier and F. Grein **2005**. MRCI Studies on the Electronic Spectrum of GeO⁺. *Chem. Phys.* **315**, 35-40.
189. P. J. Bruna and F. Grein **2005**. Theoretical study on N₂⁺, P₂⁺, As₂⁺, 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.
188. F. Grein **2005**. Electron spin resonance g tensors for complexes of Ne and Ar with AlO: Theoretical studies related to the large matrix effect observed for AlO. *J. Chem. Phys.* **122**, 124504-1 to 7.