

Publication List of Prof. Dr. Christel M. Marian

Peer-reviewed Articles in Scientific Journals and Conference Proceedings

1. Comparison of the structure and spectra of the HNO^+ and NOH^+ ions using *ab initio* SCF and CI methods. C. M. Marian, P. J. Bruna, R. J. Buenker, S. D. Peyerimhoff, *Mol. Phys* **1977**, *33*, 63-74.
2. Ab initio study on the isomers HNO^+ and NOH^+ , Vertical spectra and heat of formation. P. J. Bruna, C. M. Marian, *Chem. Phys.* **1979**, *37*, 425-444.
3. On the electronic structure of NOH (hyponitrous acid monomer) in the ground state. P. J. Bruna, C. M. Marian, *Chem. Phys. Lett.* **1979**, *67*, 109-114.
4. Ab initio CI calculation of O^+_2 predissociation phenomena induced by a spin-orbit coupling mechanism. C. M. Marian, R. Marian, S. D. Peyerimhoff, B. A. Heß, R. J. Buenker, G. Seger, *Mol. Phys.* **1982**, *46*, 779-810.
5. Ab initio calculation of the zero-field splittings of the $X^3\Sigma^-_g$ and $B^3\Pi_{g,i}$ states of the S_2 molecule. B. A. Heß, R. J. Buenker, C. M. Marian, S. D. Peyerimhoff, *Chem. Phys.* **1982**, *71*, 79-85.
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7. A theoretical study of the vibronic structure in the electronic spectrum of HNO^+ . M. Perić, M. Mladenović, J. Fejzo, C. M. Marian, P. J. Bruna, *Chem. Phys. Lett.* **1982**, *88*, 547-552.
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11. Computation of lifetimes for spin-forbidden transitions by ab initio methods: Application to the $b^1\Sigma^+$ states of NH and OH^+ . C. M. Marian, R. de Vivie, R. Klotz, *Proceedings of the 6th seminar on Computational Methods in Quantum Chemistry*, eds. W. P. Kraemer, R. Beardsworth, Max-Planck-Institut für Physik und Astrophysik, Garching **1984**, 100-110.
12. Potential energy surfaces by quantum mechanical ab initio methods. S. D. Peyerimhoff, H. Dohmann, C. M. Marian, *Proceedings of the Symposium on Atomic and Surface Physics '84*, Maria Alm / Salzburg, eds. F. Howorka, W. Lindinger, T. D. Märk, **1984**, 9-15.
13. Determination of the radiative lifetimes of the $b^1\Sigma^+$ and $a^1\Delta$ states in NH by ab initio methods. C. M. Marian, R. Klotz, *Chem. Phys.* **1985**, *95*, 213-223.
14. Ab initio study of the spin-orbit splitting of the 3P_g ground state of the selenium atom. T. Matsushita, C. M. Marian, R. Klotz, B. A. Heß, and S. D. Peyerimhoff, *Chem. Phys.* **1985**, *96*, 371-379.

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17. Spin-forbidden transitions in the presence of an intersystem crossing: Application to the b $^1\Sigma^+$ state in OH $^+$. R. de Vivie, C. M. Marian, S. D. Peyerimhoff, *Chem. Phys.* **1987**, *112*, 349-361.
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