
21. PUBLICACIONES

Algunos de los resultados que conforman este trabajo de tesis doctoral forman parte de los siguientes artículos publicados en revistas científicas:

1. "Anomeric and Mesomeric Effects in methoxycarbonylsulfonyl chloride, $CH_3OC(O)SO_2Cl$: Experimental and Theoretical Study", Erben, M. F.; Della Védova, C. O.; Romano, R. M.; Boese, R.; Oberhammer, H.; Willner, H.; Sala, O. *Inorganic Chemistry*, 2002, 41(5), 1064-1071.
2. "Dramatic changes in Geometry After Ionization: Experimental and Theoretical Studies on the Electronic Properties of Fluorocarbonyl (mono-, di- and tri-) Sulfur Compounds", Erben, M. F.; Della Védova, C. O. *Inorganic Chemistry*, 2002, 41(14), 3740-3748.
3. "Methyl Fluorocarbonyl Disulfide, $FC(O)SSCH_3$: A Theoretical Study on the Structural and Conformational Properties of its Neutral Ground State and Lowest-Lying Cationic State", Erben, M. F.; Della Védova, C. O. *Helvetica Chimica Acta*, 2003, 86(7), 2379-2395.
4. "Perfluoromethyl Fluorocarbonyl Peroxide, $CF_3OOC(O)F$: Structure, Conformations and Vibrational Spectra Studied by Experimental and Theoretical Methods", Trautner, F.; Gholivand, K.; García, P.; Willner, H.; Erben, M. F.; Della Védova, C. O.; Oberhammer, H. *Inorganic Chemistry*, 2003, 42(9), 3079-3085.
5. "Trifluoromethyl Chlorosulfonate, CF_3OSO_2Cl : Gas phase and crystal structure, conformation and vibrational analysis studied by experimental and theoretical methods", Erben, M. F.; Della Védova, C. O.; Boese, R.; Willner, H.; Leibold, C.; Oberhammer, H. *Inorganic Chemistry*, 2003, 42(22), 7297-7303.

6. "Trifluoromethyl Chloroformate, $ClC(O)OCF_3$: Structure, Conformation, and Vibrational Analysis Studied by Experimental and Theoretical Methods", Erben, M. F.; Della Védova, C. O.; Boese, R.; Willner, H.; Oberhammer, H. *The Journal of Physical Chemistry A*, 2004, 108(4), 699-706.
7. "N,N-Difluoro O-trifluoromethyl-hydroxylamine , CF_3ONF_2 : conformation and vibrational analysis studied by experimental and theoretical methods", Erben, M. F.; Della Védova, C. O.; Willner, H. *Journal of Molecular Structure*, 2004, 692(1-3), 63-70.
8. "Study of the Ionic Fragmentation of the Shallow- and Core-excited Fluorocarbonylsulfenyl Chloride, $FC(O)SCl$. Observation of a New Three-body Dissociation Mechanism", Erben, M. F.; Romano, R. M.; Della Védova, C. O. *The Journal of Physical Chemistry A*, 2004, 108(18), 3938-3946.
9. "O-O Bond Dissociation Enthalpy in Perfluoromethyl Fluorocarbonyl Peroxide, $CF_3OOC(O)F$. A Density Functional Quantum Chemical Analysis", Erben, M. F.; Della Védova, C. O. *Journal of the Argentinean Chemical Society*, 2004, 92(1/3), 133-138.
Trabajo invitado como contribución del número especial de la revista editado en homenaje al Prof. Emer. Dr. P. J. Aymonino en ocasión del 75 aniversario de su nacimiento.
10. "Factors Influencing the Conformational Behavior on Sulfenyl Carbonyl $XC(O)SY$ Compounds", Erben, M. F.; Della Védova, C. O. *Asian Chemistry Letters*, 2004, 8(2-3), 219-229.
Trabajo invitado como contribución del número especial de la revista dedicado al tema de estudios conformacionales.
11. "A theoretical investigation of the conformational space of perfluorohydroxylamine, F_2NOF ", Erben, M. F.; Pis Diez, R.; Della Védova, C. O. *Chemical Physics*, 2005, 308(1-2), 193-198.

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12. "Ionic Fragmentation on $ClC(O)SCl$. Evidence of a Highly Charged Molecular Ion and Confirmation of Unusual Dissociation Mechanisms for Halogencarbonylsulfenyl Chlorides", Erben, M. F.; Romano, R. M.; Della Védova, C. O. *The Journal of Physical Chemistry A*, 2005; 109(2), 304-313.

 13. "Fluoroformyl Trifluoroacetyl Disulfide $FC(O)SSC(O)CF_3$: Synthesis, Gas phase and crystal structure, conformation and vibrational analysis studied by experimental and theoretical methods", Erben, M. F.; Della Védova, C. O.; Boese, R.; Willner, H.; Leibold, C.; Oberhammer, H. Manuscrito en preparación.