A Quantum Chemistry Approach to the Force Fields of the Thionyl and Selenyl Halides, SOX_2 and $SeOX_2$

Lis E. Fernández[a] and Eduardo L. Varetti[b,c]

[a] Instituto de Química y Física, Facultad de Bioquímica, Química y Farmacia, Universidad, Nacional de Tucumán, San Lorenzo 456, 4000 S.M. de Tucumán, R. Argentina
[b] Centro de Química Inorgánica (CEQUINOR, CONICET-UNLP), Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C.Correo 962, 1900 La Plata, R. Argentina
[c] Member of the Carrera del Investigador Científico, CONICET, R. Argentina

Reprint requests to E. L. Varetti. E-mail: varetti@quimica.unlp.edu.ar

Z. Naturforsch. **2007**, *62b,* 1491 – 1496; received July 16, 2007

Force fields and vibrational frequencies were calculated for the molecules SOX_2 and $SeOX_2$, with X = F, Cl, Br, using DFT techniques. The previously available experimental data and assignments for the six molecules were confirmed by the theoretical results. These data were subsequently used in the definition of the corresponding scaled quantum mechanics (SQM) force fields. A comparison of the obtained internal force constants is made with results reported by other authors for the studied species.

Key words: Thionyl Halides, Selenyl Halides, Force Constants, Structure, DFT Calculations