# 29Si NMR CALCULATIONS FOR SILANES AND THEIR DERIVATIVES

Clémence Corminboeuf, Thomas Heine and Jacques Weber

Department of Physical Chemistry, University of Geneva, CH-1211 Geneva 4, Switzerland, Thomas.Heine@chiphy.unige.ch

$^{29}$Si NMR calculations for silanes and their derivatives (methyl-, hydroxy-, methoxy-, and methylmethoxysilanes and disiloxane) are performed using DFT for molecular orbitals (from the AllChem computer code [1]) and the IGLO [2] technique (as implemented in the deMon-NMR package [3]). The quality of the basis set and auxiliary functions, which are used to represent the charge density, both for geometries and chemical shift calculations, are tested. The DZVP/A2*/LDA level is found to give good results for geometries of all the classes of compounds studied here.

Chemical shift calculations are performed by using LDA and GGA (PW91, PBE) with the IGLOIII basis set and A2* auxiliary functions. The results are compared with experiment and benchmarked against GIAO [4]-DFT and ab initio calculations (LDA, PW91, HF, MP2) as implemented in Gaussian 98 [5].

[1] A.M. Köster, T. Heine and A. Vela, *AllChem* (2001) Cinvestav-IPN, Mexico.

[2] W. Kutzelnigg, *Isr. J. Chem.* 19 (1980) 193. M. Schindler and W. Kutzelnigg, *J. Chem. Phys.* 76 (1982) 1919.

[3] V.G. Malkin, O.L. Malkina, and D.R. Salahub, *Chem. Phys. Lett.* 204 (1993) 80, 87. V.G. Malkin, O.L Malkina, M.E. Casida, and D.R. Salahub, *J. Am. Chem. Soc.* 116 (1994) 5898.

[4] R. Ditchfield, *Mol. Phys.* 27 (1974) 789.

[5] Gaussian 98, Revision A.7; Gaussian Inc.: Pittsburg, PA, 1998.