Relativistic effects and orbital contributions to the electric field gradient

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The electric field gradient (EFG) is important for experimental studies, such as nuclear quadrupole resonance measurements and Mössbauer spectroscopy. It couples to the nu- clear quadrupole moment resulting in observable energy levels. The EFG has an inverse cubic distance dependence, i. e. it probes the region close to the nuclei. Relativistic ef- fects are also most pronounced in this region and so it is expected that they are important for an accurate computation of EFGs.

In the current work the EFGs of several molecules were studied using different relativistic and non-relativistic Hamiltonians. Furthermore projection analysis[1] was applied to identify the contributions of different atomic orbitals to the EFG. This will be compared to a simple model devised by by Dailey and Townes [2], which allows to relate the EFG to the ionic character and hybridization of the bond for centers with partially filled valence p-shells. An extension of this model to a relativistic framework was already presented by Pyykkö and Seth [3] and we will compare it to our approach.

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[3] P. Pyykkö, M. Seth, Theor. Chem. Acc., **96** (1997), 92–104.