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Electric field gradient calculations by quantum chemical methods

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The electric field gradient, which from the point of view of the given nucleus is a measure of the inhomogeneity of the external electric field of all other charges, is a molecular property of the first order and can be determined from the knowledge of the electronic wave function and positions of nuclei. Since for accurate calculations we have to use highly sophisticated electron correlation approximations like the Coupled Cluster Singles and Doubles with non-iterative Triples CCSD(T) method, which does not fulfill the Hellmann-Fyenman theorem, and therefore we are forced to use so-called derivatives methods instead of calculating the expectation value of the given operator. Inclusion of relativistic effects in calculation of electric field gradients is inevitable [1]. If one–or two–component relativistic methods (e.g. DKH, IOTC) are exploited, the usual method of computing, which is just a counterpart of the nonrelativistic scheme leads to the change of picture effect [2] manifested by significant inaccuracies of the calculated property values. Different techniques how to avoid the change of picture effect will be discussed [3-5].
The combination of experimental nuclear quadrupole coupling constant obtained from microwave spectra and theoretical electric field gradient provides currently the best source of nuclear quadrupole moment values, at least for light elements. A series of such determinations of nuclear quadrupole moments will be presented [6-11].
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