Walking through the exotic world of NMR

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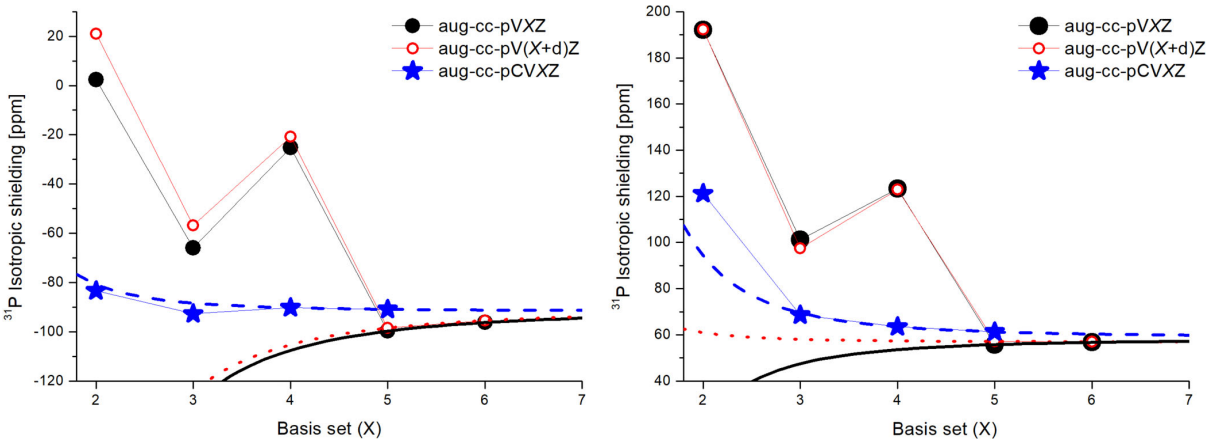
Without any doubts, NMR is the most versatile technique, which allows us to study single atoms, chemical compounds, as well as living materials. Thus, theoretical prediction of a nuclear magnetic shielding tensor or indirect spin-spin coupling constants commonly support an experiment. In this paper I will discuss problems related to theoretical predictions of NMR properties for atoms, small and middle size molecules, as well as larger molecular systems. Both complete basis set (CBS) limit assessment and locally dense basis sets (LDBS) will be described.

The quality of results, using *ab initio* and DFT approaches will be discussed, including an unusual case, where CCSD(T)/CBS nuclear shieldings are the same as these, calculated at low level of theory (RHF/CBS). Problems with aug-cc-pVXZ basis sets, applied for accurate calculation of third-row elements nuclear shieldings will be also addressed.



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