A simple comparison of several *ab initio* methods on NMR of single water molecule

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NMR is a useful method to measure the magnetic shielding of electrons on nuclear. So, for evaluating the value of NMR quantitatively and accurately, the *ab initio* methods can be applied, such as HF, MP2, and a series of DFT methods.

By the basis set of def2-TZVP, several *ab initio* methods have been analyzed for NMR. There are all of results listed in the table. The Gaussian 09 D.01 program package has been used.

def2-TZVP	O		H	
(ppm)	Isotropic	Anisotropy	Isotropic	Anisotropy
HF	329.2996	45.2775	30.9549	19.6463
MP2	349.5062	31.0156	30.9970	19.6934
B3LYP	330.2865	38.7905	31.6012	18.3505
M06-2X	330.0158	41.4742	31.3433	18.9204
PBE0	332.1298	39.4392	31.4706	18.7055
ωB97XD	330.6763	43.0584	31.4802	18.6316

With all of the data have been listed, a brief analysis can be performed. As everyone knows, it is truism the MP2 method is beneficial for predicting NMR. The computational results show that, to be compared with MP2, the results by HF, however are similar to the results of MP2 in H atom, are unreasonable obviously in O atom. On the other hand, all of the results by DFT are incorrect not only in H atom but also in O atom.