**COUPLED CLUSTER EVALUATION OF THE FREQUENCY DISPERSION OF THE FIRST AND SECOND HYPERPOLARIZABILITIES OF WATER, METHANOL AND DIMETHYL ETHER**

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The static and dynamic first (β||) and the second (γ||) hyperpolarizabilities of water, methanol, and dimethyl ether have been evaluated within the response function approach [1,2] using a hierarchy of coupled cluster levels of approximation and doubly-augmented correlation consistent atomic basis sets. For the three compounds, the electronic β|| and γ|| values calculated at the CCSD and CC3 levels are in good agreement with gas phase electric field-induced second harmonic generation (EFISHG) measurements [3,4]. In addition, for dimethyl ether, the frequency dispersion of both properties follows closely recent experimental values [5] demonstrating the reliability of these methods and levels of approximation. This also suggests that the vibrational contributions to the EFISHG responses of these molecules are small.

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