P5535: Calculations of Effective Electric Field ($\mathcal{E}_{\text{eff}}$) using Relativistic Coupled-Cluster Analytic-Gradient Theory

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- We present the development of an analytic scheme for calculations of $\mathcal{E}_{\text{eff}}$ using exact two-component coupled cluster methods:

$$\mathcal{E}_{\text{eff}} = \frac{\partial E_{\text{X2C-CC}}}{\partial d_e}|_{d_e=0} = \sum_{pq} D_{pq}^{\text{X2C-CC}} [V_{\text{eff}}]_{pq}^{\text{X2C}}$$

- Calculating $\mathcal{E}_{\text{eff}}$ as an analytic first derivative of relativistic coupled-cluster energy, the present approach is more efficient than numerical differentiation of energies and more accurate than unrelaxed formulation.

- The present approach is compatible with noniterative treatment of triple excitations.

- The next step is to extend this analytic scheme to calculations of the other symmetry-violating sensitivity parameters.

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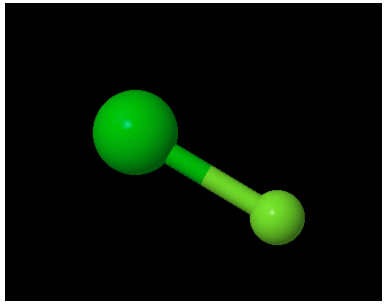
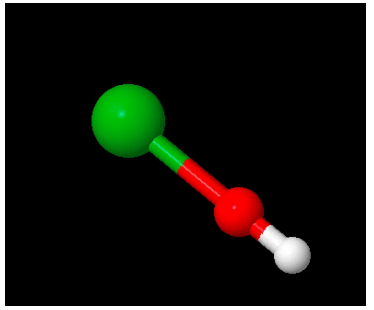
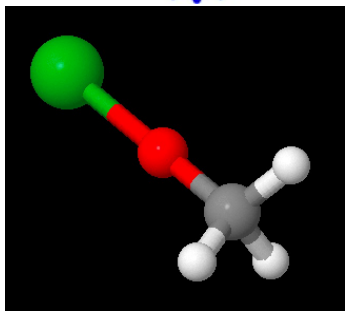


YbF
$\mathcal{E}_{\text{eff}}$ =23.5 GV/cm



YbOH
$\mathcal{E}_{\text{eff}}$ =23.7 GV/cm



$YbOCH_3$
$\mathcal{E}_{\text{eff}}$ =23.6 GV/cm

$\mathcal{E}_{\text{eff}}$ (GV/cm)	HF	CCSD	CCSD(T)
NoF	185.4	192.4	191.9
NoOH	185.2	192.4	191.7
LrO	303.3	263.9	246.5
$LrOH^+$	268.6	259.5	255.1

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