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DIPOLE MOMENT CALCULATIONS ON HCHO AND CO USING THE FLOATING SPHERICAL GAUSSIAN ORBITAL (FSGO) METHOD

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Spherical Gaussians allow an unusually simple point charge calculation of dipole moment $<m>$ of molecules. The formula used is $<m> = \sum_{v} R^{v} Z^{v} - 2 \sum_{i} R_i T_{ii} - 4 \sum_{i<j} R_{ij} S_{ij} T_{ij}$, where the first term is the nuclear contribution, R, R_i, R_{ij} are the locations of the nuclei, orbital centres and overlap centres, S_{ij} and T_{ij} are the ovelap and inverse overlap matrix elements respectively.

Two of the molecules where extensive calculations were performed are Formaldehyde (HCHO) and Carbon monoxide (CO). The fact that HCHO is quite polar (m = 2.33 D, $\vec{H_2CO}$) whereas CO is almost non-polar (m = 0.112 D, in the direction $\overleftarrow{CO}$, despite the highly electronegative Oxygen atom), makes this an interesting investigation.

The simple FSGO method, in its original form, did not give satisfactory results on either HCHO or CO. A modified FSGO procedure was therefore devised, which represented the multiple bonds in the two molecules as combinations of ' s ' and ' p ' type Gaussians and allowed them to float along the axes of the multiple bonds. This latter method gave results for m which were in agreement with the experimental value and also provided a better representation of the flexibility of the electron cloud in these two molecules.

(m = mu).