Density Functional Study of LinHm Clusters. Electric Dipole Polarizabilities

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The dipole polarizability of a series of clusters of the type LinHm has been calculated using density functional methods. The study of the trends in the mean polarizability and the anisotropy are explained in terms of the interplay between electronic and geometrical effects. The changes in the polarizability for different isomers of a given cluster as well as its variations when hydrogen atoms are added to a given cluster are also discussed. A very related quantity, the hardness, has also been calculated in the simple approximation of hardness equal to the energy gap. Their values are discussed in terms of the possible stability of the different clusters.