

Polarizability Study of Fullerene Nano-Structures C_{20} to C_{300} by Using Monopole-Dipole Interactions Theorem



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Abstract

Since the discovery of fullerenes (C_n), one of the main classes of carbon compounds, the unusual structures and physicochemical properties of these molecules have been discovered, and many potential applications and physicochemical properties have been introduced. Up to now, various empty carbon fullerenes with different numbers "n," such as C_{20} through C_{300} (like C_{60} , C_{70} , C_{76} , C_{82} , ..., C_{300}) have been obtained. The linear uniform field electric dipole polarizability tensors of 46 fullerenes in the range C_{20} through C_{240} were calculated by the Atom Monopole-Dipole Interaction (AMD) theory, using the monopole and dipole polarizabilities of the carbon atom found previously to fit polarizability tensors of aromatic hydrocarbons. The structures are taken to be those predicted by molecular dynamics energy optimization. The isotropic mean polarizabilities calculated for C_{60} and C_{70} are comparable to experimental data from solid film studies and to quantum mechanical calculations. Topological indices are digital values that are assigned based on chemical composition. These values are purported to correlate chemical structures with various chemical and physical properties. They have been successfully used to construct effective and useful mathematical methods to establish clear relationships between structural data and the physical properties of these materials. In this study were extended the calculation of the parameters concern to atom monopole-dipole moment such as Ellipsoid (α_1 to α_3 and \bar{a}), AMDI (Atom monopole-dipole interaction theory; α_1 to α_3 and \bar{a}) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, ABC α_1 to α_3) by QSAR for C_{20} through C_{300} .

Keywords: Fullerenes; Polarizability; Amdi Theory; Ellipsoid; Semi-Axes Thin Ellipsoidal Shell

Abbreviations: AMDI: Atom Monopole Dipole Interaction; FC: Ferrocene; TI: Topological Indices; Atom Monopole Dipole Interaction (AMDI); TI: Topological Indices; MLR: Modeling; MLR: Modeling Both Linear

Introduction

The electrochemical properties of the fullerene C_{60} have been studied since the early 1990s, when these materials became available in macroscopic quantities (for a review see [1]). [1-3] in 1990, have shown that C_{60} is electrochemically reducible in the CH_2Cl_2 medium to C_{60}^- and C_{60}^{2-} . In 1992, have cathodically reduced both C_{60} in six reversible one-electron steps for -0.97 vs. Fc/Fc^+ (Fc =Ferrocene). This fact, along with the absence of anodic electrochemistry of fullerenes, matches the electronic structure of fullerenes: the LUMO of C_{60} can accept up to six electrons to form C_{60}^{6-} , but the position of the HOMO does not allow for hole-doping under the usual electrochemical conditions. In 1991, Bard et al. [4-8] first reported on irreversible electrochemical and structural reorganization of solid fullerenes in acetonitrile medium. Dunsch et al. [5] have upgraded the experimental conditions by investigating highly organized C_{60}

films on HOPG in aqueous medium. The reduction of such films manifested itself by re-structuring into conductive nanoclusters of $\sim 10^2$ nm in diameter [5-9].

The linear uniform field electric dipole polarizability tensors of 46 fullerenes in the range C_{20} through C_{240} are calculated by the Olson Sundberg Atom Monopole-Dipole Interaction (AMDI) theory, using the monopole and dipole polarizabilities of the carbon atom found previously to fit polarizability tensors of aromatic hydrocarbons. The structures are taken to be those predicted by Zhang and co-workers by molecular dynamics energy optimization. The isotropic mean polarizabilities calculated for C_{60} and C_{70} are comparable to experimental data from solid film studies and to quantum mechanical calculations. Polarizability tensors are also calculated for conducting ellipsoidal shells which have the same moment of inertia tensor

as the corresponding fullerenes. These are substantially smaller than the AMDI polarizabilities for the smaller fullerenes, but the two calculations tend to converge for the larger molecules. [7-15]

Graph theory has been found to be a useful tool in assessing the QSAR (Quantitative Structure Activity Relationship) and QSPR (Quantitative Structure Property Relationship). Numerous studies in the above areas have also used what are called Topological Indices (TI). It is important to use effective mathematical methods to make good correlations between several data properties of chemicals. Numerous studies have been performed related to the above mentioned fields by using the so-called Topological Indices (TI). The numbers of carbon atoms at the structures of the fullerenes were utilized here [7-15].

In this study were extended the calculation of the parameters concern to atom monopole-dipole moment such as *Ellipsoid* (α_1 to α_3 and \bar{a}), AMDI (Atom monopole-dipole interaction theory; α_1 to α_3 and \bar{a}) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, ABC α_1 to α_3) by QSAR for C20 through C300.

Graphs And Mathematical Method

All graphing operations were performed using the *Microsoft Office Excel 2003* program. The numbers of carbon atoms at the structures of the fullerenes C_n were utilized to make the relationship and calculate the *Ellipsoid*, AMDI and thin ellipsoidal shell of uniform thickness. For Modeling, Both Linear (MLR) and nonlinear (ANN) models were used in this study.

Discussion

The polarizabilities of the ellipsoids are simply correlated with their geometry, as can be seen from the fact that the principal polarizabilities are approximately proportional to the lengths of the corresponding axes. To some extent this holds for the AMDI model as well, but for the smaller members of the series there are cases where the principal polarizabilities are not in the same ratio as the axes. This is apparently because the atom dipole contribution, which is not simply related to the axis lengths, is relatively larger for the smaller members. A further measure of the correspondence between the molecules and the ellipsoids is found in the comparison of the principal polarizability axes found by the AMDI theory with the principal geometric axes of the ellipsoids. Where the three semi-axes are distinct, the axes directions are the same to within a few tenths of a degree. The numbers of carbon atoms at the structures of the fullerenes C_n were utilized and extended the calculation of the parameters concern to atom monopole-dipole moment such as *Ellipsoid* (α_1

to α_3 and \bar{a}), AMDI (Atom monopole-dipole interaction theory; α_1 to α_3 and \bar{a}) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, ABC α_1 to α_3) by QSAR for C20 through C300.

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