Static dipole polarizabilities of icosahedral fullerenes from C_{60} to C_{2160} by all-electron density-functional theory RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso, MARK PEDERSON, Naval Research Laboratory, BRETT DUNLAP, Naval Research Laboratory — The electronic response of C_{60}, C_{180}, C_{240}, C_{540}, C_{720}, C_{960}, C_{1500}, and C_{2160} fullerenes is characterized by determining their static dipole polarizabilities by all-electron density-functional theory. We first determine the dipole polarizabilities of C_{60}, C_{180}, C_{240}, and C_{540} fullerenes by the finite-field method, using 35 basis functions per atom (NRLMOL basis set), and using the PBE-GGA. In the second set of calculations the sum-over-states (SOS) polarizabilities for all fullerenes from C_{60} through C_{2160} are determined by our fully analytic formulation of density functional theory(ADFT). The 6-311G(d,p) basis set is used in the ADFT calculation, which amounts to 38800 basis functions for the largest fullerene in this series, namely C_{2160}. The SOS polarizabilities are roughly 4 times larger than the finite-field polarizabilities. When scaled by a correction factor obtained within linear response theory, the SOS polarizabilities are within 1-3% of the finite-field polarizabilities. The polarizability per carbon atom increases from 1.34 Å^3 in C_{60} to 4 Å^3 in C_{2160} while the ratio of fullerene polarizability to its volume approaches unity pointing to quenching of quantum size effects by C_{2160}. The results show previous tight-binding calculations greatly exaggerate the electronic response of large fullerenes.

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