

Free energy of a charge distribution in a spheroidal cavity surrounded by concentric dielectric continua

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We present a theoretical treatment for the Helmholtz free energy of an arbitrary discrete charge distribution in a central prolate or oblate spheroidal cavity surrounded by two and three concentric dielectric continua of the same symmetry. The electrostatic interaction is accounted for by a multipolar expansion. This model permits us to consider in a simple way nonlinear dielectric effects and the nonsphericity of solute molecules. The results are presented in a suitable form to discuss them in terms of a virtual polarization charge distribution. Also, we give an explicit expression for the contributions coming from the zeroth-order multipole moments for any number of shells. © 1990 American Chemical Society.