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Polarizability and Kerr Constant of Proteins by Boundary Element Methods

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Abstract

A precise implementation of the Boundary Element method has been applied to the computation of the polarizability and the Kerr constant of eight soluble proteins. The method is demonstrated to be accurate and precise by comparison with analytical values for spheroids. Two different integral equations have been solved: 1) an exact equation with explicit dielectric constant dependence, and 2) an exact equation for a metallic body. The dielectric dependence for the metallic body case is built in with a generalization of the ellipsoid formula. Both methods agree quantitatively with each other for low relative dielectric constants. A full tensor expression for the Kerr constant yields perfect agreement with experiment for some proteins and badly under reports for the rest. The protein structure is obtained from a crystallographic database and is assumed rigid throughout the TEB measurement. Electrolyte effects are neglected. The Kerr constant is dominated by the protein dipole moment and is quite sensitive to the orientation of the dipole moment relative to the principal axes of the polarizability tensor. Several possible reasons for the large discrepancy between some computed and measured values are discussed.

Keywords

polarizability; Kerr constant; proteins; boundary elements

1. Introduction

The polarizability of molecules and molecular aggregates is required in order to understand measurements involving electromagnetic scattering, and the dynamics of these systems in the presence of electric fields. In addition, as emphasized in the work of Douglas, Garboczi and co workers¹, the polarizability is also essential in the description of the thermodynamic properties of mixtures since it mediates particle –particle interactions. There has been much work on the numerical computation of these quantities because analytical solutions are obtainable only for simple smooth shapes characterized by an ellipsoid. The Platonic solids have been an important challenge because despite the large amount of symmetry, no analytical solutions exist even for the cube. Two classes of numerical methods have been put forth in the study of these problems: a) Finite element¹ and boundary element methods^{2,3}, and b) random walk models or path integral methods^{1,4}. All of these numerical methods are capable of handling arbitrarily shaped objects, a requirement in the application to biomolecules such as proteins.

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Douglas and Garboczi^{1,4} have shown that the path integral method is both accurate and fast. However, that method is restricted to problems which have the electrostatic Green function as a propagator in the interaction. Some hydrodynamic problems can be approximated by the so called pre-averaging approximation in which the Oseen tensor is orientationally averaged to yield a propagator proportional to the electrostatic one. We have shown that this approximation is unsuitable for transport properties except for the case of translational diffusion⁵. We continue to emphasize the boundary element method in this work.

In our application to proteins, we will make several simplifying assumptions and determine whether these are reasonable for understanding the Kerr constant measurement. We will assume that the protein is rigid, that it is composed of electrically isotropic material, and that polyelectrolyte effects can be ignored. On the other hand, we will compute the polarizability tensor accurately and use measured dipole moments when available in order to minimize the error in the aspects that we do retain in the theory. The electrostatic problem is solved via BE with two methods, an exact and an approximate method. The approximate method computes the depolarization factors for a metallic object, and the polarizabilities are extended to arbitrary dielectric constant via an ellipsoidal ansatz. We compute the polarizability tensor of proteins from both methods and find that they are equivalent. Our work on the boundary element method applied to Platonic solids⁶ and to hydrodynamics^{7,8} is presented elsewhere.

2. Theory

The response of an object composed of isotropic material embedded in an external static electric (or magnetic) field can be formulated in terms of integral equations referring to the boundary of the object. These integral equations can be efficiently and precisely solved by the boundary element method. The exact solution to the electrical (or magnetic) response of such a dielectric object as a function of its permittivity (or permeability) has been derived by Senior^{9,10}. Let Φ_μ^t be the total potential outside the boundary B of the object, $\psi_\mu = (1 - \epsilon) \Phi_\mu^t$, for an electric field applied in the μ Cartesian direction, and a relative material dielectric constant ϵ . The integral equation satisfied by ψ_μ is given by:

$$\frac{\epsilon - 1}{\epsilon + 1} \Psi_\mu(\vec{r}_j) + \frac{1}{2\pi} \iint_B \Psi_\mu(\vec{r}) \frac{\hat{n}(\vec{r}) \cdot (\vec{r} - \vec{r}_j)}{|\vec{r} - \vec{r}_j|^3} dS = 2x_\mu^j \quad (1)$$

where, $\hat{n}(\vec{r})$ is the outward normal at point r on the particle boundary B, x_μ^j is the μ^{th} -component of an arbitrary vector $\mathbf{r}_j$ on the particle boundary B, and dS is an infinitesimal surface element. The polarizability tensor α can be readily computed as an integral over the auxiliary ψ_μ function:

$$\alpha_{\mu\nu} = \iint_B n(\vec{r}) \cdot \hat{x}_\mu \Psi_\nu(\vec{r}_j) dS \quad (2)$$

The integral equation (1) can be efficiently solved by dividing the surface in to N triangular patches and making the approximation that the function ψ_μ is constant over a patch. This approximation is removed by performing the calculation for increasing numbers of triangles, N, and extrapolating to infinity. When this procedure is implemented, there results a linear system of N equations given by:

$$\sum_{k=1}^N G_{jk} \Psi_{\mu}(\vec{r}_k) = 2x_{\mu}^j \quad (3)$$

where the NxN matrix of coefficients is given by,

$$G_{jk} = \frac{\epsilon+1}{\epsilon-1} \delta_{jk} + \frac{1}{2\pi} \hat{n}(\vec{r}_k) \cdot \vec{H}_{jk} \quad (4)$$

and the vector integrals over the k^{th} triangle Δ_k are,

$$\vec{H}_{jk} = \iint_{\Delta_k} \frac{(\vec{r}_j - \vec{r})}{|\vec{r}_j - \vec{r}|^3} dS \quad (5)$$

The linear system (3) is solved in double precision in our program POL using LAPACK with optimized BLAS for AMD Opteron processors. The vector integrals (5) are evaluated either analytically, or numerically to 16 digit precision. The details are reported elsewhere¹¹.

The integral equations presented above are exact, but the problem must be separately solved for every value of the dielectric constant of the body. We have also investigated an approximate solution based on the equations for a purely metallic body and an ellipsoid ansatz to introduce the ϵ dependence (see section 5 below). Zhou¹² has shown that the surface charge density, σ , of an arbitrarily shaped conducting particle subjected to an electric field can be determined by formulating Poisson's equation as an integral of Green's function over the surface of the molecule (omitting a factor of 4π):

$$\vec{r} = \iint_B \frac{(\hat{x}_1' \sigma_1 + \hat{x}_2' \sigma_2 + \hat{x}_3' \sigma_3)}{|\vec{r} - \vec{r}'|} dS' \quad (6)$$

and the surface charge density is expressed in terms of three auxiliary densities $\sigma_i(\mathbf{r})$. This equation can be solved in identical fashion to equation (1). For each auxiliary density, the μ^{th} component of the j^{th} surface element satisfies the linear system given by,

$$x_{\mu}^j = \sum_{k=1}^N \int_{\Delta_k} \frac{1}{|\vec{r} - \vec{r}_j|} dS \cdot \sigma_{\mu}(\vec{r}_k) \quad (7)$$

With the same super matrix G_{ij} of integrals over the Green function, one can solve 3 different linear systems to obtain the unknown surface charge densities. This is achieved in our program PBEST with the aid of LAPACK routines that call a hardware optimized BLAS library. Computations on a tetrahedron composed of 17560 triangles take less than 5 minutes on an AMD Opteron 248 machine. The integrals of the G_{kj} matrix of eq. (7) are computed essentially exactly, as a special case of those for hydrodynamics as described in Aragon⁶.

Unlike the integral equation (1), the formulation in eq (6) does not automatically ensure that there is no net charge induced on the body by the electric field. To correct for this, one must also compute the capacitance and the total charges. The computation of the capacitance

proceeds in identical fashion except that the total charge σ_c satisfies a scalar integral equation analogous to eq. (6), with “1” as the left hand side. Once the unknown surface quantities have been computed, we may easily compute the polarizability tensor and capacitance by an integration over the surface, or equivalently, by a discrete sum over the surface elements. The expressions are:

$$\alpha_{\mu\nu}^0 = 4\pi \int_B x_\mu \left(\sigma_\nu - \frac{Q_\nu \sigma_c}{C} \right) ds \quad (8)$$

$$C = 4\pi \int_B \sigma_c ds \quad ; \quad Q_\nu = 4\pi \int_B \sigma_\nu ds \quad (9)$$

A convenient set of quantities that can be used to compare the BE methodology to analytical results is the computation of the depolarization factors L_j , for a particle of volume V , from the eigenvalues of the polarizability tensor,

$$L_j = \frac{V}{4\pi \alpha_{jj}^0} \quad (10)$$

Increasing the number of boundary elements gives a better approximation to the exact surface, and therefore the exact solution, at the cost of an increase in computational time and memory requirements. To obtain the most precise values, the properties are computed for a series of values (N) of boundary elements, and then extrapolated vs. $1/N$ to an infinite number of surface triangles. In the following sections, we apply the theory to ellipsoids of revolution and to proteins.

3. Ellipsoids

In order to demonstrate the correctness of our codes, we present data for ellipsoids of revolution. The precision of our results can be observed from the linearity of the extrapolations to infinite number of surface elements. Our ellipsoids were triangulated by modifying the tessellation produced by Mathematica: every quadrilateral element was divided into two triangles. For this case, no attempt was made to more finely define the ends of a prolate or the edges of an oblate ellipsoid. In the case of an ellipsoid of revolution, Figure 1 shows that the extrapolations can be done to high precision.

For ellipsoids, the polarizability can be readily computed¹³ from the depolarization factors as a function of dielectric constant and the volume V .

$$\alpha_{jj}(\epsilon) = \frac{(\epsilon - 1) V / 4\pi}{1 + (\epsilon - 1) L_j} \quad (11)$$

The results for ellipsoids are given as a function of axial ratio for prolate (axial ratio $p < 1$) and oblate ($p > 1$) cases in Table 1. This table presents dimensionless numbers $[\sigma] = 4\pi a/V$ for convenience. The ellipsoid has two distinct eigenvalues and each of those is represented by the two rows in each data box. The errors compared to the analytical results are insignificant at a few parts per million, demonstrating that the method is both accurate and precise. The values from Pol for the metallic case were obtained by using $\epsilon = 10^5$.

For ellipsoids, either PBEST or POL should give the correct answer because the formula in eq. (11) is exact. In the case of other shapes, PBEST can only be used if we have a formula similar to eq. (11) to express the dielectric constant dependence. In this paper the “ellipsoid ansatz” is the use of a generalization of eq. (11) for arbitrary shapes. In the next section we apply it to proteins and compare with the exact calculation using POL.

4. Proteins

The triangulation method utilized for proteins has been described previously⁶. A typical triangulation with Connolly's MSROLL program, followed by coarsening with our COALESCE for xx is shown in Figure 2. The probe size used in MSROLL has some effect on the calculated values, but the difference is significant only near the metallic case. We have used a water sized probe radius of 1.5 Å and have ignored hydration. Electrically, a protein is characterized by its shape and an effective dielectric constant, ϵ . We have computed the polarizabilities of proteins using both the exact computation of POL and the ellipsoid ansatz based on the depolarization factor produced by PBEST. In the ellipsoid ansatz, the polarizability component as a function of the relative dielectric constant $\epsilon = \epsilon_b/\epsilon_m$ (where b = body, m = medium) is given by eq. (11) in the principal axes of the tensor. These results are shown in Table 2. The ellipsoid ansatz is exact in two limits, the $\epsilon = 1$ limit when the polarizability is zero, and the metallic case, when ϵ goes to infinity. The results of both calculations deviate in a minor way only in between and are essentially the same for small ϵ , the case of interest here.

A suitable experimental measurement that we can compare our results with is the Kerr constant in dilute aqueous solution. The measurement of the electric birefringence is described elsewhere¹⁴. This quantity, however also depends on the protein dipole moment, and in most of the examples below, this quantity dominates the response by comparison to the dc electric polarizability, but is directly dependent on the polarizability in the optical regime. The specific Kerr constant, K_{sp} , can be computed by a formula due to Wegener¹⁵, adapted here to the case of no electro-hydrodynamic coupling, and without the approximation that the relative index of refraction is unity. Then we have (in SI units),

$$K_{sp} = \left(\frac{n^2 + 2}{3} \right) \left(\frac{3 \text{Tr} \left[\alpha(\epsilon_{opt}) \cdot (\mu\mu + kT\alpha(\epsilon)) \right] - \text{Tr} \left[\alpha(\epsilon_{opt}) \right] \text{Tr} [\mu\mu + kT\alpha(\epsilon)]}{60n^2\epsilon_0 V k^2 T^2} \right) \quad (12)$$

The formula for K_{sp} depends on the index of refraction of the solvent, n , the relative dielectric constant for protein/water in the optical range (a laser with wavelength in the visible is used to probe the molecular orientation) $\epsilon_{opt} = 1.2 = (1.45/1.33)^2$, and the equivalent ratio in the dc or zero frequency range, $\epsilon = 4/80$. A typical value for the index of refraction of proteins was obtained from the work Willner¹⁶. For ϵ_{opt} , the calculation was done with POL, while for the dc case, we used the ellipsoid ansatz. The contribution of the dc polarizability is very small compared to the dipole moment in all cases. K_{sp} has been evaluated for a series of proteins and the data is shown in Table 3 along with a comparison with experiment. The dipole moment has been either measured, or computed with Amber 8, however, its orientation in the crystallographic frame is not known for the experimental values. The expression for K_{sp} is written in terms of tensors (and the dyadic $\mu\mu$) and is sensitive to the relative orientation of the frames defining the polarizability and the dipole moment. The polarizabilities have been computed in the crystallographic frame. The dipole moment vector in that frame has been represented by $\mu = \mu(\hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta)$.

Table 3 also shows the orientation that the dipole moment must have in crystal frame in order to have our calculation match experiment as close as possible. The results are quite mixed with

the calculation generally under-estimating the Kerr constant. Only for two proteins can we reproduce the experimental value exactly, while for the proteins with small dipole moments the error is a factor of 3 to 8. For tubulin and tropomyosin, proteins with a significant permanent moment we also have significant deviations. There are several implications to these deviations. The first is that our assumption that the electrolyte effects can be ignored is likely not correct. The fact that all proteins with small permanent dipoles are significantly lower than experiment argues for a contribution from an ion induced dipole moment which becomes less significant for proteins with large permanent dipoles. However, there are two proteins with large dipole moments that do not fit this pattern for which we also under report. Wegener¹⁵ has shown that there is an electro-hydrodynamic coupling tensor that is important when there is a screw axis (a bent molecule has one), a large permanent dipole moment and a molecular charge. This tensor adds to the $\mu\mu$ dyadic and it depends on the rotation-coupling tensor and the total charge of the body. We have calculated this effect for all the proteins and found that the value is very small compared to other terms and thus has no significant effect.

Another possibility that must be considered is a deformation of the protein structure under the influence of the electric field, generating a higher dipole moment than measured under ac conditions. If this were the case, then the rise and decay dynamics should show relaxations that are not explainable by the rotational diffusion of the protein taken as a rigid body. For most of the proteins we do not have access to the raw data to check for this effect. In addition, for tubulin, kinesin and ncd, we used an Amber calculated dipole moment which was scaled by 0.7 to account for the fact that Amber overestimated the dipole for those proteins for which we had measurements. This still represents an important source of uncertainty but we note that kinesin is one of the two cases where we do match experiment. Lastly, the very large dipole moment for tropomyosin was extracted from measurements of the Kerr constant¹⁹ using a theory applicable only for rigid rods, and so this value may be off.

The measurement of the Kerr constant is subject to systematic errors in the measurement of the raw birefringence. Extreme care must be taken to eliminate birefringence from cell windows and other components of the detection optical chain. We are comparing our calculations to data of unknown quality in this regard, for most of the proteins. Two proteins were measured in recent times by Don Eden²⁴ at San Francisco State: kinesin and ncd. We do much better on this subset than on the rest.

The fact that the Kerr constant depends sensitively on the orientation of the dipole moment also makes this quantity very difficult to predict. Fig. 3 shows the behavior of K_{sp} as a function of the dipole moment angles (in radians). The maxima and valleys occur in different locations for different proteins. When the computed value for a dipole along the z axis exceeds the experimental value, then there are an infinite number of orientations that will match the experimental value exactly. For the cases when we under report, there are generally two solutions –we report the solution for the smallest value of θ .

We began this investigation with the premise that the electrolyte effects could be ignored. The results so far appear to indicate that this may not be a reasonable assumption. The electric field will distort the ion cloud around the protein and produce an ion-induced dipole moment that adds vectorially to that of the protein itself. This is a very difficult problem to address, but it is one of great interest to us in this laboratory. Computationally, we are working on the quantification of the ion-induced dipole, taking into account that the aqueous solvent is a saturable dielectric. This is a major undertaking in this difficult field. If experimental values of the Kerr constant were available as a function of ionic strength, one could gauge the relative importance of the ion induced dipole. However, in traditional electric birefringence measurements, the salt concentration must be kept low (in the millimolar range) in order to avoid Joule heating of the sample during pulsing. This limitation can in principle be overcome

by the use of the Optical Kerr Effect²⁵, where a laser pulse substitutes for the imposed external electric field, yielding a response that depends solely on the electronic degrees of freedom. The downside of this technique is that the signal depends only on the electronic polarizability anisotropy and is expected to be very small and difficult to measure for proteins. We are nevertheless pursuing this experimental alternative in our laboratory.

4. Conclusions

In conclusion, we observe that our implementation of the BE method for the computation of the polarizability of a dielectric body is very precise and accurate by comparison to analytic values for ellipsoids of revolution. In addition, we have demonstrated that the ellipsoid ansatz is very accurate for low values of the relative dielectric constant, typical in biophysical problems. Thus, the simpler calculation of a metallic body can be substituted in most cases and the dielectric constant dependence is well expressed by the approximate formula.

When we use the polarizability tensors to predict the Kerr constants of proteins we obtain mixed results: we match experiment only in some cases and badly under report on several others. The computations assumed that the proteins are hydrated rigid structures which are unaffected by the orienting electric field, and the electro-hydrodynamic coupling was ignored. Furthermore, we assumed that the protein electrical charge and surrounding electrolyte make an insignificant contribution to the birefringence of the dilute protein solution. All of these assumptions are open to question and are being actively investigated in this laboratory. The Kerr constant also depends on the permanent protein dipole moments and there is also some uncertainty in these values. The Kerr constant is quite sensitive to the relative orientation of the dipole moment vector and the principal axes of the polarizability tensor. This feature makes the Kerr constant quite difficult to predict a-priori, but a Kerr measurement might be used to constrain the possible orientations of the dipole moment within the molecule frame.

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Figure 1.
Extrapolation to infinite number of triangles. Oblate ellipsoid with axial ratio $p=2$.

Fig 2.
The triangulated surface of lysozyme.

Fig. 3.
Dependence of the Kerr constant on the orientation of the dipole moment for tropomyosin.
Angles are given in radians ($0 < \theta < \pi$; $0 < \phi < 2\pi$).

Table 1

Ellipsoid Dielectric Polarizability ($[\sigma]_E$)

p	$\epsilon = 1.5$			$\epsilon = 10$			$\epsilon = 100000$		
	pol	pbest	exact	pol	pbest	exact	pol	pbest	exact
1/10	0.49497	0.494979	0.494979	7.61016	7.61052	7.61052	49.2615	49.2711	49.2711
	0.401628	0.401628	0.401629	1.66393	1.66395	1.66398	2.04139	2.04132	2.04137
1/9	0.494107	0.494117	0.494116	7.41113	7.41143	7.41142	41.966	41.9713	41.9714
	0.401913	0.401913	0.401914	1.66889	1.66885	1.66888	2.04877	2.0487	2.04875
1/8	0.492986	0.492994	0.492994	7.16655	7.16678	7.16679	35.1695	35.1722	35.1724
	0.402285	0.402285	0.402287	1.67533	1.67529	1.67532	2.05848	2.05841	2.05846
1/7	0.491486	0.491494	0.491495	6.86233	6.86246	6.86249	28.8847	28.886	28.8862
	0.402786	0.402786	0.402788	1.68405	1.68402	1.68405	2.07166	2.0716	2.07166
1/6	0.489414	0.489421	0.489421	6.47905	6.47915	6.47917	23.1263	23.1267	23.1269
	0.403486	0.403487	0.403489	1.69637	1.69633	1.69636	2.09032	2.09027	2.09032
1/5	0.486416	0.486424	0.486424	5.99038	5.99044	5.99046	17.911	17.911	17.9112
	0.404513	0.404514	0.404516	1.71467	1.71464	1.71468	2.11819	2.11814	2.1182
1/4	0.481826	0.481833	0.481833	5.36135	5.36138	5.3614	13.2596	13.2594	13.2596
	0.406121	0.406123	0.406125	1.74395	1.74391	1.74396	2.16306	2.163	2.16307
1/3	0.474218	0.474223	0.474224	4.54914	4.54913	4.54916	9.198	9.19785	9.19798
	0.408886	0.408888	0.40889	1.7961	1.79607	1.79612	2.24387	2.24381	2.24389
1/2	0.460069	0.460074	0.460074	3.51276	3.51273	3.51278	5.76122	5.76113	5.76123
	0.41438	0.414383	0.414384	1.90717	1.90715	1.9072	2.41993	2.41989	2.41997
1	0.428568	0.428571	0.428571	2.24997	2.24995	2.25	2.99987	2.99982	2.99991
2	0.39569	0.395692	0.395695	1.56661	1.56659	1.56663	1.89674	1.89672	1.89678
	0.447141	0.447146	0.447147	2.87758	2.87754	2.87761	4.2299	4.2298	4.22994
3	0.379448	0.379445	0.379451	1.33956	1.33954	1.33958	1.57379	1.57376	1.57381
	0.458226	0.458229	0.458231	3.40812	3.40805	3.40812	5.48502	5.4848	5.485
4	0.369868	0.369868	0.369872	1.22735	1.22732	1.22737	1.42113	1.4211	1.42116
	0.465507	0.465509	0.465511	3.85671	3.85661	3.85668	6.74826	6.74791	6.74813
5	0.363569	0.363568	0.363572	1.16062	1.1606	1.16064	1.33243	1.3324	1.33246
	0.470638	0.470641	0.470642	4.23969	4.23957	4.23964	8.01514	8.01462	8.01487
6	0.359116	0.359116	0.35912	1.11643	1.11641	1.11645	1.27453	1.27448	1.27454
	0.474445	0.474448	0.474449	4.57007	4.56993	4.56999	9.28392	9.28325	9.28354
7	0.355803	0.355803	0.355808	1.08503	1.085	1.08505	1.23376	1.23372	1.23378
	0.477379	0.477384	0.477385	4.8578	4.85766	4.85772	10.5539	10.5531	10.5533
8	0.353243	0.353243	0.353248	1.06157	1.06155	1.06159	1.20352	1.20348	1.20354
	0.479709	0.479714	0.479716	5.11055	5.11045	5.11049	11.8245	11.8236	11.8239
9	0.351205	0.351206	0.351211	1.04339	1.04336	1.04341	1.1802	1.18016	1.18022
	0.481604	0.481611	0.481613	5.33433	5.33422	5.33427	13.0955	13.0946	13.0949
10	0.349545	0.349545	0.349552	1.02887	1.02884	1.0289	1.16167	1.16162	1.16169
	0.483174	0.483186	0.483186	5.53377	5.53371	5.53376	14.3668	14.3659	14.3662

Table 2

Polarizability Tensor Eigenvalues ($\text{\AA}^3$)

ϵ	1.2			1.5			2.0			5.0			10.0		
protein	pol	pbest		pol	pbest		pol	pbest		pol	pbest		pol	pbest	
ribonuclease A	232	233		523	538		905	953		2087	2269		2854	3048	
	236	236		543	554		965	1007		2397	2599		3434	3674	
	239	240		559	574		1018	1075		2791	3106		4331	4778	
lysozyme	242	244		549	562		955	993		2214	2334		2992	3112	
	244	246		556	572		978	1023		2350	2504		3255	3423	
	249	251		583	601		1062	1121		2899	3189		4431	4844	
β -lactoglob.	636	641		1443	1482		2519	2634		5930	6323		8110	8535	
	637	643		1446	1494		2523	2672		5989	6543		8325	8942	
	655	662		1546	1600		2850	3033		8200	9230		13220	14850	
ovalbumin	770	771		1745	1777		3050	3146		7100	7446		9665	9971	
	772	775		1756	1798		3078	3210		7338	7820		10129	10654	
	796	795		1896	1912		3506	3596		9916	10588		15670	16543	
kinesin (1-349)	732	706		1671	1644		2940	2949		7130	7289		9660	9937	
	734	709		1679	1656		2963	2987		7300	7523		9980	10598	
	748	725		1756	1747		3214	3298		9100	9864		13840	14322	
ncd (335-700)	690	694		1567	1617		2740	2905		6564	7210		9202	9937	
	694	697		1589	1634		2807	2959		6907	7552		9820	10598	
	706	709		1653	1702		3013	3191		8333	9269		12990	14322	
tropomyosin	496	506		1111	1181		1905	2126		4303	5317		5857	7363	
	499	511		1120	1210		1928	2221		4422	5950		6090	8635	
	530	531		1291	1327		2498	2652		9070	10538		18800	23456	

Table 3

Protein Specific Kerr constants

Protein	Dipole		θ	ϕ	V_p $\text{\AA}^3$	$K_{sp} \times 10^{-17} \text{ m}^2/\text{V}^2$			Ref.
	Debye	Ref.				Calc	Exp		
tubulin	1443	11	90.8	0	85909.7	13.0	81.4		17
tropomyosin	6300	18	41.5	119.2	29672.0	1080	3110		18
ovalbumin	305	19	72.2	45.3	41397.5	1.34	5.16		20
lysozyme	122	21	38.4	162.5	13656.7	0.149	1.21		20
ribonuclease a	350	22	52.9	43.7	12993.0	0.94	2.13		20
β -lactoglobulin	790	23	many	many	34201.0	2.96	2.96		20
kinesin(1-349)	1042	11	many	many	36857.4	3.64	3.64		24
ncd(335-700)	331	11	51.6	80.2	35631.0	-90	-16.5		24