

Dipole-induced ordering in nematic liquid crystals fact or fiction?

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Abstract

Similar size and shape molecules with different electric multipoles are used to investigate effects of dipole and quadrupole interactions on the average orientation of solutes in nematic liquid crystals. Permanent dipoles have a negligible influence on solute orientation. Order parameters predicted from strong, short-range repulsive forces coupled with interactions between the solute quadrupole and the average electric field gradient felt by the solute $\langle \text{EFG} \rangle$ are consistent with experimental values. Calculated $\langle \text{EFG} \rangle$'s are the same sign and similar magnitude to those determined previously from D_2 and HD. For the nematic mixture 55wt% ZLI 1132 in EBBA, the contribution to solute ordering from long-range electrostatic interactions is negligible. © 1997 Elsevier Science B.V.

1. Introduction

Orientalional ordering in liquid crystals arises from anisotropic intermolecular forces. It is generally accepted that short-range repulsive forces are the dominant interactions which cause ordering [1–4]. Predictions of order parameters based on models which attempt to characterize short-range forces agree remarkably well with order parameters from computer simulations [5] and experiments [6–9]. Longer range electrostatic interactions are also important but may have a lesser influence on ordering [9,10]. There is much debate as to which electrostatic interactions are most important [9–13].

For apolar nematic phases there is no macroscopic electric field or electric field gradient. This does not

preclude the possibility that an average electric field $\langle E \rangle$ and/or an average electric field gradient $\langle \text{EFG} \rangle$ may be felt by the solute. These fields originate from the charge distribution of solvent molecules and are dependent on the structure of molecules around the solute. In this paper the long-range electrostatic contributions to solute ordering are assumed to arise from the interaction of $\langle E \rangle$ with the solute dipole and the interaction of $\langle \text{EFG} \rangle$ with the solute quadrupole. Other long-range interactions such as dispersion, induction, polarization and higher multipole interactions can influence ordering of solutes in liquid crystals. However, the relative magnitude of these interactions is expected to be much smaller than dipole and/or quadrupole interactions [4,10,13].

Emsley et al. [10] suggested that there is no contribution to solute ordering from dipole interactions because in apolar nematic phases the first rank order parameter of the liquid crystal is zero (i.e. the

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mean electric field of the nematic phase is zero). This suggestion has been criticized by Terzis, Photinos and others [11–13]. Terzis and Photinos calculated contributions to ordering from various mechanisms and concluded that, while the ordering of iodomethane is mainly due to short-range forces, dipole interactions do play an important role [13]. In another study experimental evidence of dipole induced ordering was inferred by comparing order parameters of α,ω -dibromo-*n*-alkanes and *n*-alkanes [11,12]. Dipole interactions were thought to cause C–Br chain segments to align perpendicular to the nematic director. This effect was most evident with liquid crystal molecules having dipoles perpendicular to their long axis.

Experimental evidence for a quadrupole– $\langle\text{EFG}\rangle$ interaction, as well as the value of the $\langle\text{EFG}\rangle$, was obtained from nuclear magnetic resonance (NMR) studies of H_2 , HD, HT, D_2 , DT and T_2 dissolved in nematic liquid crystals [14–21]. It was concluded that the ordering of these molecules was dominated by the quadrupole– $\langle\text{EFG}\rangle$ interaction. In addition, the unexpected negative order parameter found for acetylene [22] dissolved in the nematic liquid crystal *N*-(4-ethoxybenzylidene)-4-*n*-butylaniline (EBBA) is easily rationalized by the interaction between the positive solute quadrupole moment and the negative $\langle\text{EFG}\rangle$ in EBBA [15]. Currently there is no alternate theory which can account for this negative order parameter. Trends in experimental order parameters of benzene and hexafluorobenzene, which have similar sizes and shapes but opposite signs of quadrupole moments, are consistent with predictions from molecular quadrupole– $\langle\text{EFG}\rangle$ interactions [23]. It is very likely that this interaction is important for other probe solutes as well [18,23–25].

In this study we test the effects of permanent dipoles and quadrupoles on solute ordering. To simplify the analysis of experimental results we make and test the common assumption that in a given liquid crystal solvent all solutes feel the same average environment. Solute molecules are chosen so as to emphasize specific anisotropic interactions. Since methyl and chloro constituents have roughly the same size and shape but different electronic properties they are used in organic chemistry to distinguish between steric and electronic features of reaction mechanisms [26]; in this study, methyl and chloro substituted

benzene rings are used to distinguish between steric and electronic effects on order parameters.

2. Experiments and results

Nine samples were prepared by dissolving pairs of solutes (toluene/chlorobenzene, *p*-xylene/*p*-dichlorobenzene or *p*-chlorotoluene/*p*-dichlorobenzene) and 1,3,5-trichlorobenzene (TCB), an “orientational standard”, in three liquid crystal mixtures: Merck ZLI 1132 (see Ref. [27] for chemical composition); 55 wt% Merck ZLI 1132/EBBA; and EBBA. Proton NMR spectra were acquired at 299.6 ± 0.5 K using a Bruker AMX-500 spectrometer. Proton–proton dipolar couplings were determined from analysis of single and multiple quantum NMR spectra by a least squares minimization routine. Analysis of multiple quantum spectra provided estimates of spectral parameters which were used to analyze single quantum spectra. The predicted single quantum spectrum of the more complex spin system was subtracted from the experimental spectrum in order to identify resonances corresponding to the other solutes [28].

Using a least squares minimization routine, solute molecular order parameters and proton positions were calculated from a simultaneous fit to dipolar couplings determined for the solute in all three liquid crystal mixtures. Solute order parameters for a given liquid crystal were scaled so that different solutes in different sample tubes could be compared:

$$S_{\alpha\beta}^{\text{scaled}} = \frac{S_{\alpha\beta}}{S_{\text{TCB}}} * S'_{\text{TCB}}, \quad (1)$$

where $S_{\alpha\beta}$ and S_{TCB} are the order parameters of the solute and TCB in the same sample tube and S'_{TCB} is the order parameter of TCB in the *p*-dichlorobenzene/*p*-xylene mixture of the same liquid crystal. The *p*-dichlorobenzene/*p*-xylene mixture was arbitrarily chosen as the standard for comparison. Values obtained for scaled order parameters $S_{\alpha\beta}^{\text{scaled}}$ are given in Table 1. Dissolving several solutes in the same sample tube reduced the amount of scaling. Using this simple method, which for this study was determined to be the best scaling method [28], differences between scaled order parameters for *p*-dichlorobe-

nzene in the same liquid crystal but different sample tubes are < 1.5% (Table 1).

3. Analysis and discussion

In general, order parameters can be calculated from a mean orientational potential $U(\Omega)$:

$$S_{\alpha\beta}^{\text{calc}} = \frac{\int (3\cos\theta_{\alpha Z}\cos\theta_{\beta Z} - \delta_{\alpha\beta}) \exp(-U(\Omega)/kT) d\Omega}{2 \int \exp(-U(\Omega)/kT) d\Omega}, \quad (2)$$

where Ω denotes the Eulerian angles and $\theta_{\alpha Z}$ and $\theta_{\beta Z}$ are the angles between the molecular α and β

axes and the nematic director Z . For the molecules considered in this study, only the diagonal elements of the order matrix are non-zero. $U(\Omega)$ can be expressed in terms of short range repulsive $U(\Omega)_{\text{SR}}$ and longer range electrostatic $U(\Omega)_{\text{ES}}$ interactions between solute and an average field (due to the liquid crystal) felt by the solute:

$$U(\Omega) = U(\Omega)_{\text{SR}} + U(\Omega)_{\text{ES}}. \quad (3)$$

The orientational potential is characterized by fitting $S_{\alpha\beta}^{\text{calc}}$ to scaled experimental order parameters. For the characterization we assume that all solutes see the same average environment which is dependent only on the liquid crystal.

The short-range potential $U(\Omega)_{\text{SR}}$ can be written as an expansion in spherical harmonics. We assume that $U(\Omega)_{\text{SR}}$ is adequately approximated by the first

Table 1
Scaled and calculated order parameters^a

Solute	Order parameter	Liquid crystal		
		Merck ZLI 1132 $S_{\alpha\beta}^{\text{scaled}}/S_{\alpha\beta}^{\text{calc}}$	55 wt% 1132/EBBA $S_{\alpha\beta}^{\text{scaled}}/S_{\alpha\beta}^{\text{calc}}$	EBBA $S_{\alpha\beta}^{\text{scaled}}/S_{\alpha\beta}^{\text{calc}}$
chlorobenzene	S_{zz}	0.2251/0.2031	0.1778/0.1746	0.1769/0.1949
	S_{yy}	-0.2510/-0.2326	-0.1838/-0.1832	-0.1330/-0.1582
	S_{xx}	0.0259/0.0296	0.0060/0.0086	-0.0439/-0.0367
toluene	S_{zz}	0.2202/0.2127	0.1704/0.1746	0.1704/0.1812
	S_{yy}	-0.2477/-0.2328	-0.1853/-0.1832	-0.1537/-0.1589
	S_{xx}	0.0275/0.0195	0.0149/0.0086	-0.0167/-0.0223
<i>p</i> -dichlorobenzene ^b (with <i>p</i> -chlorotoluene)	S_{zz}	0.3072/- - -	0.2800/- - -	0.3463/- - -
	S_{yy}	-0.2706/- - -	-0.2166/- - -	-0.1972/- - -
	S_{xx}	-0.0367/- - -	-0.0634/- - -	-0.1491/- - -
<i>p</i> -dichlorobenzene (with <i>p</i> -xylene)	S_{zz}	0.3072/0.2993	0.2799/0.2830	0.3455/0.3654
	S_{yy}	-0.2701/-0.2616	-0.2163/-0.2219	-0.1976/-0.2265
	S_{xx}	-0.0372/-0.0377	-0.0636/-0.0611	-0.1479/-0.1389
<i>p</i> -chlorotoluene	S_{zz}	0.3285/0.3414	0.2863/0.2828	0.3287/0.3008
	S_{yy}	-0.2736/-0.2710	-0.2210/-0.2219	-0.2057/-0.2053
	S_{xx}	-0.0549/-0.0705	-0.0653/-0.0610	-0.1230/-0.0955
<i>p</i> -xylene	S_{zz}	0.3364/0.3645	0.2807/0.2827	0.2981/0.2641
	S_{yy}	-0.2780/-0.2747	-0.2245/-0.2219	-0.2113/-0.1974
	S_{xx}	-0.0583/-0.0898	-0.0562/-0.0609	-0.0868/-0.0667

^a For axis definitions see Fig. 1. $S_{\alpha\beta}^{\text{calc}}$ values are predicted using potential parameters from Fit # 2 (see Tables 2 and 3).

^b These order parameters were not used when determining \bar{F}_{ZZ} , $(\epsilon_Z - \epsilon_X)$, \hat{M} and k_{ZZ} and thus $S_{\alpha\beta}^{\text{calc}}$ is not reported. For these samples, scaled order parameters are shown for comparison with scaled order parameters of *p*-dichlorobenzene (with *p*-xylene). By using TCB for scaling, differences between order parameters of *p*-dichlorobenzene in the same liquid crystal, but different sample tubes are < 1.5%.

non-zero contribution to the mean orientational potential

$$U(\Omega)_{\text{SR}} = -\frac{1}{2} \sum_{\alpha, \beta=x, y, z} (M_{\alpha\beta} k_{ZZ}) \times (3\cos\theta_{\alpha Z}\cos\theta_{\beta Z} - \delta_{\alpha\beta}), \quad (4)$$

where \hat{M} is a traceless second rank tensor related to the size and shape of the molecule, and k_{ZZ} is the solvent parameter which scales this tensor among different liquid crystal solvents. Based on van der Waals' radii [29], the three para-substituted (and the two mono-substituted) molecules have similar sizes and shapes. Therefore, when characterizing $U(\Omega)_{\text{SR}}$, the same \hat{M} is used for all three para-substituted (and a different \hat{M} is used for the two mono-substituted) molecules.

The longer range electrostatic potential $U(\Omega)_{\text{ES}}$ comprises interactions of solute quadrupoles with an $\langle\text{EFG}\rangle$ and of solute dipoles with an $\langle E \rangle$. The molecular quadrupole contribution is,

$$U(\Omega)_{\text{ES}}^{\text{Quadrupole}} = -\frac{1}{6} \sum_{\alpha, \beta=x, y, z} (Q_{\alpha\beta} \bar{F}_{ZZ}) \times (3\cos\theta_{\alpha Z}\cos\theta_{\beta Z} - \delta_{\alpha\beta}), \quad (5)$$

where \bar{F}_{ZZ} is the ZZ component of the $\langle\text{EFG}\rangle$ tensor parallel to the nematic director and $Q_{\alpha\beta}$ is the $\alpha\beta$ component of the solute molecular quadrupole tensor. The $\langle\text{EFG}\rangle$ is a traceless, second-rank tensor and for a nematic phase has only one independent term. As indicated above, we follow the simplest

possible approach and assume that the $\langle\text{EFG}\rangle$ is a property of the liquid crystal only, and that it is independent of solute properties and orientation.

The interaction of a molecular dipole with an $\langle E \rangle$ is $U(\Omega)_{\text{ES}}^{\text{Dipole}} = -\mu \cdot \langle E \rangle$. Due to the apolar nature of nematic phases the average lab frame $\langle E \rangle$ must be zero. Thus, if the above approach for short-range and quadrupole effects is used (where the solute is assumed to see an average field that is constant in the lab frame), the dipole interaction is zero. To account for the possible effect of interactions involving permanent solute dipoles in a manner that is consistent with the apolar nature of nematic phases we must assume that the average field experienced by the dipole depends on its orientation. For example, if the electric field along the solute dipole direction z is assumed to vary with solute orientation as

$$\langle E_z \rangle = \frac{1}{2} \sum_{\Gamma=X, Y, Z} \epsilon_{\Gamma} \cos(2\theta_{z\Gamma}) \quad (6)$$

then the anisotropic contribution to the potential is given by

$$U(\Omega)_{\text{ES}}^{\text{Dipole}} = -\frac{1}{6} \mu_z (\epsilon_z - \epsilon_x) [3\cos(2\theta_{zZ}) + 1], \quad (7)$$

where the ϵ_{Γ} are constants and $\epsilon_y = \epsilon_x$.

Another example in which a permanent dipole can affect the orientational order of a molecule is through the field that the solute dipole induces in the sur-

Table 2
Molecular parameters^a

Solute	Dipole component ^b [30]	Quadrupole component ^c [30]			Short range parameter ^d	
	μ_z	Q_{yy}	Q_{xx}	Q_{zz}	M_{zz}	$M_{xx} - M_{yy}$
chlorobenzene	5.418	−2.418	2.369	0.049	362 (12)	542 (34)
toluene	2.022	−2.276	1.763	0.512	362 (12)	542 (34)
<i>p</i> -dichlorobenzene	0.00	−1.385	3.581	−2.196	557 (13)	558 (35)
<i>p</i> -chlorotoluene	7.093	−2.317	1.990	0.326	557 (13)	558 (35)
<i>p</i> -xylene	0.00	−2.539	0.870	1.669	557 (13)	558 (35)

^a For axis definitions see Fig. 1. For molecules considered in this study, only diagonal elements of \hat{Q} and \hat{M} are non-zero.

^b Units of 10^{-30} Cm (1Cm = 2.998×10^{29} debye).

^c Units of 10^{-39} Cm².

^d Units of 10^{-23} J. Short range parameters correspond with Fit # 2 in Table 3. Among the various fits these values varied by no more than 3.5%. Errors are reported in brackets.

rounding medium. This induced or reaction field in turn interacts with the instigating dipole. The magnitude of the reaction field depends on the solute dipole

$$\langle E_{\Delta} \rangle = \frac{1}{2} \mu_z \sum_{\Gamma=X,Y,Z} \bar{R}_{\Delta\Gamma} \cos \theta_{z\Gamma}, \quad (8)$$

where μ_z is the solute dipole moment, $\bar{R}_{\Delta\Gamma}$ is the $\Delta\Gamma$ component of the reaction tensor, and $\langle E_{\Delta} \rangle$ is the reaction field in the Δ lab fixed direction. The potential is then

$$U(\Omega)_{\text{ES}}^{\text{Dipole}} = -\frac{1}{6} \mu_z^2 (\bar{R}_{ZZ} - \bar{R}_{XX}) (3 \cos^2 \theta_{zZ} - 1), \quad (9)$$

where $\bar{R}_{YY} = \bar{R}_{XX}$ and off-diagonal elements of the reaction field tensor are zero. The difference between this case and that of Eq. (7) is that $U(\Omega)_{\text{ES}}^{\text{Dipole}}$ is now proportional to μ_z^2 . As discussed below, both approaches lead to the same general conclusions.

Molecular dipoles and quadrupoles were calculated with respect to the centre of mass using GAUSSIAN 94 [30]. The values obtained (Table 2)

are in accordance with other calculations and experiments [31,32].

The $S_{\alpha\beta}^{\text{scaled}}$ and calculated μ_z and $Q_{\alpha\beta}$ values were used to determine \bar{F}_{ZZ} , $(\epsilon_Z - \epsilon_X)$, $M_{\alpha\beta}$ and k_{ZZ} from Eqs. (2)–(5) and (7) using a non-linear least squares minimization routine (Tables 2 and 3); k_{ZZ} for the 55wt% mixture was arbitrarily set to 1 as only the product $M_{\alpha\beta} k_{ZZ}$ is important. Four different fits were done for $S_{\alpha\beta}^{\text{calc}}$ by allowing various components of $U(\Omega)$ to vary (Table 3). The $S_{\alpha\beta}^{\text{calc}}$ values predicted from Fit # 2 are given in Table 1 and agree to within $\approx 10\%$ of the largest order parameter.

Examination of Table 3 shows that inclusion of quadrupole interactions improves the quality of the fit, whereas inclusion of dipole interactions has no effect: $(\epsilon_Z - \epsilon_X)$ is zero within calculated error and does not affect parameters for short-range or quadrupole interactions. Similar fits, which are not presented in the tables, were performed using the reaction-field $\mu_z^2 (\bar{R}_{ZZ} - \bar{R}_{XX})$ potential (instead of the $\mu_z (\epsilon_Z - \epsilon_X)$ potential). Inclusion of the reaction field potential had no effect on the quality of the fit

Table 3
Liquid crystal parameters^a

Liquid crystal mixture	Scaling parameter (k_{ZZ})	Average electric field gradient ^b (\bar{F}_{ZZ})	Average electric field ^c ($\epsilon_Z - \epsilon_X$)	RMS error ^d / $\times 10^{-2}$
Fit # 1				
ZLI 1132	1.21(0.06)	0.0 ^e	0.0 ^e	2.61
55wt% 1132/EBBA	1.00 ^e	0.0 ^e	0.0 ^e	2.61
EBBA	1.06(0.06)	0.0 ^e	0.0 ^e	2.61
Fit # 2				
ZLI 1132	1.23(0.04)	8.8(1.9)	0.0 ^e	1.42
55wt% 1132/EBBA	1.00 ^e	−0.03(1.8)	0.0 ^e	1.42
EBBA	1.06(0.03)	−14.1(2.0)	0.0 ^e	1.42
Fit # 3				
ZLI 1132	1.24(0.08)	0.0 ^e	−3.9(9.1)	2.54
55wt% 1132/EBBA	1.00 ^e	0.0 ^e	1.8(8.7)	2.54
EBBA	1.02(0.08)	0.0 ^e	12.8(9.0)	2.54
Fit # 4				
ZLI 1132	1.24(0.05)	8.5(2.0)	1.5(5.2)	1.39
55wt% 1132/EBBA	1.00 ^e	−0.2(1.9)	2.6(5.0)	1.39
EBBA	1.04(0.04)	−14.0(2.0)	6.1(5.2)	1.39

^a Absolute errors are reported in brackets.

^b Units of 10^{17} Vm^{-2} ($1 \text{ Vm}^{-2} = 3.3356 \times 10^{-7} \text{ esu}$).

^c Units of 10^7 Vm^{-1} ($1 \text{ Vm}^{-1} = 3.3356 \times 10^{-5} \text{ esu}$).

^d RMS error is reported for $S_{\alpha\beta}^{\text{calc}}$.

^e Parameter was not adjusted.

between solute dipole moments and order parameters. Further, if solutes have approximately the same size and shape the correlation should be evident directly from experimental order parameters. However, the order parameters of *p*-chlorotoluene (dipole moment of 7.09×10^{-30} Cm [30]) are intermediate between those of *p*-xylene and *p*-dichlorobenzene (dipole moment = 0) (Fig. 1; Table 1). Chlorobenzene and toluene have very similar order parameters but molecular dipole moments of 5.42×10^{-30} and 2.02×10^{-30} Cm [30], respectively. For these molecules there is no correlation between order parameters and dipole moments. Thus dipole interactions seem to be of minimal importance in the anisotropic part of the electrostatic potential.

On the other hand, quadrupole- $\langle \text{EFG} \rangle$ interactions are important. In ZLI 1132 the trend for both scaled and calculated values (Fit # 2) of S_{zz} is: $S_{zz}(p\text{-xylene}) > S_{zz}(p\text{-chlorotoluene}) > S_{zz}(p\text{-dichlorobenzene})$. However, in EBBA this trend is reversed (Fig. 1 and Table 1). Since $U(\Omega)_{\text{SR}}$ is identical for all three molecules there must be a change in sign of $U(\Omega)_{\text{ES}}^{\text{Quadrupole}}$ between ZLI 1132 and EBBA and the 55wt% mixture is where $U(\Omega)_{\text{ES}}^{\text{Quadrupole}}$ happens to be ≈ 0 . The change in sign is due to \bar{F}_{zz} changing sign (Table 3). The trend in the observed order parameters is most evident with the para-substituted molecules because Q_{zz} is strongly negative for *p*-dichlorobenzene, almost zero for *p*-chlorotoluene and strongly positive for *p*-xylene. In contrast, for the mono-substituted molecules the Q_{zz} values are similar.

The value obtained from the least squares minimization of \bar{F}_{zz} in the 55wt% mixture is ≈ 0 (Table 3). Since similar size and shape molecules have similar order parameters in this liquid crystal (Fig. 1 and Table 1), it is not surprising that the electrostatic contribution to the potential is almost zero. \bar{F}_{zz} was also determined to be zero in previous studies of D_2 and HD dissolved in this liquid crystal mixture [17,19]. In other studies, order parameters of a number of solutes with various sizes, shapes and multipoles were predicted to within 10% using a potential which incorporated only short-range interactions [6,33,34]. Therefore, it seems that in this particular liquid crystal mixture, all long-range electrostatic interactions are minimal and only the short-range interactions are important.

The \bar{F}_{zz} determined from D_2 and HD experiments was $\approx 6.11 \times 10^{11}$ esu (18.44×10^{17} Vm^{-2}) for ZLI 1132 and $\approx -6.41 \times 10^{11}$ esu (-19.16×10^{17} Vm^{-2}) for EBBA [15]. \bar{F}_{zz} values for ZLI 1132 and EBBA calculated from the experiments reported here are 8.8×10^{17} and -14.1×10^{17} Vm^{-2} , respectively. These values are of the same sign, but smaller in magnitude than values from D_2 and HD experiments. Possible reasons for the smaller magnitude are: approximations in calculations of molecular quadrupole tensors; differences in sample conditions between the D_2 /HD and the present experiments (different concentrations of solutes, different reduced temperatures); or more likely, the approximation that the $\langle \text{EFG} \rangle$ is a property of the liquid crystal only, and that it is independent of solute properties. Recent Monte Carlo simulations employing point quadrupoles at the centres of solvent and solute hard ellipsoids indicate that this simplistic assumption may not be entirely valid [35]. However, these simulations were unable to rationalize the negative order parameter observed experimentally for acetylene in some nematic liquid crystal solvents.

4. Conclusions

Short-range interactions account for most of the ordering of solutes in liquid crystalline solvents. The relative importance of various electrostatic interactions on order parameters is demonstrated by using solute molecules of similar sizes and shapes. Within the reported errors $\epsilon_z - \epsilon_x$ (or $\bar{R}_{zz} - \bar{R}_{xx}$) is zero; thus for these molecules interactions involving the solute dipole moment have little or no influence on ordering.

However, trends in experimental order parameters are consistent with the $Q_{\alpha\beta}\bar{F}_{\alpha\beta}$ interaction. In addition the sign and magnitude of \bar{F}_{zz} in all liquid crystals is in accordance with previous results from D_2 and HD experiments. Since values of \bar{F}_{zz} change by no more than a factor of two between the very small solute H_2 and the larger benzene derivatives, the assumption that the solutes used in this study (all of which are of similar size and shape) feel essentially the same average environment seems reasonable. This is the only study of large molecules that

provides an estimate of the sign and magnitude of the $\langle\text{EFG}\rangle$.

A simple theory using only short-range and quadrupole– $\langle\text{EFG}\rangle$ interactions can be used to describe adequately the orientation of a variety of molecules with various electrostatic moments. More important, it has been demonstrated that the average electric field gradient ($\langle\text{EFG}\rangle$) felt by the solutes used in this study in the 55wt% mixture is ≈ 0 , indicating that these solutes feel the same average environment as does dihydrogen and its various isotopic derivatives. Not only is the $\langle\text{EFG}\rangle$ -quadrupole interaction ≈ 0 , but all other long-range interactions appear to be negligible as well. Thus liquid crystal mixtures such as 55wt% ZLI 1132/EBBA are the ideal medium for studying short-range anisotropic interactions.

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