Helical twisting power and scaled chiral indices

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Chirality of optically active liquid crystal molecules has become an important research topic and the subject of a number of theoretical and experimental studies. We present here the results of the application of a newly developed scaling method of a chiral index to a range of chiral molecules. Good agreement is found between the scaled chiral index and the helical twisting power for relatively rigid molecules. Two flexible TADDOL ($\alpha,\alpha,\alpha',\alpha'$-tetraaryl-1,3-dioxolan-4,5-dimethanol) molecules are studied to determine which conformations may give rise to their high experimental helical twisting powers. A variety of links between the moment of inertia tensor, the dihedral angles, the scaled chiral indices, the minimum energy of the optimized geometry and the experimental helical twisting power are discussed. The scaled chiral and steric indices and dihedral angles are promising as predictors of experimental helical twisting power, in particular for relatively rigid molecules, in cases where all the relevant interactions are determined by the molecular structure. © 2003 American Institute of Physics. [DOI: 10.1063/1.1590307]

I. INTRODUCTION

Experimental\textsuperscript{1–9} and simulation studies\textsuperscript{10,11} have been undertaken to create a better understanding of the concept of chirality in liquid crystals. Based on this work and similar studies, a widely accepted view is the possible inheritance of chirality in liquid crystals. Based on this work and similar undertakings to create a better understanding of the concept of structure has been investigated\textsuperscript{1} with a series of systematic studies\textsuperscript{12–25} with an extensive review by Buda et al.\textsuperscript{12} It has proved difficult to move beyond the concept that chiral molecules have no mirror symmetry to a quantitative measure of chirality for a given molecular conformation or to link this to experimental pseudoscalar quantities such as helical twisting power ($\beta_M$) or circular dichroism (CD). It is the transfer of chirality from the molecule to the phase, particularly with regard to helical twisting power that we discuss in this paper.

Linking results from experimental studies with differences in molecular structure or conformations is a complex problem. An example is the case of open-chain biaryl derivatives,\textsuperscript{2,3} where the helical twisting power was expected to change with temperature. However for some biaryls $\beta_M$ was practically constant\textsuperscript{4} whilst a pronounced increase or decrease in $\beta_M$ with increased temperature was seen for a range of bridged compounds. In addition, helical twist sign inversion can occur in compounds with single chiral centers. A phenomenological study proposed that the inversion may be due to conformational isomers or rotomers present in different concentrations at different temperatures.\textsuperscript{5} The link with spontaneous polarization, observed in ferroelectric phases of chiral liquid crystal molecules, and molecular structure has been investigated\textsuperscript{1} with a series of systematic changes in structure leading to the identification of some general trends. The polarization power often follows an inverse trend to that seen in the helical twisting power of ferroelectric liquid crystal molecules.\textsuperscript{6} Of interest are recent studies of mono- and bis-aminoanthraquinones\textsuperscript{7–9} in which a correlation of $\beta_M$ with the CD of long-wavelength charge transfer bands was shown but only for higher $\beta_M$ and CD values. It was thought that this occurred because all relevant interactions were determined by the structure of the molecules in this case.

There are three general methods that formulate a chirality measure in a mathematical definition: Buda and Mislow,\textsuperscript{12} Ruch and Schönhofer,\textsuperscript{13} Kuz'Min et al.,\textsuperscript{14} and Zabrodsky and Avnir\textsuperscript{15} use the so-called chirality functions. Liang and Mislow\textsuperscript{16} utilize an approach based on topologically chiral knots. It is the third method which utilizes chirality parameters employed by Lubensky et al.,\textsuperscript{18} Nordio et al.,\textsuperscript{19} and Osipov et al.\textsuperscript{20} that we discuss here, focusing on an extension of the latter\textsuperscript{24,25}.

Some success has been achieved in simulation studies\textsuperscript{10,11} and in a molecular surface model\textsuperscript{19} both of which link molecular structure to $\beta_M$. Recently\textsuperscript{21,22} the range of mechanisms which may link chiral molecules to chiral phases has been discussed. These mechanisms are widely varied, including for example, chiral molecular shape and chiral dispersive interactions. A mean field approximation taking into account chiral dispersion intermolecular interactions has been proposed\textsuperscript{21} to explain the experimental link observed between $\beta_M$ and CD for a special class of molecules.\textsuperscript{7–9}

The study of optically active molecular structures that we undertake here examines the link between a chiral measure of molecular structure and the pseudoscalar experimental quantity $\beta_M$. We apply the newly developed scaling...
method\textsuperscript{24,25} of a chirality measure proposed by Osipov \textit{et al.}\textsuperscript{20} that allows us to calculate a scaled chiral index measure $G_{0S}$, permitting meaningful comparison between molecules with different numbers of atoms. In the next section we briefly present the scaled chiral index. In Sec. III we discuss its application to a range of relatively rigid molecules and in Sec. IV to more flexible molecules and make comparison with experimental $\beta_M$ values. We discuss correlations between dihedral angles and both $\beta_M$ and the scaled chiral index for flexible and relatively rigid molecules. We also discuss correlations between the scaled chiral index and both the moment of inertia tensors for the optimized geometries and the associated minimized energies for the flexible molecules. Conclusions are presented in Sec. V.

\section{II. SCALED CHIRALITY MEASURE}

Osipov \textit{et al.}\textsuperscript{20} proposed a formulation for intrinsic molecular chirality developed from a basis of a simple model of optical activity, substituting the mass density for the isotropic optical activity, substituting the mass density for the isotropic optical activity, substituting the mass density for the isotropic optical activity, substituting the mass density for the isotropic optical activity, substituting the mass density for the isotropic optical activity. They developed a mathematical formulation which defines the gyration tensor $G$ for a molecule as

$$G = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) \rho(\mathbf{r}_3) \rho(\mathbf{r}_4)$$

$$\times \frac{[([\mathbf{r}_{12} \times \mathbf{r}_{34}] \cdot \mathbf{r}_{14}) ([\mathbf{r}_{12} \cdot \mathbf{r}_{23}]) ([\mathbf{r}_{23} \cdot \mathbf{r}_{34}])}{(\mathbf{r}_{12} \mathbf{r}_{23} \mathbf{r}_{34})^m r_{14}^n},$$

where each $\mathbf{r}_i$ ranges over the volume occupied by the molecule, $\rho$ is some quantity associated with the molecule, for example mass density, $\mathbf{r}_i = \mathbf{r}_{ij} - \mathbf{r}_{ij}$, and $\mathbf{r}_{ij} = \mathbf{r}_{ij} / r_{ij}$ and $n$ and $m$ are arbitrary integers. The isotropic chirality index is given by

$$G_0 = \frac{1}{3} \text{Tr} G$$

$$= \frac{1}{3} \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) \rho(\mathbf{r}_3) \rho(\mathbf{r}_4)$$

$$\times \frac{[([\mathbf{r}_{12} \times \mathbf{r}_{34}] \cdot \mathbf{r}_{14}) ([\mathbf{r}_{12} \cdot \mathbf{r}_{23}]) ([\mathbf{r}_{23} \cdot \mathbf{r}_{34}])}{(\mathbf{r}_{12} \mathbf{r}_{23} \mathbf{r}_{34})^m r_{14}^n}. \quad (3)$$

This quantity is invariant under rotation and translation, changes sign on reflection, is nonzero only for chiral objects and has properties under dilation that depend on the values of $m$ and $n$. However, it scales as $N^4$ for an $N$ point mass representation of a molecule making meaningless its application as a measure for comparison between molecules with different numbers of atoms. Some of the current authors extended this formulation [Eq. (3)] in Refs. 24, 25 for general molecular structures by calculating a scaled chiral index $G_{0S} = (4! / N^6)G_0$, that tends to a fixed value with increasing $N$ for similar shapes. The discrete form of the isotropic scaled chirality index $G_{0S}$ sums the contribution of all sets of four atoms in a numerical evaluation given by

$$G_{0S} = \frac{4!}{N^4} \frac{1}{3} \sum_{i,j,k,l=1}^{N} w_i w_j w_k w_l$$

$$(r_{ij} \times r_{kl}) \cdot (r_{ij} \cdot r_{kl} (r_{jk} \cdot r_{kl})) (r_{ij} \cdot r_{kl})$$

$$(r_{ij} \cdot r_{jk}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl})$$

$$(r_{ij} \cdot r_{jk}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl})$$

$$\times \left[ (r_{ij} \times r_{kl}) \cdot (r_{ij} \cdot r_{kl} (r_{jk} \cdot r_{kl})) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl}) \right]. \quad (4)$$

The atomic weights $w_i, w_j, w_k, w_l$ are values of physical quantities associated with atoms $i, j, k, l$. If $n = 2$ and $m = 1$ the index is dimensionless (invariant under dilation) and it is this form we shall consider. For a uniform point mass density distribution $w_i$ is set equal to 1.0.

Since the scaled chiral index $G_{0S}$ is a summation of contributions of all sets of four atoms, the contribution of any given atom to the index can be calculated separately and $G_{0S}$ can be expressed as the sum of the scaled atomic chiral indices $G_{0SA}$ through

$$G_{0SA} = G_{0S} - \frac{4!}{N^4} \times \frac{1}{3} \sum_{i,j,k,l=1}^{N} w_i w_j w_k w_l$$

$$(r_{ij} \times r_{kl}) \cdot (r_{ij} \cdot r_{kl} (r_{jk} \cdot r_{kl})) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl})$$

$$(r_{ij} \cdot r_{jk}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl})$$

$$\times \left[ (r_{ij} \times r_{kl}) \cdot (r_{ij} \cdot r_{kl} (r_{jk} \cdot r_{kl})) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl}) (r_{ij} \cdot r_{kl}) \right]. \quad (5)$$

where $i = 1, \ldots, A, \ldots, N$ indicates all values except A and

$$G_{0S} = \sum_{A=1}^{N} G_{0SA}. \quad (6)$$

The results from the previous studies were encouraging. The scaled chiral index was calculated for optimized geometries and showed good agreement with experimental $\beta_M$ for five chiral dopants.\textsuperscript{24,25} The scaled index was calculated for five ferroelectric molecules studied by Goodby\textsuperscript{1} and hinted at an inverse correlation with spontaneous polarization, agreeing with experimental results of Lemieux \textit{et al.}\textsuperscript{6} The scaled atomic index\textsuperscript{24} $G_{0SA}$ provided information with regard to the contribution of individual groups and atoms to the chirality measure and the scaling allowed meaningful comparison to be made between molecules with different numbers of atoms.

Encouraged by these results we have calculated the scaled index for three groups of rigid molecules: five disklike chiral dopants (A–E) (Ref. 10) one of which (A) is a TADDOL ($\alpha,\alpha,\alpha'$, $\alpha'$-tetraaryl-1,3-dioxolan-4,5-dimethanol) derivative with a phenyl substituent, eight binaphthyl derivatives (1–8) (Ref. 2), and four helicene derivatives ([M])1–4 (Ref. 3) allowing further comparison with experimental results. We have also calculated the scaled chiral index for a set of conformations of a flexible chiral molecule, a TADDOL derivative with a naphthyl substituent, commonly used as dopant in a nematic host; see, e.g., Ref. 26. For all the results presented here the optimized geometry of each molecular structure considered was obtained by minimizing the energy using the augmented MM3 force field in CAChE.\textsuperscript{22}

The only information utilized in the calculation of the scaled chiral index is the optimized geometry. In order to investigate the effect of the geometry further, using a uni-
form mass distribution and treating the molecules as a set of point masses, the moment of inertia tensor $I$ was obtained and diagonalized. The scaled gyration tensor $G_s = (4! / N^4) G$ [see Eq. (1)] was calculated in the principal axis system of the moment of inertia tensor. The correlation between the two tensors was investigated by evaluating a steric index $\alpha$ given by

$$\alpha = \text{Tr}(G_s - I).$$

(7)

In the following two sections we present the application of the scaled chiral index to a range of rigid and flexible chiral liquid crystal molecules which are shown in Fig. 1 and Ref. 10. We examine the correlations between the dihedral angles, the moment of inertia tensor through the steric index, and the minimized energy of the structures with the scaled chiral indices and the experimental helical twisting power and between the latter two.

### III. RELATIVELY RIGID CHIRAL MOLECULES

Chiral molecules with high helical twisting powers are often used as dopants in nonchiral nematic hosts in order to form cholesteric phases of a desired pitch, $p$. The helical twisting power ($\beta_M$) is defined as

$$\beta_M = (p / c_w r)^{-1},$$

(8)

where $c_w$ is the weight concentration of the dopant and $r$ is the enantiomeric purity of the dopant. Design of chiral dopants with high $\beta_M$ or alternatively low spontaneous polarization is vital in, for example, fast switching surface stabilized ferroelectric liquid crystal devices. A link between the scaled chiral index and $\beta_M$ would provide a vital key to molecular structure, phase property relationships.

Good correlation is seen between the experimental helical twisting power, $\beta_M$, and the scaled chiral index, $G_{OS}$, for three sets of molecules as shown in Table I. The Pearson correlation coefficient between experimental $\beta_M$ values and computational values of $-G_{OS} \times 10^4$ are presented for each set and for the total set of 17 molecules. The first set contains eight binaphthyl derivatives$^2$ and has a coefficient of 0.97. Second, following Cook and Wilson,$^10$ a set of five (A–E) dopant molecules was studied and found to have a correlation coefficient $P_\beta$ of 0.90 (Ref. 25) using a selected conformation of molecule A. The dopants B–E are more rigid than dopant A, a TADDOL derivative with a phenyl substituent, which has two main families of conformers. The selection of this conformer and its family is discussed in more detail in the next section. The third set following Nordio et al.$^{19}$ contained four helicene ([(M)-1–4] derivatives and have a coefficient of 0.80. Overall for the 17 structures the Pearson correlation coefficient $P_\beta$ is 0.95, with the correct sign predicted for the helical twist in all cases; an encouraging result. The results are presented in graphical form in Fig. 2 where it is apparent that the experimental values and the calculated values have a linear relationship.

The Pearson correlation, $P_d$, between the dihedral angles and the experimental helical twisting power, $\beta_M$, was also investigated and is presented in Fig. 3 and Table I. Figure 4 illustrates the dihedral angle chosen for binaphthyls 1 and 2, numbered 2–3–13–19. A strong correlation, $P_d$, of 0.97 was found between $\beta_M$ and the dihedral angles for the eight binaphthyl molecules but no correlation was found for the helicene molecules with a $P_d$ of $-0.03$. The contribution of each atom to the scaled chiral index for binaphthyls 1 and 2 is shown in Fig. 5. The two molecules have approximately equal and opposite experimental helical twisting power. It is
apparent that the contributions to $-G_{OS} \times 10^4$ are approximately equal and opposite from each atom for the two binaphthyls; this is also reflected in the six members not shown. No single appropriate dihedral angle is present for the dopants B–E. Dopant A is again discussed in the next section with regard to its dihedral angle.

It is interesting to note that for the four helicene derivatives the Pearson correlation coefficient with the helicity tensor of Nordio et al.19 is 0.54 for this small sample. The model formulation of the three dimensional scaled chiral index relates only to the intrinsic chirality of the dopant molecule and not to the solvent. It is remarkable that the theory of Nordio et al.,19 the aim of which was to predict the twisting power by considering the interaction between the host and the dopant, produces similar results to the scaled chiral index. It may be that in the molecules considered thus far the helical twisting power is dominated by the geometry of the dopant and insensitive to any dopant–host interaction. Some of us have investigated this lack of host sensitivity for this group of molecules through theory and further calculation in a following paper.28

Many dopant molecules are larger and more flexible than this group of 17 and it is these that we discuss in the next section.

### IV. FLEXIBLE CHIRAL MOLECULES

The values of the scaled chiral index, $G_{OS}$, calculated for the relatively rigid molecules are for one optimised configuration of the geometry in the gas phase. It is believed in many instances that it is excluded volume interactions due to molecular effects that are the driving forces that influence induced helical twist within a nematic phase. Linking experimental results to molecular structure is complex, as discussed in Sec. I, and it is likely that different mechanisms are effective for different chiral solutes and achiral solvents. It may be that certain conformers are preferentially selected in certain solvents and not others2,3 or are selected preferentially at certain temperatures.5 If we consider ferroelectric molecules with flexible tails then there are many more accessible configurations with close energy minima compared to rigid disklike molecules. It is difficult to identify which conformations are likely to influence the experimental helical twisting power.

Dopant molecule A, a TADDOL derivative with a phenyl substituent, is of particular interest and we compare it with a

![Image](https://jcp.aip.org/jcp/119/6/08/3570/fig2.jpg)

**FIG. 2.** Comparison of experimental helical twisting power, $\beta_M$, and scaled chiral index, $-G_{OS} \times 10^4$, for a range of 17 molecules, binaphthyl 1–8 (Ref. 2), (M)-1–4 (Ref. 3), and A–E (Ref. 10).
second TADDOL molecule with a naphthyl substituent (T3), the latter with a high degree of molecular flexibility and an experimental helical twisting power of approximately 180 \( \mu \text{m}^{-1} \). Table II shows results of calculations of the scaled index \(-G_{05} \times 10^4\) from 14 samples of close minimum energy configurations for molecule A and from eight samples of molecule T3(a–h). The configurations are ordered in descending magnitude of \( G_{05} \) as are the dihedral angles, the Pearson correlation, \( P_d \), between the dihedral angle and \( G_{05} \), the steric index, \( \alpha \), and the Pearson correlation, \( P_\alpha \), between \( \alpha \) and \( G_{05} \).

For molecule A it is apparent that there is a bimodal distribution in the scaled chiral index with conformations A1–A8 having a high magnitude \( G_{05} \) and conformations A9–A14 having a low magnitude \( G_{05} \). For the first eight conformations \(-G_{05} \times 10^4\) and the experimental helical twisting power all agree in sign and approximate magnitude. The steric correlation index \( P_\alpha \) is \(-0.96\) to \(-0.99\) for A1–A14 indicating a close link between the direction of the principal axes of the molecule conformation and the scaled chiral index \( G_{05} \). The correlation is negative since it is taken with \( G_{05} \) rather than \(-G_{05}\). A bimodal distribution is also seen in

![FIG. 3. Comparison of experimental helical twisting power, \( \beta_M \), and dihedral angle for a range of 12 molecules, binaphthyl 1–8 (Ref. 2), and \( (M)\)-1–4 (Ref. 3).](image)

![FIG. 4. Molecular structures of binaphthyl (a) 1 and (b) 2.](image)

![FIG. 5. Spectra of scaled atomic indices index, \(-G_{05} \times 10^4\) for binaphthyl molecules 1 and 2.](image)
the steric index \( \alpha \) itself which varies from \(-5.23 \) to \(-4.12 \) for conformations A1–A8 but drops to close to zero for conformations A9–A14. It is also interesting to note that for this sample there is a correlation between the minimum energy and \( G_{05} \) shown by a \( P_{E} \) of 0.99 for A1–A8 falling to 0.62 when A9–A14 are included.

The dihedral angles for molecules A, numbered 9–1–2–8, are shown in Fig. 6 for conformations A4 and A14 where the effect of difference of 10° on the position of the phenyl rings is apparent. We can see from Table II that for conformations A1–A8 the dihedral angles are less than 
\[ -80.5^\circ, \]
whereas those for conformations A9–A14 are greater than 
\[ -80.5^\circ. \]
The correlation between the dihedral angles and the scaled index, \( P_{d} \), is 0.89 for conformations A1–A8 and drops to 0.6–0.7 for conformations A9–A14 identifying a link between the dihedral angles and the scaled chiral index. The contribution from each atom for conformers A4 and A14 is compared in Fig. 7 where it can be seen that overall A4 has a larger negative contribution to the index from each atom than A14. Given the correlation between \( G_{05} \) and \( \beta_{m} \) found in Sec. III we propose that preferential selection of these conformers (A1–A8) in a nematic solvent may be responsible for the high experimental helical twisting powers found for this molecule. It is also interesting to note that the TADDOL3 conformation with the highest \( G_{05} \), T3a, has a similar dihedral angle to conformations A1–A8 of molecule A. Figure 8 illustrates the wide range of dihedral angles adopted by the conformations of TADDOL3 compared to the bimodal distribution adopted by conformations of molecule A. The link between the steric index \( \alpha \) and \( G_{05} \) remains high since the correlation index \( P_{a} \) is approximately 0.8 for all conformation. Again TADDOLs 3a–3e demonstrate a \( P_{E} \) of \( -0.77 \) which falls to \(-0.1 \) or less when conformations T3f, g, and h are included. The TADDOL family is studied in more detail elsewhere.

Hence the proposition is made that a good candidate for a flexible chiral dopant to induce high helical twisting power in a nematic solvent has a group of conformers with high \( G_{05} \), \( \alpha \) and similar dihedral angles. The results lend support to the proposition of Ref. 5 that conformational isomers or rotomers present in different concentrations at different temperatures determine the helical twisting power as a function of temperature.

### Table II. Values of scaled chiral indices \( G_{05} \), dihedral angles \( \theta \), the Pearson correlation index \( P_{d} \), minimum energy of structures \( E_{\text{min}} \), the Pearson correlation index \( P_{E} \), steric index \( \alpha \), and the Pearson correlation index \( P_{a} \), for conformations of the chiral dopant molecule A and for a TADDOL molecule.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>(-G_{05} ) ((\times 10^{4}))</th>
<th>(\theta) (^{\circ})</th>
<th>(P_{d})</th>
<th>(E_{\text{min}}) ((\text{kJ/mol}))</th>
<th>(P_{E})</th>
<th>(\alpha)</th>
<th>(P_{a})</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>78.1</td>
<td>(-105.6)</td>
<td>263.4</td>
<td>(-5.254)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A2</td>
<td>62.3</td>
<td>(-83.5)</td>
<td>248.4</td>
<td>(-5.227)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A3</td>
<td>62.3</td>
<td>(-83.7)</td>
<td>248.5</td>
<td>(-4.997)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A4</td>
<td>60.6</td>
<td>(-84.7)</td>
<td>249.0</td>
<td>(-5.064)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A5</td>
<td>60.5</td>
<td>(-84.3)</td>
<td>248.8</td>
<td>(-5.064)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A6</td>
<td>60.4</td>
<td>(-84.8)</td>
<td>249.0</td>
<td>(-5.037)</td>
<td></td>
<td></td>
<td>0.979</td>
</tr>
<tr>
<td>A7</td>
<td>59.4</td>
<td>(-80.5) (-0.98)</td>
<td>246.5</td>
<td>(-5.111)</td>
<td></td>
<td></td>
<td>0.999</td>
</tr>
<tr>
<td>A8</td>
<td>52.2</td>
<td>(-83.7) (-0.89)</td>
<td>246.3</td>
<td>(-4.127)</td>
<td></td>
<td></td>
<td>0.999</td>
</tr>
<tr>
<td>A9</td>
<td>1.8</td>
<td>(-78.0) (-0.60)</td>
<td>244.8</td>
<td>0.59</td>
<td>0.160</td>
<td>0.999</td>
<td></td>
</tr>
<tr>
<td>A10</td>
<td>1.4</td>
<td>(-79.7) (-0.65)</td>
<td>245.1</td>
<td>0.60</td>
<td>0.023</td>
<td>0.999</td>
<td></td>
</tr>
<tr>
<td>A11</td>
<td>(-0.2)</td>
<td>(-80.4) (-0.69)</td>
<td>244.3</td>
<td>0.63</td>
<td>0.463</td>
<td>0.999</td>
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</tr>
<tr>
<td>A12</td>
<td>(-1.2)</td>
<td>(-76.2) (-0.69)</td>
<td>248.4</td>
<td>0.57</td>
<td>0.445</td>
<td>0.999</td>
<td></td>
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<tr>
<td>A13</td>
<td>(-1.0)</td>
<td>(-75.2) (-0.72)</td>
<td>244.7</td>
<td>0.60</td>
<td>0.436</td>
<td>0.999</td>
<td></td>
</tr>
<tr>
<td>A14</td>
<td>(-2.0)</td>
<td>(-73.9)</td>
<td>244.3</td>
<td>0.62</td>
<td>0.356</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3a</td>
<td>109.94</td>
<td>(-81.3)</td>
<td>56.65</td>
<td>(-18.89)</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>T3b</td>
<td>88.87</td>
<td>(-77.7)</td>
<td>55.93</td>
<td>(-14.74)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3c</td>
<td>54.87</td>
<td>(-79.1) (-0.5)</td>
<td>56.02</td>
<td>(-15.29)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3d</td>
<td>43.64</td>
<td>(-80.9) (-0.0)</td>
<td>56.02</td>
<td>(-15.88)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3e</td>
<td>39.99</td>
<td>(-77.0) (-0.3)</td>
<td>55.72 (-0.77)</td>
<td>(-11.73) (0.891)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3f</td>
<td>31.27</td>
<td>(-76.5) (-0.5)</td>
<td>57.11 (-0.020)</td>
<td>(-7.82) (0.876)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3g</td>
<td>30.82</td>
<td>(-79.7) (-0.4)</td>
<td>55.93 (-0.108)</td>
<td>(-13.64) (0.799)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T3h</td>
<td>28.78</td>
<td>(-80.0) (-0.3)</td>
<td>57.04 (-0.096)</td>
<td>(-10.08) (0.82)</td>
<td></td>
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</tbody>
</table>
naphthyl derivative, a member of a family of a large number of derivatives used as high helical twisting power chiral dopants in nematic hosts. The same links are indicated but less strongly. The results for flexible molecules again support the proposition that these chiral and steric indices may be a useful guide to identifying derivatives which are promising candidates for chiral dopants in nematic hosts where all relevant interactions are determined by the structure of the dopants.

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