Optical activity of oriented molecular systems in terms of the magnetoelectric tensor of gyrotropy

Oriol Arteaga
Dep. Física Aplicada i Òptica, IN2UB, Barcelona, Spain
E-mail: oarteaga@ub.edu

Received 30 May 2014, revised 19 September 2014
Accepted for publication 23 September 2014
Published 27 November 2014

Abstract
The optical activity of oriented molecular systems is investigated using bianisotropic material constitutives for Maxwell’s equations. It is shown that the circular birefringence and circular dichroism for an oriented system can be conveniently expressed in terms of the two components of the symmetric magnetoelectric tensor of gyrotropy that are perpendicular to this direction of light propagation. This description establishes a direct link between the optical activity measured at a certain direction and the tensors that describe the oscillating electric and magnetic dipole and electric quadrupole moments induced by the optical wave.

Keywords: optical activity, bianisotropy, chirality

1. Introduction
The different response of a molecule to right- and left- circularly polarized light can be measured experimentally and can be explained with a semiclassical theory of multipole oscillators induced by the electric and magnetic fields of the optical wave [1]. Thanks to advances in computational chemistry calculations of the optical activity of oriented molecules are today relatively easy to do using modern software packages that do quantum-mechanical calculations of molecular property tensors [2]. Measurements of optical activity started more than two centuries ago and modern chiroptical spectroscopy techniques that exploit the intrinsic chirality of circular polarized light are widely available in chemistry laboratories. However, the experimental study of the optical activity of oriented systems is still challenging, and active research is being carried to find reliable methods to measure the typically small chiroptical contributions embedded in the large optical anisotropy of oriented system. In last few years Mueller matrix spectroscopy has emerged as a promising and powerful technique for these type of measurements [3]. Therefore, it seems that we have reached a point where the experimental and theoretical approaches to study the optical activity of oriented molecules are mature enough to be compared. One additional factor that complicates the reconciliation between these two approaches is that theoretical calculations of optical activity are typically done assuming single molecules while, in most cases, measurements are performed in macroscopic media.

Traditionally, measurements of ensembles of molecules were always done in solution, in which small molecules tend to adopt random orientations. Therefore calculations were always made under the assumption of a large collections of molecules randomly oriented. However, in recent years there is a growing interest to study the richer anisotropic spectroscopic information provided by oriented molecules. There are many strategies to orient a molecule, specially if the molecules are large. The most evident strategy consists of crystallizing them to form a molecular crystal but, in some occasions, it is also possible to incorporate the molecules during the growth of a different crystal that acts as a host [4]. In these cases the optical properties not only depend on the individual molecules but also on the symmetries of the crystal lattice. Elongated molecular aggregates are typically orientable by flows [5] and some molecules can also be oriented by simple mechanical actions such as rubbing [6]. Other methods to orient molecules use lasers pulses or other forms of electric and magnetic fields [7]. However, in this work, we will

2040-8978/14/125707+07$33.00 © 2014 IOP Publishing Ltd Printed in the UK
consider that there are no additional external fields affecting the molecules during the optical activity measurements.

In this paper we discuss the theoretical basis that permits the correlation between computations of the averaged molecular polarizability tensors and measurements. We show that the mathematical tools used to describe measurements and calculations naturally converge if a bianisotropic formulation of the material constitutive equations is considered. The key element of the analysis is to refer any measured or calculated optical activity to elements of the magnetoelectric tensor of gyration that appears in the bianisotropic constitutive equations. The results we find simplify the comparison between calculations and experiments.

2. Bianisotropic constitutive equations and multipole theory

The following form of bianisotropic constitutive equations was first given by Tellegen [8]

\[ \mathbf{D} = \varepsilon \mathbf{E} + \mu \mathbf{H}, \quad (1a) \]

\[ \mathbf{B} = \mu \mathbf{H} + \varepsilon \mathbf{E}, \quad (1b) \]

where frequency-domain fields are considered and the choice of the time dependence is given by \( \exp(i \omega t) \). \( \varepsilon \) is the permittivity dyadic, \( \mu \) the permeability dyadic and \( \mu' \) and \( \mu'' \) are the two magnetodielectric dyadics [9] and transmit the relation between the electric and magnetic field quantities \( \mathbf{E}, \mathbf{H} \) and the flux quantities \( \mathbf{D}, \mathbf{B} \). These four constitutive dyadics contain full information of the electromagnetic response of a bianisotropic medium. Lately, this form about the constitutive equations has attracted a lot of attention for the optical characterization of metamaterials [10], because these materials typically have large magnetoelectric tensors. One common simplification for equation (1) is that the specific medium should be Lorentz-reciprocal [11]. This implies

\[ \varepsilon = \varepsilon^T, \quad \mu = \mu^T, \quad \mu' = -\mu'^T, \quad (2) \]

where the superscript T indicates transposition. In this case the magnetoelectric dyadics, that in general are written as \( \mu = \mathbf{\mu} + i \mathbf{\kappa} \) and \( \mu' = \mathbf{\mu}' - i \mathbf{\kappa}' \), must satisfy \( \mathbf{\kappa} = 0 \) and \( \mathbf{\kappa}' \neq 0 \). Therefore, the constitutive equations for a bianisotropic reciprocal medium can be rewritten as

\[ \mathbf{D} = \varepsilon \mathbf{E} + i \kappa \mathbf{H}, \quad (3a) \]

\[ \mathbf{B} = \mu \mathbf{H} - i \kappa' \mathbf{E}. \quad (3b) \]

It should be indicated that, in the presence of absorption, all the tensors in this constitutive equations, i.e. \( \varepsilon, \mu, \) and \( \mu' \), become complex. For structures with uniaxial and biaxial orthorhombic crystallographic symmetries the real and imaginary parts of the tensor have the same system of principal axes. However, the situation is more complicated for media with monoclinic and triclinic symmetries, as they can lead to apparent nonreciprocal optical response, despite being reciprocal media.

Multipole theory can be used to calculate the reciprocal magnetoelectric coupling (now given by \( \kappa \)) between the electric and magnetic fields [12]. Note that equations (2) do not necessarily constraint \( \kappa \) to be a symmetric tensor. However, natural optical activity is a Lorentz reciprocal effect and only it can be contributed by the symmetric part of the magnetoelectric tensor. In this work we only consider this part of the tensor as we are interested in natural optical activity and non-magnetic media. For a complete description of natural optical activity it has been shown that, within a semiclassical theory, in addition to the mean electric dipole induced by the electric field of light it is necessary to include: the electric dipole contribution by the time-derivative of the magnetic field of the light wave, the associated mean magnetic dipole induced by the time-derivative of the electric field, the electric dipole contribution induced by the electric field gradient of the electromagnetic wave and the electric quadrupole contribution induced by the electric field [13]. When all these contributions are considered the oscillating induced moments (the electric dipole \( \hat{\mu}_i \), the magnetic dipole \( \hat{m}_i \) and the electric quadrupole \( \hat{\Theta}_{ij} \)) are the real parts of the following complex expressions [1]

\[ \hat{\mu}_i = \hat{a}_{ij} \mathbf{E}_j + \hat{G}_{ij} \mathbf{B}_j + \frac{1}{3} \hat{A}_{ij} \mathbf{V}_j \mathbf{E}_j + \ldots, \quad (4a) \]

\[ \hat{m}_i = \hat{G}_{jia} \mathbf{E}_j + \ldots, \quad (4b) \]

\[ \hat{\Theta}_{ij} = \hat{A}_{jija} \mathbf{E}_j + \ldots, \quad (4c) \]

where \( \hat{E}_j \) and \( \hat{B}_j \) the actual electric and magnetic fields of the optical wave and \( \mathbf{V}_j \mathbf{E}_j \) is the electric field gradient. \( \hat{a}_{ij} \) is the electric dipole–electric dipole polarizability tensor, \( \hat{G}_{ij} \) is the electric dipole–magnetic dipole polarizability tensor and \( \hat{A}_{ij} \) is the electric dipole–electric quadrupole polarizability tensor. Higher order polarizabilities (e.g. electric octopole, magnetic quadrupole,…) have not been specified because they do not contribute to optical activity [14]. The hats * stress that these are complex quantities. Computational software has been developed to compute all these tensors quantum mechanically by applying time-dependent perturbation theory to molecular orbitals [2]. In these calculations the electric and magnetic dipole moments and the electric quadrupole moment are usually treated as microscopic quantities that apply to single molecules. However, in this paper we discuss the optical activity of a macroscopic medium and, therefore, all the moments included in equation (4a) should be regarded as macroscopic moment densities, i.e. their statistical average multiplied by the number density. We are also assuming that local field effects are small enough to be neglected. From this point, we refer always to moment densities instead of molecular moments and to macroscopic fields instead of local fields.

In a nonmagnetic medium the molecular property tensors \( \hat{a}_{ij}, \hat{G}_{ij} \) and \( \hat{A}_{ij} \) must define the constitutive dyadics of the bianisotropic equation (3a) so that the optical response of an oriented molecule or crystal is calculated from them. Following the work of Graham and Raab [15] we find the
following relations:
\[
(f_{\alpha\beta}) = \epsilon_0 \delta_{\alpha\beta} + \tilde{a}_{\alpha\beta},
\]
\[
(b_{\alpha\beta}) = \mu_0 \delta_{\alpha\beta},
\]
\[
(k_{\alpha\beta}) = \frac{1}{2} \left( (-i\hat{G}_{\alpha\beta} - i\hat{G}_{\beta\alpha}) + \frac{\alpha}{3} (\epsilon_{\gamma\beta\delta} \hat{A}_{\gamma\alpha} + \epsilon_{\alpha\beta\gamma} \hat{A}_{\gamma\delta}) \right).
\]

where \( \epsilon_{\gamma\beta\delta} \) is the Levi–Civita operator and \( \delta_{\alpha\beta} \) is the Kronecker delta. We are using the sum over indices Einstein convention and the notation is the same as in [1, 13]. Equation (5c) can be found, apart from a numerical factor, in [13], but it is different from its equivalent appearing in [15] because here we have disregarded nonreciprocal factors. As natural optical activity is a reciprocal optical phenomena only reciprocal contributions (time-even) need to be considered and the nonreciprocal factors (time-odd) can be safely neglected. The condition \( \hat{p} = -\hat{p}^T \) is automatically satisfied because \( \tilde{a}_{\alpha\beta} \) as well as the sum \( (\hat{G}_{\alpha\beta} + \hat{G}_{\beta\alpha}) \) and \( (\epsilon_{\gamma\beta\delta} \hat{A}_{\gamma\alpha} + \epsilon_{\alpha\beta\gamma} \hat{A}_{\gamma\delta}) \) are all symmetric contributions. An additional difference compared to [15] is that we get a 1/3 factor in front of the \( \epsilon_{\gamma\beta\delta} \) as well as the sums \( (\hat{G}_{\alpha\beta} + \hat{G}_{\beta\alpha}) \) and \( (\epsilon_{\gamma\beta\delta} \hat{A}_{\gamma\alpha} + \epsilon_{\alpha\beta\gamma} \hat{A}_{\gamma\delta}) \) are all symmetric contributions. An additional difference compared to [15] is that we get a 1/3 factor in front of the \( \hat{G}_{\alpha\beta} \) terms, as opposed to the 1/2 factor obtained by Graham and Raab. This change arises because they used a so-called primitive definition of the electric quadrupole moment compared to the more extended traceless definition used for example by Buckingham and Dunn [13]. Both, the traceless and primitive definitions, are applicable because it has been shown that they allow for an origin independent description of the theoretical optical activity [12, 13, 16], i.e. its final expression is not dependent on the arbitrary choice of coordinate origin.

3. Optical activity in terms of the magnetoelectric tensor of gyrotropy

Equation (5c) is specially important because provides the connection between the molecular polarizability tensors and the magnetoelectric tensor. This equation appears in the seminal publication of Buckingham–Dunn (equation (19) in [13]) but, as far as we know, this work does not offer a clear interpretation about the meaning of \( \kappa_{\alpha\beta} \). Apparently, it was introduced as an accessory equation for their calculation of optical activity but it was not highlighted as an important result of this publication.

The elements of the magnetoelectric tensor of gyrotropy \( \kappa_{\alpha\beta} \) (from this point we omit the dyadic notation) are calculated expanding equation (5c):
\[
\kappa_{xx} = -i\hat{G}_{xx} + \frac{\omega}{3} (\hat{A}_{xx} - \hat{A}_{yy}),
\]
\[
\kappa_{yy} = -i\hat{G}_{yy} + \frac{\omega}{3} (\hat{A}_{xx} - \hat{A}_{yy}),
\]
\[
\kappa_{zz} = -i\hat{G}_{zz} + \frac{\omega}{3} (\hat{A}_{yy} - \hat{A}_{zz}).
\]
the appendix we show the results of this calculation for an uniaxial medium with crystallographic point group of symmetry 32, 422 or 622 and in which the optic axis is perpendicular to the direction of propagation of light. In practice, for media with lower symmetry it is very difficult to keep the eigenanalysis at an analytical level and it is more practical to do the calculation numerically. For constitutive tensors belonging to any crystal symmetry it is found, either analytically or numerically, that C depends only on the components of the tensor magnetoelectric tensor $\kappa_{\text{ab}}$. Therefore the optical activity of a medium is fully given by $\kappa_{\text{ab}}$ with $\epsilon_{\text{ab}}$ not playing any role.

For any crystal class, the dependence of C with $\kappa_{\text{ab}}$ follows a general rule: C can be calculated from $\kappa_{\text{ab}}$ by adding the two components of the tensor that are perpendicular to the direction of propagation of the beam. This simple result was already suggested for some particular cases in [17], but now we can generalize it with the following equations for linearly polarized components that are in the plane of wave can be decomposed into the sum of two orthogonal media with lower symmetry it is very difficult to keep the eigenanalysis at an analytical level and it is more practical to do the calculation numerically. For media with lower symmetry it is very difficult to keep the eigenanalysis at an analytical level and it is more practical to do the calculation numerically.

In all cases we have considered an incoming linearly polarized light beam propagating along the $z$ axis. Panels (a), (b) and (c) correspond to a molecule with crystallographic point group of symmetry 42 m at three different orientations. The symmetry of the magnetoelectric tensor for this molecule is

$$\tilde{\kappa} = \begin{bmatrix} -\kappa_{11} & 0 & 0 \\ 0 & \kappa_{11} & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (12)$$

This symmetry is characterized by a magnetoelectric tensor having only one independent component. Molecules belonging to this group do not have optical activity in solution because when all directions of the space are considered the magnetoelectric tensor averages to zero (which is equivalent to say that the trace of the tensor matrix is always zero) [18]. The water (H2O) molecule could be a good example of a molecule this symmetry. To describe the orientation of the molecule with respect to the laboratory reference frame we use the Euler angles $\phi$, $\theta$ and $\psi$. We stick to the convention Z-X-Z to define the rotation order around the axes. The magnetoelectric tensor then transforms as:

$$\tilde{\kappa}_{\text{lab}} = A(\phi, \theta, \psi) \tilde{\kappa} A^{-1}(\phi, \theta, \psi) \quad (13)$$

where $A$ is the 3 × 3 direction cosines matrix given by:

$$A(\phi, \theta, \psi) = \begin{bmatrix} C_{\phi} C_{\psi} - C_{\theta} S_{\phi} S_{\psi} & -C_{\theta} S_{\phi} + C_{\phi} C_{\psi} S_{\theta} & S_{\phi} S_{\theta} \\ C_{\phi} S_{\psi} + C_{\theta} S_{\phi} S_{\psi} & C_{\theta} C_{\psi} - S_{\phi} S_{\theta} & -C_{\phi} S_{\theta} \\ S_{\phi} S_{\theta} & C_{\phi} S_{\theta} & C_{\theta} \end{bmatrix}. \quad (14)$$

where we use the short-hand notation $C_{\phi} = \cos\phi$, $S_{\phi} = \sin\phi$, etc. The direction cosines matrices of panels (a), (b) and (c) are respectively given by $A(0^\circ, 0^\circ, 0^\circ)$, $A(90^\circ, 90^\circ, 90^\circ)$ and $A(90^\circ, 90^\circ, 0^\circ)$. In the orientation shown in panel (a) there is no CB, but for the orientations...
shown in (b) and (c) there exits CB and it takes opposite signs.

Panels (d), (e) and (f) show a molecule with crystallographic point group of symmetry $3, 32$ or $622$ that has a magnetoelectric tensor with two different tensor components, given by

$$\kappa_{33} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -2 \kappa \\ 0 & -2 \kappa & 0 \end{bmatrix} \Rightarrow \text{CB} = \Re(\kappa).$$

For this example we have considered that the components $\kappa_{33}$ and $\kappa_{11}$ keep a relation $-2 : 1$. Note that the trace of the magnetoelectric tensor for molecules holding this special ratio would be zero and, consequently, they would neither be optically active in solution. The direction cosines matrices of panels (d), (e) and (f) are respectively given by $A(0^\circ, n_{01})$, $A(90^\circ, n_{02})$ and $A(0^\circ, 45^\circ, n_{01})$. In all panels the CB measured along the $z$ axis is given by the real part of the sum of the tensor elements $\kappa_{xx} + \kappa_{yy}$, which is theoretically calculated using equation (9c).

### 4. Comparison with the classical tensor description for optical activity

The correspondence between calculated molecular polarizability tensors and optical activity values is treated in other works considering a different tensor, usually called gyration tensor or optical activity tensor, and represented by $g_{\alpha \beta}$ [1, 19–21]. This tensor is based in the so-called equation of the normals

$$\left( n^2 - n_{01}^2 \right) \left( n^2 - n_{02}^2 \right) = G^2,$$

where $n$ gives the possible values of the refractive index, for a given direction of the wave normal, $n_{01}$ and $n_{02}$ are the refractive indices of the eigenwaves propagating in the crystal in the absence of optical activity, and $G$ is the scalar gyration parameter

$$G = g_{\alpha \beta} N_\alpha N_\beta.$$

$N_\alpha$ and $N_\beta$ are direction cosines of the wave normal. Equation (16) is typically approximated to $(n^2 - \bar{n}^2) = G^2$ by...
assuming that the birefringence of the system is not too large \((n_{01} \approx n_{02} \approx \tilde{n} = \sqrt{n_{01}n_{02}})\). If \(G\) is assumed to be very small, the two solutions of this equation can be written as \(n = \tilde{n} \pm G/2n\) and they correspond to the refractive indices for left and right circularly polarized waves. Then, according to equation (7), the optical activity at a given direction can be written as

\[
C_{ij} = \frac{n_0 i}{nc} G = \frac{n_0 i}{nc} g_{ij} N_i N_j ,
\]

(18)

this equation is similar to equation (9a), but here there is a tensor, \(g_{ij}\) that is not the magnetoelectric.

The description of optical activity based on the tensor \(g_{ij}\) is problematic not only because it works uniquely within the approximations that we have detailed above, but also because it arises from an incorrect formulation of the constitutive equations for optical activity. To the best of our knowledge the formalism described in equation (16) was first proposed by Szigveny in 1928 [22] and it requires constitutive equations in which the permittivity tensor is perturbed by another tensor. This formulation corresponds to the classic treatment of optical activity by M Born [23], which excludes any magnetoelectric tensor and the optical activity is introduced by a modified permittivity tensor:

\[
\hat{\epsilon}_{ik} = \hat{\epsilon}_{ik}^{(0)} - i c_{ikm} g_{lm} N_m ,
\]

(19)

where \(\hat{\epsilon}_{ik}^{(0)}\) is the permittivity tensor in absence of optical activity, \(g_{lm}\) are the components of the optical activity tensor and \(N_m\) are the direction cosines of the wave normal. This form of the constitutive equations is similar to the one used for describing magneto-optical phenomena (Faraday effect and magneto-optic Kerr effect) but, despite being quite widespread in classical crystal optics texts [19, 24], it is not suitable for natural optical activity as it violates fundamental principles that natural optical activity should preserve [25] and although it can phenomenologically describe optical activity in transmission it does not work for reflection [26].

The magnetoelectric tensor \(k_{ij}\) corresponding every crystal class takes the same forms of symmetry as the gyration tensor \(g_{ij}\) (see for example the tables in [19, 24]) because the same constraints based on Neumann’s principle are applicable. However, the values of the non-vanishing elements of \(k_{ij}\) bear no relation with those of \(g_{ij}\). In general, we strongly recommend to use \(k_{ij}\) instead of \(g_{ij}\) to express the experimental or calculated optical activity of oriented systems.

5. Conclusions

We have described the optical activity of anisotropic crystals or oriented molecules by a reciprocal biaxialisotropic formulation of the constitutive equations. CB and CD measured at any molecular or crystallographic direction are fully given by the magnetoelectric tensor \(k_{ij}\) which, in turn, is expressed in terms of two molecular property tensors. These contain the effect of the mean electric and magnetic dipoles induced, respectively, by the time-derivative of the magnetic and electric fields of the light wave, as well as the electric dipole induced by the electric field gradient of the wave and the electric quadrupole induced by the electric field.

We have shown that the optical activity found by a light plane wave propagating along a certain direction of a molecule or a crystal is given by the sum of two components of \(k_{ij}\) that are perpendicular to this direction of propagation. These two tensor components describe the change of polarization of light that is due to the special interaction between the electric and magnetic fields in systems with optical activity. With biaxialisotropic constitutive equations this change in polarization is only affected by the magnetoelectric tensor and it is fully separable from the change in polarization due to the anisotropy of the permittivity tensor, which manifests in linear birefringence and linear dichroism. We expect that the use of the biaxialisotropic formalism will simplify the comparison between experiments and calculations and that it will bring the field of optical activity in molecules to a closer connection with that of artificial metamaterials, where magnetoelectric tensors are used regularly.

Acknowledgements

The author acknowledges financial support from a Marie Curie IIF Fellowship (PIIF-GA-2012-330513 Nanochirality). He is also grateful to V Murphy and B Kahr for helpful discussions.

Appendix: Optical activity in a birefringent direction of the symmetry classes 32, 422 and 622

This appendix includes an analytical calculation of the dependence of optical activity with the magnetoelectric tensor for a medium with crystallographic symmetry 32, 422 or 622. For this example we assume that light propagates in a direction perpendicular to the optical axis. For a medium with this symmetry, the dielectric tensor is \(\hat{\epsilon} = \text{diag}(\epsilon_{11}, \epsilon_{11}, \epsilon_{33})\) and the magnetoelectric tensor is \(\tilde{\beta} = \text{diag}(i\epsilon_{11}, i\epsilon_{11}, i\epsilon_{33})\).

After performing the eigenanalysis of the wave equations using the produce described in [17] we find that the refractive indices of the eigenmodes are given by

\[
\hat{n}_{\alpha,\delta} = 2^{1/2}\left[\epsilon_{11} + \epsilon_{33} + 2\kappa_1(\kappa_3 + \kappa_5) \mp \xi \right]^{1/2} / 2 ,
\]

(A1)

in which \(\xi = \sqrt{(\epsilon_{33} - \epsilon_{11})^2 + 4(\kappa_1 + \kappa_3)(\kappa_4 + \kappa_5)\epsilon_{11}}\). \(k_\alpha\) and \(k_\delta\) are obtained from the ratio of the electric field amplitudes appearing in the components of the eigenvectors associated to these eigenvalues

\[
k_\alpha = \frac{\left[\kappa_1 \epsilon_{11} + 2\kappa_3 \epsilon_{11} + \kappa_1 \epsilon_{33} - \kappa_2 \xi \right]}{(\epsilon_{33} - \epsilon_{11} + \xi)\hat{n}_\delta} ,
\]

(A2)

\[
k_\delta = \frac{\left[\kappa_1 \epsilon_{11} + 2\kappa_3 \epsilon_{11} + \kappa_1 \epsilon_{33} + \kappa_2 \xi \right]}{(\epsilon_{11} - \epsilon_{33} + \xi)\hat{n}_\delta} .
\]

(A3)

When all these equations are combined as shown in equation (8) many terms simplify and the final result is
extremely simple. The optical activity for this direction of light propagation is given by

\[ n_\perp - n_\parallel = \left( n_\alpha - n_\delta \right) \frac{1 + k_\alpha k_\delta}{k_\alpha - k_\delta} = \kappa_{11} + \kappa_{33}. \quad (A4) \]

Case (e) of figure 1 shows a visual representation of this particular relationship between optical activity and the magnetoelectric tensor (in the example \( \kappa_{11} \equiv \kappa \) and \( \kappa_{33} \equiv -2\kappa \)).

References

[1] Barron L D 2004 Molecular Light Scattering and Optical Activity (Cambridge: Cambridge University Press)
[2] Frisch M J et al 2009 Gaussian 09 Revision A.1 (Wallingford, CT: Gaussian)
[3] Arteaga O 2010 Mueller matrix polarimetry of anisotropic chiral media PhD Thesis University of Barcelona
[4] Kahr B and Gurney R W 2001 Dyeing crystals Chem. Rev. 101 893–952
[5] Arteaga O, Canillas A, Crusats J, El-Hachemi Z, Llorens J, Sorrenti A and Ribo J M 2011 Flow effects in supramolecular chirality Isr. J. Chem. 51 1007–16
[6] Wong L, Hu C, Paradise R, Zhu Z, Shukenberg A and Kahr B 2012 Relationship between tribology and optics in thin films of mechanically oriented nanocrystals J. Am. Chem. Soc. 134 12245–51
[7] Guérin S, Yatsenko L P, Jauslin H R, Faucher O and Lavorel B 2002 Orientation of polar molecules by laser induced adiabatic passage Phys. Rev. Lett. 88 233601
[8] Tellegen B D H 1948 The gyration, a new electric network element Philips Res. Rep. 3 81–101
[9] Mackay T G and Lakhtakia A 2010 Electromagnetic anisotropy and bianisotropy a field guide (Singapore: World Scientific)
[10] Zouhid S, Sihvola A and Arsalane M 2002 Advances in Electromagnetics of Complex Media and Metamaterials (Dordrecht: Kluwer)
[11] Weiglhofer W S and Lakhtakia A 2003 Introduction to Complex Mediums for Optics and Electromagnetics (Bellingham: SPIE Optical Engineering Press)
[12] Graham E B, Pierrus J and Raab R E 1992 Multipole moments and Maxwell’s equations J. Phys. B: At. Mol. Opt. Phys. 25 4673–84
[13] Buckingham A D and Dunn M B 1971 Optical activity of oriented molecules J. Chem. Soc. A 0 1988–91
[14] Raab R E and de Lange O L 2005 Multipole theory in electromagnetism: classical, quantum, and symmetry aspects with Applications (International Series of Monographs on Physics) (Oxford: Oxford University Press)
[15] Graham E B and Raab R E 1997 Covariant D and H fields for reflection from a magnetic anisotropic chiral medium J. Opt. Soc. Am. A 14 131–4
[16] Krykunov M and Autschbach J 2006 Calculation of origin-independent optical rotation tensor components in approximate time-dependent density functional theory J. Chem. Phys. 125 034102
[17] Arteaga O, Freudenthal J and Kahr B 2012 Reckoning electromagnetic principles with polarimetric measurements of anisotropic optically active crystals J. Appl. Cryst. 45 279–91
[18] Claborn K, Isborn C, Kaminsky W and Kahr B 2008 Optical rotation of achiral compounds Angew. Chem., Int. Ed. Engl. 47 5706–17
[19] Newnham R E 2005 Properties of Materials Anisotropy, Symmetry, Structure (Oxford: Oxford University Press)
[20] Graham E B and Raab R E 1990 Light propagation in cubic and other anisotropic crystals Proc. R. Soc. A 430 593–614
[21] Murphy V L and Kahr B 2011 Planar hydrocarbons more optically active than their isomeric helicenes J. Am. Chem. Soc. 133 12918–21
[22] Szivessy G 1928 Kristalloptik Handbuch der Physik 20 804–37
[23] Born M 1933 Optik: Ein Lehrbuch der Elektromagnetische Lichttheorie (Berlin: Springer)
[24] Nye J F 1985 Physical Properties of Crystals: Their Representation by Tensors and Matrices (Oxford: Oxford University Press)
[25] Lakhtakia A 2002 Optical properties of an isotropic optically active medium at oblique incidence: comment J. Opt. Soc. Am. A 19 807–8
[26] Silverman M P 1986 Reflection and refraction at the surface of a chiral medium: comparison of gyrotropic constitutive relations invariant or noninvariant under a duality transformation J. Opt. Soc. Am. A 3 830–7
[27] The tensor plots have been done with WinTensor program by W. Kaminsky. Available at http://cad4.cpac.washington.edu/WinXMorphHome/WinTensorhome/WinTensor.htm