TECHNICAL REPORT N° 37 **April 2001**

ARTIFACTS FROM LD AND LB

We want to enter this time a rather delicate argument: artifacts from LD (linear dichroism) and LB (linear birefringence).
While detailed descriptions have been available from a long time[1] it seems that many users are still not fully aware of the potential problems behind.
A few cases:
-the Ritcey & Gray publication[2] and the related strong comment by Shindo & Nishio[3]
-the paper from Maestre and coworkers[4] and the equally strong notes from Shindo and others[5]
are probably well known to most of the users.
However looking at published spectra it seems that even today several wrong data are printed in literature, regardless the level of journal involved. This phenomena is more evident in these days, when arguments related to *induced optical activity* are so popular.
It's a real fact that compensation of linear anisotropies on CD spectra is hardly possible.
As Shindo is pointing out[6] only taking into consideration the Mueller matrix[7] approach you can interpret and design experiments in polarization-modulation spectroscopy when dealing with oriented samples [8 9].

In practical terms:
-samples with linear birefringence may give apparent CD (and LD) spectra in wavelength range where no absorption is present caused by the coupling of macroscopic anisotropies with built in limitations of the optical components of the spectrometer
-samples with linear birefringence and linear dichroism will provide apparent CD spectra in the absorption wavelength range independent from rotation of the sample (see TR 38 for an example)
-samples optically active, but with macroscopic anisotropies, will provide an apparent CD signal

$$CD_r = G_0 [CD + 1/2 (LD'LB - LDLB') + (LD'\sin 2\theta - LD\cos 2\theta) \sin \alpha] \qquad (1)$$

Where:
CD is circular dichroism
G_0 is an apparatus constant
α is the residual static birefringence of modulator
θ is the angular rotation of the sample
LD is linear dichroism and LD' is 45° linear dichroism
LB is linear birefringence and LB' is 45° linear birefringence.

From equation 1 it's clear how the real CD contribution in the apparent CD spectra may be easily masked out by the LD and LB components which may be several order of magnitudes larger.
It's also clear that the common practice[10] to rotate the sample (changing θ) and take the average CD spectra will not help.

---

[1] Jensen H.P., Schellman J.A., Troxell T. *Appl.Spectrosc.* 32 (1978) 192
[2] Ritcey A.M. & Gray D.G. *Biopolymers* 27 (1988) 1363
[3] Shindo Y. & Nishio M. *Biopolymers* 30 (1990) 25
[4] Livolant F., Mickols W., Maestre M.F. *Biopolymers* 27 (1988) 1761
[5] Shindo Y., Nishio M., Maeda S. *Biopolymers* 30 (1990) 405
[6] Shindo Y. *Opt.Engineering* 34 (1995) 3369
[7] Mueller H. *J.Opt.Soc.Am.* 38 (1948) 661
[8] Schonhofer A., Kuball H.G., Puebla C. *Chem.Phys.* 76 (1983) 453
[9] Schellman J. & Jensen H.P.*Chem.Rev.* 87 (1987) 1359
[10] Tunis-Schneider M.J.B & Maestre M.F. *J.Mol.Biol.* 52 (1970) 521

E.C.S. European Chirality Services srl via Verdi 6A 23870 Cernusco Lombardone (Lc) Italy
tel/fax (0039)-039-9284368 mob 0349-6907288 e-mail ecssrl@libero.it