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*Review Article*

ECD Cotton Effect Approximated by the Gaussian Curve and Other Methods

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# *ABSTRACT* To determine the absolute conﬁguration of chiral compounds, theoreti- cal calculations of ECD spectra have been extensively carried out, where the shape of component CD Cotton effects was approximated by the Gaussian distribution curve. However, in some articles, errors are found in the equations of Gaussian curve express- ing CD Cotton effects. In this short review, the correct and general forms of the Gaus- sian equation and the approximation of the CD curve by other methods are described.

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# *KEY WORDS:* ECD Cotton effect; rotational strength; Gaussian curve; 1/*e*-bandwidth; half the bandwidth at 1/*e* peak height

INTRODUCTION

# In recent years, there have been published many articles reporting the determination of the absolute conﬁgurations of chiral compounds by the quantum chemical calculation of electronic circular dichroism (ECD).1–20 In these calcula- tions, CD Cotton effects are generally approximated by the Gaussian curve. However, in some articles, there are errors in the Gaussian equation; some are obviously trivial typos, but some are because of the disagreement between the deﬁnition of parameters and equations. Therefore, in this short review, we would like to show the correct equations together with the clear deﬁnition of parameters, and also to describe other methods for approximating CD curves.

The rotational strength *R*, a parameter representing the sign and intensity of a CD Cotton effect, is formulated in

# space, and l and *M* are operators of electric and magnetic moment vectors, respectively. The dot stands for the sca- lar product of two vectors, 0 and a are wavefunctions of ground and excited states, respectively. The rotational strength *R* is thus equal to the imaginary part of the scalar product of electric and magnetic transition moments.

The rotational strength *R* is calculable by theories suita- ble for each chiral compound; for example, the exciton theory for exciton-coupled compounds,22,25,26 the p-elec- tron SCF-CI-DV MO method for compounds with twisted p-electron systems,21,27,28 the semiempirical CNDO/S cal- culation for some chiral aromatics and hetero com- pounds,29 and the ab initio MO method of TDDFT calcula- tion for most chiral compounds1–20 have been employed.

●

# eq. (1) or (2) and is experimentally obtained from the

observed CD spectra by numerical integration.21–23

yThe original equation to obtain the rotational strength *R* from the observed CD spectrum is formulated as,21

# *R* ¼ 2:296*3*10—39 Z DeðrÞ dr cgs units ð1Þ

r

*R* ¼ ð2:296*3*10—39=roÞ Z DeðrÞdr cgs units ð2Þ

*R* ¼ ½ð3*hc*103*ln*10Þ=ð32p3*N*A Þ]

DeðrÞ dr 2:296*3*10—39

Z ¼

r

DeðrÞ dr

Z

r

ð1*a*Þ

# where r is wavenumber (cm*2*1), De is molar CD which is expressed as a function of r, and r is the central wave-

where *N*A, *h*, and *c* are Avogadro’s number, Planck’s constant, and the ve- locity of light, respectively. The term in brackets [ ] was calculated using the recently reported physical constant data (after 2003 from the Commit-

tee on Data for Science and Technology, CODATA) giving [(3*hc*103*ln*10)/

y o (32p3*N* )] *5* 2.29648 *3* 10–39. Therefore, although the value of 2.297 *3*

# number of the Cotton effect .

10*2*39

A

is used in some articles,

12,17

the value of 2.296 *3* 10

*2*39

is used here

# The quantum mechanical deﬁnition of rotational

strength, as given by Rosenfeld,24 is:

# *R* ¼ Imf<0jlja> ● <ajMj0>g ð3Þ

where Im denotes the imaginary part of the term in brack- ets { }, < > denotes the integration over conﬁgurational

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as shown in eqs. (1) and (1a).

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# If the ECD Cotton effect is approximated by the Gaus- sian distribution, the CD curve is formulated as:

DeðrÞ¼ Deext exp½—fðr — roÞ=Drg2] ð4Þ

# where Deext is the extremum value of the Cotton effect, ro is the central wavenumber of the Cotton effect, and Dr is the parameter controlling the CD bandwidth and is deﬁned as half the bandwidth at 1/*e* peak height (0.36788Deext) as shown in Figure 1{.

Substitution of eq. (4) into eq. (2) and integration gives

# eq. (6). In eq. (6), Dr can be evaluated from the corre- sponding observed UV–Vis spectra. For example, in the case of exciton-coupled CD, the bandwidth *w* (*5*2Dr) at 1/*e* of peak height is obtained from the UV spectrum of a component chromophore. In some cases, the Dr value is empirically estimated to ﬁt the calculated CD curve to the observed one.

In some articles,12,17 the Gaussian curve is formulated as a function of *w* instead of Dr. This is of course possible as shown in the next equation. The substitution of Dr with (*w*/2) in eq. (6) gives,

# *R* ¼ 2:296*3*10—39pﬃﬃﬃDe

ext

# Dr=ro

ð5Þ

# DeðrÞ¼ 2ro=ð2:296*3*10—39pp*w*Þ

*3 R* exp½—f2ðr — roÞ=*w*g2] ð7Þ

ﬃﬃﬃ }

# From eqs. (4) and (5), the CD curve is formulated as:

DeðrÞ¼ ro=ð2:296*3*10—39ppDrÞ

ﬃﬃﬃ }

# *3 R* exp½—fðr — roÞ=Drg2] ð6Þ

Therefore, if rotational strength *R* is theoretically obtain-

# where *w* is the bandwidth at 1/*e* peak height (see Fig. 1).

Both eqs. (6) and (7) give the same CD curve, but which equation is more suitable? Of course, eq. (6) using Dr is simpler and suitable. Therefore, we suggest the use of eq. (6) with Dr.

11,12,17

# able by the eq. (3), the CD spectral curve is calculable by

In some articles,

# the CD curve is expressed as a

{In the book by Harada and Nakanishi,22 the parameter Dr was errone- ously called the standparﬃﬃﬃd deviation of the Gaussian distribution. However,

it should be equal to

2 times (standard deviation).

# function De(*E*) of energy *E* instead of wavenumber r. This

is of course reasonable, and eq. (6) is reformulated as

# Deð*E*Þ¼ D*E*=ð2:296*3*10—39pﬃpﬃﬃDÞ}

§In the article by Diedrich and Grimme,12 the CD spectra were simulated by overlapping Gaussian functions for each transition:

Deð*E*Þ¼ n1=ð2:297*3*10—39pﬃﬃﬃpﬃﬃﬃrﬃﬃﬃÞoX*A*D*E R* exp½—ð*E* — D*E* =2rÞ]2 ð8*a*Þ

*i*

*i*

*i*

*i*

where r was deﬁned as the width of the band at 1/*e* height, and D*Ei* and *Ri* are the excitation energy and rotational strength for transition *i*, respec- tively.

In comparison of eq. (8a) with (7) and/or (8), there are some errors; one is obviously a typo in the Gaussian equation. The other is the disagreement between the deﬁnition of the bandwidth at 1/*e* height and

*3 R* exp½—fð*E* — D*E*Þ=Dg2] ð8Þ

# where D*E* is transition energy, and D is half the bandwidth

at 1/*e* peak height expressed in energy units§,}.

Figure 2 shows the experimental ECD curves of (1*R*,5*R*)-(*1*)-*b*-pinene together with the simulated ECD curves, where Cotton effects were approximated by the

eq. (8a).

In the article by E. Giorgio et al.,17 was corrected as;

the typo of the Gaussian equation

}One reason for errors found in the Gaussian equations may be because of the unclear deﬁnition of parameters. In the review article by Schell- man,33 the Gaussian shape function is formulated as:

Deð*E*Þ¼ n1=ð2:297*3*10—39pﬃ2ﬃﬃpﬃﬃﬃrﬃﬃﬃÞoX D*E*0*aR*0*a* exp½—fð*E* — D*E*0*a*Þ=2rg2 ]

r ðkÞ¼ 1=ðD pﬃpﬃﬃÞ} exp½—fðk — k Þ=D g2 ] ð6*a*Þ

*a*

ð8*b*Þ

where r was deﬁned as the width of the band at 1/*e* height, and D*E*0*a* and *R*0*a* are the excitation energies and rotational strengths for the transition from 0 to *a*, respectively. However, there are still errors in eq. (8b). The

correct equation is formulated as shown in eq. (8c).

m m m m

where Dm is deﬁned as the exponential half-width. This deﬁnition looks correct, but the terminology ‘‘half-width’’ is confusing, because it looks similar to ‘‘half-bandwidth’’ used in NMR spectroscopy of organic chemis- try. In the case of NMR spectroscopy, the half-bandwidth *W*1/2 is deﬁned as the bandwidth at 1/2 peak height. Therefore, the meanings of ‘‘half’’

If the bandwidth (*w*) at 1/*e* peak height is used, the reformulation of eq. (7) derives the CD De(*E*) as:

are different from each other.

In the article by Bringmann et al.,18

the corresponding parameter Gk is

D *E* 2= 2:296*3*10—39pp*w* D*E R* exp 2 *E* D*E* =*w* 2

ﬃﬃﬃ }Xeð Þ¼ ð Þ ½— ð — Þ ]f g0*a* 0*a* 0*a*

*a*

ð8*c*Þ

where *w* is the bandwidth at 1/*e* peak height and expressed in energy units. The parameters D*E*0*a* and *R*0*a* are the excitation energies and rota- tional strengths for the transition from 0 to *a*, respectively.

If the parameter D (*5w*/2) is used, eq. (8c) is transformed to:

Deð*E*Þ¼ 1=ð2:296*3*10—39ppﬃﬃﬃDÞ}X D*E*0*aR*0*a* exp½—fð*E* — D*E*0*a*Þ=Dg2 ]

deﬁned as the exponential half-width (width of the band at 1/e height).

But the deﬁnition described in parentheses is different from the deﬁnition of exponential half-width.

In the book of Lightner and Gurst,26 the corresponding parameter Dk is deﬁned as the half-width at 1/*e* times the height, and the parameter is shown in a ﬁgure. Therefore, the deﬁnition is easily understandable from the ﬁgure.

In the review chapter by Woody,34 the corresponding parameter D is called the bandwidth of the Gaussian and is deﬁned as the absolute value difference between kmax and either of the wavelengths at which the CD has decreased to De/*e*, where *e* is the base of the natural logarithms. Although the deﬁnition of the latter part is clear, the terminology of ‘‘the bandwidth of the Gaussian’’ is also confusing. In a review chapter by

*a*

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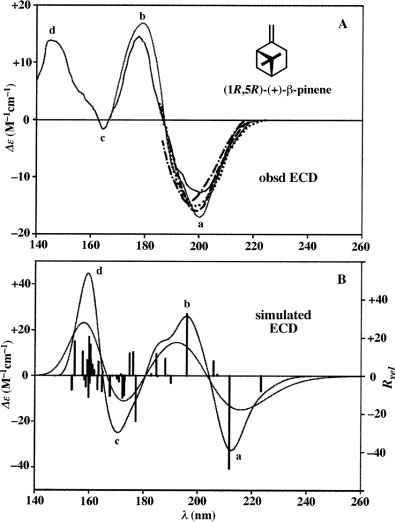
ð8*d*Þ

where D is half the bandwidth at 1/*e* peak height and expressed in energy units. The parameters D*E*0*a* and *R*0*a* are the excitation energies and rota- tional strengths for the transition from 0 to *a*, respectively.

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Koslowski et al.,35 the corresponding parameter Ga is deﬁned as the half- width of the Gaussian at 1/*e* of its maximum.

There is thus much variance and confusion in the deﬁnition. Therefore, the authors suggest the use of eqs. (6), (8), or (8d) using the parameter Dr or D (half the bandwidth at 1/*e* peak height), and the parameters should be clearly deﬁned.

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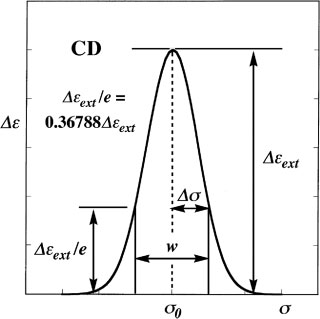


Fig. 1. ECD Cotton effect curve approximated by the Gaussian distri- bution, where Deext is the extremum value of De, r is wavenumber, ro is the central wavenumber of the Cotton effect, Dr is half the bandwidth at 1/*e* of peak height (0.36788Deext), and *w* (*5*2Dr) is the 1/*e*-bandwidth.

# Gaussian curve.4 The ECD spectrum was reproduced well by the simulation, conﬁrming the TDDFT ECD theoretical approach.

Recently it was reported that the Lorentzian equation is also useful to approximate ECD Cotton effect curves.10,13,14,16,33

# n o

DeðrÞ¼ Deext *g*2=ððr — roÞ2 þ *g*2Þ

ð9Þ

Fig. 2. (A) Experimental ECD spectra of (1*R*,5*R*)-(*1*)-*b*-pinene: solid lines, gas phase30,31; (- - -), in 3-methylpentane at 208C31; (- · -), in 3-methyl- pentane at *2*1008C31; (·· ·), in cyclohexane.32 (B) Simulated ECD spectral

curves (sharper bands, r *5* 0.2 eV: broader bands, r *5* 0.4 eV) and rota-

tional strengths by the velocity representation, where r is half the band- width at 1/*e* of peak height (Reprinted with permission from McCann

# where r is wavenumber, *g* is half the bandwidth at half peak height (expressed in wavenumber units), and ro is the central wavenumber of the Cotton effect (see Fig. 3).

The Lorentzian CD curve is also expressed as a function of wavelength k as follows.

# DeðkÞ¼ Deextn*g*2=ððk — koÞ2 þ *g*2Þo ð10Þ

where k is wavenumber, *g* is half the bandwidth at half peak height (expressed in wavelength units), and ko is the central wavelength of the Cotton effect.

# When comparing the Gaussian and Lorentzian curves with typically observed ECD curves, the Lorentzian curve is generally steeper at the peak and broader in the skirts. Furthermore, the Lorentzian curve hardly reaches the base line (zero value). On the other hand, the Gaussian curve generally ﬁts ECD spectra better than the Lorent- zian curve. Therefore, it is reasonable to use the Gaussian curve for the calculation of ECD spectra.

Both the Gaussian and Lorentzian curves are symmetri- cal in shape, but in some cases, the shape of the CD Cot- ton effect and that of the corresponding UV absorption band strongly deviate from the symmetrical pattern. For example, the UV band shape of the p-p\* transition of poly-

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and Stephens. *Journal of Organic Chemistry* 2006;71:6074–6098. © 2006

American Chemical Society).

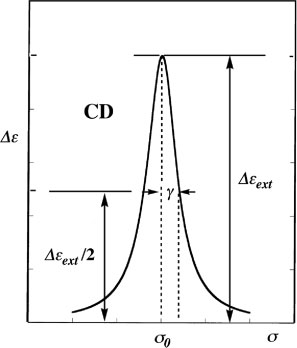


Fig. 3. CD Cotton effect curve approximated by the Lorentzian equa- tion, where Deext is the extremum value of De, r is wavenumber, ro is the central wavenumber of the Cotton effect, and *g* is half the bandwidth at

# acene, e.g.,

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Bb transition of anthracene around 250 nm, is

half peak height.

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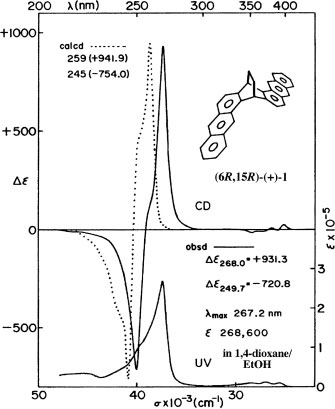


Fig. 4. Calculated and observed CD and UV spectra of chiral cage compound (6*R*,15*R*)-(*1*)-1 in 1,4-dioxane/EtOH (Adapted from Ref. 22).

# highly asymmetric, reﬂecting vibronic structure, as exem- pliﬁed by a chiral cage compound shown in Figure 4.22

In general, the longer wavelength side (smaller in wave- number) is steeper than the shorter wavelength side (larger in wavenumber). In the exciton coupling systems, such a nonsymmetric shape causes the imbalance of CD intensity between the ﬁrst and second Cotton effects. Therefore, in such a case, the Gaussian or Lorentzian approximation of the CD curve is not applicable.

# To approximate the nonsymmetrical CD curve, the shape of the corresponding UV absorption band is used as follows22:

DeðrÞ¼ Deext *f* ðrÞ ð11Þ

# where *f*(r) is the function describing the shape of CD Cot- ton effect curve and is numerically adopted from the observed UV spectra. The function *f*(r) is normalized as *f*(rext) *5* 1, where rext is the wavenumber at the CD extremum.

Then, the rotational strength *R* is formulated as,

# As seen in Figure 4, the shape of the CD curve and the imbalance of intensity between the ﬁrst and second Cotton effects are well reproduced by this method.22

In conclusion, the ECD spectral curve is approximated by several methods as described above, and the errors of equations in some articles were corrected. When the Gaussian curve is used for ECD, the present authors sug- gest the use of eqs. (6), (8), or (8d), where the parameters should be clearly deﬁned.

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# *R* ¼ 2:296*3*10—39De

ext

# Z *f* ðrÞ=r dr ð12Þ

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# where $ *f*(r)/r dr is numerically integrated.

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From eqs. (11) and (12), the CD curve is formulated as:

# DeðrÞ¼ *R*=ð2:296*3*10—39 Z *f* ðrÞ=r drÞ *f* ðrÞ ð13Þ

where the theoretically calculated value of rotational strength *R* is used.

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