Optical Activity of Intramolecular Charge-transfer Transitions

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Long wavelength optical activity is reported for a series of molecules containing both an electron donor (*e.g.* *p*-methoxyphenyl) and an electron acceptor (*e.g.* *N*-4-methoxycarbonylpyridinium) group. This optical activity is attributed to the intramolecular charge-transfer transition arising from interaction between the donor and acceptor groups. It is shown that the sign of the Cotton effects observed can be related to the absolute configuration of the systems by a simple chirality rule. The theoretical basis for this rule is discussed.

CHARGE-TRANSFER (CT) complexes show electronic transitions attributable to electron transfer from one of the constituent components (the electron donor, D) to the other (the electron acceptor, A). Briegleb *et al.*[1-3] have observed optical activity for the CT transition of complexes between chiral electron donors (*e.g.* olefins) and an achiral acceptor (*e.g.* tetracyanoethylene). This work has recently been extended to other intermolecular complexes.[4] Another well known optically active CT transition arises from interaction of the nicotinamidium ion in the coenzyme NAD$^+$ and electron donor sites (probably tryptophan) in certain enzymes.[5-8]

Theoretical evaluation and classification of the optical activity of CT transitions is hampered by the general lack of knowledge about the conformation of CT complexes in solution.

We have reported optical activity of a CT transition involving intramolecular interaction between a *p*-methoxyphenyl group as an electron donor and a 4-cyanopyridinium ion as an electron acceptor.[9] Almost simultaneously Moser [10] reported optical activity for intra- and inter-molecular CT interaction between *NN*-dimethylaniline (donor) and phthalimide-type acceptors. Intramolecular CT interactions can be studied from model compounds in which the relative orientation of the D and A portions (*i.e.* the conformation of the intramolecular 'complex') is known, thus providing the possibility of investigating the relation between (absolute) configuration of the 'complex' and the optical activity of the resulting CT transition.

In an earlier paper [11] the synthesis of a number of optically active *N*-[1-(*p*-methoxyphenyl)alkyl]- and *N*-[2-(*p*-methoxyphenyl)-alkyl and -cycloalkyl]-4-methoxycarbonylpyridinium ions *via* the so called Zincke reaction [12-14] has been described. The compounds thus obtained are compiled in the Table. All compounds from the Table contain the same two chromophores, *i.e.* a *p*-methoxyphenyl group and a 4-methoxycarbonylpyridinium ion. Although these chromophores alone do not absorb in the visible region (longest wavelength transition, ^1L_b, for both at *ca.* 275 nm) most compounds are yellow in solution and in the solid state. As shown in a previous paper,[15] this colour is caused by an intramolecular CT transition in which *p*-methoxyphenyl acts as an electron donor and 4-methoxycarbonylpyridinium as an electron acceptor. In the present paper we describe a study of the optical activity of the intramolecular CT transition.

RESULTS

For all but two compounds (1) and (2) the intramolecular CT transition shows distinct optical activity as determined by c.d. spectroscopy. The u.v. and c.d. spectroscopic data are given in the Table. As an illustration the u.v. and c.d. spectra for (−)-(1), (+)-(6), and (−)-(13) in 96% EtOH are shown in Figures 1—3 respectively.

DISCUSSION

Optically Active CT Transition.—The rotational strength *R* of the CT transition is found to vary over a wide range (see Table). For (1) and (2) the rotational strengths were not calculated, because no maximum for the Cotton effect of the CT band could be determined, but *R* is expected to be very small as is seen from Figure 1. Compounds (1) and (2) are the only examples

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[1] G. Briegleb and H. G. Kuball, *Angew. Chem.*, 1964, **76**, 228.

[2] G. Briegleb, H. G. Kuball, and K. Henschell, *Z. Phys. Chem.*, 1965, **46**, 229.

[3] G. Briegleb, H. G. Kuball, K. Henschell, and W. Euing, *Ber. Bunsengesellschaft Phys. Chem.*, 1972, **76**, 101.

[4] A. I. Scott and A. D. Wrixon, *Tetrahedron*, 1972, **28**, 933.

[5] E. Racker and I. Krimsky, *J. Biol. Chem.*, 1952, **196**, 731.

[6] G. Cilento and P. Tedeschi, *J. Biol. Chem.*, 1961, **236**, 907.

[7] S. Shifrin, *Biochim. Biophys. Acta*, 1964, **81**, 205.

[8] S. Shifrin, *Ann. New York Acad. Sci.*, 1969, **158**, 148.

[9] A. J. de Gee, J. W. Verhoeven, I. P. Dirkx, and Th. J. de Boer, *Tetrahedron*, 1969, **25**, 3407.

[10] P. Moser, *Helv. Chim. Acta*, 1968, **51**, 1831.

[11] A. J. de Gee, W. J. Sep, J. W. Verhoeven, and Th. J. de Boer, *J.C.S. Perkin I*, 1974, 676.

[12] Th. Zincke, *Annalen*, 1903, **330**, 361.

[13] Th. Zincke, G. Heuser, and W. Möller, *Annalen*, 1904, **333**, 296.

[14] Th. Zincke, *Annalen*, 1905, **341**, 369.

with D and A attached to the same carbon atom. In all other compounds D and A are connected to vicinal carbon atoms in the general arrangement D–C–C–A.

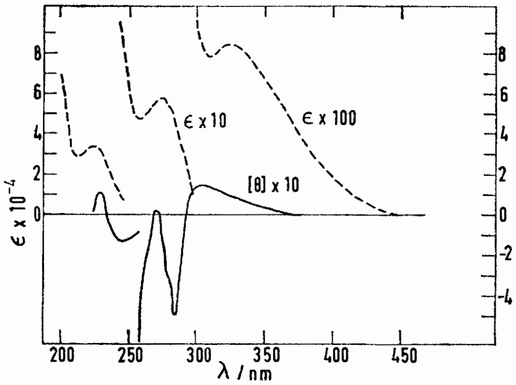


FIGURE 1 C.d. (——) and u.v. (— — —) spectra of (−)-(1) in 96% ethanol. The c.d. spectrum is corrected to 100% optical purity

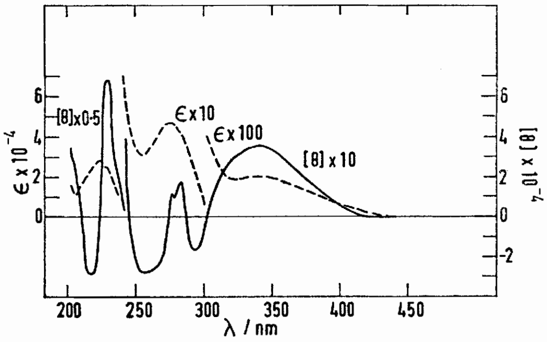


FIGURE 2 C.d. (——) and u.v. (— — —) spectra of (+)-(6) in 96% ethanol. The c.d. spectrum is corrected to 100% optical purity

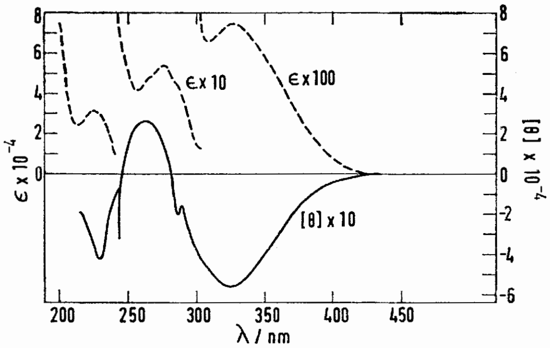
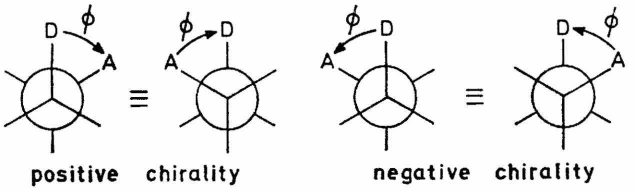
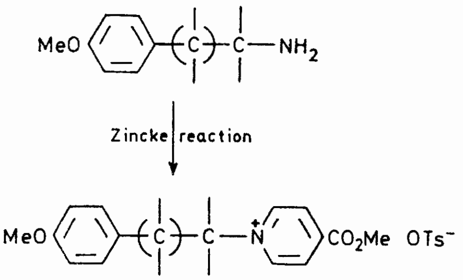


FIGURE 3 C.d. (——) and u.v. (— — —) spectra of (−)-(13) in 96% ethanol

As shown in the Theory section a general rule relating the sign of the charge-transfer Cotton effect and the chirality of the D–C–C–A system can be formulated. A positive CT Cotton effect correlates with a positive value of the dihedral angle ϕ defined by D–C–C–A.



All compounds in the Table were obtained by a completely stereospecific, one-step synthesis[11] (Zincke reaction) from the corresponding chiral *p*-methoxyphenylalkylamines. For many of these amines the absolute configuration was determined *via* independent routes as indicated in the Table. In all cases the absolute configurations arrived at *via* application of the chirality rule to the sign of the CT Cotton effect correspond with those determined for the precursor amines. Thus this chirality rule seems to be of general applicability and offers a convenient method to determine the absolute configuration of such D–A systems and of their precursor amines. The latter can be of special importance for pharmacologically interesting β-arylalkylamines of the general type $Ar{-}C^{*}{-}C^{*}{-}NH_2$.

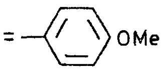
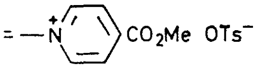


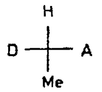
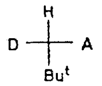
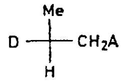
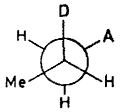
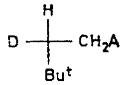
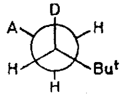
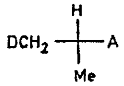
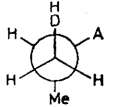
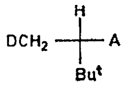
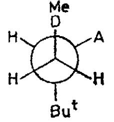
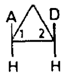
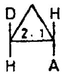
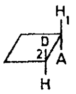
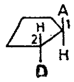
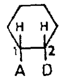
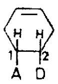
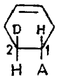
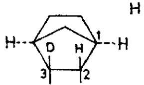
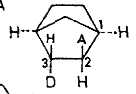
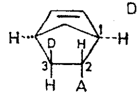
For conformationally non-rigid systems, application of the rule requires knowledge about the preferred molecular conformation. For compounds (3)—(6) it was assumed that the sign of the CT Cotton effect is determined by the most stable rotamer about the C^1–C^2 bond (see reference 15).

For the *cis*-cyclohexane and -cyclohexene derivatives *cis*-(10) and *cis*-(11) the sign of ϕ at a given absolute configuration depends on the preferred orientation, *i.e.* D axial and A equatorial or D equatorial and A axial. ^{1}H N.m.r. spectroscopy showed (see reference 15) the former conformation to be predominant for *cis*-(10), while for *cis*-(11) no clear-cut distinction could be made. Application of the chirality rule as defined above to (+)-*cis*-(10) then leads to the 1*R*,2*R* configuration, in accordance with that determined for its amine precursor. (−)-*cis*-(11), which has the same absolute configuration as (+)-*cis*-(10) (known from their chemical relation) has a negative CT Cotton effect, suggesting a preferred conformation of *cis*-(11) with D equatorial and A axial, when the chirality rule is applied.

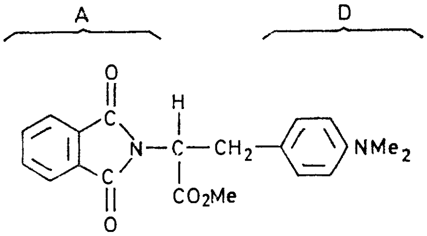
For *cis*-(7) in which the dihedral angle $\phi = 0°$ and for (1) and (2) in which D and A are both connected to the chiral centre, no conclusions about the absolute configurations can be drawn from the chirality rule applied to the observed weak CT Cotton effects. It is interesting to note that the minus sign of the intramolecular CT Cotton effect observed by Moser[10] for (15) also fulfils the chirality rule, when it is assumed that rotamer (15a), which seems sterically the more favoured of the

U.v. and c.d. data for CT transitions of compounds (1)—(14) in 96% ethanol (10^{-3}M) at 25°. $[\theta]_{max.}^{25}$ (°) and the rotational strength (*R*, c.g.s. units) are corrected to 100% optical purity

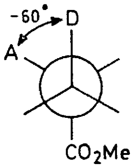
D =  A = 

				U.v.			C.d.				Precursor amines		
No.	Structure	Preferred rotamer [15]	Sign at Na D line	λ_{max} (nm)	ε_{max}	10^{36} *D*	λ_{max} (nm)	$[\theta]_{max}^{25}$	10^{40} *R*	Absolute configuration [a]	Absolute configuration [b]	Optical purity (%) [c]	Sign at Na D line
(1)			(—)	325·0	845	2·47	*d*	*d*			*S*	95	(−)
(2)			(—)	326·0	550	1·26	*d*	*d*			*S*	96	(−)
(3)			(+)	328·5	720	1·75	*e*	*e*	*e*	*R*		~30	(+)
(4)			(−)	333·0	360	0·87	332·0	−4950	−10·30	*S*	*S*	>99	(−)
(5)			(+)	324·0	700	1·94	334·0	+5710	+9·93	*S*	*S*	76	(+)
(6)			(+)	340·0	200	0·49	341·5	+3510	+6·03	*R*	*R*	95	(+)
cis-(7)			(+)	363·0	920	2·20	356·5	+2140	+3·48		1*S*,2*S*	91	(−)
trans-(7)			(+)	343·0	1715	4·23	340·5	+5290	+9·95	1*S*,2*R*	1*S*,2*R*	>99	(+)
trans-(8)			(+)	333·0	1025	2·40	328·0	+7420	+14·26	1*S*,2*R*	1*S*,2*R*	>99	(+)
trans-(9)			(−)	338·0	825	1·94	335·5	−11680	−20·14	1*R*,2*S*	1*R*,2*S*	>99	(−)
cis-(10)			(+)	340·0	535	1·24	338·0	+7320	+13·12	1*R*,2*R*	1*R*,2*R*	>99	(−)
trans-(10)			(−)	340·0	225	0·61	336·5	−3280	−6·00	1*R*,2*S*	1*R*,2*S*	>99	(−)
cis-(11)			(−)	335·0	775	1·91	*f*	−2920			1*R*,2*R*	95	(−)
trans-(11)				336sh	(240)							0	
(12)			(+)	328·5	385	0·97	328·0	+3410	+6·42	2*S*,3*R*	2*S*,3*R*	84	(+)
(13)			(−)	327·0	745	1·77	324·5	−5620	−9·75	2*R*,3*S*	2*R*,3*S*	>99	(−)
(14)			(+)	325sh	(1000)		*g*	*g*	*g*	2*S*,3*R*	2*S*,3*R*	84	(+)

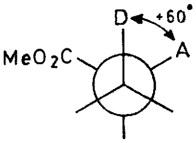
two *gauche*-rotamers, determines the sign of the CT Cotton effect, while the rotamer in which $\phi = 180°$ does not contribute to the optical activity of the CT transition.



(15)



(15a)



(15b)

Short Wavelength Optically Active Transitions.—The D and A chromophores incorporated in the molecules in the Table both exhibit local transitions in the 275 nm region [D: $\lambda_{max.}$ *ca*. 275 nm (ε *ca*. 1500) and A: $\lambda_{max.}$ *ca*. 278 nm (*ca*. 4700)] and in the 225 nm region [D: $\lambda_{max.}$ *ca*. 225 nm (ε *ca*. 11,000) and A: $\lambda_{max.}$ *ca*. 225 nm (11,000)]. The latter is attributed to the local ^1L_a transitions polarized along the long axis of the chromophores, while the former can be attributed to the local ^1L_b transitions polarized perpendicular to the ^1L_a transitions.

Optical activity in the ^1L_b transition region is observed, but the band shapes are rather complicated due to overlap with the broad CT Cotton effect and the strong Cotton effects of the ^1L_a transitons (see Figures 1—3).

The ^1L_a transitions (225 nm region) show high optical activity and for some cases it seems that these two local ^1L_a transitions (of D and A) are coupled with each other to give an exciton splitting [16] resulting in two c.d. maxima of opposite sign and approximately equal strength.

THEORY

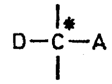
C.d. spectra are connected to electronic transitions in chiral molecules [16-19] and can be described by a quantity called the rotatory strength R, which is the imaginary part (Im) from the scalar product of the magnetic ($\vec{M}$) and the electric ($\vec{\mu}$) transition dipole moments [equation (1)].

$$R = \mathrm{Im}\vec{M}\,.\,\vec{\mu} \qquad (1)$$

In the absence of external fields, μ can be taken as a real vector while $\vec{M}$ (being out of phase with μ) is purely imaginary. Thus R is purely imaginary and its value is obtained by dropping i in the resulting formulae. Thus R depends on the magnitudes of $\vec{\mu}$ and $\vec{M}$ and on the cosine of the angle (γ) between them [equation (2)].

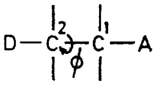
$$R = M\mu\cos\gamma \qquad (2)$$

The compounds studied in this paper contain two symmetric chromophores (D and A) connected by a chiral (cyclo)alkyl residue. The basic types are (I) and (II).



$$\mathrm{D{-}\overset{|*}{\underset{|}{C}}{-}A}$$

(I)



$$\mathrm{D{-}\overset{|_2}{\underset{|}{C}}{-}\overset{|_1}{\underset{|}{C}}{-}A}$$

(II)

The mechanism of CT in (I) has previously been shown [20] to involve homoconjugation between D and A by overlap of the p-atomic orbitals on the atoms with which they are connected to C*. In (I) the chromophore D–C*–A is intrinsically symmetric (C_s) as long as free rotation round the D–C* and C*–A bonds exists. The weak Cotton effect observed for the type (I) compounds [*e.g.* (1) and (2)] indicates that asymmetric perturbation of the chromophore by the chiral alkyl system is negligible.

For (II) we have discussed the mechanism of charge-transfer in a previous paper.[15] It essentially involves transfer of one electron from D to A through the C^2–C^1 bond. Thus as far as the intramolecular CT transition is concerned, the chromophoric part of the molecule is composed of D, A, and the C^1–C^2 bond. Even when D and A are freely rotating round D–C^2 and C^1–A the D–C^2–C^1–A array constitutes an intrinsically asymmetric chomophore for all values of ϕ except for 0 and 180°.

For a calculation of the rotational strength, the electric and magnetic transition dipole moments of the CT transition ($\vec{\mu}_{CT}$ and $\vec{M}_{CT}$ respectively) and their relative orientation have to be known. For type (II) compounds $\vec{\mu}_{CT}$

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[15] A. J. de Gee, J. W. Verhoeven, W. J. Sep, and T. J. de Boer, *J.C.S. Perkin II*, 1975, 579.

[16] J. A. Schellman, *Account Chem. Res.*, 1968, **1**, 144.

[17] R. Grinter and S. F. Mason, *Trans. Faraday Soc.*, 1964, **60**, 274.

[18] K. Mislow, E. Bunnenberg, R. Records, K. Wellman, and C. Djerassi, *J. Amer. Chem. Soc.*, 1963, **85**, 1343.

[19] R. R. Gould and R. Hoffmann, *J. Amer. Chem. Soc.*, 1970, **92**, 1813.

[20] J. W. Verhoeven, I. P. Dirkx, and Th. J. de Boer, *J. Mol. Spectroscopy*, 1972, **42**, 149.

Footnotes to Table on page 672

[a] According to the charge-transfer chirality rule (see text). [b] Based [24] on (i) literature data, (ii) the effect of a chiral solvent on the ^{1}H n.m.r. shifts according to Pirkle's rules, (W. H. Pirkle, T. G. Burlingame, and S. D. Beare, *Tetrahedron Letters*, 1968, 5849), or (iii) application of a quadrant rule (L. Verbit and H. C. Price, *J. Amer. Chem. Soc.*, 1972, **94**, 5143) to the Cotton effect observed for the ^1L_a transition of the p-methoxyphenyl chromophore or a combination of these criteria. [c] Determined [24] mostly by n.m.r. spectroscopy either through diastereomeric derivatization with (+)-α-methoxy-α-trifluoromethylphenylacetic acid according to J. A. Dale, D. L. Dull, and H. S. Mosher, *J. Org. Chem.*, 1969, **34**, 2543, or through the use of a chiral solvent [*e.g.* (S)-(+)-2,2,2-trifluoro-1-phenylethanol] according to Pirkle *et al.* [d] No CT Cotton effect maximum observed. Apparent maxima were observed for (1) at 302 nm, $[\phi]_{max.}^{25} = +1380°$ (see Figure 1) and for (2) at 314 nm, $[\theta]_{max.}^{25} = +2180°$. [e] C.d. spectrum not measured because of low optical purity. The sign at the Na D line was assumed to correspond with that of the CT Cotton effect. [f] Flattened maximum at *ca*. 325 nm. [g] CT Cotton effect maximum obscured by other absorptions. The sign at the Na D line was assumed to correspond with that of the CT Cotton effect.

was shown (reference 15) to be directed from the optical centre of A to that of D and to be proportional in magnitude to the distance between these centres ($\vec{r}_{DA}$). This $\vec{\mu}_{CT}$ can be considered to result from three linear charge displacements within the locally symmetric A–C^1, C^2–D, and C^1–C^2 parts of the molecule. The moments resulting from these linear charge displacements are $\vec{\mu}_A$, $\vec{\mu}_D$, and $\vec{\mu}_C$ centred in A, D, and the C^2–C^1 bond respectively as indicated in Figure 4. For ϕ 180° $\vec{\mu}_{CT}$ is the resultant of $\vec{\mu}_D$, $\vec{\mu}_A$, and $\vec{\mu}_C$ (see Figure 4), for all other values of ϕ the overall charge displacement contains, beside the linear part described by $\vec{\mu}_{CT}$, a circular part which results in a non-zero value of $\vec{M}_{CT}$.

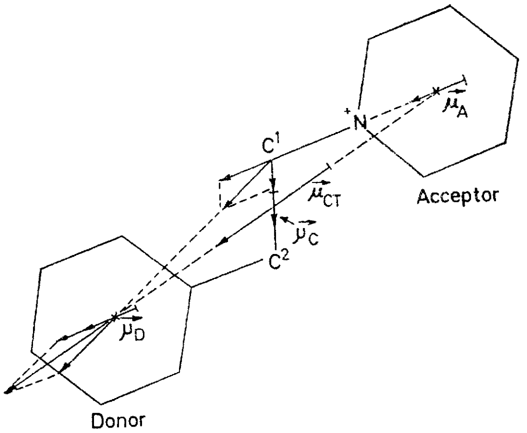

FIGURE 4 Composition of $\vec{\mu}_{CT}$ from the local moments $\vec{\mu}_D$, $\vec{\mu}_A$, and $\vec{\mu}_C$ (ϕ 180°)

A linear electric transition produces a magnetic moment given by equation (3).[16,17] In (3), ω [$= 2\pi(W_E - W_N)/h$]

$$\vec{M} = i\omega\vec{r}\vec{\mu}/2c \tag{3}$$

is the circular Bohr frequency of the transition under consideration and $\vec{r}$ is the distance vector to an arbitrarily selected origin. For a single linear charge displacement, $\vec{M}$ can be made zero by selecting the origin in its optical centre. When several linear charge displacements co-operate to produce one transition moment, $\vec{M}$ will generally be non-zero. When the origin for molecules D–C^2–C^1–A is chosen in the centre of the C^2–C^1 bond, $\vec{r}_C$ and thus $\vec{M}_C$ become zero. The moments $\vec{M}_D$ and $\vec{M}_A$ now determine $\vec{M}_{CT}$.

We take the optical centres of D and A to coincide with their respective ring centres thus $r_D \approx r_A$ and when $\mu_D \approx \mu_A = \mu_0$ also $M_D \approx M_A = M_0$. From equation (3) it follows that $\vec{M}_D$ and $\vec{M}_A$ are perpendicular to the planes determined by $\vec{r}_D/\vec{\mu}_D$ and $\vec{r}_A/\vec{\mu}_A$ respectively. In Figure 5 the situation is shown schematically. The z-axis is chosen along C^2–C^1 and A in the xz-plane. Both $\vec{M}_D$ and $\vec{M}_A$ lie in the xy plane and have the magnitude $M_0 = |i\omega\vec{r}_D\vec{\mu}_D/2c| = |i\omega\vec{r}_A\vec{\mu}_A/2c|$. Figure 6 shows the projection of the molecule in the xy plane (*e.g.* a Newman projection along C^1–C^2). $\vec{M}_D$ and $\vec{M}_A$ add up to $\vec{M}_{CT}$, which makes an angle of $(90° - \phi/2)$ with the negative x-axis and has the magnitude $2M_0 \cos \phi/2$. The electric transition moment has components perpendicular to ($\vec{\mu}_z$) and in the xy plane ($\vec{\mu}_{xy}$), the latter makes an angle $(90° - \phi/2)$ with the negative x-axis and has a magnitude $\mu_{xy} = 2\mu_0 \sin \alpha \sin \phi/2$. Thus $\vec{M}_{CT}$ and μ_{xy} are collinear and the resulting rotational strength [see equation (2)] is given by (4). Equation (4)

$$\begin{aligned} R_{CT} = \vec{M}_{CT}\vec{\mu}_{xy} &= 2M_0 \cos \phi/2 \cdot 2\mu_0 \sin \alpha \sin \phi/2 \\ &= 2M_0\mu_0 \sin \alpha \sin \phi \end{aligned} \tag{4}$$

predicts $R_{CT} = 0$ for $\phi = 0$ and 180° and at a maximum for $\phi = 90$ or 270°. Most important (4) predicts a positive R_{CT} for $0° < \phi < 180°$ (right-handed) and a negative R_{CT} for $180° < \phi < 360°$ (left-handed) in accord with the experimental data.

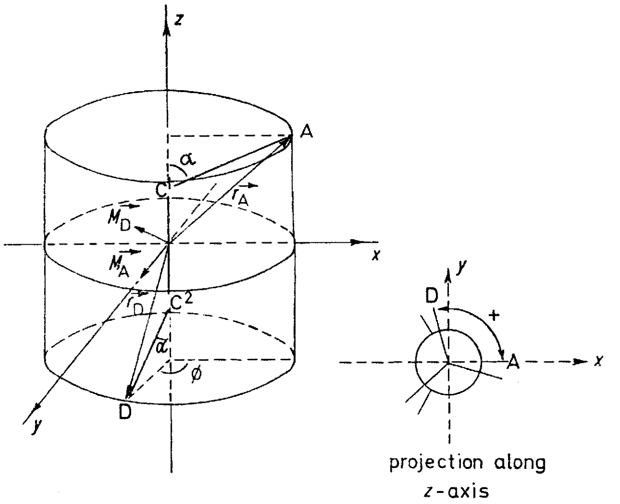

FIGURE 5 Perspective view of the A–C^1–C^2–D fragment with positive dihedral angle (ϕ) and its corresponding Newman projection

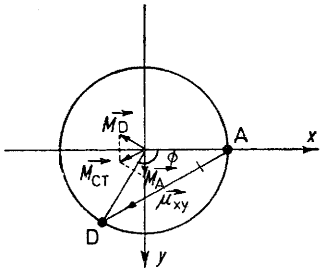

FIGURE 6 Projection of the A–C^1–C^2–D fragment with the conformation depicted in Figure 5, in the xy plane

The small R_{CT} observed for the *cis*-cyclopropyl derivative *cis*-(7) ($\phi = 0°$) indicates that R_{CT} is indeed mainly determined by the intrinsic asymmetry of the D–C^2–C^1–A array. The very large R_{CT} for the *trans*-cyclopentane system *trans*-(9) might indicate ϕ *ca.* 90°, but expression (4) is certainly too much simplified to be used for the quantitative prediction of R_{CT} values.

From the discussion given above, it seems that the sign of a CT Cotton effect is mainly determined by the relative orientation of those components of $\vec{\mu}_{CT}$, which are located in the planes of D and A. Intermolecular CT complexes between chiral molecules are also known [1-4,10] to display optical active CT transitions. From our results it seems rather certain that such optical activity can only occur when the chromophore responsible for the CT transition, *i.e.* the electron donor–acceptor complex as a whole, is intrinsically asymmetric.

For many CT complexes, the CT transition borrows a large part of its intensity,[21] from local transitions in D and A. (Note that in Figure 4, $\vec{\mu}_D$ and $\vec{\mu}_A$ are parallel to the local ^1L_a transitions in D and in A respectively.) This means that for such complexes $\vec{\mu}_{CT}$ has large components in the planes of D and A. When it is known from theoretical considerations or from experimental evidence how these components are directed, it seems reasonable to apply the chirality rule derived above to them, in order to predict the sign of the CT Cotton effect for a particular complex conformation. In our opinion this is the basis for the empirical rule derived by Scott and Wrixon [4] for the optical activity of complexes between tetracyanoethylene and chiral electron donors. It should be noted that there appears to be a strong resemblance between the chirality rule derived here for the intramolecular CT transition and the 'aromatic exciton chirality rule' [22] as it has been shown to apply to the exciton splitting resulting from interaction between the transitions of two aromatic chromophores [22,23] arranged in a chiral array. The rules differ widely however, in the predicted dependence of the rotational strength (R) on the dihedral angle (ϕ). While the CT chirality rule predicts that R should change sign only at $\phi = n\pi$ (n = 0, 1, 2, *etc.*), the exciton treatment implies a sign reversal (for the longest wavelength exciton component) at $\phi = \frac{1}{2}n\pi$.

EXPERIMENTAL

Syntheses and conformational analyses of the model compounds have been described earlier.[11,15,24] C.d. and u.v. spectra were recorded on a Cary 60 and 14 spectrophotometers respectively at 25° (96% ethanol as solvent). The rotational strength R, and the dipole strength D were calculated from $R = 22{\cdot}9 \times 10^{-40}\int\frac{\Delta\varepsilon}{\nu}\,d\nu$ and $D = 91{\cdot}8 \times 10^{-40}\int\frac{\varepsilon}{\nu}\,d\nu$, where ν is in cm^{-1} and ε is in l mol^{-1} cm^{-1}, using computerized integration of band areas with the assumption of a Gaussian band shape.

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[4/1668 *Received, 8th August,* 1974]

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