PHYSICAL METHODS IN HETEROCYCLIC CHEMISTRY

A Comprehensive Treatise in Two Volumes

Edited by A. R. KATRITZKY

VOLUME 2

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Preface

Physical methods are perhaps the most important of all the influences which have contributed to the fundamental changes of the last 50 years in the theory and practice of organic chemistry. Effective chemical research can now hardly be carried out without the aid of a variety of physical measurements.

In the advance of physical techniques into organic chemistry, two main streams may be identified: physical chemists have commenced with the study of the simplest molecules and, using methods as rigorous as practicable, have proceeded stage by stage to structures of increasing complexity. Organic chemists have, by contrast, frequently made correlations of the (usually complex) structures with which they work: such correlations being, at least at first, purely empirical. Both streams are of vital importance to the over-all development—they complement each other, and chemists of each type need to be aware of the work in both streams.

The systematic application of physical methods to heterocyclic chemistry has been slower than that to the other two traditional divisions of organic chemistry. This is probably because the molecular complexity of the heterocyclic field has hindered the advance into it by the physical chemist. A result is that most reviews and expositions of a physical method, or of a group of physical methods, deal but cursorily with its application to compounds of the heterocyclic class. The present two volumes seek to fill this gap—each chapter gives but a brief outline of the general theoretical and experimental aspects of the subject, and then gets down to surveying the literature in which the method has been applied to heterocyclic problems. This literature is often voluminous and is nearly always scattered. It is hoped that the present collection of reviews will save individual research workers much time and effort in literature searching.

As Editor, I have been fortunate in being able to enlist an international team of authors who are among the leaders in their respective fields, and my thanks go to each of them for their cooperation. We have tried to cover the literature to the beginning of 1962.

A. R. KATRITZKY

Cambridge, England, October, 1962

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Infrared Spectra

A. R. KATRITZKY AND A. P. AMBLER

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The Electronic Absorption Spectra of Heterocyclic Compounds

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I. INTRODUCTION

THE VISIBLE AND ultraviolet absorption spectrum of a molecule gives directly, in the absorption frequency, the interval between a higher occupied and a lower unoccupied electronic energy level and, in the absorption intensity, a measure of the electronic transition probability between those levels. In the analysis of the various types of electronic transitions, spectroscopy is dependent upon theoretical chemistry, and in turn, spectroscopy provides an important method of investigating the more detailed experimental consequences of chemical theory. The present chapter will be concerned primarily with these fundamentals, descriptions of the manifold applications of absorption spectroscopy being already available in a number of standard texts (see Appendix).

The applications of electronic absorption spectroscopy are of two main types. In the first, Beer's law (see below) is employed to estimate the concentration of a light-absorbing species. Since allowed electronic transitions give rise to large absorption intensities, very small concentrations may be estimated spectrophotometrically, and such measurements may be made in the presence of other species which do not absorb light of the same wavelength with the same intensity. In practice, such a condition is not unduly restrictive, and, in addition to elementary quantitative analyses, spectrophotometry has been applied to the study of the rates of a variety of chemical reactions and to the measurement of the constants governing equilibrium in a number of ionization, tautomeric, and charge transfer processes. Depending upon an empirical law, such applications do not require a knowledge of the nature of the transition giving the absorption band studied, but theory may provide a basis for the extension of the application or facilitate the interpretation of the data obtained, as in the case of the investigation of charge transfer phenomena.

The spectroscopic elucidation of molecular structures constitutes the applications of the second type. The absorption of light at certain wavelengths with given intensities indicates the presence in a molecule of a particular absorbing group or groups (chromophores), and shifts of the absorption wavelength and intensity from their standard values may be diagnostic of specific substituent or steric effects or may be indicative of a particular mode of interaction between a chromophore and its intramolecular or intermolecular environment. Empirical rules have been formulated describing the absorption wavelength and intensity changes due to substitution in a number of chromophores (27), but in general, applications of the second type require some knowledge of the character of the electronic transitions responsible for the absorption bands investigated.

II. FACTORS GOVERNING THE ABSORPTION OF LIGHT

When a molecule absorbs visible or ultraviolent light of frequency ν or wavelength λ, an electron undergoes a transition from a lower to a higher energy level in the molecule, the energy level difference ΔE being given by the well-known relationship

$$\Delta E = h\nu = hc/\lambda \tag{1}$$

where h is Planck's constant and c is the velocity of light. The insertion of the appropriate numerical values gives

$$\Delta E = 286 \times 10^3/\lambda \tag{2}$$

with ΔE in kcal/mole and λ in Ångström units. The absorption of visible and ultraviolet light corresponds to quantized energy increments of 30–300 kcal/mole. Superimposed on the electronic transition are vibrational transitions with energy quanta in the range 0.1–10 kcal/mole and, in the vapor phase, rotational transitions with energy quanta of a few calories. The rotational structure, and often the vibrational structure, is lost in the condensed phases, giving a broad and smooth absorption curve, due to intermolecular or solute-solvent interactions with the composite vibrational-electronic transition.

In general, nonbonding lone-pair electrons are the least strongly bound in a molecule, and in the bonding levels π-electrons have higher energies than corresponding σ-electrons, while in the antibonding levels that order is reversed (Fig. 1). Thus, in the spectra of simple molecules

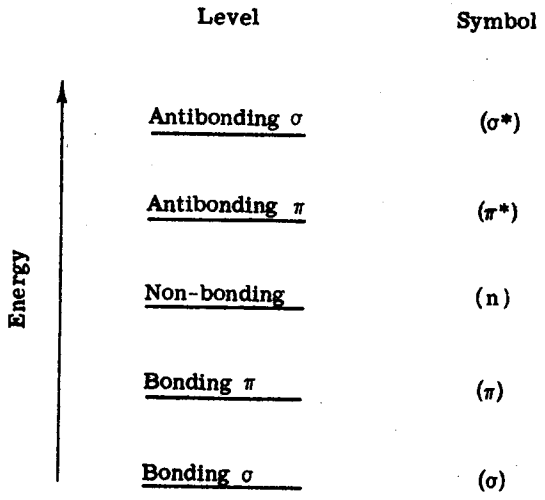

FIG. 1. Relative energies of molecular orbitals.

the bands due to $n \rightarrow \pi^*$ transitions generally lie at longer wavelengths than those arising from $\pi \rightarrow \pi^*$ excitations, the latter usually lying in the same region as the $n \rightarrow \sigma^*$ bands, while the $\sigma \rightarrow \sigma^*$ absorptions are found in the far ultraviolet (Fig. 1, Table I). In complex molecules, the highest occupied π-electron level moves to higher energies with increasing conjugation, ultimately overlying any lone-pair nonbonding electron levels, which are unaffected by conjugation, so that the $n \rightarrow \pi^*$ bands become hidden under the intrinsically stronger $\pi \rightarrow \pi^*$ absorption.

According to the Beer-Lambert law (16), the integrated fraction of

TABLE I
LONGEST WAVELENGTH ABSORPTION BANDS OF INDIVIDUAL CHROMOPHORES[a]

Compound	Solvent	Transition	λ Å	ε liter mole^{-1} cm^{-1}	Reference
$Me_3C—CH_2—CHMe_2$	Vap	$\sigma \rightarrow \sigma^*$	1540	~10,000	149
Me_3N	Vap	$n \rightarrow \sigma^*$	2270	900	146
Me_2O	Vap	$n \rightarrow \sigma^*$	1840	2520	71
Me_2S	EtOH	$n \rightarrow \sigma^*$	2100	1020	56
MeBr	Vap	$n \rightarrow \sigma^*$	2040	200	131
MeI	Pet eth	$n \rightarrow \sigma^*$	2570	365	75
$CH_2=CH_2$	Vap	$\pi \rightarrow \pi^*$	1620	~10,000	152
$H_2C=O$	Me_2CHEt	$n \rightarrow \pi^*$	3100	5	35
$(CH_2)_5—C=S$	C_6H_{14}	$n \rightarrow \pi^*$	5040	~5	83
Me—N=N—Me	EtOH	$n \rightarrow \pi^*$	3400	4.5	133
$Me_3C—N=O$	Et_2O	$n \rightarrow \pi^*$	6650	20	13
Me—NO_2	EtOH	$n \rightarrow \pi^*$	2700	20	116

[a] In the present and in subsequent tables, wavelengths are given in Ångström units (10^{-8} cm), frequencies in cm^{-1}, and decadic molar extinction coefficients in liter mole^{-1} cm^{-1}, the values, unless otherwise specified, referring to band maxima or, if given in italics, to shoulders or inflections. The following abbreviations are used for the phase or the solvent employed: Vap = vapor, EtOH = ethanol, MeOH = methanol, H_2O = water, MeCN = acetonitrile, Et_2O = diethylether, pet eth = petroleum ether, Me_2CHEt = isopentane, C_8H_{18} = isooctane, C_6H_{14} = *n*-hexane, C_6H_{12} = cyclohexane, Diox = dioxane, S = unspecified solvent.

light absorbed by an assembly of molecules is proportional to the number of absorbing systems in the light path, namely,

$$\log_{10}(I_0/I) = cd\epsilon \tag{3}$$

where I_0 and I are, respectively, the intensities of the entrant and the emergent light with a path length d of absorbing species at a concentration of c moles/liter, and the constant ϵ is the decadic molar extinction coefficient in liter mole^{-1} cm^{-1}. The fraction of light absorbed depends upon the ratio of the cross-sectional area of the absorbing molecules to the cross-sectional area of the light beam (28), so that maximum extinction coefficients should have the approximate value

$$\epsilon_{max} = 10^4 pa \tag{4}$$

if a molecule with a cross-sectional area a in Å^2 absorbs a quantum of light incident upon it with a probability p. As required by Eq. (4), strong absorption bands in the spectra of polyatomic molecules commonly have extinction coefficients of the order of 10^4 or greater.

The maximum extinction coefficient of an absorption band may be

affected markedly by a change of phase or of solvent, but the band area $A = \int \epsilon d\nu$ frequently remains constant, affording a better measure of absorption intensity. The band area is related (32) to the oscillator strength f which, in the classical vibration theory, is the number of oscillators, each of mass m and charge e, giving rise to the absorption band

$$f = (10^3 mc^2 \log_e 10/\pi e^2 N) \int \epsilon d\nu \tag{5}$$

where c is the velocity of light and N is Avogadro's number. In the case of smooth and symmetrical absorption bands, the oscillator strength may be obtained in good approximation from the experimental data by

$$f = 4.6 \times 10^{-9} \epsilon_{max} \Delta\nu \tag{6}$$

where $\Delta\nu$ is the band width at half-maximum extinction (in cm^{-1}).

In the quantum theory (113) the oscillator strength of an absorption band depends upon the absorption frequency ν and the electric transition moment length Q:

$$f = 1.085 \times 10^{-5} \nu Q^2 \tag{7}$$

with ν in cm^{-1} and Q in Å. The transition moment length is a measure of the mean displacement of the promoted electron during the transition, and it is given by

$$Q = \int \phi_n (\Sigma_i \mathbf{r}_i) \phi_m d\mathbf{r} \tag{8}$$

where ϕ_n and ϕ_m are the respective wave functions of the ground and the excited state, and $\mathbf{r}_i$ is a vector defining the position of the ith electron. For the transition of an electron from an occupied to an unoccupied orbital, with wave functions ψ_o and ψ_u, respectively, Eq. (8) becomes

$$Q = \sqrt{2} \int \psi_o(\mathbf{r}) \psi_u d\mathbf{r} \tag{9}$$

the factor $\sqrt{2}$ allowing for the promotion of either of the two electrons in the occupied orbital. Electronic displacements of 1–3 Å give oscillator strengths of the order of unity, corresponding to maximum extinction coefficients measured in solution of $\sim 10^5$.

The conditions for a finite oscillator strength and transition moment are given by the selection rules. The electric dipole transition moment is a real physical property of a molecule and as such it must be invariant with respect to any rotation, reflection, or inversion of the molecular symmetry axes. The vectors $\mathbf{r}$ have the symmetry properties of a translatory motion along one or more of the molecular axes, and so the

integrals of Eq. (8) and (9) are nonzero only if the direct product of the symmetries of the lower and the upper state wave functions $\phi_n\phi_m$ or of the orbital functions $\psi_o\psi_u$ contains a term with the symmetry properties of a translatory motion (141). The direction of that motion gives the orientation of the electric dipole transition moment. Since a molecule absorbs only that part of the incident radiation which has an electric vector parallel to the transition moment, the direction of the latter may be determined by measuring the spectrum of the orientated molecule with polarized light.

The integrals of Eqs. (8) and (9) vanish if there is a change of electron spin on excitation, and singlet-multiplet transitions occur only to the degree that the nominal singlet and multiplet states are mixtures of singlet and multiplet configurations, so that both states have components with the same spin. The spin and the orbital angular momentum of an electron are not quantized independently in the heavier atoms, and molecules containing such atoms give absorptions, due to nominal singlet-multiplet transitions, of relatively high intensity.

In molecules composed of the lighter atoms, the orbital selection rule indicates that light absorption of high intensity arises generally from an electronic transition to an upper orbital with one more nodal plane or surface than the lower orbital from which the excitation originates (22). In electronic transitions from a nodeless orbital the transition moment is directed perpendicular to the new nodal plane, and in excitations from multinodal orbitals the resultant moment is the vector sum of the component moments at the points of nodal change.

The transition of an electron from an s to a p_x orbital, for example, is allowed, electronic charge being displaced from the region of the new nodal yz-plane in the x-direction (Fig. 2). The displacement has a translatory character, and the transition moment is orientated along the x-axis. On the other hand, a transition from a p_y to a p_x orbital is forbidden, since the displacement of electronic charge would have a rotatory rather than a translatory character, and the number of nodes would not change. Thus, the $n \rightarrow \pi^*$ bands of simple carbonyl compounds are weak (Table I), since the transition involves the promotion $p_y \rightarrow p_x$ at the oxygen atom, the z-direction lying along the carbonyl bond axis. Absorption bands of the $n \rightarrow \sigma^*$ type have moderate intensities (Table I), since the transitions contain some atomic components of the $s \rightarrow p$ or $p \rightarrow s$ form which are allowed. High absorption intensity in simple molecules arises from $\sigma \rightarrow \sigma^*$ or $\pi \rightarrow \pi^*$ transitions (Table I), which are akin to the allowed atom transitions $s \rightarrow p$ and $p \rightarrow d$, respectively. In the $\pi \rightarrow \pi^*$ transition of ethylene, electronic charge is displaced linearly

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from the middle of the carbon-carbon bond, giving a transition moment parallel to the bond axis (Fig. 3).

Weak absorption results from electronic transitions to upper orbitals with more than one node additional to the number of nodes in the lower orbital, since the component transition moments tend to have opposed

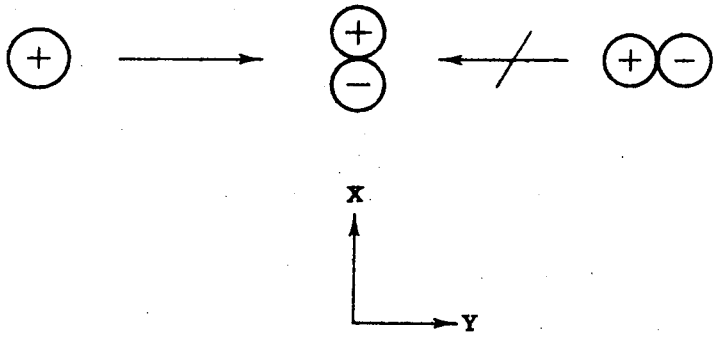


FIG. 2. Electronic transitions of the $s \rightarrow p_x$ and $p_y \rightarrow p_z$ types.

directions and partly cancel. The cancellation is particularly complete in molecules with a center of symmetry if the nodes change by an even number on excitation (parity forbidden). In the transition of an electron from the highest occupied to the highest unoccupied π-orbital of buta-

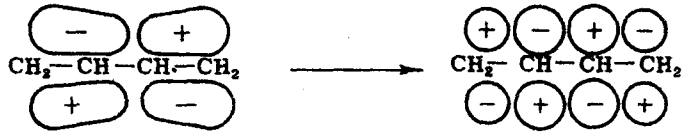
FIG. 3. Electronic transition of $\pi \rightarrow \pi^*$.

diene (Fig. 4a), the component transition moments, which have the instantaneous directions given (Fig. 4b and 4c), cancel completely in the *trans* isomer, which has a center of symmetry, but give a net resultant in the *cis* isomer (114).

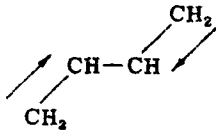
Prohibited transitions occur in polyatomic molecules with a finite probability, owing to perturbations which mix in a component of an allowed transition with the formally forbidden transition. A weak absorption band in one component of an acceptor-donor pair may develop an enhanced intensity on charge transfer complex formation, owing to the mixing of the forbidden transition with the allowed charge transfer transition. By this mechanism (78) the very weak singlet-triplet absorption bands of aromatic and *N*-heteroaromatic molecules are enhanced in

intensity by a factor as great as 10^5 (40) in the presence of paramagnetic substances, such as nitric oxide or oxygen (52).

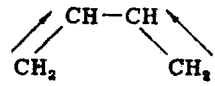
The perturbations mixing forbidden and allowed transitions may be intrachromophore as well as interchromophore. The general electronic selection rules given are based on the assumption that a molecule has a fixed shape, which remains unchanged on excitation. However, polyatomic molecules always possess some vibrations which periodically change the molecular shape, such as the bending vibrations of linear molecules. The direct product of the symmetries of the vibrational and



(a)



(b)



(c)

FIG. 4. The higher occupied and the higher unoccupied π-orbital of butadiene (*a*), and the instantaneous directions of the component moments in a transition between those orbitals for *trans*-butadiene (*b*), and *cis*-butadiene (*c*).

the electronic ground and excited state wave functions may then contain a term with the symmetry properties of a translatory motion, while the product of the electronic functions alone does not. The transition then becomes allowed to the small degree that the perturbing vibration changes the electronic wave function. Moreover, the equilibrium shapes of a molecule in the ground and the excited state may differ, so that a nominally forbidden transition becomes allowed on account of the change in symmetry. The change of electronic wave function with a gross change in molecular shape is large, but the absence of nuclear motion during an electronic transition, by the Franck-Condon principle, ensures that the resultant light absorption is usually small.

Changes of molecular shape and size on excitation, and the character of the perturbing vibrations, may be determined from the vibrational and rotational structure of an electronic band. In an allowed electronic band, the totally symmetric vibrations of the molecule, those that do not change the molecular shape, appear as progressions in the excited state frequency starting from the zero vibrational level of the electronic ground state, with weaker temperature-sensitive bands on the long wavelength side, due to transitions from the thermally populated higher vibrational levels of the ground state. The relative intensities of the vibrational bands in a progression give, by the Franck-Condon principle, a measure of the change in molecular size on excitation, and they may indicate a change of shape.

In the case of forbidden transitions made allowed by a bending or other nontotally symmetric vibration, the absorption is marked by the absence of a band origin arising from the electronic energy change without accompanying vibrational energy changes. Progressions in the totally symmetric vibrations build up on bands due to the absorption of the electronic transition energy plus or minus one quantum, or an odd number of quanta, of the energy of the perturbing vibration. The resultant absorption pattern, lacking a band origin, is characteristic of bands due to forbidden transitions.

The rotational structure of an electronic absorption band is determined by the direction of the transition moment and by the relative values of the molecular moments of inertia. The direction of the transition moment is given by the over-all appearance of the rotational structure, namely, the presence or the absence of a Q-branch in the case of linear molecules, or the predominance of J- or K-structure in the case of symmetric and slightly asymmetric tops. The degradation of the rotational structure to the red indicates a probable increase in one or more of the moments of inertia on excitation, and conversely, the less frequently observed degradation to the blue suggests a decrease in molecular dimensions. The values of one or more of the molecular moments of inertia in the ground and the excited state may be obtained from the frequency spacings in the rotational structure by the methods used in the analysis of rotational-vibrational bands (76).

III. SATURATED HETEROCYCLES

In saturated compounds with lone-pair electrons the longest wavelength absorption generally arises from the promotion of a nonbonding electron to an antibonding σ-orbital, namely, an $n \rightarrow \sigma^*$ transition (Fig. 1). Nitrogen heterocycles absorb at longer wavelengths than their oxy-

gen isomers (Table II), since lone-pair electrons have lower energies on oxygen than nitrogen, water and ammonia having ionization potentials of 12.59 and 10.23 ev, respectively (150). However, hydrogen sulfide has an ionization potential of 10.46 ev (150), and the longer wavelength absorption of the sulfur heterocycles must arise from a low-lying σ^* orbital, reflecting the weak bonding and antibonding character of the carbon-sulfur σ and σ^* orbitals, respectively.

TABLE II
SATURATED HETEROCYCLES $\square_{(CH_2)_n-X}$

X	n	Solvent	λ	ε	Reference
NH	4	Vap	1960	2000	123
	5	Vap	1980	3000	123
NMe	5	Et_2O	2130	1600	92
O	2	Vap	1713	5600	58
	3	Vap	1875; 1743	2000; 2750	58
	4	Vap	1897; 1721	600; 2500	124
	5	Vap	1890; 1760	600; 2500	124
S	2	C_6H_{12}	*2610; 2450*	34; *25*	41
	3	C_6H_{12}	2750; 2180	30; 600	69
	4	C_6H_{12}	*2400*; 2190	*50*; 800	69
	5	EtOH	*2290*; 2100	180; 1780	56

The oxygen and sulfur heterocycles, in which there are two pairs of lone-pair electrons on the heteroatom, give two absorption bands (Table II). The weaker longer wavelength band is probably due to the promotion of a p lone-pair electron, and the stronger shorter wavelength band to the excitation of an s or sp hybrid lone-pair electron. A p-electron has a higher energy than a corresponding s-electron, and since the σ^* orbital has a larger p- than s-character, $n_s \rightarrow \sigma^*$ transitions are more allowed and give rise to stronger absorption than $n_p \rightarrow \sigma^*$ transitions.

Ethylene oxide gives only the stronger shorter wavelength absorption band (Table II), and it has (150) a higher ionization potential (10.565 ev) than dimethyl ether (10.00 ev). The energy differences between these ionization potentials and between the two longer wavelength bands of the higher cyclic ethers are approximately equal, suggesting that the p lone-pair electrons in ethylene oxide are uniquely stabilized, perhaps by cyclic hyperconjugation with the methylene groups.

The $n \rightarrow \sigma^*$ absorption of piperidine shifts to longer wavelengths in the N-methyl derivative (Table II), owing to the hyperconjugating effect of the methyl group. In acid solution the nitrogen lone-pair elec-

trons become N-H bonding electrons, and the absorption band disappears (146), establishing the $n \rightarrow \sigma^*$ character of the transition involved.

Piperazine, 1,4-dioxane, and 1,4-dithiane absorb at nearly the same wavelength and with approximately twice the intensity as the corresponding monoheteroatom compounds (Table III), indicating that 1,4 interactions in saturated heterocycles are small. However, the cyclic disulfides absorb at a considerably longer wavelength than either the open-chain disulfides or the cyclic sulfides (Tables II and III). In tri-

TABLE III
POLYFUNCTIONAL SATURATED HETEROCYCLES

Compound	Solvent	λ	ε	Reference
Piperazine	Vap	1960	5000	123
1,4-Dioxane	Vap	1800	6000	124
1,4-Dithiane	EtOH	2250	350	56
1,4-Thioxane	EtOH	*2270*; 2090	*100*; 1500	56
Trimethylene disulfide	EtOH	3330	147	14
Tetramethylene disulfide	EtOH	2920	300	14
n-propyl disulfide	EtOH	2520	475	14
1,3-Dithiolane	C_6H_{12}	2470; 2070	367; 1358	33
sym-Trithiane	EtOH	2400	1350	56

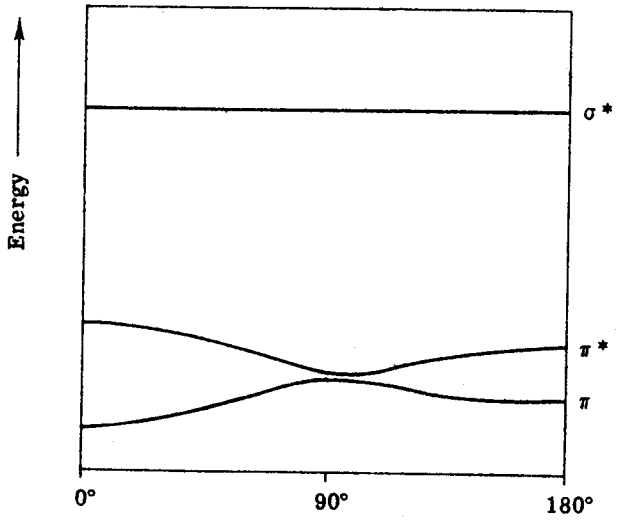


FIG. 5. The relations between the energies of the disulfide lone-pair molecular orbitals and antibonding σ-orbital, and the dihedral angle of the molecule R-S-S-R, where R is an alkyl group or a polymethylene chain.

methylene disulfide the p-electron lone-pair orbitals on the adjacent sulfur atoms overlap (18), giving rise to a bonding and an antibonding lone-pair π-type molecular orbital, both of which are filled with paired electrons (Fig. 5). The center of gravity of the lone-pair molecular orbitals has a higher energy than that of a sulfur atom p-electron lone-pair atomic orbital, and so the open chain disulfides assume a staggered conformation with a dihedral angle of $\sim$90°, the barrier to internal rotation being some 12 kcal/mole (139). The overlap between the lone-pair atomic orbitals is zero in the open-chain disulfides, and it is a maximum, about 0.129 (18) in trimethylene disulfide, but smaller in tetramethylene disulfide, owing to the conformational mobility of the six-membered ring. Transitions are allowed on symmetry grounds to the sulfur-sulfur antibonding σ^* orbital only from the higher energy π^* lone-pair molecular orbital (Fig. 5), accounting for the relative absorption wavelengths of the disulfides (Table III). The absorption spectra of 1,3-dithiolane and *sym*-trithiane suggest the presence of similar but smaller 1,3 interactions between sulfur atoms.

TABLE IV
UNSATURATED HETEROCYCLES WITHOUT CONJUGATION

Compound[a]		Solvent	λ	ε	Reference
[1]		Et_2O	2180	1700	92
[2]	$X = CH_2$	EtOH	3085; 2380	66; 15,400	90
	X = NMe	EtOH	2325	14,100	90
	$X = NMe_2^+$	EtOH	3185; 2290	37; 15,600	90
	X = S	EtOH	2300	16,000	61
	$X = SO_2$	EtOH	2290	14,800	61
	$X = SMe^+$	EtOH	2220	20,000	61
[5]	$X = CH_2$	EtOH	2830	14	93
	X = NMe	Et_2O	2250	6300	94
	X = O	EtOH	2720	16	93
	X = S	C_6H_{12}	2260	2450	93
		H_2O	2420	2780	93
[7]	$X = CH_2$	C_6H_{12}	5080; 2800	38; 15	138
	X = NCOMe	C_6H_{12}	5200; 3030	40; 80	138
	X = NH	C_6H_{12}	5500; 2800	40; 120	138
	X = O	C_6H_{12}	5620; 2800	40; 360	138
[8]		MeOH	3710; 2680	58; 260	19
[9]	$n = 2$	$CHCl_3$	3870; 2870	780; 3100	36
	$n = 3$	$CHCl_3$	3900	127	119
	$n = 4$	$CHCl_3$	3680	45	119
[10]		EtOH	3365	130	37
[11]		$CHCl_3$	3590	47	119

[a] In all tables numbers within brackets refer to structural formulas.

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