1 hr., the reaction mixture was cooled and ice water cautiously added. The reaction mixture was extracted with ether and the ethereal extracts were washed with cold dilute hydrochloric acid and a saturated solution of sodium bicarbonate, dried, and concentrated *in vacuo*. The resulting crystalline product, 180 mg., was recrystallized from acetone to yield 135 mg. of V, m.p. 102–104°, $[\alpha]^{22}_{D}$ −168 (*c*, 2), λ^{EtOH}_{max} 249 mμ, log ε 4.22.

Anal. Calcd. for $C_{29}H_{48}$: C, 87.80; H, 12.20. Found: C, 88.10; H, 12.33.

PRINCETON, N. J.

[CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, MASSACHUSETTS INSTITUTE OF TECHNOLOGY]

Labor-saving Procedures for Calculating Wave Functions for Molecules with Axes of Symmetry

C. GARDNER SWAIN AND WALTER R. THORSON

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Detailed procedures are given for calculating the first approximation LCAO-MO energies and wave functions for the π-electrons of molecules with *n* conjugated atoms and a two- or k-fold axis of rotation.

Organic chemists make increasing use of approximate calculations of resonance energy, charge distribution, bond order, force constant, free valence and localization energy (Dewar reactivity number) in correlating and predicting structures and reactivities of unsaturated systems.[1] General procedures have been described for evaluating these quantities for the π-electrons of any molecule with *n* conjugated atoms using the first-approximation LCAO-MO method.[2] These generally call for solution of an $n \times n$ determinant. When *n* is large, as in triphenylmethyl, the work involved becomes prohibitive unless a digital computer is employed. However, the work can be appreciably reduced whenever the molecule has a two- or *k*-fold axis of rotation by replacing the $n \times n$ determinant by two or more smaller determinants. This can be done by choosing trial wave functions belonging to families of different basic symmetry (Γ-types) so that no two from different families will have any resonance integrals (*i.e.*, off-diagonal elements between them in a secular determinant involving them as trial functions). Then only trial functions of the same family can interact with one another. Rules for choosing trial functions belonging to different families are given below for several kinds of molecular symmetry. Benzene will be used as an illustration in each section because it has each of these kinds of symmetry. Although the derived molecular wave functions may depend on the approach, the energies, charges, bond orders, and free valences do not. These useful procedures may be familiar or obvious to many physical chemists, but the authors know of no single source where one may find them described concisely for the cases of interest to organic chemists.

Two-fold axis. Ethylene, propene, butadiene, benzene, phenanthrene, pentadienyl, and benzyl radicals all have a two-fold axis for their π-electrons. Number all conjugated atoms of the molecule and tabulate them in a vertical column. Beside each in an adjacent column write the number of the atom it becomes after a 180° rotation about the two-fold axis. For minimum size determinants, choose the axis so that as many numbers change as possible. Now use the character table

Determinant	E	C_2^x	Family
D_1	1	1	Γ_1
D_2	1	−1	Γ_2

to generate trial wave functions ψ_1, ψ_2... for use in each determinant *D* by taking "dot products" of the *E*, C_2^x characters by the atomic wave functions corresponding to the pairs of numbers thus tabulated (see first example, which illustrates this process). Normalize each of these trial functions by dividing through by the sum of the squares of the coefficients. For each determinant *D*

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(1) R. J. Windgassen, Jr., W. H. Saunders, Jr., and V. Boekelheide, *J. Am. Chem. Soc.*, **81**, 1459 (1959); R. Breslow and C. Yuan, *J. Am. Chem. Soc.*, **80**, 5991 (1958); R. Breslow, R. Haynie, and J. Mirra, *J. Am. Chem. Soc.*, **81**, 247 (1959); F. Sondheimer and R. Wolovsky, *J. Am. Chem. Soc.*, **81**, 1771 (1959); J. H. Richards, Abstracts of Papers, 135th ACS meeting, Boston, Mass., April 5–10, 1959, p. 86-O; A. Streitwieser, Jr., and P. M. Nair, *Tetrahedron*, **5**, 149 (1959); M. M. Kreevoy, *Tetrahedron*, **2**, 354 (1958); M. J. S. Dewar, *Record Chem. Progr.* (Kresge-Hooker Sci. Lib.), **19**, 1 (1958); D. R. Augood and G. H. Williams, *Chem. Revs.*, **57**, 123 (1957); D. Peters, *J. Chem. Soc.*, 2654 (1957); E. Heilbronner, *Helv. Chim. Acta*, **37**, 913 (1954); F. L. J. Sixma, *Rec. trav. chim.*, **72**, 673 (1953); J. D. Roberts and D. A. Semenow, *J. Am. Chem. Soc.*, **77**, 3152 (1955); A. Streitwieser, Jr., *J. Am. Chem. Soc.*, **74**, 5288 (1952); J. D. Roberts, A. Streitwieser, Jr., and C. M. Regan, *J. Am. Chem. Soc.*, **74**, 4579 (1952).

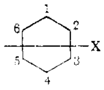
(2) C. A. Coulson and H. C. Longuet-Higgins, *Proc. Roy. Soc.* (*London*), **A191**, 39 (1947); **A192**, 16 (1948); **A193**, 447, 456 (1948); **A195**, 188 (1948); H. C. Longuet-Higgins, *J. Chem. Phys.*, **18**, 265, 275, 283 (1950); R. D. Brown, *Quart. Revs.*, **6**, 63 (1952); M. J. S. Dewar, *Progr. Org. Chem.*, **2**, 1 (1953); H. C. Longuet-Higgins, *Proc. Chem. Soc.*, 157 (1957).

$$\begin{vmatrix} H_{11} - E & H_{12} & \cdots \\ H_{21} & H_{22} - E & \cdots \\ \cdot & \cdot & \cdots \\ \cdot & \cdot & \cdots \\ \cdot & \cdot & \cdots \end{vmatrix} = 0$$

each $H_{\cdot nj} = \int \psi_m H \psi_j \mathrm{d}v$ is evaluated by expanding it in terms of atomic orbitals and setting each $\int \phi_r H \phi_s \mathrm{d}v$ equal to α when $r = s$, to β when atom r is adjacent to atom s, and to zero when it is not adjacent. Replace $\alpha - E$ by x (standing for $-\epsilon$) and β by 1 and solve each determinant for x to get $-\epsilon$ values in units of β. Substitute each value of x back into the simultaneous linear equations in $c_1, c_2 \ldots$ corresponding to the determinant from which it was derived, and solve for $c_1, c_2 \ldots$ (the coefficients of the trial functions in that molecular orbital). Expand each molecular orbital wave function in terms of the atomic orbitals and normalize.

In this first approximation overlap integrals are neglected. The coulomb integral α is the energy of a π-electron localized in a p atomic orgital of one atom. The resonance integral β is the change in energy when a π-bond is formed, and is approximately -18 kcal. for a π-bond between adjacent carbons separated by the bond distance in benzene. The binding energy ϵ is a positive multiple of β for bonding orbitals, and therefore also a negative quantity.

Example: benzene



E	C_2^x
1	4
2	3
3	2
4	1
5	6
6	5

The solution involves two 3 × 3 determinants. D_1, the first of these, is set up and solved as follows:

Unnormalized	Normalized
$\psi_1 = \phi_1 + \phi_4$	$\psi_1 = (1/\sqrt{2})(\phi_1 + \phi_4)$
$\psi_2 = \phi_2 + \phi_3$	$\psi_2 = (1/\sqrt{2})(\phi_2 + \phi_3)$
$\psi_3 = \phi_5 + \phi_6$	$\psi_3 = (1/\sqrt{2})(\phi_5 + \phi_6)$

Other combinations are duplicates of these.

$$H_{11} = \int \psi_1 H \psi_1 \mathrm{d}v = {}^1/_2(\int \phi_1 H \phi_1 \mathrm{d}v + 2\int \phi_1 H \phi_4 \mathrm{d}v + \int \phi_4 H \phi_4 \mathrm{d}v)$$
$$= {}^1/_2(\alpha + 0 + \alpha) = \alpha$$
$$H_{12} = {}^1/_2(\int \phi_1 H \phi_2 \mathrm{d}v + \int \phi_1 H \phi_3 \mathrm{d}v + \int \phi_4 H \phi_2 \mathrm{d}v + \int \phi_4 H \phi_3 \mathrm{d}v)$$
$$= {}^1/_2(\beta + 0 + 0 + \beta) = \beta = H_{21}$$
$$H_{13} = {}^1/_2(0 + \beta + \beta + 0) = \beta = H_{31}$$
$$H_{22} = {}^1/_2(\alpha + \beta + \beta + \alpha) = \alpha + \beta = H_{33}$$
$$H_{23} = {}^1/_2(0 + 0 + 0 + 0) = 0 = H_{32}$$

$$\begin{vmatrix} x & 1 & 1 \\ 1 & x+1 & 0 \\ 1 & 0 & x+1 \end{vmatrix} = 0 \qquad \begin{pmatrix} xc_1 + c_2 + c_3 = 0 \\ c_1 + (x+1)c_2 = 0 \\ c_1 + (x+1)c_3 = 0 \end{pmatrix}$$

$$x(x+1)(x+1) - (x+1) - (x+1) = 0$$
$$x^3 + 2x^2 - x - 2 = 0$$

Plotting shows that $x = +1$ is one root. Long division by $(x - 1)$ gives $x^2 + 3x + 2 = 0$ for the rest, hence $x = {}^1/_2(-3 \pm \sqrt{9-8}) = +1, -1, -2$. If $x = +1$, $\epsilon = -\beta$; the three equations are $c_1 + c_2 + c_3 = 0$, $c_1 + 2c_2 = 0$, $c_1 + 2c_3 = 0$; therefore $c_2 = c_3 = -{}^1/_2c_1$; $\psi = c_1(\psi_1 - {}^1/_2\psi_2 - {}^1/_2\psi_3) = (1/\sqrt{12})(2\phi_1 - \phi_2 - \phi_3 + 2\phi_4 - \phi_5 - \phi_6)$. Thus three of the roots are

$$x = +1, \epsilon = -\beta, \quad \Psi = (1/\sqrt{12})(2\phi_1 - \phi_2 - \phi_3 + 2\phi_4 - \phi_5 - \phi_6)$$
$$x = -1, \epsilon = \beta, \quad \Psi = {}^1/_2(\phi_2 + \phi_3 - \phi_5 - \phi_6)$$
$$x = -2, \epsilon = +2\beta, \Psi = (1/\sqrt{6})(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \phi_6)$$

D_2, the other determinant, supplies the three remaining roots.

$$\psi_1 = (1/\sqrt{2})(\phi_1 - \phi_4)$$
$$\psi_2 = (1/\sqrt{2})(\phi_2 - \phi_3)$$
$$\psi_3 = (1/\sqrt{2})(\phi_5 - \phi_6)$$

Other conditions are equivalent to these.

$$\begin{vmatrix} x & 1 & -1 \\ 1 & x-1 & 0 \\ -1 & 0 & x-1 \end{vmatrix} = 0$$

$$x = +1, \epsilon = -\beta, \quad \Psi = {}^1/_2(\phi_2 - \phi_3 + \phi_5 - \phi_6)$$
$$x = -1, \epsilon = +\beta, \quad \Psi = (1/\sqrt{12})(2\phi_1 + \phi_2 - \phi_3 - 2\phi_4 - \phi_5 + \phi_6)$$
$$x = +2, \epsilon = -2\beta, \Psi = (1/\sqrt{6})(\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6)$$

Linear conjugated polyenes $H(CH)_nH$ have roots calculable alternatively from

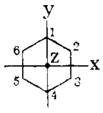
$$\epsilon_j = 2\beta \cos\left(\frac{\pi j}{n+1}\right), j = 1, 2, \ldots n$$

$$\Psi_j = \sum_r \left[\sqrt{\frac{2}{n+1}} \sin\left(\frac{\pi j r}{n+1}\right)\right] \phi_r$$

Three two-fold axes at 90°. Cyclobutadiene, benzene, stilbene, and anthracene all have this symmetry. Proceed as for one two-fold axis except consider 180° rotations about all three axes and use the character table

Determinant	E	C_2^x	C_2^y	C_2^z	Family
D_1	1	1	1	1	Γ_1
D_2	1	1	−1	−1	Γ_2
D_3	1	−1	1	−1	Γ_3
D_4	1	−1	−1	1	Γ_4

Example: benzene



E	C_2^x	C_2^y	C_2^z
1	4	1	4
2	3	6	5
3	2	5	6
4	1	4	1
5	6	3	2
6	5	2	3

The solution involves two 2 × 2 determinants and two 1 × 1 determinants.

$$D_1:\ \psi_1 = (1/\sqrt{2})(\phi_1 + \phi_4) \qquad H_{11} = \alpha$$

$$\psi_2 = {}^1/_2(\phi_2 + \phi_3 + \phi_5 + \phi_6) \qquad H_{12} = \sqrt{2}\beta = H_{21}$$

$$H_{22} = \alpha + \beta$$

$$\begin{vmatrix} x & \sqrt{2} \\ \sqrt{2} & x+1 \end{vmatrix} = 0$$

$$x = +1, \quad \epsilon = -\beta, \quad \Psi = (1/\sqrt{12})(2\phi_1 + \phi_2 + \phi_3 + 2\phi_4 + \phi_5 + \phi_6)$$

$$x = -2, \quad \epsilon = 2\beta, \quad \Psi = (1/\sqrt{6})(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \phi_6)$$

$$D_2:\ \psi_1 = {}^1/_2(\phi_2 + \phi_3 - \phi_5 - \phi_6) = \Psi$$

$$H_{11} = \alpha + \beta,\ \epsilon = +\beta$$

$$D_3:\ \psi_1 = (1/\sqrt{2})(\phi_1 - \phi_4)$$

$$\psi_2 = {}^1/_2(\phi_2 - \phi_3 - \phi_5 + \phi_6)$$

$$\begin{vmatrix} x & \sqrt{2} \\ \sqrt{2} & x-1 \end{vmatrix} = 0$$

$$x = +2, \quad \epsilon = -2\beta, \quad \Psi = (1/\sqrt{6})(\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6)$$

$$x = -1, \quad \epsilon = \beta, \quad \Psi = (1/\sqrt{12})(2\phi_1 + \phi_2 - \phi_3 - 2\phi_4 - \phi_5 + \phi_6)$$

$$D_4:\ \psi_1 = {}^1/_2(\phi_2 - \phi_3 + \phi_5 - \phi_6) = \Psi$$

$$H_{11} = \alpha - \beta, \quad \epsilon = -\beta$$

A k-fold axis. Benzene, 1,3,5-trivinylbenzene, cyclopropenyl, and triphenylmethyl radicals all have a three-fold axis for their π-electrons. Benzene and toluene have six-fold axes for their π-electrons. Tropilium ion has a seven-fold axis. Number all conjugated atoms. Generate as many trial functions as atoms (n). For each atom e on the axis (e.g., the central carbon of triphenylmethyl), use one trial function of the form

$$\psi = \phi_e$$

When there is a k-fold axis, for each group of k equivalent atoms f, g, h, . . . (*e.g.*, the 3 p-carbons of triphenylmethyl or the 6 of benzene), use k trial functions of the form

$$\psi = (1/\sqrt{k})(\phi_f + \phi_g + \phi_h + \ldots) \qquad \Gamma_1$$

$$\psi = (1/\sqrt{k})(\omega^1\phi_f + \omega^2\phi_g + \omega^3\phi_h + \ldots) \qquad \Gamma_3$$

$$\psi = (1/\sqrt{k})(\omega^{-1}\phi_f + \omega^{-2}\phi_g + \omega^{-3}\phi_h + \ldots) \qquad \Gamma_3$$

$$\psi = (1/\sqrt{k})(\omega^2\phi_f + \omega^4\phi_g + \omega^6\phi_h + \ldots) \qquad \Gamma_3$$

$$\psi = (1/\sqrt{k})(\omega^{-2}\phi_f + \omega^{-4}\phi_g + \omega^{-6}\phi_h + \ldots) \qquad \Gamma_3$$

$$\cdots\cdots$$

$$\cdots\cdots$$

$$\psi = (1/\sqrt{k})(\phi_f - \phi_g + \phi_h - \ldots) \qquad \Gamma_2$$

where $\omega = e^{2\pi i/k}$ and $i = \sqrt{-1}$. Note that the Γ_3 trial functions occur always as degenerate pairs (complex and complex conjugate). The Γ_2 orbital is missing if k is odd. Only the first 3 apply if k is 3.

When k is 3 but cannot be 6, for each group of 6 equivalent atoms o, p, q, r, s, t (e.g., the 6 o-carbons of triphenylmethyl), use the 6 trial functions

$$\psi = (1/\sqrt{6})(\phi_o + \phi_p + \phi_q + \phi_r + \phi_s + \phi_t) \qquad \Gamma_1$$

$$\psi = (1/\sqrt{6})[\omega^1(\phi_o + \phi_p) + \omega^2(\phi_q + \phi_r) + \omega^3(\phi_s + \phi_t)] \qquad \Gamma_3$$

$$\psi = (1/\sqrt{6})[\omega^{-1}(\phi_o + \phi_p) + \omega^{-2}(\phi_q + \phi_r) + \omega^{-3}(\phi_s + \phi_t)] \qquad \Gamma_3$$

$$\psi = (1/\sqrt{6})[\omega^1(\phi_o - \phi_p) + \omega^2(\phi_q - \phi_r) + \omega^3(\phi_s - \phi_t)] \qquad \Gamma_3$$

$$\psi = (1/\sqrt{6})[\omega^{-1}(\phi_o - \phi_p) + \omega^{-2}(\phi_q - \phi_r) + \omega^{-3}(\phi_s - \phi_t)] \qquad \Gamma_3$$

$$\psi = (1/\sqrt{6})(\phi_o - \phi_p + \phi_q - \phi_r + \phi_s - \phi_t) \qquad \Gamma_2$$

All trial functions of a given family are combined in one determinant and solved for energies and molecular orbital wave functions by expanding each H_{mj} in terms of atomic orbitals using the rules given before. If trial functions of all three families (Γ_1, Γ_2, and Γ_3) have been generated, there will therefore be three determinants. The family designations used in this section (k-fold axis) have nothing in common with the same designations in other sections.

Monocyclic polyenes $(CH)_n$ (*e.g.*, benzene, cyclopropenyl radical, or tropilium ion) have all conjugated atoms equivalent. For monocyclic polyenes, the trial wave functions are the final molecular orbital wave functions directly.

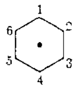
$$\epsilon_j = 2\beta \cos\left(\frac{2\pi j}{n}\right), j = 0, 1, \ldots n - 1$$

$$\Psi_j = \sum_r \left[\frac{1}{\sqrt{n}}\, e^{i2\pi jr/n}\right] \phi_r$$

Because the Γ_3 trial functions are chosen as complex conjugate pairs ψ, ψ^*, it happens that their determinant reduces to two noninteracting determinants with the same roots, so that only one needs to be solved. Let $H_{11} = \int \psi_1^* H\psi_1 dv$, $H_{12} = \int \psi_1^* H\psi_2 dv$, $H_{21} = \int \psi_2^* H\psi_1 dv$, ... Whenever the off-diagonal elements are complex (involve i), $H_{jm} = H_{mj}^*$, where * means complex conjugate (i replaced by $-i$). The ϵ values obtained are then each doubly degenerate, with corresponding complex conjugate molecular orbital wave functions for the other roots (from the other determinant). For triphenylmethyl a 19 × 19 determinant is thus replaced by one 5 × 5 (Γ_1), one 2 × 2 (Γ_2), and one 6 × 6 (Γ_3) determinant (since the other 6 × 6 (Γ_3) determinant need not be solved).

The rules for evaluating imaginary exponentials are as follows: $e^{ix} = \cos x + i \sin x$; $e^{-ix} = \cos x - i \sin x$; $e^{i(2\pi + x)} = e^{ix}$; $e^{i(2\pi - x)} = e^{-ix}$; $e^{ix} + e^{-ix} = 2 \cos x$. For example, $e^{2\pi i/3} + e^{4\pi i/3} = e^{2\pi i/3} + e^{-2\pi i/3} = 2 \cos (2\pi/3) = -1$. Imaginary parts will all vanish when energies or charges are computed.

Example: benzene



The highest symmetry axis is 6-fold. There are 6 equivalent atoms. Hence the molecular orbital wave functions are

$$\Psi = (1/\sqrt{6})(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \psi_6) \qquad \epsilon = 2\beta$$

$$\Psi = (1/\sqrt{6})(e^{\pi i/3}\phi_1 + e^{2\pi i/3}\phi_2 + e^{\pi i}\phi_3 + e^{-2\pi i/3}\phi_4 + e^{-\pi i/3}\phi_5 + \phi_6) \quad \epsilon = \beta$$

$$\Psi = (1/\sqrt{6})(e^{-\pi i/3}\phi_1 + e^{-2\pi i/3}\phi_2 + e^{-\pi i}\phi_3 + e^{2\pi i/3}\phi_4 + e^{\pi i/3}\phi_5 + \phi_6) \quad \epsilon = \beta$$

$$\Psi = (1/\sqrt{6})[e^{2\pi i/3}(\phi_1 + \phi_4) + e^{-2\pi i/3}(\phi_2 + \phi_5) + (\phi_3 + \phi_6)] \quad \epsilon = -\beta$$

$$\Psi = (1/\sqrt{6})[e^{-2\pi i/3}(\phi_1 + \phi_4) + e^{2\pi i/3}(\phi_2 + \phi_5) + (\phi_3 + \phi_6)] \quad \epsilon = -\beta$$

$$\Psi = (1/\sqrt{6})(\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6) \qquad \epsilon = -2\beta$$

Quantities derivable from wave functions. From the normalized molecular orbital wave functions

$$\Psi_j = a_1\phi_1 + a_2\phi_2 + \ldots a_n\,\phi_n,\ j = 1, 2, \ldots n$$

and the number of electrons ν_j in each molecular orbital j, one may calculate in the usual way the total energy of the π-electrons:

$$E = \sum \nu_j(\epsilon_j + \alpha) = \sum_j \nu_j \int (\Psi_j H \Psi_j \mathrm{d}v)$$

the resonance (delocalization) energy relative to a localized structure with d double bonds:

$$\text{R.E.} = \sum_j \nu_j\epsilon_j - d(2\beta)$$

the π-electron density q_r or the net positive charge Q_r on any atom r:

$$q_r = \sum_j \nu_j a_{jr}^2 = 1 - Q_r$$

the π-bond order p_{rs} or the total bond order N_{rs} of the bond between atoms r and s:

$$p_{rs} = \sum_j \nu_j a_{jr} a_{js} = N_{rs} - (\text{No. of } \sigma\text{-bonds})$$

and the free valence on any atom:

$$F_r = 4.732 - \sum_s N_{rs}$$

CAMBRIDGE 39, MASS.

[RESEARCH LABORATORY OF RESOURCES UTILIZATION, TOKYO INSTITUTE OF TECHNOLOGY]

Isomerization of *N*-Substituted Glycidyl Carbamates

YOSHIO IWAKURA AND YASUO TANEDA

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Glycidyl aryl- or alkylcarbamate undergoes a pyrolytic rearrangement to give 3-aryl- or alkyl-5-hydroxytetrahydro-1,3-oxazine-2-one in good yields.

In connection with a research on the addition reaction of glycidyl *N*-aryl- or alkylcarbamates, it happened that they thermally isomerized to give *N*-substituted 5-hydroxytetrahydro-1,3-oxazine-2-one (*N*-substituted 5-hydroxy-2-pentoxazolidone). On the isomerization of three- membered ring compounds, it was reported that *N*-acyl-[1,2] or *N*-phenylthiocarbamyl ethyleneimine[3] and their derivatives[4] underwent a rearrangement to give 2-substituted oxazoline-2 or thiazoline-2. No literature was found, however, on the ring expansion of *N*-substituted glycidyl carbamates. In the first place from the reactivity of epoxy ring to imino group, it is considered that the isomerization of glycidyl carbamate to substituted tetrahydro-1,3-oxazine-2-one will be caused by intramolecular addition reaction of epoxy ring to urethane linkage.

To confirm the structure of isomers, isomerization of glycidyl phenylcarbamate and some of the alkylcarbamates prepared from phenyl or alkyl isocyanate and glycidol were studied in detail.

When glycidyl phenylcarbamate (I) was heated without solvent in a test tube at 125° for 1 hr., crystalline II was obtained in 95% yield, the molecular weight and microanalysis of which were found to be similar to those of I. Phenyl isocyanate or acetic anhydride reacts with II to give phenylcarbamate (III) or acetate (IV) of II. II was also obtained from 1-chloro-2-hydroxy-3-phenylcarbamyloxypropane (V), prepared from I and hydrogen chloride.[5] This confirms II to be 3-phenyl-5-hydroxytetrahydro - 1,3 - oxazine - 2 - one. From 1-chloro - 2,3 - bis(phenylcarbamyloxy)propane (VI), 3 - phenyl - 5 - phenylcarbamyloxymethyl- 2 - oxazolidone (VII) was obtained without forming III. This might be because of the fact that five-membered cyclic urethane was more stable and easier to form than six membered one.[6-8] An attempt to obtain IV from 1-chloro-2-acetoxy-3-phenylcarbamyloxypropane by ring closure with sodium methoxide, gave unexpectedly 10% yield of II and 90% yield of oily polymeric substance.

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