

[CONTRIBUTION FROM THE DEPARTMENT OF PHARMACEUTICAL CHEMISTRY, SCHOOL OF PHARMACY, UNIVERSITY OF CALIFORNIA, SAN FRANCISCO MEDICAL CENTER, SAN FRANCISCO, CALIF.]

## The Dipole Moment and Structure of the Imide Group. I. Five- and Six-membered Cyclic Imides

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The free imide group could be present in three conformations, namely, *cis-cis*-I, *cis-trans*-II or *trans-trans*-III. Calculations indicate moments would increase I < II < III. The determination of the dipole moments of six-membered cyclic imides, in which the only possible conformation is the *cis-cis*, gives values of 2.6–2.9 D. The five-membered ring imides have lower dipole moments of 1.5–2.2 D., as the angle between the carbonyl groups is greater and the resultant of the N<sup>+</sup>O<sup>-</sup> contributions are opposed to the resultant of the carbonyl dipoles. The effect of replacing >N-H by >N-CH<sub>3</sub> on dipole moments, ultraviolet and infrared spectra is discussed.

### Introduction

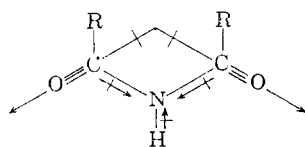
One would expect the free imide group  $\text{O}=\text{C}-\text{N}-\text{C}=\text{O}$  to be present in three different conformations (Fig. 1). These conformations are named for the position of the carbonyl groups, relative to the group on the nitrogen, as the *cis-cis*-I, the *cis-trans*-II and the *trans-trans*-III. Because of resonance the group is essentially planar facilitating our calculations. We have studied the dipole moments, ultraviolet and infrared spectra of cyclic, semi-cyclic, straight chain and aromatic imides to see which of the conformations are favored in each case.

The *cis-cis* conformation I would be expected to be the favored conformation when R is small as the carbonyl groups are farthest apart (about 5.6 Å. measured from the centers of Stuart-Briegleb models), and electrostatic repulsion least. One may try to predict the relative magnitudes of the imide moments in the three conformations, but the use of bond moments for quantitative determination is risky due to resonance and inductive effects. The three dipoles to be considered are the

$\text{>C}=\text{O}$  dipole, the C-N dipole and the H-N dipole.

If we take all angles to be 120°, the C-N resultant is in the same direction as the carbonyl resultant

with the H-N dipole 180° to the two resultants. Smyth<sup>1</sup> gives values of 0.2 and 1.3 D. as the bond



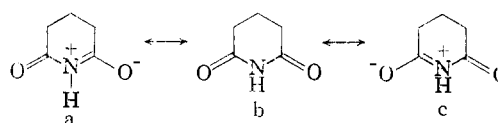
*cis-cis*-I

moments for C-N and H-N, respectively. Popov

and Holm<sup>2</sup> suggest that the H-N moment is 0.7

D. and the C-N moment 0.3 D. One would expect the H-N bond moment to be less than in methylamine<sup>1</sup> because the normal imide resonance (a ↔

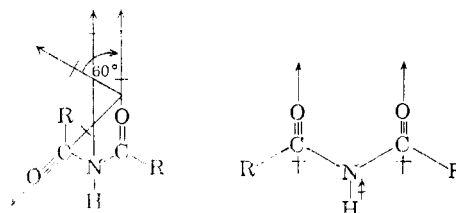
b ↔ c) places a plus charge on the nitrogen. In any case, the H-N moment is greater than the



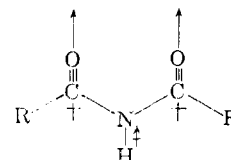
resultant and the difference is 180° from the carbonyl resultant. In the *cis-cis* and *cis-trans* conformations, the carbonyl resultant is equal to one carbonyl bond moment since the two carbonyl groups make an angle of 120° with each other. One would predict a low moment for the *cis-cis* conformation because the two resultants are subtracted from each other. Furthermore, the additional contribution to the moment from the usual imide resonance (a ↔ b ↔ c) is not present because the N<sup>+</sup>O<sup>-</sup> dipoles are 180° to each other. Both considerations lead to a prediction that the *cis-cis* conformation would have a low dipole moment.

If R is large, the *cis-trans* conformation II is favored. There is little interference here between the R groups and the distance between the carbonyl groups is about 4.8 Å. The difference between the

C-N resultant and the H-N dipole makes an angle of 60° with the carbonyl resultant. Normal imide resonance would tend to increase the moment. Thus the *cis-trans* conformation would be expected to have a higher moment than the *cis-cis* conformation as both resultants and the N<sup>+</sup>O<sup>-</sup> dipoles are in the same direction.



*cis-trans*-II



*trans-trans*-III

From the point of view of electrostatic repulsion, the *trans-trans* conformation III is the least

(1) C. P. Smyth, "Dielectric Behavior and Structure," McGraw-Hill Book Co., Inc., New York, N. Y., 1955, pp. 244, 311.

(2) A. Popov and R. D. Holm, *J. Phys. Chem.*, **65**, 774 (1961).

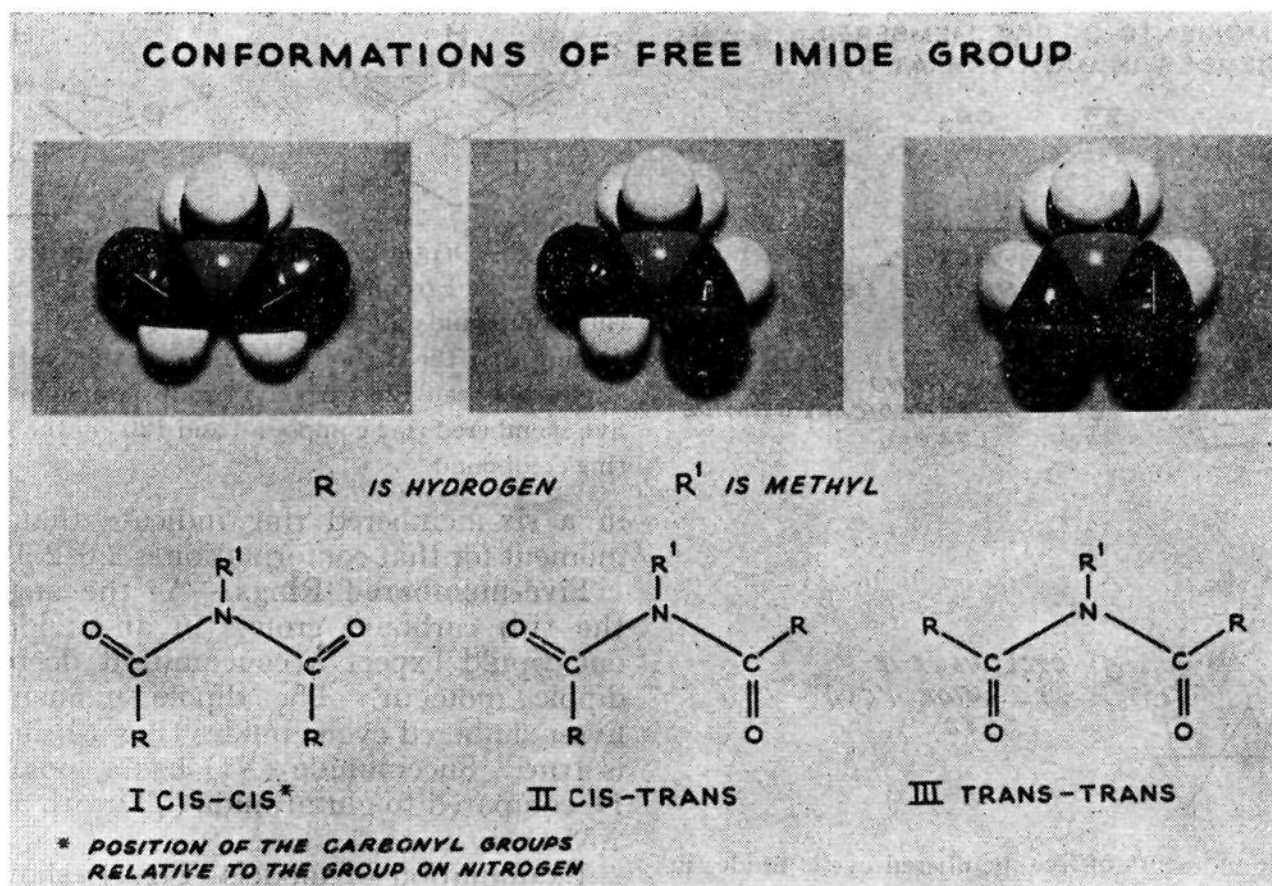


Fig. 1.—Conformation of the free imide group.

avored. The distance between the centers of the carbonyl groups is about 2.5 Å. and one can see (Fig. 1) that the groups are almost touching. Since the two carbonyl dipoles are almost parallel and in the same direction, they add up and their contribution would be twice the bond moment of the carbonyl group. The difference between the

$$\begin{array}{c} \text{N} \\ \diagup \quad \diagdown \\ \text{C} \quad \text{C} \end{array} \quad \begin{array}{c} + \\ \rightarrow \end{array}$$
 resultant and the H-N moment and the resultant of the N<sup>+</sup>O<sup>-</sup> dipoles are also in the same direction so one would predict a high moment for this conformation.

From the preceding considerations, one may predict that the dipole moments of the three possible conformations of imides would increase in the order *cis-cis* < *cis-trans* < *trans-trans*.

### Results and Discussion

**Six-membered Rings.**—In cyclic imides with five- and six-membered rings, only the *cis-cis* conformation I is permitted. Figure 2 shows the dipole moment of the six-membered ring compounds is, as expected, lower than that of the usual amide moment of 3.8 D. In cyclohexane-1,3-imide (IV), the imide group is attached to two axial positions and is rigidly held.

Glutarimide (VI) and N-methylglutarimide (VII) have slightly lower dipole moments, 2.58 and 2.70 D., respectively, than the more rigidly held cyclohexane-1,3-imides. The greater flexibility of this setting allows the bond angles to become greater and the moment slightly lower. (Between two dipoles each of 3.8 D., a difference of only 5° changes the dipole moment by 0.3 D.)

Bemegrade, a CNS stimulant, has about the same dipole moment as the cyclohexane-1,3-imides, 2.92 D. The inductive effect of the methyl and ethyl groups serves to increase the dipole moment over that of the unsubstituted glutarimide (2.92 com-

### DIPOLE MOMENTS OF SIX MEMBERED CYCLIC IMIDES IN DIOXANE AT 30°

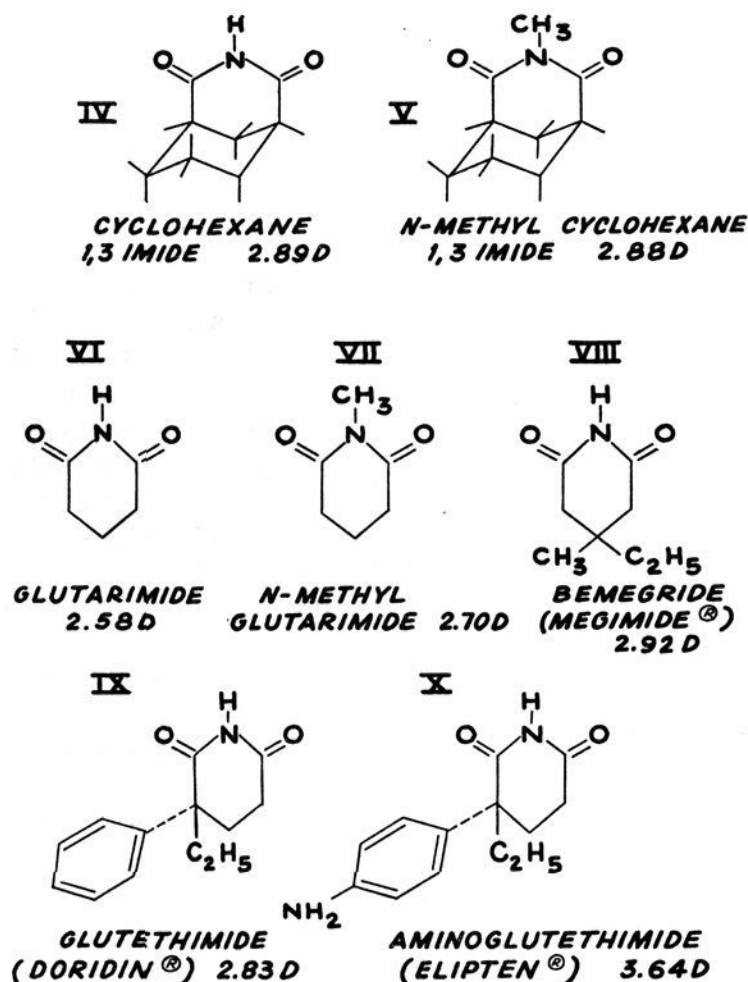


Fig. 2.—Dipole moments of six-membered cyclic imides in dioxane at 30°.

pared with 2.58 D.). Popov and Holm<sup>2</sup> recently measured the moment of bemegrade in benzene at 25° and obtained a value of 2.84 D.

Glutethimide (IX), a CNS depressant, shows a slight increase (0.2 D.) due to both the inductive effect of the ethyl group and the resonance effect of the phenyl group. The insertion of an amino group into the benzene ring in aminoglutethimide

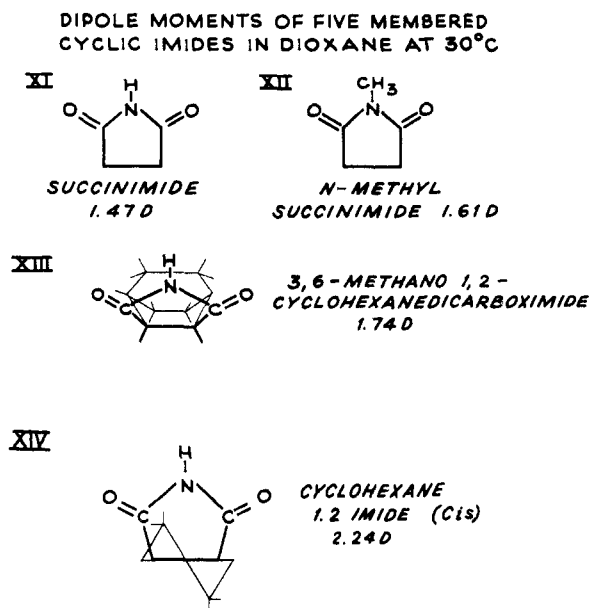
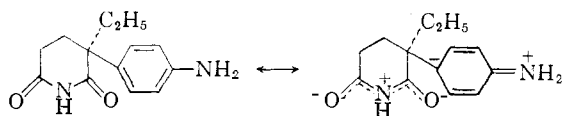


Fig. 3.—Dipole moments of five-membered cyclic imides in dioxane at 30°.

(X) greatly increases the resonance effect. As the benzene ring is in the quasi-equatorial position, the additional moment adds to the original resultant.



The angle between the *p*-aminophenyl groups and the resultant *cis-cis* dipole is about 120°. The dipole moment of aniline is 1.5 D., and using the moment of glutarimide (VI), 2.58 D., one calculates a moment of 3.56 D. for aminoglutethimide. This is a good approximation to the experimental value 3.64 D. and one would expect the value to be higher due to the inductive effect of the ethyl group. Using the moment of glutethimide (IX), 2.83 D., one calculates a dipole moment of 3.83 D. for aminoglutethimide.

The ultraviolet spectra of cyclohexane-1,3-imide (IV), glutarimide (VI), bemegride (VIII) and glutethimide (IX) show a sharp peak between 203 and 206  $m\mu$  (Table I) with extinctions of 11,000 to 15,000. Glutethimide (IX) shows the usual imide absorption at 206  $m\mu$ ,  $\epsilon$  17,700, and the benzene fine structure between 250 and 260  $m\mu$ . Aminoglutethimide has a broad band at 244  $m\mu$ ,  $\epsilon$  11,600, and one low band at 292  $m\mu$ ,  $\epsilon$  1800, quite different from glutethimide itself. The same solution plus acid shows a marked change with the usual sharp imide peak at 206  $m\mu$ ,  $\epsilon$  17,700, and the benzene fine structure between 250 and 260  $m\mu$ . In the salt form, the amino group cannot resonate with the benzene ring and the spectrum is that of the imide group and the benzene ring.<sup>3</sup>

The five examples (IV - VIII) we have examined where the imide is locked in the *cis-cis* conformation

(3) W. D. Kumler and L. A. Strait, *J. Am. Chem. Soc.*, **65**, 2349 (1943).

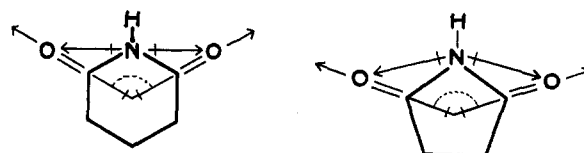


Fig. 4.—Diagram illustrating the difference in the angle between the carbonyl groups in the five- and six-membered ring compounds and the position of the N<sup>+</sup>O<sup>-</sup>dipoles. Assuming that the carbonyl groups and the N-H are flat, the angles between the carbonyl groups would be 154° in the five-membered ring compound and 120° in the six-membered ring compound.

in a six-membered ring indicate that the dipole moment for that conformation is 2.6–2.9 D.

**Five-membered Rings.**—As the angle between the two carbonyl groups in an amide increases, one would expect a concomitant decrease in the dipole moment. The dipole moments for the five-membered cyclic imides (Fig. 3) show that this is true. Succinimide (XI) has a moment of 1.47 D. compared to glutarimide (VI) with a moment of 2.58 D.<sup>4</sup>

Examination of models (Fig. 4) shows that the angle between the carbonyl groups in the five-

TABLE I  
ULTRAVIOLET, INFRARED SPECTRA AND SOURCES OF FIVE-  
AND SIX-MEMBERED RING IMIDES

Compound	U.v. spectra in ethanol		Carbonyl band, KBr, cm. <sup>-1</sup>	Source
	$\lambda_{max}$ , $m\mu$	$\epsilon$		
IV Cyclohexane-1,3- imide ( <i>cis</i> )	206	14,000	1701	<i>a, b</i>
V Cyclohexane-N- methyl-1,3- imide ( <i>cis</i> )	212	15,000	1724, 1672	<i>a, b</i>
VI Glutarimide	204	14,700	1695, (1661) <sup>d</sup>	<i>a</i>
VII N-Methyl- glutarimide	210	15,600	1721, 1667	<i>a, c</i>
VIII Bemegride	203?	15,400	1718, 1667	<i>d</i>
IX Glutethimide	206	11,600	1718, 1691	<i>e</i>
	252	390		
	258	430		
	263	330		
X Aminogluteth- imide	244	11,600	(1715), 1689	<i>e</i>
	292	1,800		
	Above plus acid			
	206	17,700		
260	350			
XI Succinimide	194?	12,000	1770, 1689	
XII N-Methyl succinimide	204	13,000	1757, (1718), 1686	<i>a, c</i>
	242	110		
XIII 3,6-Methano-1,2- cyclohexanedi- carboximide	223	200	1754, 1695	<i>a</i>
	248	100		
XIV Cyclohexane-1,2- imide ( <i>cis</i> )	255	90	1748, 1692	<i>a</i>

<sup>a</sup> Courtesy of Dr. H. K. Hall, Jr., du Pont. <sup>b</sup> H. K. Hall, Jr., *J. Am. Chem. Soc.*, **80**, 6412 (1958). <sup>c</sup> H. K. Hall, Jr., M. K. Brandt and R. M. Mason, *ibid.*, **80**, 6420 (1958). <sup>d</sup> Courtesy of Dr. A. O. Geiszler, Abbott Laboratories. <sup>e</sup> Courtesy of Dr. Albert J. Plummer, Ciba Pharmaceutical Products. <sup>f</sup> Eastman Kodak Co. <sup>g</sup> Parentheses indicate shoulders.

membered ring is about 154°, contrasted to about 120° in the six-membered ring glutarimide. The N<sup>+</sup>O<sup>-</sup> dipoles do not cancel as in the six-membered ring, but subtract from the moment as its resultant is opposite to that of the carbonyl resultant.

(4) E. G. Cowley and J. R. Partington, *J. Chem. Soc.*, 47 (1936), give a value of 1.54 D for succinimide in dioxane at 20°.

Theoretically one can 1,2-*cis* fuse an imide group to either the boat or chair form of cyclohexane. Compound XIII with the bridge must be in the boat form with the five-membered ring fused to two  $\beta$ -positions. The slight increase in the moment (0.2 g. over succinimide) may be due to the inductive effect of the attached ring.

If cyclohexane-1,2 imide (XIV) is in the boat form, one would not expect its moment to differ from XIII. Its dipole moment is 0.5 D. higher than XIII which indicates that it is not in the boat form, but in the chair form attached to one equatorial and one axial bond of cyclohexane. This would be expected, for the chair form has fewer bond oppositions; the greater flexibility and skewing of angles in the five-membered ring of this structure would cause the dipole moment to increase.

The ultraviolet spectrum of compounds XIII and XIV show weak bands around 250  $m\mu$  with extinctions of about 100. There is also evidence of an intense band below 200  $m\mu$  beyond the range of the instrument.

The four examples of five-membered ring imides show the large effect ring size has on dipole moment. Five-membered ring imides have moments lower than six-membered ring imides. The moments of the five-membered ring imides vary and increase from 1.47 D. in succinimide to 1.61, 1.74 and 2.24 D., depending on substitution of an alkyl on nitrogen, fusion of a boat six-membered ring and fusion of a chair six-membered ring to the five-membered imide ring.

**The Effect of an N-Methyl Group on the Dipole Moment, Ultraviolet and Infrared Spectra of Imides.**—One would expect the substitution of a methyl group for a hydrogen on the imide nitrogen to increase the dipole moment of the compound. Two effects are at work here: one effect is due to

$\begin{array}{ccc} & \text{+} \rightarrow & \text{+} \rightarrow \\ & | & | \\ \text{H} & - \text{N} & \text{C} - \text{N} \\ & | & | \\ & \text{+} \rightarrow & \text{+} \rightarrow \end{array}$

the replacement of a H-N dipole by a C-N dipole; the other is an inductive effect of methyl group in stabilizing the imide resonance.

Fischer<sup>5</sup> suggested that the presence of an N-methyl group would decrease the dipole moment of lactams, but he later showed<sup>6</sup> that this was not true. The three sets of data of the *cis-cis* conformation show either no change or a slight increase in dipole moment. This effect will be discussed further in subsequent papers.

It has been reported that the bond moment of  $\text{H} \rightarrow \text{N}$  dipole is greater than the bond moment of  $\text{C} \rightarrow \text{N}$  dipole. This being the case, the substitution of a  $\text{C} \rightarrow \text{N}$  bond moment for the  $\text{H} \rightarrow \text{N}$  bond moment would be expected to give a resultant moment of zero and the moment of the N-methyl compound would increase. Both the  $\text{C} \rightarrow \text{N}$  and  $\text{H} \rightarrow \text{N}$  bond moments are decreased due to the imide resonance ( $\text{a} \leftrightarrow \text{b} \leftrightarrow \text{c}$ ) putting a partial positive charge on the nitrogen while the bond

TABLE II  
DIPOLE MOMENTS OF SIX-MEMBERED RING IMIDES AT 30° IN DIOXANE

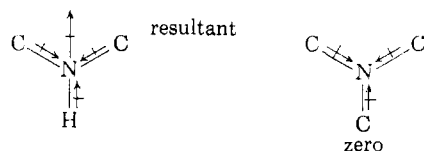
		$\mu_{12}$	$\mu_{13}$	$\mu_{12}$
IV	Cyclohexane-1,3-imide ( <i>cis</i> )	0.00	2.20309	.....
	$\mu = 2.89 \pm 0.05$ D.	.0009241	2.20884	0.97830
		.0019445	2.21607	.97812
		.0028799	2.22209	.97795
	Mol. wt. = 153.11	.0033730	2.22557	.97786
	$\epsilon_1 = 2.20257$	$\nu_1 = 0.97845$	$P_{20} = 206.71$	
	$\alpha = 6.74156$	$\beta = -0.17588$	$P_E = 38.67$ calcd.	
V	Cyclohexane-N-methyl-1,3-imide ( <i>cis</i> )	0.00	2.21321	0.97397
	$\mu = 2.88 \pm 0.05$ D.	.0114083	2.22134	.97379
		.0020958	2.22664	.97397
		.0026660	2.22810	.97397
		.0034518	2.23375	.97397
	Mol. wt. = 167.2	.0058754	2.24240	.97397
	$\epsilon_1 = 2.21317$	$\nu_1 = 0.97397$	$P_{20} = 211.45$	
	$\alpha = 5.96025$	$\beta = 0.00$	$P_E = 43.51$ calcd.	
VI	Glutarimide	0.0011553	2.21564	0.97793
	$\mu = 2.58 \pm 0.04$ D.	.0016230	2.21825	.97781
		.0020406	2.22174	.97774
		.0024879	2.22522	.97765
		.0028277	2.22793	.97757
	Mol. wt. = 113.13	.0034202	2.23141	.97743
	$\epsilon_1 = 2.20706$	$\nu_1 = 0.97817$	$P_{20} = 160.23$	
	$\alpha = 7.21768$	$\beta = -0.21263$	$P_E = 26.58$ calcd.	
VII	N-Methylglutarimide	0.00	2.20143	.....
	$\mu = 2.70 \pm 0.04$ D.	.0014604	2.21206	0.97819
		.0020203	2.21477	.97810
		.0026944	2.22000	.97803
		.0029938	2.22261	.97796
	Mol. wt. = 127.16	.0033931	2.22522	.97790
	$\epsilon_1 = 2.20139$	$\nu_1 = 0.97841$	$P_{20} = 177.87$	
	$\alpha = 6.9845$	$\beta = -0.14832$	$P_E = 31.37$ calcd.	
VIII	Bemigrade	0.00	2.20248	.....
	$\mu = 2.92 \pm 0.05$ D.	.0011107	2.21041	0.97814
		.0014547	2.21302	.97812
		.0019656	2.21477	.97811
		.0025988	2.22000	.97805
		.0030646	2.22313	.97803
	Mol. wt. = 155.21	.0032705	2.22444	.97798
	$\epsilon_1 = 2.20269$	$\nu_1 = 0.97822$	$P_{20} = 211.72$	
	$\alpha = 6.6386$	$\beta = -0.06584$	$P_E = 40.34$ calcd.	
IX	Glutethimide	0.00	2.20640	.....
	$\mu = 2.83 \pm 0.03$ D.	.0010554	2.21163	0.97877
		.0015121	2.21433	.97875
		.0018778	2.21564	.97867
		.0022988	2.21782	.97861
		.0032333	2.22217	.97846
	Mol. wt. = 219.03	.0035159	2.22348	.97841
	$\epsilon_1 = 2.20642$	$\nu_1 = 0.97895$	$P_{20} = 228.02$	
	$\alpha = 4.8428$	$\beta = -0.15174$	$P_D = 66.74$ calcd.	
X	Aminoglutethimide	0.00	2.20160	.....
	$\mu = 3.64 \pm 0.03$ D.	.0017033	2.21346	0.97793
		.0020296	2.21599	.97781
		.0025263	2.21965	.97774
		.0031314	2.22444	.97758
	Mol. wt. = 234.03	.003249	2.22488	.97754
	$\epsilon_1 = 2.20143$	$\nu_1 = 0.97833$	$P_{20} = 331.10$	
	$\alpha = 7.23886$	$\beta = -0.23978$	$P_E = 65.36$ calcd.	

moment places a partial negative charge on the nitrogen.

The inductive effect of the methyl group, as shown in the ultraviolet and infrared spectra, is

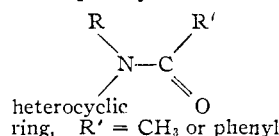
(5) E. Fischer, *J. Chem. Soc.*, 4525 (1952).

(6) E. Fischer, *ibid.*, 1382 (1955).



probably more important. The electron-repelling nature of the methyl group neutralizes the partial positive charge on the nitrogen enabling it to absorb more positive charge. Consequently, there is resonance stabilization of ionic forms a and c. This effect is shown in the ultraviolet spectra. The electron-repelling effect of the methyl group facilitates the electronic transition so the maximum is shifted to low frequency or long wave length and there is a higher extinction (*cf.* Table I: IV and V, VI and VII, XI and XII.)

In the infrared similar effects have been noted. Katritzky and Jones<sup>7</sup> showed in compounds in which R is changed from hydrogen to methyl that there is an increase in the conjugation of the carbonyl group. They attribute this to the favorable inductive effect of the methyl group and to partial steric inhibition of resonance between the nitrogen atom and the heterocyclic ring; the frequency is lowered by  $35 \pm 6 \text{ cm.}^{-1}$ . This is not due to loss of hydrogen bonding for the shifts would be to higher not lower frequency.



Ogata<sup>8</sup> reported that N-alkyl substitution in amides causes shifts of carbonyl absorption toward lower frequencies and relates this to the increasing contribution of the ionic structures to the resonance of the amide group. He also noted doublets or triplets in the infrared carbonyl frequency of N-methyl lactams as compared to the unsubstituted compounds. N-Methylimides generally have two sharp bands as compared with the unsubstituted imide with only one broad band (Table I).

### Experimental

The dipole moments were measured using an apparatus described previously<sup>9</sup> and the dioxane was purified as before.<sup>9</sup> The dipole moments were calculated using the equation and method of Halverstadt and Kumler.<sup>10</sup>

$$p_{20} = \frac{3\alpha v_1}{(\epsilon_1 + 2)^2} + (v_1 + \beta) \frac{(\epsilon_1 - 1)}{(\epsilon_1 + 2)}$$

$$P_{20} = p_{20} M$$

$$\mu = 0.01281 \sqrt{(P_{20} - P_E) T}$$

The plots of  $\epsilon_{12}$  versus  $\omega_2$  and  $\nu_{12}$  versus  $\omega_2$  were straight lines within the limits of experimental error. The values

(7) A. R. Katritzky and R. A. Jones, *J. Chem. Soc.*, 2096 (1959).

(8) N. Ogata, *Bull. Chem. Soc. Japan*, **34**, 245 (1961).

(9) W. D. Kumler, *J. Am. Chem. Soc.*, **62**, 3292 (1940).

(10) I. F. Halverstadt and W. D. Kumler, *ibid.*, **64**, 2933 (1942).

TABLE III  
DIPOLE MOMENTS OF FIVE-MEMBERED-RING IMIDES AT 30°  
IN DIOXANE

		$\omega_{12}$	$\epsilon_{12}$	$\nu_{12}$	
XI	Succinimide	0.00	2.20700	0.97435	
		.0015400	2.21106	.97395	
		.0050932	2.21517	.97347	
		$\mu = 1.47 \pm 0.01 \text{ D.}$	.0051131	2.22091	.97270
			.0067462	2.22587	.97222
			.0081739	2.22990	.97193
			.0097516	2.23461	.97146
	Mol. wt. = 99.09				
	$\epsilon_1 = 2.20660$	$\nu_1 = 0.97436$	$P_{20} = 65.70$		
	$\alpha = 2.84132$	$\beta = -0.30315$	$P_E = 22.02$	calcd.	
XII	N-Methyl succinimide	0.00	2.20700	0.97433	
		.0014991	2.21149	.97395	
		.0030260	2.21569	.97376	
		$\mu = 1.61 \pm 0.02 \text{ D.}$	.0039579	2.21911	.97347
			.0046743	2.22082	.97328
			.0051255	2.22236	.97308
			.0051255	2.22236	.97308
	Mol. wt. = 111.10				
	$\epsilon_1 = 2.20696$	$\nu_1 = 0.97435$	$P_{20} = 78.79$		
	$\alpha = 2.99353$	$\beta = -0.23043$	$P_E = 28.86$	calcd.	
XIII	3,6-Methano-1,2-cyclohexane-dicarboximide	0.00	2.20160	0.97810	
		.0008731	2.20322	.97810	
		.0014792	2.20640	.97797	
		.0018389	2.20771	.97787	
		$\mu = 2.24 \pm 0.03 \text{ D.}$	.0022817	2.20945	.97779
			.0027383	2.21119	.97771
			.0033336	2.21346	.97758
	Mol. wt. = 179.12				
	$\epsilon_1 = 2.20128$	$\nu_1 = 0.97828$	$P_{20} = 146.38$		
	$\alpha = 3.5951$	$\beta = -0.21087$	$P_E = 45.64$	calcd.	
XIV	Cyclohexane-1,2-imide	0.00	2.20160	0.97840	
		.0009560	2.20422	.97826	
		.0020727	2.20683	.97807	
		$\mu = 1.74 \pm 0.02 \text{ D.}$	.0024253	2.20771	.97800
			.0029501	2.20901	.97790
			.0032637	2.20988	.97787
			.0032637	2.20988	.97787
	Mol. wt. = 153.18				
	$\epsilon_1 = 2.20168$	$\nu_1 = 0.97841$	$P_{20} = 99.049$		
	$\alpha = 24.99313$	$\beta = -0.16851$	$P_E = 38.47$	calcd.	

of  $\epsilon_1$  and  $\nu_1$  were obtained by the method of least squares. The standard errors in the dipole moments were calculated from the equation  $\delta\mu = \pm 0.0046 \frac{M}{\mu} \delta\alpha^{11}$  and the standard error in  $\alpha$  from the equation<sup>11,12</sup>

$$\delta\alpha = \pm \left[ \frac{n}{n-2} \left( \frac{\sum(\epsilon_1 - \epsilon_{12})^2}{n\sum(\omega_2)^2 - (\sum\omega_2)^2} \right) \right]^{1/2}$$

The errors from scatter of the points for specific volume do not need to be considered since even large errors in  $\beta$  produce only very small errors in the dipole moment.<sup>13</sup>

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