Infrared Spectra of Acyclic Imides. V. Infrared Spectra and Structure of Acyclic Imides in Solutions

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(Received January 11, 1962)

In earlier papers of this series[1-4], it has been shown that the infrared spectra of saturated acyclic imides in the crystalline state are closely related to the configuration of the -CONHCO- group. Some higher homologs of diacetamide (R-CONHCO-R′, R=CH_3, C_2H_5 and n-C_3H_7; R′=C_2H_5 and n-C_3H_7) have been proved to be crystallized in a stable form taking the trans-trans configuration[2,3]. The characteristic frequencies of the trans-trans -CONHCO- group have been assigned, and their similarity to the characteristic frequencies of the trans -CONH- group has been pointed out[2]. No example of the trans-cis -CONHCO- group, however, has been found to exist in the crystalline state except for the stable form (form A) of diacetamide[1], the first member of the homologous series. In connection with these results, the present paper deals with the infrared spectra (4000 to 900 cm^{-1}) of these acyclic imides dissolved in various non-polar solvents. It will be shown that the higher homologs, as well as diacetamide itself, take the trans-cis configuration when dissolved in a non-polar solvent, such as carbon tetrachloride, tetrachloroethylene or carbon disulfide. The characteristic frequencies of the trans-cis -CONHCO- and -CONDCO- groups in the rock salt region will also be discussed in detail.

Results and Discussion

Diacetamide in Non-polar Solvents.—In the infrared measurements of the solutions of diacetamide, the three non-polar solvents, carbon tetrachloride, tetrachloroethylene and carbon disulfide, lead to nearly identical spectra except for covering the regions where their own absorptions arise. By using these solvents in turn, an almost complete range of the spectra of diacetamide dissolved in a non-polar solvent at a concentration between 0.25 and 0.01 mol./l. can be recorded from 4000 to 900 cm^{-1}. The infrared spectra thus obtained for several solutions of diacetamide and diacetamide-*d* are shown in Fig. 1[5].

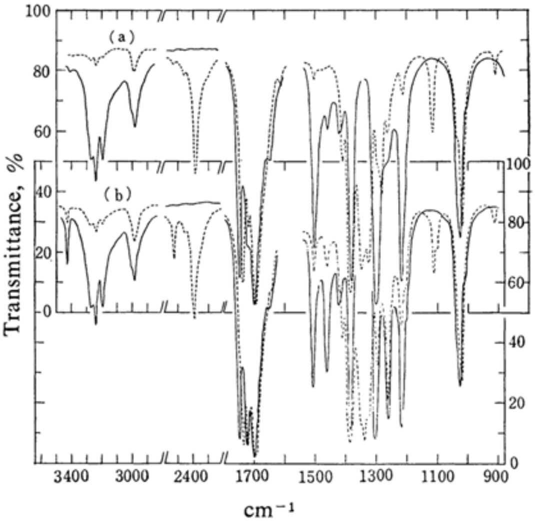

Fig. 1. Infrared spectra of diacetamide (solid line) and diacetamide-d (broken line); (a) 0.34 mol./l., (b) 0.012 mol./l.

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[1] T. Uno and K. Machida, This Bulletin, **34**, 545 (1961).
[2] T. Uno and K. Machida, ibid., **34**, 551 (1961).
[3] T. Uno and K. Machida, ibid., **34**, 821 (1961).
[4] T. Uno, K. Machida and I. Hamanaka, ibid., **34**, 1448 (1961).

[5] The infrared spectra shown in Figs. 1, 2, 4 and 5 were recorded with the use of the following cell length and solvents: (a) 0.1 mm.; CCl_4: (b) 2.85 mm.; 3500~1600 and 1480~1300 cm^{-1}, CCl_4: 1550~1480 cm^{-1}, C_2Cl_4; 1300~900 cm^{-1}, CS_2.

TABLE I. THE INFRARED FREQUENCIES (cm^{-1}) DUE TO ASSOCIATED MOLECULES

	Diacetamide	*N*-Acetylpropionamide	Dipropionamide	*N*-Propionyl-*n*-butyramide	Di-*n*-Butyramide
R	CH_3	CH_3	C_2H_5	C_2H_5	*n*-C_3H_7
R′	CH_3	C_2H_5	C_2H_5	*n*-C_3H_7	*n*-C_3H_7
R-CONHCO-R′					
Imide Ia+Imide II	3277 sh[b]	3275 sh	3273 sh	3273 sh	3269 sh
ν_{N-H}[a]	3222 m	3220 m	3220 m	3219 m	3218 m
Imide Ib+Imide II	3170 m	3168 m	3160 m	3157 m	3152 m
ν_{C-H}	2998 w	2988 m	2985 m	2980 m	2969 s
	—	2948 sh	2942 w	2942 sh	2937 sh
	—	2889 w	2886 sh	2883 w	2879 w
Imide Ia ($\nu_{C=O}$ free)	1747 s	1747 s	1747 s	1746 s	1743 s
Imide Ib ($\nu_{C=O}$ bonded)	1698 vs	1698 vs	1694 vs	1694 vs	1690 vs
Imide II (δ_{N-H}, ν_{C-N-C} antisym.)	1503 s	1502 s	1498 s	1496 s	1495 s
CH_3 asym. deform., CH_2 bend.	—	1462 w	1461 m	1461 m	1461 m
	1423 w	1423 w	1421 w	1420 w	1420 sh
CH_3 sym. deform.	1383 s	1382 s	1383 s	1382 s	1394 s 1377 sh
CH_2 twist., CH_2 wag.	—	—	1301 w	1337 sh 1300 w	1321 w 1295 w
Imide III					
(ν_{C-N-C} sym.)	1301 s	1302 s 1220 s	1214 s	1215 s	1205 s
(δ_{N-H}, ν_{C-N-C} antisym.)	1216 s	1159 m	1160 m	1160 m	1160 m
$\nu_{skeletal}$, CH_3 rock., CH_2 rock.	—	—	—	—	1100 m
	—	1075 w	1083 m	1081 m	1054 w
	1028 s	1030 w	1060 sh	1063 sh	1041 w
	—	—	—	—	990 w
	—	924 w	931 w	933 w	973 w
R-CONDCO-R′[c]					
ν_{N-D}	2390 m	2390 m	2385 m	2380 m	2380 m
Imide Ia ($\nu_{C=O}$ free)	1737 s	1737 s	1736 s	1735 s	1733 s
Imide Ib ($\nu_{C=O}$ bonded)	1695 vs	1694 vs	1689 vs	1688 vs	1687 vs
CH_3 asym. deform., CH_2 bend.	—	1463 w	1462 m	1462 m	1462 m
	1418 w	1420 sh	1435 w	1434 w	1435 w
CH_3 sym. deform.	1385 s	1384 s 1357 sh	1385 vs 1359 sh	1397 sh 1386 s	1397 s 1380 sh
Imide II′					
(ν_{C-N-C} antisym.)	1350 1326 db, s	1328 sh 1314 s	1300 s	1304 s	1335 s 1312 m
(ν_{C-N-C} sym.)	1286 m	1211 m	1208 m	1208 m	1200 m
δ_{N-D}, $\nu_{skeletal}$, CH_3 rock., CH_2 rock.	1112 m	1109 w	—	—	1103
	—	1078 m	1079 s[d]	1078 s[d]	1086 db, m
	—	—	1059 sh	1060 w	1058 w
	1024 s	1034 s[d]	1025 w	1026 w	1043 w
	—	980 w	984 w	981 w	1007 m[d]
	913 w	959 w	959 w	961 w	994 w

a) ν, stretching; δ, in-plane deformation.

b) vs, very strong; s, strong; m, medium; w, weak; sh, shoulder; db, doublet.

c) The ν_{C-H} frequencies are the same as the corresponding undeuterated compounds.

d) Probably the imide III′ frequencies.

Most of the bands observed for the concentrated solution show, in intensities as well as in frequencies, marked correspondences with the bands of the crystal of diacetamide in form A[1] (see Table I). The N–H stretching band appears near 3220 cm^{-1}, indicating the presence of hydrogen bonds. The complicated feature of this band is quite analogous to that of the triplet observed in the same region for the crystal in form A. The 0.34 mol./l. solution shows two C=O stretching (imide I) bands, at 1747 and 1698 cm^{-1}, of which the band with the lower frequency is stronger than the other, as in the case of form A. The analogy in infrared spectra between the concentrated solution and the crystal in form A is preserved

TABLE II. THE CHARACTERISTIC FREQUENCIES (cm^{-1}) DUE TO THE MONOMERS[a]

	Diacetamide	*N*-Acetylpropionamide	Dipropionamide	*N*-Propionyl-*n*-butyramide	Di-*n*-butyramide
R-CONHCO-R′					
ν_{N-H}	3416	3416	3416	3416	3416
Imide I	1720	1718	1718	1718	1715
Imide II	1465	1462[b]	1461[b]	1461[b]	1461[b]
Imide III	1263	1265 1187	1187	1186	1180
R-CONDCO-R′					
ν_{N-D}	2523	2523	2523	2523	2523
Imide I	1717	1717	1715	1715	1712
Imide II′	1339 1260	1183	1183	1180	1177

a) Only the frequencies were listed which differ appreciably from those of the associated molecules.

b) Overlapped by the CH_3 asymmetric deformation bands.

on deuteration. For instance, the bands at 1503, 1301 and 1216 cm^{-1} observed for diacetamide in the solution disappear on deuteration. Instead, diacetamid-*d* shows a strong doublet near 1340 cm^{-1} and a weak band at 1286 cm^{-1}. These features of spectral change have also been observed for form A in a quite similar way[1].

It has been pointed out previously[1] that the difference in the configurations of the N–H and the C=O bonds in the –CONHCO– group results in the marked difference in the characteristic bands of this group. In this connection, the present results strongly suggest that the configuration of the –CONHCC– group of diacetamide in the concentrated solution in the non-polar solvents is similar to that involved in the crystal in form A, that is, it is similar to the trans-cis configuration. The dimeric association of diacetamide dissolved in nitrobenzene has been suggested on the basis of the cryoscopic study[6]. Although the difference in the nature of the solvents must be taken into account, it seems quite probable that the association of diacetamide dissolved in the non-polar solvents is also dimeric, the two molecules involved being in the trans-cis configuration. If this is valid, the characteristic bands of the –CONHCO– group observed for the concentrated solution must be given reasonable assignments on the basis of the trans-cis configuration. Taking into account the spectral change on deuteration, we can pick up several characteristic bands of the –CONHCO– group besides the C=O stretching (imide I) bands, which may be assigned without question. Thus, the imide II, III and II′ frequencies shown in Table I were determined by analogy with the corresponding characteristic frequencies of the trans-trans configuration[2]. In the following sections, the nature of these characteristic bands will be discussed in relation to the configuration of the –CONHCO– group.

The frequency shifts on the change from the crystal in form A to the concentrated solution in the non-polar solvents are rather small for these characteristic bands. This is analogous to the case of *N*-methylacetamide, the characteristic bands of which have been reported to show small frequency shifts on the change from the crystal in the stable form above the transition point to the concentrated solution in carbon tetrachloride[7]. The characteristic bands of diacetamide dissolved in the non-polar solvents undergo marked changes on the change in concentration. The N–H stretching and the imide II bands (3222 and 1503 cm^{-1}) of the associated molecules are replaced gradually by the monomer bands at 3416 and 1465 cm^{-1} respectively on successive dilution. The directions of these frequency shifts are in agreement with those of the corresponding characteristic bands of monosubstiuted amides[7]. On the other hand, the imide I and III bands of the monomers are observed at 1720 and 1263 cm^{-1} respectively for the solutions at a concentration below 0.1 mol./l. Thus, it is seen that a monomer band appears between the two dimer bands for each of these characteristic vibrations (see Tables I and II). In this respect, the situation for diacetamide, involving two C=O, and two C–N bonds, seems to be different from the case of monosubstituted amides.

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6) L. Hunter and N. Raynolds, *J. Chem. Soc.*, **1950**, 2857.

7) T. Miyazawa, *J. Chem. Soc. Japan, Pure Chem. Sec.* (*Nippon Kagaku Zassi*), **77**, 171, 321 (1956); T. Miyazawa, T. Shimanouchi and S. Mizushima, *J. Chem. Phys.*, **24**, 408 (1956).

Besides the characteristic bands described above, all the bands due to the CH_3 deformation vibrations are easily assigned, except for those due to the CH_3 rocking modes. The bands at 1424 and 1383 cm^{-1} are assigned to the CH_3 asymmetric and symmetric deformation vibrations respectively. Appreciable frequency shifts for these bands do not occur on either deuteration or dilution.

Higher Homologs in Non-polar Solvents.— The infrared spectra of the higher homologs of diacetamide dissolved in the three non-polar solvents are shown in Figs 2−5[5]. In some cases, the concentrations of the saturated solutions at room temperature are so small that the observed band intensities are not sufficient for the 0.1 mm. cell. Thus, infrared spectra in which the monomer bands are absent could not be recorded for some of these higher homologs. It is seen, however, that these higher homologs show, at a variety of concentrations, infrared spectra resembling that of diacetamide at the corresponding concentration. This fact is in marked contrast with the case of the crystalline state, in which the stable form (form A) of diacetamide shows a quite different spectrum from those of the higher homologs[2]. The spectral difference between diacetamide and the higher homologs in the crystalline state was explained as resulting from the difference in the configuration of the

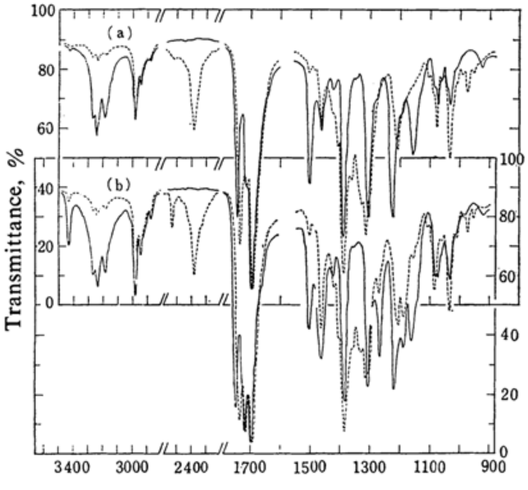


Fig. 2. Infrared spectra of *N*-acetylpropionamide (solid line) and *N*-acetylpropionamide-d (broken line); (a) 0.20 mol./l. (b) 0.01 mol./l.

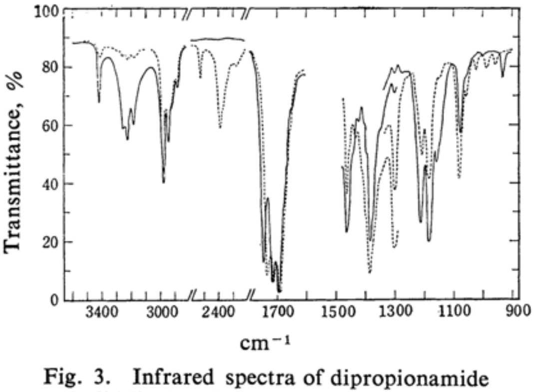


Fig. 3. Infrared spectra of dipropionamide (solid line) and dipropionamide-d (broken line); 2.85 mm. cell; 3500∼1300 cm^{-1}, 0.01 mol./l. in CCl_4; 1300∼900 cm^{-1}, 0.007 mol./l. in CS_2.

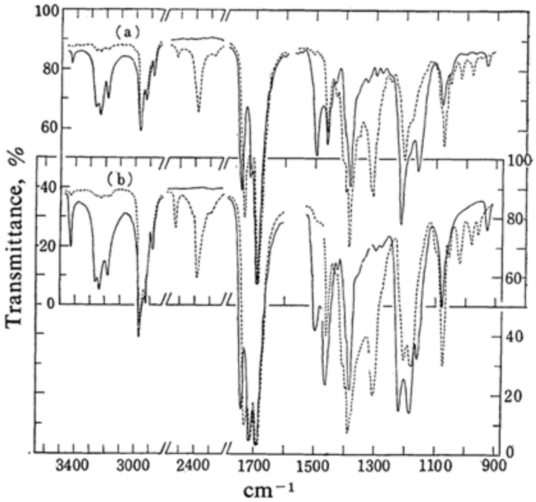


Fig. 4. Infrared spectra of *N*-propionyl-*n*-butyramide (solid line) and *N*-propionyl-*n*-butyramide-d (broken line); (a) 0.14 mol./l. (b) 0.01 mol./l.

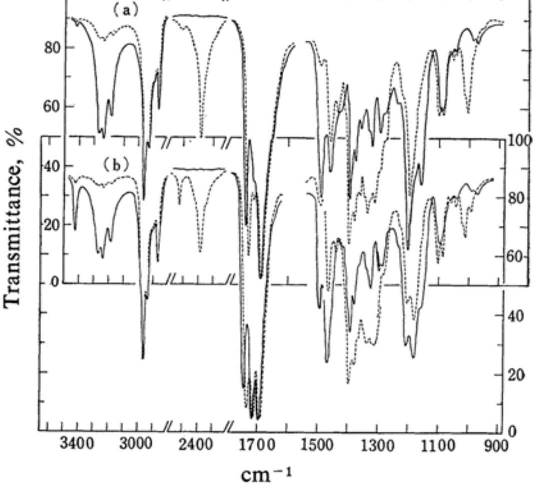
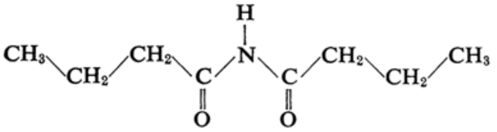


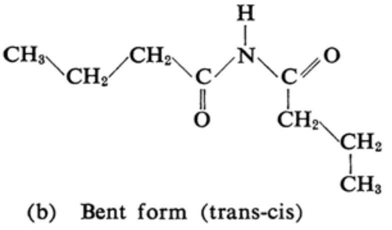
Fig. 5. Infrared spectra of di-*n*-butyramide (solid line) and di-*n*-butyramide-d (broken line); (a) 0.30 mol./l. (b) 0.01 mol./l.

–CONHCO– group[1,2]. That is to say, diacetamide in form A takes the trans-cis configuration, while the higher homologs are in the trans-trans configuration. The present results suggest, however, that the higher homologs take the same configuration as diacetamide takes when dissolved in the non-polar solvents. In other words, the higher homologs undergo an inversion of the –CONHCO– group from the trans-trans to the trans-cis configuration in going from the crystals to the solutions in the non-polar solvents. Previously[4] we found that the addition of some alkali halides to diacetamide in form A gives rise to the inversion from the trans-cis to the trans-trans configuration and pointed out that this inversion is due to the electrostatic and steric effects of the cations and of the anions of the alkali halide added. Similarly, the above inversion of the higher homologs suggested as taking place on the change of state can be interpreted in terms of the analogous effects of the functional group and of the alkyl residues of these molecules.

With respect to an isolated molecule, the trans-trans configuration is expected to be less stable than the trans-cis configuration since the strong electrostatic dipole-dipole interaction between the two C=O groups may be involved in the former. On the other hand, if the alkyl chains of the higher homologs are assumed to be in the trans zigzag arrangement, the molecules involving the trans-trans and the trans-cis –CONHCO– group may be considered to take the linear and the bent form respectively. Di-*n*-butyramide in these two forms is illustrated in Fig. 6. With respect to the packing of the molecules in a unit cell, the linear form is expected to have greater advantages than the bent form. Thus, in the case of the higher homologs in the crystalline state, the advantage for the molecular packing overcomes the electrostatic interaction. In the case of diacetamide, however, difference between the linear and the bent form is not so distinct as in the higher homologs. Thus, the electrostatic interaction determines the configuration of diacetamide in the crystalline state; the trans-cis –CONHCO– group is therefore involved in the stable form (form A). On the other hand, diacetamide as well as the higher homologs takes the trans-cis configuration when dissolved in the non-polar solvents; in this case the advantage for the packing is not required, so only the electrostatic interaction may determine the configuration. The trans-cis acyclic imides dissolved in the non-polar solvents may be associated to construct the cyclic dimers involving the two equivalent hydrogen bonds of the N–H···O type. From the above considerations, it may be seen that both the electrostatic and the steric effects play important roles in determining the configuration of the –CONHCO– group.



(a) Linear form (trans-trans)



(b) Bent form (trans-cis)

Fig. 6. The configurations of di-*n*-butyramide with the trans zigzag alkyl groups.

The Characteristic Bands of the trans-cis Imides.—The characteristic bands of the associated trans-cis –CONHCO– group in the rock salt region are listed in Table I. The assignment of these bands will now be discussed in comparison with the results for the trans-trans[2] and the cis-cis[8] –CONHCO– groups.

Imide I Bands.—Since the –CONHCO– group contains two C=O and two C–N bonds, we may expect two bands for each of the C=O and the C–N stretching vibrations. It has been pointed out, however, that the symmetric arrangement of atoms in the trans-trans configuration results in a decrease in intensity or even in the vanishing of the C=O out-of-phase and the C–N–C symmetric stretching bands[2]. On the other hand, the reduced symmetry of the trans-cis configuration may result in agreement between the number of possible stretching modes and the number of observed bands. In fact, as shown in Fig. 1, two C=O stretching bands are observed for the 0.34 mol./l. solution of diacetamide. For convenience, the weaker band at 1747 cm^{-1} and the stronger band at 1698 cm^{-1} will be called the imide Ia and Ib band respectively. The higher homologs show these bands in a quite similar way. As the first approximation, the Ia and Ib bands are attributable to the free and the bonded C=O stretching vibration respectively, although the coupling between the two C=O stretching vibrations is more or less expected[9]. With respect to the features of the C=O stretching bands, the trans-cis –CONHCO– group of these

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[8] T. Uno and K. Machida, This Bulletin, **35**, 276 (1962).

[9] R. A. Abramovitch, *J. Chem. Soc.*, **1957**, 1413; H. K. Hall, Jr. and R. Zwinden, *J. Am. Chem. Soc.*, **80**, 6428 (1958).

acyclic imides is rather similar to the cis-cis –CONHCO– group of succinimide and maleimide[8], except that the ring strain raises the free C=O stretching frequency of these cyclic imides by about 30 cm^{-1} in comparison with acyclic imides. This may be related to the similarity in the hydrogen bonds resulting from these two configurations. By X-ray diffraction study[10], the crystal of succinimide has been proved to consist of ring dimers involving both the bonded and the free C=O bonds.

Imide II Band.—In contrast with the case of the imide I bands, the presence of the imide II band near 1500 cm^{-1} differentiates the infrared spectra of the trans-cis –CONHCO– group from those of the cis-cis group. This band results from the coupling between the N–H in-plane deformation and the C–N stretching vibrations of the –CONHCO– group containing the trans –CONH– group. Thus, the imide II band is characteristic of the trans-cis and the trans-trans –CONHCO– group, although the vibrational modes involved may be different for these two configurations. Table I shows that the difference in the alkyl frameworks hardly affects the imide II frequency, suggesting that the vibration is almost localized in the –CONHCO– group.

Imide III Bands.—As has been seen for the imide I bands previously, the features of the imide III bands are also affected by the difference in symmetry between the trans-trans and the trans-cis –CONHCO– group. The two strong bands at 1301 and 1216 cm^{-1} observed for diacetamide dissolved in the non-polar solvents disappear on deuteration. This fact may be well elucidated since the trans-cis –CONHCO– group, for which all the in-plane vibrations belong to the same symmetry species, A′, involves two C–N stretching modes being allowed to couple with the N–H in-plane deformation vibration. The imide III frequencies of the trans-cis –CONHCO– group, as in the case of the trans-trans group, vary with the change in alkyl framework. This means that the coupling between the vibrations of the functional group and the alkyl frameworks is appreciable with respect to the imide III bands. The higher homologs other than *N*-acetylpropionamide show the two imide III bands, consistent with the above consideration for diacetamide. On the other hand, the three imide III bands of *N*-acetylpropionamide (Fig. 2) seem to indicate the presence of the rotational isomers. The trans-cis –CONHCO– group of *N*-acetylpropionamide differentiates the two configurations in which the C=O bond in the acetyl group takes the trans and the cis position with respect to the N–H bond. In the infrared spectra of fatty acid esters, the acetyl group is distinguished from other acyl groups with respect to the C–O–C antisymmetric stretching frequency[11]. A similar peculiarity of the acetyl group was observed for the imide III frequencies of acyclic imides in the trans-trans configuration[2]. Thus, the imide III frequencies may be different for the two trans-cis configurations of *N*-acetylpropionamide, so that in carbon tetrachloride solutions this compound shows more than two bands related to the C–N stretching vibrations in the region 1350 to 1100 cm^{-1}.

Imide II′ and III′ Bands.—The difference in the alkyl framework affects the imide II′ and III′ frequencies of the *N*-deuterated compounds. Each of the acyclic imides investigated has turned out to show the two imide II′ bands in the region 1360 to 1150 cm^{-1} on deuteration. These bands are due to the two C–N stretching vibrations released from the coupling with the N–H in-plane deformation vibration. The contribution of the framework vibrations seems to remain on deuteration, since in some cases the band with the higher frequency shows a complicated feature with several peaks. This band is always stronger than the other band with the lower frequency. The frequency of the weaker band for each compound is 10 to 20 cm^{-1} lower than the higher imide III frequency of the corresponding undeuterated compound (see Table I). On the basis of these results, it is suggested that the antisymmetric and the symmetric C–N–C stretching vibrations are related to the stronger and the weaker band respectively. For the former band, however, the amplitude of the stretching coordinate of the shorter C–N bond may be greater than that of the longer bond, and vice versa for the latter band. As with the related compounds[7,12], the N–D in-plane deformation vibration seems to couple appreciably with the framework vibrations. The two bands at 1112 and 913 cm^{-1} of diacetamide-d are considered to result from such a coupling, in which an in-plane vibration contributing to the band at 1028 cm^{-1} of diacetamide is expected to be involved on deuteration. In fact, the features of the band at 1028 cm^{-1} are also changed on deuteration. This interpretation is consistent with the product rule applied to diacetamide in the trans-cis configuration. For the in-plane (A′) frequencies below 2000 cm^{-1}, the observed and the theoretical ratios,

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[10] R. Mason, *Acta Cryst.*, **9**, 405 (1956).

[11] H. W. Thompson and P. Torkington, *J. Chem. Soc.*, **1945**, 640; the recent investigation by K. Toriyama and T. Shimanouchi (unpublished) must also be referred to.

[12] T. Miyazawa, *J. Mol. Spectroscopy*, **4**, 155 (1960).

$II(\nu_H/\nu_D)$, are 1.41[13] and 1.44 respectively. Here, the theoretical ratio has been calculated from the same molecular constants as those used in the calculation of the A'' ratio[1]. The high-frequency separation has been made in analogy with that applied to succinimide[8]. For the solution of the higher homologs of diacetamide, the bands in the 1100 to 900 cm^{-1} region are much obscured by the destruction of the trans-zigzag arrangement of the alkyl chains. As with the imide III' band, however, each *N*-deuterated compound shows a fairly strong band in this region which is not observed for the corresponding undeuterated compound. Although this band results mainly from the N–D in-plane deformation vibration, the varying of the frequency with the alkyl groups seems to indicate some contribution of the framework vibrations.

N–H and N–D Stretching Bands.—As has been seen for the trans-trans[3] and the cis-cis[8] configurations, the features of the N–H and N–D stretching bands of the trans-cis configuration may well be elucidated in terms of Fermi resonance. All the in-plane vibrations of the trans-cis configuration belong to a single symmetry species, A', of the point group C_s. Thus, the imide Ia and Ib vibrations of this configuration can combine with the imide II vibration to give rise to two combination tones, which take part in the Fermi resonance with the N–H stretching vibration. The three peaks in the 3280 to 3150 cm^{-1} region observed for each undeuterated compound are attributed to this Fermi resonance (see Table I). It is seen from Figs. 1—5 that the vanishing of the resonance on deuteration leads to a single peak near 2390 cm^{-1} for the N–D stretching band of the trans-cis –CONDCO– group. It may be noted here that the intermolecular interaction is improbable as the cause of the splitting of the N–H stretching band in this case, since the symmetry of the associated ring dimer in the solution leads to only one infrared active N–H stretching vibration.

Conclusion

The infrared spectra of the aliphatic acyclic imides dissolved in the non-polar solvents indicate that the –CONHCO– group of these compounds takes the trans-cis configuration in the associated molecules. This means that the higher homologs of diacetamide (trans-trans in the crystalline state) undergo an inversion of the configuration of the –CONHCO– group upon the change of state. One of the anomalous features observed for the infrared spectra of the higher homologs of diacetamide is the marked decrease (30～40 cm^{-1}) in the frequencies of the strongest C=O stretching band on going from the crystals to the solutions in the non-polar solvents. This may result not only from the change in the vibrational modes due to the change in the configuration, but also from the change in the force constants due to the change in the type of hydrogen bond.

Experimental

The samples used in the present study are the same as those reported previously[1,2]. Commercially available, guaranteed-pure grade carbon tetrachloride, tetrachloroethylene and carbon disulfide were dried with silica gel and redistilled before use. The infrared measurements were made with a Perkin Elmer Model 221 spectrophotometer equipped with a lithium fluoride prism (4000～2600 cm^{-1}) and a Koken DS-301 spectrophotometer equipped with two rock salt prisms (2600～900 cm^{-1}). The water vapor and the polystyrene bands were used for the wave number calibration.

The authors wish to express their thanks to Dr. Tatsuo Miyazawa of Osaka University and to Dr. Kiyoshi Nakamura of the Research Laboratory, Dainippon & Co., Ltd., for their helpful advice throughout this work. Thanks are also due to Dr. Kunio Fukushima of Osaka University for his measurement in the 4000 to 2600 cm^{-1} region.

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[13] Calculated from the following frequencies: diacetamide, 1747, 1698, 1503, 1301, 1216, 1028; diacetamide-d, 1737, 1695, 1338 (the mean value of 1350 and 1326), 1286, 1112, 913.