IR-Spectroscopy of Aqueous Solutions of Monoethanolamine

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Abstract: The monoethanolamine (MEA)-water system has been studied by IR spectroscopy and quantum-chemical calculations (DFT B3LYP). It was found that spatial networks both of water and MEA are continuously rearranging depending on the content of the system components. Water molecules are embedded into the net of MEA, and molecules of MEA into the water net, thereby forming a mixed network of hydrogen bonds.

Keywords: IR spectroscopy, spatial hydrogen bond networks, monoethanolamine, water

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1. INTRODUCTION (169)

Aqueous solutions of amino alcohols are widely used in cryobiology, in particular, for long-term preservation of living organs and cells, due to the large hypothermia of the liquid phase [1-3]. Monoethanolamine (MEA) is the first representative of aliphatic amino alcohols, similar to water, possesses a spatial network of hydrogen bonds [4]. It mixes with water in all proportions, forming a mixed network of H-bonds in solution. It is the presence of spatial networks of hydrogen bonds in aqueous MEA solutions that explains the strong supercooling of the H₂O-MEA liquid system. These networks were described by the method of molecular dynamics [5], and their local F-structure - by the methods of quantum chemistry [6,7]. It was of interest to study hydrogen bonds in the H₂O-MEA system by vibrational spectroscopy. This work is devoted to this.

The MEA molecule, which has hydroxyl and amine groups, has a large number of conformers [8]. The most stable conformers MEA are shown at Fig. 1. The MEA molecule can form intramolecular H-bond OH⋯N and NH⋯O and intermolecular hydrogen

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bonds of OH⋯N, OH⋯O, NH⋯O and NH⋯N types. The bond strength depends on how the OH or NH₂ groups act: as a donor or as an acceptor of the hydrogen bond proton. In addition, the hindered internal rotation of the –CH₂OH and –CH₂NH₂ groups provides a different mutual orientation of intermolecular H-bonds, which is reflected in the local structural organization of macroscopic particles, based on MEA or with its participation. The variety of conformers of the MEA molecule, their transition into each other, and their stability depending on the phases is described in detail in [8]. In the gas phase MEA molecules were found to be in the gauche conformation of the NCCO angle (60°, −60°). It is mainly stabilized by intramolecular bonds OH⋯N in conformer g'Gg' and by bonds NH⋯O in conformer gGt. The hydrogen bond of OH⋯N type was shown to be energetically more preferable. During the transition from gas to liquid, most of intramolecular H-bonds are broken, new intermolecular bonds are formed; nevertheless the gauche conformation of the dihydral angle is mainly retained. According to MD calculations [9], at room temperature, among 1000 MEA molecules, only ~90 molecules have an intramolecular H-bond, mainly of OH⋯N type, which number grows with the temperature increase.

In crystalline MEA, chains of bent molecular chains, consisting of g'Tg isomers formed and stabilized due to strong intermolecular NH⋯O bonds [10] were found. Probably, the transition from the gauche conformation of the dihydral angle of the MEA molecule to trans occurs during the phase transition from the liquid to the crystalline phase. The reverse transition of trans conformers into gauche upon crystal melting was considered in [11].

We will be interested in the MEA liquid phase at a temperature of 298K. According to [9], the number of intermolecular NH⋯O bonds in a cell of 1000 MEA molecules is almost 2 times greater than the OH⋯N H-bonds, and the number of intramolecular bonds is 20 times less.

2. IR SPECTRA OF MEA-WATER MIXTURES

IR spectra of liquids were recorded in the spectral range 4000-400 cm⁻¹ on a Bruker Tensor 37 FT-IR spectrometer in a thin layer between the CaF₂ and KRS windows.

Earlier, dilute solutions of MEA in inert solvents were studied by vibrational spectroscopy [12,13]. It was demonstrated that the MEA molecules are predominantly in the gauche conformation, though can easily transform into the trans conformation. The aim of our study was not so much in the study of the MEA behavior in a polar solvent (water-MEA system), as in the study of the interaction of the system components, characterized by spatial network of hydrogen bonds.

The IR spectrum of pure MEA in the range of OH, NH₂ and CH stretching vibrations (4000-2400 cm⁻¹) exhibits several intense bands: 3366 cm⁻¹, 3289 cm⁻¹, 3178 cm⁻¹, 2930 cm⁻¹, 2862 cm⁻¹ (Fig. 2).

First two bands correspond to antisymmetric and symmetric vibrations of NH₂ group. This is evidenced by the fact that they satisfy the previously established empirical equation that is used to identify the vibrational frequency of the free NH₂ group: ν_symm = 345.53 + 0.876 ν_antisymm [14]. Bands at 2930, 2862 cm⁻¹ are assigned to stretching vibrations of CH-groups. The broad intense band at 3178 cm⁻¹...
can be attributed to vibrations of intermolecular H-bonds. When studying hydrogen bonds, the differentiation between intermolecular and intramolecular H-bonds is carried out by decreasing the concentration of the associated substance. It is considered that during dilution the intermolecular H-bonds are broken, while intramolecular are retained. Though the study of the MEA-water system by the IR method is complicated by the overlapping of the MEA and water bands in the range 4000-2400 cm\(^{-1}\), nevertheless, it is noticeable that with a decrease of MEA content to 50 mol % in the MEA-water mixture, the band at 3178 cm\(^{-1}\) becomes practically invisible (Fig. 2). This allows it to be attributed to the intermolecular H-bonds of pure MEA.

It should be noted that the low frequency wing of the combination band of stretching vibrations of OH\(\cdot\), NH\(\cdot\) and CH-groups reaches 2400 cm\(^{-1}\), indicating the presence of additional absorption bands lower than 2700 cm\(^{-1}\) (\(\nu\)CH). This may signify the presence in MEA of intermolecular associates characterized by a rather strong H-bonding.

Dilution of MEA with water (Fig. 3) leads to a slight upshift of the bands assigned to antisymmetric and symmetric vibrations of the NH\(\cdot\) groups, which indicates their participation in intermolecular hydrogen bonds in pure MEA and the H-bond weakening in the MEA-water system.

The intensity of the \(\nu\)CH bands gradually decreases due to a decrease in the MEA content in the MEA-water system. Along with this the broadening of the absorption band in the 4000-2400 cm\(^{-1}\) range is observed due to upshifting of the high frequency wing. This is caused by several processes: the appearance of bulk water in the system, which has a broad absorption band in the IR spectrum with a maximum at 3400 cm\(^{-1}\), retaining some of the associates of MEA, as well as the possible arising of new ones with the participation of water molecules.

An uneven decrease in the intensity of two \(\nu\)CH bands (in pure MEA they have practically the same intensity, while upon dilution the band at 2930 cm\(^{-1}\) gradually becomes more intense than that at 2862 cm\(^{-1}\)) can have two explanations. First, this may be due to the structural isomerism of MEA molecules. Second, the contribution to their intensity can be made by bands related to intermolecular associates with absorption in the same spectral region.

In this regard, an attempt was made to decompose the contour of absorption bands in the region 4000-2400 cm\(^{-1}\) (Figs. 4 and 5). The data are given in Table 1.

The table clearly shows that the spectral contour of the combined band in the range 4000-2400 cm\(^{-1}\) is a superposition of a large number of absorption bands. Their amount depends on the ratio of water and MEA content in the mixture. In the MEA-water system with the MEA: water ratio of 1:1 and 1:2 (50 mol % MEA and 33 mol % MEA), the number of bands is maximum, which should be expected. These solutions can already have molecules of bulk water (3496, 3523 cm\(^{-1}\)), still keep associates available in pure

![Fig. 3. IR spectra of an MEA-water mixture with an MEA content of 33 mol. %, 21 mol. %, 11 mol %, 6 mol % in the range 4000-2400 cm\(^{-1}\).](image)

![Fig. 4. Decomposition of the spectral contour of pure MEA in the range 4000-2400 cm\(^{-1}\).](image)

![Fig. 5. Decomposition of the spectral contour of an MEA-water mixture with an MEA content of 50 mol % in the range 4000-2400 cm\(^{-1}\).](image)
MEÅ, and also the formation of some H-bonded MEÅ-water associates of various compositions can be expected. The absorption maxima of bands related to $\nu$CH with an increase in the water content in the MEÅ-water system undergo a high-frequency shift (from 2931 and 2862 cm$^{-1}$ in pure MEÅ to 2952 and 2884 cm$^{-1}$ with an MEÅ content of 6 mol %). The ratio of the band intensities at 2931 cm$^{-1}$ and at 2862 cm$^{-1}$ with increasing of water content in the system really gradually changes thus indicating a change in geometry of MEÅ molecules.

A special attention should be attracted to the presence of absorption bands with frequencies below the frequencies of $\nu$CH, the number of which also depends on the composition of the system: there are two of them at an MEÅ content of 100 mol% - 2787 and 2624 cm$^{-1}$; two at 50 mol% - 2799, 2644 and 2496 cm$^{-1}$; two at 33 mol% - 2819 and 2621 cm$^{-1}$, and at 21% and 11% MEÅ only one such band is observed (2827 cm$^{-1}$; 2848 cm$^{-1}$, respectively). For a mixture with 6 mol % MEÅ content, the presence of such bands is no longer observed. These bands, as well as $\nu$CH, undergo frequency upshift with increasing water content in the system. They can be attributed to vibrations of the intermolecular hydrogen bonds of MEÅ associates in pure MEÅ and to H-bonds vibrations of MEÅ-water associates, for which the weakening of MEÅ-MEÅ intermolecular hydrogen bonding is quite predictable when water molecules introducing into them. However, it should be noted that the decrease in the number of these bands with an increase in the water content in the MEÅ-water system can be associated both with the disappearance of some type of associate and with the fact that, due to a decrease in its concentration in the mixture their amount becomes insufficient for detection by IR method.

The presence of water in the system leads to the appearance of absorption bands of bulk water with frequencies above 3400 cm$^{-1}$. Bands at 3623 cm$^{-1}$ (11 mol % and 6 mol % MEÅ) correspond to the vibrations of free OH groups.

### 3. QUANTUM-CHEMICAL CALCULATIONS OF THE GEOMETRY AND VIBRATIONAL FREQUENCIES

To interpret the IR spectroscopy data, quantum chemical calculations were performed using the DFT method (B3LYP).

Earlier in [15] for one molecule of MEÅ by DFT (B3 LYP) was shown, that the influence of a water molecule to intramolecular H-bond in MEÅ depends both on the type of conformer and water molecules location related to the MEÅ molecule. However, in all cases, the presence of a water molecule led to an increase in the intramolecular H-bond (downshift of the $\nu$OH absorption band by approximately 100 cm$^{-1}$). The value of the frequency shift of $\nu$OH band of water molecules interacting with MEÅ significantly depends on the location of its oxygen atom relative to the NH$_2$-group of MEÅ molecule. The largest shift (about 500 cm$^{-1}$) is observed when the NH$_2$···O bond is formed. From these results, it can be concluded that upon mixing MEÅ with water, one can expect destruction of only intermolecular bonds of the spatial MEÅ network without breaking the intramolecular H-bond of MEÅ.

In [16] the possibility of the formation of MEÅ$\cdot$nH$_2$O clusters at $n = 1-4$ was shown. A water molecule is coordinated via O-H groups both with the nitrogen atom and with the oxygen atom of MEÅ, while the second water molecule forms H-bond of type O···O-H with the first molecule of water, thus forming a hydrophobic particle.

In the work [17] by DFT (B3 LYP) it was demonstrated that MEÅ in condensed phase may also exist as dimers, both of open and cyclic type.
However, as in the presence of a polar solvent (water as well) one can expect the formation of a spatial network, dimers of open type should be more preferable.

Taking into account these data for understanding of the experimental IR spectra of pure MEA and mixtures MEA-water the geometry of MEA open dimers of two types were optimized.

The first type is characterized by the formation of a contact of the NH$_2$-group of one MEA molecule with the O atom of another MEA molecule.

The second type is distinguished by the presence of an H-bond between two OH-groups of two MEA molecules.

The starting geometry of monomers composing dimer was chosen as g’Gg’, as the most stable. The optimization of geometries of MEA dimmers and their geometries in the presence of one and two water molecules as well as vibrational frequencies of these entities were carried out by DFT (B3LYP 3-21+G*) using the complex of programs G03W [18]. It should be noted that the calculated frequencies of the OH- and NH$_2$-groups are usually notably overestimated in comparison with their experimental values due to the difficulties in taking into account the anharmonicity of vibrations with the participation of hydrogen atoms.

3.1. Dimer of the 1st type (contact of the NH$_2$-group of one molecule with the O atom of another molecule)

According to the calculation data, upon the formation of a 1st type of dimer, one of the MEA molecules retains the intramolecular H-bond, while in the second, its breaking is observed as a result of the OH-group reversal in the opposite direction to the nitrogen atom (Fig. 6). Similar results for the formation of intermolecular bonds for MEA were obtained in [13]. The length of the N-H bond (1.02789 Å) directed to the oxygen atom of the second MEA molecule increases in comparison with the monomer (1.02224 Å), elongation is also found for the OH-group of MEA (1.00727 Å), in which the oxygen atom is coordinated with the NH$_2$-group.

Without coordination, this distance is 0.9913 Å. The frequency value of the symmetric vibration of NH$_2$-group involved in the intermolecular H-bonding NH$_2$-···OMEA is equal to 3553 cm$^{-1}$, which is 91 cm$^{-1}$ lower than that of a symmetrical vibration of the free NH$_2$-groups (3444 cm$^{-1}$). The frequency of the antisymmetric vibration of the NH$_2$-group participating in the intermolecular H-bond NH$_2$-···O is 3510 cm$^{-1}$, which is 41 cm$^{-1}$ lower than the frequency of the analogous vibration of the free NH$_2$-group.

Frequencies of stretching vibrations of dimer of 1st type.

| vibration | formula | frequency (cm$^{-1}$) | change (cm$^{-1}$) |
|-----------|---------|----------------------|------------------|
| νNH$_2$ antisymm. free | 3551 | | |
| νOH free | 3527 | | |
| νNH$_2$ antisymm. H···O MEA (intermolecular H-bond) | 3510 | Δ = 41 | |
| νNH$_2$ symm. free | 3444 | | |
| νNH$_2$ symm.··· O MEA (intermolecular H-bond), | 3353 | | |
| νOH (intermolecular H-bond) | 3305 | | |

3.2. Frequencies of stretching vibrations of MEA dimer of 1st type coordinated with one and two water molecules

Coordination of one water molecule with a dimer (Fig. 7) leads to a change in the mutual arrangement of molecules in the dimer. A structure similar to a cycle is formed, consisting of two MEA molecules and a water molecule. This is manifested in the coordination of a water molecule with three functional groups at once: two OH-groups (one from each MEA molecule) and one NH$_2$-group (one MEA molecule). As a result of a change in the geometry of MEA molecules, no intramolecular H-bond is retained in any of the molecules.

Fig. 6. Optimized geometry of MEA dimer of the 1st type (contact of NH$_2$-group of one molecule with the O atom of another molecule).

Fig. 7. Optimized geometry of the 1st type of MEA dimer coordinated with one water molecule.
The frequencies of stretching vibrations of a dimmer of the 1st type coordinated with one water molecule.

- $\nu_{\text{NH}}$ antisymm. free: 3539, 3528 cm$^{-1}$
- $\nu_{\text{OH}}$ free: 3527 cm$^{-1}$
- $\nu_{\text{NH}}$ antisymm. $\text{NH} \cdots \text{O}$ water: 3385 cm$^{-1}$, $\Delta = 140$ cm$^{-1}$
- $\nu_{\text{NH}}$ antisymm. $\text{NH} \cdots \text{O}_{\text{MEA}}$ (intermolecular H-bond): 3225 cm$^{-1}$, $\Delta = 130$ cm$^{-1}$
- $\nu_{\text{OH}}$ $\text{MEA} \cdots \text{O}$ water: 3064 cm$^{-1}$

Thus, the coordination of a dimer of this type with one water molecule leads to an increase in the strength of intermolecular $\text{N-H} \cdots \text{O}$ bond, and to the destruction of the intramolecular H-bond.

The introduction of the second water molecule leads to another change in the geometry of the MEA molecules (Fig. 8). In one of them, the appearance of an intramolecular H-bond is again observed. The coordination of two water molecules by two MEA molecules is also carried out by three functional groups: two $\text{OH}$-groups (one from each MEA molecule) and one $\text{NH}_2$-group (one MEA molecule). According to calculations, the introduction of a second molecule of water (unlike one molecule) leads to a weakening of the intermolecular H-bond $\text{NH}_2 \cdots \text{O}_{\text{MEA}}$ (3375 cm$^{-1}$) and H-bond strengthening of $\text{NH}_2 \cdots \text{O}$ water bond (3147 cm$^{-1}$) and the appearance of new H-bonds of the type $\text{OH}_{\text{MEA}} \cdots \text{N}_{\text{MEA}}$ (intramolecular) 3219 cm$^{-1}$, and the intermolecular $\text{OH}_{\text{MEA}} \cdots \text{O}_{\text{MEA}}$ is 3090 cm$^{-1}$.

3.3. Dimer of MEA of the 2nd type (coordination O-H⋯O) Similarly to a 1st type dimer, in a dimer of the 2nd type an intramolecular H-bond is retained in one of the MEA molecules, while in the second one, its break is observed as a result of a turn of the $\text{OH}$-group towards the oxygen atom of the second MEA molecule and in the opposite direction to nitrogen atom (Fig. 9). An elongation of the O-H bond (1.0144 Å), coordinated with the oxygen atom of the second MEA molecule, was found. Without coordination, this distance is 0.9913 Å. The length of the O-H bond participated in the MEA intramolecular bond is 1.0138 Å. The vibration frequency of the intramolecular OH-bond $\text{OH}_{\text{MEA}} \cdots \text{N}_{\text{MEA}}$ is 3219 cm$^{-1}$, and the intermolecular $\text{OH}_{\text{MEA}} \cdots \text{O}_{\text{MEA}}$ is 3090 cm$^{-1}$.

3.4. Frequencies of stretching vibrations of MEA dimer of the 2nd type coordinated with one and two water molecules

The introduction of one water molecule leads to its coordination with two $\text{OH}$-groups of two MEA molecules and the rupture of the intermolecular...
OH$_{\text{MEA}}$···O$_{\text{MEA}}$ (Fig. 10). Intermolecular H-bonds of the type OH$_{\text{MEA}}$···O water (2945 cm$^{-1}$) and OH water···O$_{\text{MEA}}$ (2777 cm$^{-1}$, 2621 cm$^{-1}$) are formed. The frequency values of the last three vibrations correspond to the transfer of a proton from a water molecule to the oxygen atom of MEA.

Frequencies of stretching vibrations of MEA dimmer of the 2nd type coordinated with one water molecule

- $\nu$OH water free 3658 cm$^{-1}$
- $\nu$NH$_2$ antisymm. free. 3543, 3539 cm$^{-1}$
- $\nu$NH$_2$ symm. free 3437, 3427 cm$^{-1}$
- $\nu$OH$_{\text{MEA}}$···O water (intermolecular H-bond), 2945 cm$^{-1}$
- $\nu$OH water···O$_{\text{MEA}}$ (intermolecular H-bond), 2777 cm$^{-1}$, 2621 cm$^{-1}$.

The introduction of the second water molecule leads to its insertion between two NH$_2$-groups and one of the OH-groups of MEA. In this case, the formation of a not very strong H-bond between NH$_2$-groups and the oxygen atom of water is observed (Fig. 11). The frequencies of the vibrational bands corresponding to the $\nu$NH$_2$ antisymm. are equal to 3531 and 3519 cm$^{-1}$, and $\nu$NH$_2$ symm.-3392 and 3179 cm$^{-1}$. Much stronger interaction of water molecules with the MEA observed during the formation of H-bonding of type OH water···O$_{\text{MEA}}$ and OH$_{\text{MEA}}$···O water, where the values of vibrational frequencies of OH-groups both water and MEA downshift to 2656 cm$^{-1}$, 2452 cm$^{-1}$, 2413 cm$^{-1}$ and 2231 cm$^{-1}$, indicating the formation of nearly symmetric intermolecular bonds O···H···O.

Thus, based on the results of calculations in mixing process of MEA with water in the case of dimers of the 2nd type the break of the intermolecular bonds OH$_{\text{MEA}}$···O$_{\text{MEA}}$, the formation of very strong H-bonds OH$_{\text{MEA}}$···O water and OH water···O$_{\text{MEA}}$ can be expected.

In the case of dimers of the 1st type (NH$_2$···O$_{\text{MEA}}$) character of the influence of water molecules in the structure depends on its amount. The presence of one water molecule should lead to strengthening of the intermolecular H-bond NH$_2$···O$_{\text{MEA}}$ and the simultaneous formation of new bonds NH$_2$···O water and OH$_{\text{MEA}}$···O water. Two water molecules cause weakening of intermolecular H-bond in dimmers of type NH$_2$···O$_{\text{MEA}}$ (3375 cm$^{-1}$), strengthening of NH$_2$···O water bonding (3147 cm$^{-1}$) and appearance of new OH$_{\text{MEA}}$···O water (2785 cm$^{-1}$, 2605 cm$^{-1}$, 2379 cm$^{-1}$, 2131 cm$^{-1}$).

Thus, strengthening of intermolecular hydrogen bonds between molecules of the MEA can be expected only for dimers of the 1st type (bond NH$_2$···O$_{\text{MEA}}$) and only when a ratio H$_2$O:MEA is not more than 1:2. With a further increase in the water content, the intermolecular bond in dimers will weaken, since water molecules act as competitors and gradually all MEA atoms capable of forming H-bonds will be coordinated with water molecules.

In the case of dimers containing an H-bond OH$_{\text{MEA}}$···O$_{\text{MEA}}$ appearance of water will immediately lead to their destruction.

4. CONCLUSION

Thus, according to quantum-chemical calculations made for MEA dimers the presence of absorption bands in the region 2800-2400 cm$^{-1}$ are attributed to formation of associates of the type MEA-MEA and mixed water-MEA ones, characterized by very strong H-bonds. However, an unambiguous interpretation of the IR spectra is difficult due to band overlapping, as well as the probability of simultaneous existence in the MEA-water system of associates of different structures such as MEA with itself, MEA-water clusters, and also single MEA...
molecules bound to water molecules demonstrated in [5]. In this case, the formation of intermolecular H-bonds both between MEA molecules and MEA and water can lead to the rupture of intramolecular bonds in MEA. Nevertheless, the data obtained indicate the incorporation of water molecules into the spatial MEA network and molecules of MEA into the spatial water network, with the formation of a mixed MEA–water network, which is consistent with the MD results [5].

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