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## Description of the hydrogen bond network in liquid 3-amino-1-propanol by graph theory and percolation methods

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**Abstract.** Using the molecular dynamics method, vibrationally averaged V-structures of liquid 3-amino-1-propanol (3-AP) were obtained at three temperatures of 293, 323 and 373 K. The structure was described using the methods of graph theory and percolation. The description is based on the hydrogen bond criterion. The adjacency matrix is constructed and the conclusion is about presence in liquid 3-AP in the temperature range 293–373K a spatial network of hydrogen bonds, which includes almost all the molecules of the structure in question. Her characteristics are given. The hydrogen bond lifetimes are determined and the percolation threshold is considered. Comparison of the obtained data with similar results for monoethanolamine (MEA) shows a greater stability of the spatial network, a longer lifetime of hydrogen bonds, and a larger percolation threshold. A comparison is made with similar calculations in a series of diols.

**Keywords:** hydrogen bonds, spatial networks, aminopropanol, molecular dynamics, percolation threshold

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### 1. INTRODUCTION

Aliphatic amino alcohols with a small bridge of CH<sub>2</sub> groups in the molecule can be used as inhibitors of crystallization of aqueous solutions; therefore,

they are used in cryobiology as cryoprotectants for vitrification of biological materials [1]. They have a wide temperature range of the liquid phase and its strong hypothermia [2]. We attribute this feature of amino alcohols to the presence of a spatial network of H-bonds in their liquid phase [3]. The spatial network of hydrogen bonds has a number of features, in particular, stability — the ability to transmit perturbation to the entire volume. This network feature is associated with strong supercooling of the liquid phase of alkyl

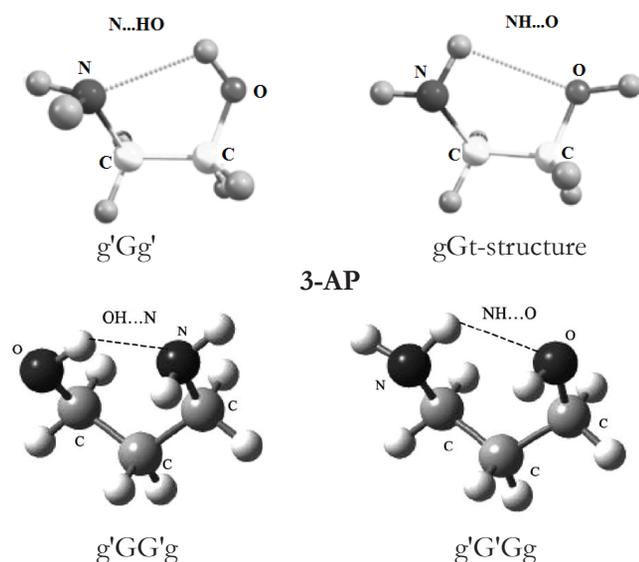
amino alcohols. 3-amino-1-propanol (3-AP) has the greatest supercooling [2], due to the greater stability of the spatial network of H-bonds in this compound compared to monoethanolamine and 4-amino-1-butanol [4].

The objective of this work was to describe the spatial network of hydrogen bonds of liquid 3-amino-1-propanol using graph theory and percolation and compare the data with the results of a similar description of monoethanolamine (MEA), which we obtained earlier [5], as well as with similar calculations in the series of diols.

**Fig. 1** shows the diagrams of 3-AP and MEA molecules in the gas and liquid phases in the most stable conformations of gosh (MEA) and gosh-gosh (3-AP), with intramolecular (OH ... N) and (O ... HN) hydrogen bonds [6, 7]. Note that the 3-AP molecule, in contrast to the MEA molecule, has a mobile bridge —CH<sub>2</sub>—CH<sub>2</sub>—CH<sub>2</sub>—, which determines the best distance for the intramolecular H bond [6] and the greater stability of the spatial network of H bonds in this compound when comparing with the MEA [4].

Physico-chemical properties of 3-AP and MEA are shown in **Table 1**. This table presents for comparison the similar data for ethylene glycol (EG) and 1,3-propanediol (1,3-PD).

It was shown in [4] that the pressure dependence of the isothermal compressibility



**Fig. 1.** Scheme of the molecules of monoethanolamine and 3-aminopropanol in most likely gosh conformations

**Table 1**  
Physico-chemical properties of diols and amino alcohols at 298 K.

	EG	1,3-PD	MEA	3-AP
M	62	76	61	75
$T_{\text{melt}}^*$ , °C [8]	-12.9	-32	10.3	11
$T_{\text{boiling}}^*$ , °C [8]	197	214	170	187
$T_{\text{overcool}}^*$ , °C [9]	31	40	38	43
$\Delta_{\text{vap}}H$ , kJ/mol [10]	50	57.2	49.83	49.59
$\mu^{(25^\circ\text{C})}$ , D [11]	2.88	2.5	2.27	2.67
$DN_{\text{SbCl}_5}$	18.5 [12]	-	41 [12]	43 [13]
$\rho^{(25^\circ\text{C})}$ , (kg/m <sup>3</sup> ·10 <sup>3</sup> ) [8]	1.113	1.052	1.012	0.982
$\eta^{(25^\circ\text{C})}$ , (Pa·c·10 <sup>-3</sup> )	16.16 [14]	40.07 [15]	18.95 [13]	27.70 [13]
$\beta_T \times 10^{11}$ , Pa <sup>-1</sup> [4]	37.4	40.4	39.6	38.9

can be considered as a measure of the stability of the network of H bonds in a liquid. The smaller the absolute value of the quantity ( $-\Delta\beta/\Delta P$ ), the greater the network stability. The stability of the network is greater in 3-AP than in MEA, which is reflected in the higher supercooling temperature of the liquid phase.

## 2. TOPOLOGY OF A SPATIAL NETWORK OF HYDROGEN BONDS IN A LIQUID 3-AP

**CALCULATION DETAILS AND DISCUSSION OF RESULTS**  
Using the molecular dynamics method in NPT mode, trajectories averaged over 0.1 ps were made to obtain vibrationally averaged V-structures of 3-AP at three temperatures of 293, 323 and 373 K and a pressure of 1 bar. A model of liquid 3-AP with 1000 molecules in a rectangular cell with periodic boundary conditions was constructed using the molecular dynamics method [16, 17]. The interaction parameters and partial charges on the atoms were the same as for the MEA [17]. Other details are in [17]. For numerical integration, the Verlet velocity algorithm [18] was used. The integration step was 1 fs. The temperature in the system was maintained with the help of a collision thermostat [19, 20], and pressure with the help of a Berendsen barostat [21].

From the molecular distribution functions obtained by the molecular dynamics method, the hydrogen bonding criterion was determined, both intermolecular and intramolecular. The distance between the coordinating atoms (O ... O, O ... N

and N ... N) should not exceed 3.5 Å, and between OH ... N, O ... HN and NH ... N should not exceed 2.5 Å.

Based on the criteria of hydrogen bonding, an adjacency matrix was constructed for V-trajectories obtained by averaging the coordinates of atoms over 0.1 ps. At each moment of time, the V-trajectory contains a structure of 1000 molecules in the computational cell with periodic boundary conditions.

An element with an index (*i, j*) of the adjacency matrix contains 1 if the *i* molecule is bonded to *j* by a hydrogen bond (satisfies the H-bond criterion) and 0 if the molecules are not bonded. This applies to both intermolecular and intramolecular H-bonds.

The main parameter that evaluates the network of hydrogen bonds within the structure is the size of the maximum connectivity component of the graph described by the constructed adjacency matrix. To find the connected components of the graph, the Taryan algorithm [22], which analyzes the adjacency matrix, was used. The result of his work is the number of connected components in the graph and their size, as well as a list of the vertices of the graph indicating their belonging to one or another connected component.

The results of calculating the characteristics of V-structures obtained by the graph theory method for 3-AP are presented in **Table 2** for three temperatures of 293, 323, and 373 K along with similar data for MEA. In parentheses are the minimum and maximum sizes of the parameter in question.

The number of pairs of molecules having at least one hydrogen bond is equal to the total number of edges in the graph. The number of connected components of the graph and the size of the maximum connected component are the result of the Taryan algorithm [23]. The numbers in parentheses are the minimum and maximum values of the parameter in question.

The main result of the analysis of the table is the conclusion that almost all molecules in all the studied trajectories of 3-AP, like MEA, form a

**Table 2**  
Characteristics of V structures obtained by graph theory methods for three temperatures 293, 323 and 373 K

Characteristic	MEA	3-AP
<b>293 K</b>		
Number of structures examined	100	100
The number of pairs of molecules in 1 structure having at least one hydrogen bond	2286.5 [2247, 2324]	2306.9 [2266,2356]
The number of connected components in 1 structure	1.03 [1, 2]	1.01 [1, 2]
The number of intramolecular bonds in 1 structure	43.17 [30, 60]	34.91 [30, 43]
The size of the maximum connected component in 1 structure	999.97 [999, 1000]	999.99 [999, 1000]
<b>323 K</b>		
Number of structures examined	100	100
The number of pairs of molecules in 1 structure having at least one hydrogen bond	2162.8 [2112, 2223]	2216.9 [2164, 2268]
The number of connected components in 1 structure	1.11 [1, 2]	1.18 [1,3]
The number of intramolecular bonds in 1 structure	49.02 [29, 69]	48.33 [38, 57]
The size of the maximum connected component in 1 structure	999.89 [999, 1000]	999.82 [998, 1000]
<b>373 K</b>		
Number of structures examined	100	100
The number of pairs of molecules in 1 structure having at least one hydrogen bond	1932.1 [1871, 1991]	2011.3 [1962, 2055]
The number of connected components in 1 structure	1.71 [1, 4]	1.73 [1, 4]
The number of intramolecular bonds in 1 structure	63.68 [45, 83]	65.75 [52, 79]
The size of the maximum connected component in 1 structure	999.28 [997, 1000]	999.25 [997,1000]

three-dimensional network of hydrogen bonds at all studied temperatures. Note that the number of intramolecular hydrogen bonds slightly increases

with temperature, to a greater extent with 3-AP, which is consistent with our IR data [24].

The most important characteristic of the spatial network of H-bonds is the lifetime of the hydrogen bond. Consider the total trajectory lifetime of the hydrogen bond in 3-AP and MEA. To do this, we construct adjacency matrices in each time frame of 0.1 ps and sum them along the entire trajectory of the V-structures. The main characteristics of the obtained matrix for both substances at temperatures of 293, 323, 373K are shown in **Table 3**.

The table discusses intermolecular H-bonds. The trajectory length is the duration of the V structures calculated by the molecular dynamics method. There are 1000 molecules in each structure.

The number of pairs of molecules that form a hydrogen bond is the total number of pairs of molecules between which the hydrogen bond criterion has been carried out at least once along the trajectory.

The number of H-bonds per molecule is the number of H-bonds averaged over the structure per molecule. As before, the table shows three values: the first is the average value over all structures, and in square brackets the minimum and maximum values of the parameter over all structures of the trajectory are given.

The lifetime of the H-bond was calculated as follows. If the hydrogen bond criterion turned out to be carried out for a certain pair of molecules in the structure, then, since the V trajectories were averaged over 0.1 ps, we believe that the criterion was carried out for 0.1 ps. Summing up for the selected pair of molecules time of fulfilling the hydrogen bond criterion along the entire trajectory for, we obtain the hydrogen bond lifetime.

The number of other molecules having H-bonds with a given molecule on the trajectory is the total number of molecules that have at least once formed a hydrogen bond with the selected molecule over the duration of the trajectory.

**Table 3**

Characteristics of summed adjacency matrices along the trajectory of V-structures with a duration of 600 ps for monoethanolamine and 3-amino-1-propanol at 293, 323, and 373 K

Characteristic	MEA	3-AP
<b>293 K</b>		
Trajectory length (ps)	600 ps	600 ps
The number of different pairs of molecules forming a hydrogen bond on the trajectory	8291	6101
H-bonds number per molecule	5.08 [4.95, 5.22]	4.69 [4.56, 4.83]
Hydrogen bond lifetime (ps)	165.59 [0.1, 600]	226.70 [0.1, 600]
The number of other molecules having H-bonds with this molecule on the trajectory	16.58 [10, 26]	12.20 [7, 20]
<b>323 K</b>		
Trajectory length (ps)	600 ps	600 ps
The number of different pairs of molecules forming a hydrogen bond on the trajectory	13786	8168
H-bonds number per molecule	4.8 [4.66, 4.95]	4.51 [4.38, 4.66]
Hydrogen bond lifetime (ps)	93.83 [0.1, 596.6]	162.9 [0.1, 600]
The number of other molecules having H-bonds with this molecule on the trajectory	27.57 [19, 38]	16.34 [8, 25]
<b>373 K</b>		
Trajectory length (ps)	600 ps	600 ps
The number of different pairs of molecules forming a hydrogen bond on the trajectory	34113	14830
H-bonds number per molecule	4.3 [4.15, 4.46]	4.11 [3.97, 4.27]
Hydrogen bond lifetime (ps)	34 [0.1, 358.5]	81.47 [0.1, 595.1]
The number of other molecules having H-bonds with this molecule on the trajectory	68.23 [50, 97]	29.66 [19, 44]

The duration of the considered trajectories is 600 ps. At 293 K, the number of pairs of molecules forming a hydrogen bond in MEA is approximately 1.36 times greater than in 3-AP. The amount of EG in relation to 1,3-PD is 1.55 times greater, but on a longer trajectory of at least 1000 ps [25]. With

increasing temperature, this ratio changes and at 373 K it is 2.3 for MEA to 3-AP and 1.9 for EG to 1,3-PD.

The number of hydrogen bonds per molecule decreases with increasing temperature for all pairs under consideration, while the value of the indicator itself is slightly larger in MEA than in 3-AP and in EG than in 1,3-PD. Note that at all temperatures, this indicator is greater in amino alcohols than in diols.

The hydrogen bond lifetime with increasing temperature drops significantly for all the cases we have examined: 4.9 times for MEA, 2.8 times for 3-AP (5 times for EG, and 4 times for 1,3-PD).

The average lifetime of H-bonds at 293 K in 3-AP is 1.37 times longer than in the MEA (1,3-PD is 1.5 times longer than in the EG), and at 373 K it is already 2.4 times (1.9 times for 1,3-PD to the EG).

To determine the lifetime of a specific H-bond, the Voloshin approach was chosen [24]. Following this approach and proceeding from the hydrogen bond criterion, we obtained the characteristics of the continuous lifetime of the H-bond — the time until its first break with respect to the time chosen by us  $t_0$ , both in the continuation in the interval from  $t_0$  to  $t_0 + \Delta t$ , and in the opposite direction from  $t_0$  to  $t_0 - \Delta t$ . In our calculations,  $\Delta t = 200$  ps. This continuous lifetime of H-bonds was the basis for the percolation analysis of spatial networks for the selected configurations – H-bond structures at time  $t_0$  with a special adjacency matrix. The calculation procedure is presented in [25].

We call a graph edge colored if the lifetime of the corresponding H-bond is not less than some time  $t^*$ . We consider a subgraph containing only colored bonds on the condition of “leakage”, i.e. does this subgraph form a three-dimensional network of H-bonds, taking into account the periodic boundary conditions for our structure? If the “leakage” condition is satisfied, then the largest possible value  $t^* = t^*_{cr}$  will be called the percolation threshold. A connected subgraph forming a three-dimensional network at the percolation threshold is called a percolation cluster.

The results of calculating the percolation threshold and the power of the percolation

cluster at three temperatures of 293, 323, and 373 K for 3-AP and MEA are shown in **Table 4**.

Table 4  
Percolation analysis results at temperatures of 293, 323 K

Characteristic	MEA	3-AP
<b>293 K</b>		
Bonds average number per molecule	5.09 [5.05, 5.13]	4.683 [4.654, 4.73]
Maximum lifetime of continuous communication in configuration (ps).	398.2 [388.1, 400.1]	400.1 [400.1, 400.1]
Average lifetime of a continuous connection (ps)	23.7 [22.02, 26.05]	43.22 [41.77, 46.36]
Percolation threshold (ps)	10.39 [8.4, 12.8]	18.78 [16.7, 22.8]
Average lifetime of the colored bonds at the percolation threshold (ps)	57.22 [52.33, 61.55]	108.3 [100.9, 120.19]
Proportion of colored bonds on the threshold of flow	0.38 [0.36, 0.41]	0.37 [0.36, 0.4]
Proportion of molecules in percolation cluster	0.63 [0.5, 0.78]	0.6 [0.4, 0.74]
Percentage of colored bonds in percolation cluster	0.45 [0.43, 0.47]	0.45 [0.44, 0.46]
Average lifetime of colored bonds in percolation cluster (ps).	56.01 [51.61, 60.95]	107.3 [98.85, 121.69]
<b>323 K</b>		
Bonds average number per molecule	4.82 [4.796, 4.884]	4.52 [4.47, 4.56]
Maximum lifetime of continuous communication in configuration (ps).	256.72 [210.7, 343.8]	400.1 [400.1, 400.1]
Average lifetime of a continuous connection (ps)	1 1.32 [9.86, 12.41]	22.83 [21.76, 24.63]
Percolation threshold (ps)	5.48 [4.5, 6.1]	10.43 [8.6, 11.6]
Average lifetime of the colored bonds at the percolation threshold (ps)	25.72 [22.61, 28.08]	55.98 [51.6, 59.72]
Proportion of colored bonds on the threshold of flow	0.4 [0.37, 0.42]	0.37 [0.36, 0.39]
Proportion of molecules in percolation cluster	0.59 [0.45, 0.73]	0.57 [0.39, 0.65]
Percentage of colored bonds in percolation cluster	0.47 [0.46, 0.49]	0.46 [0.44, 0.46]
Average lifetime of colored bonds in percolation cluster (ps)	25.16 [22.73, 28.25]	55.73 [51.62, 59.34]

Table 4 (continued)  
Percolation analysis results  
at temperatures of 373 K

Characteristic	MEA	3-AP
<b>373 K</b>		
Bonds average number per molecule	4.29 [4.22, 4.37]	4.12 [4.08, 4.18]
Maximum lifetime of continuous communication in configuration (ps)	96.12 [65.9, 133]	190.4 [137.9, 238.2]
Average lifetime of a continuous connection (ps)	4.75 [4.37, 5.04]	8.72 [8.37, 9.24]
Percolation threshold (ps)	2.66 [2.4, 3]	4.22 [3.3, 4.8]
Average lifetime of the colored bonds at the percolation threshold (ps)	9.41 [8.3, 10.37]	18.51 [16.46, 20.17]
Proportion of colored bonds on the threshold of flow	0.44 [0.41, 0.47]	0.42 [0.4, 0.47]
Proportion of molecules in percolation cluster	0.59 [0.49, 0.71]	0.6 [0.42, 0.78]
Percentage of colored bonds in percolation cluster	0.52 [0.5, 0.53]	0.5 [0.48, 0.52]
Average lifetime of colored bonds in percolation cluster (ps)	9.22 [8.17, 9.8]	18.29 [15.94, 20.46]

The percolation analysis was averaged over 10 independently selected instants of time  $t_0$  and configurations corresponding to these times.

Table 4 shows the following characteristics of the considered configurations:

The average number of bonds per molecule - this characteristic is calculated as the double ratio of the total number of H-bonds to the number of molecules in the configuration.

The maximum lifetime of a continuous communication in a configuration is the largest value of the lifetime of a continuous communication obtained in this configuration.

The average lifetime of a continuous bond is the value averaged over all H-bonds in the configuration.

The percolation threshold is such a maximum value of time  $t^*$  for which a subgraph containing only hydrogen bonds with a continuous life of at least  $t^* = t_{cr}^*$  forms a three-dimensional infinite

network of H-bonds, but for large  $t^*$  it does not form.

The average lifetime of colored bonds at the percolation threshold is the average value of the time of continuous H bonds that existed in time longer than the percolation threshold.

The proportion of colored bonds at the percolation threshold is the ratio of the number of bonds existing longer than the percolation threshold to the total number of bonds in the configuration.

The fraction of molecules in a percolation cluster is the ratio of the number of molecules in the percolation cluster to the total number of molecules.

The proportion of colored bonds in the percolation cluster is an indicator similar to the proportion of colored bonds at the percolation threshold, but in calculating this indicator only those H-bonds that are included in the percolation cluster are considered. The same applies to the other two indicators: the average life time of the colored bonds in the percolation cluster and the average life time of the colored bonds at the percolation threshold.

The average number of bonds per molecule for MEA and 3-AP decreases by about 10% with increasing temperature (292 K-373 K) as well as in EG and 1,3-PD. And, as in diols, this indicator is lower for the propane derivative than for the ethane derivative. The average number of H-bonds per molecule in 3-AP is less than in MEA. It decreases slightly with increasing temperature.

All temporal characteristics are greater for 3-AP than for MEA. The percolation threshold at 293 K is 18.78 ps for 3-AP and 10.39 ps for MEA. In diols, the same picture — the percolation threshold is 11.02 ps for 1,3-PD and 8.12 ps for EG [25].

The fraction of colored bonds at the percolation threshold and the fraction of colored bonds in the percolation cluster with increasing temperature for 3-AP and MEA somewhat increase (as in diols).

### 3. CONCLUSION

Description of vibrationally averaged V-structures of 3-AP and MEA for 0.1 ps, obtained by the molecular dynamics method at three temperatures of 293, 323 and 373 K, was carried out using graph theory and percolation methods. In both liquid amino alcohols, the presence of a three-dimensional network of hydrogen bonds is shown, which includes almost all the molecules of the structures under consideration. The characteristics of the structures are obtained. It is emphasized that the most important characteristic of the structure is the hydrogen bond lifetime. According to all temporal characteristics, the hydrogen bond in 3-AP is more long-lived than in the MEA structure. This explains the wider interval of the liquid phase and the higher viscosity in 3-AP than in MEA. The number of intramolecular bonds in 3-AP at a temperature of 293 K is on average less than that of MEA, however, with increasing temperature, the growth dynamics of this indicator is higher than that of MEA, and at 373 K it exceeds the MEA. Despite the greater number of CH<sub>2</sub> groups in the 3-AP molecule, which are considered as network defects [3], both networks are stable and similar. Maybe because the 3-AP molecule is more flexible than the MEA molecule, due to the fact that there are three rather than two CH<sub>2</sub> groups in it, as in MEA.

A similar pattern is observed in diols. All time characteristics are greater for the propane derivative. Despite the similarity of the ratios of the characteristics of the MEA – 3-AP and EG – 1,3-PD, we note the greater compressibility of 1,3-PD compared to the EG, and hence the greater brittleness (higher absolute value  $\Delta\beta_T/\Delta P$ ). The application of topological methods together with the molecular dynamics method to the description of spatial hydrogen bond networks in liquids and solutions allows one to obtain structural and temporal characteristics of these networks, explaining the physicochemical properties of liquids with these networks, characteristics that cannot be obtained by direct experiment.

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