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The Structure of Liquid Alcohols by Neutron Diffraction. II. Molecular Structure of Ethyl Alcohol

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The structure factor $S_m(Q)$ for liquid ethyl alcohol (C_2D_5OD) at room temperature was obtained by means of the time-of-flight (TOF) neutron diffraction method using electron LINAC. An analysis of the diffraction data was carried out and the molecular structure in liquid phase was determined as follows: the O-D, C-O, and C-C bond lengths are 0.960±0.010 Å, 1.410±0.010 Å and 1.510±0.010 Å, respectively.

In the preceding papers,[1-3] the structure of liquid water (D_2O) and the molecular conformation of liquid methyl alcohol (CD_3OD) were determined successfully by means of the LINAC-TOF neutron diffraction method. Then, as a part of a series of studies for hydrogen-bonded liquids, we have investigated the molecular structure of ethyl alcohol C_2D_5OD in liquid phase.

Several authors have performed studies of gaseous ethyl alcohol. Concerning molecular geometries, the coexistence of two molecular conformations has been reported, which are the hydroxyl trans form and the gauche one.[4-8] The O-H groups in liquid ethyl alcohol are known to be concerned with hydrogen bond.[9-11] But, due to the lack of experimental techniques, there is very scarce information of the molecular structure of ethyl alcohol in liquid phase, which is fundamental to the consideration on the hydrogen-bonded liquid structure. Because the molecular conformation of ethyl alcohol in liquid phase may be subjected to the effect of its comparatively large alkyl group as well as to that of hydrogen bonding, its geometry in liquid phase is very interesting in comparison with the cases of water[1,2] and methyl alcohol.[3]

These circumstances add special interest to the investigation of molecular conformations in liquid ethyl alcohol. The objective of the present work is not only to determine the molecular structure of ethyl alcohol C_2D_5OD in liquid phase but also to examine that of a series of hydrogen-bonded liquids, D_2O, CD_3OD, and C_2D_5OD. Then, we have carried out a LINAC-TOF neutron diffraction measurement on liquid ethyl alcohol and have made an analysis of the data to determine its molecular structure.

Experimental

The experiment was performed by means of the TOF neutron diffraction method using electron LINAC at Hokkaido University. Neutron scattering intensities were measured for liquid ethyl alcohol C_2D_5OD (purity of deuteration 99%, Commissariat à l' Energie Atomique (CEA), France) at room temperature at five different scattering angles: 2θ=30.0°, 40.0°, and 65.0° at 24.0±0.5 °C, 2θ=90.0° at 20.0±0.5 °C, and, 2θ=120.0 at 22.0±0.5 °C. A thin-walled cylindrical quartz vessel was used to contain the sample. Detailed experimental apparatus and procedures were reported elsewhere.[3,12] After all corrections (background, absorption, multiple scattering, inelastic scattering and incoherent scattering), absolute normalizations and Q-scale calibrations, we obtained structure factors $S_m(Q)$ for five different scattering angles as shown in Fig. 1. The coincidence of the values from different angles in each overlapping region of Q is quite well as seen in the figure, and, combining these data set, we obtained the final $S_m(Q)$ curve of wide Q range. The statistical error for values of the $S_m(Q)$ is smaller than 1.0%, and the resolving power $\Delta Q/Q$ less than a few % in the whole range of Q.

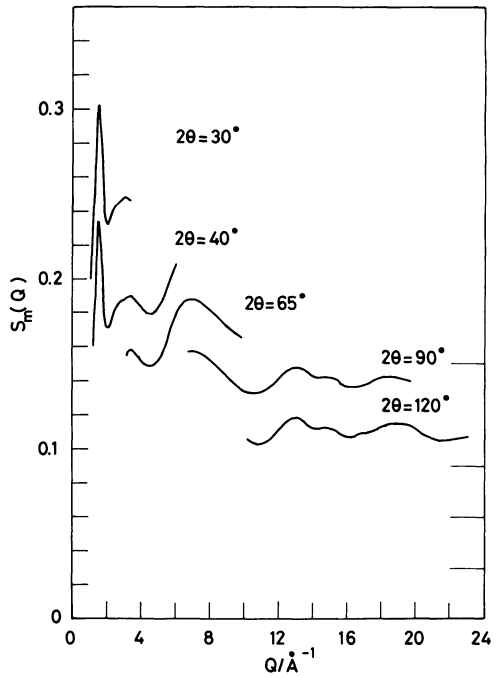

Fig. 1. Observed neutron structure factors $S_m(Q)$ for deutrated ethyl alcohol at various scattering angles.

Procedures of Analysis

Theoretical framework and procedures for determining the molecular structure from observed $S_m(Q)$ data have been stated previously,[3,13] and only a brief description is given here.

The intramolecular structure factor $f_1(Q)$, which is a dominant part of $S_m(Q)$ at higher Q, is written as,

$$f_1(Q) = \left(\sum_i b_i\right)^{-2} \sum_{ij} b_i b_j j_0(Qr_{ij}) \exp(-\gamma_{ij}Q^2), \quad (1)$$

where b_i is the coherent scattering length of i-th nucleus in the molecule, r_{ij} the distance between i-th and j-th nucleus, $2\gamma_{ij}$ the mean square variation to the distance r_{ij} and $j_0(x)=\sin x/x$ a zeroth order spherical Bessel function. $\sum$ is over all the nuclei in the molecule. With

respect to the mean square variation $2\gamma_{ij}$, we assume that $\gamma_{ij}=1/2D_{ij}^2r_{ij}$, where D_{ij} is estimated to be 0.03 Å$^{1/2}$ per Å for distances between carbon and oxygen atoms, 0.036 Å$^{1/2}$ for that between carbon atoms and 0.06 Å$^{1/2}$ for other distances in the molecule.[13]

The structure of ethyl alcohol molecule C_2D_5OD is shown in Fig. 2. The methyl group can rotate about the C-C axis in Fig. 2, and it is assumed that the three C-D bonds and the three DCD angles in the methyl group are all identical, respectively. It is also assumed that the deuterium atoms in the methylene group are located in plane symmetry about the CCO plane. The hydroxyl group can rotate about the C-O axis (Fig. 2). Then, we characterize the molecular structure by twelve structural parameters, *i.e.*, the bond lengths r_{OD}, r_{CO}, r_{CC}, r_{CD_M}, and r_{CD_N}, and, the angles COD, CCO, DCD_M, DCD_N, CCD_N, τ, and ϕ (Fig. 2). In order to determine these molecular parameters, $f_1(Q)$ were calculated for more than 15000 models by using Eq. 1 and the curves obtained were compared with the observed $S_m(Q)$ data in the higher Q region ($Q\gtrsim 6$ Å^{-1}).[3,13] The magnitudes of the parameters were varied in reference to the values given in Table 1.

Determination of the Molecular Structure

Observed Structure Factor Data. The structure factor data $S_m(Q)$ obtained for liquid ethyl alcohol C_2D_5OD is shown in Fig. 3. Comparing this $S_m(Q)$ data with those obtained for liquid water D_2O (Fig. 1 in Ref. 1 and Fig. 5 in Ref. 2), liquid methyl alcohol CD_3OD (Fig. 3 in Ref. 3) and liquid acetyl chloride CD_3COCl (Fig. 3 in Ref. 13) at room temperatures, we can point out several distinctive features as follows.

(1) With respect to the first peaks for the series of hydrogen-bonded systems, D_2O, CD_3OD, and C_2D_5OD, ratios of the heights to its $S_m(Q)$ values at $Q\to\infty$ decrease monotonously in the order of D_2O (≈2.0), CD_3OD (≈1.7), and C_2D_5OD (≈1.4). The same trend is seen for the peak positions (≈2.0 Å^{-1}, ≈1.8 Å^{-1}, and ≈1.5 Å^{-1} for D_2O, CD_3OD, and C_2D_5OD, respectively) as well as for their width as clearly seen.

(2) In the case of methyl alcohol CD_3OD, there is a doublet hump at *ca.* Q=4 Å^{-1}, and the similar but more subtle trend is observed for C_2D_5OD. On the other hand, for heavy water, there is a singlet hump at *ca.* Q=4 Å^{-1} of its $S_m(Q)$ curve. In the preceding paper of D_2O,[1,2] it is elucidated from the analysis of $S_m(Q)$ data that the hump is originated in the existence of the hydrogen-bonded liquid structure. Hydrogen-bonded structures are also expected in liquid CD_3OD and C_2D_5OD.[9-11] In addition to that, the calculated $f_1(Q)$ curves of these fluids have a peak at *ca.* Q=4 Å^{-1} (Ref. 3 for CD_3OD and Fig. 3 in this paper as seen in the next item), which is not seen in the case of water.[1,2] Then, these humps at *ca.* 4 Å^{-1} for CD_3OD and C_2D_5OD systems are due to the superposition of the two contributions: one of them is its intramolecular conformation and the other its intermolecular hydrogen-bonded structure.

(3) Concerning the second peaks at *ca.* Q=7 Å^{-1}, its intensity for CD_3OD and C_2D_5OD is distinctive, being in contrast to the broad second peak at *ca.* Q=8 Å^{-1} in the $S_m(Q)$ curve for D_2O. And, further, the position of each second peak is seen to shift to smaller Q side in the order of D_2O, CD_3OD, and C_2D_5OD (≈8.3 Å^{-1}, ≈7.1 Å^{-1}, and ≈6.8 Å^{-1}).

(4) Concerning the third peaks at *ca.* 13 Å^{-1}, the shoulder at *ca.* 14—15 Å^{-1} for C_2D_5OD is distinctive, being in contrast to the cases of D_2O and CD_3OD. It is noticeable that the nearly identical feature is seen in the data for liquid acetyl chloride.

(5) There are marked forth peaks at *ca.* Q=19 Å^{-1} of the data for CD_3OD and C_2D_5OD. These features are also seen in the case of liquid CD_3COCl.

Determination of Intramolecular Parameters for Liquid Ethyl Alcohol. By making the calculated $f_1(Q)$ curves fit with the observed $S_m(Q)$ data, we have determined the best structural parameters of liquid ethyl alcohol C_2D_5OD at room temperature as follows: r_{OD}=0.960±0.010 Å, r_{CO}=1.410±0.010 Å, r_{CC}=1.510±0.010 Å, r_{CD_M}=1.080±0.005 Å, r_{CD_N}=1.085±0.005 Å, COD=120.0±5.0°, CCO=105.0±1.0°, DCD_M=110.0±0.5DCD_N=112.0±3.0°, CCD_N=106.0±1.0°, and ϕ=12.0±5.0°.

Two structural models shown in Table 2, which differ only in the magnitudes of parameter τ determining the rotation angle of O-D bond, are found to give the best $f_1(Q)$ curves: τ=0.0°, the trans conformation and 160.0°, the gauche one. As seen in Fig. 3, the coincidence between the calculated $f_1(Q)$ curves for these models and the observed $S_m(Q)$ values is satisfactory

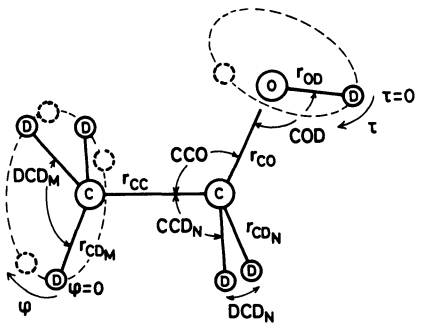

Fig. 2. The structure of deuterated ethyl alcohol (C_2D_5OD) molecule.

TABLE 1. RANGE OF PARAMETERS

Parameter	Range	Interval of variation
r_{OD}/Å	0.930—1.010	0.010
r_{CO}/Å	1.380—1.445	0.005
r_{CC}/Å	1.480—1.540	0.010
r_{CD_M}/Å	1.070—1.100	0.005
r_{CD_N}/Å	1.070—1.100	0.005
COD/°	100.0—130.0	1.0
CCO/°	100.0—120.0	1.0
DCD_M/°	102.0—118.0	1.0
DCD_N/°	100.0—125.0	1.0
CCD_N/°	100.0—120.0	1.0
τ/°	0.0—360.0	5.0
ϕ/°	0.0—120.0	5.0
	free rotation	—

in the higher Q region ($Q \gtrsim 6$ Å^{-1}). The best structural parameters determined are tabulated in Table 3, together with those by other workers.[5,6,14]

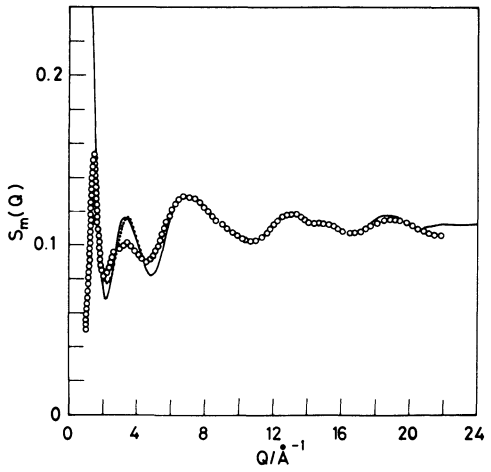

Fig. 3. Comparison between observed neutron structure factor $S_m(Q)$ and present $f_1(Q)$ curves calculated. ○: observed $S_m(Q)$, ——: calculated $f_1(Q)$ for the gauche conformation ($\tau = 160.0°$, Table 2), ($\varepsilon = 0.003327$), ·····: calculated $f_1(Q)$ for the trans conformation ($\tau = 0.0°$, Table 2), ($\varepsilon = 0.003328$).
ε is a measure for indicating the deviations of $f_1(Q)$ from the experimental data, and is expressed as,

$$\varepsilon = (\sum_i^N \{S_m(Q)_{obsd} - f_1(Q)_{calcd}\}^2)^{1/2} / \sum_i^N S_m(Q)_{obsd},$$

where N is the number of data points in the fitting range of Q, 6—18 Å^{-1}.

Structure of Molecules in Liquid State Compared with That in Gaseous One. By using microwave techniques, the geometrical parameters of ethyl alcohol molecules in gaseous phase were given by Sasada *et al.* for the trans and gauche conformations[5] and by Culot for the trans conformation[6] (Table 3). We have calculated the $f_1(Q)$ curves by using their parameters[5,6] and those are compared with the present $S_m(Q)$ curve in Fig. 4. Significant discrepancies between the present data and the $f_1(Q)$ curves calculated are seen on the whole range of Q. The disagreement at higher Q regions ($Q \gtrsim 6$ Å^{-1})[3,14] is ascribed to the variation of the intramolecular structure of molecules from gaseous to liquid states, as seen in Table 3.

One of the most interesting parameters of the molecule in liquid phase is the O-D distance, because a stretching of the bond length from gaseous to liquid phase gives a criterion for the strength of hydrogen bonds. As seen in Table 3, the present value of O-D distance obtained is 0.960±0.010 Å, and is nearly identical with that in gaseous state. It is distinguished from the cases of D_2O (0.98 Å)[1,2] and CD_3OD (0.99 Å),[3] and this trend suggests that the strength of hydrogen bonds for these fluid systems follows in the order of $C_2D_5OD \lesssim CD_3OD \lesssim D_2O$. The trend is also seen in the coordination numbers of these systems obtained by computer experiments.[11,15,16]

Concerning the C-O distance, we obtained the value of 1.410±0.010 Å. This is nearly identical with those obtained for gaseous dimethyl ether (1.410 Å)[17] and gaseous diethyl ether (1.408 Å),[18] and shorter than that obtained for gaseous ethyl alcohol by Culot (1.431 Å)[6]

Table 2. Geometrical parameters of best structural models determined by neutron diffraction method

r_{OD}/Å	r_{CO}/Å	r_{CC}/Å	r_{CD_M}/Å	r_{CD_N}/Å	COD/°	CCO/°	DCD_M/°	DCD_N/°	CCD_N/°	τ/°	ϕ/°	$\varepsilon \times 10^3$
0.960	1.410	1.510	1.080	1.085	117.0	105.0	109.5	112.0	106.0	160.0	10.0	3.327
0.960	1.410	1.500	1.080	1.085	123.0	105.0	110.5	112.0	106.0	0.0	15.0	3.328

With respect to ε, see Fig. 3.

Table 3. Comparison of intramolecular parameters obtained for ehtyl alcohol molecule in the present study with those by other workers

	Present (liquid)	Montague *et al.*[a] ($\lambda = 0.5$ Å liquid	Montague *et al.*[a] $\lambda = 0.7$ Å)	Culot[b] (gas)	Sasada *et al.*[c] (gas)	Sasada *et al.*[c] (gas)
r_{OD}/Å	0.960±0.010	0.966±0.010	0.931±0.006	0.971	(0.9451)	(0.9451)
r_{CO}/Å	1.410±0.010	1.571±0.016	1.416±0.009	1.431	(1.4247)	(1.4273)
r_{CC}/Å	1.510±0.010	(1.5297)	(1.5297)	1.512	(1.5297)	(1.5297)
r_{CD_M}/Å	1.080±0.005	(1.0936)	(1.0936)	1.088—1.091[d]	(1.0936)	(1.0936)
r_{CD_N}/Å	1.085±0.005	(1.0936)	(1.0936)	1.098	(1.0936)	(1.0936)
COD/°	120.0°±5.0°	106.4°±1.7°	107.3°±1.2°	105.4°	108°32′±29′	108°32′±29′
CCO/°	105.0°±1.0°	111.1°±1.6°	113.3°±0.9°	107.8°	107°20′±14′	112°21′±30′
DCD_M/°	110.0°±0.5°	(108°38′)	(108°38′)	108.4—108.9°[d]	108°38′±42′	108°38′±42′
DCD_N/°	112.0°±3.0°	(109°30′)	(109°30′)	108.0°	109°05′±33′	109°05′±33′
CCD_N/°	106.0°±1.0°	(109°30′)	(109°30′)	110.7°	110°18′±42′	110°18′±42′
τ/°	{0.0° {160.0°±10.0°	—	—	0.0°	0.0°	126.0°±6.0°
ϕ/°	12.0°±5.0°	—	—	0.0°	0.0°	0.0°
Shape	trans/gauche	—	—	trans	trans	gauche

a) Neutron diffraction at reactor, Ref. 14. b) Microwave, Ref. 6. c) Microwave, Ref. 5. d) This author obtaines different values for each geometrical parameter. The values in parentheses were assumed.

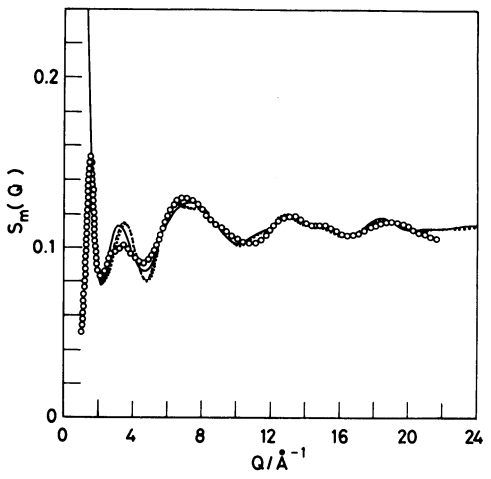

Fig. 4. Comparison between observed neutron structure factor $S_m(Q)$ and calculated $f_1(Q)$ curves for the models given by Sasada *et al.* and by Culot in gaseous phase.
○: observed $S_m(Q)$, ——: calculated $f_1(Q)$ for the gauche conformation by Sasada *et al.*[5] ($\tau=126.0°$, Table 3), ($\varepsilon=0.007080$), ----: calculated $f_1(Q)$ for the trans conformation by Sasada *et al.*[5] ($\tau=0.0°$, Table 3), ($\varepsilon=0.007084$), ·····: calculated $f_1(Q)$ for the trans conformation by Culot[6] ($\tau=0.0°$, Table 3), ($\varepsilon=0.006429$).
With respect to ε, see Fig. 3.

and that by Sasada *et al.* (1.4247 Å, assumed value).[5] The Montague's value of the C-O bond, 1.571 Å in liquid phase is too large, as mentioned in their article.[14] The C-C distance obtained is 1.510±0.010 Å, being in good agreement with that by Culot (1.512 Å) in gaseous phase.[6] With respect to the methyl group, a slight shortening of the C-D distance and a slight increase of the DCDM angles are observed in comparison with those in gaseous state, and the same trend is also observed in the case of methyl alcohol.[3] The methyl rotation angle obtained is 12.0±5.0° and is nearly identical with that for liquid methyl alcohol.[3] Concerning the models with freely-rotating methyl group, the $f_1(Q)$ calculated is found to disagree with the observed $S_m(Q)$ ($Q\gtrsim6$ Å^{-1}) in contrast to the case of CD_3OD.[3] With respect to the angular parameters in the ethylene group, DCDN and CCDN angles are 112.0±3.0° and 106.0±1.0°, respectively, and is different from those in gaseous phase, about 108.0—110.7° for both angular parameters (Table 3). The C-D bonds in the ethylene group are 1.085±0.005 Å, and are shorter than those in gaseous phase, 1.094—1.098 Å (Table 3). With respect to the hydroxyl rotation angle τ for the gauche ethyl alcohol molecule, the present value is 160.0±10.0° and larger than that in gaseous state, 126.0±6.0°.[5]

Trans and Gauche Conformations with Respect to the Hydroxyl Internal Rotation. As stated in the preceding item, two conformations concerning the rotation of the OD radical, trans and gauche forms, are expected to exist in gaseous phase. With respect to the energy difference between the two conformations, Radom *et al.* gave the value of 0.63 kcal/mol by *ab initio* calculations.[19] In a recent microwave study on ethyl alcohol, Kakar and Quade showed that the energy difference is only 41.2 cm^{-1} (=0.12 kcal/mol).[8] The number ratio of trans to gauche molecules in the vapour phase at room temperature was estimated to be 2:1 by Barnes and Hallam.[4]

Jönssen reported the coexistence of the two conformers in solid phase by means of the X-ray diffraction.[20] According to the results the number ratio of the two conformers becomes 1:1. On the other hand there is no information concerning the rotational isomers in liquid phase. Considering the interaction between molecules within liquid, we can expect that the energy difference between the conformers of the trans and gauche types in liquid phase is small, and that the two types coexist in liquid phase as well as in gaseous and solid phases. Due to the small energy difference, the main frame of molecules won't be affected strongly by the hydroxyl rotation angle. Then, the present results that the two geometrical models of trans and gauche types fit with the observed $S_m(Q)$ data (Table 2 and Fig. 3) suggest the coexistence of the two conformers in liquid ethyl alcohol. The $f_1(Q)$ curves calculated for these two models are undiscriminated with each other at higher Q region ($Q\gtrsim6$ Å^{-1}, Fig. 3), and show a slight difference at the lower ($Q<6$ Å^{-1}), where intermolecular contributions appear as well as intermolecular ones. And, the number ratio of the two conformers in liquids is not determined in the present study.

On the Intermolecular Contribution to the Total Structure Factor $S_m(Q)$— the Effect of Debye-Waller Factors for Intermolecular Atomic Pairs.

In the present series of studies of liquid alcohols,[3] we have determined intramolecular structures within liquids by making calculated structure factors fit with observed diffraction data in the higher Q region ($Q\gtrsim6$ Å^{-1}), as described above. The procedure of analysis has been applied by several workers[1-3,13,21,22] including us for determining molecular structures from neutron diffraction data of liquids. For its successful application, the following fact is presupposed as the one established empirically for those molecular fluids treated (D_2O, CD_3OD, C_2D_5OD, CD_3COCl, C_3O_2, *etc.*): the $S_m(Q)$ is practically identical with $f_1(Q)$ (Eq. (1)) in the higher Q region ($Q\gtrsim6$ Å^{-1}) as the result of comparatively rapid decay of the intermolecular terms with increasing Q. We consider, here, why the intermolecular contributions decay so rapidly with increasing Q in these liquids. The most deterministic factor of that behavior of intermolecular terms at the high Q region may be tentatively considered to be the Debye-Waller factor of atomic pair between two molecules, and we concentrate our present concern to this problem.

Concerning the Debye-Waller factors for intermolecular atomic distances, which is expressed as exp ($-\gamma_{ij}Q^2$) ($2\gamma_{ij}$: the mean-square amplitude for the variation of the distance), a few discussions will be given below. The mean-square amplitude for the variation of the distance between atoms i and j in molecles p and

q ($p \neq q$) can be expressed as,

$$2\gamma_{ij} = \langle \Delta r_{cip}^2 \rangle + \langle \Delta r_{cpq}^2 \rangle + \langle \Delta r_{cjq}^2 \rangle. \quad (2)$$

$\langle \Delta r_{cip}^2 \rangle$ is the mean-square amplitude for the variation of the distance between the center of molecule p and its i-th atom, and $\langle \Delta r_{cpq}^2 \rangle$ is that for the distance between the centers of the p-th and q-th molecules. In the expression described above, the thermal vibration of atoms within a molecule and the thermal Brownian motion of the molecule on the whole are safely considered to be independent with each other, and the simple sum formula consists. The term $\langle \Delta r_{cpq}^2 \rangle$ is expressed as,

$$\langle \Delta r_{cpq}^2 \rangle = \langle \Delta r_{cp}^2 \rangle + \langle \Delta r_{cq}^2 \rangle = 2\langle \Delta r_{cp}^2 \rangle, \quad (3)$$

where $\langle \Delta r_{cp}^2 \rangle$ is the term due to the Brownian motion of the center of the molecule p. Then,

$$\gamma_{ij} = \langle \Delta r_{cp}^2 \rangle + \frac{1}{2}(\langle \Delta r_{cip}^2 \rangle + \langle \Delta r_{cjq}^2 \rangle). \quad (4)$$

The term $\langle \Delta r_{cp}^2 \rangle$ can be determined approximately from the effective free volume v_f (the statistical average of fluctuational void space[23,24]) and the effective hard-sphere diameter of molecules. The magnitude of the effective hard-sphere diameter is estimated from the first peak region of the $S_m(Q)_{obsd}$ by using the Percus-Yevick equation, that is, by making the theoretial $S(Q)$ fit with the observed first peak of $S_m(Q)$.[25-28] At the same time, we can obtain the packing fraction ξ, and can estimate the magnitude of v_f by the use of the Percus-Yevick equation.[23-24] Thus, for CD_3OD and C_2D_5OD, the magnitude of $\langle \Delta r_{cp}^2 \rangle^{1/2}$ becomes nearly equal at room temperature: 0.12 Å (the magnitudes of ξ also become nearly equal for these two alcohols, 0.36). The γ_{ij} for the intermolecular D···D pair in CD_3OD and C_2D_5OD becomes $(0.12)^2 + \langle \Delta r_{cD}^2 \rangle$, and $\langle \Delta r_{cD}^2 \rangle \gtrsim (0.06)^2$. Thus, for the intermolecular D···D pair, the term $\exp(-\gamma_{ij}Q^2)$ is found to decay to e^{-1} at about $Q \sim 7$ Å^{-1}. As clearly seen in the above rough estimation, the γ_{ij} for the intermolecular atomic pair is dominated by the contribution from the thermal Brownian motion of molecules, and this is expected to be the dominant factor for the rapid decay of the intermolecular contribution to the $S_m(Q)$ at about 6—7 Å^{-1} (Fig. 5) in sharp contrast to the case of the intramolecular terms. This is considered to be the main support of the adequacy of determining the intramolecular parameters from the observed $S_m(Q)$ in the higher Q region ($Q \gtrsim 6$ Å^{-1}).

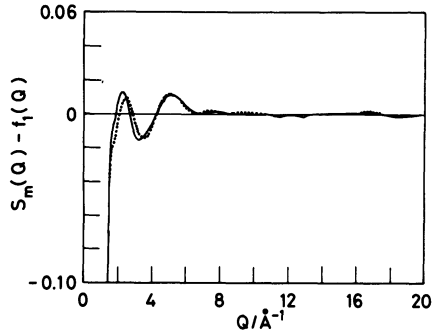

Fig. 5. Intermolecular contributions $S_m(Q)_{obsd} - f_1(Q)_{calcd}$ for the present two models.
——: intermolecular factor for the gauche conformation ($\tau = 160.0°$, Table 2), ·····: intermolecular factor for the trans conformation ($\tau = 0.0°$, Table 2).

Concluding Remarks

A neutron diffraction study of liquid ethyl alcohol (C_2D_5OD) by means of the LINAC-TOF method was performed and the structure of molecules within liquids was determined. The present result is primarilly due to the success in securing the structure factor data for wide Q range with sufficient accuracy. Then the result as well as the preceding one of CD_3OD[3] confirms the usefulness of the present LINAC-TOF neutron diffraction method to the structural study of polyatomic molecular fluids.

References

1) N. Ohtomo, K. Tokiwano, and K. Arakawa, *Bull. Chem. Soc. Jpn.*, **54**, 1802 (1981).
2) N. Ohtomo, K. Tokiwano, and K. Arakawa, *Bull. Chem. Soc. Jpn.*, **55**, 2788 (1982).
3) Y. Tanaka, N. Ohtomo, and K. Arakawa, *Bull. Chem. Soc. Jpn.*, **57**, 644 (1984).
4) A. J. Barnes and H. E. Hallam, *Trans. Faraday Soc.*, **66**, 1932 (1970).
5) Y. Sasada, M. Takano, and T. Satoh, *J. Mol. Spectrosc.*, **38**, 33 (1971).
6) J. P. Culot, Fourth Austin Symposium on Gas Phase Molecular Structure, Austin, Texas, 1972, Paper T8; through *J. Phys. Chem. Ref. Data*, **8**, 619 (1979).
7) J. R. During, W. E. Bucy, C. J. Wurrey, and L. A. Carreira, *J. Phys. Chem.*, **79**, 988 (1975).
8) R. K. Kakar and C. R. Quade, *J. Chem. Phys.*, **72**, 4300 (1980).
9) W. A. P. Luck, "Water", ed by F. Franks, Plenum, New York (1973) Vol. 2, Chap. 4.
10) A. N. Fletcher, *J. Phys. Chem.*, **76**, 2562 (1972).
11) W. L. Jorgensen, *J. Am. Chem. Soc.*, **103**, 345 (1981).
12) N. Ohtomo, Y. Tanaka, and K. Arakawa, *Bull. Faculty Eng. Hokkaido Univ.*, **109**, 43 (1982).
13) N. Ohtomo, and K. Arakawa, *Bull. Chem. Soc. Jpn.*, **53**, 1510 (1980).
14) D. G. Montague, I. P. Gibson, and J. C. Dore, *Mol. Phys.*, **47**, 1405 (1982).
15) R. H. Stillinger, *Science*, **209**, 451 (1980).
16) W. L. Jorgensen, *J. Am. Chem. Soc.*, **103**, 341 (1981).
17) U. Blukis, P. H. Kasai, and R. J. Myers, *J. Chem. Phys.*, **38**, 2753 (1963).
18) M. Hayashi and K. Kuwada, *Bull. Chem. Soc. Jpn.*, **47**, 3006 (1974); M. Hayashi, H. Imaishi, K. Ohno, and H. Murata, *ibid.*, **44**, 299 (1971).
19) L. Radom, W. J. Hehre, and J. A. Pople, *J. Am. Chem. Soc.*, **94**, 2371 (1972).
20) P.-G. Jönsson, *Acta Crystallogr., Sect. B*, **32**, 232 (1976).
21) R. Triolo and A. H. Narten, *J. Chem. Phys.*, **63**, 3624 (1975).
22) G. Walford, J. H. Clarke, and J. C. Dore, *Mol. Phys.*, **36**, 1581 (1978).
23) K. Arakawa and K. Kojima, *Bull. Chem. Soc. Jpn.*, **48**, 26 (1975).
24) K. Arakawa, K. Tokiwano, and K. Kojima, *Bull. Chem. Soc. Jpn.*, **50**, 65 (1977).
25) N. W. Ashcroft and J. Lekner, *Phys. Rev.*, **145**, 83 (1966).
26) N. W. Ashcroft and D. C. Langreth, *Phys. Rev.*, **156**, 685 (1967).
27) J. E. Enderby and D. M. North, *Phys. Chem. Liquids*, **1**, 1 (1968).
28) Y. Tanaka, N. Ohtomo, and K. Arakawa, *J. Phys. Soc. Jpn.*, **52**, 2093 (1983).