

水溶液の差分空間分布関数による解析 III：
直鎖及び分岐型アルキル基を有する
アルコールとエーテルの水和構造

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Difference Spatial Distribution Function Analysis of Aqueous Solutions. III. Hydration Structures of Alcohol and Ether Solutions Having Straight Chain and Branched Alkyl Groups

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ABSTRACT: Spatial distribution functions (SDFs) obtained from Monte Carlo simulations were applied to characterize the anisotropic structure of infinitely dilute aqueous solutions of alcohols and ethers having straight chain and branched alkyl groups. In spite of the different size and shape of the hydrophobic groups, the spatial orientation of the hydrogen-bonded water molecules was found to be of linear type with a triple layer structure in the hydrogen acceptor (HA) region and a double layer structure in the hydrogen donor (HD) region. The volumes and the coordination number in the HA region were essentially identical for all alcohol and ether solutions. In the hydrophobic hydration (HH) region, these values increased with increasing size and shape of hydrophobic groups, except of isopropyl alcohol and isopropyl methyl ether solutions. These results indicated that the hydration structures around the isopropyl group in alcohol and ether solutions differed from those in other solutions. From the results of the difference SDF (DSDF), it was apparent that the distribution of hydration water molecules in the HA region for ether solution was characterized by the increase of the distribution in the direction of lone pair electrons on the oxygen atom of the solute molecule with increasing hydrophobicity.

抄録 直鎖型及び分岐型アルキル基を有するアルコールとエーテルの無限希釈水溶液の構造異方性を特徴付けるために空間分布関数を利用した。その結果、疎水性基の違い

によらず水素原子受容体 (HA) 領域では三層構造、水素原子供与体領域 (HD) では二層構造であった。イソプロピル基を持つアルコール及びエーテルを除き、HA領域の分布体積と配位数はアルコール水溶液とエーテル水溶液の結果がほぼ一致し、疎水性水和 (HH) 領域では、これらの値は疎水性基が大きくなると増加した。この結果はイソプロピル基の周辺の水和構造が他の疎水性基の水溶液と異なっていることを示した。差分空間分布関数の結果より、エーテル水溶液のHA領域の水分子の分布が疎水性の増加とともにエーテル酸素原子のローソペア方向に水和水の分布の増加をもたらすことが明らかとなった。