水溶液の差分空間分布関数による解析 IV：
エチレングリコールのgGg'からtGg'への
配座変換過程における水和構造変化

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Difference Spatial Distribution Function Analysis of Aqueous Solutions. IV. Hydration Structure Changes of Ethylene Glycol Solutions throughout Conformational Change Process from gGg' to tGg' Conformers

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ABSTRUCT： Monte Carlo simulations were carried out for an infinitely dilute aqueous solution of two stable conformers (gGg' and tGg') and of three conformations between gGg' and tGg' conformers of ethylene glycol (EG). Based on the spatial distribution function (SDF) obtained from the MC simulation in the above conformations in liquid water, the high distribution of hydration water molecules could be divided into hydrogen acceptor (HA), hydrogen donor (HD), MIX (overlapped distribution of HA and HD), and hydrophobic hydration (HH) regions. The spatial orientations of hydrogen-bonded water molecules were found to be of a linear type with a triple-layer structure in the HA region and HA part (in the MIX region), and double-layer structures in the HD region and HD part (in the MIX region). In addition, it was apparent that the spatial orientations of these water molecules were of the linear type throughout the conformational change process from gGg' to tGg' conformers in liquid water. From the difference SDF (DSDF) between the SDFs of two conformations, we concluded that the distribution of hydration water molecules in the HA and HD parts of the MIX region are governed by the competition of internal hydrogen bonds between the hydrogen atom and two lone-pair electrons on the oxygen atom of an EG molecule.

抄録 エチレングリコール（EG）の２つの安定配座とこれらの間の３つの配座の無限希釈水溶液のモンテカルロシミュレーションを行った。空間分布関数の解析から、すべての配座の水和水の分布が水素原子受容体（HA）領域と水素原子供与体（HD）領域、MIX領域（HAとHDが重なった）及び疎水性水和（HH）領域に分けられた。このうちHA領域とMIX領域のHA部分は配座変換過程を通じても常に三層構造であり、水分子の配向は直線型を保持していた。差分空間分布関数の解析からMIX領域のHAとHD部分の水和水の分布はEGの水素原子とEGの酸素原子の２つのlone-pair間の分子内水素結合の競合によって支配されていることが明らかとなった。