

研究论文

## $A_{a1}D_{d1}-A_{a2}D_{d2}$ 型氢键体系的网络结构参数

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**摘要** 利用溶胶-凝胶分配理论对氢键溶液的模型体系进行研究, 给出了体系的凝胶化条件以及凝胶点后氢键网络中各类结构参数的计算方案, 并进行了相应的数值计算. 结果表明, 当两类质子受体基团的活性不同时, 质子受体基团的竞争作用对网络结构有一定影响. 这为控制氢键网络结构特征提供了可能的理论线索.

**关键词** [氢键网络](#) [结构参数](#) [溶胶-凝胶相变](#)

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## Structural Parameters for Hydrogen Bonding Networks Formed in Systems of $A_{a1}D_{d1}-A_{a2}D_{d2}$ Type

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**Abstract** Structural parameters of hydrogen bonded network formed in a model system of hydrogen bonding solutions were studied on the basis of the sol-gel partition theory. With the proposed method, the gelation condition, the theoretical and numerical results of these structural parameters were presented in the cases that there exist the activity differences between the proton-donors and proton-accepters. It is shown that the activity difference can give rise to influence on the hydrogen bonded networks. This provides a possible theoretical clue to control of the hydrogen bonded networks.

**Key words** [Hydrogen bonded network](#) [Structural parameters](#) [Sol-gel phase transition](#)

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