液体内聚能的统计热力学研究

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摘要
用统计热力学方法建立了一个液体内聚能模型。它能用来计算各种液体的内聚能和溶解度参数。考虑到液体分子间的强相互作用，引入了一个阻障因子，以修正其转动和振动对内配分函数的贡献。这个因子依赖于液体的密度，它与密度间的关系也在模型中导得。对溶解度参数的计算结果表明，与文献值的一致性令人满意。
关键词　　内聚能　溶解度　热力学研究　统计力学

分类号　0642

Statstical thermodynamic study on cohesive energy of liquids

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Abstract a model of the cohesive energy of liquids, which can be used to calculate the cohesive energy and solubility parameters of various liquids, has been established using a statistical thermodynamic method. In consideration of the strong intermolecular interactions in liquids, a hindering factor is introduced to modify the contribution of their rotation and vibration to the internal partition function. The factor is dependent on the density of liquids. The relationship between this factor and density is also derived. The results of calculation for the solubility parameters are consistent with the literature values.

Key words COHESIVE ENERGY SOLUBILITY STATISTICAL MECHANICS

DOI:

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