用于计算机模拟的**ab initio N2-H2O势**

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摘要　　用6-31G^*^*基组对N2-H2O体系作了量子化学ab initio计算研究。采用模拟褪火(Simulated anneal)算法将所得的计算结果用于拟合一个适用于计算机模拟的解析势能函数。函数的形式为10-6的Lennard-Jones势加指数项校正。鉴于非极性溶质的排斥能对第一水合层的形成起着重要作用,在拟合过程中对势能的排斥部分和吸引部分作了等权考虑。

关键词　　水　氮　计算机模拟　从头计算法　国家教委高等学校博士学科点专项科研基金　解析势函数

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An ab initio N2-H2O potential for computer simulations

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Abstract　N2-H2O system was studied by ab initio SCF calculations with a 6-31G^*^* basis set. The resulted 200 data were fitted to an analytical function assuming pairwise additivity for the interaction between individual centres. The analytical functions were Lennard- Jones 10-6 and exponential form. A satisfactory fitting result was achieved by the simulated anneal algorithm. Special care was paid to repulsive region, which gives the important contributions to the formation of the first solvation shell of apoler solutes.

Key words　WATER　NITROGEN　COMPUTERIZED SIMULATION　AB INITIO CALCULATION

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