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Full Paper

应用**ABEEM/MM**方法研究**Co^{3+}**离子水溶液的性质

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摘要 应用原子一键电负性均衡方法融合进分子力场（ABEEM/MM）对Co^{3+}水溶液在室温（298.15K）时进行了细致的分子动力学模拟研究。通过模拟获得了Co^{3+}水溶液的各种性质，例如：静态性质，包括径向分布函数，角度分布函数，ABEEM电荷分布，水分子的结构和平均氢键个数等；动力学性质，包括扩散系数和振动光谱；和溶剂化能等热力学性质。结果表明，ABEEM/MM模型能够较准确地描述Co^{3+}水溶液的各种性质。

关键词 分子动力学模拟,ABEEM/MM模型,Co^{3+}水溶液

分类号

Theoretical Study on Co^{3+} in Aqueous Solution in Terms of ABEEM/MM Model

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Abstract A detailed theoretical investigation on Co^{3+} hydration in aqueous solution has been carried out by means of molecular dynamics (MD) simulations based on the atom-bond electronegativity equalization method fused into molecular mechanics (ABEEM/MM). The effective Co^{3+} ion-water potential has been constructed by fitting to *ab initio* structures and binding energies for ionic clusters. And then the ion-water interaction potential was applied in combination with the ABEEM-7P water model to molecular dynamics simulations of single Co^{3+}(aq.) solution, managing to reproduce many experimental structural and dynamical properties of the solution. Here, not only the common properties (radial distribution function, angular distribution function and solvation energy) obtained for Co^{3+} in ABEEM-7P water solution were in good agreement with those from the experimental methods and other molecular dynamics simulations but also very interesting properties of charge distributions, geometries of water molecules, hydrogen bond, diffusion coefficients, vibrational spectra are investigated by ABEEM/MM model.

Key words molecular dynamics simulation ABEEM/MM model Co^{3+} hydration in aqueous solution

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