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Full Papers

TiO_2和Mg-Fe型类水滑石特征电离/络合平衡常数研究

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摘要 采用改进的双外推法（MDE）分别研究了不带结构电荷的TiO_2和带结构电荷的Mg-Fe型类水滑石的特征界面电离平衡常数（pK_{a1}^{int}和pK_{a2}^{int}）和络合平衡常数（$p*K_C^{int}$和$p*K_A^{int}$）。将TiO_2的结果与文献中采用经典双外推法（CDE）所得结果对比表明，MDE法获得的pK_{a1}^{int}和pK_{a2}^{int}值与CDE法一致，而$p*K_C^{int}$和$p*K_A^{int}$值有很大差别，理论上分析认为MDE法结果更准确。采用MDE法获得的电离/络合平衡常数值对TiO_2和Mg-Fe型类水滑石的荷电曲线进行了数值模拟，证明结果是可信的。

关键词 界面络合模型；双电层；酸-碱化学；两性界面
分类号

Evaluation of Intrinsic Ionization and Complexation Constants of TiO_2 and Mg-Fe Hydrotalcite-like Compounds

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Abstract The intrinsic surface reaction constants, pK^{int}_{a1}, pK^{int}_{a2}, $p^*K^{int}_C$ and $p^*K^{int}_A$, were evaluated by a modified double extrapolation (MDE) for TiO_2 without structural charge and Mg-Fe hydrotalcite-like compounds (HTlc) with structural charge, respectively. The results of intrinsic surface reaction constants for TiO_2 were compared with those obtained by class double extrapolation (CDE) in literature. Furthermore, the values of intrinsic surface reaction constants obtained by MDE were used to simulate the charging behaviors of the materials. The following conclusions were obtained. For TiO_2 without structural charge, the pK^{int}_{a1} and pK^{int}_{a2} evaluated by MDE are equal to those by CDE, however the $p^*K^{int}_C$ and $p^*K^{int}_A$ evaluated by MDE are much different from those by CDE. In principle, the results of the $p^*K^{int}_C$ and $p^*K^{int}_A$ evaluated by MDE are more accurate than those by CDE. The values of intrinsic surface reaction constants obtained by MDE can excellently simulate the charging curves for TiO_2 with the triple layer model (TLM). For HTlc with positive structural charge, the results of $p^*K^{int}_C=0$ and $p^*K^{int}_A\rightarrow\infty$ were obtained by MDE, which means the inert electrolyte chemical binding does not exist; the point of zero net charge (PZNC) of *c*-independence also exist as the same as solid without structural charge, and the pH_{PZNC} obtained by the acid-base titration can excellently be simulated and the surface charging tendency can be simulated to a great extent using the pK^{int}_{a1} and pK^{int}_{a2} evaluated by MDE and the diffuse layer model (DLM).

Key words **Keywords** surface complexation electric double layers acid-base chemistry amphoteric surface

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