

定量结构-性质相关原理在阴离子表面活性剂临界胶束浓度预测中的应用

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**摘要** 利用定量结构-性能相关(QSPR)原理,建立起了8类不同结构,计40个阴离子表面活性剂临界胶束浓度(cmc)的定量模型。所得到的最佳模型包括:分子总能量(E<sub>T</sub>)、分子生成热(ΔH<sub>f</sub>)、分子偶极矩(D)、前线分子轨道能量(E<sub>(LUMO)</sub>,E<sub>(HOMO)</sub>)及憎水基0级Kier & Hall指数(KHO),计6个描述符,复相关系数R<sup>2</sup> = 0.9778。

**关键词** [结构与性能关系](#) [胶束](#) [表面活性剂](#) [前线轨道理论](#)

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## Prediction on Critical Micelle Concentration of Anionic Surfactants in Aqueous Solution: Quantitative Structure-Property Relationship Approach

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**Abstract** To predict critical micelle concentration (cmc) of anionic surfactants in aqueous solution, a quantitative structure-property relationship (QSPR) has been found the descriptors of eight series including 40 anionic surfactants. The best-regressed model includes six descriptors: the Kier & Hall index of zero order KHO of the hydrophobic fragment of the surfactant, the total molecular energy E<sub>T</sub>, the heat of molecular formation ΔH<sub>f</sub>, the molecular dipole moment D and the energies of frontier molecular orbits E<sub>(LUMO)</sub> and E<sub>(HOMO)</sub> of the surfactant. The established best general QSPR between lg cmc and the descriptors produces the relevant coefficient of multiple determination high up to 0.9778.

**Key words** [STRUCTURE AND PROPERTY CORRELATION](#) [MICELLE](#) [SURFACTANTS](#) [FRONTIER ORBITAL THEORY](#)

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