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硝基苯类化合物的**FMO**位电荷密度能**S_(Ei)~(HO)**与生物毒性的**QSAR**研究

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摘要　应用简易的量化方法计算了20多种硝基苯衍生物中的64个芳环FMO位电荷密度 能S_(Ei)~(HO)，用回归法建立了一个新的生物毒性评价方程，-lg LC_(50)=0. 6191log K_(ow)+0.1881S_(Ei)~(HO)+4.0894，应用所得方程，预测有机物的生物 毒性，方程对大多数化合物拟和很好。结果表明，所研究的有机物生物毒性同S_ (Ei)~(HO)和log K_(ow)密切相关，同化合物与酶的活性点复合或反应是生物中毒的主要因素。

关键词　硝基苯 P　电荷密度　毒性　定量构效关系

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Study on the QSAR of Biiodegradationh Toxicol of Nitrobenzene Derivatives with Their FMO Potential Charge Density Energies S_(Ei)~ (HO)

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Abstract　Sixty-four FMO potential charge density energies S? were calculated by the simplified quantum chemical method. The new biological toxic evaluation equation, - lg LC50 = 0.61911og Km + 0.1881S? + 4.0894 was set up by the application of regressive method. The QSAR equations were used to calculate biodegradability and it was found that most compounds fit well. It has been shown that the biodegradability of studied compounds has a close relationship with SfP and log Kow. The chief factor of biodegradability is that the reaction or complecation of compound with the active site of enzyme.

Key words　NITROBENZENE P　CHARGE DENSITY　TOXICITY　QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP

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