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N-取代吩噻嗪衍生物分子的结构和二阶非线性光学性质的理论研究

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摘要 在ZINDO方法基础上, 按完全态求和(SOS)公式,
编制了计算分子二阶非线性光学系数βijk的程序。研究了各种取代基在吩噻嗪的氮上取代后衍生物的结构和二阶非线性光学系数。结论是N上取代推电子基对增大二阶光学非线性有利,
N上取代吸电子基对增大二阶光学非线性不利。扩大共轭范围对增大二阶光学非线性有利。对上述结果在微观上给予了解释。

关键词 光学性质 非线性光学 吩噻嗪 P 光学系数 国家教委高等学校博士学科点专项科研基金

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The studies on the structures and nonlinear second-order optical properties of N-substituted phenothiazine derivatives

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Abstract On the basis of ZINDO methods, according to the sum-over-states (SOS) expression, a program for the calculation of nonlinear second-order optical susceptibilities βijk has been devised. The structures and nonlinear second-order optical properties of phenothiazine derivatives substituted at nitrogen by different substituents have been studied. The conclusion is that electron donating groups substituted at N facilitate the nonlinear second-order optical susceptibility, whereas electron with drawing groups substituted at N decrease the nonlinear second-order optical susceptibility. Extending the conjugated area increases the nonlinear second-orer optical susceptibility. The calculated results have been explained micromechanically.

Key words OPTICAL PROPERTIES NON LINEAR OPTICS PHENOTHIAZINE P

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