

## 一水甲酸锂晶体三阶非线性光学性质理论研究

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**摘要** 用含时耦合微扰Hartree-Fock (CPHF) 方法,有限场MP2理方法以及有向气体方法,首次分别在分子和晶体水平上计算了一水甲酸锂晶体三次谐波极化率,表明超分子 $\chi^{(3)}(-3\omega; \omega, \omega, \omega)$ 数值与超分子链长有线性关系;晶体 $\chi^{(3)}(-3\omega; \omega, \omega, \omega)$ 计算值主要受到电子相关影响,其次受到基组和局域场影响,在非共振条件下,频率色散的影响甚小最后,估算了一水甲酸锂的三次谐波系数.

**关键词** [非线性光学](#) [甲酸锂](#) [极化率](#) [谐波分析](#)

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## Theoretical Studies of Third-order Susceptibilities of Lithium Formate Monohydrate (HCOOLi·H<sub>2</sub>O) Crystals

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**Abstract** The theoretical investigations of third-harmonic susceptibilities of lithium formate monohydrate crystals with chemical formula of HCOOLi·H<sub>2</sub>O have been performed for the first time, by using the time-dependent coupled-perturbed Hartree-Fock (CPHF) method, the finite-field MP2 approach and the oriented-gas approximation at both molecular and crystalline levels. It has been found that the elements of  $\chi^{(3)}(-3\omega; \omega, \omega, \omega)$  tensors of supermolecules depend linearly on chain lengths. The calculated magnitudes of  $\chi^{(3)}(-3\omega; \omega, \omega, \omega)$  tensor components of lithium formate monohydrate crystals are influenced by electron correlation, frequency, basis set and the local field factor, of which electron correlation is the most important and frequency dispersion is negligible at the off-resonant frequencies. Finally, the third-harmonic coefficients have been estimated.

**Key words** [NON LINEAR OPTICS](#) [lithium formate](#) [POLARIZABILITIES](#) [HARMONIC ANALYSIS](#)

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