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离子晶体透红外截止波长的拓扑研究

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摘要 基于邻接矩阵和离子结合力参数(b_i)概念, 建立了新的连接性指数(m_B); 用其0、1阶指数${}^0B$和${}^1B$与23种常见透红外离子晶体的晶格能(U)和透红外截止波长(λ)关联, 拟合所得的回归方程的相关系数分别为0.96904、0.98523、0.99185、0.97635, 满足优级或良级标准, 可作为设计透红外离子晶体截止波长的参考.

关键词 透红外截止波长 晶格能 结合力参数 连接性指数

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Topological Research on Long Wavelength Limit of Transparent Ionic Crystals in Infrared Range

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Abstract A novel connectivity topological index(${}^mB$) based on the adjacency matrix and the ionic parameter of binding force(b_i) was derived in the present paper. The 0 and 1 order indexes${}^0B$ and ${}^1B$ of ${}^mB$ were derived to correlate the long wavelength limit(λ) and the lattice energy (U) of 23 different types of transparent ionic crystals in infrared range. The relative coefficients (R=0.96904, 0.98523, 0.99185, 0.97635) of the derived equations are all in the range of higher level standards. Therefore, the results of present research could be useful for the design and evaluation of the long wavelength limit of ionic crystals.

Key words long wavelength limit binding force parameter lattice energy connectivity index

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