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标题: THz Spectroscopic Investigation of Energetic Ion Salt

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摘要: In order to further explore the terahertz spectrum characteristics of energetic ion salts on the basis of the research on traditional nitro energetic materials, and extend applicable scope of terahertz wave technology in the study of safety testing field, experimental measurement and theoretical analysis of THz spectrum for new energetic ion salts (5-ATN and BMDATHBT) were introduced. The absorption coefficient of the samples was measured in the region of 0.5 similar to 2.0 THz by time-domain spectroscopy and by Fourier transform infrared spectroscopy in the 2.0-8.0 THz region. Using the density functional theory methods, the vibration characteristics were simulated by Gaussian 03 and Materials Studio 4.3. The simulated spectrum of samples is in agreement with the experimental data. The result showed that ion salts have the typical absorption peaks that have close relation with the tribal structure, and the interaction between particles and the single skeleton vibrations of individual ion are the main reason for energetic ion salt to form absorption peak in terahertz band, which provides references for detecting high nitrogen compounds by terahertz technique.

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