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Accession number:12991245
Title:Study on the Terahertz Time Domain Spectrum of P-chloroaniline
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Source title:Advanced Materials Research
Abbreviated source title:Adv. Mater. Res. (Switzerland)
Volume:441
Publication date:2012
Pages:741-5
Language:English
ISSN:1022-6680
Document type:Journal article (JA)
Publisher:Trans Tech Publications Ltd.
Country of publication:Switzerland
Material Identity Number:GC91-2012-079
Abstract:P-chloroaniline is one of the most important azo dye intermediates. It is a highly desired research on the identification of P-chloroaniline. Terahertz time domain spectroscopy (THz-TDS) is sensitive to the molecule structure of compound. In this paper, the spectra of P-chloroaniline located at the region from 0.1 to 3 THz were tested by THz-TDS system, and then the geometry structure of p-chloroaniline at the range of 0 THz to 10 THz was optimized, resonance frequency was calculated by Gussian03 software based on the density functional theory (DFT). The results showed that the absorbance peaks at 1.96 THz and 2.20 THz were caused by the hydrogen bonding force or crystal phonon mode, and suggested that it is feasible to identify P-chloroaniline by THz-TDS, which is of great value to the examination of banned azo dyes in the future.
Number of references:14
Inspec controlled terms:density functional theory - dyes - geometry - hydrogen bonds - terahertz spectroscopy - textile technology
Uncontrolled terms:terahertz time domain spectrum - P-chloroaniline - azo dye intermediates - terahertz time domain spectroscopy - molecule structure - THz-TDS system - geometry structure - resonance frequency - Gussian03 software - density functional theory - DFT - absorbance peak - hydrogen bonding force - crystal phonon mode - frequency 0 THz to 10 THz
Inspec classification codes:E3606 Textile industry - E1780 Products and commodities - E1710 Engineering materials - E1525 Industrial processes - E0210E Combinatorial mathematics
Numerical data indexing:frequency 0.0E+00 1.0E+13 Hz
Treatment:Practical (PRA); Theoretical or Mathematical (THR); Experimental (EXP)
Discipline:Manufacturing and production engineering (E)
DOI:10.4028/www.scientific.net/AMR.441.741
Database:Inspec