

IR Absorption Peaks Assignments of LLM-105 by Temperature-Dependent FT-IR Spectroscopy

LI Jing-you^{1,2}, ZHANG Hao-bin², XU Jin-jiang², SUN Jie²

(1. School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang 621010, China; 2. Institute of Chemical Materials, CAEP, Mianyang 621999, China)

Abstract: To accurately determine the assignments of IR absorption peaks for 2, 6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105), the process of change in IR absorption peaks of LLM-105 under the heating conditions was investigated by temperature-dependent FT-IR spectroscopy. The positions of various IR absorption peaks at different temperatures were determined. Results show that with increasing the temperature, the strength of intermolecular hydrogen bond for LLM-105 is significantly weakened. IR absorption peak positions of amino group ($-\text{NH}_2$) and nitro group ($-\text{NO}_2$) participated in forming hydrogen bonds shift at least 4 cm^{-1} . The pyrazine ring and C—N bond do not participate in the formation of hydrogen bonds, their peak positions shift about 1 cm^{-1} .

Key words: 2, 6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105); temperature-dependent IR spectroscopy; hydrogen bond; vibration frequency

CLC number: TJ55; O65

Document code: A

DOI: 10.11943/j.issn.1006-9941.2015.05.019



《含能材料》“观点”征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了“观点”栏目。“观点”栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要研究工作介绍。

《含能材料》高效毁伤弹药专栏征稿

高效毁伤弹药以“利用最小化成本获得最大化效果”为目标,对含能材料的性能和能量提出了更高的要求。为进一步促进高效毁伤弹药及其技术的研究,本刊将于2015年增设高效毁伤弹药专栏,内容涉及(1)传统含能材料的优化和改进以及先进含能材料的开发和应用,包括:传统含能材料合成、制造、处理和应用的新技术与新技术,新的CHON含能材料的开发和应用,金属化炸药,非传统概念炸药(如燃料空气炸药、温压炸药),高能量密度材料;(2)含能材料能量的控制输出研究,包括:能量输出增强(如组合装药),能量输出聚焦/定向,能量输出模式可控(如多模装药),能量输出范围可控(如低附带毁伤炸药)。欢迎广大学者投稿,来稿时请选择对应的专栏。

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