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Crystal Structure and Thermodynamic Properties of 1-Methyl-2,4-dinitroimidazole

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Abstract: 1-Methyl-2, 4-dinitroimidazole(2,4-MDNI) was synthesized via nitration, thermal rearrangement and methylation with imidazole as primary material. The single crystal of 1-methyl-2, 4-MDNI was cultivated in acetone and its crystal structure was determined by a four-circle X-ray diffractometer. The results indicate that the crystal is orthorhombic, space group P_{212121}, with crystal parameters: a=6.215(12)Å, b=9.431(19)Å, c=23.531(5)Å, V=1379.3(5)Å^3, $\alpha=\beta=\gamma=90°$, D_c=1.658 g·cm^{-3}, Z=8, $F(000)$=704 and μ=0.149 mm^{-1}. The results reveal that 2,4-MDNI has good thermal stability, and exhibits different thermodynamic behavior under different conditions.

Key words: physics chemistry; energetic material; 1-methyl-2,4-dinitroimidazole(2,4-MDNI); crystal structure; thermal properties

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国家能源新材料技术研发中心揭牌仪式暨能源材料发展研讨会在绵举行

2012年10月25日,国家能源新材料技术研发中心揭牌仪式暨能源材料发展研讨会在四川绵阳顺利举行。此次揭牌仪式暨研讨会由国家能源局和中国工程物理研究院共同主办,化工材料研究所承办。

国家能源局能源节约与科技装备司副司长修炳林和中国工程物理研究院院长赵宪庚为中心揭牌并先后向大会致贺词。会上,化工材料研究所与深圳智惠科技有限公司共同签署了共建先进功能材料实验室协议。深圳智惠科技有限公司将出资与化工材料研究所共建实验室。杜祥琬院士主持召开了能源材料发展研讨会,针对美国三大核武器实验室能源材料研究情况等议题组织了深入的讨论交流。

国家能源新材料技术研发中心于2011年9月由国家能源局批准成立,依托中国工程物理研究院建设。它是国家能源局批复的唯一一个以"新材料技术"命名的研发中心。

(中国工程物理研究院化工材料研究所 张 赟 供稿)