

Synthesis and Properties of Dihydroxylammonium 5,5'-Bistetrazole-1,1'-diolate

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Abstract: Using dichloro-glyoxime, sodium azide and dimethyl formamide (DMF) as primary materials, the 1,1'-dihydroxy-5,5'-bistetrazole (1,1'-BTO) was synthesized. Then, it was reacted with the hydroxylamine hydrochloride to form the target compound dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50) with a yield of 73.2%. Its structure was simulated by Gaussian software at the B3LYP/6-31++G level. Results show that there are strong inter- and intra-molecular hydrogen bonds in the solid crystal. These hydrogen bonds effectively improve the density of TKX-50 to 1.918 g · cm⁻³. Based on this density, detonation parameters were calculated. The detonation velocity reaches 9698 m · s⁻¹, the detonation pressure is 42.4 GPa, friction sensitivity is 120 N, and impact sensitivity is 20 J.

Key words: organic chemistry; energetic salt; dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50); synthesis; property

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读者·作者·编者

本刊于2014年第2期组织的“液体推进剂研究”专栏,受到了业内人士的关注。中国航天液体推进剂研究中心的禹天福老师在给本刊的来信中写到“本期选题很好,大多是热点问题。为了感谢编辑部发来目录,写了一点读后感,仅供参考。”为感谢禹天福老师的关心,本刊特别刊出信函全文,希望这些问题也能引起本刊作者及相关学者的重视,在今后撰写/评审论文时予以注意。

对几篇文章的意见

一、新型乙炔氨推进剂热力性能计算分析(文章编号:1006-9941(2014)02-0161-04)

1. “能源机械”科研生产集团

应译为“格鲁什科动力机械科研生产联合体”。原文“НПО Энергомаш имени академика В. П. Глушко”,英文“Energomash Scientific Production Association Glushko”。

(1) 张婵。俄罗斯的液体火箭发动机研制企业——动力机械科研生产联合体。《飞航导弹》2000年11期。

(2) 格鲁什科动力机械制造科研生产联合体。载人航天信息数据库。中国载人航天工程网站。

2. “阿采塔姆”

原文“Ацетам”。

乙炔俄文“ацетилен”,氨俄文“аммиак”。将乙炔和氨两个词的前缀组合在一起,形成这个词。建议将“阿采塔姆”改为“乙炔氨”后面标注俄文。不要采用音译的方法。

3. 乙炔氨的优点

乙炔氨比冲并不高。俄罗斯最看中的是乙炔氨价格低廉,

液氢2000卢布/kg,乙炔氨100卢布/kg。可以降低发射成本的1/3。

4. 表1 煤油、甲烷、乙烷、丙烷、乙炔氨的基本参数和部分理化性能比较

(1) 未标明此处煤油是民用煤油、航空煤油、美国火箭煤油还是俄罗斯火箭煤油。

(2) 该表指煤油分子式为C₁₂H_{24.74}。文章未标明这个数据是作者的测试结果,还是引用哪篇文献。

根据AIAA 2002-3874 “Kerosene” Fuels for Aerospace Propulsion-Composition and Properties

美国火箭煤油和俄罗斯火箭煤油分子式均为C₁₂H_{23.4}。



格鲁什科动力机械科研生产联合体

推进剂组合	热值, kJ/kg
液氧/乙炔	11346
液氧/甲烷	9504
液氧/煤油	9211
液氧/氨	6908

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Crystal Structure and Molecular Structure of Hexabenzylhexaazaisowurtzitane

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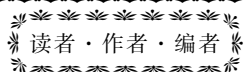
Abstract: The single crystal structure of hexabenzylhexaazaisowurtzitane (HBIW) was determined by X-ray single crystal diffractometer, the characteristics of NMR spectra of HBIW were studied in CDCl_3 , acetone- d_6 and DMSO- d_6 , respectively, and the molecular structure of HBIW was identified by a combination of 1D (^1H NMR, ^{13}C NMR and ^{15}N NMR) and 2D (gHSQC and gHMBC) NMR techniques. Results show that the crystal belongs to orthorhombic system with space group $Pca2(1)$ and the unit cell parameters $a=0.10724(2)$ nm, $b=0.37001(7)$ nm, $c=0.20476(4)$ nm, $\alpha=\beta=\gamma=90^\circ$, $V=8.125(3)\times 10^3$ nm 3 , $Z=4$, $D_c=1.159$ g \cdot cm $^{-3}$, $F(000)=3024$. The chemical shifts of H atoms from high field to low field are assigned to CH on the bridge head, CH_2 bonded to six-membered ring, CH_2 bonded to five-membered ring, CH in six-membered ring and CH in benzene, respectively, while the chemical shifts of C atoms from high field to low field are assigned to CH_2 bonded to five-membered ring, CH_2 bonded to six-membered ring, CH in six-membered ring, CH on the bridge head, and C in benzene. The chemical shifts of N atoms in five-membered ring and six-membered ring were found at $\delta=-317.0$ and $\delta=-297.1$, respectively.

Key words: analytical chemistry; hexabenzylhexaazaisowurtzitane (HBIW); characterization; crystal structure; NMR

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5. 热力计算

г. Химки. Ацетам как новое перспективное горючее ЖРД. ОАО «НПО Энергомаш» имени академика В. П. Глушко»等文章中,已进行了详细计算,比本文详细。

6. “1950年, Winternitz等[5]”

参考文献[5] ЛихванцевА. ААЦЕТАМ :новооеракетногорючее[Ж]. труды НПО Энергомаш ,2012, T29, 132-134

正文是1950年,参考文献是2012年,相差甚远。

这篇文章的作者有7名之多。如果每位作者校对一遍,不至于出现这些差错。看来,很多作者是挂名的。挂名作者得到了“名”,但是影响了刊物的“名”。

审稿人也不够负责任。

二、高浓度过氧化氢分解用 $\text{MnO}_x/\text{CeO}_2\text{-Al}_2\text{O}_3$ 整体催化剂(文章编号:1006-9941(2014)02-0148-07)

“肼单组元推进剂有毒,能致癌”。

根据国家职业卫生标准 GBZ 2.1-2007“工作场所所有害因素职业接触限值 化学有害因素”,无水肼是人体可疑致癌物质。现在国内外职业卫生部门都没有确认无水肼能致癌。

根据 ICSC(International Chemical Safety Cards) 0281 hydrazine (November 25, 2009 Validated) “Suspected of causing cancer”。

三、硝酸酯液体推进剂长时储存性能(文章编号:1006-9941(2014)02-0165-05)

1. “长时”宜改为“长期”。

“储存”应改为“贮存”。短期,叫“储存”;长期,叫“贮存”。“长时”和“储存”组配在一起,不妥。

(1) 储存

GB 17914-2013 易燃易爆性商品储存养护技术条件

GB 17915-2013 腐蚀性商品储存养护技术条件

GB 17916-2013 毒害性商品储存养护技术条件

商品要流通,所以叫“储存”。

(2) “贮存”

沈伟等. 长期贮存固体火箭发动机安全性评估. 航空动力学报 2013, 28(4)

罗俊等. 半导体器件的长期贮存失效机理及加速模型. 微电子学 2013, 43(4)

2. 稳定性预测方法

北大西洋公约组织有标准可供参考

NATO STANAG 4582: EXPLOSIVES, NITROCELLULOSE BASED PROPELLANTS, STABILITY TEST PROCEDURE AND REQUIREMENTS USING HEAT FLOW CALORIMETRY