4 结 论

（1）呋咱及其自由基环的共轭性较弱，分子共轭性强弱及其稳定性次序为呋咱 > 单自由基 > 双自由基，且 N—O 键可能是分子热安定性的“薄弱环节”。

（2）呋咱环能够从与之相连的氢原子上转移电子，环获得一定量的电子以后，环的稳定度增加。

（3）双自由基对亲核、亲电及自由基反应均有一定的活性，单自由基次之，而呋咱较稳定；所有分子上的 N 原子可能对反应有一定活性。

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Theoretical Study on Structures and Properties of Furazan and its Radicals

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Abstract: The structures and properties (geometrical optimization, molecular vibration, thermodynamics, activation of reaction and stability) of furazan and its radicals are studied theoretically by using $DMol^3$. The calculated results show that there are weak conjugated effects on rings of furazan and its radicals, the N—O bonds are the weakest on rings; the order of molecular stability is furazan > single-radical > double-radical; the rings have a certain ability to accept electrons from H atoms which connect with them and become more stable consequently; the double-radical has some electrophilic, nucleophilic and radical ability, single-radical takes the second place and furazan is the most inertial; N atoms on all molecules probably have certain activations of reactions.

Key words: physical chemistry; $DMol^3$; furazan and its radical; molecular structure and property

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为建立读者、作者、编者之间更广泛地联系，加强学术交流，提高编辑部工作质量，《含能材料》将设立"读者·作者·编者"栏目，刊登读者对刊载文章的不同看法、意见及其建议，作者对编辑部工作意见、建议，编辑部工作的相关说明等内容。编辑部全体工作人员期望通过这个栏目能与全国的读者、作者协力搭建起百家争鸣、共同进步的平台。

热情欢迎全国的读者、作者的来信！

《含能材料》编辑部：

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Application of Acoustic Emission Technique in Energetic Materials

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Abstract: The development of acoustic emission (AE) technique and its application in the field of researching energetic materials have been reviewed. From the research of AE features and the performance experimentation, the method and application of AE testing in the field of energetic materials have been analyzed and compared. The results show that AE testing, as a dynamic non-destructive testing technique, has unique reliability and advantages in the research of energetic materials, such as quality control, performance research, the monitor and evaluation of the inner damage, safety control during processing of energetic materials, etc.

Key words: acoustics; acoustic emission; energetic materials; non-destructive testing; damage

读者·作者·编者

编辑同志：

感谢您们的辛苦工作。

我们对清样进行了认真核对，……。

对您们的辛苦、高效的工作再次表示诚挚的谢意！

祝工作顺利。

卢芳云(国防科技大学)

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