

化学结构中互变键、交替键和芳香键的自动识别

姚建华,李丰,罗时玮,袁身刚,陈海峰,李强,郑崇直

中国科学院上海有机化学研究所.上海(200032)

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摘要 化学结构计算机处理中最常遇到的困难是互变现象、交替键和芳香键的处理,尽管解决这些问题的方法早有报道,但它们都有仅考虑计算机处理的方便,而很少注意其化学应用的不足。本工作在环系识别算法的基础上,设计了新的识别算法,使得识别的整体性能更好,形成了拥有自主知识产权的软件。简要介绍了这些算法,并通过例子说明了它们的可能应用。

关键词 [化学键](#) [计算机应用](#)

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Automatic Identification of Tautomeric, Alternating and Aromatic Bonds in Chemical Structures

Yao Jianhua,Li Feng,Luo Shiwei,Yuan Shengang,Chen Haifeng,Li Qiang,Zheng Chongzhi

Key Laboratory of Computer Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences,Shanghai(200032)

Abstract The most usual problems encountered in the structure handling are tautomerism, alternating and aromatic systems. Though a number of methods have been reported in the literature, a common disadvantage is that only the convenience for processing were taken into account, but their chemical sense was rarely considered. Thus their application is limited. Based on the identification of ring system, novel algorithms have been devised in order to enhance the overall performance and a software with copyright has been developed. This paper introduces these algorithms and their potential applications by examples.

Key words [CHEMICAL BONDS](#) [COMPUTER APPLICATIONS](#)

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