

图书基本信息

书名：<<高等有机化学-结构与机理(第五版)>>

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内容概要

自从1997年面世以来,《高等有机化学》作为学科首选教材的地位一直没有动摇过,广泛地覆盖了有机化合物的结构、反应活性及合成。

她的第五版相对2001年出版的第四版进行了大幅度的修订,更新了学科发展的相关资料,内容组织更加清晰明朗,特别是计算化学部分。

Part A从化合物结构和立体化学基础概念讲起,涉及有机化学反应热力学和动力学的方方面面。

主要反应类型涵盖亲核取代反应、加成反应、碳负离子和羰基化学反应、芳环取代反应、周环反应、自由基反应和光化学反应。

每章后附有习题精选及解答习题的推荐参考文献。

本书可供有机化学、药物化学和生物化学等专业的高年级本科生、研究生以及相关领域的科研人员参考。

作者简介

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章节摘录

插图：The stabilization provided by various functional groups contributes to reduced BDEs for bonds to the stabilized radical center. Computational methods can be used to assess these effects. The BDE can be calculated by comparing the total energy of the dissociated radicals with the reactant. Differences in bond dissociation energies relative to methane (ΔBDE) can be taken as a measure of the stabilizing effect of the substituent on the radical. Some computed ΔBDE values are given in Table 3.19 and compared with experimental values. As an example of the substituent effect on BDEs, it can be seen that the primary C-H bonds in acetonitrile (12 kcal/mol) and acetone (11 kcal/mol) are significantly weaker than a primary C-H bond in methane. The data show that both electron-releasing and electron-withdrawing functional groups stabilize radicals. The strong bond-weakening effect of amino substituents is noteworthy, both in its size and the apparent underestimation of this effect by the computations. A recent reevaluation of the ΔBDE for amines arrived at a value of 13 ± 1 kcal/mol, which is in better agreement with the calculations. 102b

编辑推荐

《高等有机化学:结构与机理(第5版)》可供有机化学、药物化学和生物化学等专业的高年级本科生、研究生以及相关领域的科研人员参考。

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