

有机质谱人工智能(AI)解释-邻位效应重排在鉴别位置异构体及几何异构体中的应用

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摘要 本文对一些典型化合物(如芳香类化合物、杂环化合物、含双键链状化合物等)中的邻位效应重排离子及异构体鉴别进行简述和讨论。

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Abstract AI Interpretation of OMS-Ortho Effect Rearrangement and its Application to identify the Positional and Geometric Isomers\$Li Xinming(Dalian Institute of Chemical Physics,Chinese Academy of Sciences,Dalian 116012, China)Abstract:The ortho effect rearrangements have been applied to identify positional isomers and geometric isomers in artificial intelligence(AI)interpretation of organic mass spectra(OMS). The ortho effect rearrangements form typical ions for elucidating molecular structure, so that the correct rate of the computer program output is raised by these typical ions of ortho effect rearrangements.In this paper, producing processes of ortho effect rearrangements have been discussed for the aromatic compounds,heterocyclic compounds and unsaturated acyclic compounds.Keywords:AIMS,ortho effect rearrangement,positional and geometric isomers

Key words

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