

硫醇和硫醚的沸点与分子结构之间关系的拓扑化学研究

王克强,胡英

华东理工大学化学系

收稿日期 修回日期 网络版发布日期 接受日期

**摘要** 根据分子拓扑学原理,用染色因子标识原子性质的差异,发展了一种适用于含原子分子体系结构性能关系研究的新方法。据此探讨了硫醇和硫醚的沸点与分子结构之间的关系,提出一个既能合理表征结构性能关系,又能预测沸点的定量关系式。

**关键词** [硫醇](#) [分子结构](#) [硫醚](#) [结构与性能关系](#) [拓扑](#) [沸点](#)

分类号 [O621](#)

## Studies on the relationship between boiling point of mercaptan and thioether and their molecular structure

WANG KEQIANG,HU YING

**Abstract** Based on the chemical topology, a new method is developed which can be used to study the structure-property relationship of molecules containing heteroatoms. In this paper distance matrix is used to describe molecules structure and dyeing factors are proposed to distinguish the difference among the atoms in molecular. The method is used to study the relationship between boiling point and molecular structure of mercaptan and thioether, and a quantitative relation is proposed that can be used to characterize the structure-property relationship and to predict the boiling point. The calculated results show that the predicted boiling points are in good agreement with the experimental data, and the mean relative deviation is 0.240%. Not only can the quantitative relation predict the boiling points of mercaptan and thioether, but can help to understand the structure-property relationship of matter.

**Key words** [MERCAPTAN](#) [MOLECULAR STRUCTURE](#) [SULFUR ETHER](#) [STRUCTURE AND PROPERTY CORRELATION](#) [TOPOLOGY](#) [BOILING POINTS](#)

DOI:

通讯作者

扩展功能

本文信息

▶ [Supporting info](#)

▶ [PDF\(0KB\)](#)

▶ [\[HTML全文\]\(0KB\)](#)

▶ [参考文献](#)

服务与反馈

▶ [把本文推荐给朋友](#)

▶ [加入我的书架](#)

▶ [加入引用管理器](#)

▶ [复制索引](#)

▶ [Email Alert](#)

▶ [文章反馈](#)

▶ [浏览反馈信息](#)

相关信息

▶ [本刊中包含“硫醇”的相关文章](#)

▶ 本文作者相关文章

· [王克强](#)

· [胡英](#)