

四溴四苯基卟啉及其金属配合物的电子结构和四溴四苯基卟啉Ni(II)的晶体结构

邹建忠,李明,徐正,游效曾,王化勤

南京大学配位化学研究所;南京大学配位化学国家重点实验室;南京大学分析测试中心

收稿日期 修回日期 网络版发布日期 接受日期

摘要 本文合成了7, 8, 17, 18-四溴-5, 10, 15, 20-四苯基-21, 23(H)-卟啉(H~2TPPBr~4)及其金属配合物MTPPBr~4 [M=Cu(II), Ni(II), Co(II)和Zn(II)]。测定了它们的可见紫外光谱和循环伏安,用四轨道模型(Four Orbital Model)计算了MTPPBr~4的相对前线轨道,并解释了配合物的可见紫外光谱及电化学性质。测定了NiTPPBr~4的晶体结构,晶体属单斜晶系,空间群C2/c, a=2.6077(7), b=1.0414(4), c=1.9312(3)nm, $\beta=137.1(7)^\circ$, Z=4, 最后偏离因子R=0.067, 晶体结构直接证明了卟啉亲电溴化反应具有区域选择性, 四个溴分布在相对两个吡咯环上。

关键词 [紫外分光光度法](#) [晶体结构测定](#) [金属络合物](#) [电子结构](#) [镍络合物](#) [前沿轨道理论](#) [区域选择性](#) [电化学性质](#) [四苯基卟啉](#)

分类号 [0611.662](#)

The electronic structure of tetrabromotetraphenylporphyrin and its metalloporphyrins [M=Cu(II), Co(II), Ni(II), Zr(II)] and the crystal structure of Ni(II)TPPBr~4

ZOU JIANZHONG, LI MING, XU ZHENG, YOU XIAOZENG, WANG HUAQIN

Abstract MTPPBr₄ (M = Cu, Co, Ni, Zn) were synthesized. Their UV-visible spectra and cyclic voltammetry were determined. The relative energy of frontier orbital of metalloporphyrins, which explained the characters of UV-visible spectra and electrochem., were calculated according to four orbital parameters. The crystal structure of NiTPPBr₄ was determined by a CAD4 diffractometer. Crystallog. parameters were as follows: monoclinic, space group C2/c with a 2.6077(7), b 1.0414(4), c 1.9312(3) nm; β 137.1(7)°; Z = 4, F(000) = 2048, final R = 0.067. This structure directly verified that electrophilic bromination occurred regioselectively at the antipodal pyrrolic ring of free base porphyrins.

Key words [ULTRAVIOLET SPECTROPHOTOMETRY](#) [CRYSTAL STRUCTURE DETERMINATION](#) [METAL COMPLEX](#) [ELECTRONIC STRUCTURE](#) [NICKEL COMPLEX](#) [FRONTIER ORBITAL THEORY](#) [REGIOSELECTIVITY](#) [FUEL CELL](#)

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“紫外分光光度法” 的相关文章](#)

▶ [本文作者相关文章](#)

- [邹建忠](#)
- [李明](#)
- [徐正](#)
- [游效曾](#)
- [王化勤](#)