

三(3,5-二甲基吡唑)氢合硼酸钾及双[三(3,5-二甲基吡唑)]氢合硼酸根合铜(II)的合成和晶体结构

王瑾玲,汪大伟,缪方明

天津师范大学化学系

收稿日期 修回日期 网络版发布日期 接受日期

摘要 为研究吡唑硼类配体的配位行为,合成了三(3,5-二甲基吡唑)氢合硼酸钾[KHB(C~5H~7N~2)~3],简称(KL)和双[三(3,5-二甲基吡唑)氢合硼酸根]合铜(II){Cu[HB(C~5H~7N~2)~3]~2},简称(CuL~2),

并测定了它们的晶体结构。化合物KL属空间群P2~1/n。a=1.0527(8),b=0.9464(3),c=1.7730(9)nm,β=94.51(5)°,Z=4,D~c=1.268g.cm~3,R=0.079。化合物CuL~2属空间群P1,a=0.8768(1),b=1.0170(2),c=1.0859(1)nm,

α=62.45(1),β=83.78(1),γ=78.52(1)°,Z=2,D~c=1.298g.cm~3,R=0.062。晶体结构测定结果表明:

化合物KL由钾离子和配体负离子组成,K~+与配体L中的B原子相距0.3634nm,

在配体负离子中B原子与三个吡唑环的N原子及H原子形成四面体构型。化合物CuL~2由孤立分子组成,铜离子处于分子的对称中心且与两个配体分子中的六个N原子形成六配位的八面体构型,并表现出明显的Jahn-Teller效应。

关键词 [晶体结构测定](#) [吡唑 P](#) [铜络合物](#) [硼酸盐 P](#) [钾络合物](#) [杨-特勒效应](#) [配位](#)

分类号 [0611.662](#)

Synthesis and crystal structures of [Hydridotris (3,5-dimethylpyrazol-1-yl)borato]K and bis-[hydridotris (3,5-dimethylpyrazol-1-yl)borato] Cu(II)

WANG JINLING,WANG DAWEI,MIAO FANGMING

Abstract To study the coordination action of pyrazolyborato ligands, KBHR3 (R = 3,5-dimethylpyrazol-1-yl) and Cu (BHR3)2 were prepared, and their crystal structures were determined by x-ray anal. The crystallog. data are as follows: KBHR3, monoclinic, space group P21/n, and R = 0.079; Cu(BHR3)2 triclinic, space group P1, Z = 2, and R = 0.062. The distance between atom K(1) and B(1) is 0.3634 nm. Atom B(1) in BHR3- is tetrahedrally coordinated by one H atom and three N atoms from three pyrazole rings. The bond distances B(1)-N(12), B(1)-N(22) and B(1)-N(32) are 0.1587, 0.1586 and 0.1509 nm, resp. In Cu(BHR3)2, the Cu atom is located about a crystallog. center of symmetry and coordinated octahedrally by six N atoms which are from two BHR3- ligands. The bond distances Cu(1)-N(11), Cu(1)-N(21) and Cu (1)-N(31) are 0.2153, 0.2344 and 0.2035 nm, resp. An obvious Jahn-Teller effect is displayed.

Key words [CRYSTAL STRUCTURE DETERMINATION](#) [PYRAZOLE P](#) [COPPER COMPLEX](#) [BORATES P](#) [POTASSIUM COMPLEX](#) [JAHN-TELLER EFFECT](#) [COORDINATION](#)

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“晶体结构测定” 的相关文章](#)

▶ 本文作者相关文章

· [王瑾玲](#)

· [汪大伟](#)

· [缪方明](#)