

钴原子簇化合物研究 V. 含硫脲桥基三钴硫羰基簇化合物的合成和结构

刘树堂, 燕红, 胡襄, 刘启旺

内蒙古大学化学系

收稿日期 修回日期 网络版发布日期 接受日期

摘要 本文通过 $\text{Co}_2(\text{CO})_8$ 与5个取代硫脲 $\text{R}^1\text{NHC}(\text{S})\text{NHR}^2$ 反应,制得了通式 $\text{Co}_3(\text{CO})_7(\mu\text{-}3\text{-S})[\mu\text{-}\eta^2\text{-R}^1\text{NC}(\text{S})\text{NHR}^2]_5$ 个新簇合物.除用碳氢氮元素分析、IR、 ^1H NMR和MS表征它们的结构外,还用X光衍射法测得 $\text{R}^1=\text{Ph}, \text{R}^2=\text{CH}_2\text{Ph}$ 簇合物的单晶结构.该簇合物属三斜晶系,PI空间群.晶胞参数如下: $a=0.9116(1), b=1.2289(2), c=1.2518(2)\text{nm}, \alpha=115.56(1), \beta=100.92(2), \gamma=93.29(1)^\circ; z=2, V=1226.2 \times 10^{-5}\text{nm}^3; D_c=1.75\text{g}\cdot\text{cm}^{-3}; \mu=22.099\text{cm}^{-1}, F(000)=646$.结构分析表明,该分子中的 Co_3S 原子构成三角锥分子骨架,所有CO为钴原子的端羰配体,而 $\text{PhNC}(\text{S})\text{NHCH}_2\text{Ph}$ 以S原子和与苯基相连的N原子分别与两个钴原子配位,形成 Co_2NCS 五圆环结构.

关键词 [晶体结构测定](#) [X射线衍射分析](#) [硫脲类](#) [羰基化合物](#) [簇状化合物](#) [钴络合物](#) [桥环化合物](#)

分类号 [0627](#)

Studies on cobalt clusters. V. syntheses and structures of sulfur-capped trinuclear cobalt carbonyl clusters containing bridged thiourea moiety

LIU SHUTANG, YAN HONG, HU XIANG, LIU QIWANG

Abstract Through the reaction of $\text{Co}_2(\text{CO})_8$ with 5 thioureas $\text{R}^1\text{NHC}(\text{S})\text{NHR}^2$, $\text{Co}_3(\text{CO})_7(\mu\text{-}3\text{-S})[\mu\text{-}\eta^2\text{-RNC}(\text{S})\text{NHR}^2]_5$ were prepared and characterized by elemental anal., IR, ^1H NMR, and mass spectroscopy. The crystal structure of the cluster with $\text{R}^1 = \text{Ph}$ and $\text{R}^2 = \text{CH}_2\text{Ph}$ was determined by x-ray single crystal diffraction: triclinic, space group P1, $a = 0.9116(1), b = 1.2289(2), c = 1.2518(2)\text{ nm}, \alpha = 115.56(1), \beta = 100.94(2), \gamma = 93.39(1)^\circ; Z = 2, R = 0.033, R_w = 0.046$. The mol. contains a tetrahedral cluster framework Co_3S ; all carbonyls are terminal ligands of 3 Co atoms; and $\text{PhNC}(\text{S})\text{NHCH}_2\text{Ph}$ as bridging ligand links up with 2 Co atoms of the framework by S and N atom-a 5-membered ring of Co_2NCS was formed.

Key words [CRYSTAL STRUCTURE DETERMINATION](#) [X-RAY DIFFRACTION ANALYSIS](#) [SULFOCARBAMIDES](#) [CARBONYL COMPOUNDS](#) [CLUSTER COMPOUND](#) [COBALT COMPLEX](#) [BRIDGE COMPOUNDS](#)

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](#)

- [刘树堂](#)
- [燕红](#)
- [胡襄](#)
- [刘启旺](#)