{[(K·TPPO·DB~1~8C~6)~2(C~4H~8O~2)](HgI~3)~2}·3C~4H~8O~2单晶的合成、性质和结构表征

蒋德华,刘学勇,孙大岩,沈静兰

山东大学化学学院

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用二苯并-18-冠-6(DB18C6)和三苯基氧化膦(TPPO)的三氯甲烷溶液从KI介质中萃取Hg(II), 先制得固体协萃配合物,在二氧六环(C~4H~8O~2)中重结晶得标题物单晶,对单晶进行了熔点测定、 热重和红外光谱分析, 测定了结构。晶体属P1空间群, 晶胞参数a=1.4211(2), b=1.4488(4), c=1.4934(4)nm; α=113.61 ▶把本文推荐给朋友 (2),β=110.78(1),γ=87.29(2)°。晶体中每个K与一个DB18C6上的六个O和一个TPPO上的一个O配位的同时, 每两个K还与一个C~4H~8O~2上的两个O配位, 桥连成中心对称的二聚[(K·TPPO·DB18C6)~2(C~4H~8O~2)] ^2^+配阳离子; 每两个Hg通过两个I桥连成二聚[HgI~3]~2^2^-配阴离子; 阴阳离子相间排列。另外三个C~4H~8O~2 分子填充于晶格间隙中。

晶体结构 汞络合物 冠式化合物 萃取 二氧六环 三苯基氧化膦 关键词 分类号 074

Studies on synthesis, characterization and structure of the compounds {[(K·TPPO·DB~1~8C~6)] ~2(C~4H~8O~2)](HgI~3)~2}·3C~4H~8O~2

JIANG DEHUA,LIU XUEYONG,SUN DAYAN,SHEN JINGLAN

Abstract The crystals of the title compounds were synthesized by solvent extraction of Hg(II) with DB18C6 and TPPO in CHCl~3 solution from KI media, and recrystallization in C~4H~8O~2. They have been studied by melting point determination and TG, IR analysis, and have been structurally characterized by singlecrystal X-ray diffraction techniques. Crystals of the complexes are triclinic, space group P1 with a=1.4211(2), b=1.4488(4), c=1.4934(4)nm; α =113.61(2), β =110.78(1), γ =87.29(2)°. In the crystals, every K is corrdinated by the six oxygen atoms of the DB18C6, one oxygen atom of the TPPO, and every two K are coordinated by two oxygen atoms of the C~4H~8O~2. Dipolymer [(K·TPPO·DB18C6)~2(C~4H~8O~2)]^2^+ cations can be considered to be based on a centrosymmetric bridged dimetric arrangement. Every two Hg were halogen-bridged by two I to be a dipolymer (HgI~3)~2^2- anions. The anions and the cations arrange in order every other. The other three C~4H~8O~2 fill in the gap of the lattices.

Key words CRYSTAL STRUCTURE MERCURY COMPLEX CROWN ETHER COMPOUNDS EXTRACTION DIOXANE

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