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二维网状结构双核配合物**[Ca_2(C_(10)H_8N_2O_4)_2(DMSO)_2(H_2O)_4]·2DMSO**的合成、热分解及晶体结构

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摘要 以2-羰基丙酸水杨酰腙(C_(10)H_(10)N_2O_4)作为配体与碳酸钙在水中反应， 在DMF(N,N'-二甲基甲酰胺)和DMSO（二甲基亚砜）的混合溶剂中培养了单晶，其组 成为 [Ca_2(C_(10)H_8N_2O_4)_2(DMSO)_2(H_2O)_4]·2DMSO [C_(10)H_8N_2O~2- _4为2-羰基丙酸水杨酰腙负离子]。测字了单晶的结构，该单晶为黄色，属单斜晶 系，空间群为P2(1)/C，晶胞参数a=1.0634(3)nm, b=1.7035(5)nm, c=1.2183(3) nm, β=106.180(5)°, V=2.1192(10)nm!, Dc=1.412Mg·m~(-3), Z=2, F(000) =944, μ=0.534m~(-1), GOF=0.867。所测单晶是以2-卷曲在丙酸水杨酰腙羧基上 的一个氧原子作为桥联的双核钙（II）配合物，两个Ca~(2+)均处于五角双锥的七 配位环境中，锥底为配体2-羰基丙酸水杨酰腙中的三个配位原子，以及另一2-羰基 丙酸水杨酰腙羧基上的桥联氧原子和一个水分子的配位氧原子，锥顶为一配位水和一想位的DMSO分子，即溶剂DMSO也参也了配位，从晶胞结构看，晶体中除配位的 DMSO分子外，还有自由的DMSO溶剂分子，它们与配位水以氢键连接存在于晶格之中 ，在空间形成的二维网状结构。通过TG-DTG还测定了配合物的热稳定性。

关键词 钙络合物 腙 P 二甲基甲酰胺 网状结构 热分解 晶体结构 稳定性

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Synthesis, thermal Decomposition and Crystal Structure of Two- Dimensional Network Binuclear Complex [Ca_2(C_(10)H_8N_2O_4)_2(DMSO)_2 (H_2O)_4]·2DMSO

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Abstract In water, a calcium(II) complex with 2-oxo-propionic acid salicyloyl hydrazon (C_(10)H_(10)N_2O_4) has been synthesized. The yellow wystals of the calcium (H) complex was obtained in a mixed solvent of DMF and DMSO. The formula of the complex is [Ca_2(C_(10) H_8N_2O_4)_2(DMSO)_2(H_2O)_4] ·2DMSO (C_(10)H_8N_2O_4~(2-) is the dinegative ion of 2-oxo-propionic acid salicyloyl hydrazone) . The crystal structure was determined by X-ray single crystal diffraction analysis. The results show that the complex is monoclinic of space group P2(1)/c, the cell parameters are as follows: a = 1.0634(3) nm, b = 1.7035(5) nm, c = 1.2183(3) nm, β = 106.180(5)°, V = 2.1192(10) nm~3, D_c= 1.412 Mg·m~(-3), Z = 2, F(000)=944, μ =0.534 mm~(-1), GOF = 0.861. The complex is a binuclear Ca complex, with one O atom of the carboxyl of 2-oxo-propionic acid salicyloyl hydrazone bridging two Ca. Each Ca atom is pentagonal bipyramid coordinated by two O atoms and one N atom of tridentates C_(10)H_8N_2O_4~(2-) ligand, one O atom of DMSO molecule and the O atoms of two H_2O. One H_2O and one DMSO locate at the apical position. In the crystal cell, there are free DMSO which are connected with H2O by hydrogen bonds. Because of the hydrogen bonds the complex formed a two-dimensional network structure in space. The thermal stability of the complex was studied by TG-DTG analysis.

Key words CALCIUM COMPLEX HYDRAZONE P DIMETHYLFORMAMIDE RETICULAR FORMATION THERMAL DECOMPOSITION CRYSTAL STRUCTURE STABILITY

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