

论文

配合物{[Cu(hmtade)][Ni(dmit)₂]}₂·4DMSO的合成、表征及晶体结构

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摘要:

合成了配合物{[Cu(hmtade)][Ni(dmit)₂]}₂·4DMSO(1)(hmtade为5,7,7,12,14,14-六甲基-1,4,8,11-四氮杂环十四-4,11-二烯; dmit为1,3-二硫杂环戊二烯-2-硫酮-4,5-二硫醇; DMSO为二甲亚砜), 采用元素分析、红外光谱和紫外-可见光谱进行了表征, 并用X射线衍射法测定了晶体结构. 该晶体属于单斜晶系, *P*₂₁/*n*空间群; 晶胞参数: *a*=1.49952(6) nm, *b*=1.77229(7) nm, *c*=3.1275(1) nm, β=102.442(1)°, *V*=8.1163(5) nm³, *D*_c=1.558 Mg/m³, *Z*=8, *F*(000)=3944, μ(Mo *K*α)=1.637 mm⁻¹, *S*=1.016, (Δ/σ)_{max}=0.001, *R*₁=0.0673, *wR*₂=0.1672 [*I*>2σ(*I*)]. 晶体结构研究表明, 配合物{[Cu(hmtade)][Ni(dmit)₂]}₂·4DMSO包含2个[Cu(hmtade)][Ni(dmit)₂]子单元. 每个子单元中, 1个dmit中的1个S原子与Cu及Ni配位, 形成异双核Cu—Ni配合物. 其中Cu(II)为五配位的四方锥形, Cu—N键长在0.1949(5)~0.2007(4) nm范围内, Cu—S键长分别为0.28913(18)和0.28952(18) nm; 配阴离子[Ni(dmit)₂]²⁻为畸变四方, Ni—S键长在0.21729(16)~0.21905(17) nm范围内. 溶剂分子DMSO与配体hmtade形成了N—H...O氢键. 通过分子内S...S和S...H短接触形成了二聚体, 二聚体之间通过S...S短接触形成一维链状结构, 并通过S...S, S...H和C...H短接触进一步形成二维和三维结构.

关键词: 1,3-二硫杂环戊二烯-2-硫酮-4,5-二硫醇; 四氮杂大环; 配合物; 晶体结构

Synthesis, Characterization and Crystal Structure of Complex { [Cu(hmtade)][Ni(dmit)₂]}₂·4DMSO

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Abstract:

A new complex { [Cu(hmtade)][Ni(dmit)₂]}₂·4DMSO(1)(hmtade=5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene, dmit=4,5-dimercapto-1,3-dithiole-2-thione, DMSO=dimethyl sulfoxide) was synthesized and characterized by means of elemental analysis, Infrared, Ultraviolet-visible spectroscopy, and X-ray structure analysis. Complex 1 belongs to monoclinic system, space group *P*₂₁/*n* with *a*=1.49952(6) nm, *b*=1.77229(7) nm, *c*=3.1275(1) nm, β=102.442(1)°, *V*=8.1163(5) nm³, *D*_c=1.558 Mg/m³, *Z*=8, *F*(000)=3944, μ(Mo *K*α)=1.637 mm⁻¹, *S*=1.016, (Δ/σ)_{max}=0.001, and final *R*₁=0.0673, *wR*₂=0.1672 [*I*>2σ(*I*)]. Two independent structural units of [Cu(hmtade)][Ni(dmit)₂] are found in an asymmetric unit along with four DMSO solvent molecules. Sulfur-bridged heterometal Cu—Ni complex is formed by one dmit ligand of [Cu(hmtade)][Ni(dmit)₂]. The copper(II) ion is a five coordinated square pyramidal environment, with Cu—N distances in the region of 0.1949(5)—0.2007(4) nm and Cu—S distances of 0.28913(18)—0.28952(18) nm. The nickel(II) ion which is coordinated by four sulfur atoms of two dmit ligands is in the distorted square geometry, and the dimmer is formed through intramolecular S...S and S...H short contacts. Finally, one-dimensional zigzag chain, two-dimensional and three-dimensional networks are formed via S...S, S...C or C...H short contacts.

Keywords: 4,5-Dimercapto-1,3-dithiole-2-thione; Tetraazamacrocyclic; Complex; Crystal structure

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