

[ReO(MPMEP)(BMPBA)][ReO(MPMEP)(BMPBA)]的合成和结构

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摘要 合成了未见文献报道的[ReO(MPMEP)(BMPBA)][ReO(MPMEP)(BMPBA)]配合物,其中MPMEP = 1-(2-甲氧基苯基)-4-(2-巯基乙基)哌嗪, BMPBA = N,N-二(2-巯基乙基)苄胺,并在适当的溶剂中培养出单晶,用X射线单晶衍射法测定了单晶结构,晶体属三斜晶系,空间群P1,晶胞参数 $a = 0.93604(19)$ nm, $b = 1.1044(2)$ nm, $c = 1.3823(3)$ nm; $\alpha = 89.19(3)^\circ$, $\beta = 74.50(3)^\circ$, $\gamma = 75.04(3)^\circ$; $Z = 1$, $V = 1.3281(5)$ nm³, $\mu = 4.836$ mm⁻¹, $F(000) = 677$, $R = 0.0403$, $wR = 0.0673$ 。配合物的两个[ReO(MPMEP)(BMPBA)]部分均采取扭曲的三角双锥几何结构,基底面由三齿配体的两个硫原子与氧原子构成,三齿配体的一个氮原子和单齿配体的一个硫原子分别占取两个顶角位置,硫原子的离子化致使配合物呈电中性。

关键词 [铼](#) [晶体结构](#) [哌嗪](#) [P](#) [巯基化合物](#) [苄胺](#) [P](#)

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Synthesis and Crystal Structure of [ReO(MPMEP)(BMPBA)][ReO(MPMEP)(BMPBA)]

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Abstract A new rhenium SNS/S mixed ligand complex [ReO(MPMEP)(BMPBA)][ReO(MPMEP)(BMPBA)] [MPMEP = 1-(2-methoxyphenyl)-(4-mercaptoethyl)-piperazine, BMPBA = N,N-bis(2-mercaptoethyl)-benzylamine] has been prepared. The single crystal structure of the complex was determined by X-ray diffraction method. It belongs to triclinic crystal system, space group P1 with $a = 0.93604(19)$ nm, $b = 1.1044(2)$ nm, $c = 1.3823(3)$ nm; $\alpha = 89.19(3)^\circ$, $\beta = 74.50(3)^\circ$, $\gamma = 75.04(3)^\circ$; $Z = 1$, $V = 1.3281(5)$ nm³, $\mu = 4.836$ mm⁻¹, $F(000) = 677$, $R = 0.0403$, $wR = 0.0673$. Both [ReO(MPMEP)(BMPBA)] of the complex adopt distorted trigonal bipyramidal geometry, with the basal plane defined by the SS atoms of the tridentate ligand and the oxo-group. The N of the tridentate ligand and the S of the monodentate ligand occupy two apical positions. Ionization of the sulphur atoms leads to a neutral compound.

Key words [RHENIUM](#) [CRYSTAL STRUCTURE](#) [PIPERAZINE](#) [P](#) [MERCAPTO COMPOUNDS](#) [BENZENEMETHANAMIUM](#)

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