

异丙氧基-羟肟酸-氧钒(V)配合物的合成、晶体结构和量子化学研究

杨频,韩广业,金祥林,陈世荣

山西大学分子科学研究所,太原(030006);北京大学化学与分子工程学院,北京(100871)

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摘要 以苯甲酰羟肟酸为配体,首先合成四价氧钒化合物,以此为基础合成了标题化合物,并用元素分析,红外光谱, ^1H NMR, ^{13}C NMR, ^{15}V NMR, 电子吸收光谱等,分别对它进行了表征,其结构用单晶X射线衍射法测定,晶体属三斜晶系, $P1\bar{1}$ 空间群,所得晶体学参数为 $a = 1.1119(3)$ nm, $b = 1.1735(3)$ nm, $c = 0.8660(2)$ nm, $\alpha = 96.84(1)^\circ$, $\beta = 106.93(1)^\circ$, $\gamma = 88.97(1)^\circ$, $V = 1.0731(2)$ nm 3 , $D_c = 1.415$ g/cm 3 , $Z = 2$, $F(000) = 478$, $\mu = 5.06$ cm $^{-1}$ 。采取ab initio(GTO-6-31d)方法对标题化合物的结构单元的成键情况进行了分析,讨论了化合物的稳定性、分子轨道能量、原子静电荷分布等情况。

关键词 [钒络合物](#) [羟肟酸 P](#) [晶体结构](#) [从头计算法](#)

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Synthesis, Crystal Structure and ab initio Study of Bis- (benzohydroxamato) oxoisopropoxovanadium(V)

Yang Pin,Han Guangye,Jin Xianglin,Chen Shirong

Institute of Molecular Science, Shanxi University,Taiyuan(030006);College of Chemical and Molecular Engineering, Peking University. Beijing(100871)

Abstract On the basis of synthesis of bis-(benzohydroxamato) oxoisopropoxovanadium(IV) compound containing bezohydroxamatic acid, the titled complex has been synthesized and characterized by elemental analyses and IR, ^1H NMR, ^{13}C NMR, ^{15}V NMR and UV-vis spectroscopies. The X-ray structure of titled complex has been determined to be in triclinic, $P1\bar{1}$ with $a = 1.1119(3)$ nm, $b = 1.1735(3)$ nm, $c = 0.8660(2)$ nm, $\alpha = 96.84(1)^\circ$, $\beta = 106.93(1)^\circ$, $\gamma = 88.97(1)^\circ$, $V = 1.0731(2)$ nm 3 , $D_c = 1.415$ g/cm 3 , $Z = 2$, $F(000) = 478$, $\mu = 5.06$ cm $^{-1}$. The investigation of the titled complex as structural unit has been performed by ab initio (GTO-6-31d) calculation and the stability of the complex, molecular orbitals, the population regularities of the atomic net charges have been discussed.

Key words [VANADIUM COMPLEX](#) [HYDROXIMIC ACID P](#) [CRYSTAL STRUCTURE](#) [AB INITIO CALCULATION](#)

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