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混合配体配合物**[Pd(bpy)(L-asp)]·3**。**5H_2O**的晶体结构及其稳定性研究

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摘要 合成了混合配体配合物单晶[Pd(bpy)(L-asp)·]3.5H_2O(bpy=2,2'-联吡啶， L-asp~2=L-天冬氨酸根)。用红外光谱和元素分析对配合物的成键及组成进行了表 征。用X射线单晶衍射仪（CCD）测定配合物的结构，晶体属四方晶系，为P4（1） 2（1）2空间群。配合物为平面四边形结构，分子内存在氢键作用，其晶胞靠氢键和芳环堆砌等弱相互作用力形成。用电位滴定法测定了配合物稳定常数lgK[Pd~ (2+)+bpy+L-asp~2<->Pd(bpy)(L-asp)]、表征常数△lgK[Pd(bpy)~(2+)Pd(L-asp) <->Pd(bpy)(L-asp)+Pd~(2+)]和lgX[Pd(bpy)_2~(2+)+Pd(L-asp)_2~(2-)<->2Pd (bpy)(L-asp)]，各常数均大于相应的统计期望值，从分子内d-pπ电子效应和电性中和角度对配合物额外稳定性进行了讨论。

关键词 联吡啶 P 天冬氨酸 钯化合物 元素分析 红外分光光度法 X射线衍射分析 晶体结构

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Studies on the Crystal Structure and Stability in Solution of Mixed Ligand Complex of Palladium (II) with 2,2'-Bipyridine and L-Aspartic Acid

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Abstract The mixed ligand complex [Pd(bpy)(Z,-asp)*3.5H2O (bpy = 2,2'- bipyridine, L-asp= L-aspaitic acid) (1) has been synthesized and characterized by IR spectra, elemental analysis and electroconductivity. The molecular structure and the packing of 1 have been determined by single crystal X-ray structure analysis. The results show that the Pd(II) in 1 has a square planar coordination geometry and the molecules of 1 are assembled via hydrogen bond and intermolecular aromatic ring stacking. The crystal of 1 belongs to tetragonal, space group P4(l)2(l)2, a - h - 1.5979(3) nm, c = 1.3749(5) ran, Z = %, V- 3.5105(15) ran3. The stability of the mixed ligand complex was determined by the pH potentiometric titration technique in water at 37 °C and 0.10 ionic strength (NaCl). The results show that the complex is quite stable, The higher scale values of relative stability AlgX and lgZ demonstrate that the complex possesses enhanced stability. The reasons that lead to these results were discussed in terms of 7r-electron back donation and electroneutralization.

Key words BIPYRIDINE P ASPARTIC ACID PALLADIUM COMPOUNDS ELEMENTAL ANALYSIS IR XRD CRYSTAL STRUCTURE

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