

C-取代二氧三胺大环配体合成及其Cu(II)配合物性质研究

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摘要 本文合成了1, 4, 7-三氮杂环十烷-8, 10-二酮(td)和9-(2'-羟基苄基)-1, 4, 7-三氮杂环十烷-8, 10-二酮(btd)两个新型二氧三胺大环配体, 经元素分析, IR, ¹H

NMR以及MS等方法表征。采用分子力学方法探讨了取代基对配体合成的影响。利用pH法, 在25.0±0.1℃, I=0.1mol/L KNO₃条件下, 测定了配体btd的质子化常数及其与Cu(II)

配位的平衡常数。结合光谱滴定及配合物EPR结果, 讨论了二氧三胺大环配体与Cu(II)离子的配位方式。

关键词 [红外分光光度法](#) [元素分析](#) [质谱法](#) [氮杂环化合物](#) [铜络合物](#) [质子磁共振谱法](#) [二元酮](#) [酰胺 P](#)

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Synthesis of C-functionalized macrocycles and properties of its copper(II) complex

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Abstract Two novel dioxotriamine macrocycles (1, 4, 7-triazacyclodecane-8, 10-dione (td), 9-(2'-hydroxybenzyl)-1, 4, 7-triazacyclodecane-8, 10-dione (btd)) have been synthesized and characterized by elemental analysis, IR, ¹H NMR and MS. The introduced substituent has considerable effect on ligand synthesis, which was explained through molecular mechanics. By pH potentiometric titration at 25±0.1℃, I=0.1mol/L KNO₃, the ligand (btd) protonation constants and its complexation equilibrium constants with Cu(II) have been determined, and the complexation form of this kind of ligands with Cu(II) was postulated together with the results obtained by spectra titration and EPR of the complexes. We concluded that dioxotriamine macrocycles would be regarded as a new kind of ligands different from both saturated N₃ macrocycle and dioxotetraamine.

Key words [INFRARED SPECTROPHOTOMETRY](#) [ELEMENTAL ANALYSIS](#) [MASS SPECTROGRAPHY](#) [NITROGEN HETEROCYCLICS](#) [COPPER COMPLEX](#) [PROTON MAGNETIC RESONANCE SPECTROMETRY](#) [DIKETONE](#) [AMIDES P](#)

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