

苯并15-冠-5与Na₂[M(SCN)₄](M=Pd,Pt)配合物的合成与结构

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摘要 合成了苯并15-冠-5与Na₂[M(SCN)₄] (M = Pd, Pt)生成的配合物: [Na(B15-C-5)]₂[Pd(SCN)₄] (1), {[Na(B15-C-5)][Na(B15-C-5)(H₂O)]}[Pt(SCN)₄] (2)。1为单斜晶系, 空间群P2₁/n, a = 1.0164(6) nm, b = 1.3743(3) nm, c = 1.4987(7) nm, β = 95.248(6)°, V = 2.0847 nm³, Z = 2, D_(calcd) = 1.47 g/cm³, F(000) = 944, R = 0.053, wR = 0.072。2为三斜晶系, 空间群P(1- $\bar{3}$), a = 1.1484(2) nm, b = 1.4210(3) nm, c = 1.5026(3) nm, α = 62.500(3)°, β = 72.393(3)°, γ = 73.106(4)°, V = 2.0398(7) nm³, Z = 2, D_(calcd) = 1.674 g/cm³, F(000) = 1028, R₁ = 0.0327, wR₂ = 0.0885。1由两个[Na(B15-C-5)]⁺配阳离子和一个[Pd(SCN)₄]²⁻配阴离子组成, 两者通过Na-N键形成中性配合物, [Na(B15-C-5)]⁺相对钯原子呈反式排列。2由[Na(B15-C-5)]⁺和[Na(B15-C-5)(H₂O)]⁺配阳离子和一个[Pt(SCN)₄]²⁻配阴离子组成, 它们也通过Na-N键形成中性配合物, 配阳离子相对铂原子呈顺式排列。2的两个分子通过氢键形成二聚结构。

关键词 [冠式化合物](#) [铂化合物](#) [钯化合物](#) [晶体结构](#)

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Synthesis and Structure of Benzo-15-Crown-5 Complexes with Na₂[M(SCN)₄] (M = Pd, Pt)

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Abstract Two benzo-15-crown-5 (B15-C-5) complexes: [Na(B15-C-5)]₂[Pd(SCN)₄] (1) and {[Na(B15-C-5)][Na(B15-C-5)(H₂O)]}[Pt(SCN)₄] (2) have been synthesized and characterized by IR, elemental analysis, X-ray diffraction analysis. 1 belongs to monoclinic, space group P2₁/n with cell dimensions: a = 1.0164(6) nm, b = 1.3743(3) nm, c = 1.4987(7) nm, β = 95.248(6)°, V = 2.0847 nm³, Z = 2, D_(calcd) = 1.47 g/cm³, F(000) = 944, R = 0.053, wR = 0.072. 2 is triclinic crystal system, space group P(1- $\bar{3}$) with cell dimensions: a = 1.1484(2) nm, b = 1.4210(3) nm, c = 1.5026(3) nm, α = 62.500(3)°, β = 72.393(3)°, γ = 73.106(4)°, V = 2.0398(7) nm³, Z = 2, D_(calcd) = 1.674 g/cm³, F(000) = 1028, R₁ = 0.0327, wR₂ = 0.0885. 1 is composed of two [Na(B15-C-5)]⁺ complex cations and one [Pd(SCN)₄]²⁻ complex anion. Complex cations and complex anion form neutral complex through Na-N interactions. Two [Na(B15-C-5)]⁺ are trans-orientation with respect to Pd atom. 2 is made up of [Na(B15-C-5)]⁺ and [Na(B15-C-5)(H₂O)]⁺ complex cations and one [Pt(SCN)₄]²⁻ complex anion. They also form neutral complex through Na-N interactions. [Na(B15-C-5)]⁺ and [Na(B15-C-5)(H₂O)]⁺ are cis-orientation with respect to Pt atom. Two molecules of 2 form dimer structure though hydrogen bonds of H₂O and N atom of SCN group.

Key words [CROWN ETHER COMPOUNDS](#) [PLATINUM COMPOUND](#) [PALLADIUM COMPOUNDS](#) [CRYSTAL STRUCTURE](#)

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