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Molecular Structure of Metal Complexes of Certain Benzimidazole Derivatives

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Keywords: Molecular structure of bis [2-(4-methylsulfanylphenyl)-1H-benzimidazole] dibromidocadmium (II) ethanol (1) and 2-(p-thiomethyl-phenyl)benzimidazole tetrabromidocadmate (II) ethanol (2)

Introduction

Transition metal complexes containing imidazole and their derivatives have been shown to possess pharmacological activity [1,2] and have been used as antitumor and antimicrobial agents. Nitrogen heterocycles in general, and benzimidazole and their derivatives in particular, have been investigated for their antitumor, antibacterial, anti fungicidal, anticarcinogenic, anti-tubercular, anti-allergic and poliovirus inhibitor properties. Benzimidazole has a planar ring structure and is mainly used as an anticancer drug [3,4]. Nitrogen heterocycles are an interesting class of chelating agents and are capable of coordinating to one or more metal ions and thus forming mononuclear as well as polynuclear metal complexes. They find applications in analytical chemistry and also serve as biochemical models. Some of the first-row transition metal complexes of N-heterocycles containing benzimidazole moiety exhibit antifungal and antiviral activities [5,6]. Metal complexes containing N-heterocycles are also known to be good catalysts for hydrogenation, hydroformylation, transfer hydrogenation and related reactions involving organic substrates [7].

Single Crystal X-ray Analysis and Refinement

Single crystal X-ray diffraction data for the compounds **1** and **2** were collected on a Bruker Smart CCD Area Detector System [8], using MoKα (0.71073Å) radiation for the crystal. Intensity data was collected up to a max of 26.81° for the compound in the w–ϕ scan mode. The data was reduced using SAINTPLUS [8].

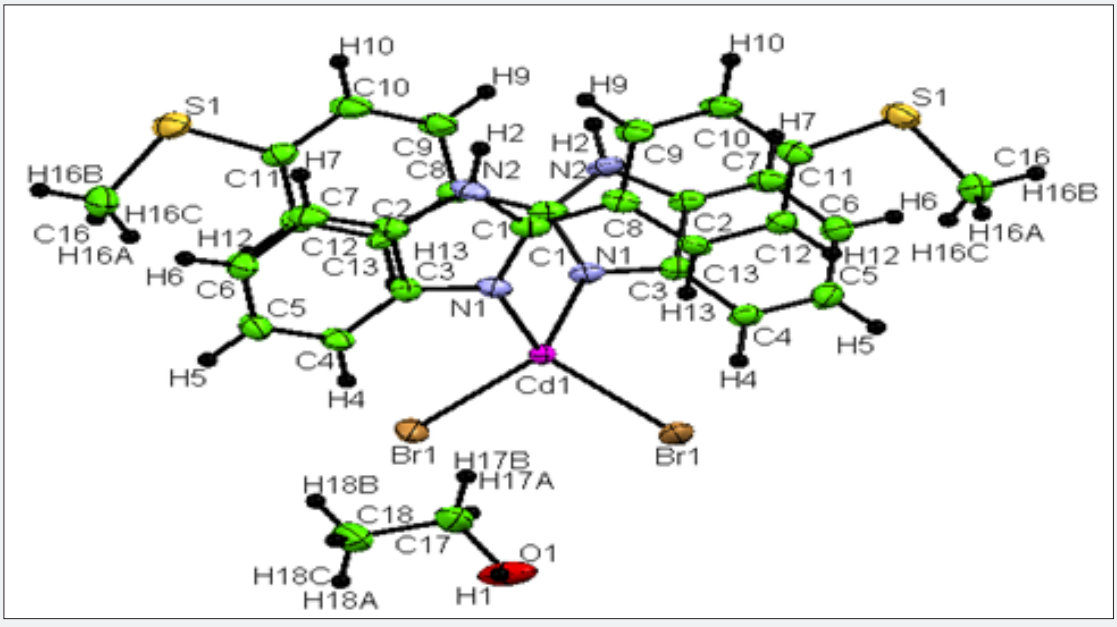

Figure 1: ORTEP diagram of compound 1, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

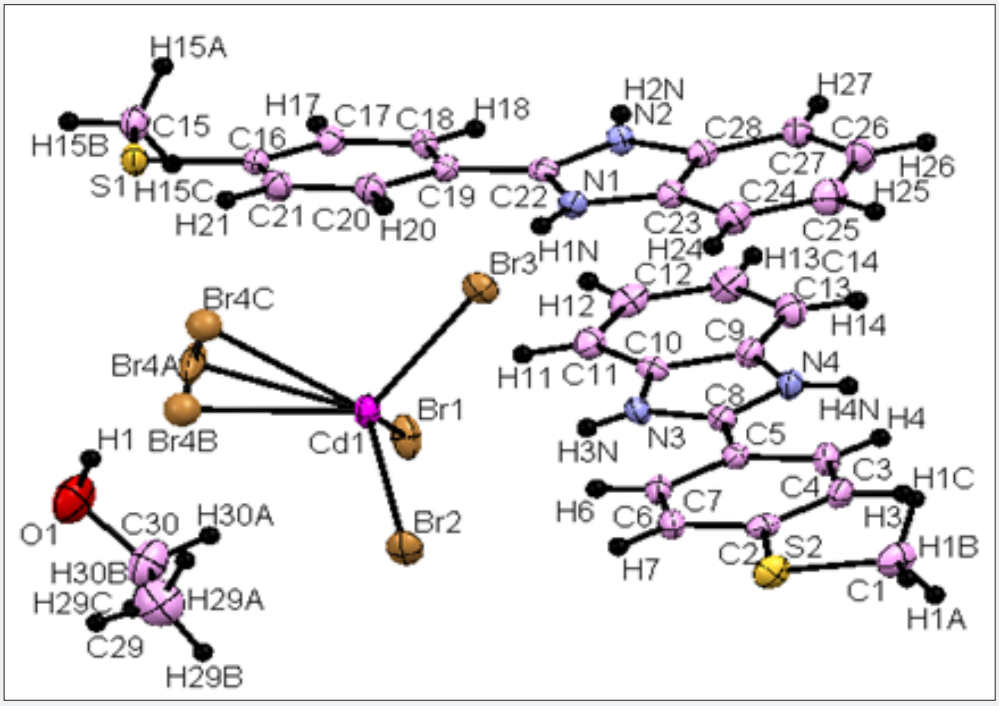

Figure 2: ORTEP diagram of compound 2, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Compound **1**: A total of 7272 reflections were collected, resulting in 7272 independent reflections of which the number of reflections satisfying $I>2\ \sigma(I)$ criteria were 6210. These were treated as observed. Corrections for Lorentz and Polarization effects were applied. It was confirmed that the crystal belongs to monoclinic crystal system and the space group is *C2/c* (Figure 1). Compound **2**: A total of 93968 reflections were collected, resulting in 7467 independent reflections of which the number of reflections satisfying $I>2\ \sigma(I)$ criteria were 5951. These were treated as observed. Corrections for Lorentz and Polarization effects were applied. It was confirmed that the crystal belongs to monoclinic crystal system and the space group is *Pbca* (Figure 2).

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