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Research paper

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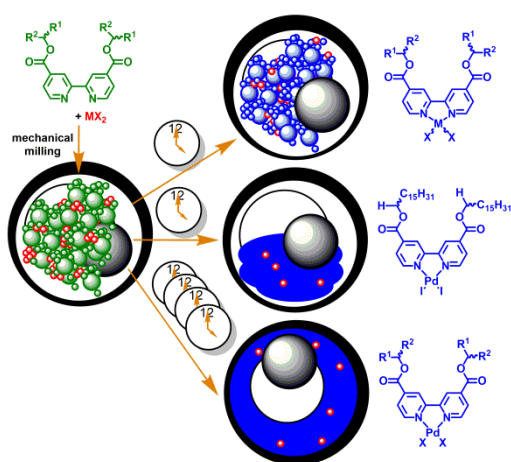
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# Mechanochemical synthesis of zinc and palladium complexes of dialkyl 2,2'-bipyridine-4,4'-dicarboxylate and analysis of solid-state reaction kinetics.

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Mechanochemical synthesis of a series of Zn and Pd dialkyl 2,2'-bipyridine-4,4'-dicarboxylate complexes ( $L^n$ , where  $n$  specifies the number of carbons in the  $\alpha$ - or  $\beta$ -substituted alkyl chains) including  $ZnL^{\beta 12}Cl_2$ ,  $ZnL^{\beta 14}Cl_2$ ,  $ZnL^{\alpha 14}Cl_2$ ,  $ZnL^{\alpha 14}I_2$ , and  $PdL^{\alpha 14}Cl_2$  is explored through a variety of linear and sigmoidal reaction models. The Johnson-Mehl-Avrami-Yerofeev-Kolmogorov (JMAYK) and Finke-Watzky (FW) models are largely equivalent as demonstrated through analysis of Akaike weights. This analysis was extended to the previously reported syntheses of  $PdL^{\beta 10}I_2$ ,  $PdL^{\alpha 16}I_2$ , and  $PdL^{\beta 16}I_2$  with similar results,

except that the JMAYK model is significantly superior to the FW model for  $PdL^{\beta 16}I_2$ . The physical properties of the reaction mixture, most prominently whether the product phase is easily mixed, is a major factor in determining the rate of reaction.

**Keywords:** mechanochemistry; ball mill; solid-state synthesis; kinetics; transition metal complexes

## 1. Introduction

Mechanochemical synthesis, although not a new technology, is currently being used to prepare many more types of compounds than the oxides, alloys, and compounds that were the previously the focus of the technique [1, 2]. Sustainability drives much of this research as the mechanical force used in these syntheses can be applied in the absence of solvent, drastically reducing the waste in these reactions [3]. From the perspective of researchers at less well-resourced institutions, mechanochemistry also provides a method for highly cost-effective preparation of transition metal complexes; an area of study only recently emerged in mechanochemical synthesis [4]. However, in order for mechanochemical synthesis to be utilized for routine small molecule and

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