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Farhad Shirini, Mohaddeseh Safarpoor Nikoo Langarudi, Nader Daneshvar

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ACCEPTED MANUSCRIPT

Preparation of a new DABCO-based ionic liquid [H₂-DABCO][H₂PO₄]₂} and its application in the synthesis of tetrahydrobenzo[b]pyran and pyrano[2,3-d]pyrimidinone derivatives

Farhad Shirini, a,b* Mohaddeseh Safarpoor Nikoo Langarudia, Nader Daneshvarb

^a Department of Chemistry, College of Sciences, Guilan University, Rasht, 41335-19141, Iran

Abstract— A new acidic ionic liquid, 1,4-diazabicyclo[2.2.2]octane-1,4-diium dihydrogen phosphate {[H₂-DABCO][H₂PO₄]₂}, was prepared in a quick and straightforward process and characterized by using different methods such as FT-IR, NMR and Mass analysis. Then it was used as a reusable and new catalyst to promote the synthesis of tetrahydrobenzo[b]pyran and pyrano[2,3-d]pyrimidinone derivatives as important biologically active compounds that they are used in pharmaceutical industry. This adequate procedure possess some advantages like producing target compounds in high yields, short reaction times, simple work-up procedure and use of chief and easily preparable catalyst.

Keywords: DABCO, ionicliquids, tetrahydrobenzo[b]pyrans, pyrano[2,3-d]pyrimidinones.

1. Introduction

In recent years, organocatalysts have been paid much attention because of their specific and characteristic properties. These reagents are often based on nontoxic organic compounds originating from biological materials and they can be Lewis bases, Lewis acids, Brønsted bases, and Brønsted acids. 1,4-Diazabicyclo[2.2.2]octane (DABCO) is a small diazabicyclic molecule with weak alkalescence and medium-hindrance that is used as an organocatalyst in the synthesis of many biological compounds [1-4] and recently, it has been used in the preparation of some DABCO-based ionic liquids like [DABCO(C₄H₈SO₃H)₂][HSO₄]₂ [5], [DABCO](SO₃H)₂(Cl)₂ [6, 7], [DABCO-PDO][OAc] [8, 9], and [DABCO](SO₃H)₂(HSO₄)₂ [10]. These reagents were able to promote some organic transformations such as oxathioacetalization [5], Knoevenagel condensation [8], and Aza-Michael addition [9], and the synthesis of dihydropyrimidinones [6], 1,8-dioxo-octahydro-xanthene and 5-arylmethylenepyrimidine-2,4,6-trione derivatives [7], 2*H*-indazolo[2,1-*b*]phthalazine-1,6,11(13*H*)-triones [10] and pyrano[2,3-*d*]-pyrimidinones [11].

Tetrahydrobenzo[b]pyran derivatives belong to an important class of heterocyclic compounds having important pharmaceutical and biological activities. Some drugs which possess antianaphylactin, anticoagulant, anticancer, diuretic, and spasmolitic properties [12, 13] are a part of tetrahydrobenzo[b]pyran derivatives. Also, they can be used as cognition-enhancing drugs for the treatment of neurodegenerative disease, including Alzheimer's disease, Huntington's disease, Parkinson's disease, Down's syndrome and schizophrenia [14, 15]. On the other hand, pyrano[2,3-d]-pyrimidinones are regular structural subunits in some important natural products, including carbohydrates, alkaloids, polyether antibiotics, pheromones, and iridoids (Fig. 1) [16, 17].

^b Department of Chemistry, College of Science, University of Guilan, University Campus 2, Rasht, Iran

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