Book of Abstracts

UNIVERSIDADE DE ÉVORA

SOCIEDADE PORTUGUESA DE QUÍMICA

New triazine-phosphonate dopants for proton exchange membranes (PEM)

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The establishment of a new paradigm for energy is underway demanding new energy sources for the increasing needs of society with none or lower environmental impact. To reach the ambitious and well-defined targets for decarbonized energy systems it is needed new clean technologies. Some of them rely on well-established or emerging electrochemical devices, including batteries, fuel cells and CO_2 and water electrolysers, whose applications and performances depend on key components such as their separators/ion-exchange membranes.[1,2] The most studied and already commercialized membranes go by the brand name of Nafion, which showed great chemical stability, but their high proton conduction depends on their water content, markedly limiting their operating temperature range. Our previous studies have demonstrated that the incorporation of aryl or heterocyclic phosphonic acid dopants into Nafion, by casting, results in an enhancement of the proton conductivity[1-4] and stability[5] of the Nafion doped membranes.

This work reports the synthesis and characterization of a new series of triazine-phosphonate derivatives for use as dopants in the preparation of Nafion modified membranes. Several arylphosphonate compounds were prepared bearing an amino or a hydroxy functional group at the *para*-position of the aryl ring. These compounds react with 2,4,5-trichloro-1,3,5-triazine through a nucleophilic substitution reaction to obtain the 2,4,6-(*p*-substituted)phosphonate-1,3,5-triazine dopants (**Figure 1**). The new compounds were characterized by NMR, IR spectroscopy and mass spectrometry, allowing the assignment of their structure.

Figure 1: Syntheis of new triazine-phosphonates.

In the anticipation that these synthesized phosphonates can act both as a source of protons and proton acceptors, facilitating the intermolecular proton conduction throughout the modified membranes, new Nafion modified membranes were prepared by casting, through the incorporation of these synthesized 1,3,5-triazine-phosphonate derivatives. The new membranes were characterized, and their proton conduction properties were evaluated by electrochemical impedance spectroscopy (EIS), at different temperature and relative humidity (RH) conditions.

Acknowledgements: This work was financed by national funds through FCT – Fundação para a Ciência e a Tecnologia, I.P., within the scope of the project PTDC/EQU-EPQ/2195/2021 - CO2RED, and LAQV-REQUIMTE, project UIDB/50006/2020 and UIDP/50006/2020. We also acknowledge the project "HYLANTIC" - EAPA_204/2016, co-financed by the European Regional Development Fund in the framework of the INTERREG ATLANTIC program.

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Ficha Técnica:

Título: ISySyCat – International Symposium on Synthesis and Catalysis, Évora, 2023
Editores: Carolina S. Marques, Elisabete P. Carreiro, Anthony J. Burke
Impressão: Cromotema
Tiragem: 228 exemplares
Designer Capa: Susana Oliveira, Gabinete de Comunicação, Universidade de Évora
ISBN: 978-972-778-309-0 (printed edition)
978-972-778-310-6 (digital edition)