

MS44-P5 The use of polystyrene organic-based gels for the diffraction quality single crystal growth of small molecules. L. Menéndez-Taboada^a, L. Rocés^{a,b}, A. Presa Soto^a, S. García-Granda^a, ^aPhysical and Analytical and Organic and Inorganic Chemistry Department, Faculty of Chemistry, University of Oviedo, Spain, ^bScientific and Technological Services, University of Oviedo, Spain
E-mail: menendezlaura.uo@uniovi.es

The use of gels for the crystallization of small molecules and proteins has been studied during the last decades. Gel media removes convection and sedimentation controlling the transport processes by diffusion, and providing higher crystal quality [1,2]. Crystallisation of small molecules in gel media has been broadly described for hydrogels and, recently, it has been reported the use of organic solvent-based gels using poly(ethylene oxide) (PEO), a synthetic polymer soluble in water and organic solvents [3]. Nevertheless, the usability of PEO gels is restricted to the limited number of solvents on which this polymer is soluble.

Polystyrene (PS) is a linear polymer, well known and characterized, cheap and accessible. We have studied the suitability of PS gels as media for diffraction quality small-molecule crystal growth. Herein, we report the detailed method for the preparation of PS gels, including a list of solvents, recommended PS concentrations in function of the crystallisation method employed and crystal extraction from the gel.

Acknowledgements

Financial support given by Spanish MICINN (MAT2006—01997, MAT2010-15094, PTA-2009-2346-I and Factoría de Cristalización Consolider Ingenio 2010), Ficyt grant (ref.: BP-060).

- [1] García-Ruiz, J. M., Novella, M. L., Moreno, R. & Gavira, J. A., *J. Cryst. Growth*, 2001, 232, 165-172.
- [2] García-Ruiz, J. M., Otálora, F. *Crystal Growth – Form Fundamentals to Technology*, 2004, edited by G. Müller, J.-J. Métois & P. Rudolph, pp. 369-375.
- [3] Choquesillo-Lazarte, D., García-Ruiz, J. M., *J. Appl. Cryst.*, 2011, 44, 172-176.

Keywords: gels, crystal growth, polymers

MS44-P6 Broad solvent compatibility of polystyrene functionalised polystyrene gels for single crystal growth of small molecules. Laura Rocés^{ab}, Laura Menéndez Taboada,^a Alejandro Presa Soto,^c Santiago García-Granda,^a ^aPhysical and Analytical Chemistry Department, Faculty of Chemistry, University of Oviedo, Spain, ^bScientific and Technological Services, University of Oviedo, Spain, ^cOrganic and Inorganic Chemistry Department, Faculty of Chemistry, University of Oviedo, Spain.
E-mail: roceslaura@uniovi.es

Obtention of diffraction quality single crystals is usually the limiting step of single crystal X ray structure determination. The use of gels as crystallisation media has been proved to present many advantages, leading to the obtention of high quality single crystals[1-3]. We report in this conference the use of polystyrene (PS) organic gels for the single crystal growth of small molecules (see contribution by Menéndez-Taboada et al.).

The use of PS as gel media has many advantages: PS is a well-known and characterized polymer; it is cheap and accessible; it is soluble in a large list of organic solvents. A minor disadvantage of PS as gel media is that there are still a number of solvents in which PS will not dissolve and the formation of a gel will never be reached. This issue can be overcome by the introduction of functionality onto the polymer support [4]. In fact, functionalized PS show a broad solvent compatibility range. In this way, it is possible to obtain gels of PS and functionalized PS with almost any solvent or solvent combination needed for small molecule crystallisation.

In this communication we will describe the method for the preparation of functionalized-PS hydrogels and organic gels, including a table of adequate solvents. Three successful crystallization experiments of different nature compounds (organic, organometallic and ionic) demonstrate the feasibility of this method for high quality single crystal obtention.

Acknowledgements

Financial support given by Spanish MICINN (MAT2006—01997, MAT2010-15094, PTA-2009-2346-I and Factoría de Cristalización Consolider Ingenio 2010), Ficyt grant (ref.: BP-060).

- [1] García-Ruiz, J. M., Novella, M. L., Moreno, R. & Gavira, J. A. (2001). *J. Cryst. Growth*, **232**, 165-172.
- [2] García-Ruiz, J. M., Otálora, F. *Crystal Growth – Form Fundamentals to Technology*, (2004), edited by G. Müller, J.-J. Métois & P. Rudolph, pp. 369-375.
- [3] Choquesillo-Lazarte, D., García-Ruiz, J. M. (2011) *J. Appl. Cryst.*, **44**, 172-176. [4] Zinck, P., Bonnet, F., Mortreux, A., Visseaux M. (2009) *Prog. Polym. Sci.* **34**, 369-392.

Keywords: crystal growth; gel; polymer