

# LECTURE

## prof. Delia Haynes

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University of Stellenbosch

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**VISITING  
PROFESSOR  
PROGRAMME**

will deliver a lecture titled:

### *Towards functional materials from multi-component crystals*

DATE: Tuesday, 9 July 2019 | 15:30  
VENUE: CNBCh UW, sem. room: 0.38

#### ABSTRACT:

Multi-component crystals, which include both salts and co-crystals, offer several advantages in the development of organic materials. Properties such as flexibility and solubility, as well as the possibility of including desirable physical properties in a material without altering key molecular properties, make multi-component crystals attractive targets. This lecture will describe efforts in our group to develop multi-component crystalline materials with interesting physical properties.

Co-crystallisation has been investigated as a means of overcoming dimerization in 1,2,3,5-dithiadiazolyl radicals (hereafter DTDA). DTDA are of considerable interest due to their potential as building blocks for organic magnetic or conducting materials, but they frequently dimerise in the solid state, rendering them diamagnetic. Co-crystallisation initially seemed a promising route to overcoming dimerisation in DTDA radicals, however this has proven to be more challenging than expected. A computational investigation, as well as experimental charge density studies, have been carried out on some DTDA and DTDA co-crystals in order to better understand the dimerisation interaction. Insight gained from these studies will be discussed.

Porous organic salts offer several advantages over metal-organic frameworks and covalent organic frameworks; for example these materials can be dissolved and re-assembled from solution. We have investigated the use of the pamoate ion in the design of porous organic salts. The interesting properties of several salts, including selectivity and guest exchange, will be presented. Recent results involving a series of zwitterionic building blocks will also be discussed.



#### Activity at Home University:

Prof Haynes' research focusses on crystal engineering with multi-component crystals. She has experience both with thiazyl radicals as building blocks for molecular materials, and with organic salts and co-crystals. Delia was a Fulbright Scholar at the University of California, Berkeley in 2010, a visiting professor at the University of Strasbourg in 2013, and was the 2015 recipient of the Jan Boeyens medal. She is a member of the Executive Committee of the European Crystallographic Association, and the chair of the Steering Committee for the African Crystallographic Association.



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