

# The role of transition metals in the structure and reactivity of astrochemicals

WCPM/CSC joint seminar

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Monday, 5th June, 1 p.m.

D2.02 Seminar room, Engineering

**Abstract:** The field of astrochemistry is growing rapidly. There are yearly, impactful discoveries of new gas phase molecules in the interstellar medium, and a growing interest experimentally and theoretically on the surface interactions of molecules with interstellar ices and grains. Most research in the field of astrochemistry has focused on the structure and reactivity of organic molecules. Deciphering the electronic structure of small gas phase inorganic radicals is extraordinarily challenging. These challenges downplay the roles that these transient molecules may play in the composition of ices and grains, and the catalysis of molecules implicated in origin-of-life chemical processes. The part that computational chemistry is playing in guiding observational and terrestrial detection of new gas phase inorganic astrochemicals will be discussed. Specifically, the interplay between theory and experiment in the discovery of the first organometallic astrochemical, iron monocyanoide (FeCN), and surprising aspects of the electronic structure and spectroscopy of titanium dicarbide ( $TiC_2$ ) will be featured.



A buffet lunch will be available from 12:45 pm.

More info: <http://warwick.ac.uk/wcpm/seminars>

