

AVVISO DI SEMINARIO

Lunedì **28 giugno 2010** alle ore **11.30**
presso l'aula **A1** del Dipartimento di Scienze Chimiche,

il prof. **JAN MOCÁK**

Department of Chemistry, Faculty of Natural Sciences, University of Ss. Cyril
and Methodius, Slovak Republic

Terrà un seminario dal titolo:

RECURRENT RELATIONS AND CHEMOMETRIC CALCULATIONS

Many physicochemical constants of organic compounds (bp, mp, ri, permittivity, relative density, dynamic viscosity, surface tension, etc) are widely used in characterization and prediction of analytical properties like retention indices in gc. Even though there exist electronic databases and many exploitable handbooks containing detailed information on the constants of organic substances, still not all compounds are described by reliable values.

Recurrent equations, discovered in mathematics many centuries ago, may be used for a very precise calculation used in chemistry, particularly in organic, physical organic and analytical chemistry. Implementation of recurrent equations is very simple and can be performed by any spreadsheet programs. Typical applications will be demonstrated in the lecture. Two dimensional recurrences are important in transforming divergent infinite series into converging sequences, which enables precise calculations of current – potential signals in voltammetry.

Several applications of chemometric techniques may demonstrate their potentialities in various border chemical disciplines, like environmental, pharmaceutical and clinical chemistry. Several examples will be shortly presented: the applications of principal component analysis, cluster analysis, discriminant analysis, artificial neural networks, QSAR and QSRR (quantitative structure – retention relationships). The studied objects have been various series of organic compounds characterized by a large amount of chemical, physical and biological properties.

Tutti gli interessati sono cordialmente invitati

Il Direttore
del Dipartimento
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