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# 12th International Conference Processes in Isotopes and Molecules

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## Topics:

- T1: Stable Isotopes Labeled Compounds and Analytical Techniques
- T2: Molecules, Biomolecules and Green Technologies
- T3: Energy Efficiency and High-Tech Engineering
- T4: Nanostructured Materials Nanocomposites and Hybrid Materials

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## **Section T1:**

Stable Isotopes, Labeled Compounds and Analytical Techniques

#### Plenary Pl-13

## Aspects of structural investigations of 'Core-Shall' structures, Fe<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub>, by X-Ray and Neutron Scattering

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Abstract. Synthesis of magnetic nanoparticles (MNPs), such as Fe<sub>3</sub>O<sub>4</sub>, CoFe<sub>2</sub>O<sub>3</sub> etc., are of great interest because of the possibility of their wide using in technology and science, especially in medicine. For medical applications MNPs have to be nanosized, monodispersed, nontoxic and have stability to aggregation. The structural aspects of powders Fe<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub> magnetic nanoparticles with the anticipated "core-shell" structure have been analysed by comparison with individual Fe<sub>3</sub>O<sub>4</sub> and CoFe<sub>2</sub>O<sub>4</sub> particles using X-ray powder diffraction, small-angle neutron and X-ray (synchrotron) scattering. It is shown that MNPs in the powders are strongly polydisperse and form complex aggregates. The characteristic sizes of the crystallites, as well as the ratio between magnetite and cobalt ferrite in the composition of the Fe<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub> particles are estimated based on analysis of the diffraction peaks. Analysing the small-angle scattering data, the characteristics particles' size and aggregates are obtained. The fractal dimensions of the aggregates are determined. A significant difference between scattering at Fe<sub>3</sub>O<sub>4</sub>/CoFe<sub>2</sub>O<sub>4</sub> particles and the total scattering derived from the partial contributions of scattering events at powders of separate magnetite and cobalt ferrite particles is observed, which suggests the formation of a "core-shell" structure.

### Plenary Pl-14

# Caracterization of pharmaceuticals, cosmetics and supplements using Stable Isotope Ratio Analysis

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Abstract. Stable isotope ratio analysis of bio-elements (hydrogen, carbon, nitrogen, oxygen and sulphur) has been used since the 1990s to check food authenticity and traceability of a wide variety of food commodities. In the last years, examples of applications also in the pharmaceutical and cosmetic field have been reported. The use of stable isotope analysis for products authentication purposes is possible thanks to isotopic fractionation occurring in several processes and reactions (biological, biochemical, physical, chemical etc.) which generates unique isotopic signatures. For this reason, the application of this technique on the bulk samples as well as on specific components (e.g. aroma compounds) can be used to detect the origin of an ingredient (synthetic or natural), the substitution of one ingredient for another, as well as the geographical and/or botanical origin of the products. The  $\delta^{13}$ C and  $\delta^{2}$ H values of vanillin can determine whether the product is natural (deriving from the expensive CAM plant Vanilla), biotechnologically derived or synthetic. Moreover, the  $\delta^{13}$ C values of specific components of Rosa damascene mill., one of the most expensive essential oils in the market world, can indicate the fraudulent addition of cheaper oil from a C4 plant (e.g. Cymbopogon martinii, palmarosa). In pharmaceutical and cosmetic formulations,  $\delta^{13}$ C analysis is a suitable tool to discriminate between squalene and squalane from shark (illegal) and from olive oil (expensive) as well as between monacolin K (contained in the fermented dietary supplement red yeast rice) and the commercially marketed statin, lovastatin. It's possible to combine different isotopic signatures to guarantee the natural origin of curcumin, caffeine, tartaric acid and its derivatives. These examples demonstrate that the isotopic fingerprint represent an effective tool for the authenticity assessment of economically important pharmaceutical, cosmetic and supplement products.