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Increasing the radial distance, the accuracy of the Sievert Integration Model (SIM) decreases in a non-linear manner, adding errors up of 10% into the dose rate calculations; a similar fact occurs to the 2D anisotropy function where the errors may achieve 30% as already related. For that reason, this paper sought an innovative approach to optimize the error variance and its biases of dose rate calculations around a Nucletron brachytherapy source of ^{192}Ir from 0 to 10 cm taken in the radial distance, using an improved SIM through a hybrid coupling of Artificial Neural Networks (ANN) and Inverse Problem Theory (IPT). Since the traditional approach relies into the use of a small data set of dose rate, the ANN generalized these doses, making possible to search more broadly optimum parameters to SIM using the IPT. The results showed excellent accuracy evaluated with the Root Mean Square Percentage Error (RMSPE). In conclusion, the low RMSPE values indicate that the methodology is a consistent methodology, showing an excellent agreement with the state of art of dosimetric measurement techniques.

Determination of Si content in Fe-doped HfSiO₄ nanoparticles by neutron activation analysis

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New synthesis method of Fe-doped hafnium silicate nanoparticles (NPs) with tetragonal structure is reported. The procedure implies auto-controlled incorporation of Si from the quartz to the iron-doped hafnium oxide NPs. X-ray diffraction data has shown that lattice parameters of Fe-HfSiO₄ thus obtained are very close to those previously known for hafnon. It was established that the hafnon-like phase has stabilized at T=1173K which is ~500K lower than the corresponding transition of bare bulk hafnium silicate. The

fractions of Si and Fe in the composite matrix were evaluated via neutron activation analysis (NAA). Delayed gamma NAA results allowed to assume that (i) Fe initially substituted Hf in the HfO₂ lattice; (ii) there was no migration of iron atoms from Hf to Si sites throughout the formation of hafnon-like phase; (iii) Fe-doped hafnium oxide has taken as much Si from the quartz as was needed for the arrangement of Fe_{1-x}Hf_xSiO₄ tetragonal system. Our results are consistent with those observed for similar materials, such as metal (Fe,V) doped zircon, where metal has also demonstrated catalytic effect on phase stabilization.

Structural characterization of a novel anti-inflammatory parent compound

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LASSBio-1860 is an inhibitor of phosphodiesterase type 4 (PDE4). This enzyme plays a major role in modulating the activity of virtually all cells involved in the inflammatory process acting in the control of cAMP levels [1]. This compound was planned and synthesized in Laboratory of Evaluation and Synthesis of Bioactive Substances – LASSBio® as part of a research program to develop a series of compounds with anti-inflammatory activities. As important as the planning and synthesis of new drugs is its structural characterization, since its structure may be related to a biological activity. In many cases suitable single crystals cannot be prepared, and the most used technique that is the single crystal X-ray diffraction (XRD) is not a viable approach for structure determination. Under such circumstances, structure determination must be tackled instead from X-ray powder diffraction (XRPD) data and that is considerably more challenging than structure determination from single-crystal XRD data. In this work we determined the crystal structure of LASSBio-1860 compound using XRPD that has been a very important tool in the structural determination of new synthesized compounds. LASSBio-1860 crystallized in a monoclinic system (P2₁/c) and the crystal structure consists of four formula units per unit cell ($Z = 4$), thus accommodating one molecule in the asymmetric unit ($Z' = 1$). The Rietveld method was used to refine the crystal structure and the goodness-of-fit indicator as well as R-factors were $\chi^2 = 1.131$, $R_{\text{Bragg}} = 0.856\%$, $R_{\text{wp}} = 4.174\%$ and $R_{\text{exp}} = 3.692\%$.

Test enclosure design, construction, and tests for the CNEC well-logging benchmark tool

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