DETERMINATION OF $K_{\alpha,\beta}$ EXCITATION FACTORS FOR Cd, Sb AND La

R. DURAK (ATATÜRK UNIVERSITY), M.F. TURHAN, and F. AKMAN
rdurak@atauni.edu.tr

Kα and Kβ excitation factors were measured for the elements Cd, Sb and La. To determine the Kα and Kβ excitation factors, the experimental values of K shell fluorescence yields, K shell absorption jump factors and theoretical values of the fractional ratio of the Kα,β X-rays were used. To determine the K shell fluorescence yields, the targets were excited using photons of 59.54 keV emitted from an Am-241 radioactive source. Also, the K shell absorption jump factor measurements done in a transmission geometry utilizing the Kα2, Kα1, Kβ1 and Kβ2 X-rays from some selected elements in the atomic range $39 \leq Z \leq 68$. Emitted K X-ray photons from targets were collected by means of a Si(Li) detector with resolution of 160 eV at 5.9 keV. The present results are generally in a good agreement with theoretical calculations and the other results obtained in the literature.

STRUCTURAL AND CONFORMATIONAL STUDY OF DIENOGEST

G. YILMAZ (ISTANBUL UNIVERSITY), S.CELİK, , A.E. OZEL
gzdektrn@hotmail.com

The present study on the conformational and structural behaviors of dienogest molecule with the chemical formula 17-hydroxy-3-oxo-19-nor-17α-pregna-4,9-dien-21-nitrile 17-α-cyanomethyl-17β-hydroxy-estra-4,9(10)-dien-3-one ($C_{20}H_{25}NO_2$), which is an orally-active semisynthetic and steriodal progestogen were investigated. Dienogest given in isolation is available for the treatment of endometriosis which is a gyneacological disease and its main symptoms are pelvic pain and infertility. It is a non-ethinylated progestin which is structurally related to testosterone.

In this work, the molecular conformations of free title molecule were searched by means of torsion potential energy surfaces scan studies, through two dihedral angles in electronically ground state. Afterwards, the most stable optimized structural geometry and energetically preferred conformations of dienogest molecule were determined using DFT method at B3LYP/631++ G(d,p) level of theory with the help of Gaussian09 packed program.