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PROGRAMME

(*Session on Molecular Atom and quantum optics*)

4rd International Conference on

"HIGH LEVEL PHYSICS AND APPROPRIATE SOLUTIONS TO REAL LIFE PROBLEMS IN DEVELOPING COUNTRIES"

Plus a special session on the state of physics in Africa

24 – 28 November 2015

Yaounde, Cameroon

Organised by

Cameroon Physical Society

With the support of

INTERNATIONAL YEAR OF LIGHT 2015

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Thursday, 26 November 2015

Hotel Franco - Conference Hall FOVU

Session on Molecular Atom and quantum optics - Programme

First part (Chairman: Prof. Nsangou Mama)

08h00-08h30: ETINDELE Anne Justine, *Investigation and modelling of off-center endohedral fullerenes,* Université de Douala

08h30-09h00: TCHAKOUA Théophile, *Rotational excitation of some molecular anions of astrophysical interest,* Université de Douala

09h00-09h30: MAIMOUNATOU BOUBAKARI, *Comparative study of the quasi-phonons and the mode electric field in the $LiTaO_3$ and $LiNbO_3$ single crystals,* Université de Maroua

09h30-10h00:ALHADJI MALLOUM, *Solvatation du proton dans l'ammoniac,* Université de Ngaoundéré

10h00-10h30:HOLTOMO Olivier, *Structure and kinetic study of the antioxidant mechanism of phenylethyl-3,4-dihydroxyhydrocinnamate,* Université de Bamenda

10h30-11h00:EPEE EPEE Michel Douglas, *Reactive collision of very low-energy electron with D2+ and CH+ molecular cations: Dissociative recombination and rotational transition,* Université de Douala

11h00-11h30:TCHODIMOU Carolle, *Alphabetic character recognition of national languages through an Associative Memory: Hopfield Neural Network,* Université de Ngaoundéré

11h30-12h00:MELINGUI MELONO Robert Landry, *Electronic structure of hydrogenic impurity in quantum dots and quantum nanowires: energy levels and dipole polarizability,* Université de Douala

12h00-13h30: Pause-café

Second part (Chairman: Prof. Motapon Ousmanou)

13h30-14h00: TCHAPET NJAFA Jean-Pierre, *Quantum associative memory for the diagnosis of some tropical diseases,* Université de Ngaoundéré

14h00-14h30: DJORWE Philippe, *Molecular cavity optomechanics,* Université de Yaoundé I

14h30-15h00: NGOA ENGOLA Louis, *Environmental pollution survey using XRF spectrometry in the Gold Mining Region of East-Cameroon,*University of Douala

15h00-15h30:NDJANA NKOULOU II Emmanuel Joseph, *Natural radiation monitoring using gamma spectrometry in the Gold Mining Region of East- Cameroon,*Institute of Geological and Mining Research

15h30-16h00: BINENG Guillaume Samuel, *Indoor radon and thoron measurements in the Nyong Ekelle Division, Centre Region, Cameroon,* Université de Yaoundé I

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BOOK OF ABSTRACT

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Investigation and modelling of off-center endohedral fullerenes

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ABSTRACT

The necessity of building a model potential of fullerene cages C_n, felt by an atoms *A* trapped inside ($A@C_n$) is relevant. Indeed, these systems have a wide range of potential applications in promising areas like drugs delivering in medicine[1-3], or they can be used as building blocks of new electronic devices[4]. These kinds of applications require a good knowledge of the way the cage and the confined system interact together. There exist some potential models that caracterise the effect of the presence of C_{60} on the confined atom. The simplest and most used one, the square square well potential, has been first proposed by Pushka and Niemenen[5] and next by Xu *et al*.[6], and has been successfully used by several authors to describe the properties of centered confined atoms. Up to date, the have never been used to describe metal atoms that are known to be stable off-center.

We are investigating the applicability of square well potential model of C60 fullerene to the case of off-center endohedrally confined alkali atoms. We use a similar method to the one of Ting *et al.*[7] to handle the the spherical symmetry breaking due to the displacement of atom from the center. The sake of simplicity of the alkali Schrödinger equation, we consider the external electron moving the central field of the core electrons and the nucleus modeled by a core potential of Schweizer[8].

We found that the energies obtained as a function of the distance from the center of the cage show that Li and Na atoms are off-center stable whereas K is stable at the center of the cage as it is predicted in the literature. The study the influence of square potential parameters on the equilibrium position of the alkali in the cage shows the possibility of perceiving an effective radius of the cage. The impact of the asymmetry induced by the off-center displacement on the static and dynamic polarizabilities is studied.

Key words: endohedral cavity, endofullerene, model potential, off-center atom.

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Rotational excitation of some molecular anions of astrophysical interest

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ABSTRACT

The progress brought to the instruments used in astronomy during this last decades (HERSCHEL ET ALMA), allow the observation of new molecules in stellar and interstellar clouds, and this was done with high precision as revealed by various spectra. These data obtained using these instruments, could be interpreted theoretically through the computation of the collisional rate coefficients, the latter being derived from state-to-state cross sections of these observed molecules. In fact, collision rate or reaction rate, can be defined as the probability that a molecule goes through collision, from a less excited level to a more excited level at a given temperature of the medium. The accuracy of these collisional rate coefficients is the key objective of this presentation, particularly for negatively molecules with high electron affinity (anions) such as NCO− , NCS− , C3 N− , C5 − .

Key words: Molecular anion, collision cross sections, rate coefficients, rotational transitions.

Directional dependence of optical polar phonons in LiNbO3 single crystals

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Abstract

The present work reports the analysis of both experimental and theoretical angular dispersion of the Raman frequencies of the optical polar phonons in LiNbO3 single crystal. This analysis allows the determination of the complete set of the normal frequencies assignment of phonons frequencies. The coherency of such couples assignment is assessed by the computed oscillator strengths that are revealed to be satisfactory agreement with literature. Finally the directional behavior of the normal vector has been established and permit to a quantitative determination of the electro-optic coefficients.

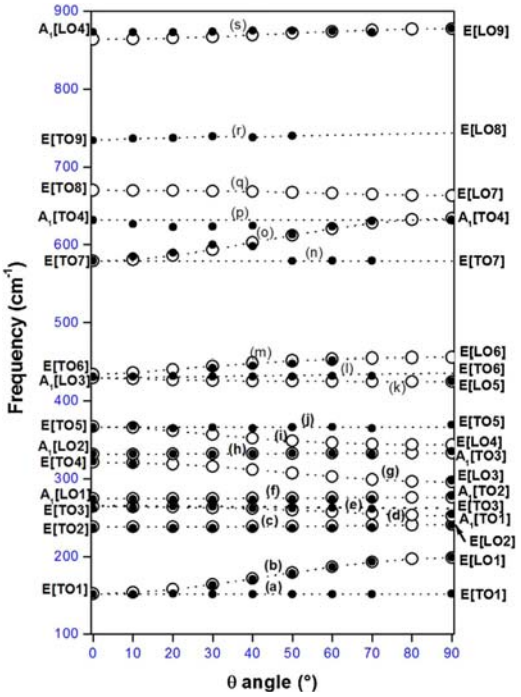

Figure: Angular dispersion branches of phonons in the LN crystal: the theoretically computed angle-dependent frequencies are plotted as open circles and the experimentally determined frequencies are illustrated by scatter points; the dotted lines are the expected angular dispersion curves.

Keywords: LiNbO3, optical phonon, phonon dispersion, Raman spectra.

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Structures and Relative Stabilities of ammonia clusters at different temperatures: Ab-Initio Vs DFT

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Key words: Neutral ammonia clusters, *Ab-initio*, DFT, Relative stability, Temperature effects, Infra-Red Spectra

Abstract

Hydrogen bond network in ammonia clusters is very important to understand properties of species embedded in ammonia. This network is dictated by the structures of neutral ammonia clusters. Structures of neutral ammonia clusters *(NH3)n=2-10* , have been studied at *M06-2X/6-31++G(d,p)* and *MP2/6-31++g(d,p)* levels of theory. We noted that *M06-2X* provides lower electronic energies, greater binding energies and higher structural resolution than *MP2*. We also noted that at the *M06-2X* level of theory, the binding energy ΔEn converges to the experimental vaporization enthalpy faster than at the MP2 level of theory. As a result, *M06-2X* functional must be more suitable than *MP2ab initio* method in the study of structures and energies of ammonia clusters. However, we found a very good correlation between electronic energies computed at *M06-2X* and those computed at *MP2*, for the most stable isomers. The difference between these two energies exhibits a linear variation with *n* (number of ammonia molecules in a cluster). As far as the structures of ammonia clusters are concerned, we proposed new ”significant” isomers that have not been reported previously. The most remarkable is the global minimum electronic energy structure of ammonia hexamer, which has an inversion center and confirms experimental observation. Moreover, we reported the most favored isomers of neutral ammonia clusters for temperatures ranging from 25 to 400 K. The stability of isomers changes with the increase of the temperature. As a result, the branched and less bounded isomers were most favored at high temperatures and disfavored at low temperatures, while compact and symmetric isomers dominate the population of clusters at low temperatures. In fine, from this work, the global minimum energy structures of ammonia clusters are known for the first time at a given temperature (T □ 0 − 400 K) at a reliable computational level of theory.

Structure and kinetic study of the antioxidant mechanism of phenylethyl-3,4-dihydroxyhydrocinnamate

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/mol and 301.93kJ/mol. The corresponding free energy of bond dissociation (BDFE) were 308.76kJ/mol and 268.59kJ/mol. Thus site O_3-H_3 was the propitious site of radical attack. Then we were interested

ABSTRACT

In this work, we investigated the structure of phenylethyl-3,4-dihydroxyhydrocinnamate (PDH) using B3LYP/6-31+G(d,p) level of DFT. With the lack of the experimental results, the data were compared to those of caffeic acid phenethyl ester (CAPE). The molecular skeleton of the two compounds were almost similar. The bond lengths and angles of the two compounds were closer together (1.1%), except the C_7=C_8 double bond of CAPE which was a single bond in PDH. The bond dissociation enthalpy (BDE) of the two site of radical attack O_3-H_3 and O_4-H_4 are respectively 343.15kJ by the effect of scavenging the alkoxyl radicals C_nH_{2n+1}-$O^\bullet$, n=0,1,2,3,4,5. We took six radicals: $OH^\bullet$, CH_3-$O^\bullet$, C_2H_5-$O^\bullet$, C_3H_7-$O^\bullet$, C_4H_7-$O^\bullet$ and C_5H_{11}-$O^\bullet$. The results showed that the free energy required for hydrogen atom transfer (HAT) in terms of the number of carbon n, follows: $0<1<2<3$, but $2\approx4\approx5$.

Keywords: PDH, DFT, BDE, alkoxyl radical, scavenging, HAT.

Reactive collision of very low-energy electron with D_2^+ and CH^+ molecular cations: Dissociative recombination and rotational transition

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Abstract

We have performed high precision computations for the cross sections and rate coefficients of Dissociative recombination and Rotational Transitions at very low collision energies for some diatomic molecular ions of astrophysical interest or relevant for the modelling of fusion plasma. The study is based on the stepwise Multichannel Quantum Defect Theory (MQDT)[1-3], which is time independent approach that has been proven to be appropriate for such investigations. The results will be presented for H_2^+ and its isotopologues (see Figure 1 for example)[4] as well as CH^+.

Key words: **Reactive collision, Dissociative Recombination, Rotational Transition, Molecular ion, Multichannel Quantum Defect Theory**

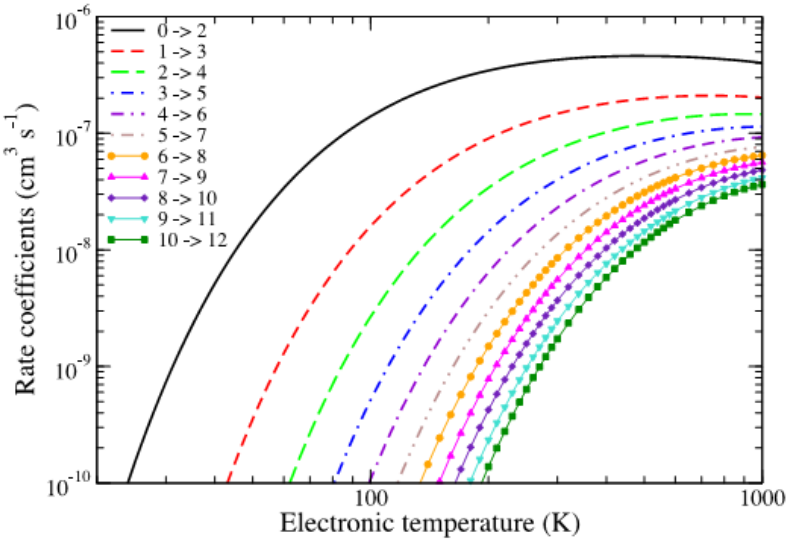

Figure: Rate coefficients for $N_i^+ \rightarrow N_i^+ + 2$ transitions in the ground vibrational state of $H_2^+(X^2\Sigma_g^+)$, with $N_i^+ = 0$ to 10 (From Ref.[4]).

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Alphabetic character recognition of national languages through an Associative Memory: Hopfield Neural Network

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Abstract

The artificial neural networks are excellent tools for character recognition. Here, we use an Associative Memory for the recognition of special alphabetic characters which are specific to our Cameroonian languages.The algorithm used for the Associative Memory is the Hopfield algorithm. The process consists to teach to the neural network all special alphabetic characters. The artificial neural network is able to return the characters that he has stored as will the brain of a human being. The Hopfield Neural Network minimizes an energy function. It would allow the convergence to a stable state. Each stable state of the network corresponds to the desired output. The Hopfield network gives satisfactory results when we stored a number of characters inferior to the number of neuron.

Keywords: neural network, alphabetical character, associative memory, Hopfield neural network, recognizing.

Electronic structure of hydrogenic impurity in quantum dots and quantum nanowires: energy levels and dipole polarizability

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Abstract

Due to their many technological applications such as fabrications of opto- and electro-optical devices which operate in the green-ultraviolet region in the visible spectrum, quantum nanowires (QNWs) and quantum dots (QDs) have, in recent years become an area of intense research.[1-5] Recent improvements in the nanostructure technology have made possible the preparation of these small scale semiconductors, through different methods such as etching or molecular-beam epitaxy (MBE).[6] An impurity in quantum dots and quantum nanowires is very important because it increases the ability of this system. If a donor impurity has one additional electron, such an impurity is said to be hydrogenic one because it is very similar to a hydrogen atom.[7] In this new interesting research axis we study how a confined hydrogenic impurity in quantum dots and quantum nanowires reacts to an external electric field via the calculation of non-relativistic static and dynamic dipole polarizabilities. The more general case where the impurity is located out of center of the nanostructure is also considered and new numerical approaches inspired by some recent works [8-9]in spherically and cylindrically confined system are used.

Key words: **quantum dots, quantum nanowires, hydrogenic impurity, dipole polarizability, off center.**

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Eigenvectors of the fractional Schrodinger-like equation with non local term

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Abstract

We investigate eigenfunctions of time-dependent fractional Schrödinger equation in presence of a nonlocal term by using the method of fractional Fourier transform. We analyze the fractional Fourier transform and give some of its new properties in the case of the Riesz derivative. As an application, we study the problem of eigenfunctions of the time-dependent fractional Schrödinger equation in presence of a nonlocal term. Some results for the free particle and delta potential energy function are presented. The obtained results for the considered Schrödinger-like equation may be transformed to those for the probability distribution function of a diffusion-like equation with memory kernel and could eventually be used to explain quantum effects in nano electromechanical systems.

Quantum associative memory with linear and non-linear algorithms for the diagnosis of some tropical diseases

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Abstract

In this work we present a model of Quantum Associative Memory (QAM) which can be a helpful tool for physicians without experience or laboratory facilities, for the diagnosis of four tropical diseases (malaria, typhoid fever, yellow fever and dengue) which have several similar symptoms. The memory can distinguish single infection from multi-infection. The two algorithms used for the Quantum Associative Memory are improve models of original linear algorithm made by Ventura for Quantum Associative Memory and the nonlinear quantum search algorithm of Abrams and Lloyd. From the simulation results given, it appears that the efficiency of recognition is good when a particular symptom of a disease with the similar symptoms are inserted as linear algorithm is the main algorithm. The non-linear algorithm allows to confirm the diagnosis or to give some advices to the physician. So our QAM which have a graphical user interface for desktop and smartphone is a sensitive, low-cost diagnostic tools that enable rapid and accurate detection of some tropical diseases.

Molecular cavity optomechanics

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Abstract

The enhancement of Raman scattering cross-section by localized plasmonic resonances has enabled spectroscopic fingerprinting of single molecules and is widely used in material, chemical and biomedical analysis. Here we present the plasmon-enhanced Raman scattering based on parametric amplification in optomechanics. This enhancement mechanism is efficient when the mechanical effective damping hits the negative values, in the blue-sideband, corresponding to the parametric instability.

The Raman cross section is derived from the optomechanical coupling rate, which is computed from the molecules Raman activities and the plasmonic field distribution. Following the optomechanical theory, a quantitative framework for the calculation of enhanced cross-sections is provided, recovering known results, and enabling the design of novel systems that leverage dynamical backaction to achieve additional, mode-selective enhancement. It yields a new understanding of plasmon-enhanced Raman scattering and opens a route to molecular quantum optomechanics.

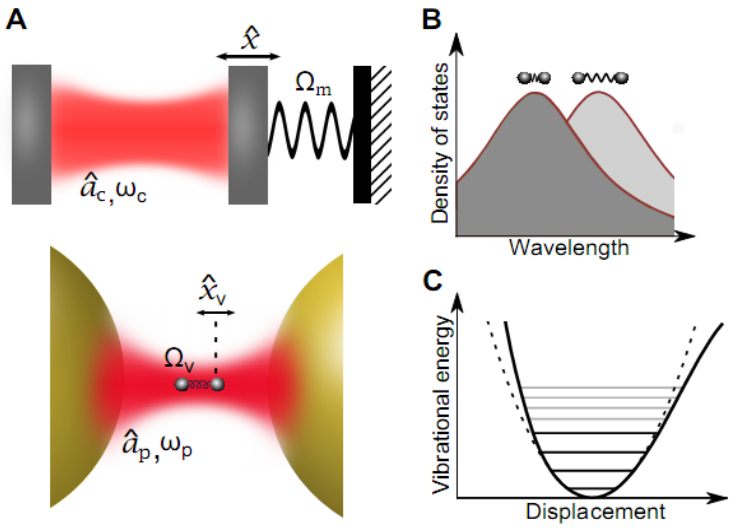

Figure: Cavity-optomechanical model of the interaction between plasmon and molecular vibration. (**A**) Schematic mapping between (upper panel) an optical cavity with a mechanically compliant mirror and (lower panel) a plasmonic hot spot and a molecule with internal vibrational mode (sketched as two masses connected by a spring). (**B**) During vibrational motion the change in polarizability of the molecule leads to a shift of the plasmon resonance frequency at the origin of the parametric optomechanical coupling. (**C**) Schematic molecular potential as a function of the vibrational coordinate. The harmonic oscillator description is valid for small amplitudes (low excitation numbers, dark lines) but anharmonicity must be taken into account under high amplification (higher levels, gray lines).

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Environmental pollution monitoring using xrf-spectrometry in the gold mining region of east Cameroon

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Abstract

The main objective of this study is to assess the level of heavy metals pollution in soil collected around gold mines located in Betaré Oya (BO) and Batouri (BA) in Eastern Cameroon. Elemental analysis of soil samples was carried out by Quant´X EDXRF spectrometer and its sensitivity and accuracy was increased by using the Fundamental Parameter approach for quantification of the results. The results obtained show a predominance of iron (39285.7±188.4 ppm) and the presence on a high level of manganese (725.7±62.8 ppm), arsenic (4.1±1.9 ppm), zirconium (313.8±4.0 ppm) and lead (78.9±8.6 ppm) as compared to worldwide average soil values. To assess if the heavy metals levels found in the soil derive from natural or anthropogenic sources, the parameters such asIndex of Geoaccumulation (Igeo), Enrichment Factors (EF), Contamination Factors (CF) and Degree of Contamination (Cdeg) were calculated.The mean enrichment factors decrease as Pb>As>Zr>Mn>Fe>Y>Ga>Zn>Cu>Ni>Rb>Sr>Sn>Ba in agreement with the CF. The Cdegcompared to the sites shows that BO5>BO4>BA1>BO3>BO1>BO2>BA2. Results of this study revealed that soil pollution by metals stems from anthropogenic sources such as gold mining activities. Consequently, there is an exposure to potential threat for humans and critical environmental media such as food chain, dust and water.

Key words: gold mine, soil, X-ray fluorescence, heavy metals, enrichment factor.

Natural radiation monitoring using gamma spectrometry in the Gold Mining Region Of Cast-Cameroon

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Abstract

The objective of the present study, is to carry out natural radioactivity measurements and to assess radiological exposure of the public in the gold mining areas of Eastern Cameroon. For this purpose sodium iodide (NaI) detector spectrometer was used to determine activity concentrations of natural radionuclides in soil samples collected from the mining areas. The average activity concentrations determined for ^{226}Ra, ^{232}Th, and ^{40}K are 40.2 Bq kg^{-1}, 29.4 Bq kg^{-1}, and 186.2 Bq kg^{-1}, respectively. ^{226}Ra is identified as major natural radionuclide with the activity concentrations slightly higher than the world average value given by UNSCEAR. The averaged external annual effective dose due to radioactivity in soil is 0.34 mSv.yr^{-1}. The average external hazard index is less than unity. Consequently, soils from mining sites may be used for building constructions. Nevertheless, there is an exposure to potential threat for humans and environmental media such as food chain, dust and water. Some recommendations are drawn to strengthen the environmental protection of mining areas.

Key words: gold mine, soil, natural radioactivity, external hazard index

Indoor radon and thoron measurements in the Nyong Ekelle Division, Centre Region, Cameroon

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Abstract

The objective of this work is to carry out indoor radon and thoron measurements in Eséka and Ngombas II in the uranium region of Lolodorf. The indoor radon and thoron concentration were measured in 28 dwellings with RADUET detectors. Indoor radon and thoron distributions follow the lognormal law. Radon and thoron concentrations were determined using Image-J and Microscope Methods track evaluation. Their concentrations ranged respectively 54±4 $Bq.m^{-3}$ to 254±6 $Bq.m^{-3}$ and 91±88 $Bq.m^{-3}$ to 386±0 $Bq.m^{-3}$. The arithmetic means of radon and thoron were 100 $Bq.m^{-3}$ and 209 $Bq.m^{-3.}$ Less than 13% of houses have indoor radon above the directive level of 200$Bq.m^{-3}$; 10% and 50% of have indoor thoron respectively above the reference level of 300$Bq.m^{-3}$ and 200$Bq.m^{-3}$. Inhalation doses due to radon and thoron range respectively between 1.02-4.8$mSv.yr^{-1}$ and 0.38-1.6$mSv.yr^{-1}$ with the mean values of 1.9$mSv.yr^{-1}$ and 0.9$mSv.yr^{-1}$. The estimate annual effective doses are below 1$mSv.yr^{-1}$, the limit value for the public. Thus radon and thoron cannot be neglected when assessing radiation dose.