X-RAY SPECTROSCOPY OF BROMINE COMPOUNDS AND BIOMEDICAL APPLICATIONS

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In conventional biomedical applications intense and broadband high energy X-rays are used in therapy and diagnostics (theranostics) to ensure sufficient tissue penetration for imaging or treatment. To avoid damages incurred by these, our proposed method, *Resonant Theranostics^{b,c}*, aims to find narrow energy regions that corresponds to *resonant* absorption or emission. We show that such energy bands lie *below* the K-shell ionization energy, contrary to the research focus on the K-shell ionization energy itself. Targeting these energy bands, Auger processes can be initiated to produce a number of photons and electrons from each atomic/molecular species via photon fluorescence and electron ejections.

We will report our study on the bromine compound bromodeoxyuridyne (BUdR), widely used as radiological contrast agent in radiation imaging. The active system is Br^o - Br^+ combination, which can emit or absorb X-rays in the relative narrow energy range of 12 to 13.6 keV, through 1s-np transitions. We will present the oscillator strengths and transition probabilities for various Auger or K-shell 1s-np transitions. We will show that the corresponding cross sections and attenuation coefficients per unit mass, are orders of magnitude higher than the background and that at K-shell ionization energy. Employing these attenuation coefficients in the Monte Carlo simulation program Geant4, we study the intensities of photon and electron emission spectra. ^{*a b c*}

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^b"Resonant X-Ray Enhancement of the Auger Effect in High-Z atoms, molecules, and Nanoparticles: Biomedical Applications", A.K. Pradhan, S.N. Nahar, M. Montenegro, Yan Yu, H.L. Zhang, C. Sur, M. Mrozik, R.M. Pitzer, J. of Phys. Chem. A, 113 (2009), 12356.

^c"Monte Carlo Simulations and Atomic Calculations for Auger Processes in Biomedical Nanotheranostics", M. Montenegro, S. N. Nahar, A. K. Pradhan, Ke Huang, Yan Yu, J. of Phys. Chem. A, 113 (2009), 12364.