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Research Article

Comparison of the Effective Atomic Numbers of Some Contrast Agents Compounds Used in Medical Imaging

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Abstract

Contrast agents are frequently used in medical imaging such as computed tomography (CT) and magnetic resonance (MR) to reveal the final state of the body or organs. The states of the organs examined are obtained according to the absorption principle of x or gamma rays interacting with contrast agents. In this study, $C_{17}H_{22}I_3N_3O_8$ (Iopamidol), $C_{11}H_9I_3N_2O_4$ (Diatrizoic acid), $BaSO_4$ (Barium sulfate) and $C_7H_6O_2$ (Benzoic acid) compounds are examined to calculate effective atomic number (Z_{eff}). Auto-Z_{eff} and Direc-Z_{eff} software were used for calculation in an energy range of 100 keV to 10 MV. According to the calculation results obtained have been compared with each other for each compound. According to these results, it was seen that the results were compatible with each other in low energy regions.

Keywords: Iopamidol; Diatrizoic Acid; Barium Sulfate; Benzoic Acid; Contrast Agent; Z_{eff}

Medikal Görüntülemede Kullanılan Bazı Kontrast Madde Bileşiklerinin Etkin Atom Numaralarının Karşılaştırılması

Öz

Bilgisayarlı Tomografi (CT) ve Manyetik Rezonans (MR) gibi medikal görüntülemede vücudun veya organların son durumunu ortaya çıkarmak için sıklıkla kontrast ajanlar kullanılır. İncelenen organların durumları, kontrast maddelerle etkileşime giren x veya gama ışınlarının soğurma prensiplerine göre elde edilir. Bu çalışmada, $C_{17}H_{22}I_3N_3O_8$ (iyopamidol), $C_{11}H_9I_3N_2O_4$ (Diatrizoik Asit), $BaSO_4$ (Baryum sülfat) ve $C_7H_6O_2$ (Benzoik asit) bileşikleri incelenerek etkin atom numarası (Z_{eff}) hesaplanmıştır. 100 keV ile 10 MV enerji aralığında gerçekleştirilen hesaplamalar için Auto-Z_{eff} ve Direc-Z_{eff} yazılımları kullanılmıştır. Elde edilen hesaplama sonuçlarına göre, her bileşik için birbiriyle karşılaştırılmıştır. Bu sonuçlara göre düşük enerjili bölgelerde sonuçların birbiriyle uyumlu olduğu görülmüştür.

Anahtar kelimeler: İyopamidol; Diatrizoik Asit; Baryum Sülfat; Benzoik Asit; Kontrast Madde; Z_{eff}

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1.Introduction

Radiology is one of the areas where the development in Medical Technology is seen most effectively. Because, thanks to the development of radiology technology, radiological imaging methods are increasingly included in diagnosis and interventional applications day by day. Thus, it is important to research and develop contrast agents used in this field(Neutze, 2020 ; William Herring, 2019).

Contrast agents are substances that are actively used in radiology and used to increase the contrast of structures or fluids in the body. In order to an organ or system to be radiographically displayed, it must be surrounded by matter of different density. In this way, various structures such as bone tissue, which are surrounded by adipose tissue, kidneys, lungs, which naturally contain gas, are surrounded by soft tissues, can be seen easily(William Herring, 2019)(Krause Werner, 2002).

Contrast agents can be classified into two groups as radiolucent and radiopaque substances(Krause Werner, 2002). The density of radiolucent substances is lower than the air and because they pass x-rays more than the tissues, they cause darker images to form on the film. Radiopaque substances are called substances whose density is higher than the tissue density. their atomic weight is high and therefore absorb more X-rays from tissues(Singh and Neutze, 2012).

Iodine and barium compounds, which are among the radiopaque contrast agents, are one of the most used contrast agents(Neutze, 2020). All iodinated contrast agents contain 3 iodinated benzene rings. Benzene is a toxic, water-insoluble molecule. Benzoic acid formed by adding the acid group to the 1st carbon of the 6-carbon benzene ring, it provides water solubility by providing the formation of salts and amides. The 3 iodinated benzene ring is formed by the addition of iodine at positions 2, 4 and 6 of the benzene ring (such as $C_7H_6O_2$)(Singh and Neutze, 2012).

Iodine-containing contrast agents (such as $C_{17}H_{22}I_3N_3O_8$ and $C_{11}H_9I_3N_2O_4$) are opaque for X-rays and they are pharmacologically inert(Thomsen et al., 2014)(Çakır, 2020). Because they are water soluble, they can be injected even at high concentrations. Since they are chemically stable, they do not react in the body. The vast majority are rapidly excreted through the kidneys(Çakır, 2020).

The Barium sulfate ($BaSO_4$) compound is odorless, in the form of a white powder, toxic but not soluble in water and thus not dissolved by digestive tract secretions. Barium sulfate is used orally or rectally as a solution in the esophagus, stomach, duodenum, small and large intestine graphies. For this, it is excreted from the digestive tract without being absorbed and changed. It is the most suitable contrast agent for the digestive system since it adheres to the mucosa very easily due to its high viscosity(William Herring, 2019; Thomsen et al., 2014).

There is a strong relationship between atomic number and absorption coefficient in medical imaging applications (Kurudirek, 2014). Photon attenuation in the environment can be increased with the high density contrast agents used (Sayyed, 2016). Z_{eff} can be used to

determine the radiation response of multi-element materials consisting of elements with different atomic numbers. Determination of Z_{eff} values can potentially contribute to the prediction of contrast agent distribution and material separation in clinical data(Çakır, 2020)(Özpolat et al., 2020).

In this study, Iopamidol ($C_{17}H_{22}I_3N_3O_8$), Diatrizoic acid ($C_{11}H_9I_3N_2O_4$), Barium sulfate ($BaSO_4$) and Benzoic acid ($C_7H_6O_2$) compounds(Krause Werner, 2002) are examined to calculate effective atomic number (Z_{eff}). Auto-Z_{eff} (Taylor et al., 2012) and Direc-Z_{eff} (Un and Caner, 2014)software have been used for calculation in an energy range from 100 keV to 10 MeV. These obtained results have been compared with each other for each compound.

2. Material and Method

In the scope of this study, Iopamidol ($C_{17}H_{22}I_3N_3O_8$)(Çakır, 2020), Diatrizoic acid ($C_{11}H_9I_3N_2O_4$), Barium sulfate ($BaSO_4$) and Benzoic acid ($C_7H_6O_2$) compounds(Krause Werner, 2002) as used contrast agent have been investigated. To obtain of these contrast agents' effective atomic number (Z_{eff}), Auto-Z_{eff} and Direc Z_{eff} software have been used.

Auto-Z_{eff} is developed by Taylor et al. (2012)(Taylor et al., 2012) using Microsoft Visual Basic language. During the compiling of this program, pre-calculated data files loads that is occurred by internal source. The mass attenuation coefficients and cross section matrices as a function of photon energy for the first 100 elements are found in these pre-calculated files. The mass attenuation coefficient data (μ/ρ (cm^2/g)), files for each corresponding element in the selected material are first selected by the program. Based on the mass fraction of each element in the material, the total attenuation coefficient is calculated by linear summation. The cross section for each energy is calculated and the effective atomic number is determined using these calculated cross sections, using the preloaded cross section matrix for each element as a lookup table. The program compares the calculated cross sections with matrix data at each energy and the corresponding atomic number is determined by interpolation. This calculated effective atomic number data is displayed under the Z_{eff} (E) tab and as an exportable table.

Direct-Z_{eff} have been developed by Un and Caner (2014) (Un and Caner, 2014) using Fortran77 programming language. By using Direct-Z_{eff}, the mass attenuation coefficient, effective atomic number and effective electron number per unit mass of any element, compound or mixture on a standard energy grid can be calculated. These calculations have been done for total photon interaction with and without coherent interaction as well as partial photon interactions including characteristic X-ray energies of elements. The mass attenuation coefficients that is used in the program as a function of photon energy is taken from WinXCom (Gerward, L., 2012) for pre-calculated data files. After defined as weight fractions or amounts of mole for material, the effective atomic number Z_{eff} is calculated. To calculate Z_{eff} is effective atomic cross section and effective electronic cross section can be used. σ_a is effective atomic cross section and it can be used for the Zeff calculation that is given in eq. 1:

$$\sigma_a = \frac{1}{N_A}\sum f_i A_i \left(\frac{\mu}{\rho}\right)_i$$

(1)

f_i is the fractional abundance of the element and effective electronic cross section is given in eq.2 as follows:

$$\sigma_e = \frac{1}{N_A}\sum \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i$$

(2)

Z_i is the atomic number of ith element and effective atomic number can be calculated by using eq.3 (Un and Caner, 2014):

$$Z_{eff} = \frac{\sigma_a}{\sigma_e}$$

(3)

3. Result and Discussion

$C_7H_6O_2$, $BaSO_4$, $C_{17}H_{22}I_3N_3O_8$ and $C_{11}H_9I_3N_2O_4$ contrast agent compounds have been investigated in this study to obtain effective atomic number (Z_{eff}) by using Auto-Zeff and Direc-Zeff software. Percent composition of compounds have been given in Table 1. In the calculations made with the Auto-Z_{eff} program for $C_7H_6O_2$ (Figure 1), the value obtained as 5.843 at 0.01 keV energy decreased to 4.484 until 10 MeV done by Auto-Z_{eff} software. But, in the calculations made with Direct-Z_{eff}, it changes from 6.606 to 4.53 respectively. In the calculations made with the Auto-Z_{eff} program for the $BaSO_4$ compound as seen in Figure 2, 36.350 value is obtained for 0.01 keV and decreases to 19.606 up to 4 MeV. However, after this energy value, it rises to 21.775 up to 10 MeV. But, For the Direc Z_{eff} program, 45.57 value is obtained for 0.01 keV and it decreases 19.847 up to 4 MeV. After this value it increases again up to 10 MeV as 24.251. As seen in Figure 3, there is a fluctuation in the $C_{17}H_{22}I_3N_3O_8$ calculations by done Auto-Z_{eff}. firstly, the value of 14.814 increased to 24.705 and then decreased to 7.634 again. It increased again up to 9.994. But in the Direc-Z_{eff} calculations, these fluctuations changed between 46.044 to 11.017 value. Lastly as seen Figure 4, for the $C_{11}H_9I_3N_2O_4$ compound, similarly, there is a fluctuation between 17.270 to 13.986 that is calculated values by Auto-Z_{eff} in the 0.01 keV to 10 Mev energy range. 48.742 to 15.863 values have been obtained respectively by using Direc-Z_{eff} for 0.01 keV and 10 MeV energies.

Table 1. Percent composition of compounds(Krause Werner, 2002; Thomsen et al., 2014)

Compound	Molar Mass (g/mol)	Symbol	Atomic Mass (g/mol)	Atoms	Mass Percent(%)
$C_7H_6O_2$	122.121				
		H	1.007	6	4.952
		C	12.010	7	68.845
		O	15.999	2	26.202
$BaSO_4$	233.389				
		Ba	137.327	1	58.840
		O	15.999	4	27.421
		S	32.065	1	13.739
$C_{17}H_{22}I_3N_3O_8$	777.085				
		H	1.007	22	2.854
		C	12.010	17	26.275
		N	14.006	3	5.407
		O	15.999	8	16.471
		I	126.904	3	48.992
$C_{11}H_9I_3N_2O_4$	613.913				
		H	1.007	9	1.478
		C	12.010	11	21.521
		N	14.006	2	4.563
		O	15.999	4	10.425
		I	126.904	3	62.014

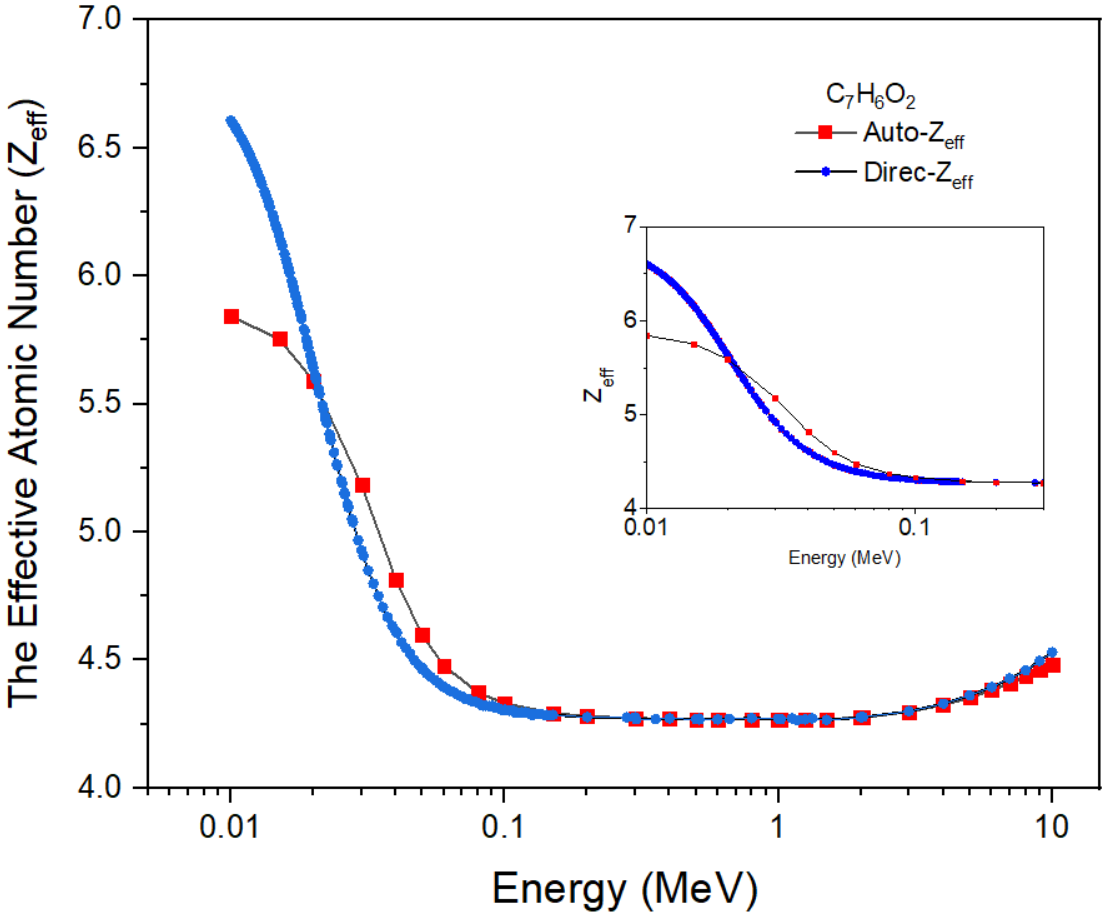

Figure 1. The Effective Number (Z_{eff}) comparation of $C_7H_6O_2$

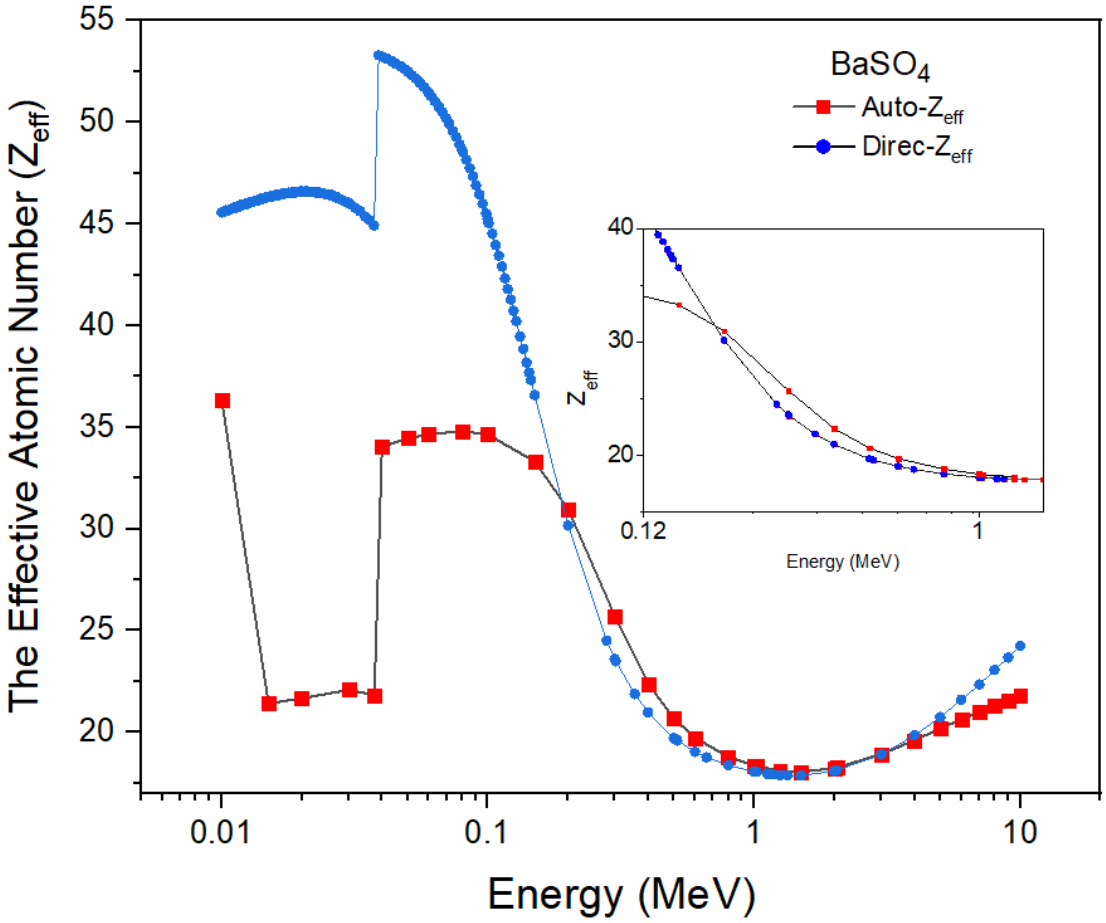

Figure 2. The Effective Number (Z_{eff}) comparation of $BaSO_4$

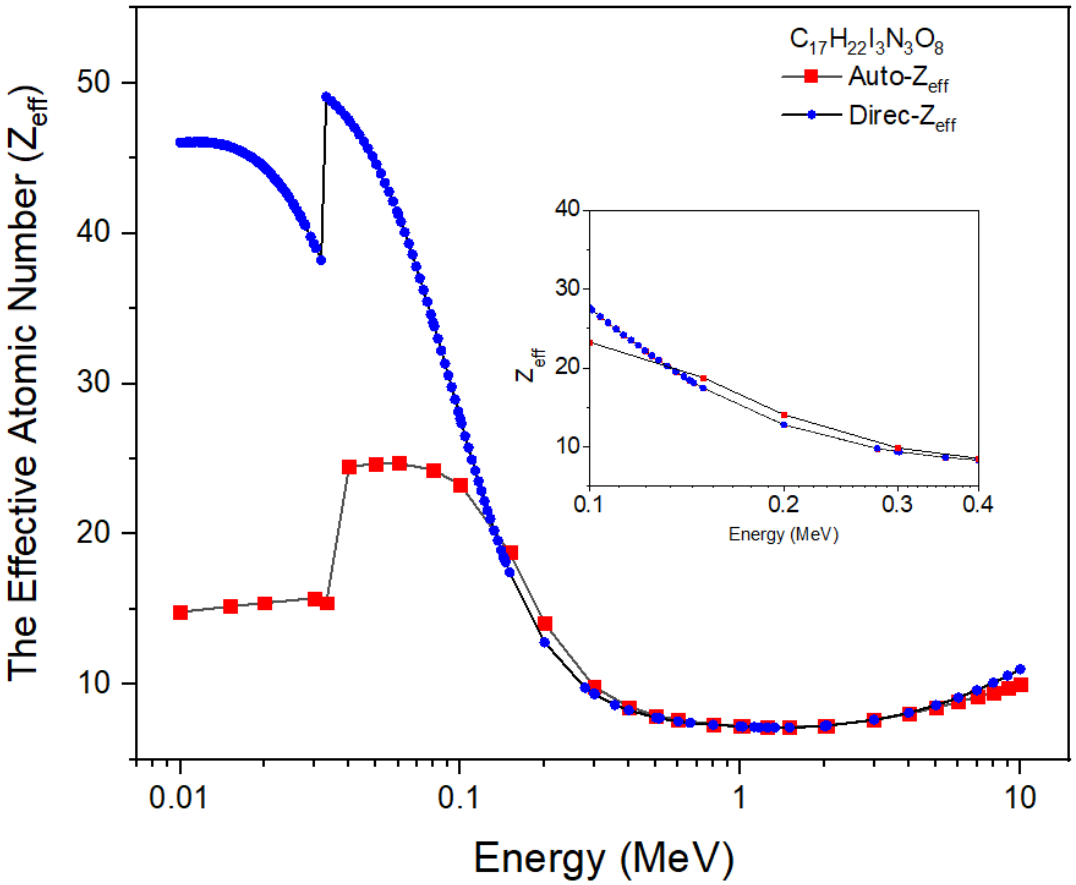

Figure 3. The Effective Number (Z_{eff}) comparation of $C_{17}H_{22}I_3N_3O_8$

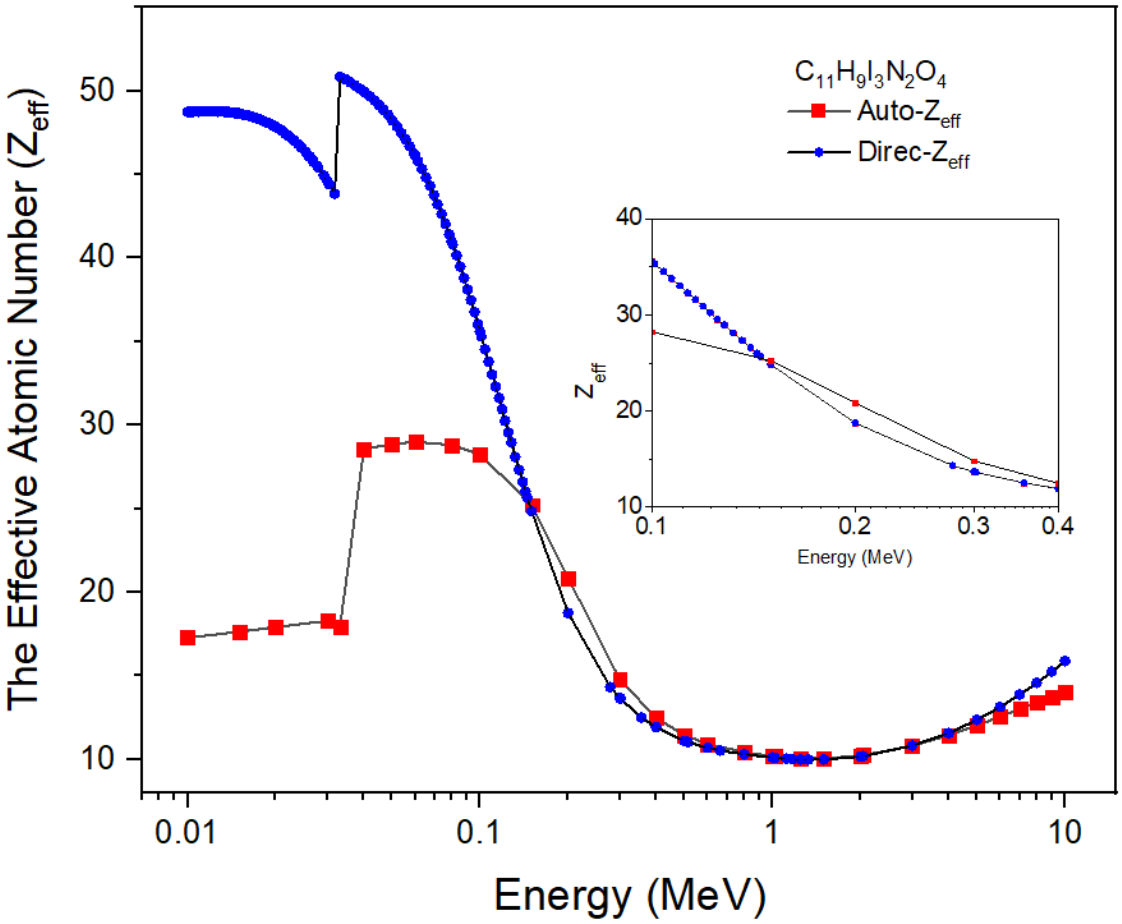

Figure 4. The Effective Number (Z_{eff}) comparation of $C_{11}H_9I_3N_2O_4$

4. Conclusion

The present study was carried out to investigate the effective atomic number parameter of selected, Iopamidol ($C_{17}H_{22}I_3N_3O_8$), Diatrizoic acid ($C_{11}H_9I_3N_2O_4$), Barium sulfate ($BaSO_4$) and Benzoic acid ($C_7H_6O_2$) contrast agents. The Z_{eff} values have been calculated between 0.01 keV to 10 MeV energy range by using the Auto-Z_{eff} and Direc-Z_{eff} software. The obtained Z_{eff} values have been compared each other and these comparisons have been shown in Figure 1-4. These results are in agreement with previous similar studies (Sıngh and Badıger, 2016) (Teklemariam et al., 2019). Firstly, obtained data are generally compatible each other for Benzoic acid up to 7 MeV as seen in figure 1. But these values are not similar in figure 2 for Barium sulfate compound. Z_{eff} values is not compatible except 1-4 MeV energy range. Between 150 keV to 5 Mev, the obtained data similar compatibility with each other in figure 3 for Iopamidol compound. In the same way as Figure 3, between the energy range of 180 keV to 4 MeV, there have similar compatibility for Diatrizoic acid Z_{eff} data in figure 4. Based on these compatibilities and values in energy ranges, these compounds can be used as contrast agents in the appropriate energy range.

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