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Effective Atomic Number and Kerma for Photon Energy Absorption of Organic Scintillators

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Abstract

An attempt has been made to calculate the effective atomic number and Kerma for photon energy absorption of organic scintillators in the energy region 1 keV to 20 MeV. We have chosen seven organic scintillators viz., anthracene, stilbene, naphthalene, *p*-terphenyl, PPO, butyl PBD and PBD. The $Z_{PEA,\ eff}$ and Kerma values are calculated by using mass-energy absorption coefficient from Hubbell and Seltzer. We also calculated $Z_{PI,\ eff}$ for total photon interaction with coherent scattering by using WinXCom and compared with the $Z_{PEA,\ eff.}$

1. Introduction

The understanding of interaction of photon with matter is very important in various fields of radiation application and radiation protection such as nuclear and medical physics, space physics etc. The principal modes by which photon interact with matter, get attenuated and deposit energy are photoelectric effect, Compton effect, and pair production. Although photons also undergo Rayleigh scattering, Bragg's scattering, photo-disintegration and nuclear resonance scattering, however these modes of interaction result in negligible attenuation or energy deposition and are generally ignored in many applications of radiation and radiation protection. The photoelectric absorption coefficient τ, Compton interaction coefficient σ, and the pair production interaction

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coefficient κ, of a material are all related to the atomic number of the material.

An important quantity characterizing the penetration and scattering of gamma or X-rays in a medium is the linear attenuation coefficient (μ). The ratio of the linear attenuation coefficient to the density is called the mass attenuation coefficient, μ/ρ (ρ- density of the material). The amount of energy that is actually deposited in the medium is important in evaluating biological effects, explaining the response of a radiation detector and other applications. For this purpose, one can define a linear energy-absorption coefficient (μ_{en}). This coefficient includes only the energy absorbed in the medium from photoelectrons, Compton electrons, and the electron-positron pair. But, energy carried away by scattered Compton photons, annihilation radiation and bremsstrahlung radiation is not included.

A more detailed version of the energy-deposition quantity is the mass energy-absorption coefficient, μ_{en}/ρ, and can be described more clearly through the use of an intermediate quantity called mass energy-transfer coefficient. The mass energy-transfer coefficient, μ_{tr}/ρ, is the mass attenuation coefficient multiplied by the fraction of energy of the interacting photons which is transferred to charged particles as kinetic energy. Hence μ_{tr}/ρ is a measure of the average fractional amount of incident photon energy transferred to charged particles as kinetic energy due to all types of interactions of photons with matter.

The mass energy-absorption coefficient, μ_{en}/ρ, takes into account the fraction of the kinetic energy that is subsequently lost in radiative energy-loss processes like bremsstrahlung, annihilation in flight etc, as the charged particles come to rest in the absorbing medium. Therefore, μ_{en}/ρ has an essential role in estimating the absorbed dose in medical and health physics. The μ/ρ and μ_{en}/ρ are basic quantities used in calculations of the penetration and the energy deposition by photons in biological, shielding and other materials [1-2].

Organic scintillators are aromatic hydrocarbon compounds which contain benzene ring structures interlinked in various ways. Their luminescence typically decays within a few nanoseconds. Some

organic scintillators are pure crystals. The most common types are anthracene ($C_{14}H_{10}$), stilbene ($C_{14}H_{12}$), and naphthalene ($C_{10}H_8$). They are very durable, but their response is anisotropic (which spoils energy resolution when the source is not collimated), and they cannot be easily machined, nor can they be grown in large sizes; hence they are not very often used. Therefore, one can dissolve organic scintillator, in neutral solvents to have liquid scintillator. The typical solutes are *p*-terphenyl ($C_{18}H_{14}$), PBD ($C_{20}H_{14}N_2O$), butyl PBD ($C_{24}H_{22}N_2O$) and PPO ($C_{15}H_{11}NO$). The selected organic compounds are widely used in several fields. Anthracene is used as a scintillator for detectors of high energy photons, electrons and alpha particles. Plastics, such as polyvinyl toluene, can be doped with anthracene to produce plastic scintillators that is approximately water-equivalent for use in radiation therapy dosimetry. It is also used in wood preservatives, insecticides, and coating materials. Stilbene is used in manufacture of dyes and optical brighteners, and also as a phosphor and scintillators. Stilbene is one of the gain mediums used in dye lasers. Naphthalene is used as dispersants in synthetic and natural rubbers, and as tanning agents in leather industries, agricultural formulations (dispersants for pesticides), and dyes. The other organic compounds are used as laser dye.

Various investigators have [3–7] carried out broad investigation on $Z_{PI,\ eff}$ in a variety of composite materials like alloys, polymers, thermoluminescent and dosimetric compounds, semiconductors, superconductors, tissues, and equivalent materials for photon interaction. Corresponding studies for $Z_{PEA,eff}$ appear to be limited [8-10]. In the literature, there are no reports on the study of $Z_{PEA,eff}$ and Kerma of selected organic scintillators. This inspired us to carry out the present work. In the present work, the $Z_{PEA,eff}$ has been calculated for organic scintillators in the energy region of 1 keV to 20 MeV using the μ_{en}/ρ values from the compilation of Hubbell and Seltzer [11] and also calculated $Z_{PI,\ eff}$ for total photon interaction with coherent scattering by using WinXCom programme [12-13]. The Kerma relative to air has also been computed and reported in the present work.

2. Estimation of Parameters

2.1. Effective Atomic Number

The effective atomic number for photon-energy absorption can be obtained by using mass energy-absorption coefficients of the scintillators. The values of mass energy-absorption coefficients of scintillators, μ_{en}/ρ, are evaluated by using the Bragg's additive law.

$$\left(\frac{\mu_{en}}{\rho}\right) = \sum_i w_i \left(\frac{\mu_{en}}{\rho}\right)_i \tag{1}$$

where w_i and $(\mu_{en}/\rho)_i$ are the weight fraction and mass energy-absorption coefficients of the i^{th} constituent element, respectively.

Several investigators have been used the detailed steps to calculate the effective atomic number for photon energy absorption [14] is given as.

$$Z_{PEA,eff} = \frac{\sigma_{a,en}}{\sigma_{e,en}} \tag{2}$$

where σ_a is effective (average) atomic cross section and σ_e is effective (average) electronic cross section.

2.2. Kinetic Energy Release per Unit Mass (Kerma)

The word Kerma is an acronym for "kinetic energy released per unit mass" or "kinetic energy released in material". Two useful quantities for describing the interaction and absorption of high energy photons in a medium, for example, in cancer radiotherapy, are Kerma (K_a) and absorbed dose (D). The Kerma is proportional to the mass energy-transfer coefficient, which is a function of the photon energy and atomic number of the medium. Kerma is defined as the sum of the initial kinetic energies of all those primary charged particles released due to the transfer of energy by uncharged ionizing radiation (i.e. indirectly ionizing radiation) per unit mass.

Kerma (K_a) has been estimated by using the known mass energy absorption coefficient of the compound $(\mu_{en}/\rho)_{comp}$ and mass

energy absorption coefficient values of air $(\mu_{en}/\rho)_{air}$ with the following expression:

$$K_a = \frac{(\mu_{en}/\rho)_{comp}}{(\mu_{en}/\rho)_{air}} \quad (3)$$

(μ_{en}/ρ) of both compound and air are estimated using equation (1).

3. **Results and Discussion**

The variations of $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ with energy are shown in Figures 1 to 7 and energy dependence of Kerma is shown in Figure 8. The calculated values of $Z_{PI,\ eff}$, $Z_{PEA,\ eff}$ and Kerma for the energy range 1 keV to 20 MeV using the μ_{en}/ρ values from the compilation of Hubbell and Seltzer [12] are given in Tables 1, 2 and 3 respectively. From Figures 1 to 7 it is clear that, the effective atomic numbers for photon energy absorption and photon interaction varies with energy. The values of $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ with energy depends upon relative proportion and the range of atomic numbers of the elements of which organic scintillators are composed off.

For anthracene, stilbene, naphthalene and *p*-terphenyl, the $Z_{PEA,\ eff}$ is almost same in the energy range 1 keV- 10 keV and decreases rapidly from 15 to 150 keV then after it remains constant up to 2 MeV and then again increases steadily up to 20 MeV. The variation of $Z_{PEA,\ eff}$ with energy confirms the dominance of different processes, that is photoelectric absorption, Compton scattering, pair production (Nuclear field and electric field). It is observed that the variation in $Z_{PEA,\ eff}$ also depends upon relative proportion and the range of atomic numbers of the elements of which scintillators is composed. The PPO, Butyl PBD and PBD contain more number of elements when compared with anthracene, stilbene, naphthalene and *p*-terphenyl. Therefore the change of effective atomic number for photon energy absorption with energy is more for compounds which consists of nitrogen and oxygen. For PPO, Butyl PBD and PBD the $Z_{PEA,\ eff}$ increases slowly from 1 to 8 keV and exactly same behavior as for rest of the scintillators.

The K_a values estimated using expression (3) is plotted as a function of energy in Figure 8. The qualitative variation of Kerma with energy is almost same for all organic scintillators. The energy

dependence of Kerma indicates the relative importance of photoelectric absorption, Compton scattering and pair production. At and above 3 keV, it is photoelectric absorption dominant interaction process. This can be observed in the energy region 3 to 40 keV. In the energy region 40 to 200 keV, Compton scattering dominates and we can see that the Kerma value increases sharply. Kerma is almost constant in the energy region from 200 keV to 2 MeV and then slowly decreases where the pair production process dominates.

Table 1. Energy Dependence of Effective Atomic Numbers for Total Photon Interaction (Coherent Scattering)

Energy (MeV)	anthracene	stilbene	naphthalene	*p*-terphenyl	PPO	Butyl PBD	PBD
0.001	5.99	5.99	5.99	5.99	6.30	6.24	6.28
0.0015	5.99	5.99	5.99	5.99	6.31	6.25	6.29
0.002	5.99	5.99	5.99	5.99	6.32	6.26	6.30
0.003	5.99	5.99	5.99	5.99	6.33	6.26	6.30
0.004	5.98	5.97	5.98	5.98	6.32	6.25	6.30
0.005	5.96	5.95	5.96	5.96	6.31	6.24	6.29
0.006	5.93	5.92	5.93	5.93	6.29	6.21	6.27
0.008	5.85	5.82	5.83	5.84	6.22	6.12	6.20
0.01	5.72	5.67	5.69	5.70	6.11	5.98	6.10
0.015	5.28	5.16	5.21	5.23	5.62	5.47	5.69
0.02	4.85	4.68	4.74	4.77	5.22	4.96	5.26
0.03	4.33	4.12	4.20	4.23	4.64	4.34	4.70
0.04	4.13	3.91	3.99	4.03	4.40	4.09	4.47
0.05	4.04	3.82	3.90	3.93	4.29	3.98	4.364
0.06	3.99	3.77	3.86	3.89	4.24	3.93	.31
0.08	3.96	3.73	3.82	3.85	4.19	3.89	4.26
0.1	3.94	3.72	3.80	3.84	4.17	3.87	4.24
0.15	3.93	3.71	3.79	3.83	4.16	3.85	4.23
0.2	3.92	3.70	3.78	3.82	4.15	3.84	4.22
0.3	3.93	3.70	3.79	3.82	4.15	3.85	4.22
0.4	3.92	3.70	3.78	3.82	4.15	3.84	4.22
0.5	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.6	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.8	3.92	3.70	3.78	3.82	4.15	3.84	4.22
1	3.92	3.70	3.78	3.82	4.15	3.84	4.22
1.25	3.92	3.69	3.78	3.81	4.14	3.84	4.22
1.5	3.92	3.69	3.78	3.81	4.14	3.84	4.21
2	3.92	3.70	3.78	3.82	4.15	3.84	4.22
3	3.94	3.72	3.80	3.84	4.17	3.87	4.24
4	3.97	3.74	3.83	3.86	4.20	3.89	4.27
5	3.99	3.77	3.86	3.89	4.23	3.92	4.30
6	4.02	3.80	3.88	3.92	4.25	3.95	4.33
8	4.07	3.85	3.94	3.97	4.31	4.01	4.38
10	4.13	3.91	4.00	4.03	4.37	4.07	4.44
15	4.25	4.04	4.12	4.15	4.50	4.21	4.57
20	4.36	4.15	4.23	4.26	4.61	4.32	4.67

Table 2. Energy Dependence of Effective Atomic Numbers for Photon Energy Absorption

Energy (MeV)	anthracene	stilbene	naphthalene	*p*-terphenyl	PPO	Butyl PBD	PBD
0.001	5.99	5.99	5.99	5.99	6.30	6.24	6.28
0.0015	6.00	5.99	5.99	6.00	6.31	6.25	6.29
0.002	6.00	6.00	6.00	6.00	6.32	6.26	6.30
0.003	6.00	6.00	6.00	6.00	6.34	6.27	6.31
0.004	6.00	6.00	6.00	6.00	6.34	6.27	6.32
0.005	6.00	6.00	6.00	6.00	6.35	6.28	6.32
0.006	6.00	6.00	6.00	6.00	6.35	6.28	6.33
0.008	6.00	5.99	5.99	5.99	6.36	6.28	6.33
0.01	5.99	5.99	5.99	5.99	6.36	6.28	6.33
0.015	5.97	5.96	5.96	5.96	6.34	6.26	6.31
0.02	5.89	5.87	5.88	5.88	6.28	6.18	6.26
0.03	5.54	5.46	5.49	5.50	5.96	5.79	5.95
0.04	5.00	4.85	4.91	4.93	5.42	5.16	5.44
0.05	4.56	4.36	4.44	4.47	4.93	4.63	4.97
0.06	4.28	4.07	4.15	4.19	4.61	4.30	4.66
0.08	4.05	3.83	3.92	3.95	4.32	4.01	4.38
0.1	3.98	3.75	3.84	3.87	4.22	3.91	4.29
0.15	3.93	3.71	3.79	3.83	4.16	3.85	4.23
0.2	3.92	3.70	3.79	3.82	4.15	3.85	4.22
0.3	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.4	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.5	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.6	3.92	3.69	3.78	3.81	4.14	3.84	4.22
0.8	3.92	3.69	3.78	3.81	4.14	3.84	4.22
1	3.91	3.69	3.77	3.81	4.14	3.83	4.21
1.25	3.91	3.69	3.78	3.81	4.14	3.83	4.21
1.5	3.91	3.69	3.77	3.81	4.14	3.83	4.21
2	3.92	3.70	3.78	3.82	4.15	3.84	4.22
3	3.94	3.72	3.80	3.84	4.17	3.86	4.24
4	3.97	3.75	3.83	3.87	4.20	3.89	4.27
5	4.00	3.78	3.86	3.90	4.23	3.93	4.30
6	4.03	3.81	3.89	3.93	4.26	3.96	4.34
8	4.09	3.87	3.96	3.99	4.33	4.03	4.40
10	4.15	3.93	4.02	4.05	4.39	4.10	4.46
15	4.28	4.07	4.15	4.18	4.53	4.24	4.59
20	4.37	4.17	4.25	4.28	4.63	4.34	4.69

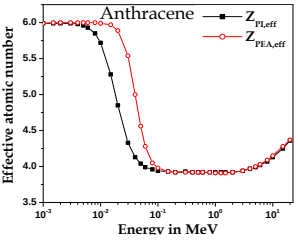

Fig. 1 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for Anthracene

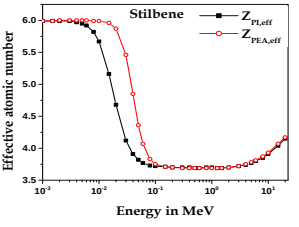

Fig. 2 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for Stilbene

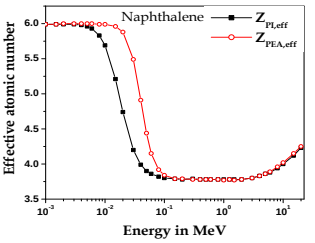

Fig. 3 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for Naphthalene

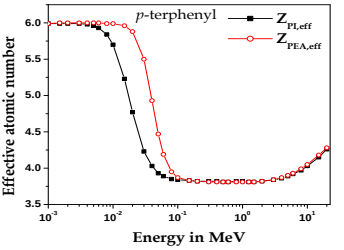

Fig. 4 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for *p*-terphenyl

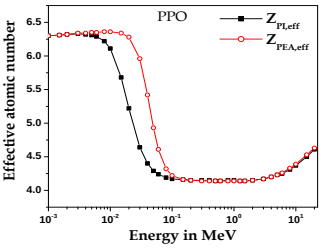

Fig. 5 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for PPO

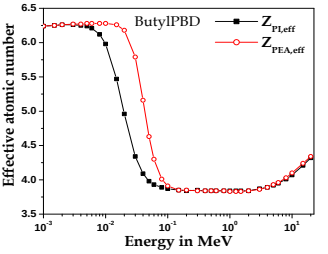

Fig. 6 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for Butyl PBD

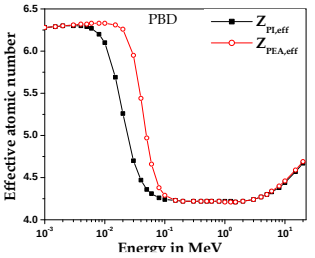

Fig. 7 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for PBD

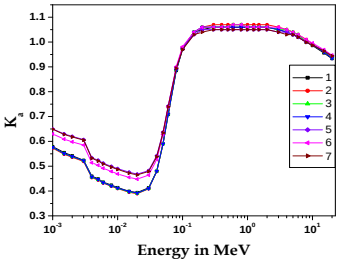

Fig. 8 Energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ for scintillators

Notations in Figure 8: 1- Anthracene; 2- Stilbene; 3-Naphthalene; 4-*p*-terphenyl; 5- PP0; 6-Butyl PBD; 7-PBD

The energy dependence of $Z_{PEA,eff}$ and $Z_{PI,eff}$ reflects the dominating absorption processes, which are changing from photoelectric absorption in the low-energy range (<10 keV)to Compton scattering in the medium energy range and pair production in the high energy (>5 MeV) range. The notable differences exist among $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ in the energy range 6 to 100 keV for all organic

scintillators. The maximum difference is observed at 30 keV for all the scintillators studied. A maximum difference of 21%, 25.5%, 23.4%, 23%, 22%, 25% and 21% is observed for anthracene, stilbene, naphthalene, *p*-terphenyl, PPO, Butyl PBD and PBD respectively. The notable differences occur in the range 6 to 100 keV because, major part of the Compton scattered radiation escapes from the absorbing medium. Thus, while contributing significantly to the attenuation of the incident beam, Compton scattering contributes only a little to the energy absorption.

Table 3. Energy Dependence of Kerma for Photon Energy Absorption

Energy (MeV)	anthracene	stilbene	naphthalene	p-terphenyl	PPO	Butyl PBD	PBD
0.001	0.58	0.57	0.58	0.58	0.65	0.63	0.65
0.0015	0.56	0.55	0.55	0.55	0.63	0.61	0.63
0.002	0.54	0.54	0.54	0.54	0.62	0.60	0.62
0.003	0.52	0.52	0.52	0.52	0.61	0.58	0.60
0.004	0.46	0.45	0.46	0.46	0.53	0.51	0.53
0.005	0.45	0.44	0.45	0.45	0.52	0.50	0.52
0.006	0.44	0.43	0.43	0.43	0.51	0.49	0.51
0.008	0.42	0.42	0.42	0.42	0.50	0.48	0.50
0.01	0.41	0.41	0.41	0.41	0.49	0.47	0.49
0.015	0.40	0.40	0.40	0.40	0.48	0.46	0.47
0.02	0.39	0.39	0.39	0.39	0.47	0.45	0.46
0.03	0.41	0.41	0.41	0.41	0.48	0.46	0.48
0.04	0.48	0.48	0.48	0.48	0.54	0.53	0.54
0.05	0.59	0.59	0.59	0.59	0.64	0.63	0.63
0.06	0.71	0.71	0.71	0.71	0.74	0.74	0.74
0.08	0.88	0.89	0.89	0.89	0.90	0.90	0.89
0.1	0.97	0.98	0.97	0.97	0.97	0.98	0.97
0.15	1.04	1.04	1.04	1.04	1.03	1.04	1.03
0.2	1.05	1.06	1.06	1.06	1.05	1.06	1.04
0.3	1.06	1.07	1.06	1.06	1.05	1.06	1.05
0.4	1.06	1.07	1.06	1.06	1.05	1.06	1.05
0.5	1.06	1.07	1.06	1.06	1.05	1.06	1.05
0.6	1.06	1.07	1.07	1.06	1.05	1.07	1.05
0.8	1.06	1.07	1.07	1.06	1.05	1.07	1.05
1	1.06	1.07	1.06	1.06	1.05	1.06	1.05
1.25	1.06	1.07	1.06	1.06	1.05	1.06	1.05
1.5	1.06	1.07	1.06	1.06	1.05	1.06	1.05
2	1.06	1.07	1.06	1.06	1.05	1.06	1.05
3	1.05	1.06	1.05	1.05	1.04	1.06	1.04
4	1.04	1.05	1.05	1.04	1.04	1.05	1.03
5	1.03	1.04	1.04	1.03	1.03	1.04	1.03
6	1.02	1.03	1.03	1.02	1.02	1.03	1.02
8	1.00	1.01	1.00	1.00	1.00	1.01	1.00
10	0.99	0.99	0.99	0.99	0.99	1.00	0.99
15	0.96	0.96	0.96	0.96	0.97	0.97	0.96
20	0.93	0.94	0.94	0.94	0.94	0.95	0.94

Therefore, the transition from photoelectric absorption to Compton scattering as the dominating absorption process is shifted toward higher energies for the mass energy-absorption coefficient as compared with the mass attenuation coefficient.

It has been shown that the substantial change occurs between $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ for scintillators is insignificant (1%) for the photon energy less than 6 keV and above 100 keV. Radiotherapy is usually performed with photons in the MeV energy range, where the difference between $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ is insignificant as discussed above. Thus, it follows from the present work that in radiotherapy one can use $Z_{PI,\ eff}$ instead of $Z_{PEA,\ eff}$. This has the advantage that $Z_{PI,\ eff}$ can easily be measured experimentally for different tissues. No experimental data on $Z_{PEA,\ eff}$ are available in the literature for comparison with the present results.

4. Conclusion

It is seen that the values of $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ with energy depends upon relative proportion and the range of atomic numbers of the elements of which organic scintillators are composed off. The Kerma value decreases for all scintillators from 1 keV to 20 keV then increases sharply up to 200 keV. From 300 keV to 2 MeV it remains constant and then gradually decreases up to 20 MeV.

The significant differences exist among $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ in the energy range 6-100 keV for all organic scintillators. It has been shown that the substantial change occurs between $Z_{PEA,\ eff}$ and $Z_{PI,\ eff}$ for scintillators is insignificant (1%) for the photon energy less than 6 keV and above 100 keV. The use of $Z_{PEA,\ eff}$ is important in dealing with the absorbed dose due to photons of range 6–100 keV. To the best of our knowledge, the results reported are the first of their kind and have not been reported earlier.

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