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Change of ^{7}Be decay rate in exohedral and endohedral C_{60} fullerene compounds and its implications

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The half-life of exohedral ^{7}Be-C_{60} complex and that of ^{7}Be implanted in a gold foil have been found to be about the same within ≈0.2%. Using a radiochemical technique, we also measured that the probability of formation of endohedral ^{7}Be@C_{60} complex by nuclear implantation technique was (5.6 ± 0.45)%. We also find that the half-life of endohedral ^{7}Be@C_{60} complex is shorter than that of exohedral complex by more than 1%. An analysis of these results using linear muffin-tin orbital method calculations indicates that most of the implanted ^{7}Be ions in fullerene C_{60} stay at a distance of ≈5.3 Å from the centers of nearest C_{60} molecules forming exohedral compounds and those who enter the fullerene cages go to the centers of the cages forming endohedral ^{7}Be@C_{60} compounds.

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I. INTRODUCTION

It is known from earlier works [1–6] that the rate of orbital electron capture of ^{7}Be is susceptible to the surrounding environment and depends on both the lattice structure and electron affinity of the host atoms. Calculations [2,5,6] also showed that the decay rate of ^{7}Be should depend on its position in the host lattice. So the decay rate of ^{7}Be in an atomic cluster such as fullerene C_{60} or large biomolecule should also depend on its position with respect to the molecule and could be used as a tool to learn about the position of the implanted radioactive ion in the atomic cluster. In the future, this kind of study might also tell us about any abnormal change of DNA molecule in a living cell.

It is already well-known [7–9] that different types of metal atoms (Be, Kr, Xe, etc.) can be inserted into C_{60} fullerene cage-forming endohedral compounds by nuclear implantation techniques. Many theoretical studies [10–14] have been done regarding the charge and equilibrium positions of the implanted ion in both endohedral and exohedral fullerene complexes, but there is no corresponding experimental measurement. So it is important to address these questions experimentally. By comparing the measured half-lives of exohedral ^{7}Be-C_{60} and endohedral ^{7}Be@C_{60} with that of implanted ^{7}Be in another well-understood material such as gold, we can learn about the charge and equilibrium positions of ^{7}Be in endohedral and exohedral fullerene C_{60} complexes.

II. EXPERIMENT AND RESULTS

In this work, we have measured the difference of half-lives of ^{7}Be implanted in a gold (Au) foil and fullerene (C_{60}) pellet. A 25-μm-thick gold (Au) foil and a 500 μm-thick fullerene (C_{60}) pellet were bombarded by an 18-MeV ^{7}Be beam from Nuclear Science Center (New Delhi, India). The ranges of 18-MeV ^{7}Be in Au and C_{60} are 12 μm and 40 μm respectively. The intensity of the ^{7}Be beam was about 40,000 particles/s and the duration of the irradiation 24 hr for each sample. To obtain an 18-MeV ^{7}Be beam, a liquid-nitrogen-cooled hydrogen gas cell at one atmospheric pressure was bombarded with a 15-pnA 21-MeV ^{7}Li beam obtained from the pelletron machine of Nuclear Science Center (New Delhi, India). The ^{7}Be nuclei produced by the reaction $^1\mathrm{H}(^7\mathrm{Li},^7\mathrm{Be})^1n$ at 0° were separated from the primary ^{7}Li beam by using a recoil mass spectrometer called Heavy Ion Reaction Analyzer (HIRA) [15] operated in a suitable ion optical mode [16]. Primary ^{7}Li beam particles were rejected by a slit system installed at the intermediate focal plane of the spectrometer. The primary beam rejection factor was about 10^{12} and the purity of the separated ^{7}Be beam was about 92%. The advantages of rejecting the primary ^{7}Li beam and using only a high purity ^{7}Be beam for implantation are to minimize the radiation damage of the sample and avoid production of unwanted radioactivity.

The ^{7}Be implanted samples were brought to Variable Energy Cyclotron Center (Kolkata, India) for off-line counting. Following electron capture, a ^{7}Be nucleus has a 10.4% probability [17] of populating the first excited state of ^{7}Li, which decays subsequently to its ground state, emitting a 478-keV γ-ray photon. The half-life of ^{7}Be was determined by monitoring the intensity of this 478-keV γ-ray line with time. Two HPGe detectors (detector 1 and detector 2) having efficiency ≈30% were used to count the samples (^{7}Be-implanted Au foil and ^{7}Be-implanted fullerene pellet). In addition, a standard ^{133}Ba source was also placed in front of each HPGe detector. The detectors were well shielded by lead bricks to avoid any cross-talk between them and also to reduce the background level. A typical γ-ray spectrum (for ^{7}Be in C_{60} fullerene) as recorded by detector 1 is shown in Fig. 1. Apart from the 478-keV γ-ray line coming from the decay of ^{7}Be and other γ-ray lines from ^{133}Ba, we also see standard background γ rays such as 239-, 511-, 583-, 609-, 727-, and

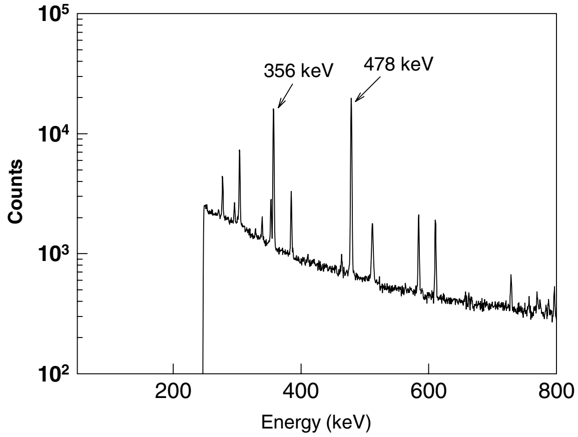

FIG. 1. γ-ray spectrum from the decay of ^{7}Be implanted in C_{60} fullerene

911-keV lines, but there was no other contaminant. The γ-ray spectrum of ^{7}Be in Au is very similar to that in Fig. 1.

The count rate of the 478-keV γ-ray was about 1 count per second at the beginning of the run. Both the HPGe detectors were started at the same time, data were accumulated for 24 hr and stored in a computer, and the spectra were cleared and the counting was restarted. After counting for 7 days, the positions of the samples were interchanged and counted again. This was done to take care of any systematic error. The counting was continued for about 6 months.

From each day's spectra, we determined the counts under 478-keV [$N_\gamma(478)$] and 356-keV [$N_\gamma(356)$] photopeaks coming from ^{7}Be and ^{133}Ba respectively. The ratio $N_\gamma(478)/N_\gamma(356)$ should be independent of computer dead time and systematic errors and decay exponentially with time. In the case of data sets for ^{7}Be in fullerene C_{60} and ^{7}Be in Au samples taken with detector 1, the reduced chi-square values of the exponential fits are 1.5 and 1.6, respectively. We also have similar data taken by detector 2 for ^{7}Be in fullerene C_{60} and Au and the reduced chi-square values of these exponential fits are 2.7 and 2.9, respectively. The γ-ray line shape of detector 2 showed slight tailings on both sides and this is probably responsible for obtaining comparatively poor exponential fit from the data set recorded by detector 2. So we compared data sets taken by the same detector and analyzed the same way with similar quality of fits (reduced chi-square values) to cancel out the effect of any systematic error. We obtain the percentage difference of the two decay rates, i.e., $\lambda(\mathrm{Au}) - \lambda(C_{60})/\lambda(\mathrm{Au}) = (0.060 \pm 0.405)\%$ and $(0.087 \pm 0.264)\%$ for detector 1 and detector 2, respectively, where only statistical errors have been considered. Taking the weighted average, we finally obtain the percentage difference in decay rates of ^{7}Be in gold and fullerene to be $\lambda(\mathrm{Au}) - \lambda(C_{60})/\lambda(\mathrm{Au}) = (0.079 \pm 0.221)\%$. So we find that the half-life of ^{7}Be in gold and fullerene is about the same within $\approx 0.2\%$.

To determine the half-life of ^{7}Be in Au, we used known half-life [17] of $^{133}\mathrm{Ba} = (3836 \pm 15)$ days and only the data set taken by detector 1. The absolute half-life of ^{7}Be in Au as obtained from the data set (reduced chi-square value = 1.6 for exponential fit) taken by detector 1 is = (53.60 ± 0.19) days, where only statistical errors have been considered. The half-life of ^{7}Be in Au as obtained from the data set taken by detector 2 agrees very well with that obtained from detector 1. However, we think it would not be appropriate to reduce the error bar on the absolute value of the half-life by combining results from two data sets that give significantly different reduced chi-square values when fitted with exponential functions. Norman *et al.* [3] obtained the half-life of ^{7}Be in Au = (53.311 ± 0.041) days and the reduced chi-square value for exponential fit of their data set was = 1.04. However, in their experiment, a primary ^{7}Li beam was incident on a Au foil and so some radiation damage of the Au lattice was expected. We also performed a similar experiment by bombarding a kapton foil with a 48-MeV ^{7}Li beam from BARC-TIFR pelletron machine (Mumbai, India) and implanting recoiled ^{7}Be ions emitted at 0° in a Au foil placed behind the target. The implanted sample along with a ^{133}Ba source were counted using a HPGe detector for about 2 months and the half-life of ^{7}Be was determined by monitoring the ratio of counts under 478- and 356-keV γ-ray photopeaks with time. The reduced chi-square of the exponential fit was 1.45 and taking the half-life [17] of $^{133}\mathrm{Ba} = (3836 \pm 15)$ days, we obtained the half-life of ^{7}Be in Au = (53.328 ± 0.082) days, in good agreement with Norman *et al.*'s [3] result. So we think the radiation damage of Au lattice caused by a high-flux incident primary heavy-ion beam might be responsible [18] for slightly lowering $(0.54 \pm 0.36)\%$ the half-life of ^{7}Be in Au.

In a subsequent experiment, we performed a radiochemical separation of endohedral $^7\mathrm{Be@C}_{60}$ compound. ^{7}Be implanted fullerene C_{60} catcher was dissolved in 5 ml 1, 2, 4-trichlorobenzene. An equal volume of 6N hydrochloric acid containing carriers was added to the solution and the mixture was thoroughly shaken for 5 min in a separating funnel. The organic and the aqueous phases were separated and the activities of both the phases were determined accurately by γ spectroscopy using a 20% HPGe detector. The aqueous fraction was again mixed with equal volume of organic solvent and a second extraction was carried out. The second organic fraction contained $\leqslant 4\%$ of radioactivity compared to the first extraction. The organic fraction was also filtered through a millipore filter (pore size = 0.45 mm) to remove any insoluble material. No activity could be detected in the filter paper fraction. It is known [7] from Ohtsuki *et al.*'s high-pressure liquid chromatography (HPLC) work that the ^{7}Be radioactivities observed in the organic phase come from molecules having similar mobility as C_{60} molecules implying ^{7}Be is somehow attached to fullerene C_{60} molecule. So the possibilities are ^{7}Be activities in organic phase are coming from either endohedral $^7\mathrm{Be@C}_{60}$ complex or heterofullerene complex or exohedral $^7\mathrm{Be}\text{-}C_{60}$ complex. Because only elements of group IVb and Vb of periodic table are known [9] to form heterofullerene compounds, so beryllium is not expected to form a heterofullerene compound with C_{60}. ^{7}Be ions stopped in the interstitial positions forming exohedral complex with C_{60} fullerene are not expected to form strong covalent bond with carbon atoms of C_{60} and should be readily dissolved in the hydrochloric acid and remain in the aqueous fraction. Therefore, as concluded earlier [7], the ^{7}Be activities observed in the organic phase should be associated only with the formation of endohedral ^{7}Be@C$_{60}$ fullerene complex. So the yield of radioactive endofullerene can be accurately determined from the ratio of activities present in the organic and aqueous fractions. We found that the yield of endohedral ^{7}Be@C$_{60}$, i.e., the probability of insertion of ^{7}Be in C$_{60}$ by nuclear implantation technique is $(5.6 \pm 0.45)\%$, where the estimated uncertainty includes both the statistical and systematic errors. ^{7}Be ions remain at interstitial space forming exohedral ^{7}Be-C$_{60}$ complexes for the remaining 94.4% of the time.

The radiochemically separated organic fraction containing endohedral ^{7}Be@C$_{60}$ complex was dried in a plastic crucible. Two HPGe detectors having efficiency $\approx$30% were used to count endohedral ^{7}Be@C$_{60}$ and ^{7}Be in Au samples along with a ^{133}Ba source for 3 months following identical procedure as described earlier. However, the amount of extracted endohedral ^{7}Be@C$_{60}$ complex was only 5.6% and so the statistical uncertainty on one day count of 478 keV γ-ray from endohedral complex was rather large (initially about 4.5% and 14% at the end of the run) for each detector. We finally obtained from our measurement that the half-life of endohedral ^{7}Be@C$_{60}$ complex is shorter than that of ^{7}Be in Au by $(3.3 \pm 2.3)\%$. Recently Ohtsuki *et al.* [19] measured the half-life (52.68 ± 0.05 days) of an endohedral ^{7}Be@C$_{60}$ complex with high accuracy. Comparing their number with our measured half-life (53.60 ± 0.19 days) of ^{7}Be in Au, we find that the half-life of an endohedral ^{7}Be@C$_{60}$ complex is shorter than that of ^{7}Be in Au by $(1.71 \pm 0.37)\%$. If we compare Ohtsuki *et al.*'s measured half-life [19] of endohedral ^{7}Be@C$_{60}$ complex with that of ^{7}Be in Au as measured by Norman *et al.* [3], then the half-life of endohedral complex is shorter by $(1.20 \pm 0.12)\%$. All these results agree with one another within about one standard deviation. The lower difference seen in the case of comparison with Norman *et al.*'s measured half-life of ^{7}Be in Au might be because of radiation damage of Au lattice in Norman *et al.*'s experiment [3] as discussed before. We also conclude that the half-life of exohedral ^{7}Be-C$_{60}$ complex and that of ^{7}Be implanted in Au foil are about the same within $\approx$0.2%. So the half-life of endohedral ^{7}Be@C$_{60}$ complex is significantly (more than 1%) shorter than that of exohedral complex.

III. DISCUSSION AND INTERPRETATION

Let us first try to get a qualitative understanding of our results in terms of electron affinity. We have found experimentally that an implanted ^{7}Be ion has a very low probability $(5.6 \pm 0.45)\%$ of entering the fullerene cage and they mostly stay in interstitial space forming the exohedral ^{7}Be-C$_{60}$ complex. The electron affinities of a fullerene molecule (C$_{60}$) and gold atom are 2.6 eV [20] and 2.3 eV [21] respectively. Both gold and fullerene have face-centered cubic (FCC) lattice structure, but the lattice parameter of fullerene C$_{60}$ lattice is much larger (14.17 Å) than that(4.08 Å) of Au lattice. So if an implanted ^{7}Be ion occupies the same geometrical position in both C$_{60}$ and Au lattices, then its distance from the center of the nearest Au atom and C$_{60}$ molecule would be very different. When ^{7}Be would occupy the octahedral site of Au lattice, then its distance from the nearest Au atom would be $\approx$2Å, whereas in the case of C$_{60}$ lattice, the corresponding distance would be $\approx$7Å and the distance from the nearest carbon atom of C$_{60}$ molecule would be $\approx$3.7Å. Hence ^{7}Be should retain a significantly higher fraction of its 2*s* electrons in C$_{60}$ lattice and so the decay rate of ^{7}Be should be significantly faster in C$_{60}$ lattice than in Au lattice. So the observation of the same (within 0.2%) half-life of ^{7}Be in C$_{60}$ and Au lattices should imply different geometrical positions for the implanted ^{7}Be ions in the two lattices. It should also imply that the bond lengths of ^{7}Be-C$_{60}$ (i.e., the distance between ^{7}Be and the nearest carbon atom of C$_{60}$) and ^{7}Be-Au are about equal.

To understand the results quantitatively, we have done tight binding linear muffin-tin orbital (TB-LMTO) method calculations [2,5,6,22] to determine the average number of 2*s* electrons of ^{7}Be for both endohedral and exohedral fullerene complexes. A fullerene molecule consists of 60 carbon atoms placed on a sphere of radius 3.54 Å. These fullerene C$_{60}$ molecules are arranged in a face-centered cubic structure with 14.17 Å lattice constant. For both the endohedral and exohedral complexes, ^{7}Be should go to equilibrium positions where the total energy of the system has local minima and the calculated decay rate of ^{7}Be at those positions should agree with the experimental results.

However, we found that the TB-LMTO code [22] was not very suitable for the determination of equilibrium positions in the fullerene C$_{60}$ lattice, because its spheridization of potential requires filling up of the available empty space with close packed empty spheres and because such a division is not unique, it introduces an uncertainty in the determination of the total energy of the system. In the case of fullerene C$_{60}$ lattice, this uncertainty could be of the order of 0.4% in some cases and this is unacceptably large because the differences in binding energies of ^{7}Be at different sites are very small (of the order of 10 eV). The uncertainty in the determination of the charge density and number of 2*s* electrons of ^{7}Be could be up to 20% in some cases, but this is acceptable for the purpose of estimating the change in half-life of ^{7}Be and comparing with the experimental results. So the equilibrium position of ^{7}Be in endohedral ^{7}Be@C$_{60}$ was taken from a previous density functional calculation [13] and TB-LMTO code was used to determine the average number of 2*s* electrons of ^{7}Be at that position.

Lu *et al.* [13] performed density functional calculations for endohedral Be@C$_{60}$ and found that the equilibrium position of beryllium ion should be exactly at the center of C$_{60}$ cage. So we performed a TB-LMTO calculation placing a ^{7}Be atom atom exactly at the center of fullerene C$_{60}$ cage. The calculation was performed assuming such endofullerenes will form a face-centered cubic lattice with lattice parameter 14.17 Å. Empty spheres were placed in the interstitial space and one inside the cage for close packing. The TB-LMTO calculation shows that the radius of the muffin-tin sphere of the ^{7}Be atom at the center of C$_{60}$ cage is $\approx$3 Å and it almost fills up the entire space inside the C$_{60}$ cage. Let Ψ_{total} be the complete electronic wave function and $\Psi_{\text{Be}2s}$ be beryllium 2*s* state wave function. Then the square of the overlap of Ψ_{total} with $\Psi_{\text{Be}2s}$, i.e., $|\langle\Psi_{\text{total}}|\Psi_{\text{Be}2s}\rangle|^2$ represents the average number of $2s$ electrons in beryllium ion. Our TB-LMTO calculation shows that the average number of $2s$ valence electrons of ^{7}Be atom placed at the center of a C_{60} cage is = 1.07. However, the convergence of the code for this calculation was not very good and the total energy was determined within 10 eV. The uncertainty on the average number of $2s$ valence electrons of ^{7}Be atom is not expected to be better than 20%.

We also calculated the average number of $2s$ electrons of ^{7}Be in Au. As shown earlier [6], in the case of implantation of ^{7}Be in Au lattice, ^{7}Be should go to octahedral and tetrahedral sites of the Au lattice. TB-LMTO calculations were performed by placing a ^{7}Be atom at octahedral and tetrahedral positions of a face-centered cubic Au lattice having a lattice parameter of 4.08 Å. The average number of $2s$ electrons $|\langle\Psi_{\text{total}}|\Psi_{\text{Be}2s}\rangle|^2$ was found to be 0.54 and 0.36 for ^{7}Be occupying octahedral and tetrahedral positions of gold lattice, respectively. The convergences of these calculations were excellent and the uncertainties in the number of $2s$ electrons should not be more than a few percentages [6]. We expect that as a result of random implantations, the number of ^{7}Be atoms occupying tetrahedral sites would be twice that of occupying octahedral sites, because the number of tetrahedral sites are twice that of octahedral sites in a face-centered cubic lattice. Hence, taking a weighted average, we found ^{7}Be would have 0.42 electrons in its $2s$ orbital when implanted in Au. So the decay rate of ^{7}Be in endohedral ^{7}Be@C_{60} should be faster than that of ^{7}Be in Au. According to Hartree and Hartree's calculation [23], the overlap of valence $2s$ electrons to the total electronic overlap at the beryllium nucleus is only 3.32% for a neutral beryllium atom. As shown in Ref [6], there is a linear relationship between the decay rate of ^{7}Be and its number of valence $2s$ electrons. Using Hartree and Hartree's result [23] along with the linear relationship found earlier [6], we obtain that the decay rate of endohedral ^{7}Be@C_{60} should be faster by $\approx$1.1% compared to that of ^{7}Be in Au lattice. The uncertainty on this calculated number is around 20% because of the poor convergence of the TB-LMTO calculation for the endohedral ^{7}Be@C_{60} complex, as discussed earlier. This result is in reasonable agreement with the result that the decay rate of endohedral ^{7}Be@C_{60} complex is faster than that of ^{7}Be in Au by (1.71 ± 0.37)%.

To calculate the decay rate of ^{7}Be when it goes to interstitial space of C_{60} lattice forming exohedral complex, we have to first determine its equilibrium positions in the fullerene C_{60} lattice. Although we have not come across any calculation for determining equilibrium positions of ^{7}Be in a fullerene C_{60} lattice, there are a large number of calculations [10–12,14] for equilibrium geometries of the isolated exohedral fullerene C_{60} complex. From those calculations, it is known that the typical bond length between a carbon and the other ion forming the exohedral fullerene C_{60} complex is $\approx$2 Å. The distance of the other ion from the center of the C_{60} cage is usually [10–12,14] around 5.5 Å and the equilibrium position of the other ion is most likely to be along a line bisecting normally a C-C bond of C_{60} molecule. Using this information, we carried out TB-LMTO calculations for beryllium in C_{60} lattice and found that there were total energy minima postions when beryllium was on any face of the face-centered cubic C_{60} lattice between a corner C_{60} molecule and a face-centered C_{60} molecule along a line bisecting normally C-C bond of a C_{60} molecule. At equilibrium position, the distance of beryllium ion from the center of C_{60} molecule is about 5.3 Å and C-Be bond length comes out around 2 Å. We find from TB-LMTO calculation that at this position, the average number of valence $2s$ electrons of beryllium ion is 0.44. The uncertainty on this number is around 20% because of comparatively poor convergence of the code for these calculations. So using Hartree and Hartree's result [23], the decay rate of exohedral ^{7}Be-C_{60} complex should be faster by $\approx$0.03 % compared to that of ^{7}Be in Au. This result agrees with our experimental observation that the decay rate of exohedral ^{7}Be-C_{60} and that of ^{7}Be in Au are equal within 0.2%.

If we assume that ^{7}Be ions go to the octahedral or tetrahedral sites of face-centered cubic C_{60} lattice, then according to TB-LMTO calculations, the average number of $2s$ electrons of ^{7}Be should be 1.12 and 1.51, respectively. So using the method of Ref. [6], the decay rate of ^{7}Be should be faster than that of ^{7}Be in Au by 1.16 and 1.8%, respectively, in complete disagreement with our experimental observation. Moreover, if ^{7}Be is at octahedral site, then its distance from the center of the nearest C_{60} molecule would be about 7 Å and so the length of shortest C-Be bond would be about 3.7 Å. Similarly, when ^{7}Be is at the tetrahedral site of the C_{60} lattice, then its distance from the center of the nearest C_{60} molecule is 6.1 Å and the length of shortest C-Be bond is about 3 Å. At this position, the line joining the center of the C_{60} molecule and ^{7}Be ion does not bisect C-C bond of C_{60} molecule, but passes through the center of the hexagonal opening of C_{60} molecule. It is also expected [14] that for most stable exohedral configuration, a beryllium atom should go to a site of high electron density. Our TB-LMTO calculations show that the electron density at a tetrahedral site of C_{60} lattice should be about 50% more than that at octahedral site. However, the electron density on a face of the lattice midway between two C_{60} molecules is about 5 times the electron density at the octahedral site. So from these qualitative arguments, we expect that the octahedral and tetrahedral sites should not be the equilibrium positions of ^{7}Be in fullerene C_{60} lattice. However our TB-LMTO calculations for the total energy of the system do not support this expectation, perhaps because of the model limitations mentioned above.

In the case of endohedral ^{7}Be@C_{60} complex formation, although C-Be bond length would be 3.54 Å because ^{7}Be is expected to be at the center of fullerene C_{60} cage; however, at that position, ^{7}Be is equidistant from all 60 carbon ions and is held there by 60 C-Be bonds. So even if each bond is weak, there are 60 such bonds holding the beryllium ion.

In summary, we have found experimentally that the decay rate of exohedral ^{7}Be-C_{60} complex is equal to that of ^{7}Be implanted in Au within 0.2%. A radiochemical analysis of the irradiated sample shows that only 5.6% of the implanted ^{7}Be ions form endohedral ^{7}Be@C_{60} complexes and the remaining 94.4% of the ^{7}Be ions form exohedral ^{7}Be-C_{60} complexes. The measured decay rate of endohedral ^{7}Be@C_{60} complex is in agreement with recent accurate measurement of Ohtsuki *et al.* [19]. It is interesting to note that the half-life of the endohedral ^{7}Be@C$_{60}$ complex is shorter than that of the exohedral complex by more than 1%. Our TB-LMTO analysis shows that for the endohedral ^{7}Be@C$_{60}$ complex, ^{7}Be ion should go to the center of C$_{60}$ cage. For the exohedral ^{7}Be-C$_{60}$ complex, we expect that ^{7}Be should go to one of the faces of face-centered cubic C$_{60}$ lattice forming exohedral complex with C-Be bond length ≈2Å.

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