Determination of Internal Conversion Coefficients in Mercury Isotopes

Rishita Gudapati

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1 Initial Estimation

A primary estimation of the conversion coefficients of seven Mercury isotopes was determined through peak fitting the experimental data. The data was sorted with grsisort and fit using jRoot. Locations to this software is provided in the Appendix to this report. The data that was used in this fitting is stored in `/data3/rgudapati/`, and the resulting estimates from peak fitting (including gamma summing corrections) are found in the directory provided with this report under `/mcc/fitting_estimates.ods`

2 Corrections to the Hg-198 K-Peak

2.1 Background

In this analysis, we are looking at the decay of Tl-198 → Hg-198(2+) → Hg-198(g.s.). We will consider both the Tl-198(7+) isomer and Tl-198(g.s.) decays.

The purpose of the following analysis is to determine whether all corrections to the data have been identified by simulating the decay in Geant4 and normalizing the Tl isomer and ground state K-peaks to a spherically uniform electron beam at the energy of a K-electron for the Hg 2+ → 0+ transition. Having identified all corrections, we will be more accurately able to calculate the internal conversion coefficients for this transition. The exercise will also provide some insight and a starting point for which corrections need to be made to the other mass transitions for this experiment.

In this report, we focus on the Hg 2+ → 0+ transition: (all energies in keV)

Level Energy	411.80
Transition Energy	411.80
K-Binding Energy Hg	83.102
K-Electron Energy	328.7

Table 1: Hg-198 2+ → 0+ Transition

Almost all decays to the Hg 0+ g.s. are through the first 2+ state described above. Using the electron capture branching ratios (I_{EC}) and gamma branching ratios (I_γ) in the Geant4 v.10.01 RadioactiveDecay and PhotonEvaporation modules, respectively, we use the following method to determine the fraction of decays that bypass this level.

$$\sum_i^n (I_{EC}^i \times I_\gamma^i) + \sum_j^m \left[(I_{EC}^j + I_\gamma^j) \times I_\gamma^{1087} \right]$$

Where we sum over n direct decays to the Hg-198 ground state and m direct decays to Hg-198(2_2+) ($E_L = 1087$) from the Tl-198 ground state. This second level can decay directly to the ground state or to Hg(2+). To determine the equivalent value for the Tl-198 isomer decay, we multiply the ground state value by the internal transition probability 44.1%.

In the Tl ground state decay, only about 0.50% of decays bypass the first 2+ state. In the isomer decay, only 0.20% bypass this 2+ state. We can therefore assume that the corrections due to these transitions are small and focus soley on the Hg 2+ $\rightarrow$ 0+ decay for the rest of our corrections. See the file `bypasses.ods` included with this report.

Furthermore, simulations were run both with fluorescence on and with it off. The effects of fluorescence was found to be minimal in all cases. In this report, we include only the analysis for fluorescence off.

2.2 Tl-198(2−) Ground State Decay

Peak area before normalization: $N_e(K) = 2876.3 \pm 71$
† taken from nuclear data sheets for A=198. All other values taken from Geant4 RDM and PE modules.

$$\frac{\alpha_K}{\alpha} = 0.6823$$

$$\alpha = 0.0439 \quad \text{total conversion coefficient}$$

$$\begin{aligned}
I_\gamma &= 750^\dagger \times 0.00106^\dagger \\
&= 0.795 \\
I_T &= 0.83^\dagger \\
I_{e^-} &= I_T - I_\gamma \\
&= 0.83 - 0.795 \\
&= 0.035 \\
I_{e^-}(K) &= I_{e^-} \times \frac{\alpha_K}{\alpha} \\
&= 0.035 \times 0.6823 \\
&= 0.0238805
\end{aligned}$$

Per decay we have 0.0239 ±15.6% K electrons produced by this decay.

A note on error propagation: the errors for values taken from Geant4 are unknown, so all errors are taken from the NDS for a rough estimation.

Normalization gives us: $\quad N_e(K)/0.0239 = 120,347 \ \pm 15.8\%$

2.3 Tl-198(7+) Isomer Decay

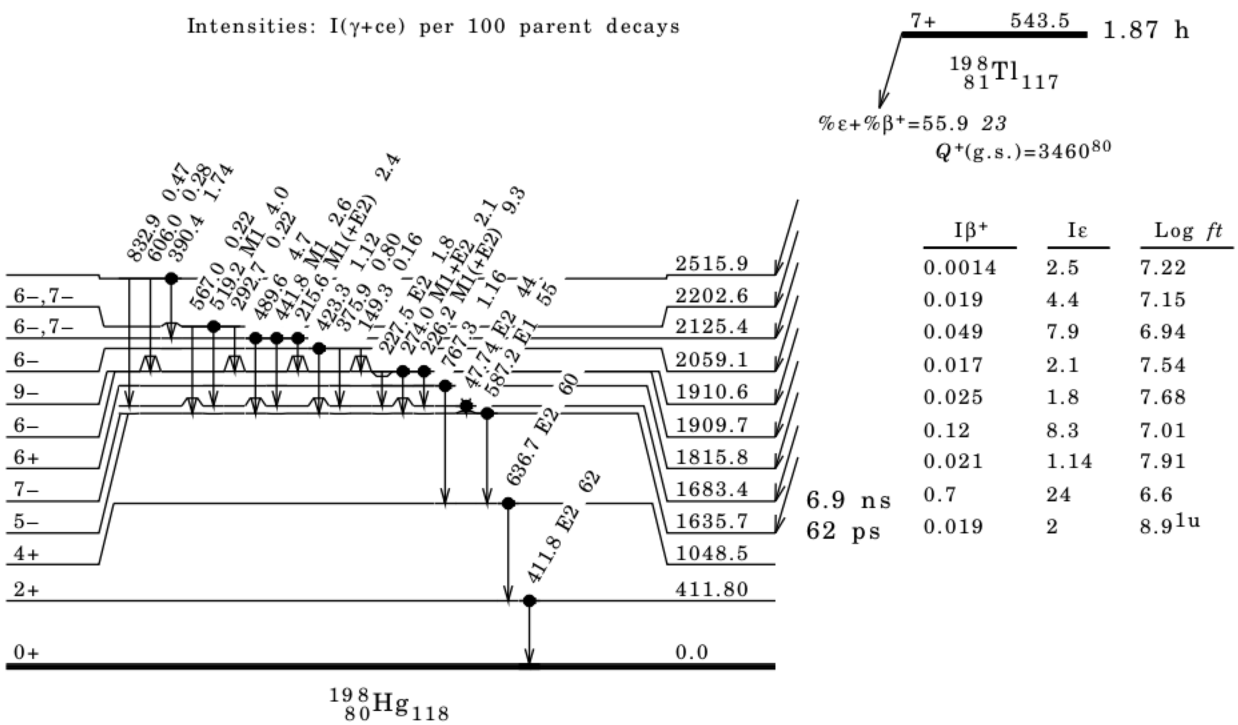

Figure 1: Tl-198(7+) $\rightarrow$ Hg-198 $\beta+$ decay

Peak area before normalization: $N_e(K) = 2560.22 \pm 153$

$$
\begin{aligned}
I_T &= 0.62^{\dagger} \text{ per decay} \\
I_\gamma &= 109^{\dagger} \times 0.00544^{\dagger} \\
&= 0.59296 \\
I_e &= I_T - I_\gamma \\
&= 0.02704 \\
I_e(K) &= 0.68 \times 0.02704 \\
&= 0.01839
\end{aligned}
$$

Per decay, we produce 0.01839 $\pm 18\%$ K-electrons.

Normalization gives us: $N_e(K)/0.01839 = 139,218 \ \pm 19\%$

2.4 Hg-198(2+) Decay

$N_e(K)$ before normalization $= 15807 \pm 207$

$$\frac{\left[(\alpha_K/\alpha) \times \alpha\right]}{1+\alpha} = \frac{\left[(0.0300/0.0439) \times 0.0439\right]}{1+0.0439}$$
$$= 0.0287383849$$

Per decay, we produce 0.0287 $\pm 3.22\%$ K-electrons.

Normalization gives us $N_e(K)/0.0287 = 550,766 \pm 3.48\%$

2.5 e^- Beam

This is a simple detector simulation where all particles are electrons at 330 keV emitted as a spherically symmetric beam. Therefore, the normalized values for all $N_e(K)$ above should match the raw area for the peak in this simulation: 558,044 $\pm$ 8114.

2.6 Summary: Corrections to Detector Simulations

DETECTOR SIM	$N_e(K)$ unnormalized	$N_e(K)$ normalized	electron beam / norm. $N_e(K)$
Tl-198(g.s.)	2876.3 $\pm$ 2.5%	120,347 $\pm$ 15.8%	4.63 $\pm$ 15.9%
Tl-198(7+)	2560.22 $\pm$ 6.0%	139,218 $\pm$ 19.0 %	4.02 $\pm$ 19.1%
Hg-198(2+)	15807 $\pm$ 1.3%	550,766 $\pm$ 3.48 %	1.01 $\pm$ 3.8%

So, there are still missing corrections which need to be identified before we can calculate the true values of the conversion coefficients. The missing corrections will only apply to the Tl-198 decays.

3 Comparison to Pure Simulation

The simulations above were repeated without detector geometry. *All* simulations referred to in this report were done for 10 million particles.

Below is a sample normalization using the pure simulation of the ground state decay.

$N_e(K,p) = 52752$ before normalization (pure).
$N_e(K,d) = 2876.3$ before normalization (detector).

We use the pure normalization factor A_p to find the detector normalization factor A_d:

$$\begin{aligned} A_p &= 52,752/10,000,000 = 0.0052752 \\ A_d &= A_p^{-1} \\ &= 189.57 \end{aligned}$$

Therefore $N_e(K,d) = 2876.3 \times 189.57 = 545,260$ after normalization.

I present a summary of the comparisons between the detector simulations and the pure simulations for each case:

SIMULATION	$N_e(K)$ unnorm. (pure)	$N_e(K)$ unnorm. (detector)	A_d factor	$N_e(K)$ norm. (detector)
Tl-198(g.s.)	52752 ± 2.5%	2876.3 ± 2.5%	189.57	545,260 ± 13,632
Tl-198(7+)	52763 ± 6.0%	2560.22 ± 6.0%	189.53	485,238 ± 29,114
Hg-198(2+)	287506 ± 1.3%	15807 ± 1.3%	34.78	549,767 ± 7147
e^- beam	558,044 ± 1.5%	558,044 ± 1.5%	1.0	558,044 ± 8114

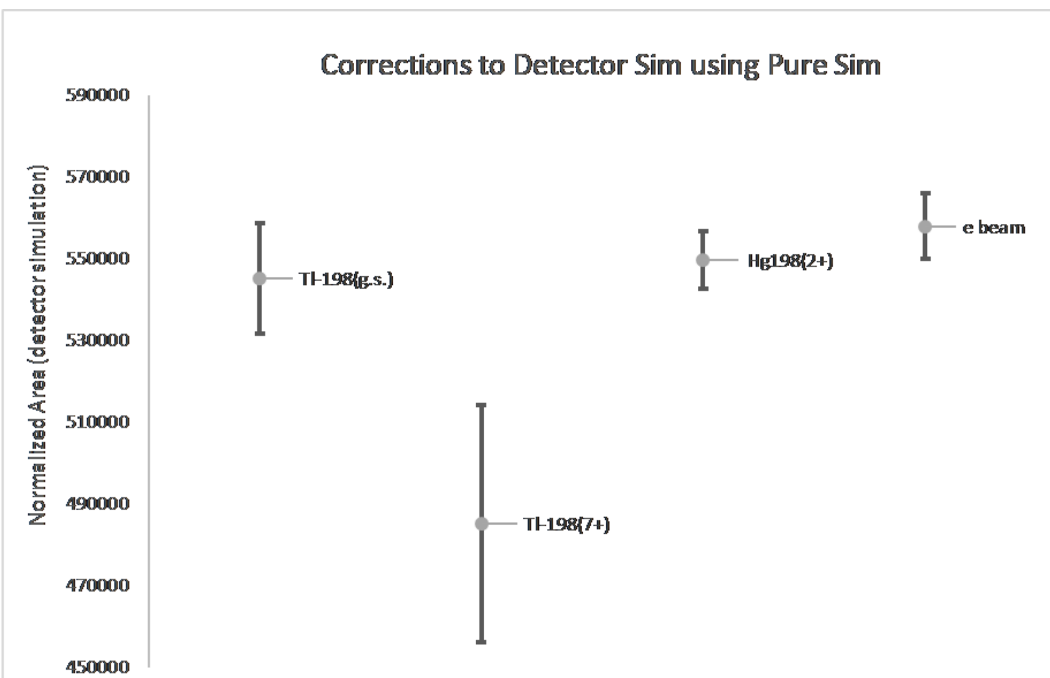

Figure 2: visual comparison of $N_e(K,d)$ normalized to pure simulation for each decay

4 Next Steps

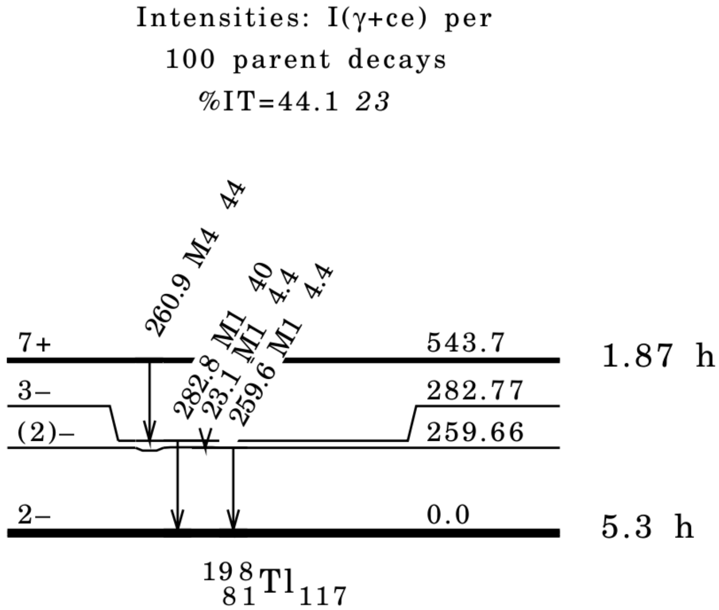

Figure 3: internal transition in the Tl-198 nucleus

The data still needs to be corrected for electron summing effects. This is slightly more complicated than the gamma case. Furthermore, it is necessary to determine the isomeric ratio of Tl-198 to determine the relative contribution of the 2− ground state and 7+ state to the electron and gamma peaks retrieved from the experimental data. This ratio is largely dependent on the reaction mechanism and may be very difficult to attain.

Appendix

Refer to the `mcc` directory provided with this report. A full list of files in this directory is provided below, with important text files in red:

```
mcc
├── selectors
│   ├── selector_info
│   ├── ICSelector.h
│   ├── ICSelector.C
│   ├── gamma_summing.h
│   └── gamma_summing.C
├── sorting
│   ├── calibrate.C
│   ├── run1989.cal
│   ├── RunSummary.xlsx
│   ├── sorted_runs
│   ├── sorting_howto
│   └── UnPack198
├── efficiency_curves
│   ├── paces_curve.pdf
│   └── griffin_curve.xlsx
├── fitting_estimates.ods
└── bypasses.ods
```

`fitting_estimates.ods` is a spreadsheet with the results of peak fitting used to determine an initial estimation of the internal conversion coefficients for seven Mercury isotopes. No corrections are made to the values (ie. no summing corrections), and the estimates are compared to the BrIcc values for three different transitions ([E2] $4^+ \rightarrow 2^+$, [E2/M1] $2^+ \rightarrow 2^+$, [E2] $2^+ \rightarrow 2^+$). There should be a total of $7 \times 3 = 21$ coefficient estimations in this file. However, there are only 20; the Hg-196 $2^+ \rightarrow 2^+$ transition is difficult to see in the spectra and extra gating may be required to obtain a satisfactory peak for fitting.

Data which has already been unpacked and sorted is available for all seven isotopes in `/data3/rgudapati/`

NDS values taken from Nuclear Data Sheets A = 198 (2009).