## Supplemental Material for "Theory of Coulomb Excitation of the <sup>229</sup>Th Nucleus by Protons"

Tao Li,<sup>1, \*</sup> Hanxu Zhang,<sup>1, \*</sup> and Xu Wang<sup>1, 2, †</sup>

<sup>1</sup>Graduate School, China Academy of Engineering Physics, Beijing 100193, China

<sup>2</sup>Southern Center for Nuclear-Science Theory, Institute of Modern Physics,

Chinese Academy of Sciences, Huizhou, Guangdong 516000, China

(Dated: September 27, 2023)

More details of the SRIM simulation. — In the main text, we mostly focus on the situation with proton energy 10 MeV and target thickness 100  $\mu$ m. Such a parameter selection is based on comprehensive considerations from SRIM simulations.

(i) In this situation, there is almost no residual proton in the target. As shown in Fig. S1, the incident protons have enough energy to penetrate through 100  $\mu$ m thickness. Except for very rare cases of large-angle scattering, almost all protons are deposited beyond 500  $\mu$ m.



FIG. S1: Trajectories of 10 MeV incident protons with (a) 600  $\mu$ m target thickness and (b) 100  $\mu$ m target thickness, simulated by the SRIM software.

(ii) Within 100  $\mu$ m, the stopping power is relatively small, as shown in Fig. S2. Small stopping power results in less energy deposition and defects, decreasing the likelihood of the internal-conversion process.



FIG. S2: Stopping power as a function of penetration depth for proton incident energy of 10 MeV.

(iii) Such parameters can simultaneously lead to efficient excitation and limit the number of vacancy defects. As shown in Fig. S3(a), the residual proton energy does not change much within 100  $\mu$ m, ensuring relatively large excitation cross sections. Meanwhile, the simulated number of vacancy defects caused by each proton within 100  $\mu$ m

is only about 6 for 10 MeV. For proton irradiation dose of  $6 \times 10^{17}$  cm<sup>-2</sup> as considered in the main text, the vacancy density would be  $10^{18}$  cm<sup>-3</sup>. In real experiments this number could be smaller because of the thermal annealing effect, which is not considered in the SRIM simulation. Indeed, latest experimental research shows that the defects caused by each proton of energy 3.5 MeV is on the orders of 0.1 to 1 [S1], much lower than the corresponding SRIM simulation results [Fig. S3(b)]. Therefore higher proton irradiation doses might be used than the value considered in the main text, yielding even higher isomeric excitation probabilities.



FIG. S3: Residual proton energy and vacancy numbers simulated by the SRIM software for (a) 10 MeV and (b) 3.5 MeV incident energy. The black solid curve is the residual energy of the proton in the  $CaF_2$  target. The red dotted curve represents the number of vacancies caused by each incident proton as a function of the penetration depth.

Calculation of  $\alpha$  particle-induced Coulomb excitation.— The theoretical approach developed in the main text can also be applied to other positive projectiles, like  $\alpha$  particles. As an example, we calculate the Coulomb excitation cross sections (by  $\alpha$  particles) of two energy levels in <sup>19</sup>F, and compare them to the experimental results [S2]. As shown in Fig. S4, our results agree well with the experimental data. This comparison provides support for the reliability of our theory and calculations.



FIG. S4: Coulomb excitation cross sections by  $\alpha$  particles from the nuclear ground state to the 109-keV and the 196-keV energy levels in <sup>19</sup>F. The transition types are electric dipole and electric quadrupole, respectively. The experimental data points are extracted from Ref. [S2]. The theoretical curves are calculated by the approach presented in the main text, and are normalized to the experimental data at 1.55 MeV.

- \* T. L. and H. Z. contributed equally to this work.
- <sup>†</sup> Corresponding author: xwang@gscaep.ac.cn
- [S1] R. Hazem and M. Izerrouken, Radiat. Phys. Chem. 204, 110643 (2023).
- [S2] R. Sherr, C. W. Li and R. F. Christy, Phys. Rev. 96, 1258 (1954).