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Nuclear Data Matters - The obvious case of a bad mixing ratio for 58Co

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Nuclear Data Matters – The obvious case of a bad mixing ratio for ^{58}Co

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Abstract: We present results of modeled cross sections for neutron- and proton-induced reactions leading to the final product nucleus ^{58}Co. In each case the gamma-cascade branching ratios given in the ENSDF database circa 2014 predict modeled nuclear cross sections leading to the ground and first excited metastable state that are incompatible with measured cross sections found in the NNDC experimental cross section database EXFOR. We show that exploring the uncertainty in the mixing ratio used to calculate the gamma-cascade branching ratios for the 53.15 keV 2nd excited state leads to changes in the predicted partial cross sections by amounts that give good agreement with measured data.

Introduction

Precise knowledge of excitation functions and isomeric cross section ratios of neutron induced reactions from threshold to 20 MeV are of considerable importance in many areas, including reactor technology, the production of medical isotopes, radiation damage in semi-conductors, and national security. Many different reaction channels are open in this range, some of the more important being (n,f), (n,γ), (n,n'), (n,2n), (n,p), (n,α), etc. Of particular interest is the product nucleus ^{58}Co. We consider three specific reactions for which measured cross sections are known for the activation (total) cross section and the partial cross sections to its 2+ ground state and its 5+ (9.10 h) metastable state: ^{59}Co(n,2n)^{58}Co, ^{58}Ni(n,p)^{58}Co, and ^{58}Fe(p,n)^{58}Co.

Figure 1 shows our modeled cross sections (b) vs. incident particle energy (MeV) for these three reactions calculated with the Hauser-Feshbach code STAPRE. Details of the input to various quantities affecting the calculations such as nuclear structure and spectroscopic decay data, level densities, gamma-ray strength functions, pre-equilibrium models, etc. are given in Ref. 1. In all cross section plots, the black solid line is the activation (total) cross section, the grey data with error bars show the total cross section results as measured by the many experiments listed for each reaction in the EXFOR database (Ref. 2). We find in each case the agreement with the total cross section is very good. The solid red and blue lines (and their uncertainties given by the extent of the shaded regions) give the cross sections to the ground (GS) and first metastable (M1) states, respectively, assuming a mixing ratio δ=-0.33 for the 53.15 keV 4+ second excited state. The red and blue data with error bars represent measured cross sections for each reaction from the EXFOR database. In each case the cross section to the metastable state (blue) is *under*-estimated while that to the ground state is *over*-estimated compared to the EXFOR data.

We will carry out a sensitivity study to determine the effect of the mixing ratio for the 2nd excited state in ^{58}Co on the predicted partial cross sections to the ground and first excited meta-stable states.

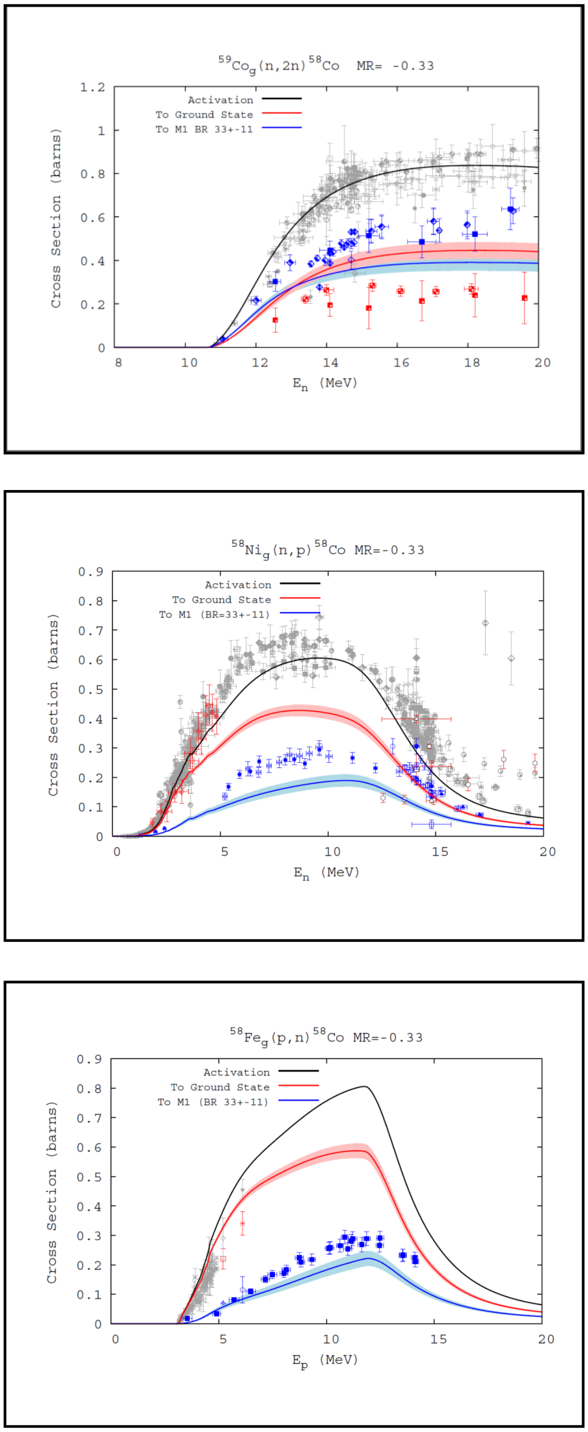

Fig. 1. STAPRE calculated cross sections for ^{59}Co(n,2n)^{58}Co, ^{58}Ni(n,p)^{58}Co, and ^{58}Fe(p,n)^{58}Co showing the total (black) and partial cross sections to the ground state (red) and metastable state (blue) compared to measured data from EXFOR. Here δ=-0.33.

Calculating Decay Branching Ratios

The adopted levels for ^{58}Co with the isomer at level 53.15 keV and its gamma decays are shown in Figure 2 below. In the STAPRE calculation the first 12 levels in the ENSDF level scheme were used.

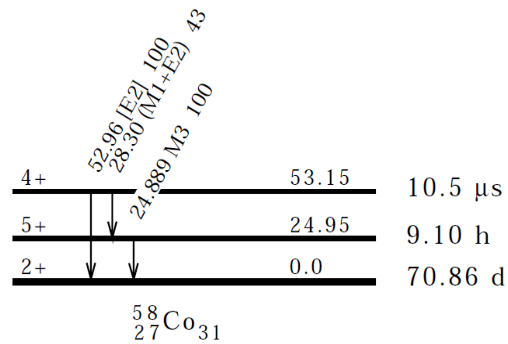

Fig. 2. Simplified decay scheme of ^{58}Co

In the current version of ENSDF (Ref. 3), the 53.15 keV, 4+ state in ^{58}Co decays to the 24.95 keV, 5+ state and to the ground, 2+ state. The latter transition has an E2 multipole character while both M1 and E2 multipolarities are favored for the former. In the work by Bertschat *et. al.* (Ref. 4), the authors have suggested two possible mixing ratio (δ) values of - 0.33 (6) (90% M1, 10% E2) or -2.3 (4) (16% M1, 84% E2) for the 24.95 γ transition.

The mixing ratio value of -0.33 was considered more likely by the evaluators in Ref. 3 based on the other mixed transition in the levels scheme that are mainly M1 in character.

However, our model calculations (Fig. 1) show a deviation from experimental cross sections of ^{59}Co(n,2n)^{58m,g}Co to the ground and metastable states due to the branching ratios that were used based on this lower mixing ratio. Since these low energy transitions (53 γ and the 24 γ) are highly converted, the internal conversion coefficients (α), will have a strong effect on the total branching ratios.

The transition intensity (TI) which takes into account the gamma intensities and the internal conversion electrons is defined as (TI)= Iγ x (1 + α_{tot}) where Iγ is the relative gamma intensity and α_{tot} is the total internal conversion coefficient.

The total internal conversion coefficient (α_{tot}) was calculated using the BrICC program (Ref. 5) with calculations using the so called "Frozen Orbital" approximation, that take into account the effect of atomic vacancies created in the conversion process.

The total internal conversion coefficient (α_{tot}) for 28.30 keV, (M1+ E2) with δ=-2.3= 51 (4) and for 52.96 keV, E2 =5.97 (10)

Hence the total transition intensity is

i) Eγ=28.30 (15) keV and Iγ=43 (5), TI=2236 (407)

ii) Eγ=52.96 (13) keV and Iγ=100, TI=697 (12)

Branching ratios (BR) can then be calculated (TI/Total TI) x 100%: BR(28.30 γ)= 76 (17)% and BR (52.96 γ)= 24 (3)%.

Figure 3 shows our results when adopting the higher value mixing ratio δ=-2.3 for the 53.15 keV 2^{nd} excited state and its affect on the cross sections to the ground and meta-stable state in ^{58}Co. For each reaction the agreement with measured cross section data is greatly improved. We recommend that the value for the mixing ratio for the 53.15 MeV 2^{nd} excited state in ^{58}Co be changed from δ=-0.33 to δ=-2.3.

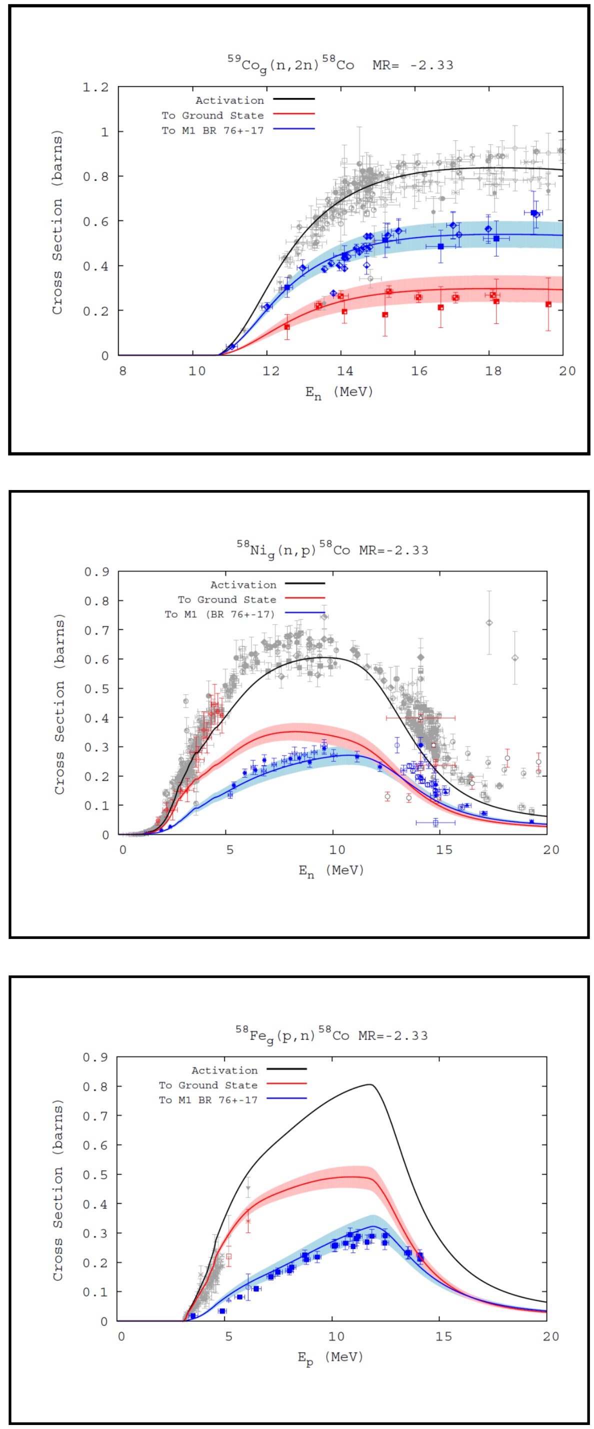

Fig. 3. STAPRE calculated cross sections for ^{59}Co(n,2n)^{58}Co, ^{58}Ni(n,p)^{58}Co, and ^{58}Fe(p,n)^{58}Co showing the total (black) and partial cross sections to the ground state (red) and metastable state (blue) compared to measured data from EXFOR. Here δ=-2.3.

Conclusions

The effort that goes into an NNDC evaluation for a given mass chain involves the consideration of many available published results. Sometime various results get missed or become available at the end of an evaluation effort. And sometimes conflicting data is deemed not pertinent or "experience" leads to choices that seem reasonable at the time. Our small survey suggests in this particular case that a choice within estimated uncertainty led to a modeling result that was incompatible with experiment, but consideration of its upper limit could address the modeled inconsistency leading to very good agreement. Here is a fine example where evaluation is guided by theory, experiment, and modeling, to the benefit of all.

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