frescoPRC

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The tool frescoPRC has been created to easily generate inputs for the nuclear reaction program FRESCO¹ [3] that describe the scattering of neutrons by even and odd actinides using a dispersive optical model with effective couplings between bands presented in [1]. In said article, calculations were done with the nuclear reaction program OPTMAN [2] but its use is limited compared to others more popular like FRESCO, so it could be useful for the nuclear physics community to be able to do this kind of calculations in a more widely used program. The tool frescoPRC uses as input the parameters that define the dispersive optical potential given in Table I of [1]. In addition to this, the effective parameters of the target, presented in the Table IV of [1] for ²³⁸U and in Table VI for ²³⁹Pu, as well as the energy scheme of the target are part of frescoPRC's input. Beside this, the energy of the neutron and some integration parameters also have to be included in the tool's input.

Volume	Surface	Spin-orbit	Coulomb
$V_0 = 50.41 + 0.0292 \text{ (A - 238) MeV}$		$V_{\rm spo} = 5.64 \; {\rm MeV}$	$C_{coul} = 1.36 \text{ MeV}$
$\lambda_{\rm HF} = 0.00977~{ m MeV}^{-1}$	-	$\lambda_{\rm so} = 0.005~\rm MeV^{-1}$	
$C_{\rm viso} = 17.5 \ {\rm MeV}$			
$A_v = 11.91 \text{ MeV}$	$W_0 = 17.70 \text{ MeV}$	$W_{\rm spo} = -3.1 \; {\rm MeV}$	
$B_v = 81.86 \text{ MeV}$	$B_s = 10.85 \text{ MeV}$	$B_{\rm so}=160~{ m MeV}$	
$E_a = 55 \text{ MeV}$	$C_s = 0.01331 \text{ MeV}^{-1}$		
$\alpha_v = 0.355 \text{ MeV}^{1/2}$	$C_{\rm wiso} = 29.0 {\rm \ MeV}$		
$r_{\rm HF} = 1.2490$ - 0.00171 (A - 238) fm	$r_s = 1.1701 + 0.0041 \text{ (A - 238) fm}$	$r_{\rm so} = 1.1214 \; {\rm fm}$	
$a_{\rm HF} = 0.638 + 0.002190 \text{ (A - 238) fm}$	$a_s = 0.617 \text{ fm}$	$a_{\rm so} = 0.59 \; {\rm fm}$	
$r_v = 1.2657 \text{ fm}$			$r_c = 1.12894 \text{ fm}$
$a_v = 0.6960 - 0.00021 \text{ (A - 238) fm}$			$a_c = 0.547 \text{ fm}$

Table I: Dispersive optical-model parameters for dispersion of neutrons by actinides presented in [1].

Target	β_{20}	β_{40}	β_{60}
$^{238}\mathrm{U}$	0.231	0.062	-0.0096
²³⁹ Pu	0.236	0.086	-0.0310

Table II: Static axial deformation parameters for ²³⁸U and ²³⁹Pu given in [1].

 $^{^{1}}$ More specifically, it has been created to be compatible with the version frxy6j of FRESCO modified to be able to define states grouped by bands.

Bands	Deformation parameters
β -band	$[\beta_2]_{\text{eff}} = 0.1039$
γ -band	$[\gamma_{20}]_{\rm eff} = 0.0476$
Octupole band	$[\beta_{30}]_{\text{eff}} = 0.2684$
γ -band (non-axial)	$[\gamma_{22}]_{\rm eff} = 0.3030$

Table III: Effective deformation parameters for 238 U. This numerical values do not coincide with ones presented in the table IV of [1] because they are multiplied by β_{20} to meet OPTMAN's convention. With this said, effective parameters in table IV of [1] are actually $\beta_{20} \times [\beta_{\lambda}]^{\text{eff}}$.

Bands	Deformation parameters
Octupole band (axial)	$\alpha(1/2, 1/2) \times [\beta_{30}]_{\text{eff}} = 0.2627$
γ -band (non-axial)	$\alpha(5/2, 1/2) \times [\gamma_{22}]_{\text{eff}} = 0.1059$

Table IV: Effective deformation parameters for 239 Pu. Like in Table III, this numerical values are different from ones presented in table VI of [1] because they are multiplied by β_{20} to meet OPTMAN's convention. In addition, the non-axial band is a γ -band instead of a octupole band because there is not change of parity in the transition from G.S band to the non-axial band.

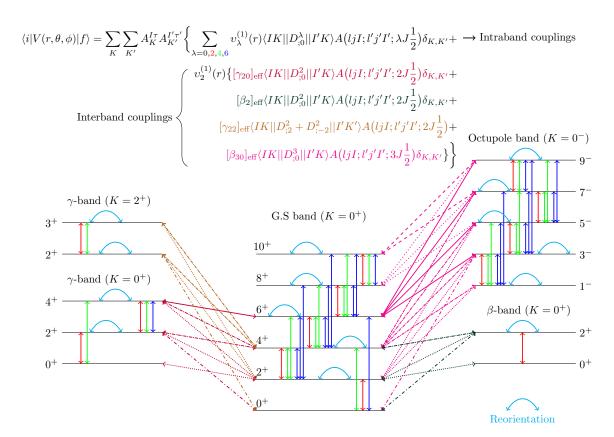


Figure 1: Coupling scheme for $n+^{238}U$ (energy levels are not in scale) showing intraband and interband couplings due to different terms in the coupling matrix elements expression B.12 from [1].

frescoPRC's input in NAMELIST format is :

• &TARGET namelist

Z, A, eferm, β_{20} , β_{40} , β_{60} , nstat

Target's information including atomic and mass number, fermi energy (*eferm*), static axial deformation parameters (e.g. parameters from Table II for ²³⁸U or ²³⁹Pu) and number of coupled levels considered (*nstat*).

• &STATE namelist

Et, Jval, Kval, NBAND, COEFF

One &STATE per level considered. The level is characterised by an energy Et in keV, an angular momentum Jval and a projection Kval. NBAND is a integer that is common to all states in a same band [all states from G.S band must have NBAND = 1 while any other integer identify an excited band] and its sign determines the parity of the band. For states of G.S band COEFF is β_{20} and for states of excited bands COEFF is $\beta_{20} \times [\beta_{\lambda}]^{\text{eff}}$ where $[\beta_{\lambda}]^{\text{eff}}$ is the effective deformation parameter (e.g. parameters from Tables III and IV for 238 U and 239 Pu).

• &FRESCO namelist

hcm, rmatch, Jmax, Ngrid, pythonFlag, Nenergy

rmatch is the matching radius in fm, hcm is the integration step for coupled equations in fm, Jmax is maximum value of angular momentum for a coupled-channels sets and Nenergy is the number of energies for which the calculation is performed (incident neutron's energies). External form factors (fort.4) are calculated from r=0 to r=rmatch with a total number of points Ngrid (Ngrid > 1). If pythonFlag = 1 then graphs for elastic, absorption and total cross section will be generated using Python at the end of the run (matplotlib library and the bash script runall.sh are required). Set pythonFlag to any other integer to do not generate any graph (default option).

• &Energies namelist

elab(1:Nenergy) = elab1, elab2,...

elab is an array with incident neutron's energies in MeV.

• &Potential namelist

v0a, v0b, lambdhf, cviso, vspo, lambdso, ccoul, av, bv, w0, bs, wspo, bso, ea, alphav, cs, cwiso, adv, rhfa, rhfb, ahfa, ahfb, rv, ava, avb, rsa, rsb, as, rso, aso, rc, ac

All parameters in & Potential are dispersive optical-model parameters given in Table I. Parameters that depend on the mass number A are characterised by two components (e.g. v0 = v0a + v0b(A - adv)).

Calculations for 238 U and 239 Pu using level schemes presented in Tables IV and VI of [1] are presented in Figures 2 and 3 comparing FRESCO and OPTMAN results².

²In order to compare results from both programs, OPTMAN's results are for the case of MEAPP=1 [i.e., no potential dependency on level energy losses], so small differences for low energies are expected for MEAPP=0. Besides, results presented in Figures 2 and 3 were obtained using a different version of OPTMAN (OPTMAN v.16) than the used in [1] (OPTMAN v.15) because the last one had some bugs that caused an incorrect coupling between G.S band and octupole and non-axial bands. Because of this, a new parameters adjustment is required.

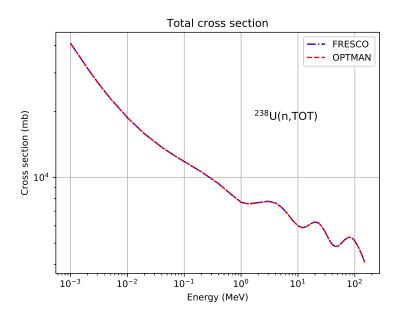


Figure 2: Total cross section for $n+^{238}U$ using parameters from Tables III and I calculated with FRESCO and OPTMAN.

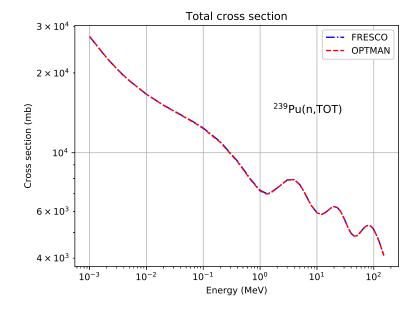


Figure 3: Total cross section for $n+^{239}$ Pu using parameters from Tables IV and I calculated with FRESCO and OPTMAN.

References

[1] E. Sh. Soukhovitskiï, R. Capote, J. M. Quesada, S. Chiba, and D. S. Martyanov. "Nucleon scattering on actinides using a dispersive optical model with extended couplings". *Phys. Rev. C* 94 (6 2016), 064605. DOI: 10.1103/PhysRevC.94.064605.

- [2] E.Sh. Soukhovitskiï, G.B. Morogovskiï, R. Capote Noy, S. Chiba, and J. M Quesada. *Program OPTMAN Version 14 (2013), User's Guide Coupled-Channel Optical Model Code Based on Rigid- or Soft-Rotator Models, Compatible with the Empire Nuclear Data Evaluation System.* International Atomic Energy Agency (IAEA), 2013.
- [3] Ian J. Thompson. FRESCO, coupled reaction channels calculations. http://www.fresco.org.uk/.