EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Crystal field excitations in the Kondo insulator CeRu4Sn6	**Experiment number**: HC3005
Beamline: ID32	**Date of experiment**: from: 07.04.2017 to: 11.04.2017	**Date of report**: 16.03.2020
Shifts: 12	**Local contact(s)**: Nick Brokks	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

We took RIXS data of the Kondo inuslator $CeRu_4Sn_6$, plus some test data of SmB_6. Both data sets resulted in a publication.

Ref. 1)
Amorese, K. Kummer. N.B. Brooks, O. Stockter, D. T Adroja, A. M. Strydom, A. Sidorenko, H. Winkler, D. A. Zocco, A. Prokoviev, S. Paschen, M- W. Haverokrt, L.H. Tjeng, A. Severing
Phys. Rev. B **98**, 08116(R) (2018)

Ref. 2)
Amroese, O. Stocktert, K. Kummer, N.B. Brookes, D.-J. Kim, Z. Gisk, M-H. Haverokrt, P- Thal,meier, L.H. Tjeng, A. Severing
Phys. Rev. B **100**, 241107(R) (2019)

RIXS data and simulation of CeRu4Sn6, taken from Ref. 1)

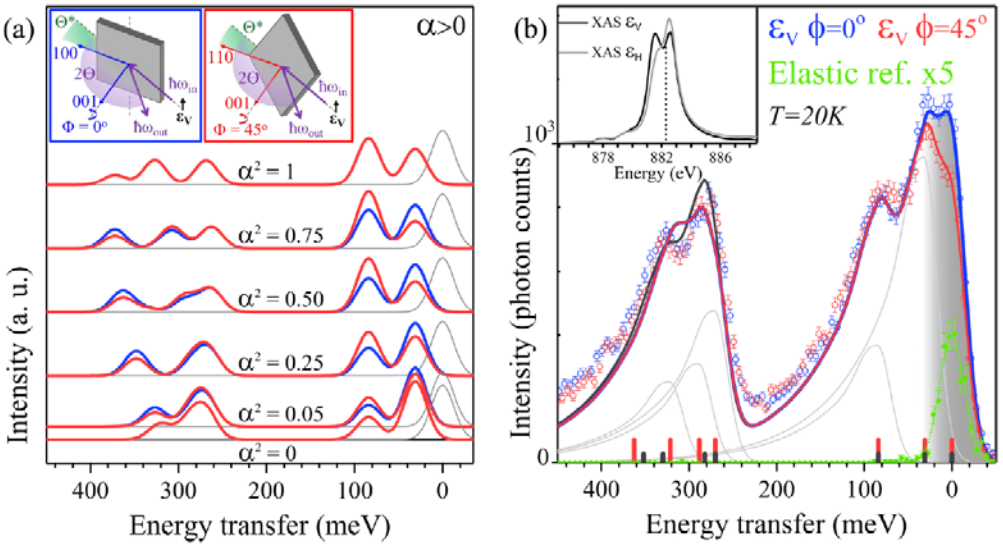

FIG. 2. (a) Calculated RIXS spectra at $T = 20$ K as a function of the mixing parameter α^2 for $\alpha > 0$, with vertical polarization, for the two geometries $\phi = 0°$ and $\phi = 45°$ (see inset). (b) Experimental RIXS data (circles) with statistical error bars with the same scattering geometry as in the calculated RIXS spectra on the right. The red and blue lines (black line) show the full multiplet simulation with three (four) crystal-field parameters (the fourth being $\tilde{A}_6^0 = 200$ meV) using an asymmetric line shape for the CEF excitations [see red (black) ticks and gray lines]. The respective CEF parameters are given in Table S1 in the Supplemental Material [17]. Note, the highest transition at ≈ 360 meV corresponds to a $\Delta J_z = \pm 3$ transition and therefore has no spectral weight. The gray shading indicates the elastic region (see text). The elastic reference (green) shows the Gaussian response function of the beamline. XAS M_5 edge and incident energy (dotted line) shown in the inset.

RIXS data and simulation of SmB6, taken from Ref. 2)

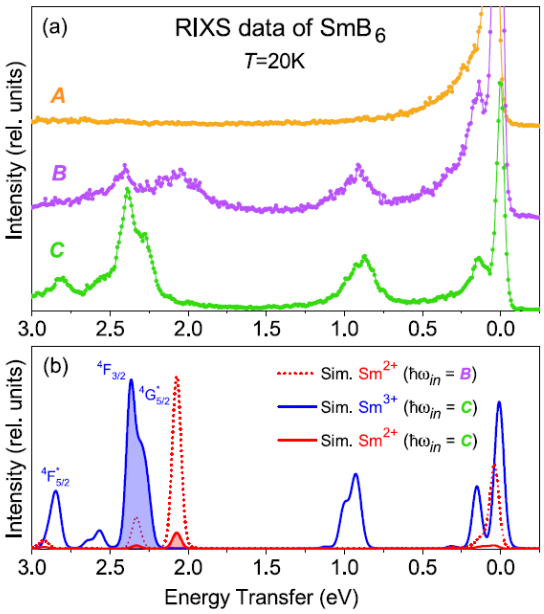

FIG. 3. (a) RIXS data of SmB_6 for incident energies $\hbar\omega_{in}$ $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$ as defined in Fig. 1(a) (see text for the scattering geometry). (b) RIXS simulation for Sm^{3+} (solid blue line) with $\hbar\omega_{in} = \boldsymbol{C}$ and for Sm^{2+} with $\hbar\omega_{in} = \boldsymbol{B}$ (dashed red line) and $\boldsymbol{C}$ (solid red line) (simulation, see text).

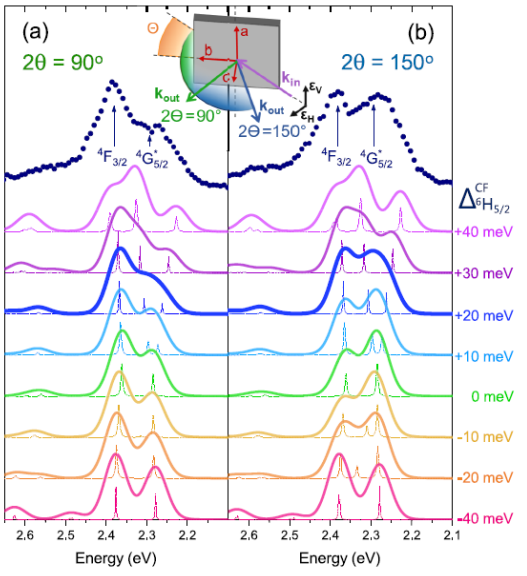

FIG. 4. Data and simulations of RIXS spectra with $\hbar\omega_{in} = \boldsymbol{C}$ (dark-blue dots) with horizontal polarization (π) for two scattering angles $2\Theta = 90°$ (a) and $2\Theta = 150°$ (b) (see inset). Different colors are simulations with different crystal-field splittings; thin dotted lines with an unrealistic narrow resolution and solid thick lines taking into account the resolution function. The numbers refer to the respective Hund's rule ground-state splitting $\Delta^{CF}_{^6H_{5/2}}$, positive numbers refer to a Γ_8, and negative numbers to a Γ_7 ground state. Note, $\Delta^{CF}_{^4G^*_{5/2}} \approx 2.2\Delta^{CF}_{^6H_{5/2}}$.