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## Supplementary Materials for

### Orbital symmetries of charge density wave order in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

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Published 6 November 2020, *Sci. Adv.* **6**, eaay0345 (2020)  
DOI: 10.1126/sciadv.aay0345

#### **This PDF file includes:**

Supplementary Text  
Figs. S1 to S3

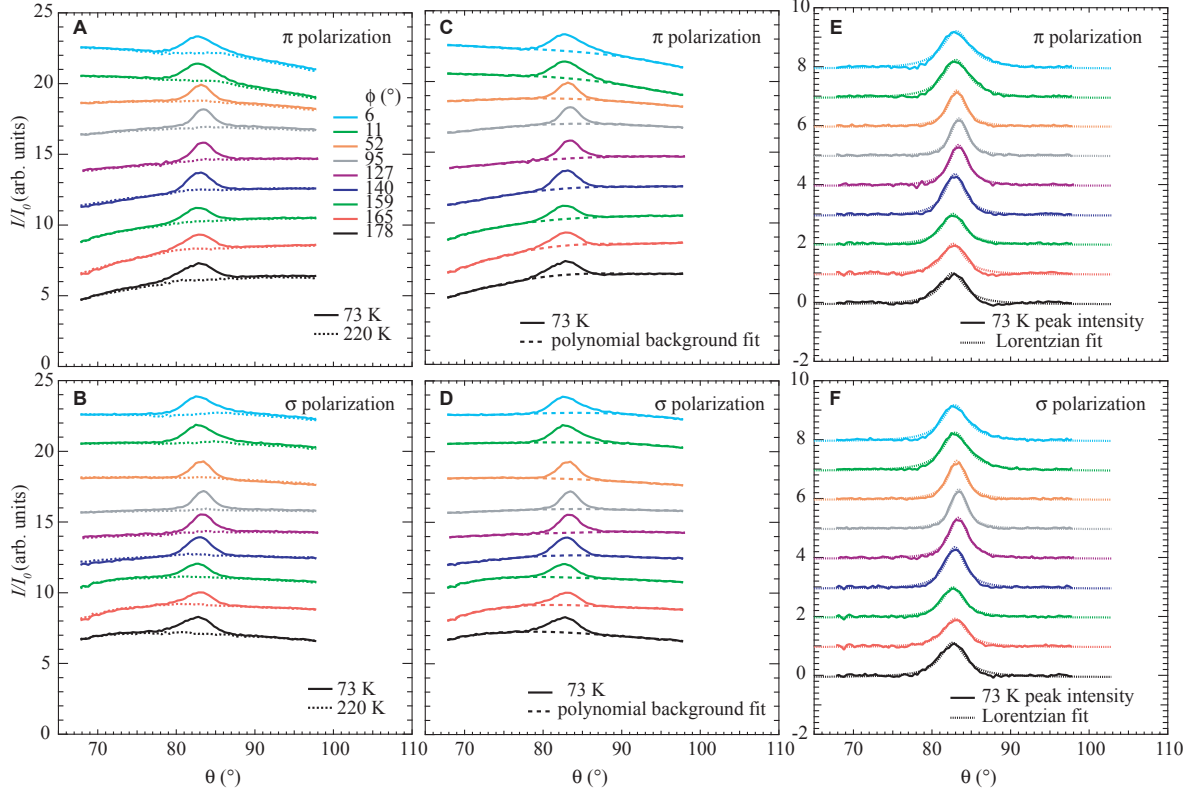


Figure S1: **Example of the measurement and extraction of peak intensities.**  $\theta$  scans at various  $\phi$  values through the CDW peak in the  $\text{YBa}_2\text{Cu}_3\text{O}_{6.75}$  sample at  $(0.31 \ 0 \ 1.48)$  for A)  $\pi$  and B)  $\sigma$  incident photon polarization. For clarity, data at different  $\phi$  values are offset in the y-axis increments of 2 (Measurements at  $\phi = 178^\circ$  are not offset. C) and D) fits to the fluorescent background of the data at 73 K using a 5th order polynomial. E) and F) The peak intensity for various  $\phi$  values after subtraction of a polynomial background along with Lorentzian fits to the peaks.

## Assessment of the quality of fits and range of parameters that agree with the measurements.

For the  $(0 \ 0.31 \ 0 \ L)$  peak, the measured ratio  $I_\sigma/I_\pi$  was fit to a model with;

$$\hat{F}(\vec{Q}, \hbar\omega) \sim \begin{bmatrix} F_{aa} & 0 & 0 \\ 0 & F_{bb} & 0 \\ 0 & 0 & F_{cc} \end{bmatrix} \quad (\text{S1})$$

The best fit to the data was achieved with  $F_{bb}/F_{aa} = 0.998 \pm 0.020$  and  $F_{cc}/F_{aa} = 0.049 \pm 0.041$ . The standard deviation, however, does not adequately represent the uncertainty

in the parameters. This is because  $F_{bb}/F_{aa}$  and  $F_{cc}/F_{aa}$  are not completely independent fitting parameters. Rather, variation in one parameter can be offset with variation in the other in order to improve the fit. A better assessment of the range of parameters that provide good agreement with the data can be achieved by examining the dependence on fit parameters of the reduced  $\chi^2$  statistic, as shown in Figure S2 A). Good fits to the data are found in an elliptical range of parameters around the best fit value, where  $F_{aa} \simeq F_{bb} \ll F_{cc}$  with a level of agreement comparable to the scatter in the data are roughly found for range of parameters inside the  $\chi_0^2 = 5$  contour. A comparison between the measurement and model calculations with selected parameters (shown by the solid circles in fig. S2 A) that have different values of  $\chi_0^2$  is shown in Fig. S2 B and C.

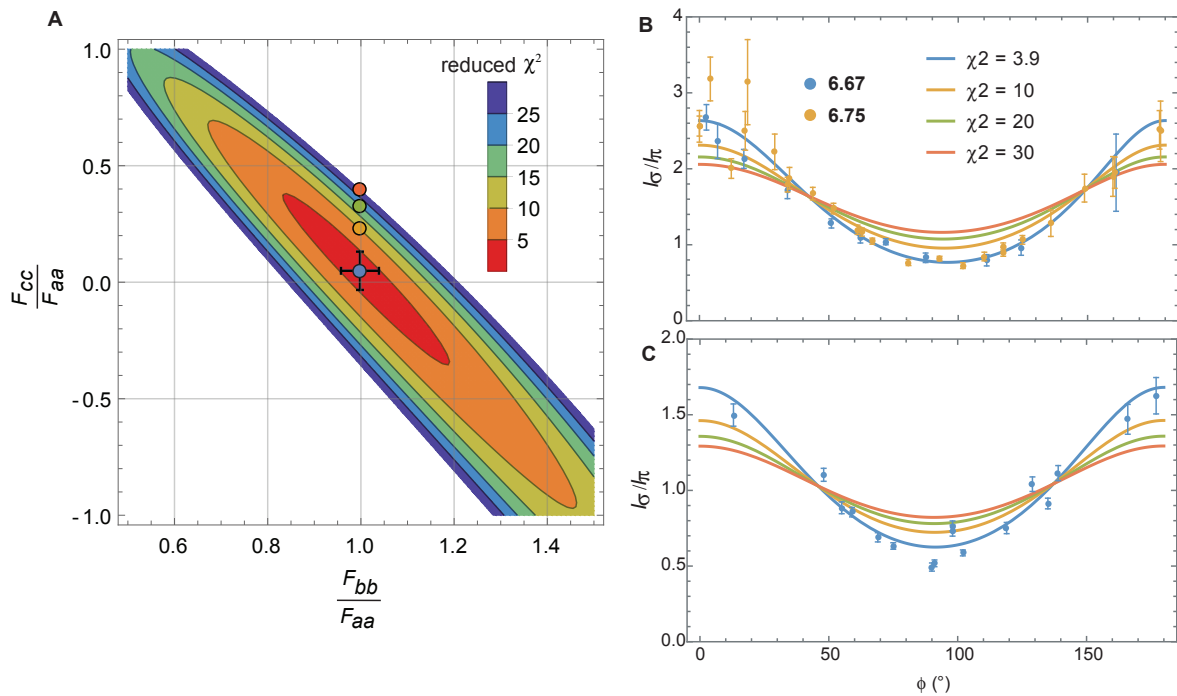


Figure S2: **Assessment of the fit quality for the (0 0.31 L) peak.** **A** A map of the reduced  $\chi^2$  from fits to data at both (0.31 0 1.48) and (0.31 0 1.32) vs.  $F_{cc}/F_{aa}$ , and  $F_{bb}/F_{aa}$ . The blue circle represents the best fit value. **B** and **C** Examples of  $I_\sigma/I_\pi$  vs.  $\phi$  calculated for different reduced  $\chi^2$  values. The curves in **B** and **C** were calculated using parameters given by the point in **A** of the same colour as the curve.

For the (0.31 0 0  $L$ ) peak, the measured ratio  $I_\sigma/I_\pi$  was fit to a more a general model with off-diagonal terms  $F_{ac} = F_{ca}$ , indicative of broken  $bc$  and  $ab$  plane mirror symmetries:

$$\hat{F}(\vec{Q}, \hbar\omega) \sim \begin{bmatrix} F_{aa} & 0 & F_{ac} \\ 0 & F_{bb} & 0 \\ F_{ac} & 0 & F_{cc} \end{bmatrix} \quad (\text{S2})$$

The best fit to the data on the 6.75 sample gave  $F_{ac}/F_{bb} = -0.073$ ,  $F_{cc}/F_{bb} = 0.183$ , and  $F_{aa}/F_{bb} = 1.172$ . In figure S3 we present the variation of reduced  $\chi^2$  statistic with model parameters. As shown, a range of model parameters provide good agreement with the data with fits with reduced  $\chi^2 < 10$  all provide similar quality, comparable to the scattering in the data. This region with  $\chi^2 < 10$  includes models with  $F_{ac} = 0$  and  $F_{aa}/F_{bb}$  significantly greater than 1, models that retain  $ab$  and  $bc$  plane mirror symmetries but has significant in-plane asymmetry. However, it also includes a model with  $F_{aa} \simeq F_{bb}$  and  $F_{ac} = -0.22$ , a model that breaks  $ab$  and  $bc$  plane mirror symmetries but retains approximate in-plane asymmetry of the diagonal elements, similar to the (0 0.31  $L$ ) peak.

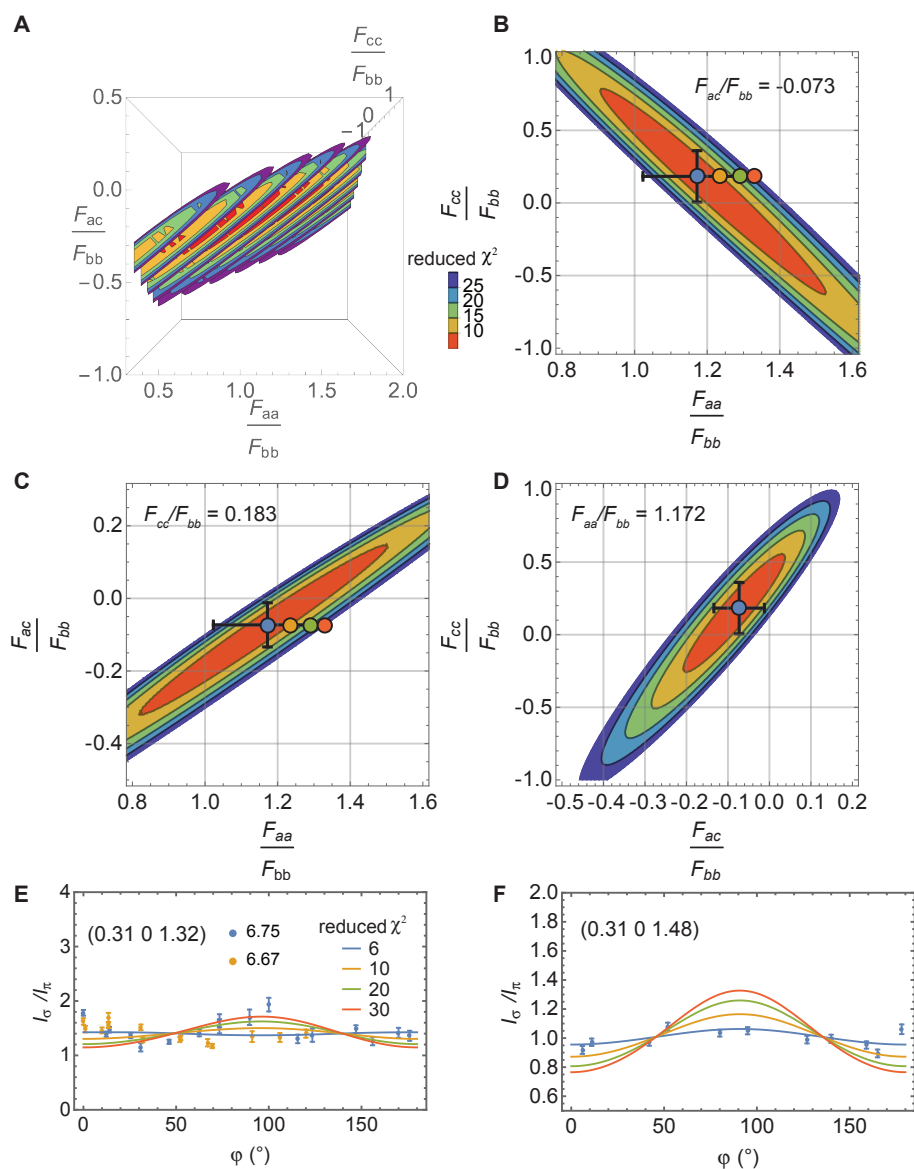


Figure S3: **Assessment of the fit quality for the (0.31 0 L) peak.** **A** A map of the reduced  $\chi^2$  from fits to the 6.75 data at both (0.31 0 1.48) and (0.31 0 1.32) vs.  $F_{ac}/F_{bb}$ ,  $F_{cc}/F_{bb}$ , and  $F_{aa}/F_{bb}$ . Contours of constant  $\chi^2$  are shown as slices through the 3D parameter space. **B**, **C** and **D** 2D slices of reduced- $\chi^2$  through the best fit value  $F_{ac}/F_{bb} = -0.073$ ,  $F_{cc}/F_{bb} = 0.183$ , and  $F_{aa}/F_{bb} = 1.172$ . The blue circle represents the best fit value and the error bars denote the 95% confidence interval of the fit. **E** and **F** Examples of  $I_\sigma/I_\pi$  vs.  $\phi$  calculated for different reduced  $\chi^2$  values. The curves in **E** and **F** were calculated using parameters given by the point in **C** and **D** of the same colour as the curve.