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Supporting information for article:

K-space algorithmic reconstruction (KAREN): a robust statistical methodology to separate Bragg and diffuse scattering

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S1. A movie of the 3-D reciprocal space neutron diffraction data for CBr_4 is given as 3-D-diffraction-CBr4.mp4

Movies of the 3-D Δ-PDF of CBr_4 are given as:

KAREN-negative-correlations.mp4

KAREN-positive-correlations.mp4

fixed-punch-only-negative-correlations.mp4

fixed-punch-only-positive-correlations.mp4

variable-punch-only-negative-correlations.mp4

variable-punch-only-positive-correlations.mp4

punch-HC-fill-8-pixels_negative-correlations.mp4

punch-HC-fill-8-pixels_positive-correlations.mp4

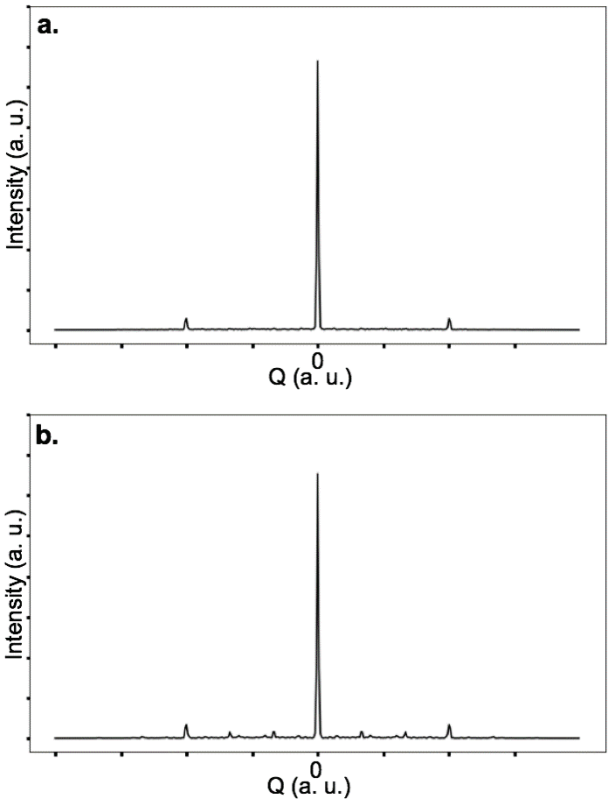

Figure S1 Full intensity diffraction pattern corresponding to the expanded view given in Fig. 2g and h for the images with a. filled pixels randomly distributed on 10.5 % of the odd values of a square spiral, and b. for an Ulum spiral with an equivalent number of pixels.

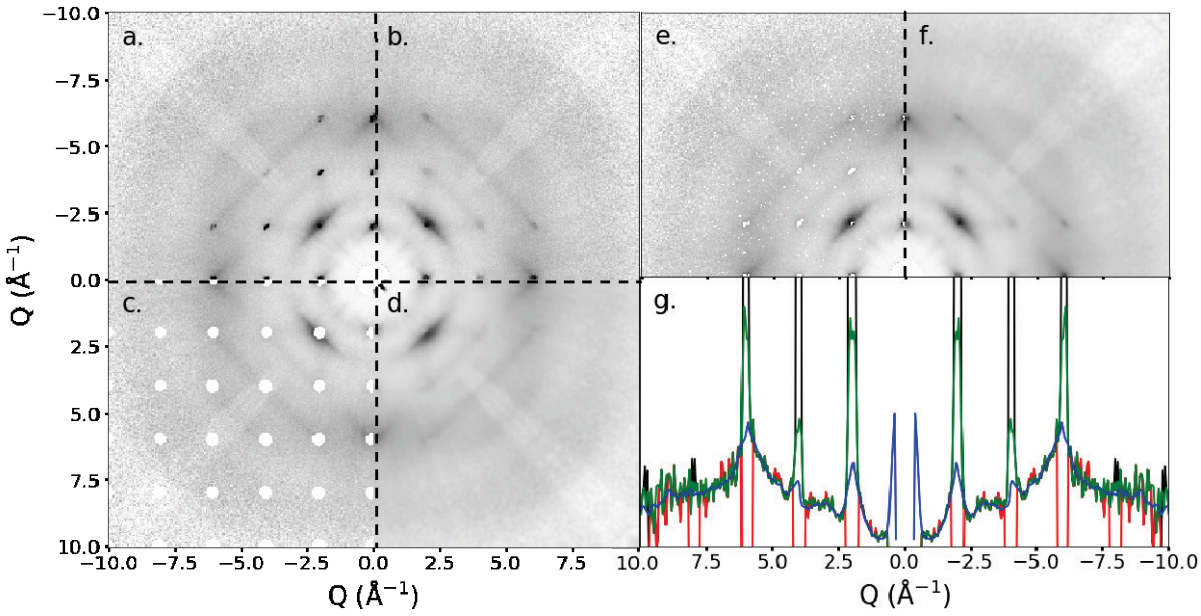

Figure S2 (200)* cross section of the diffuse scattering of CBr_4. **a.** Original data. **b.** KAREN reconstructed diffuse scattering. **c.** Bragg scattering removed with a 8-pixel fixed-punch function, **d.** 8-pixel fixed punch and filled with Astropy Gaussian interpolation using the MANTID punch-and-fill method, **e.** Bragg scattering removed with variable punch based on outlier definition, **f.** variable punch filled with Astropy Gaussian interpolation, and **g.** 1-D plot along the [100]* vector with the total scattering represented as a black line, the Bragg scattering fixed punch data (red), the variable punch-and-filled with Gaussian interpolation (blue), and the KAREN reconstructed diffuse (green).

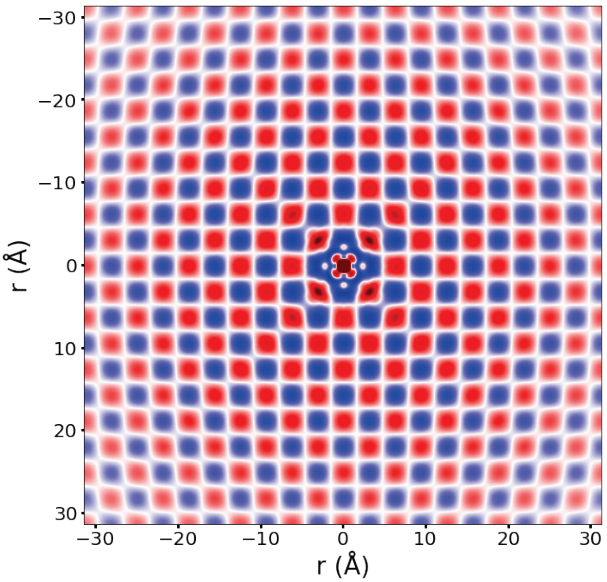

Figure S3 Checkerboard pattern of artifacts that results from a 6-pixel fixed punch with a $\sigma = 1$ Gaussian kernel using the punch-HC-fill method.

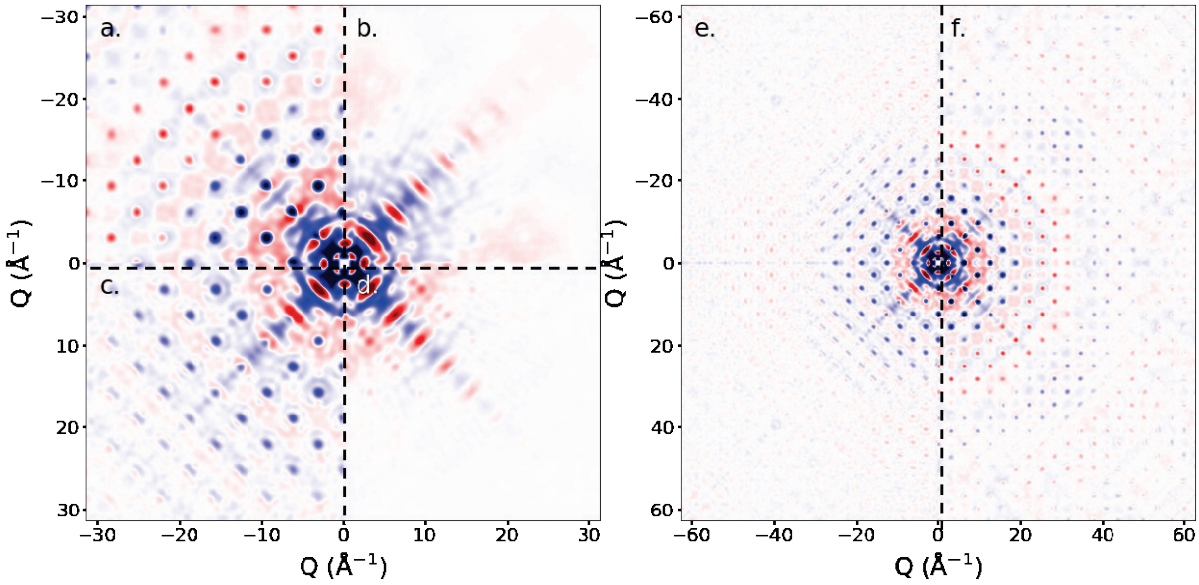

Figure S4 100 cross section of the Δ-PDF of plastic crystalline CBr_4 calculated to r = 30 Å from neutron scattering data after removal of the Bragg scattering and reconstruction of the diffuse scattering using: **a.** 8 pixel fixed punch-only, **b.** fixed punch-and-fill using the MANTID punch-and-fill implementation with whole pattern Astropy Gaussian convolution, **c.** variable punch-only and **d.** variable punch with whole pattern Astropy Gaussian convolution to fill methods, respectively. Δ-PDF calculated to r = 60 Å for **e.** variable punch-only and **f.** fixed punch-only methods. Intensity is plotted on a log scale, with positive correlations as red and negative correlations blue.