# On average structures of the disordered β-phase of Pigment Red 170: A single crystal X-ray diffraction study

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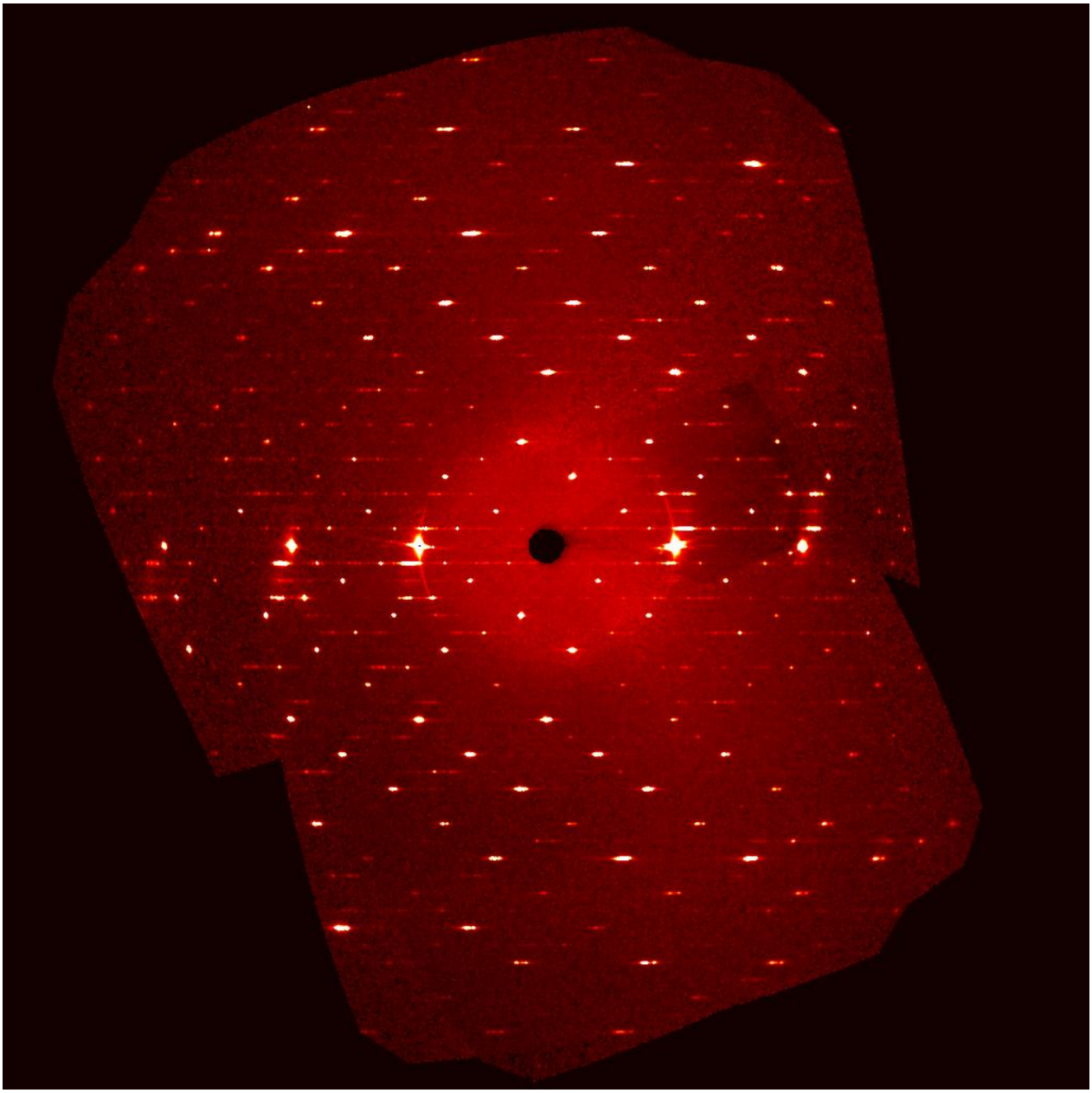
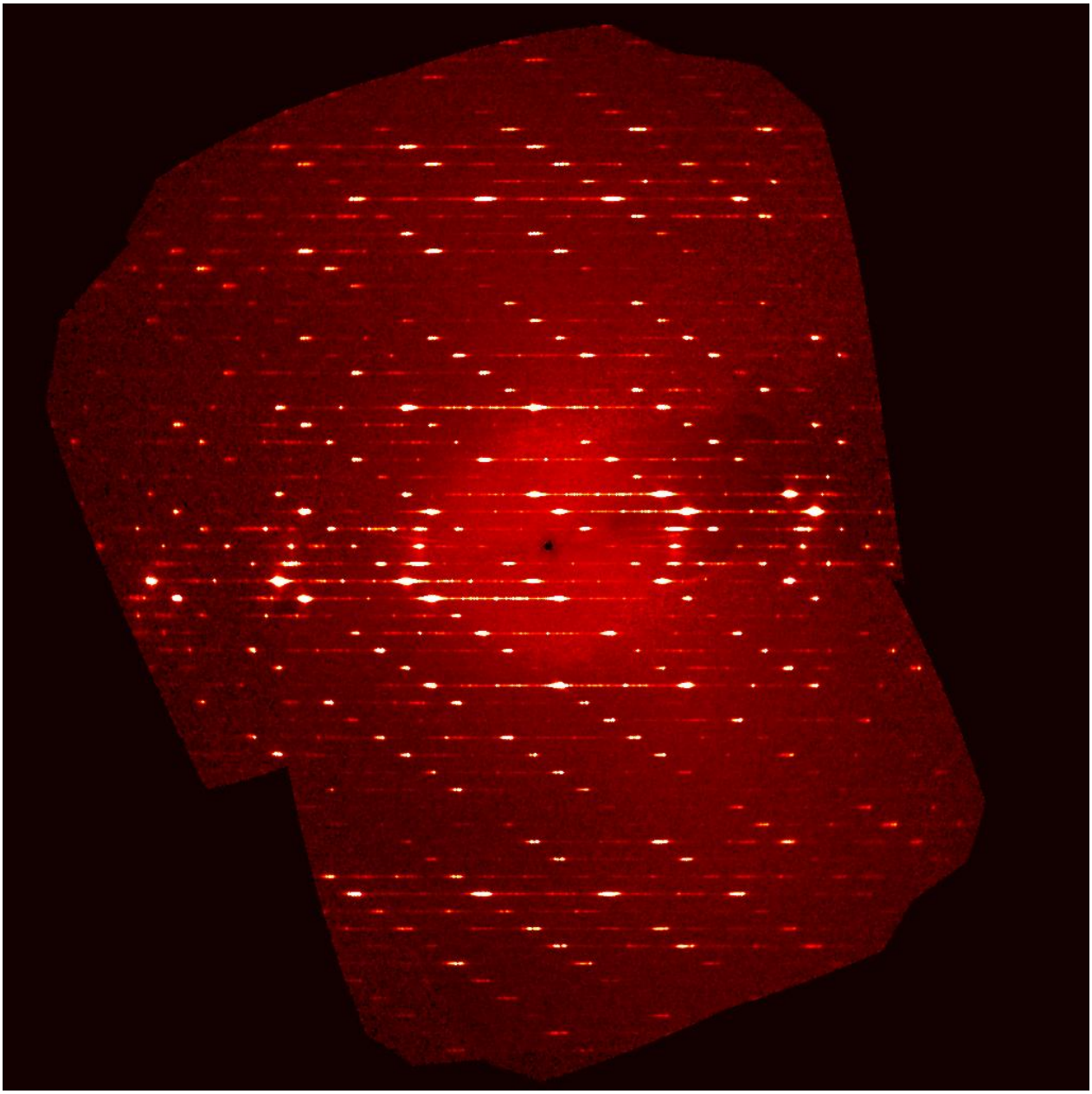
## SUPPLEMENTARY MATERIALS

Fig. S1. Reciprocal lattice layer reconstructions (*h*0*l* to *h*20*l*) for β-Pigment Red 170

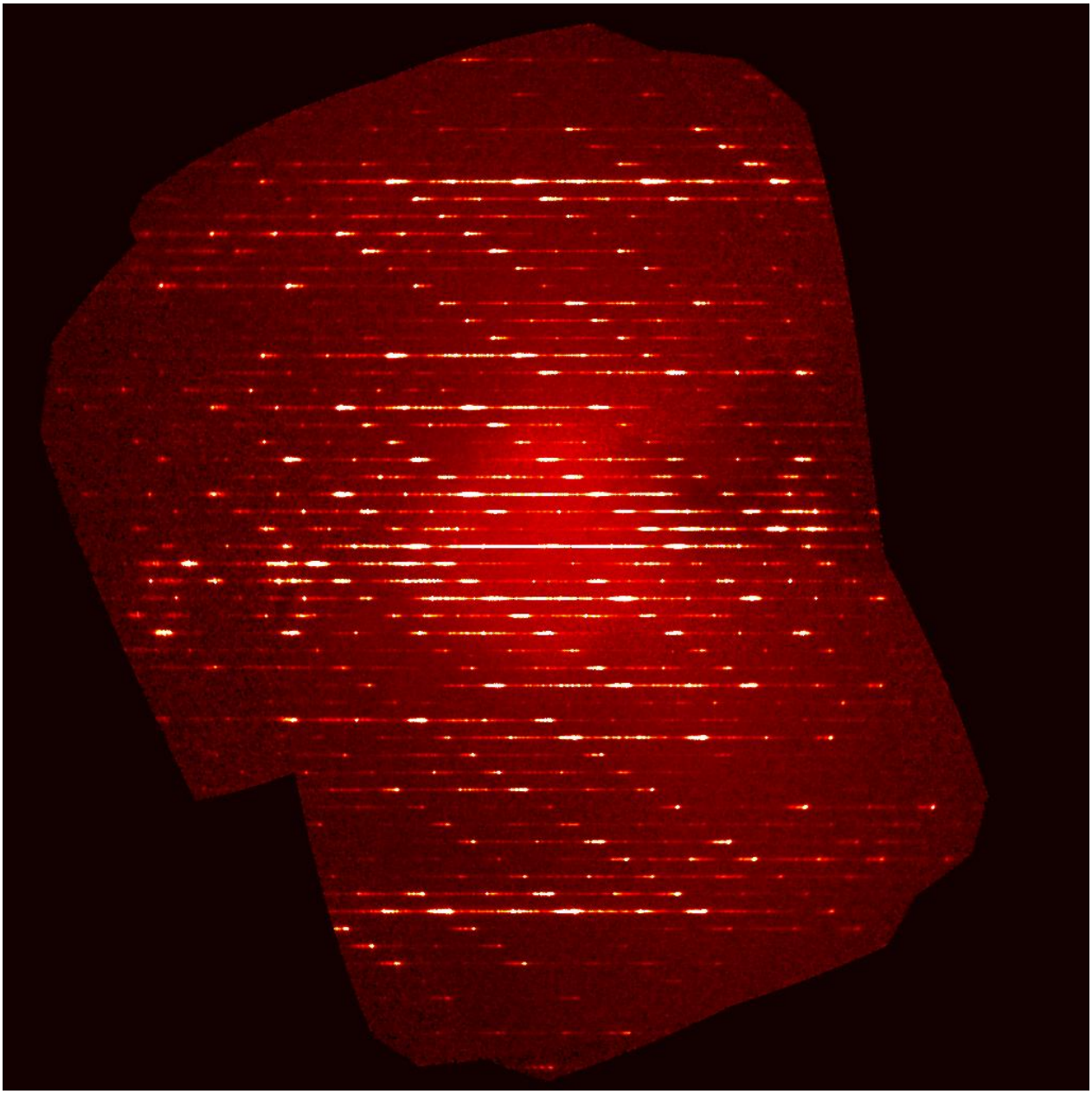
*h*0*l* layer:



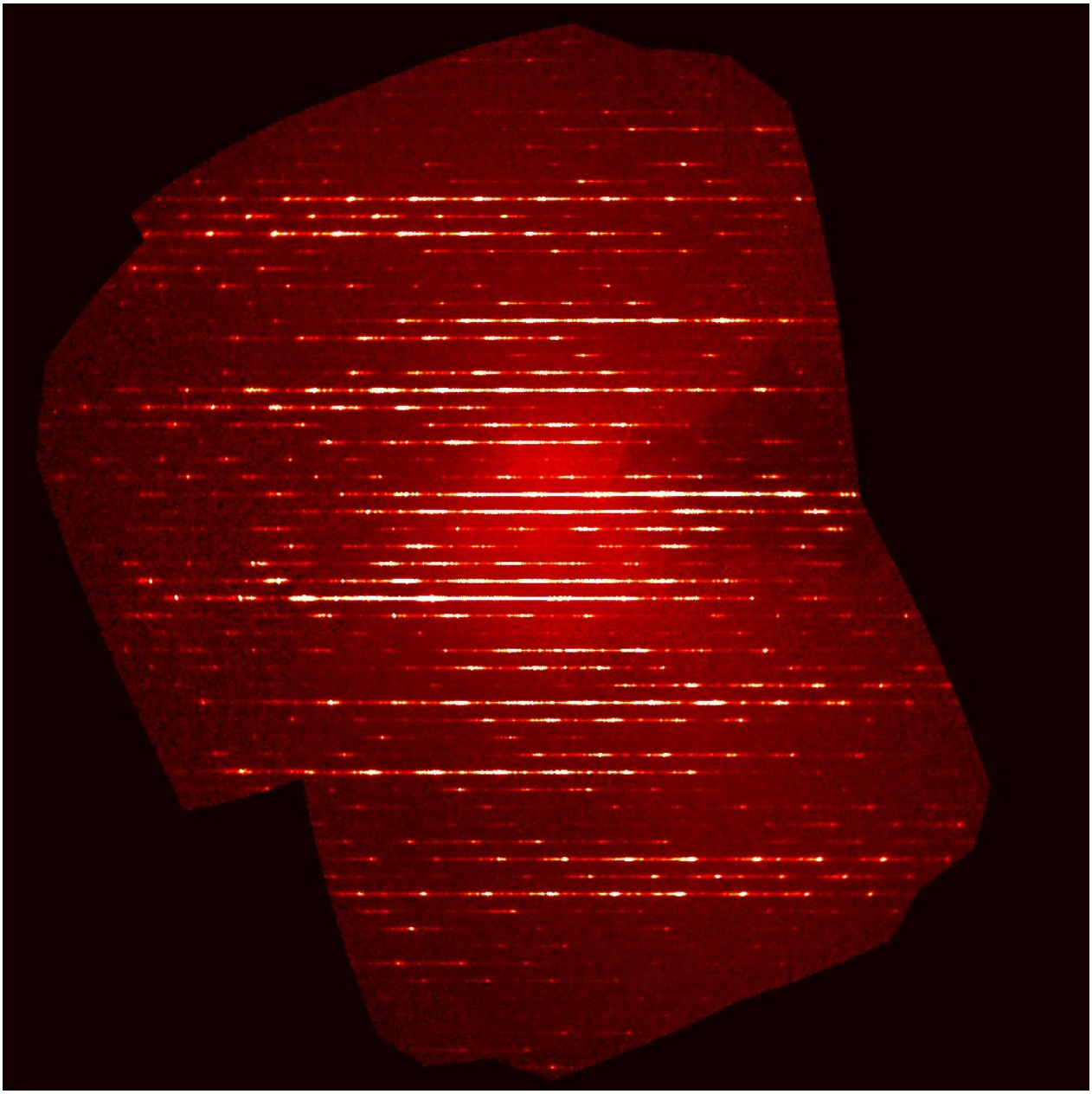
*h*1*l* layer:



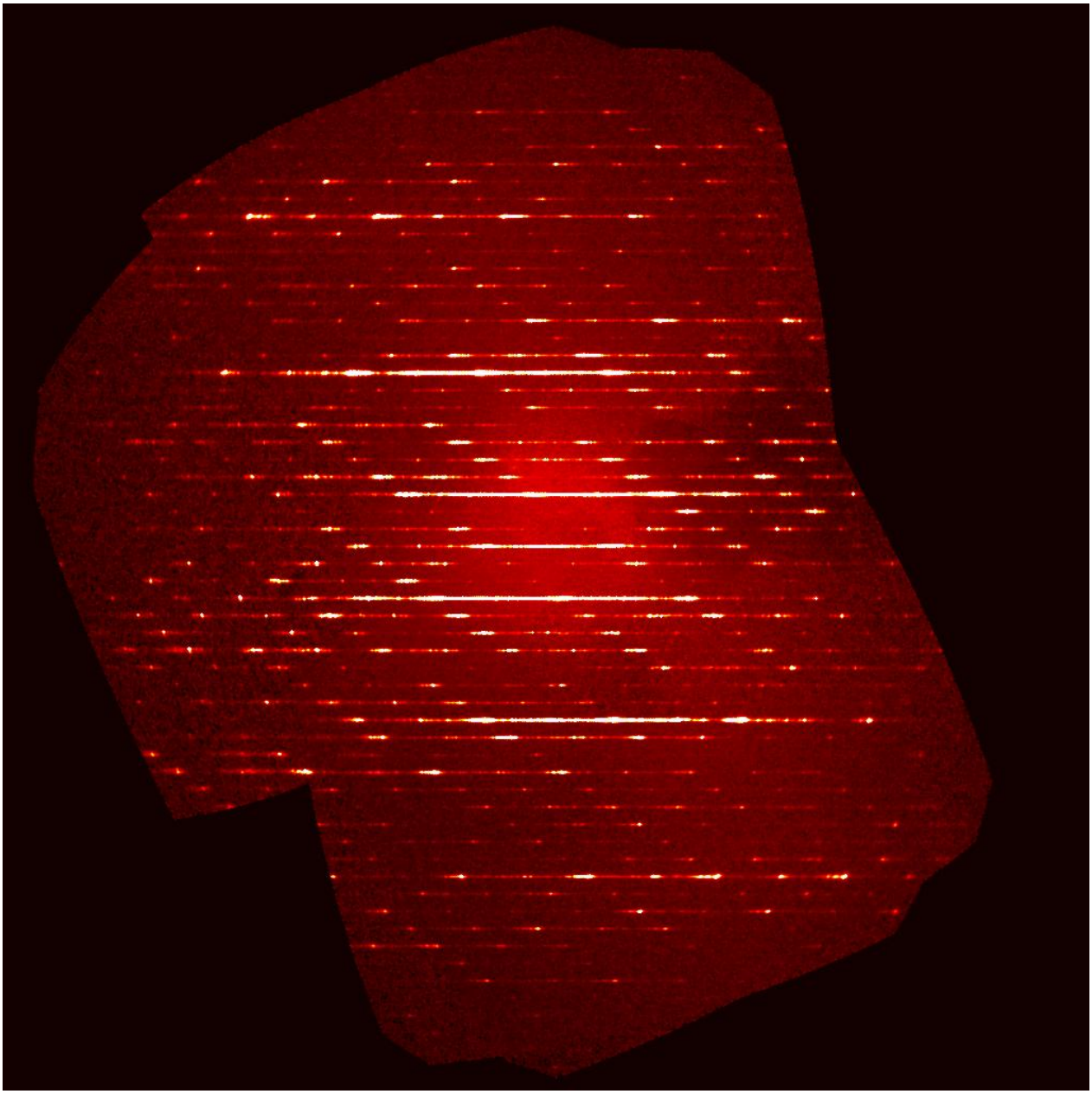
*h*2*l* layer:



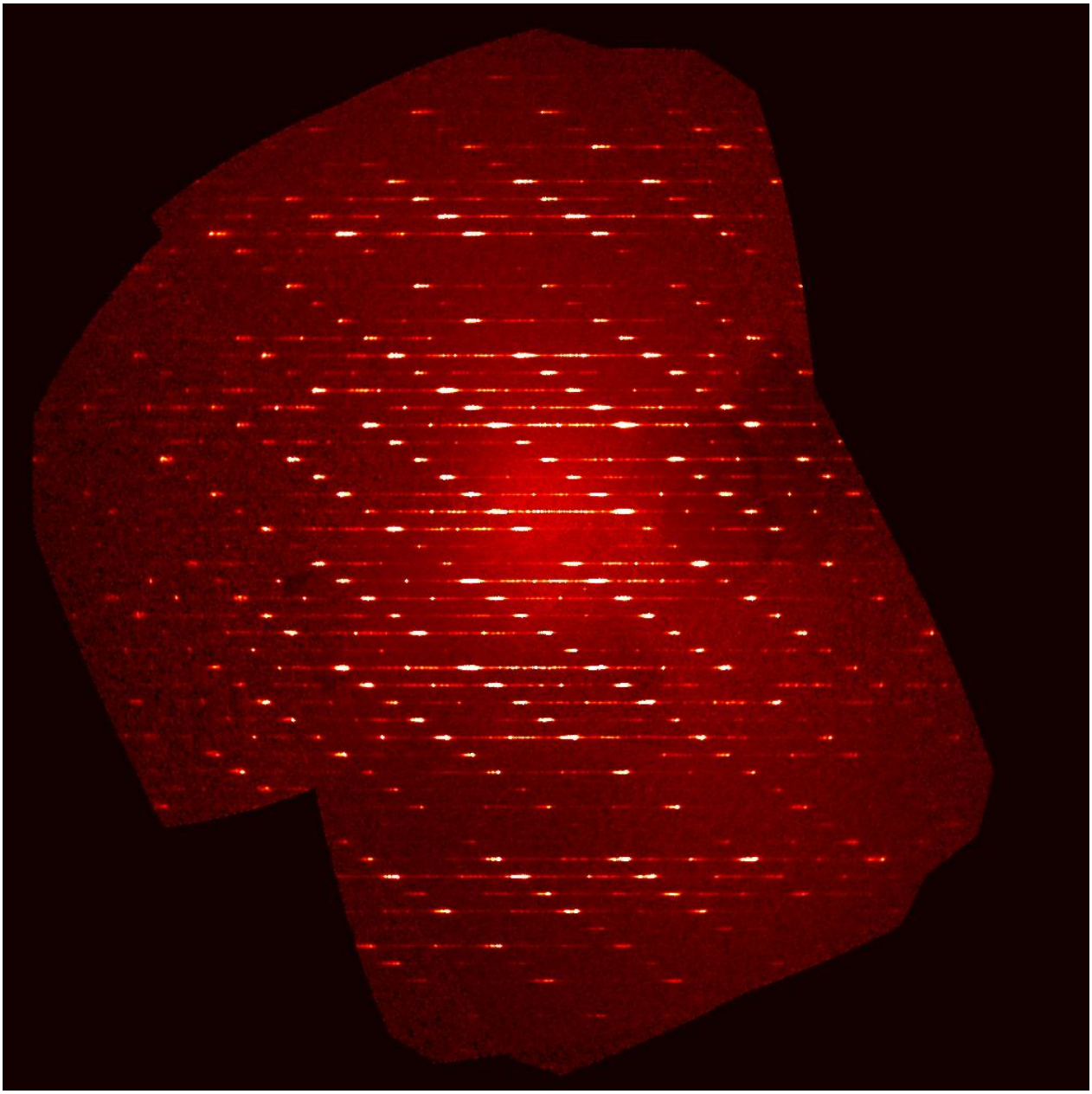
*h*3*l* layer:



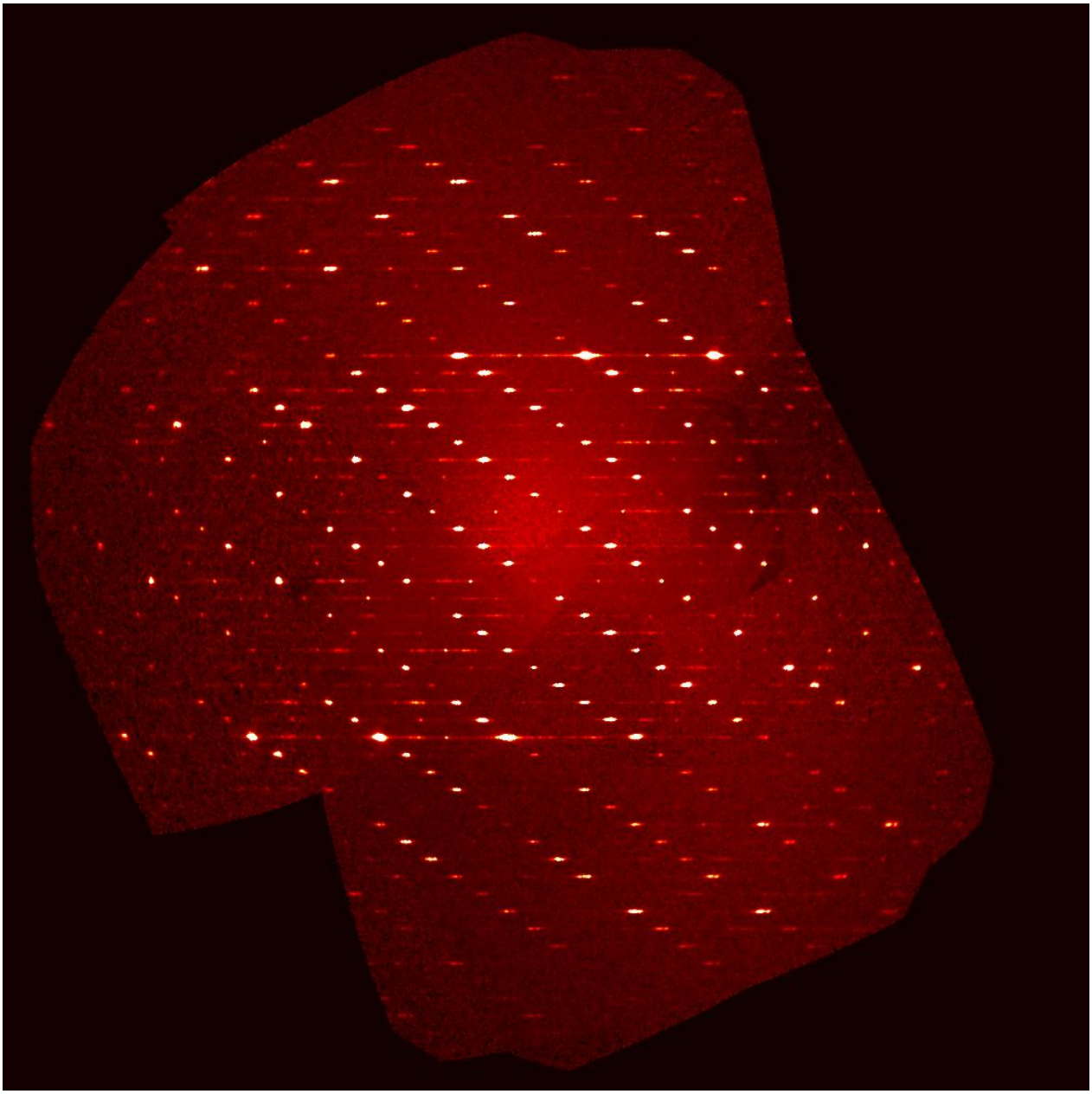
*h*4*l* layer:



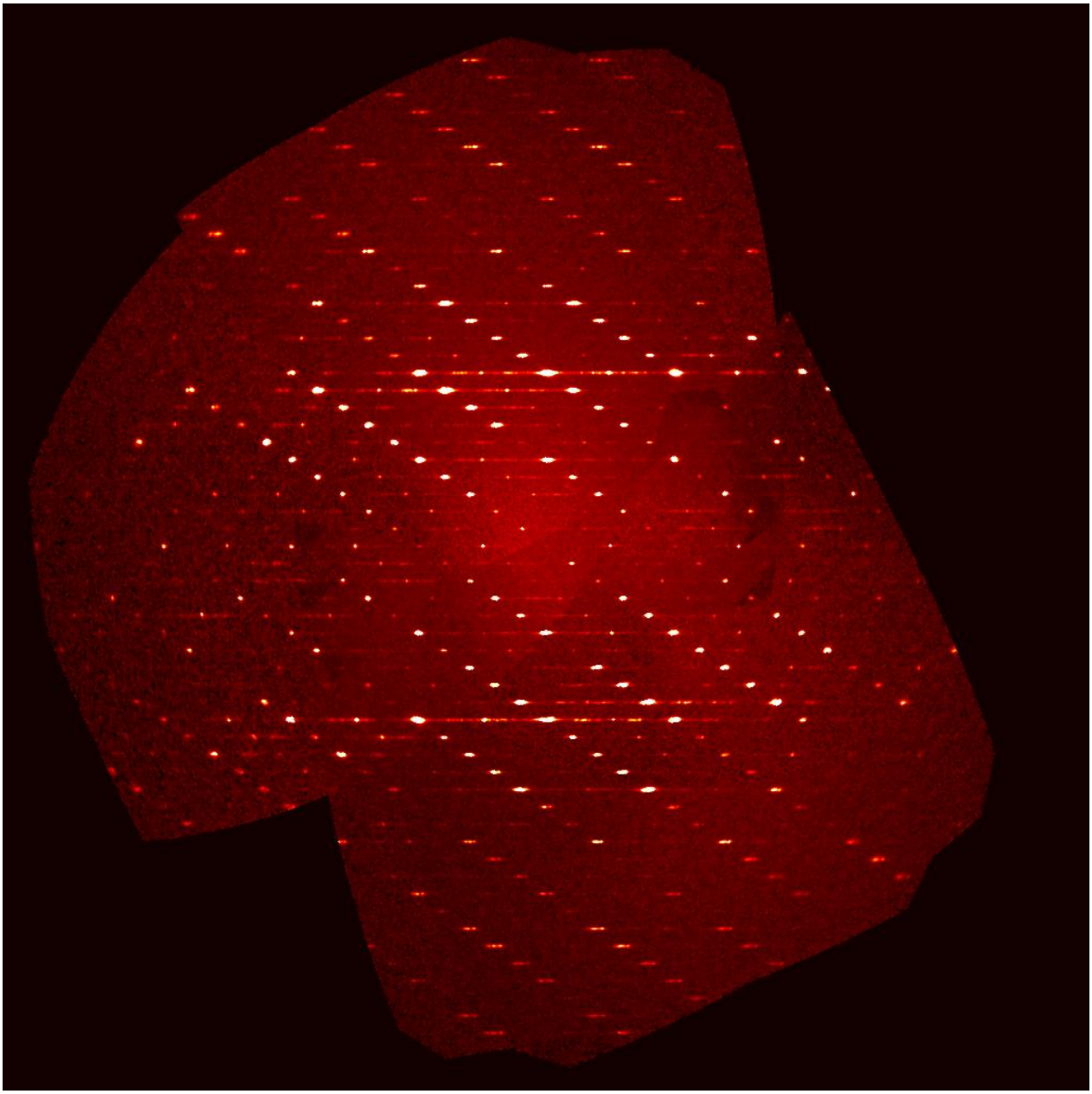
*h*5*l* layer:



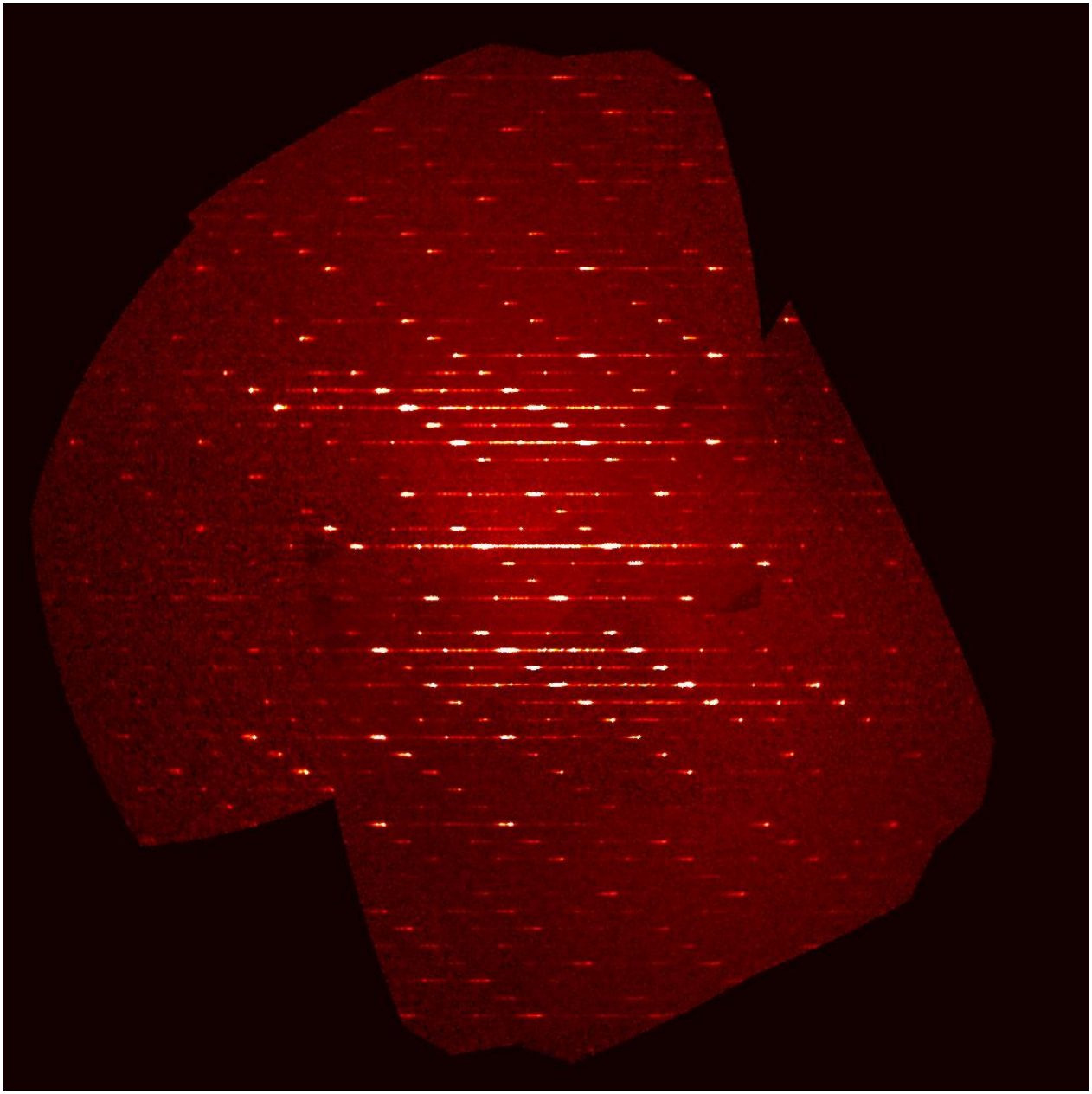
*h*6*l* layer:



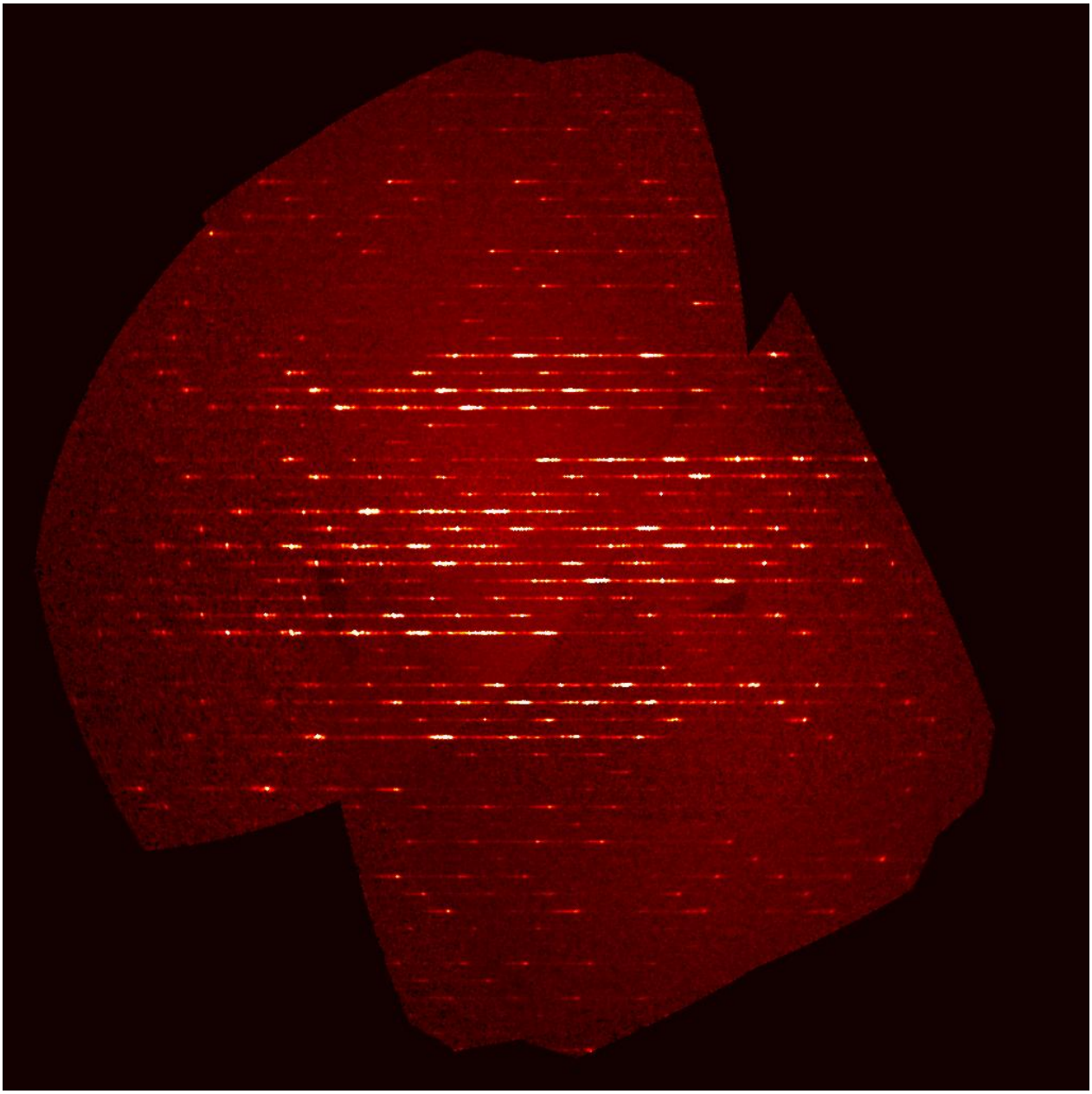
*h7l* layer:



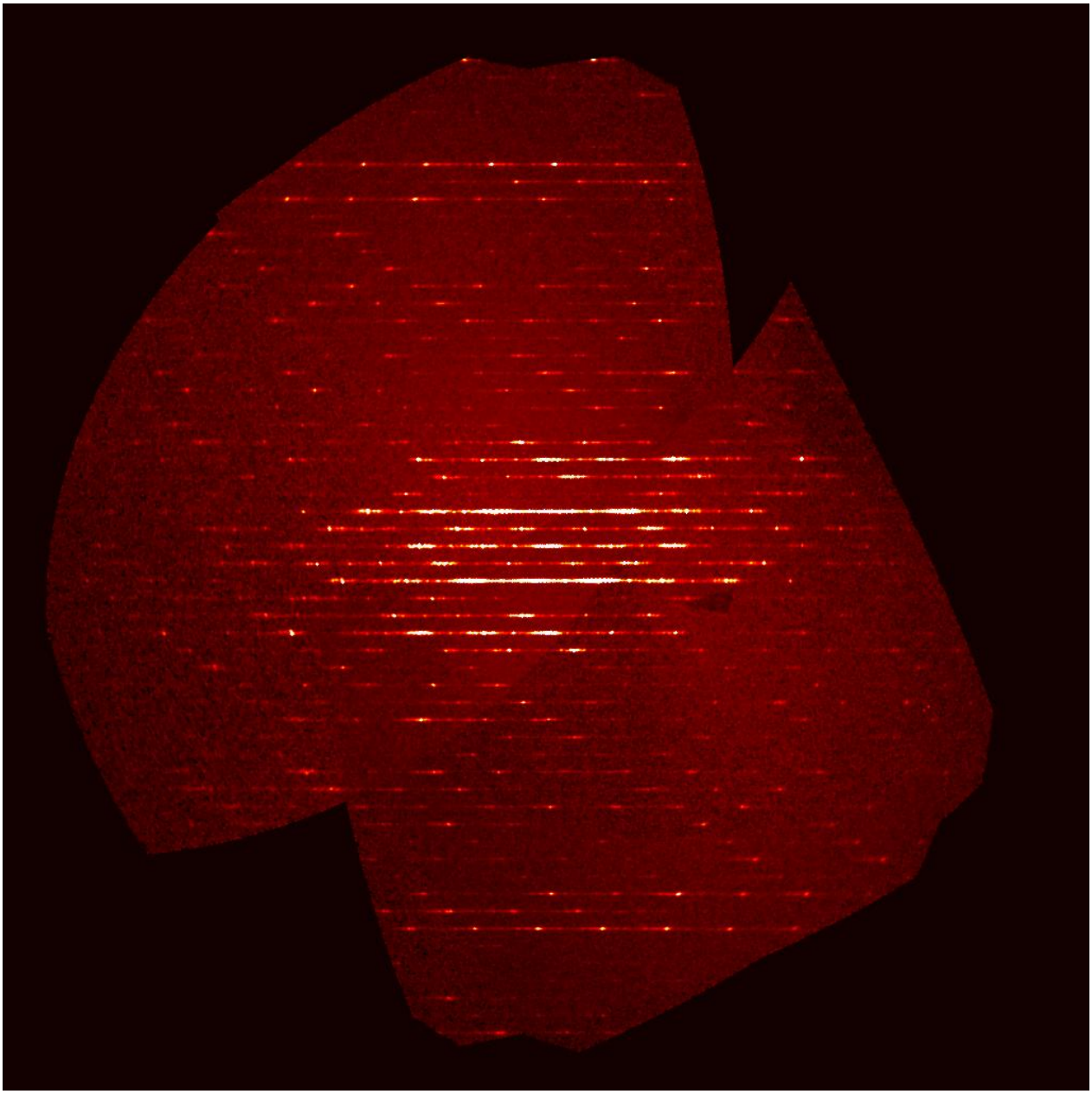
*h*8*l* layer:



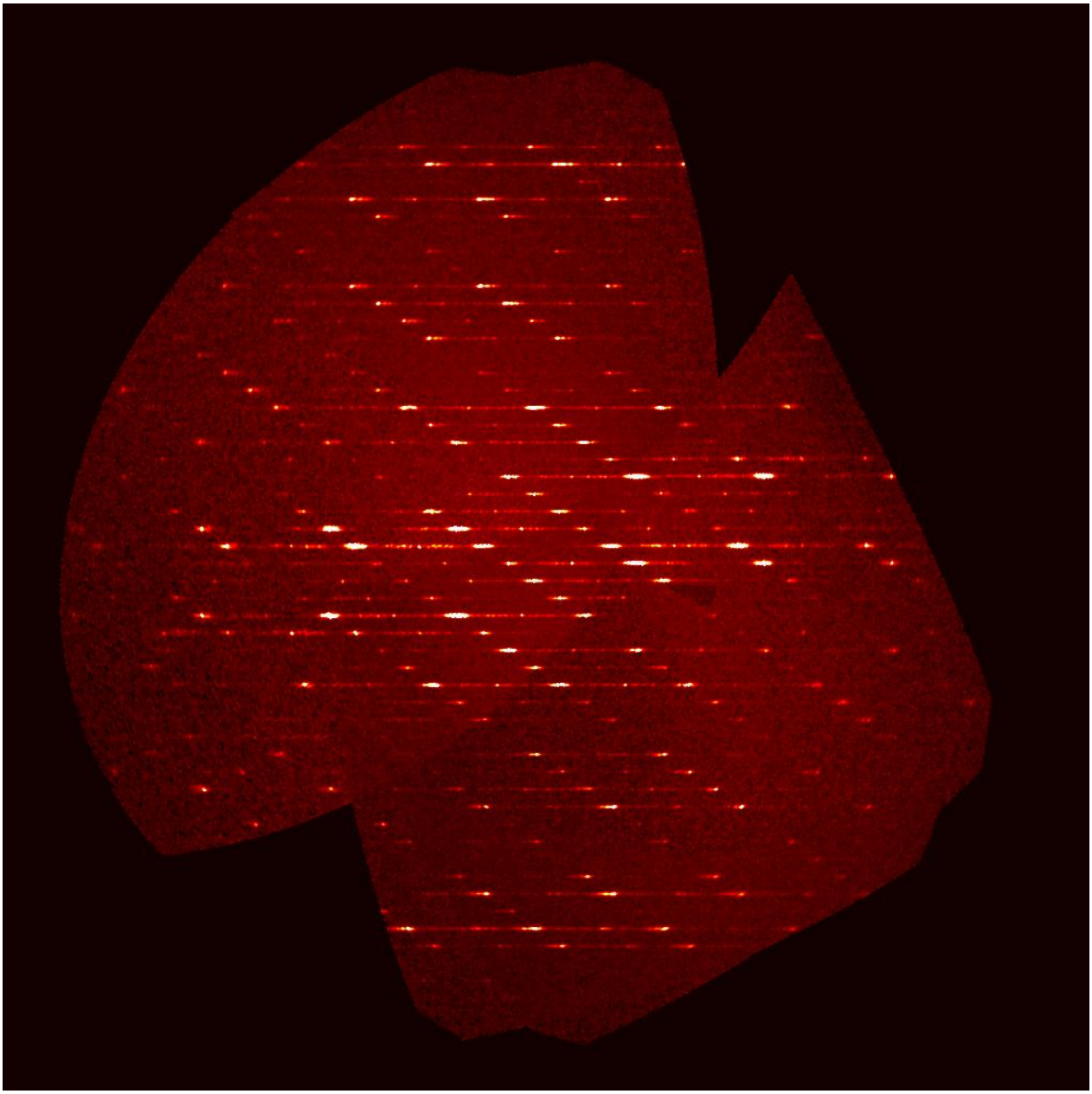
*h*9*l* layer:



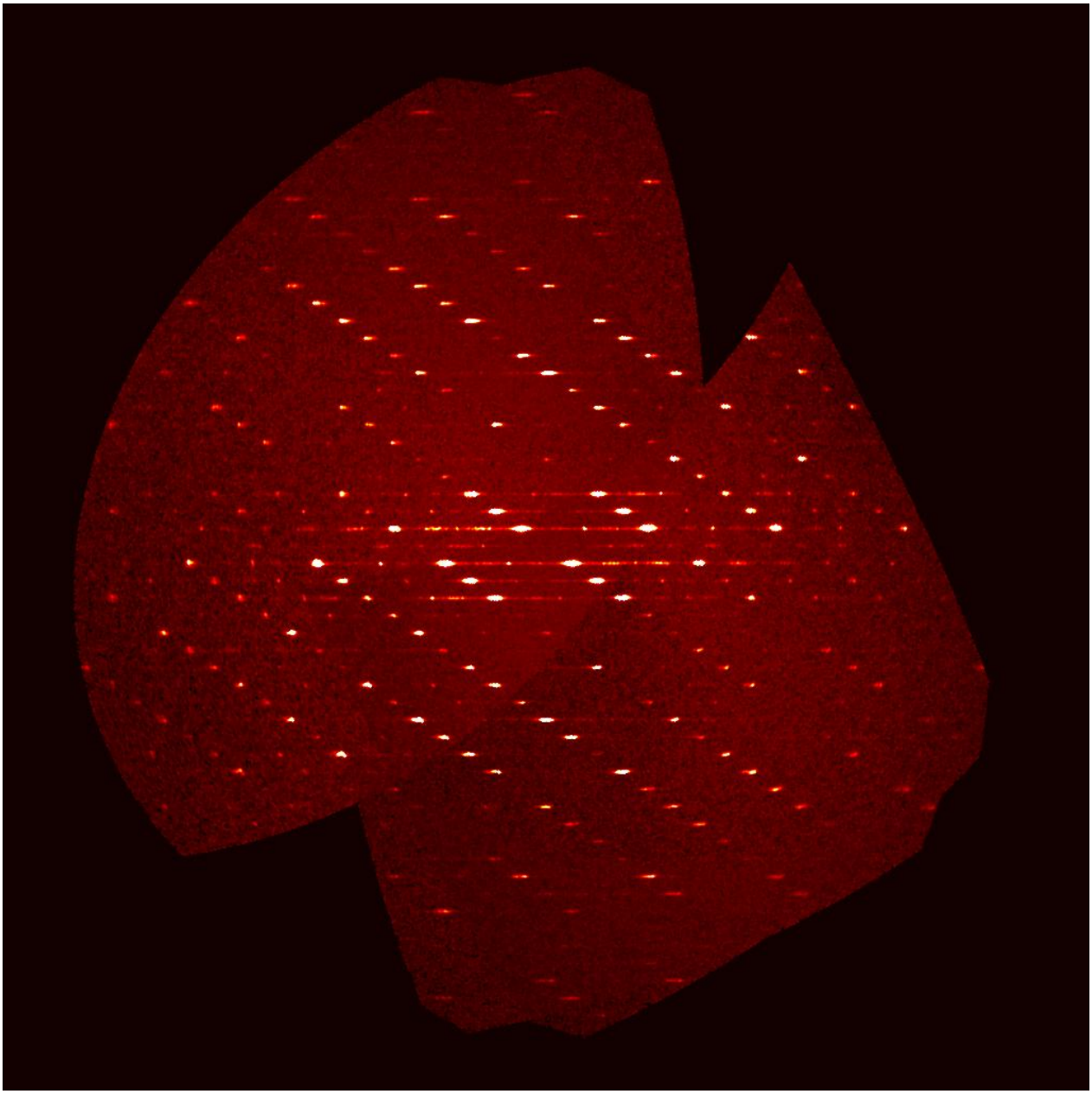
*h*10*l* layer:



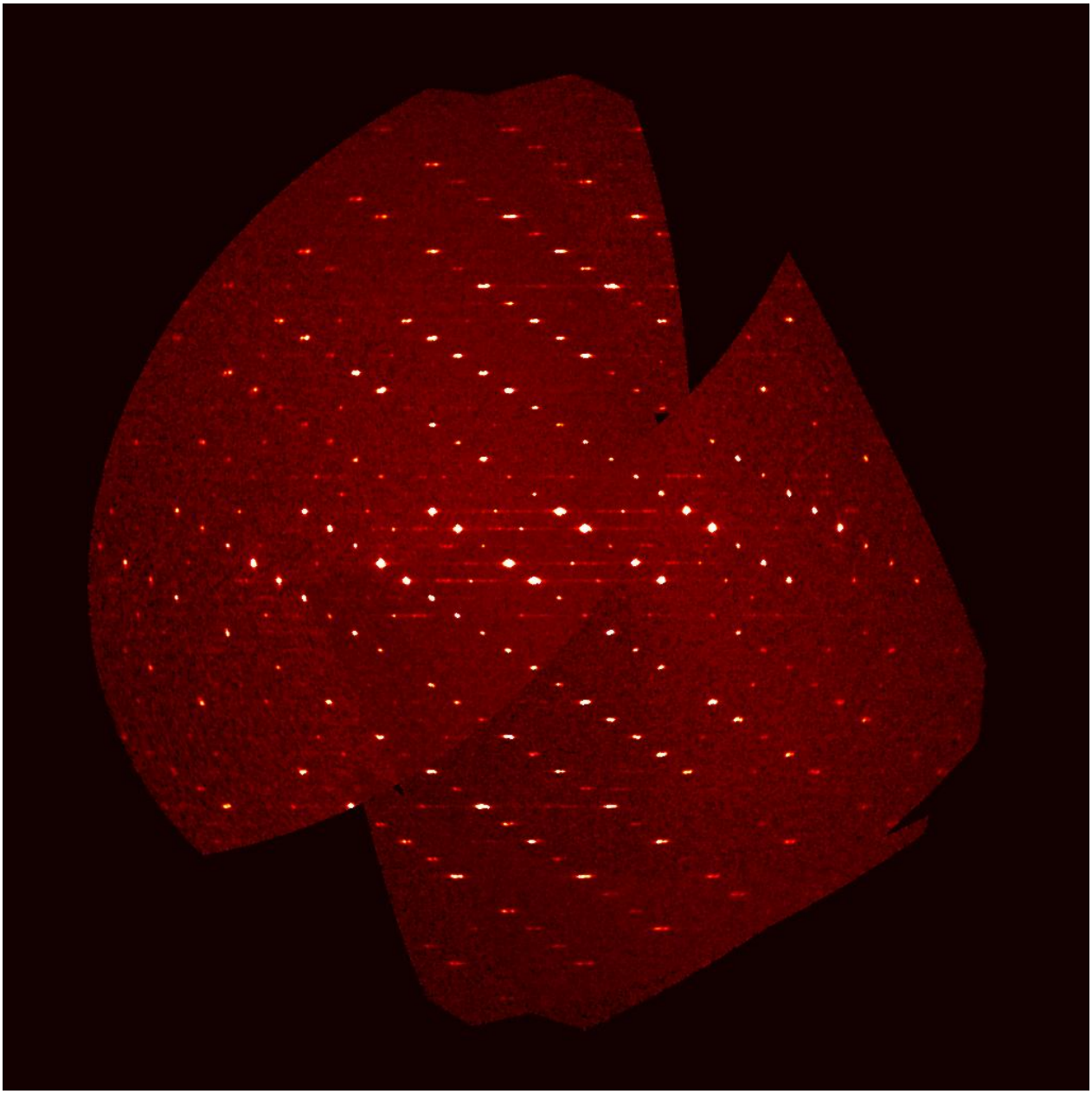
*h*11*l* layer:



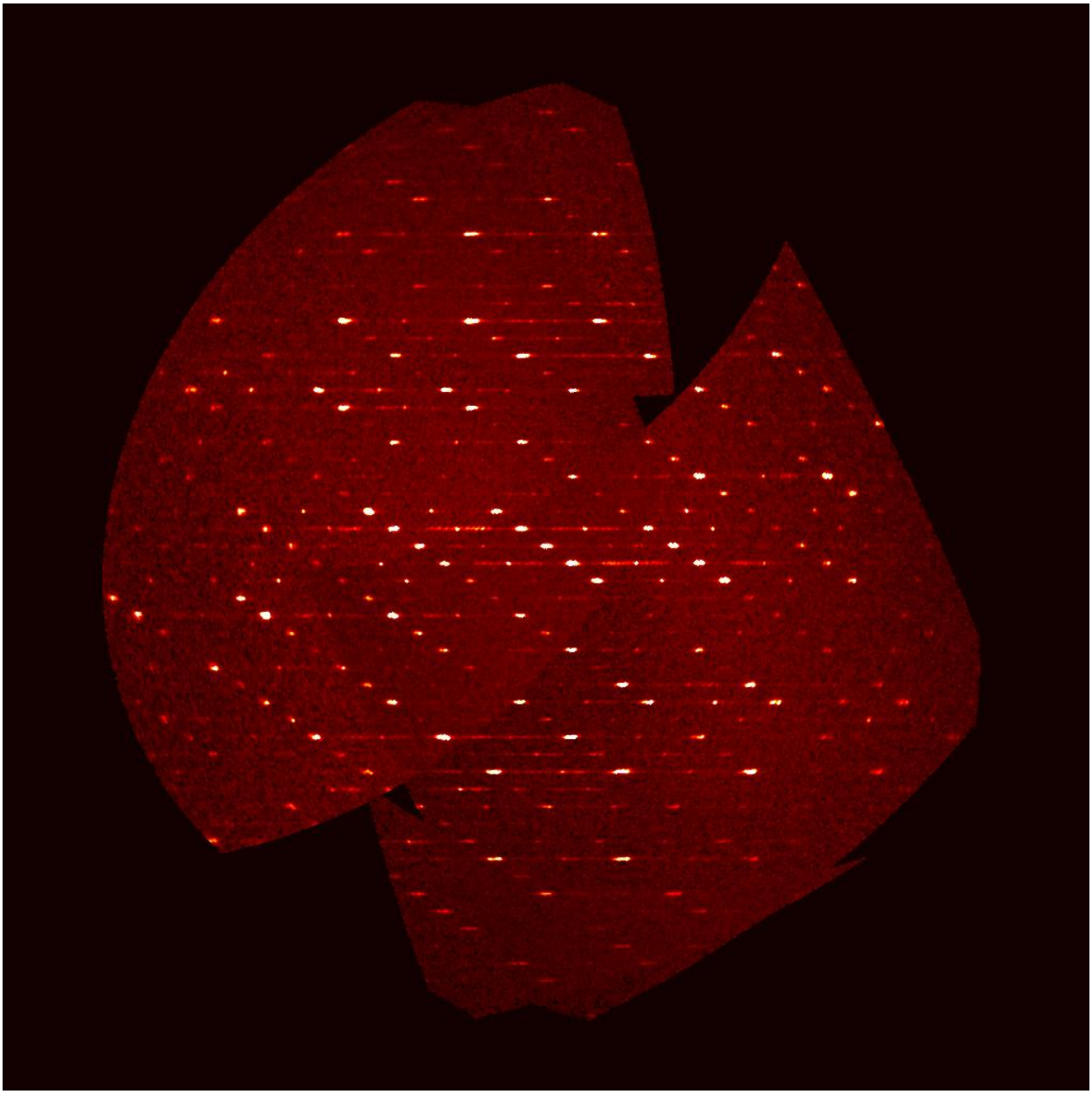
*h*12*l* layer:



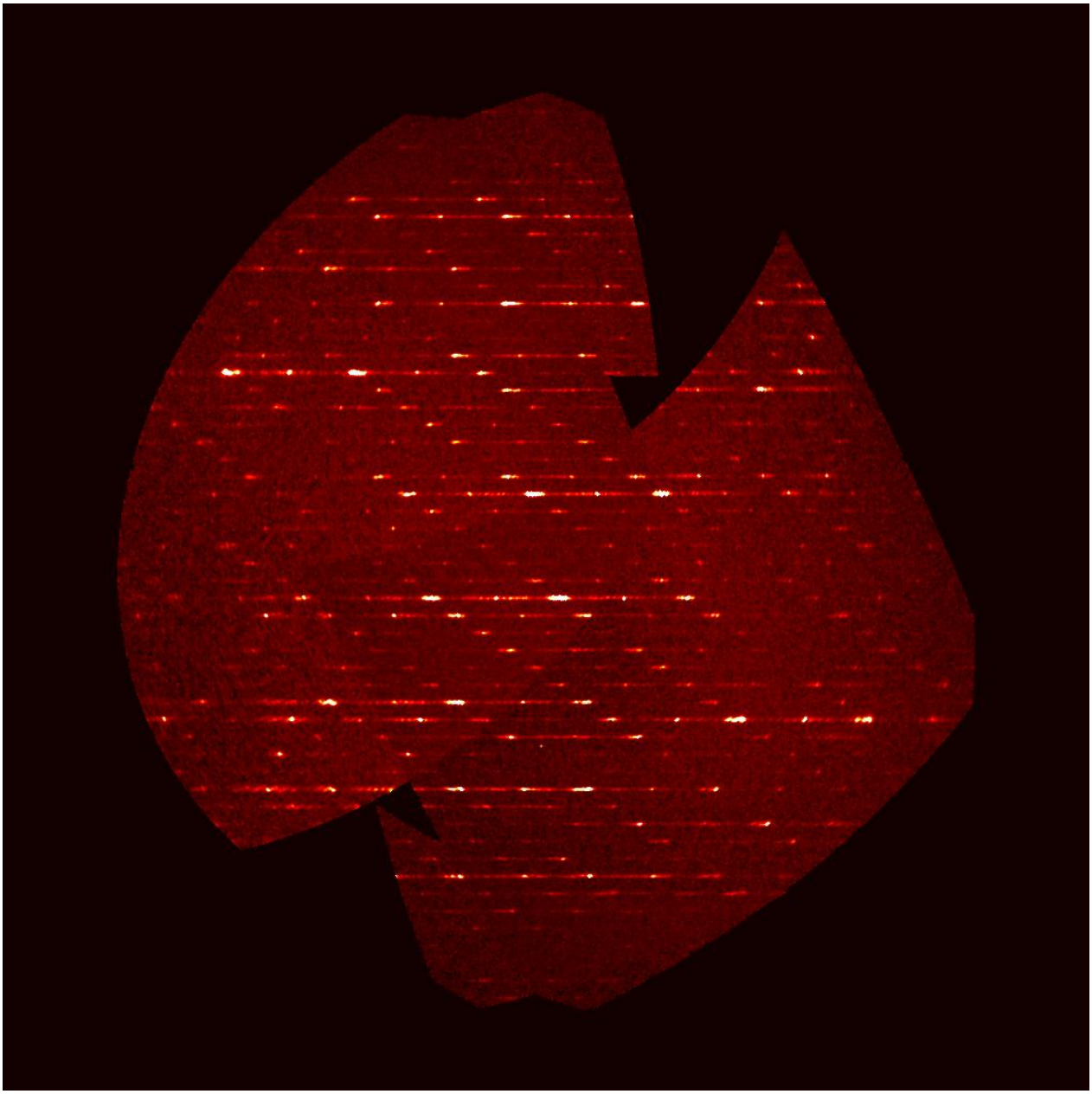
*h*13*l* layer:



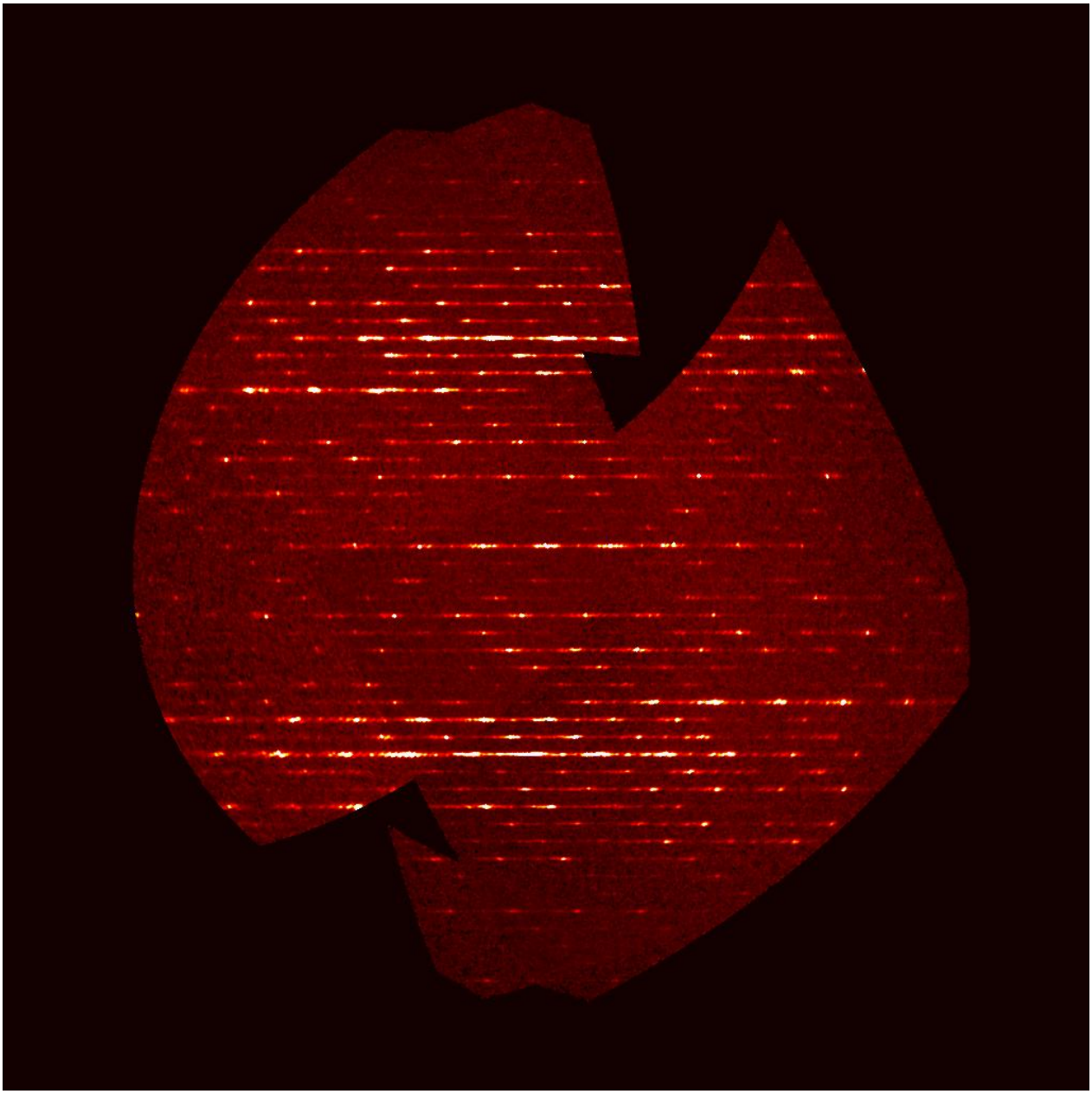
*h*14*l* layer:



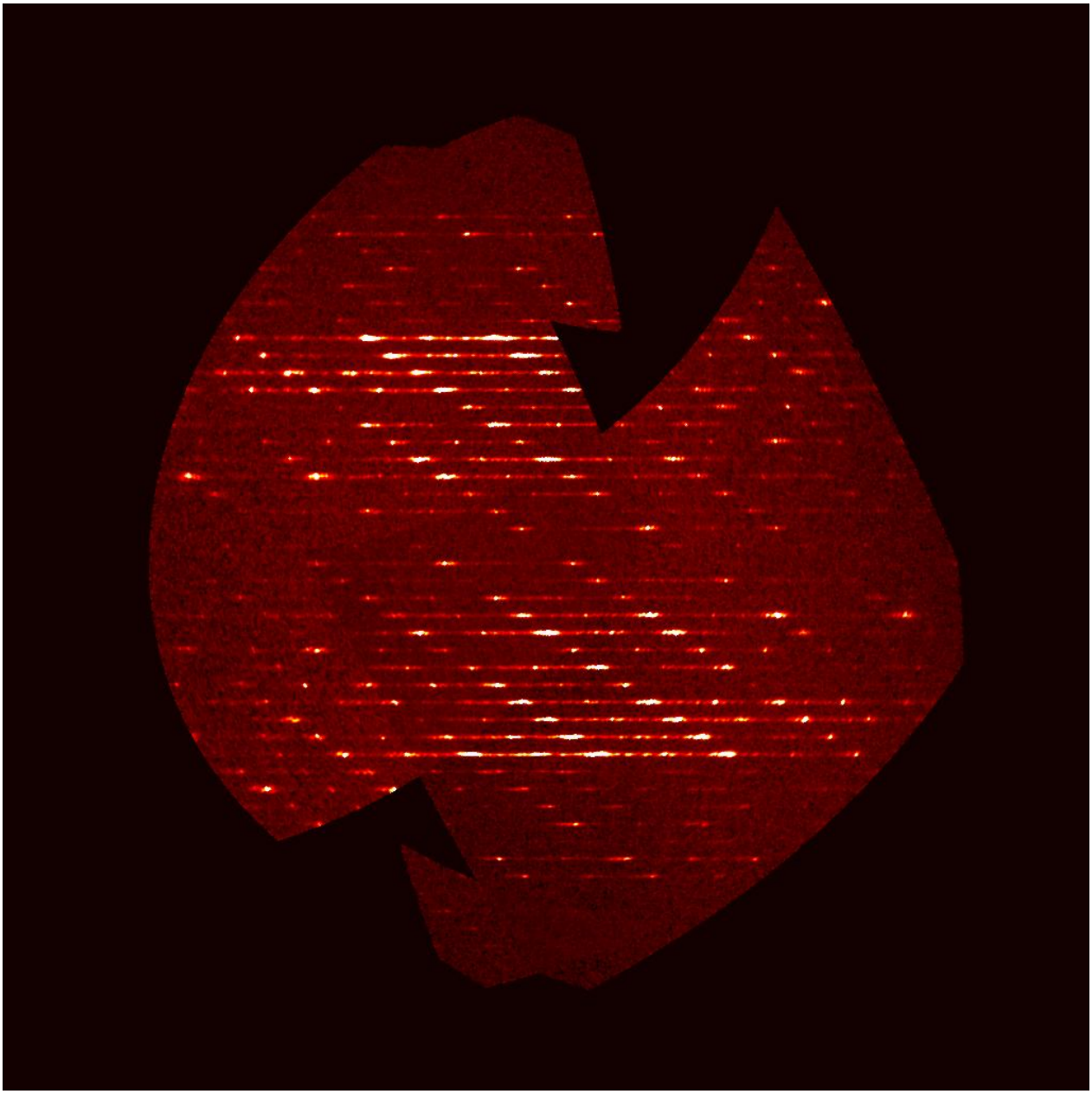
*h*15*l* layer:



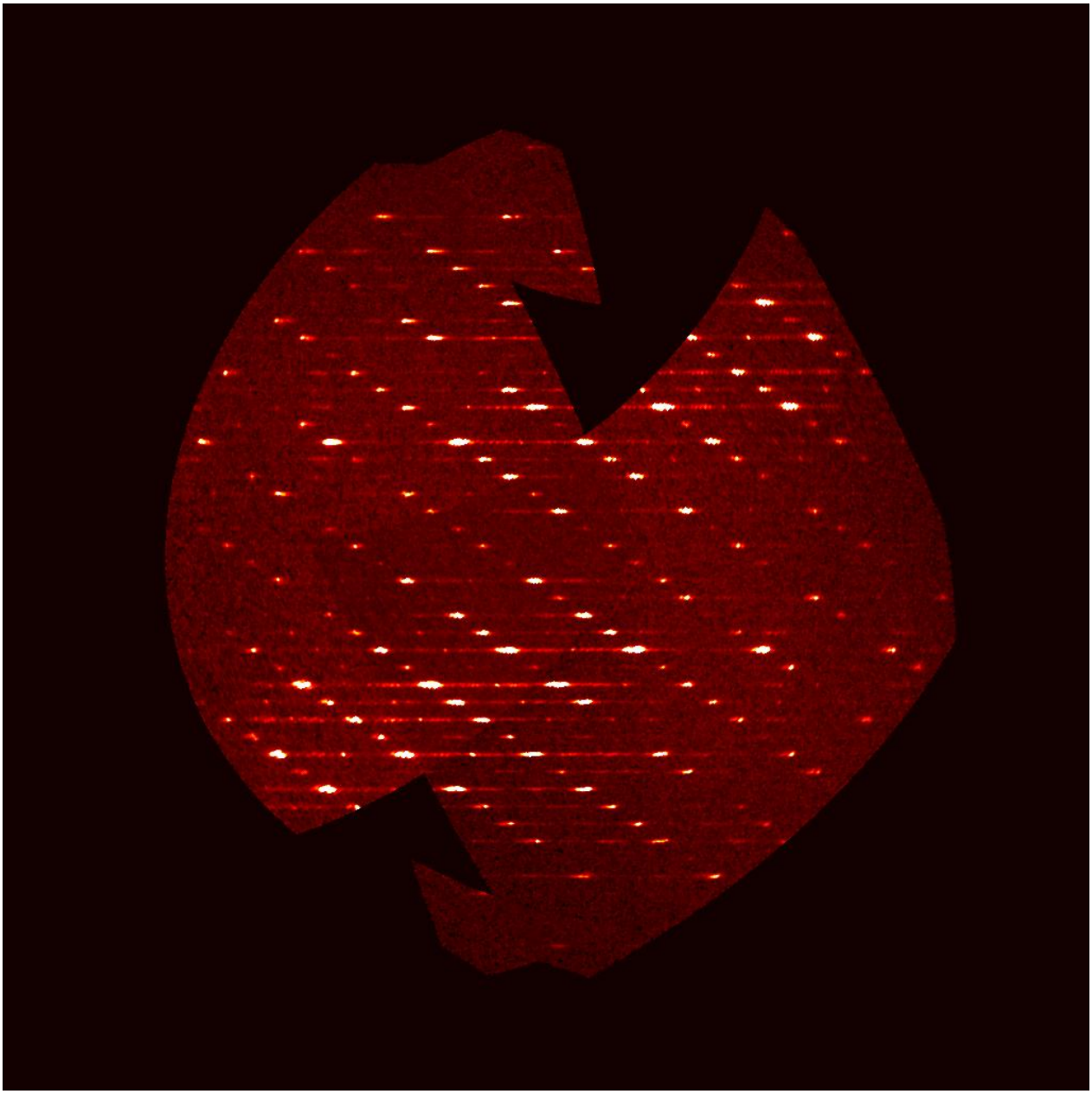
*h*16*l* layer:



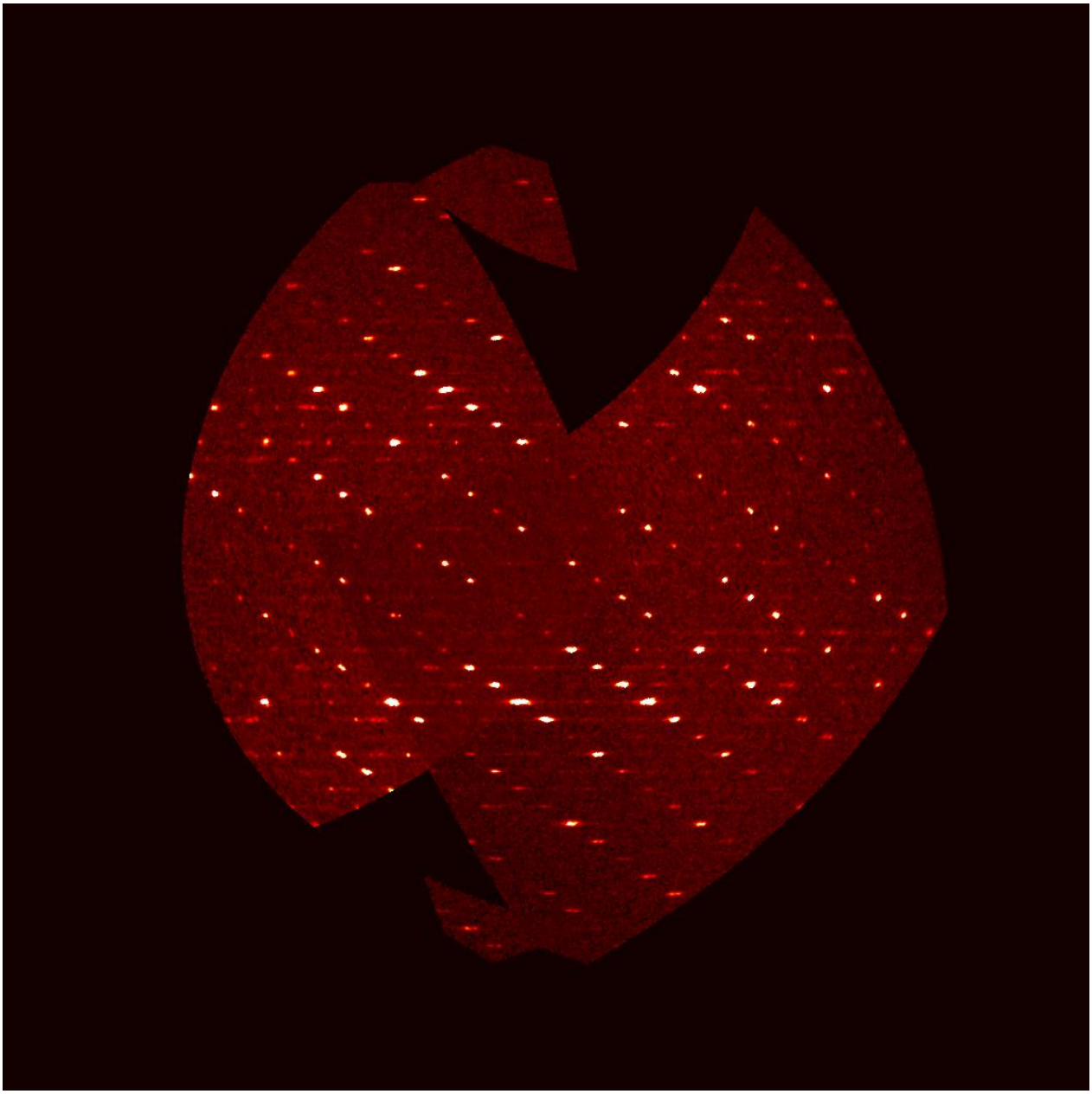
*h*17*l* layer:



*h*18*l* layer:



*h*19*l* layer:



*h*20*l* layer:

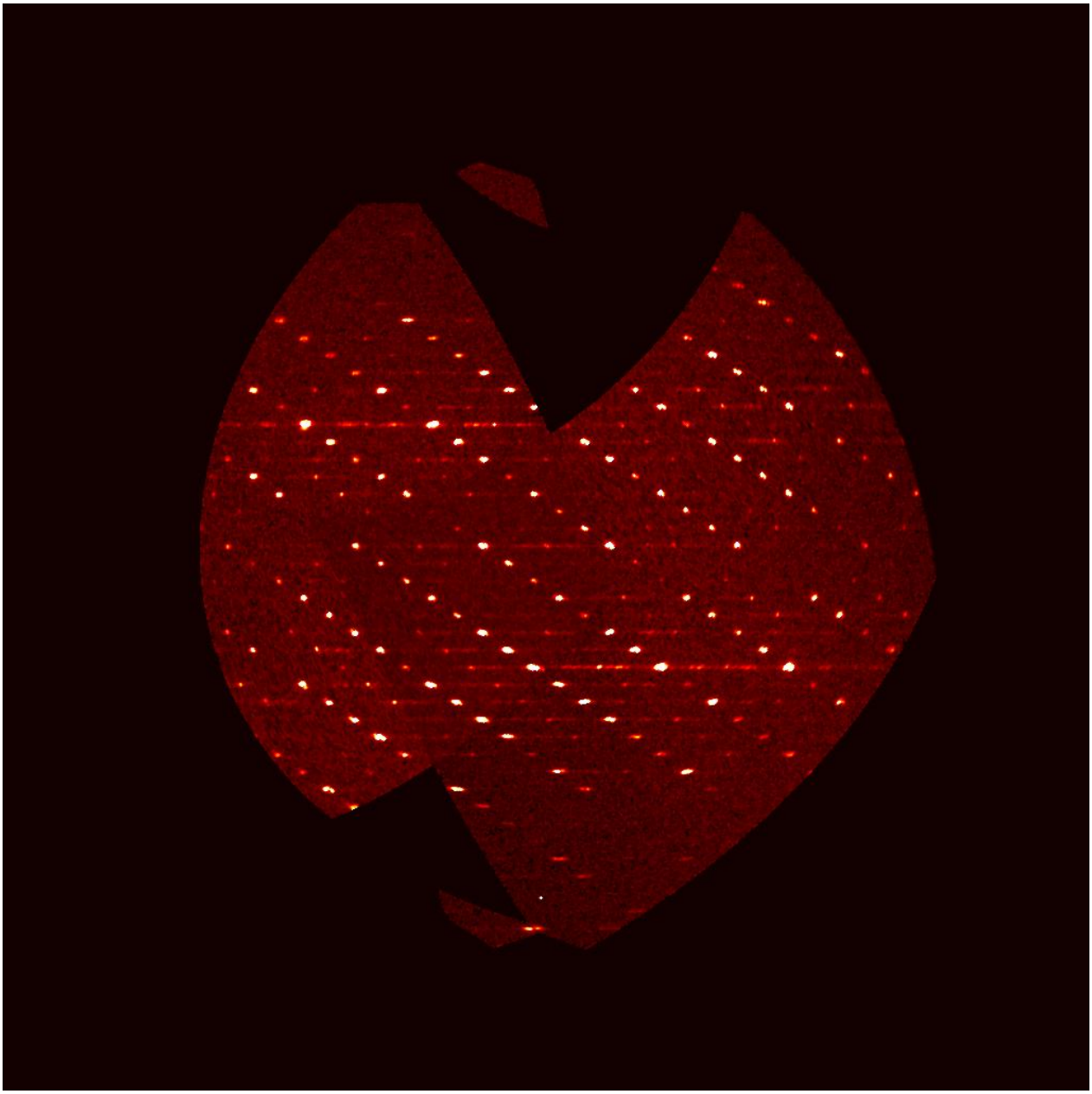


**Table S1: Important parameters from the subgroup analysis of the two models.**

| Subgroup | Origin shift | Unique ref. | *R*(int) | *R*1 (Fo >4σ) | *R*1 (all) |
|---|---|---|---|---|---|
| Model 1 subgroups | | | | | |
| *P*1 | ¼, 0, ¼ | 101466 | 0.081 | 0.1268 (47470) | 0.1947 (101466) |
| $P\bar{1}$ | ¼, 0, ¼ | 101466 | 0.081 | 0.1525 (47470) | 0.2191 (101466) |
| $P\bar{1}$ | 0, 0, 0 | 101466 | 0.081 | 0.1504 (47470) | 0.2174 (101466) |
| $P2_1$ | ⅜, 0, ⅛ | 56141 | 0.085 | 0.1291 (28583) | 0.1875 (56141) |
| $P2_1$ | ⅛, 0, -⅛ | 56141 | 0.085 | 0.1266 (28583) | 0.1854 (56141) |
| *B*1 | ¼, 0, ¼ | 50680 | 0.066 | 0.1188 (33855) | 0.1479 (50680) |
| $B\bar{1}$ | ¼, 0, ¼ | 50680 | 0.066 | 0.1333 (33855) | 0.1609 (50680) |
| $B2_1$ | ⅜, 0, ⅝ | 28066 | 0.070 | 0.1197 (19769) | 0.1445 (28066) |
| *Bg* | ¼, -½, ¾ | 27639 | 0.070 | 0.1203 (19696) | 0.1445 (27639) |
| $B2_1/g$ | 0, 0, 0 | 27617 | 0.070 | 0.1319 (19694) | 0.1543 (27617) |
| Model 2 subgroups (**a** and **c** interchanged in TC2) | | | | | |
| *P*1 | 0, 0, 0 | 101466 | 0.081 | 0.1252 (47470) | 0.1929 (101466) |
| $P\bar{1}$ | 0, 0, 0 | 101466 | 0.081 | 0.1938 (47470) | 0.2600 (101466) |
| $P2_1$ | ¼, 0, 0 | 56141 | 0.085 | 0.1259 (28583) | 0.1844 (56141) |
| *Pc* | 0, ¼, 0 | 55271 | 0.085 | 0.1719 (28316) | 0.2319 (55271) |
| $P2_1/c$ | 0, 0, 0 | 55249 | 0.085 | 0.1948 (28314) | 0.2504 (55249) |