

Table 1. Indexing of power diffraction maxima of GNNQQNY microcrystals: Comparison of observed and calculated peak positions

| | h | k | l | $s, 1/\text{\AA}$ | $d, \text{\AA}$ | $r_{\text{calc}}, \text{pixels}$ | $r_{\text{obs}}, \text{pixels}$ |
|---|-----|-----|-----|-------------------|-----------------|----------------------------------|---------------------------------|
| A | 0 | 1 | 0 | 0.025 | 39.437 | 95.8 | SYS ABS |
| B | 1 | 0 | 0 | 0.044 | 22.634 | 167.1 | 166.2 |
| C | 0 | 2 | 0 | 0.051 | 19.719 | 191.8 | 191.9 |
| C | 1 | 1 | 0 | 0.051 | 19.630 | 192.7 | 191.9 |
| D | 1 | 2 | 0 | 0.067 | 14.868 | 254.6 | 254.4 |
| E | 0 | 3 | 0 | 0.076 | 13.146 | 288.1 | SYS ABS |
| F | 1 | 3 | 0 | 0.088 | 11.367 | 333.4 | 333.5 |
| F | 2 | 0 | 0 | 0.088 | 11.317 | 334.9 | 333.5 |
| G | 2 | 1 | 0 | 0.092 | 10.878 | 348.6 | 348.2 |
| H | 0 | 4 | 0 | 0.101 | 9.859 | 384.8 | 385.2 |
| H | 2 | 2 | 0 | 0.102 | 9.815 | 386.6 | 385.2 |
| I | 1 | 4 | 0 | 0.111 | 9.039 | 420.1 | 420.1 |
| J | 2 | 3 | 0 | 0.117 | 8.576 | 443.0 | 442.8 |
| K | 0 | 5 | 0 | 0.127 | 7.887 | 482.2 | SYS ABS |
| L | 3 | 0 | 0 | 0.133 | 7.545 | 504.4 | 512.3 |
| L | 1 | 5 | 0 | 0.134 | 7.448 | 511.0 | 512.3 |
| L | 2 | 4 | 0 | 0.135 | 7.434 | 512.0 | 512.3 |
| L | 3 | 1 | 0 | 0.135 | 7.410 | 513.7 | 512.3 |
| M | 3 | 2 | 0 | 0.142 | 7.046 | 540.6 | 540.6 |
| N | 0 | 6 | 0 | 0.152 | 6.573 | 580.3 | 581.2 |
| N | 3 | 3 | 0 | 0.153 | 6.543 | 582.9 | 581.2 |
| N | 2 | 5 | 0 | 0.155 | 6.471 | 589.6 | 581.2 |
| O | 1 | 6 | 0 | 0.158 | 6.312 | 604.7 | 605.0 |
| P | 3 | 4 | 0 | 0.167 | 5.992 | 637.8 | 637.8 |
| Q | 2 | 6 | 0 | 0.176 | 5.684 | 673.2 | 674.4 |
| Q | 4 | 0 | 0 | 0.177 | 5.658 | 676.3 | 674.4 |
| Q | 0 | 7 | 0 | 0.177 | 5.634 | 679.3 | SYS ABS |
| Q | 4 | 1 | 0 | 0.179 | 5.601 | 683.4 | 674.4 |
| R | 1 | 7 | 0 | 0.183 | 5.467 | 700.6 | 701.4 |
| R | 3 | 5 | 0 | 0.183 | 5.452 | 702.6 | 701.4 |
| R | 4 | 2 | 0 | 0.184 | 5.439 | 704.3 | 701.4 |
| S | 4 | 3 | 0 | 0.192 | 5.197 | 738.0 | 738.0 |
| T | 2 | 7 | 0 | 0.198 | 5.043 | 761.2 | 777.5 |
| U | 3 | 6 | 0 | 0.202 | 4.956 | 775.1 | 777.5 |
| U | 0 | 8 | 0 | 0.203 | 4.930 | 779.4 | 777.5 |
| U | 4 | 4 | 0 | 0.204 | 4.908 | 783.0 | 777.5 |
| V | 0 | 0 | 1 | 0.207 | 4.825 | 796.9 | 798.2 |
| V | 1 | 8 | 0 | 0.208 | 4.817 | 798.3 | 798.2 |

| | | | | | | | |
|---|---|----|---|-------|-------|--------|---------|
| V | 0 | 1 | 1 | 0.209 | 4.789 | 803.0 | 798.2 |
| W | 1 | 0 | 1 | 0.212 | 4.719 | 815.4 | 815.1 |
| W | 0 | 2 | 1 | 0.213 | 4.687 | 821.2 | 815.1 |
| W | 1 | 1 | 1 | 0.213 | 4.686 | 821.5 | 815.1 |
| X | 4 | 5 | 0 | 0.218 | 4.598 | 837.8 | 837.5 |
| X | 1 | 2 | 1 | 0.218 | 4.590 | 839.3 | 837.5 |
| Y | 0 | 3 | 1 | 0.221 | 4.530 | 850.9 | 855.4 |
| Y | 5 | 0 | 0 | 0.221 | 4.527 | 851.5 | 855.4 |
| Y | 2 | 8 | 0 | 0.221 | 4.519 | 852.9 | 855.4 |
| Y | 3 | 7 | 0 | 0.222 | 4.514 | 853.9 | 855.4 |
| Y | 5 | 1 | 0 | 0.222 | 4.497 | 857.3 | 855.4 |
| Z | 1 | 3 | 1 | 0.225 | 4.442 | 868.4 | 873.7 |
| Z | 2 | 0 | 1 | 0.225 | 4.439 | 869.1 | 873.7 |
| Z | 5 | 2 | 0 | 0.227 | 4.412 | 874.5 | 873.7 |
| Z | 2 | 1 | 1 | 0.227 | 4.411 | 874.8 | 873.7 |
| a | 0 | 9 | 0 | 0.228 | 4.382 | 880.8 | SYS ABS |
| b | 0 | 4 | 1 | 0.231 | 4.334 | 891.0 | 900.9 |
| b | 2 | 2 | 1 | 0.231 | 4.330 | 891.8 | 900.9 |
| c | 1 | 9 | 0 | 0.232 | 4.302 | 897.9 | 900.9 |
| c | 4 | 6 | 0 | 0.233 | 4.288 | 900.9 | 900.9 |
| c | 5 | 3 | 0 | 0.234 | 4.280 | 902.7 | 900.9 |
| d | 1 | 4 | 1 | 0.235 | 4.257 | 907.9 | 900.9 |
| e | 2 | 3 | 1 | 0.238 | 4.205 | 919.5 | 917.1 |
| f | 3 | 8 | 0 | 0.242 | 4.127 | 937.8 | 941.2 |
| f | 0 | 5 | 1 | 0.243 | 4.116 | 940.4 | 941.2 |
| f | 5 | 4 | 0 | 0.243 | 4.114 | 940.9 | 941.2 |
| g | 2 | 9 | 0 | 0.245 | 4.086 | 947.6 | 947.7 |
| h | 3 | 0 | 1 | 0.246 | 4.065 | 952.8 | 947.7 |
| h | 1 | 5 | 1 | 0.247 | 4.050 | 956.6 | 947.7 |
| h | 2 | 4 | 1 | 0.247 | 4.047 | 957.2 | 947.7 |
| h | 3 | 1 | 1 | 0.247 | 4.044 | 958.1 | 947.7 |
| i | 4 | 7 | 0 | 0.250 | 3.992 | 971.0 | 971.3 |
| i | 3 | 2 | 1 | 0.251 | 3.981 | 973.9 | 971.3 |
| j | 0 | 10 | 0 | 0.254 | 3.944 | 983.6 | 989.7 |
| j | 5 | 5 | 0 | 0.255 | 3.926 | 988.3 | 989.7 |
| k | 0 | 6 | 1 | 0.257 | 3.890 | 998.1 | 997.9 |
| k | 1 | 10 | 0 | 0.257 | 3.885 | 999.3 | 997.9 |
| k | 3 | 3 | 1 | 0.258 | 3.884 | 999.7 | 997.9 |
| k | 2 | 5 | 1 | 0.259 | 3.868 | 1003.9 | 997.9 |
| k | 1 | 6 | 1 | 0.261 | 3.833 | 1013.5 | 997.9 |
| l | 3 | 9 | 0 | 0.264 | 3.789 | 1026.1 | 1031.0 |
| l | 6 | 0 | 0 | 0.265 | 3.772 | 1030.9 | 1031.0 |
| l | 3 | 4 | 1 | 0.266 | 3.758 | 1035.0 | 1031.0 |
| l | 6 | 1 | 0 | 0.266 | 3.755 | 1035.9 | 1031.0 |
| m | 5 | 6 | 0 | 0.268 | 3.728 | 1043.9 | 1046.7 |

| | | | | | | | |
|---|---|----|---|-------|-------|--------|---------|
| m | 2 | 10 | 0 | 0.269 | 3.724 | 1045.1 | 1046.7 |
| m | 4 | 8 | 0 | 0.269 | 3.717 | 1047.2 | 1046.7 |
| m | 6 | 2 | 0 | 0.270 | 3.705 | 1050.7 | 1046.7 |
| n | 2 | 6 | 1 | 0.272 | 3.678 | 1058.8 | 1063.5 |
| n | 4 | 0 | 1 | 0.272 | 3.672 | 1060.9 | 1063.5 |
| n | 0 | 7 | 1 | 0.273 | 3.665 | 1063.0 | 1063.5 |
| n | 4 | 1 | 1 | 0.274 | 3.656 | 1065.8 | 1063.5 |
| o | 6 | 3 | 0 | 0.276 | 3.626 | 1075.1 | 1063.5 |
| o | 1 | 7 | 1 | 0.276 | 3.618 | 1077.7 | 1063.5 |
| o | 3 | 5 | 1 | 0.277 | 3.613 | 1079.1 | 1063.5 |
| o | 4 | 2 | 1 | 0.277 | 3.609 | 1080.3 | 1063.5 |
| p | 0 | 11 | 0 | 0.279 | 3.585 | 1088.1 | SYS ABS |
| q | 1 | 11 | 0 | 0.282 | 3.541 | 1102.6 | 1104.5 |
| q | 4 | 3 | 1 | 0.283 | 3.536 | 1104.2 | 1104.5 |
| q | 5 | 7 | 0 | 0.283 | 3.529 | 1106.7 | 1104.5 |
| q | 6 | 4 | 0 | 0.284 | 3.523 | 1108.6 | 1104.5 |
| r | 3 | 10 | 0 | 0.286 | 3.495 | 1118.1 | 1122.4 |
| r | 2 | 7 | 1 | 0.287 | 3.487 | 1121.0 | 1122.4 |
| s | 4 | 9 | 0 | 0.289 | 3.465 | 1128.7 | 1131.4 |
| s | 3 | 6 | 1 | 0.289 | 3.457 | 1131.2 | 1131.4 |
| s | 0 | 8 | 1 | 0.290 | 3.448 | 1134.4 | 1131.4 |
| t | 4 | 4 | 1 | 0.291 | 3.441 | 1137.0 | 1137.8 |
| u | 2 | 11 | 0 | 0.293 | 3.418 | 1145.2 | 1137.8 |
| u | 1 | 8 | 1 | 0.293 | 3.409 | 1148.4 | 1137.8 |
| u | 6 | 5 | 0 | 0.294 | 3.403 | 1150.5 | 1137.8 |

Table contents correspond to data from Figure 3. The first column corresponds to peak labels in Figure 3. Other columns are labeled in the table.