**Table 5. Anisotropic Displacement Parameters for four samples of F-Cl apatite.**

|  |
| --- |
| Anisotropic atomic displacement parameters (Å2) for HNF5CL5. |
|  |
| The anisotropic atomic displacement factor exponent takes the form: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ] |

|  | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| --- | --- | --- | --- | --- | --- | --- |
| Ca1 | 0.01440(10) | 0.01440(10) | 0.00749(15) | 0 | 0 | 0.00720(5) |
| P | 0.00718(14) | 0.01007(14) | 0.00797(14) | 0 | 0 | 0.00424(11) |
| Ca2 | 0.01227(13) | 0.02261(15) | 0.01011(13) | 0 | 0 | 0.00562(10) |
| O1 | 0.0077(4) | 0.0201(5) | 0.0141(4) | 0 | 0 | 0.0067(3) |
| O2 | 0.0136(4) | 0.0107(4) | 0.0262(6) | 0 | 0 | 0.0037(3) |
| O3 | 0.0108(12) | 0.0268(19) | 0.0112(11) | 0.0056(12) | -0.0016(9) | 0.0092(13) |
| O3' | 0.0108(12) | 0.0268(19) | 0.0112(11) | 0.0056(12) | -0.0016(9) | 0.0092(13) |

|  |
| --- |
| Anisotropic atomic displacement parameters (Å2) for HNF5CL58. |
| The anisotropic atomic displacement factor exponent takes the form: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ] |

|  | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| --- | --- | --- | --- | --- | --- | --- |
| Ca1 | 0.01578(10) | 0.01578(10) | 0.00861(14) | 0 | 0 | 0.00789(5) |
| P | 0.00853(13) | 0.01141(14) | 0.00918(14) | 0 | 0 | 0.00489(10) |
| Ca2 | 0.01366(12) | 0.02398(14) | 0.01123(12) | 0 | 0 | 0.00630(10) |
| O1 | 0.0159(4) | 0.0094(4) | 0.0149(4) | 0 | 0 | 0.0019(3) |
| O2 | 0.0151(4) | 0.0120(4) | 0.0272(5) | 0 | 0 | 0.0043(3) |
| O3 | 0.0112(13) | 0.0248(19) | 0.0134(10) | 0.0053(11) | -0.0013(8) | 0.0082(13) |
| O3' | 0.0112(13) | 0.0248(19) | 0.0134(10) | 0.0053(11) | -0.0013(8) | 0.0082(13) |

|  |
| --- |
| Anisotropic atomic displacement parameters (Å2) for HNF5CL59. |
|  |
| The anisotropic atomic displacement factor exponent takes the form: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ] |

|  | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| --- | --- | --- | --- | --- | --- | --- |
| Ca1 | 0.01447(11) | 0.01447(11) | 0.00747(15) | 0 | 0 | 0.00724(5) |
| P | 0.00711(14) | 0.01009(14) | 0.00806(14) | 0 | 0 | 0.00420(11) |
| Ca3 | 0.01232(13) | 0.02260(15) | 0.01007(13) | 0 | 0 | 0.00562(10) |
| O1 | 0.0078(4) | 0.0203(5) | 0.0138(4) | 0 | 0 | 0.0068(3) |
| O2 | 0.0139(4) | 0.0105(4) | 0.0264(6) | 0 | 0 | 0.0037(3) |
| O3 | 0.0108(12) | 0.0262(18) | 0.0113(10) | 0.0056(11) | -0.0016(8) | 0.0091(13) |
| O3' | 0.0108(12) | 0.0262(18) | 0.0113(10) | 0.0056(11) | -0.0016(8) | 0.0091(13) |

|  |
| --- |
| Anisotropic atomic displacement parameters (Å2) for HNF5CL510. |
|  |
| The anisotropic atomic displacement factor exponent takes the form: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ] |

|  | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| --- | --- | --- | --- | --- | --- | --- |
| Ca1 | 0.01451(11) | 0.01451(11) | 0.00750(14) | 0 | 0 | 0.00725(5) |
| Ca2 | 0.01235(13) | 0.02266(15) | 0.01014(13) | 0 | 0 | 0.00563(10) |
| P | 0.00719(14) | 0.01007(14) | 0.00810(14) | 0 | 0 | 0.00424(11) |
| O1 | 0.0077(4) | 0.0201(5) | 0.0141(4) | 0 | 0 | 0.0067(3) |
| O2 | 0.0140(4) | 0.0105(4) | 0.0262(5) | 0 | 0 | 0.0037(3) |
| O3 | 0.0108(12) | 0.0268(18) | 0.0111(11) | 0.0054(11) | -0.0017(9) | 0.0093(13) |
| O3' | 0.0108(12) | 0.0268(18) | 0.0111(11) | 0.0054(11) | -0.0017(9) | 0.0093(13) |

**Table 6a: FoFc for sample HNFCL5**

#

# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag

#

data\_hnf5cl5\_0m

\_shelx\_title ' HNF5CL5\_0m in P6(3)/m'

\_shelx\_refln\_list\_code 4

\_shelx\_F\_calc\_maximum 200.56

\_exptl\_crystal\_F\_000 508.00

\_reflns\_d\_resolution\_high 0.6543

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-y, x-y, z'

'-x+y, -x, z'

'-x, -y, z+1/2'

'y, -x+y, z+1/2'

'x-y, x, z+1/2'

'-x, -y, -z'

'y, -x+y, -z'

'x-y, x, -z'

'x, y, -z-1/2'

'-y, x-y, -z-1/2'

'-x+y, -x, -z-1/2'

\_cell\_length\_a 9.5104

\_cell\_length\_b 9.5104

\_cell\_length\_c 6.8311

\_cell\_angle\_alpha 90.000

\_cell\_angle\_beta 90.000

\_cell\_angle\_gamma 120.000

\_shelx\_F\_squared\_multiplier 1.000

loop\_

\_refln\_index\_h

\_refln\_index\_k

\_refln\_index\_l

\_refln\_F\_squared\_calc

\_refln\_F\_squared\_meas

\_refln\_F\_squared\_sigma

\_refln\_observed\_status

0 1 0 277.26 283.13 1.34 o

-1 2 0 48.35 51.45 0.56 o

0 2 0 257.89 265.93 1.37 o

-2 3 0 44.60 26.77 0.55 o

-1 3 0 2656.86 2575.03 10.01 o

0 3 0 21464.28 21217.83 89.06 o

-3 4 0 8109.78 9063.53 37.35 o

-2 4 0 174.49 155.37 1.16 o

-1 4 0 1214.37 1265.45 5.10 o

0 4 0 728.10 683.48 3.13 o

-4 5 0 5387.06 5258.31 18.18 o

-3 5 0 2937.07 3050.39 11.91 o

-2 5 0 28.17 23.92 0.58 o

-1 5 0 6309.12 6341.48 22.31 o

0 5 0 216.97 193.95 1.32 o

-5 6 0 20.88 27.80 0.61 o

-4 6 0 4292.81 4390.21 15.60 o

-3 6 0 1470.55 1509.44 6.34 o

-2 6 0 114.09 104.99 1.11 o

-1 6 0 1862.20 1865.67 7.10 o

0 6 0 700.09 652.36 3.16 o

-6 7 0 1101.14 1028.34 4.74 o

-5 7 0 1538.30 1522.27 6.11 o

-4 7 0 474.92 462.72 2.47 o

-3 7 0 365.06 352.74 2.23 o

-2 7 0 5401.08 5362.27 18.88 o

-1 7 0 1478.71 1498.87 6.42 o

0 7 0 38.55 33.93 1.15 o

-7 8 0 4864.60 4909.35 19.10 o

-6 8 0 431.45 440.24 2.87 o

-5 8 0 1186.77 1178.06 5.35 o

-4 8 0 4736.90 4771.39 19.08 o

-3 8 0 141.78 144.32 1.53 o

-2 8 0 28.50 22.59 0.79 o

-1 8 0 766.98 812.12 4.35 o

0 8 0 2745.23 2720.93 11.44 o

-8 9 0 51.93 41.47 1.14 o

-7 9 0 609.42 614.51 3.95 o

-6 9 0 34.38 37.65 1.00 o

-5 9 0 139.24 131.93 1.56 o

-4 9 0 108.87 100.45 1.39 o

-3 9 0 1.26 2.57 0.55 o

-2 9 0 721.71 702.18 4.06 o

-1 9 0 188.48 180.62 2.00 o

0 9 0 534.83 514.62 3.67 o

-9 10 0 315.27 314.72 2.86 o

-8 10 0 380.90 392.58 3.17 o

-7 10 0 32.06 31.14 1.37 o

-6 10 0 406.45 394.02 2.93 o

-5 10 0 1712.23 1657.99 9.03 o

-4 10 0 95.69 96.05 1.46 o

-3 10 0 712.79 704.40 4.21 o

-2 10 0 1595.70 1576.93 9.49 o

-1 10 0 181.35 174.35 2.08 o

0 10 0 102.78 110.97 2.27 o

-10 11 0 2259.45 2226.36 12.88 o

-9 11 0 591.53 596.40 4.95 o

-8 11 0 388.70 389.47 3.50 o

-7 11 0 2407.53 2349.91 12.31 o

-6 11 0 1026.12 1023.31 6.23 o

-5 11 0 23.24 20.45 1.03 o

-4 11 0 1021.67 1005.78 5.53 o

-3 11 0 11.91 10.04 0.82 o

-2 11 0 149.96 137.98 2.24 o

-1 11 0 8.19 8.59 1.16 o

0 11 0 26.47 19.89 1.29 o

-11 12 0 2.39 2.93 0.95 o

-10 12 0 721.30 710.37 5.96 o

-9 12 0 346.05 343.81 3.89 o

-8 12 0 127.38 125.60 2.37 o

-7 12 0 23.22 22.80 1.22 o

-6 12 0 278.09 272.88 3.12 o

-5 12 0 458.05 473.46 3.96 o

-4 12 0 618.26 606.63 5.23 o

-3 12 0 811.40 816.97 5.95 o

-2 12 0 287.26 293.28 3.91 o

-1 12 0 153.17 144.28 2.86 o

0 12 0 1308.48 1325.73 10.00 o

-12 13 0 335.06 345.08 12.84 o

-11 13 0 3.92 3.47 1.07 o

-10 13 0 70.87 65.20 2.37 o

-9 13 0 8.60 11.05 1.16 o

-8 13 0 299.95 315.39 3.81 o

-7 13 0 582.89 574.30 5.68 o

-6 13 0 414.57 405.41 4.29 o

-5 13 0 1122.24 1134.92 8.07 o

-4 13 0 663.58 673.91 5.80 o

-3 13 0 346.21 332.35 4.67 o

-2 13 0 354.63 350.14 4.76 o

-10 14 0 426.41 440.41 9.70 o

-9 14 0 225.19 224.22 4.77 o

-8 14 0 49.76 51.16 2.46 o

-7 14 0 131.50 131.26 2.79 o

-6 14 0 471.47 475.77 6.38 o

-5 14 0 239.99 227.12 10.09 o

-4 14 0 29.13 32.68 4.70 o

0 1 1 178.56 186.95 0.76 o

-1 2 1 310.84 323.56 1.11 o

0 2 1 268.85 296.26 1.09 o

-2 3 1 4385.30 4355.78 11.22 o

-1 3 1 9662.28 9639.18 23.53 o

0 3 1 713.03 800.32 2.57 o

-3 4 1 1400.49 1428.04 3.96 o

-2 4 1 214.47 187.17 0.97 o

-1 4 1 219.53 270.95 1.04 o

0 4 1 111.90 95.84 0.63 o

-4 5 1 34.67 34.59 0.52 o

-3 5 1 3357.01 3366.89 8.33 o

-2 5 1 2985.10 3010.16 7.54 o

-1 5 1 36.48 38.89 0.47 o

0 5 1 941.43 1026.82 2.98 o

-5 6 1 681.62 696.46 2.17 o

-4 6 1 1489.99 1454.86 4.03 o

-3 6 1 1839.96 1772.61 4.86 o

-2 6 1 603.23 630.81 2.05 o

-1 6 1 5063.06 5173.60 12.91 o

0 6 1 9.58 9.75 0.34 o

-6 7 1 333.97 313.69 1.49 o

-5 7 1 263.71 266.90 1.31 o

-4 7 1 84.28 97.35 0.80 o

-3 7 1 3142.45 3086.95 8.45 o

-2 7 1 1085.55 1063.43 3.42 o

-1 7 1 120.46 121.38 0.93 o

0 7 1 5.43 8.70 0.44 o

-7 8 1 25.05 24.46 0.61 o

-6 8 1 38.55 30.56 0.68 o

-5 8 1 48.82 43.62 0.69 o

-4 8 1 1145.43 1125.16 3.73 o

-3 8 1 101.12 100.50 0.91 o

-2 8 1 62.94 68.11 0.90 o

-1 8 1 195.56 203.60 1.30 o

0 8 1 18.00 18.44 0.57 o

-8 9 1 122.70 117.01 1.26 o

-7 9 1 14.02 16.04 0.63 o

-6 9 1 490.40 462.80 2.25 o

-5 9 1 670.79 656.93 2.66 o

-4 9 1 849.96 847.53 3.09 o

-3 9 1 2754.33 2684.48 7.94 o

-2 9 1 377.95 374.26 1.94 o

-1 9 1 286.87 289.65 1.90 o

0 9 1 541.63 537.93 2.83 o

-9 10 1 34.31 36.45 0.90 o

-8 10 1 386.09 396.85 2.41 o

-7 10 1 242.88 232.10 1.77 o

-6 10 1 296.31 300.35 1.94 o

-5 10 1 688.07 671.07 3.10 o

-4 10 1 5.37 7.28 0.48 o

-3 10 1 380.26 389.94 2.19 o

-2 10 1 118.00 120.08 1.39 o

-1 10 1 352.26 348.78 2.40 o

0 10 1 74.29 71.59 1.24 o

-10 11 1 131.56 134.41 1.61 o

-9 11 1 1232.66 1221.80 5.17 o

-8 11 1 8.00 7.43 0.62 o

-7 11 1 1.91 1.89 0.50 o

-6 11 1 867.53 872.85 4.06 o

-5 11 1 282.94 284.67 2.02 o

-4 11 1 224.57 221.03 1.73 o

-3 11 1 273.45 276.68 2.02 o

-2 11 1 9.16 12.14 0.68 o

-1 11 1 1571.16 1560.27 6.96 o

0 11 1 155.52 142.94 1.75 o

-11 12 1 37.24 38.87 1.24 o

-10 12 1 64.53 55.70 1.27 o

-9 12 1 190.42 201.83 1.98 o

-8 12 1 501.97 500.05 3.23 o

-7 12 1 146.42 157.54 1.76 o

-6 12 1 77.79 69.60 1.21 o

-5 12 1 462.93 445.92 2.79 o

-4 12 1 0.12 0.81 0.57 o

-3 12 1 226.28 209.41 1.97 o

-2 12 1 339.49 322.73 2.59 o

-1 12 1 11.76 18.44 0.99 o

0 12 1 136.38 134.77 2.49 o

-12 13 1 13.39 11.26 2.01 o

-11 13 1 117.87 118.35 3.16 o

-10 13 1 332.18 326.40 4.29 o

-9 13 1 44.06 44.17 1.25 o

-8 13 1 1.34 2.21 0.66 o

-7 13 1 125.58 123.05 1.72 o

-6 13 1 230.95 223.88 2.24 o

-5 13 1 81.73 82.89 1.58 o

-4 13 1 76.46 81.47 2.14 o

-3 13 1 31.27 29.88 1.21 o

-2 13 1 52.38 54.00 1.78 o

-1 13 1 98.14 102.62 6.89 o

-10 14 1 44.74 54.18 6.36 o

-9 14 1 932.76 960.64 8.08 o

-8 14 1 78.65 74.40 1.98 o

-7 14 1 359.84 375.28 3.69 o

-6 14 1 334.34 331.39 4.58 o

-5 14 1 0.82 0.91 1.19 o

-4 14 1 82.27 89.56 5.92 o

0 0 2 17357.67 17676.08 113.00 o

0 1 2 586.01 540.66 1.76 o

-1 2 2 8354.62 8096.99 20.64 o

0 2 2 3262.81 3566.58 8.66 o

-2 3 2 599.61 709.35 2.22 o

-1 3 2 669.52 798.14 2.44 o

0 3 2 417.95 475.54 1.61 o

-3 4 2 2268.99 2373.66 5.89 o

-2 4 2 10739.35 10735.89 26.57 o

-1 4 2 1912.68 2008.50 5.14 o

0 4 2 4479.66 4406.76 10.56 o

-4 5 2 100.59 104.19 0.70 o

-3 5 2 15.44 18.35 0.35 o

-2 5 2 2930.59 2930.20 7.11 o

-1 5 2 717.03 709.57 2.28 o

0 5 2 5143.07 5112.62 12.25 o

-5 6 2 536.91 543.34 1.96 o

-4 6 2 637.13 645.67 2.18 o

-3 6 2 1126.10 1092.01 3.20 o

-2 6 2 839.96 849.42 2.65 o

-1 6 2 1204.59 1190.91 3.56 o

0 6 2 1041.24 1070.50 3.32 o

-6 7 2 616.76 583.69 2.32 o

-5 7 2 5822.20 5768.07 14.79 o

-4 7 2 3276.45 3300.04 8.80 o

-3 7 2 64.39 66.62 0.68 o

-2 7 2 614.17 618.76 2.28 o

-1 7 2 0.75 1.63 0.33 o

0 7 2 1623.06 1580.66 5.19 o

-7 8 2 251.07 252.45 2.02 o

-6 8 2 111.91 114.64 1.07 o

-5 8 2 3585.74 3563.54 10.05 o

-4 8 2 170.52 176.50 1.19 o

-3 8 2 1654.88 1646.07 5.31 o

-2 8 2 983.33 985.16 3.70 o

-1 8 2 1889.86 1787.32 6.28 o

0 8 2 3857.30 3795.23 13.02 o

-8 9 2 535.90 554.04 2.85 o

-7 9 2 3.51 5.05 0.50 o

-6 9 2 2562.99 2527.28 8.43 o

-5 9 2 147.40 153.09 1.28 o

-4 9 2 98.20 97.89 1.12 o

-3 9 2 2625.36 2591.81 9.64 o

-2 9 2 38.09 36.86 0.79 o

-1 9 2 36.05 34.57 0.85 o

0 9 2 753.69 747.60 3.74 o

-9 10 2 59.26 63.67 1.17 o

-8 10 2 1815.06 1759.02 6.71 o

-7 10 2 201.01 202.85 1.71 o

-6 10 2 44.99 44.56 0.93 o

-5 10 2 900.05 882.09 3.84 o

-4 10 2 214.21 212.48 1.67 o

-3 10 2 8.80 9.47 0.55 o

-2 10 2 110.81 108.71 1.28 o

-1 10 2 2.92 3.56 0.56 o

0 10 2 66.66 67.73 1.24 o

-10 11 2 60.08 59.14 1.20 o

-9 11 2 171.66 174.21 1.81 o

-8 11 2 357.29 349.16 2.49 o

-7 11 2 58.79 54.44 1.06 o

-6 11 2 121.14 121.38 1.41 o

-5 11 2 92.29 89.43 1.23 o

-4 11 2 62.99 67.64 1.12 o

-3 11 2 293.32 294.56 2.19 o

-2 11 2 49.37 46.86 1.13 o

-1 11 2 1103.08 1137.35 5.45 o

0 11 2 31.94 28.68 1.01 o

-11 12 2 88.33 86.49 1.53 o

-10 12 2 53.58 62.22 1.35 o

-9 12 2 472.29 472.44 3.33 o

-8 12 2 983.39 1002.05 5.18 o

-7 12 2 129.63 125.02 1.61 o

-6 12 2 789.24 792.44 4.12 o

-5 12 2 4.78 4.41 0.63 o

-4 12 2 957.58 933.78 4.76 o

-3 12 2 508.63 500.82 3.39 o

-2 12 2 12.86 16.14 0.85 o

-1 12 2 470.26 469.81 3.40 o

0 12 2 35.33 37.72 1.62 o

-11 13 2 774.18 814.28 8.51 o

-10 13 2 221.46 223.43 2.45 o

-9 13 2 317.67 336.90 2.86 o

-8 13 2 267.30 254.89 2.36 o

-7 13 2 465.62 479.92 3.40 o

-6 13 2 50.61 53.98 1.39 o

-5 13 2 0.98 3.93 0.70 o

-4 13 2 769.09 798.68 4.62 o

-3 13 2 39.43 41.44 1.23 o

-2 13 2 85.47 84.96 2.70 o

-9 14 2 1.25 6.22 3.12 o

-8 14 2 0.37 2.00 1.28 o

-7 14 2 563.33 591.97 9.09 o

-6 14 2 22.29 19.95 1.92 o

-5 14 2 25.15 28.32 2.53 o

0 1 3 52.30 64.95 0.45 o

-1 2 3 1525.24 1626.16 4.24 o

0 2 3 985.78 1077.01 3.00 o

-2 3 3 4081.54 4157.48 10.36 o

-1 3 3 8046.29 8174.11 20.57 o

0 3 3 521.22 548.70 1.94 o

-3 4 3 1189.23 1238.46 3.61 o

-2 4 3 11.57 19.83 0.35 o

-1 4 3 1324.47 1405.54 3.94 o

0 4 3 21.36 14.54 0.36 o

-4 5 3 450.56 448.25 1.78 o

-3 5 3 318.10 305.17 1.38 o

-2 5 3 3388.54 3416.34 8.76 o

-1 5 3 165.93 155.76 0.89 o

0 5 3 126.78 118.79 0.85 o

-5 6 3 164.02 177.54 1.09 o

-4 6 3 3128.52 3124.17 8.43 o

-3 6 3 233.71 225.38 1.19 o

-2 6 3 430.35 441.85 1.84 o

-1 6 3 3970.37 4000.61 11.02 o

0 6 3 195.72 195.14 1.25 o

-6 7 3 204.13 198.45 1.33 o

-5 7 3 281.37 286.96 1.56 o

-4 7 3 1.68 2.46 0.37 o

-3 7 3 4110.61 4002.81 11.28 o

-2 7 3 1298.73 1278.46 4.20 o

-1 7 3 9.11 10.37 0.44 o

0 7 3 502.56 490.36 2.35 o

-7 8 3 381.25 376.68 2.18 o

-6 8 3 35.37 33.05 0.77 o

-5 8 3 46.23 44.09 0.87 o

-4 8 3 45.05 43.96 0.77 o

-3 8 3 249.79 242.41 1.60 o

-2 8 3 101.58 94.03 1.08 o

-1 8 3 51.89 52.89 0.90 o

0 8 3 45.50 44.05 0.93 o

-8 9 3 0.04 0.79 0.49 o

-7 9 3 115.47 120.06 1.36 o

-6 9 3 4.77 7.65 0.52 o

-5 9 3 375.80 365.33 2.16 o

-4 9 3 546.64 537.97 2.83 o

-3 9 3 1346.98 1300.64 5.03 o

-2 9 3 232.25 230.09 1.83 o

-1 9 3 206.72 194.02 1.71 o

0 9 3 640.45 624.06 3.39 o

-9 10 3 187.90 184.98 1.97 o

-8 10 3 395.88 387.96 2.69 o

-7 10 3 37.07 35.91 1.01 o

-6 10 3 206.92 213.61 1.82 o

-5 10 3 458.25 461.66 2.76 o

-4 10 3 0.57 1.15 0.54 o

-3 10 3 970.14 956.27 4.42 o

-2 10 3 169.64 175.23 1.68 o

-1 10 3 692.70 687.02 3.81 o

0 10 3 1.15 0.85 0.67 o

-10 11 3 210.50 219.13 2.29 o

-9 11 3 844.88 865.33 4.87 o

-8 11 3 11.56 13.21 0.77 o

-7 11 3 17.97 21.17 0.88 o

-6 11 3 298.71 300.71 2.46 o

-5 11 3 473.49 464.71 2.89 o

-4 11 3 184.24 185.39 1.81 o

-3 11 3 42.99 43.11 1.06 o

-2 11 3 110.28 113.37 1.66 o

-1 11 3 1868.67 1886.38 8.17 o

0 11 3 191.41 194.44 2.31 o

-11 12 3 28.00 29.24 1.18 o

-10 12 3 322.61 312.57 2.73 o

-9 12 3 148.70 153.22 1.90 o

-8 12 3 200.18 204.87 2.24 o

-7 12 3 7.78 11.09 0.80 o

-6 12 3 31.65 30.61 1.01 o

-5 12 3 91.57 87.87 1.47 o

-4 12 3 4.23 4.57 0.64 o

-3 12 3 179.11 172.51 1.99 o

-2 12 3 233.74 217.36 2.26 o

-1 12 3 1.15 2.96 0.73 o

0 12 3 79.85 92.80 7.25 o

-10 13 3 320.19 326.38 4.07 o

-9 13 3 1.90 2.12 0.70 o

-8 13 3 5.29 7.76 0.82 o

-7 13 3 103.91 99.77 1.68 o

-6 13 3 143.35 142.05 1.87 o

-5 13 3 16.90 18.97 0.95 o

-4 13 3 95.42 96.84 1.67 o

-3 13 3 32.02 28.97 1.52 o

0 0 4 40225.92 39372.32 224.68 o

0 1 4 634.67 667.48 2.09 o

-1 2 4 47.73 49.22 0.55 o

0 2 4 98.01 78.72 0.64 o

-2 3 4 1779.51 1833.48 4.81 o

-1 3 4 1129.06 1089.93 3.25 o

0 3 4 5592.78 5559.40 13.78 o

-3 4 4 20.71 17.06 0.41 o

-2 4 4 14.85 12.14 0.46 o

-1 4 4 243.62 237.40 1.23 o

0 4 4 126.46 121.83 0.88 o

-4 5 4 2819.25 2823.27 7.69 o

-3 5 4 1479.45 1438.08 4.16 o

-2 5 4 52.17 52.37 0.66 o

-1 5 4 2095.66 2071.58 5.91 o

0 5 4 442.93 434.42 1.84 o

-5 6 4 66.11 75.49 0.87 o

-4 6 4 2800.40 2796.88 7.90 o

-3 6 4 878.60 867.31 3.19 o

-2 6 4 1847.95 1877.32 6.04 o

-1 6 4 3029.25 2996.16 8.71 o

0 6 4 557.97 533.99 2.23 o

-6 7 4 2065.45 2023.22 6.82 o

-5 7 4 2.22 3.98 0.52 o

-4 7 4 226.58 237.10 1.47 o

-3 7 4 600.99 585.25 2.60 o

-2 7 4 1207.88 1207.88 4.35 o

-1 7 4 1045.29 1043.18 3.94 o

0 7 4 27.49 27.68 0.67 o

-7 8 4 3255.57 3205.18 10.56 o

-6 8 4 1297.19 1287.79 5.11 o

-5 8 4 546.95 535.55 2.62 o

-4 8 4 3585.52 3510.87 11.11 o

-3 8 4 34.88 34.72 0.87 o

-2 8 4 6.67 8.45 0.53 o

-1 8 4 224.20 229.07 1.77 o

0 8 4 1180.57 1168.82 5.69 o

-8 9 4 14.18 19.13 1.23 o

-7 9 4 626.49 639.82 3.50 o

-6 9 4 9.95 12.46 0.70 o

-5 9 4 160.54 164.15 1.58 o

-4 9 4 64.55 64.55 1.04 o

-3 9 4 1.65 2.63 0.48 o

-2 9 4 843.99 831.21 3.90 o

-1 9 4 105.69 102.60 1.43 o

0 9 4 190.99 185.14 1.98 o

-9 10 4 217.54 210.59 2.13 o

-8 10 4 24.02 28.65 1.02 o

-7 10 4 14.24 15.12 0.79 o

-6 10 4 356.77 346.85 2.62 o

-5 10 4 331.05 325.02 2.34 o

-4 10 4 35.18 38.85 0.95 o

-3 10 4 464.87 461.37 2.95 o

-2 10 4 779.36 773.10 3.97 o

-1 10 4 410.72 407.39 2.98 o

0 10 4 118.33 117.91 1.63 o

-10 11 4 1497.62 1497.04 7.06 o

-9 11 4 912.41 923.35 5.54 o

-8 11 4 2.96 3.51 0.68 o

-7 11 4 1732.92 1691.19 7.73 o

-6 11 4 979.73 998.39 5.14 o

-5 11 4 171.64 168.27 1.87 o

-4 11 4 744.01 735.46 4.04 o

-3 11 4 0.80 1.68 0.59 o

-2 11 4 189.47 189.97 2.07 o

-1 11 4 3.50 3.33 0.69 o

0 11 4 28.30 35.67 1.24 o

-11 12 4 36.60 37.00 4.35 o

-10 12 4 625.01 633.22 4.81 o

-9 12 4 108.73 115.15 1.93 o

-8 12 4 76.66 77.47 1.51 o

-7 12 4 32.87 34.11 1.16 o

-6 12 4 83.26 78.80 1.49 o

-5 12 4 311.72 313.06 2.86 o

-4 12 4 220.04 225.90 2.21 o

-3 12 4 217.97 227.32 2.56 o

-2 12 4 214.37 212.32 2.96 o

-1 12 4 24.14 23.32 4.44 o

-9 13 4 1.17 5.39 3.44 o

-8 13 4 193.84 211.03 4.12 o

-7 13 4 71.27 75.52 2.27 o

-6 13 4 468.78 466.96 5.25 o

-5 13 4 767.56 833.27 8.63 o

-4 13 4 127.79 133.68 5.09 o

0 1 5 47.89 46.82 0.56 o

-1 2 5 233.01 222.29 1.21 o

0 2 5 269.18 253.03 1.30 o

-2 3 5 1530.33 1542.38 4.76 o

-1 3 5 3591.02 3572.26 9.92 o

0 3 5 95.42 96.03 0.86 o

-3 4 5 622.08 645.70 2.54 o

-2 4 5 206.47 185.76 1.23 o

-1 4 5 92.68 73.68 0.83 o

0 4 5 176.87 170.47 1.47 o

-4 5 5 5.83 5.74 0.39 o

-3 5 5 2196.74 2132.43 6.59 o

-2 5 5 1043.92 1058.32 3.67 o

-1 5 5 12.37 10.10 0.44 o

0 5 5 554.38 544.25 2.49 o

-5 6 5 376.30 389.72 2.13 o

-4 6 5 797.78 810.22 3.28 o

-3 6 5 1066.16 1059.31 4.17 o

-2 6 5 180.19 183.07 1.50 o

-1 6 5 2973.48 2924.56 9.41 o

0 6 5 0.38 1.24 0.43 o

-6 7 5 117.09 107.03 1.25 o

-5 7 5 168.57 167.98 1.49 o

-4 7 5 67.76 62.16 0.98 o

-3 7 5 1154.30 1110.50 4.43 o

-2 7 5 471.62 469.91 2.44 o

-1 7 5 86.82 85.35 1.30 o

0 7 5 0.18 1.58 0.49 o

-7 8 5 4.33 5.91 0.61 o

-6 8 5 11.59 13.85 0.72 o

-5 8 5 31.59 29.95 0.80 o

-4 8 5 734.81 728.37 3.44 o

-3 8 5 19.45 22.68 0.73 o

-2 8 5 100.07 109.30 1.23 o

-1 8 5 159.84 159.97 1.66 o

0 8 5 1.02 2.20 0.62 o

-8 9 5 48.08 45.41 1.31 o

-7 9 5 0.19 1.04 0.55 o

-6 9 5 489.53 492.12 2.97 o

-5 9 5 481.36 478.09 3.01 o

-4 9 5 575.27 567.98 3.24 o

-3 9 5 1670.68 1653.11 6.70 o

-2 9 5 261.79 271.34 2.23 o

-1 9 5 165.47 165.27 1.86 o

0 9 5 252.77 257.20 2.50 o

-9 10 5 12.09 15.40 1.02 o

-8 10 5 233.58 240.97 2.55 o

-7 10 5 206.86 208.77 2.20 o

-6 10 5 135.01 145.02 1.71 o

-5 10 5 428.72 432.26 2.96 o

-4 10 5 4.92 5.23 0.64 o

-3 10 5 126.70 135.28 1.73 o

-2 10 5 51.26 52.87 1.25 o

-1 10 5 143.73 140.27 1.88 o

0 10 5 93.91 98.72 1.67 o

-10 11 5 101.25 108.43 2.07 o

-9 11 5 854.88 867.02 5.72 o

-8 11 5 9.46 8.84 0.91 o

-7 11 5 7.86 7.66 0.81 o

-6 11 5 731.14 732.70 4.34 o

-5 11 5 144.50 151.15 1.81 o

-4 11 5 122.15 124.30 1.79 o

-3 11 5 172.18 179.77 2.22 o

-2 11 5 1.36 1.42 0.71 o

-1 11 5 925.37 924.37 5.56 o

0 11 5 110.60 106.35 7.67 o

-8 12 5 472.88 465.36 4.92 o

-7 12 5 110.66 117.91 1.91 o

-6 12 5 61.06 59.55 1.44 o

-5 12 5 422.22 424.52 3.49 o

-4 12 5 1.97 2.16 0.85 o

-3 12 5 162.04 157.11 3.56 o

0 0 6 10401.45 10054.25 64.88 o

0 1 6 439.58 429.61 1.94 o

-1 2 6 4769.13 4688.27 13.17 o

0 2 6 303.79 318.55 1.71 o

-2 3 6 259.20 250.65 1.58 o

-1 3 6 11.85 11.38 0.68 o

0 3 6 93.92 95.56 1.03 o

-3 4 6 2416.87 2364.76 7.69 o

-2 4 6 3068.39 2978.98 8.91 o

-1 4 6 56.90 60.48 0.88 o

0 4 6 1501.23 1482.06 5.31 o

-4 5 6 189.22 188.37 1.48 o

-3 5 6 11.06 9.73 0.67 o

-2 5 6 849.85 838.20 3.60 o

-1 5 6 398.66 400.95 2.21 o

0 5 6 1383.93 1368.75 5.23 o

-5 6 6 331.64 312.03 2.12 o

-4 6 6 374.04 373.45 2.37 o

-3 6 6 1065.64 1057.77 4.57 o

-2 6 6 44.42 37.62 0.93 o

-1 6 6 97.71 98.27 1.21 o

0 6 6 1141.57 1130.07 5.07 o

-6 7 6 25.38 26.97 1.06 o

-5 7 6 937.53 924.49 4.60 o

-4 7 6 1058.38 1080.10 4.93 o

-3 7 6 69.83 72.24 1.15 o

-2 7 6 49.67 44.10 1.01 o

-1 7 6 31.53 32.20 0.90 o

0 7 6 462.42 455.22 3.04 o

-7 8 6 43.05 47.20 1.18 o

-6 8 6 0.02 0.54 0.56 o

-5 8 6 1752.74 1725.31 7.32 o

-4 8 6 1.41 1.78 0.55 o

-3 8 6 659.92 657.63 3.65 o

-2 8 6 242.95 237.85 2.08 o

-1 8 6 699.66 693.37 4.64 o

0 8 6 2603.28 2619.72 11.14 o

-8 9 6 134.48 138.94 2.09 o

-7 9 6 11.33 14.78 0.93 o

-6 9 6 1994.55 1995.30 8.64 o

-5 9 6 66.25 65.57 1.38 o

-4 9 6 335.76 339.04 2.76 o

-3 9 6 1738.00 1726.53 8.07 o

-2 9 6 33.87 35.30 1.14 o

-1 9 6 479.57 483.29 3.60 o

0 9 6 414.20 416.10 3.65 o

-9 10 6 1.39 1.51 0.79 o

-8 10 6 686.29 682.59 5.12 o

-7 10 6 284.83 284.90 2.98 o

-6 10 6 0.29 1.90 0.71 o

-5 10 6 124.89 125.68 1.92 o

-4 10 6 417.11 419.73 3.33 o

-3 10 6 14.39 15.85 0.95 o

-2 10 6 54.20 57.36 1.54 o

-1 10 6 10.48 12.05 1.04 o

0 10 6 17.43 19.31 2.27 o

-8 11 6 693.29 711.40 8.95 o

-7 11 6 4.57 5.49 0.87 o

-6 11 6 89.57 88.82 1.84 o

-5 11 6 89.99 91.03 1.83 o

-4 11 6 128.67 140.71 2.11 o

-3 11 6 203.22 213.08 3.49 o

0 1 7 12.31 14.04 0.73 o

-1 2 7 1.80 2.53 0.50 o

0 2 7 5.56 7.11 0.54 o

-2 3 7 1226.46 1203.28 4.65 o

-1 3 7 1691.43 1654.23 6.23 o

0 3 7 69.84 68.53 1.09 o

-3 4 7 546.01 551.25 2.86 o

-2 4 7 48.28 44.35 0.90 o

-1 4 7 33.41 40.62 0.91 o

0 4 7 94.55 95.16 1.19 o

-4 5 7 66.07 66.54 1.06 o

-3 5 7 426.83 417.25 2.52 o

-2 5 7 781.73 768.45 3.79 o

-1 5 7 6.66 5.71 0.61 o

0 5 7 10.57 9.95 0.68 o

-5 6 7 279.28 281.74 2.27 o

-4 6 7 618.99 627.78 3.65 o

-3 6 7 412.56 401.83 2.71 o

-2 6 7 162.99 164.50 1.79 o

-1 6 7 1484.81 1455.88 6.45 o

0 6 7 101.37 108.36 1.52 o

-6 7 7 24.93 23.72 0.94 o

-5 7 7 127.37 125.41 1.69 o

-4 7 7 4.01 4.39 0.67 o

-3 7 7 1297.95 1254.21 5.68 o

-2 7 7 492.35 492.01 3.36 o

-1 7 7 32.42 34.90 1.08 o

0 7 7 62.48 61.65 1.35 o

-7 8 7 52.19 54.35 1.31 o

-6 8 7 25.74 27.05 1.04 o

-5 8 7 13.34 13.49 0.85 o

-4 8 7 174.24 174.27 1.95 o

-3 8 7 99.08 101.10 1.59 o

-2 8 7 3.98 5.91 0.71 o

-1 8 7 108.30 105.52 1.74 o

0 8 7 26.77 27.57 1.19 o

-8 9 7 45.08 47.85 1.61 o

-7 9 7 34.49 38.53 1.33 o

-6 9 7 94.93 105.35 1.81 o

-5 9 7 109.37 111.71 1.78 o

-4 9 7 284.27 277.04 2.70 o

-3 9 7 1024.00 1020.01 6.23 o

-2 9 7 179.26 184.46 2.57 o

-1 9 7 77.22 76.44 1.69 o

0 9 7 300.44 301.07 6.33 o

-8 10 7 144.22 145.82 5.38 o

-7 10 7 84.95 86.51 2.74 o

-6 10 7 209.41 215.34 2.57 o

-5 10 7 239.38 248.20 2.74 o

-4 10 7 1.45 1.53 0.79 o

-3 10 7 429.76 446.25 5.73 o

-2 10 7 35.20 37.05 3.72 o

0 0 8 7983.04 7677.09 60.66 o

0 1 8 134.05 140.59 1.75 o

-1 2 8 50.33 47.38 1.17 o

0 2 8 25.12 25.80 0.96 o

-2 3 8 793.06 774.43 4.43 o

-1 3 8 381.62 382.51 2.90 o

0 3 8 1883.11 1864.26 7.88 o

-3 4 8 87.95 90.11 1.38 o

-2 4 8 0.20 1.35 0.60 o

-1 4 8 32.89 34.47 0.99 o

0 4 8 97.44 94.23 1.41 o

-4 5 8 1390.57 1369.52 6.37 o

-3 5 8 327.75 331.67 2.83 o

-2 5 8 26.80 29.18 1.03 o

-1 5 8 578.84 584.39 3.76 o

0 5 8 302.96 289.07 2.67 o

-5 6 8 114.42 112.68 1.84 o

-4 6 8 1088.22 1080.43 5.63 o

-3 6 8 411.70 412.95 3.01 o

-2 6 8 1198.45 1198.51 5.85 o

-1 6 8 1436.80 1451.53 7.20 o

0 6 8 359.18 355.16 3.20 o

-6 7 8 957.22 955.68 5.74 o

-5 7 8 26.25 30.62 1.19 o

-4 7 8 94.64 100.00 1.64 o

-3 7 8 157.29 153.46 1.97 o

-2 7 8 437.73 445.54 3.35 o

-1 7 8 336.55 338.41 3.03 o

0 7 8 19.48 22.90 1.15 o

-7 8 8 1854.19 1902.38 11.09 o

-6 8 8 615.17 616.48 4.45 o

-5 8 8 250.00 241.69 2.48 o

-4 8 8 1898.66 1929.27 9.05 o

-3 8 8 31.76 32.05 1.21 o

-2 8 8 1.85 2.15 0.79 o

-1 8 8 72.64 79.20 1.96 o

0 8 8 378.09 399.18 13.32 o

-6 9 8 9.73 12.59 1.99 o

-5 9 8 66.31 64.21 2.01 o

-4 9 8 164.52 162.16 5.33 o

-3 9 8 5.13 4.54 1.74 o

0 1 9 9.29 9.92 0.82 o

-1 2 9 36.19 33.72 1.18 o

0 2 9 2.77 3.63 0.82 o

-2 3 9 590.29 586.46 4.42 o

-1 3 9 1476.94 1449.23 7.31 o

0 3 9 21.10 22.04 1.00 o

-3 4 9 184.74 190.66 2.27 o

-2 4 9 9.31 9.01 0.85 o

-1 4 9 175.98 186.09 2.37 o

0 4 9 27.81 31.07 1.25 o

-4 5 9 53.96 52.12 1.85 o

-3 5 9 335.62 340.46 3.55 o

-2 5 9 443.96 440.37 4.14 o

-1 5 9 19.27 17.95 1.12 o

0 5 9 0.01 0.94 0.91 o

-5 6 9 50.54 52.05 1.94 o

-4 6 9 701.87 717.41 5.65 o

-3 6 9 126.47 122.17 2.10 o

-2 6 9 24.44 26.87 1.21 o

-1 6 9 1238.90 1230.65 8.81 o

0 6 9 30.10 29.69 2.95 o

-4 7 9 0.00 1.42 1.40 o

-3 7 9 553.50 565.22 6.92 o

-2 7 9 270.68 274.76 7.01 o

0 0 10 1627.18 1639.95 21.70 o

0 1 10 128.94 129.06 2.18 o

-1 2 10 1463.83 1477.88 9.09 o

0 2 10 107.19 106.89 2.67 o

-2 3 10 47.75 54.23 2.51 o

-1 3 10 1.14 1.07 1.14 o

0 3 10 1.57 -0.55 1.86 o

-2 4 10 1206.24 1241.10 18.23 o

**Table 6b: FoFc for sample HNFCL8**

#

# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag

#

data\_hnf5cl58\_0m

\_shelx\_title ' HNF5CL58\_0m in P6(3)/m'

\_shelx\_refln\_list\_code 4

\_shelx\_F\_calc\_maximum 199.25

\_exptl\_crystal\_F\_000 508.00

\_reflns\_d\_resolution\_high 0.6510

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-y, x-y, z'

'-x+y, -x, z'

'-x, -y, z+1/2'

'y, -x+y, z+1/2'

'x-y, x, z+1/2'

'-x, -y, -z'

'y, -x+y, -z'

'x-y, x, -z'

'x, y, -z-1/2'

'-y, x-y, -z-1/2'

'-x+y, -x, -z-1/2'

\_cell\_length\_a 9.5101

\_cell\_length\_b 9.5101

\_cell\_length\_c 6.8300

\_cell\_angle\_alpha 90.000

\_cell\_angle\_beta 90.000

\_cell\_angle\_gamma 120.000

\_shelx\_F\_squared\_multiplier 1.000

loop\_

\_refln\_index\_h

\_refln\_index\_k

\_refln\_index\_l

\_refln\_F\_squared\_calc

\_refln\_F\_squared\_meas

\_refln\_F\_squared\_sigma

\_refln\_observed\_status

0 1 0 268.18 254.02 1.74 o

-1 2 0 45.23 47.05 0.47 o

0 2 0 250.76 249.05 1.64 o

-2 3 0 41.30 27.44 0.77 o

-1 3 0 2627.21 2445.26 14.48 o

0 3 0 21366.28 21752.96 148.38 o

-2 4 0 178.29 147.49 1.12 o

-1 4 0 1191.33 1188.93 7.15 o

0 4 0 723.93 652.47 4.03 o

-4 5 0 5301.93 5134.66 29.23 o

-3 5 0 2883.56 2981.80 16.83 o

-2 5 0 28.36 24.47 0.61 o

-1 5 0 6219.33 6244.71 37.04 o

0 5 0 215.39 186.51 1.32 o

-5 6 0 21.28 26.59 0.49 o

-4 6 0 4185.90 4279.40 24.13 o

-3 6 0 1443.82 1470.46 8.88 o

-2 6 0 107.87 102.21 0.95 o

-1 6 0 1800.11 1776.37 11.80 o

0 6 0 677.40 622.06 3.75 o

-6 7 0 1056.01 996.30 6.72 o

-5 7 0 1504.46 1489.91 9.09 o

-4 7 0 463.08 449.04 2.92 o

-3 7 0 351.75 336.50 2.30 o

-2 7 0 5245.61 5234.04 36.94 o

-1 7 0 1425.61 1442.80 10.32 o

0 7 0 37.18 32.38 0.65 o

-7 8 0 4655.49 4744.94 29.21 o

-6 8 0 413.38 425.80 3.16 o

-5 8 0 1143.64 1157.94 7.23 o

-4 8 0 4565.68 4633.39 27.28 o

-3 8 0 134.41 135.36 1.27 o

-2 8 0 26.95 20.99 0.56 o

-1 8 0 736.32 775.23 6.49 o

0 8 0 2609.30 2601.28 17.08 o

-8 9 0 49.17 37.42 0.79 o

-7 9 0 579.21 580.55 4.19 o

-6 9 0 32.64 37.44 0.72 o

-5 9 0 132.70 127.95 1.50 o

-4 9 0 104.84 99.79 1.25 o

-3 9 0 1.10 2.28 0.58 o

-2 9 0 681.36 672.48 5.25 o

-1 9 0 179.81 178.83 1.93 o

0 9 0 500.96 485.00 4.29 o

-9 10 0 296.22 287.56 3.13 o

-8 10 0 356.13 366.26 3.48 o

-7 10 0 31.51 30.04 0.86 o

-6 10 0 381.30 375.81 3.52 o

-5 10 0 1613.40 1610.93 12.84 o

-4 10 0 92.79 91.20 1.47 o

-3 10 0 675.39 677.15 5.99 o

-2 10 0 1493.29 1512.96 12.20 o

-1 10 0 167.74 164.55 2.15 o

0 10 0 95.55 103.21 1.80 o

-10 11 0 2071.03 2053.08 18.87 o

-9 11 0 542.09 564.42 5.68 o

-8 11 0 360.50 366.28 3.80 o

-7 11 0 2230.11 2237.68 17.73 o

-6 11 0 953.61 972.92 7.85 o

-5 11 0 21.61 19.05 1.05 o

-4 11 0 942.91 943.65 8.69 o

-3 11 0 10.98 9.99 0.67 o

-2 11 0 136.89 125.36 2.03 o

-1 11 0 7.38 6.37 0.67 o

0 11 0 24.24 17.39 1.01 o

-11 12 0 2.43 2.76 0.74 o

-10 12 0 648.92 645.76 7.73 o

-9 12 0 313.84 315.89 4.09 o

-8 12 0 113.12 115.63 2.23 o

-7 12 0 21.55 20.19 0.87 o

-6 12 0 255.83 247.26 3.14 o

-5 12 0 419.25 440.11 5.05 o

-4 12 0 565.13 562.56 7.49 o

-3 12 0 738.44 733.88 7.77 o

-2 12 0 263.19 264.75 3.63 o

-1 12 0 138.07 131.74 2.60 o

0 12 0 1160.69 1158.28 11.46 o

-11 13 0 4.05 6.80 1.74 o

-10 13 0 63.32 58.76 1.77 o

-9 13 0 8.26 10.77 0.90 o

-8 13 0 267.88 278.71 3.76 o

-7 13 0 524.77 516.74 5.92 o

-6 13 0 372.04 355.17 4.48 o

-5 13 0 1010.13 1030.87 10.24 o

-4 13 0 594.20 609.01 6.75 o

-3 13 0 311.82 298.36 4.04 o

-2 13 0 312.09 302.73 5.07 o

-1 13 0 64.79 59.10 2.91 o

-10 14 0 379.14 368.56 8.11 o

-9 14 0 198.51 190.20 5.46 o

-8 14 0 45.01 44.08 1.57 o

-7 14 0 116.19 112.17 2.24 o

-6 14 0 423.58 424.02 6.40 o

-5 14 0 211.24 192.20 5.76 o

-4 14 0 25.96 28.55 2.14 o

0 1 1 178.29 168.40 0.93 o

-1 2 1 309.03 302.39 1.57 o

0 2 1 267.71 277.23 1.43 o

-2 3 1 4358.89 4202.01 16.75 o

-1 3 1 9606.28 9487.79 38.65 o

0 3 1 707.43 759.35 3.32 o

-3 4 1 1384.73 1369.07 5.60 o

-2 4 1 212.33 176.19 0.94 o

-1 4 1 217.49 261.90 1.31 o

0 4 1 110.59 91.05 0.58 o

-4 5 1 34.09 33.91 0.35 o

-3 5 1 3305.63 3280.75 13.35 o

-2 5 1 2935.04 2926.65 12.13 o

-1 5 1 36.00 36.61 0.35 o

0 5 1 923.99 986.60 3.99 o

-5 6 1 665.76 670.14 2.99 o

-4 6 1 1449.61 1399.52 6.01 o

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-6 7 1 322.64 302.28 1.58 o

-5 7 1 254.12 257.62 1.38 o

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-1 6 3 3842.99 3911.11 17.14 o

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-2 6 7 151.42 152.27 1.45 o

-1 6 7 1386.05 1392.77 7.76 o

0 6 7 92.66 101.50 1.22 o

-6 7 7 24.12 22.41 0.71 o

-5 7 7 118.21 115.02 1.28 o

-4 7 7 4.11 4.49 0.43 o

-3 7 7 1202.41 1186.71 6.73 o

-2 7 7 452.89 450.01 2.98 o

-1 7 7 31.02 31.14 0.80 o

0 7 7 57.31 55.37 0.95 o

-7 8 7 47.30 48.38 0.91 o

-6 8 7 23.03 25.16 0.73 o

-5 8 7 12.49 12.76 0.58 o

-4 8 7 160.98 159.81 1.60 o

-3 8 7 89.49 93.28 1.15 o

-2 8 7 3.65 5.28 0.47 o

-1 8 7 98.55 94.69 1.28 o

0 8 7 23.98 25.88 0.75 o

-8 9 7 41.10 41.83 0.97 o

-7 9 7 31.98 32.49 0.86 o

-6 9 7 87.00 88.94 1.21 o

-5 9 7 99.05 100.32 1.28 o

-4 9 7 257.61 257.61 2.27 o

-3 9 7 927.25 910.27 5.51 o

-2 9 7 163.01 168.11 1.71 o

-1 9 7 68.93 67.90 1.12 o

0 9 7 265.23 264.84 5.25 o

-8 10 7 126.94 121.91 3.32 o

-7 10 7 76.25 77.65 1.67 o

-6 10 7 186.53 187.38 1.89 o

-5 10 7 214.60 213.55 1.98 o

-4 10 7 1.40 1.65 0.42 o

-3 10 7 382.25 388.17 4.26 o

-2 10 7 32.33 36.08 2.59 o

0 0 8 7532.52 7557.64 109.68 o

0 1 8 126.61 131.09 1.34 o

-1 2 8 47.19 46.35 0.83 o

0 2 8 23.83 25.29 0.67 o

-2 3 8 735.84 735.97 4.90 o

-1 3 8 355.78 359.66 2.81 o

0 3 8 1754.55 1776.92 11.12 o

-3 4 8 80.48 85.24 1.20 o

-2 4 8 0.19 1.10 0.41 o

-1 4 8 31.07 32.09 0.81 o

0 4 8 88.65 88.13 1.25 o

-4 5 8 1280.03 1271.30 8.38 o

-3 5 8 307.25 302.51 2.47 o

-2 5 8 24.70 27.26 0.75 o

-1 5 8 541.93 535.78 3.83 o

0 5 8 275.81 265.74 2.40 o

-5 6 8 103.97 105.63 1.48 o

-4 6 8 995.59 986.95 6.78 o

-3 6 8 376.10 370.60 2.84 o

-2 6 8 1094.39 1107.56 6.80 o

-1 6 8 1311.58 1340.92 8.28 o

0 6 8 327.21 327.10 2.82 o

-6 7 8 871.84 857.30 6.13 o

-5 7 8 22.61 27.67 0.87 o

-4 7 8 86.79 90.46 1.22 o

-3 7 8 146.45 138.81 1.53 o

-2 7 8 395.30 406.09 3.19 o

-1 7 8 306.31 306.04 2.62 o

0 7 8 17.40 19.73 0.76 o

-7 8 8 1650.88 1596.83 21.48 o

-6 8 8 558.68 539.62 4.26 o

-5 8 8 224.79 212.05 2.09 o

-4 8 8 1717.26 1718.17 10.03 o

-3 8 8 27.59 29.13 0.86 o

-2 8 8 1.43 2.46 0.47 o

-1 8 8 67.12 68.86 1.80 o

-7 9 8 247.22 236.82 8.32 o

-6 9 8 8.55 6.71 1.92 o

-5 9 8 59.02 56.99 1.62 o

-4 9 8 144.38 131.78 3.44 o

0 1 9 8.65 9.63 0.91 o

-1 2 9 33.79 35.61 1.00 o

0 2 9 2.44 4.55 0.60 o

-2 3 9 544.30 545.43 5.22 o

-1 3 9 1357.52 1345.47 10.99 o

0 3 9 19.17 19.39 0.88 o

-3 4 9 167.49 170.49 2.15 o

-2 4 9 7.99 9.22 0.67 o

-1 4 9 158.59 163.54 1.89 o

0 4 9 24.75 27.69 1.00 o

-4 5 9 47.81 50.64 1.13 o

-3 5 9 305.52 304.39 3.13 o

-2 5 9 407.46 403.96 3.64 o

-1 5 9 17.39 18.07 0.74 o

0 5 9 0.02 0.81 0.45 o

-5 6 9 45.42 45.62 1.27 o

-4 6 9 633.45 629.51 5.20 o

-3 6 9 115.07 110.29 1.78 o

-2 6 9 21.79 23.70 0.84 o

-1 6 9 1117.73 1097.01 8.95 o

0 6 9 26.13 24.89 2.14 o

-5 7 9 97.42 84.44 4.80 o

-4 7 9 0.00 -0.46 0.93 o

-3 7 9 493.60 468.85 6.79 o

-2 7 9 242.81 238.09 6.72 o

0 0 10 1465.78 1432.08 32.80 o

0 1 10 116.09 117.37 2.59 o

-1 2 10 1324.65 1292.85 13.45 o

0 2 10 95.90 95.82 2.01 o

-2 3 10 40.30 44.49 2.14 o

-1 3 10 0.94 1.63 0.89 o

0 3 10 1.06 0.92 0.80 o

-3 4 10 306.38 301.97 7.02 o

-1 4 10 44.72 42.53 3.20 o

**Table 6c: FoFc for sample HNFCL9**

# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag

#

data\_hnf5cl59\_0m

\_shelx\_title ' HNF5CL59\_0m in P6(3)/m'

\_shelx\_refln\_list\_code 4

\_shelx\_F\_calc\_maximum 146.50

\_exptl\_crystal\_F\_000 508.00

\_reflns\_d\_resolution\_high 0.6543

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-y, x-y, z'

'-x+y, -x, z'

'-x, -y, z+1/2'

'y, -x+y, z+1/2'

'x-y, x, z+1/2'

'-x, -y, -z'

'y, -x+y, -z'

'x-y, x, -z'

'x, y, -z-1/2'

'-y, x-y, -z-1/2'

'-x+y, -x, -z-1/2'

\_cell\_length\_a 9.5100

\_cell\_length\_b 9.5100

\_cell\_length\_c 6.8289

\_cell\_angle\_alpha 90.000

\_cell\_angle\_beta 90.000

\_cell\_angle\_gamma 120.000

\_shelx\_F\_squared\_multiplier 1.000

loop\_

\_refln\_index\_h

\_refln\_index\_k

\_refln\_index\_l

\_refln\_F\_squared\_calc

\_refln\_F\_squared\_meas

\_refln\_F\_squared\_sigma

\_refln\_observed\_status

0 1 0 277.45 282.38 1.31 o

-1 2 0 48.10 50.34 0.38 o

0 2 0 257.59 264.14 1.28 o

-2 3 0 44.64 28.30 0.37 o

-1 3 0 2659.42 2548.47 9.94 o

0 3 0 21462.26 21353.48 88.70 o

-3 4 0 8105.25 9167.68 31.96 o

-2 4 0 174.54 156.43 0.97 o

-1 4 0 1206.67 1257.07 5.61 o

0 4 0 729.33 684.69 2.84 o

-4 5 0 5370.28 5250.48 27.60 o

-3 5 0 2941.69 3072.15 10.60 o

-2 5 0 28.08 24.42 0.40 o

-1 5 0 6308.48 6318.62 25.87 o

0 5 0 218.77 193.86 1.22 o

-5 6 0 20.93 27.84 0.55 o

-4 6 0 4279.16 4402.44 16.42 o

-3 6 0 1471.01 1512.20 6.35 o

-2 6 0 114.39 109.00 1.31 o

-1 6 0 1860.93 1867.39 7.63 o

0 6 0 694.79 653.53 3.13 o

-6 7 0 1100.85 1039.33 4.37 o

-5 7 0 1538.29 1533.34 6.01 o

-4 7 0 477.48 474.49 2.22 o

-3 7 0 364.30 352.89 2.18 o

-2 7 0 5397.73 5372.52 20.75 o

-1 7 0 1475.42 1501.54 6.58 o

0 7 0 39.75 35.78 0.81 o

-7 8 0 4861.88 4890.55 20.17 o

-6 8 0 431.08 441.62 2.61 o

-5 8 0 1187.99 1202.30 5.76 o

-4 8 0 4739.20 4795.30 20.53 o

-3 8 0 140.41 140.09 1.38 o

-2 8 0 28.44 23.50 0.69 o

-1 8 0 769.43 802.92 4.38 o

0 8 0 2746.75 2712.67 11.92 o

-8 9 0 51.54 39.71 1.00 o

-7 9 0 611.05 615.14 4.17 o

-6 9 0 34.34 38.07 0.97 o

-5 9 0 139.58 130.44 1.70 o

-4 9 0 109.44 102.40 1.33 o

-3 9 0 1.20 2.41 0.47 o

-2 9 0 717.77 701.35 4.07 o

-1 9 0 188.56 181.29 1.80 o

0 9 0 530.21 511.59 3.40 o

-9 10 0 315.17 311.90 3.08 o

-8 10 0 379.28 384.03 3.44 o

-7 10 0 33.96 31.65 1.07 o

-6 10 0 405.34 386.36 3.35 o

-5 10 0 1703.05 1658.10 9.40 o

-4 10 0 96.58 92.17 1.50 o

-3 10 0 714.83 702.65 4.38 o

-2 10 0 1592.41 1595.16 8.84 o

-1 10 0 180.36 175.80 1.90 o

0 10 0 102.60 109.28 1.88 o

-10 11 0 2259.27 2233.88 12.62 o

-9 11 0 590.68 597.99 4.80 o

-8 11 0 390.53 392.87 3.62 o

-7 11 0 2401.21 2346.74 13.90 o

-6 11 0 1024.74 1007.98 7.21 o

-5 11 0 22.33 21.61 0.95 o

-4 11 0 1017.82 990.79 6.56 o

-3 11 0 12.31 12.21 0.94 o

-2 11 0 147.76 139.61 1.76 o

-1 11 0 8.11 8.80 1.06 o

0 11 0 27.10 22.19 1.14 o

-11 12 0 2.35 3.83 0.82 o

-10 12 0 716.76 717.38 6.07 o

-9 12 0 346.82 341.01 3.81 o

-8 12 0 125.93 124.24 2.23 o

-7 12 0 22.79 23.39 1.21 o

-6 12 0 278.42 262.07 3.02 o

-5 12 0 454.79 473.39 4.51 o

-4 12 0 619.28 610.24 4.63 o

-3 12 0 806.94 814.26 5.64 o

-2 12 0 285.68 290.14 3.49 o

-1 12 0 154.79 147.62 2.55 o

0 12 0 1300.53 1324.60 12.09 o

-12 13 0 333.13 353.96 6.40 o

-11 13 0 4.23 5.55 0.91 o

-10 13 0 71.43 66.75 1.85 o

-9 13 0 8.89 11.64 1.02 o

-8 13 0 295.52 318.98 3.79 o

-7 13 0 583.21 575.11 5.32 o

-6 13 0 411.57 402.45 4.29 o

-5 13 0 1117.79 1158.74 7.96 o

-4 13 0 661.13 670.44 5.10 o

-3 13 0 347.78 337.83 3.67 o

-2 13 0 353.66 353.22 4.47 o

-1 13 0 74.29 71.15 2.99 o

-10 14 0 427.57 447.39 12.58 o

-9 14 0 224.18 224.99 6.28 o

-8 14 0 49.52 46.02 2.08 o

-7 14 0 130.84 128.36 2.53 o

-6 14 0 471.15 487.62 5.42 o

-5 14 0 238.42 231.85 3.59 o

-4 14 0 29.36 31.35 2.88 o

0 1 1 179.04 189.61 1.33 o

-1 2 1 310.35 324.76 1.08 o

0 2 1 269.94 299.61 1.05 o

-2 3 1 4386.72 4377.45 11.09 o

-1 3 1 9652.55 9579.58 26.09 o

0 3 1 712.83 801.01 2.42 o

-3 4 1 1401.95 1430.31 3.71 o

-2 4 1 213.11 185.22 0.76 o

-1 4 1 218.80 271.70 1.11 o

0 4 1 111.71 96.41 0.58 o

-4 5 1 34.37 35.09 0.36 o

-3 5 1 3358.25 3379.74 9.45 o

-2 5 1 2978.33 3000.23 7.78 o

-1 5 1 36.04 37.82 0.42 o

0 5 1 943.44 1032.24 3.08 o

-5 6 1 681.74 705.99 2.20 o

-4 6 1 1484.32 1457.77 4.02 o

-3 6 1 1837.50 1790.27 4.79 o

-2 6 1 605.32 629.74 2.21 o

-1 6 1 5064.39 5161.25 14.34 o

0 6 1 10.13 11.35 0.40 o

-6 7 1 332.63 318.20 1.42 o

-5 7 1 262.82 268.98 1.20 o

-4 7 1 84.15 98.13 0.65 o

-3 7 1 3135.20 3093.55 8.70 o

-2 7 1 1084.06 1059.15 3.50 o

-1 7 1 119.56 118.20 0.97 o

0 7 1 5.72 9.46 0.48 o

-7 8 1 25.74 25.33 0.52 o

-6 8 1 38.30 30.99 0.58 o

-5 8 1 49.24 44.11 0.61 o

-4 8 1 1143.49 1118.19 3.58 o

-3 8 1 101.57 98.94 0.85 o

-2 8 1 63.15 68.65 0.77 o

-1 8 1 197.67 202.84 1.24 o

0 8 1 17.46 18.95 0.51 o

-8 9 1 122.12 114.54 1.08 o

-7 9 1 14.17 15.05 0.53 o

-6 9 1 486.86 464.67 2.32 o

-5 9 1 669.30 651.21 2.98 o

-4 9 1 846.96 845.68 3.51 o

-3 9 1 2759.76 2677.85 8.48 o

-2 9 1 376.68 369.51 1.94 o

-1 9 1 288.17 287.02 1.66 o

0 9 1 542.86 541.14 2.72 o

-9 10 1 34.39 36.17 0.85 o

-8 10 1 386.66 395.74 2.40 o

-7 10 1 243.77 230.25 1.87 o

-6 10 1 293.01 297.75 2.03 o

-5 10 1 689.03 681.56 3.11 o

-4 10 1 5.31 5.62 0.43 o

-3 10 1 380.10 381.51 2.11 o

-2 10 1 116.20 120.05 1.08 o

-1 10 1 350.53 343.20 2.17 o

0 10 1 72.27 71.93 1.09 o

-10 11 1 131.58 134.17 1.52 o

-9 11 1 1229.40 1222.21 5.77 o

-8 11 1 8.08 7.23 0.58 o

-7 11 1 1.87 1.55 0.44 o

-6 11 1 867.78 875.37 4.29 o

-5 11 1 279.58 278.50 2.15 o

-4 11 1 222.82 221.29 1.74 o

-3 11 1 273.53 278.77 1.91 o

-2 11 1 9.47 13.39 0.68 o

-1 11 1 1568.98 1574.74 6.38 o

0 11 1 154.01 143.45 1.61 o

-11 12 1 36.83 40.16 1.13 o

-10 12 1 66.33 56.45 1.18 o

-9 12 1 191.44 199.74 2.02 o

-8 12 1 502.58 492.43 3.45 o

-7 12 1 145.74 154.87 1.75 o

-6 12 1 77.09 68.41 1.22 o

-5 12 1 461.47 443.82 2.95 o

-4 12 1 0.17 1.50 0.46 o

-3 12 1 228.30 211.49 1.86 o

-2 12 1 339.72 325.28 2.46 o

-1 12 1 12.03 15.93 0.78 o

0 12 1 136.68 133.41 1.92 o

-12 13 1 13.42 9.99 2.96 o

-11 13 1 118.64 120.07 2.19 o

-10 13 1 329.86 319.67 2.85 o

-9 13 1 42.87 41.91 1.14 o

-8 13 1 1.27 3.55 0.57 o

-7 13 1 126.86 123.93 1.67 o

-6 13 1 231.00 221.34 2.18 o

-5 13 1 82.55 83.64 1.31 o

-4 13 1 76.05 82.38 1.31 o

-3 13 1 31.13 30.96 0.97 o

-2 13 1 52.17 55.50 1.59 o

-1 13 1 98.33 99.51 5.92 o

-10 14 1 45.50 55.12 5.18 o

-9 14 1 934.14 956.30 27.58 o

-8 14 1 78.61 71.19 2.11 o

-7 14 1 358.91 378.01 3.62 o

-6 14 1 335.09 327.73 3.30 o

-5 14 1 0.86 2.49 0.73 o

-4 14 1 80.63 76.93 2.59 o

0 0 2 17320.03 17001.85 162.82 o

0 1 2 579.84 536.46 1.55 o

-1 2 2 8371.03 8117.00 19.49 o

0 2 2 3249.46 3527.71 8.44 o

-2 3 2 605.41 710.79 2.08 o

-1 3 2 663.15 787.10 2.28 o

0 3 2 420.91 476.89 1.67 o

-3 4 2 2259.24 2373.48 6.00 o

-2 4 2 10746.05 10714.24 27.52 o

-1 4 2 1911.70 2003.05 5.45 o

0 4 2 4466.27 4364.21 11.75 o

-4 5 2 103.10 106.50 0.64 o

-3 5 2 14.69 17.08 0.30 o

-2 5 2 2923.11 2940.51 7.68 o

-1 5 2 721.48 712.37 2.31 o

0 5 2 5132.77 5104.83 13.65 o

-5 6 2 532.87 538.56 1.93 o

-4 6 2 638.86 645.13 2.13 o

-3 6 2 1127.24 1102.52 3.14 o

-2 6 2 844.81 851.72 2.84 o

-1 6 2 1208.79 1193.27 3.77 o

0 6 2 1043.99 1078.61 3.52 o

-6 7 2 619.57 585.97 2.24 o

-5 7 2 5821.71 5788.10 15.81 o

-4 7 2 3270.24 3312.46 8.79 o

-3 7 2 63.30 65.88 0.63 o

-2 7 2 613.23 612.79 2.35 o

-1 7 2 0.71 2.10 0.28 o

0 7 2 1620.04 1624.17 9.94 o

-7 8 2 249.63 250.62 1.41 o

-6 8 2 112.29 114.08 0.90 o

-5 8 2 3585.56 3594.24 10.96 o

-4 8 2 170.94 175.78 1.14 o

-3 8 2 1639.13 1624.65 5.44 o

-2 8 2 979.94 984.37 3.49 o

-1 8 2 1885.11 1777.91 5.81 o

0 8 2 3840.42 3811.59 11.45 o

-8 9 2 533.93 553.80 2.71 o

-7 9 2 3.98 6.91 0.40 o

-6 9 2 2556.95 2547.03 8.19 o

-5 9 2 146.43 154.10 1.23 o

-4 9 2 96.06 93.03 0.97 o

-3 9 2 2624.01 2586.37 8.42 o

-2 9 2 37.85 36.29 1.03 o

-1 9 2 35.65 35.60 0.68 o

0 9 2 751.73 761.89 3.36 o

-9 10 2 58.97 64.45 1.07 o

-8 10 2 1813.65 1759.70 7.21 o

-7 10 2 201.14 204.04 1.69 o

-6 10 2 44.04 43.08 0.83 o

-5 10 2 901.21 886.80 4.05 o

-4 10 2 214.55 213.22 1.59 o

-3 10 2 8.38 8.98 0.46 o

-2 10 2 110.83 107.74 1.16 o

-1 10 2 2.99 4.63 0.51 o

0 10 2 65.99 69.43 1.12 o

-10 11 2 59.62 56.42 1.17 o

-9 11 2 172.27 173.67 1.77 o

-8 11 2 358.51 350.77 2.62 o

-7 11 2 58.61 54.92 1.03 o

-6 11 2 122.66 120.91 1.37 o

-5 11 2 93.58 90.88 1.16 o

-4 11 2 61.79 64.29 1.09 o

-3 11 2 290.35 290.53 1.97 o

-2 11 2 48.41 48.03 0.92 o

-1 11 2 1098.49 1133.80 5.16 o

0 11 2 31.46 27.50 0.98 o

-11 12 2 87.35 83.78 1.49 o

-10 12 2 53.95 62.90 1.33 o

-9 12 2 466.22 469.86 3.64 o

-8 12 2 981.60 980.40 5.21 o

-7 12 2 128.89 122.47 1.65 o

-6 12 2 790.32 791.39 4.47 o

-5 12 2 4.86 4.49 0.54 o

-4 12 2 956.10 936.44 4.68 o

-3 12 2 510.77 504.54 3.24 o

-2 12 2 12.92 15.89 0.75 o

-1 12 2 472.24 473.76 3.48 o

0 12 2 34.63 37.02 1.42 o

-11 13 2 771.38 791.32 8.69 o

-10 13 2 219.08 220.02 2.27 o

-9 13 2 315.92 332.85 2.92 o

-8 13 2 267.28 253.68 2.51 o

-7 13 2 462.54 477.99 3.69 o

-6 13 2 50.94 55.35 1.30 o

-5 13 2 1.06 3.31 0.58 o

-4 13 2 766.82 790.06 4.85 o

-3 13 2 39.50 40.70 1.19 o

-2 13 2 84.28 89.11 2.29 o

-8 14 2 0.35 0.74 2.22 o

-7 14 2 556.45 586.23 13.69 o

-6 14 2 22.55 23.51 2.47 o

-5 14 2 25.81 24.41 3.33 o

0 1 3 52.43 65.40 0.49 o

-1 2 3 1524.95 1623.93 4.26 o

0 2 3 983.05 1068.03 2.80 o

-2 3 3 4086.83 4121.90 9.75 o

-1 3 3 8040.56 8083.09 19.73 o

0 3 3 520.85 546.66 1.74 o

-3 4 3 1190.41 1235.05 3.38 o

-2 4 3 11.79 20.64 0.40 o

-1 4 3 1323.55 1402.77 3.97 o

0 4 3 21.38 14.44 0.34 o

-4 5 3 450.68 444.54 1.62 o

-3 5 3 319.63 305.17 1.15 o

-2 5 3 3381.35 3406.66 8.74 o

-1 5 3 165.33 154.48 0.85 o

0 5 3 125.49 119.92 0.76 o

-5 6 3 164.98 177.51 1.00 o

-4 6 3 3121.08 3096.43 7.96 o

-3 6 3 233.74 226.66 1.12 o

-2 6 3 430.01 442.22 1.68 o

-1 6 3 3976.48 3990.10 10.87 o

0 6 3 197.61 196.35 1.11 o

-6 7 3 203.81 195.23 1.21 o

-5 7 3 282.21 290.03 1.43 o

-4 7 3 1.74 2.90 0.29 o

-3 7 3 4106.92 4008.12 10.98 o

-2 7 3 1298.21 1266.29 4.22 o

-1 7 3 8.89 9.43 0.36 o

0 7 3 503.92 490.42 2.15 o

-7 8 3 384.29 377.57 1.92 o

-6 8 3 34.46 32.96 0.69 o

-5 8 3 46.31 44.94 0.72 o

-4 8 3 45.13 45.67 0.69 o

-3 8 3 249.43 242.69 1.36 o

-2 8 3 101.22 95.98 0.94 o

-1 8 3 52.36 52.11 0.71 o

0 8 3 44.53 43.48 0.70 o

-8 9 3 0.04 0.98 0.37 o

-7 9 3 116.08 121.25 1.18 o

-6 9 3 4.69 5.89 0.43 o

-5 9 3 374.55 367.23 2.13 o

-4 9 3 545.29 534.19 2.70 o

-3 9 3 1349.86 1313.75 4.79 o

-2 9 3 233.58 235.11 1.50 o

-1 9 3 206.86 196.61 1.48 o

0 9 3 638.82 626.55 2.90 o

-9 10 3 188.37 187.47 1.74 o

-8 10 3 393.74 391.28 2.47 o

-7 10 3 37.01 35.31 0.80 o

-6 10 3 205.30 208.11 1.68 o

-5 10 3 456.97 458.91 2.73 o

-4 10 3 0.68 1.73 0.38 o

-3 10 3 967.88 945.70 4.16 o

-2 10 3 168.42 173.15 1.48 o

-1 10 3 693.70 688.03 3.45 o

0 10 3 1.26 0.87 0.49 o

-10 11 3 210.03 215.07 2.14 o

-9 11 3 839.78 861.15 4.60 o

-8 11 3 11.77 12.59 0.71 o

-7 11 3 17.69 21.83 0.77 o

-6 11 3 297.07 297.13 2.30 o

-5 11 3 469.39 457.44 2.86 o

-4 11 3 184.34 182.93 1.78 o

-3 11 3 43.19 42.26 1.05 o

-2 11 3 111.33 113.97 1.36 o

-1 11 3 1862.44 1880.14 8.18 o

0 11 3 191.38 194.43 2.17 o

-11 12 3 27.51 28.75 1.08 o

-10 12 3 326.33 309.70 2.77 o

-9 12 3 147.87 150.26 1.88 o

-8 12 3 200.10 200.51 2.14 o

-7 12 3 7.93 10.11 0.68 o

-6 12 3 31.24 29.49 0.93 o

-5 12 3 91.70 85.52 1.38 o

-4 12 3 4.17 3.88 0.60 o

-3 12 3 180.19 173.02 2.00 o

-2 12 3 234.55 223.98 2.31 o

-1 12 3 1.07 1.83 0.60 o

0 12 3 79.62 91.02 4.19 o

-10 13 3 316.85 321.87 5.84 o

-9 13 3 2.02 2.32 0.61 o

-8 13 3 5.06 7.56 0.75 o

-7 13 3 104.51 104.43 1.66 o

-6 13 3 142.65 140.83 1.86 o

-5 13 3 16.59 16.90 0.89 o

-4 13 3 94.37 100.07 1.62 o

-3 13 3 30.93 28.77 1.40 o

0 1 4 631.96 668.89 1.94 o

-1 2 4 48.61 48.92 0.44 o

0 2 4 97.11 77.17 0.54 o

-2 3 4 1774.39 1815.44 4.56 o

-1 3 4 1124.62 1086.97 2.99 o

0 3 4 5601.64 5540.40 13.54 o

-3 4 4 20.99 17.85 0.37 o

-2 4 4 14.61 12.29 0.44 o

-1 4 4 240.47 233.81 1.03 o

0 4 4 127.46 121.43 0.77 o

-4 5 4 2813.40 2782.85 7.66 o

-3 5 4 1480.15 1435.40 4.20 o

-2 5 4 53.02 52.56 0.58 o

-1 5 4 2098.36 2068.46 5.90 o

0 5 4 443.59 433.46 1.79 o

-5 6 4 65.37 75.74 0.74 o

-4 6 4 2790.61 2772.52 8.27 o

-3 6 4 880.44 873.24 3.00 o

-2 6 4 1840.30 1880.46 5.76 o

-1 6 4 3025.26 2979.29 8.42 o

0 6 4 558.27 531.85 2.25 o

-6 7 4 2058.74 2003.80 6.81 o

-5 7 4 2.36 3.89 0.35 o

-4 7 4 228.49 238.50 1.44 o

-3 7 4 598.98 582.41 2.36 o

-2 7 4 1206.08 1206.44 4.27 o

-1 7 4 1041.50 1036.45 3.90 o

0 7 4 28.14 28.28 0.60 o

-7 8 4 3246.70 3213.92 10.42 o

-6 8 4 1296.31 1273.30 4.80 o

-5 8 4 548.08 536.61 2.71 o

-4 8 4 3587.25 3497.92 10.89 o

-3 8 4 33.90 33.54 0.64 o

-2 8 4 6.61 7.52 0.41 o

-1 8 4 226.90 231.53 1.57 o

0 8 4 1178.94 1179.75 4.88 o

-8 9 4 13.93 14.48 0.62 o

-7 9 4 627.20 639.95 3.19 o

-6 9 4 9.87 11.43 0.55 o

-5 9 4 158.39 162.69 1.46 o

-4 9 4 64.01 63.51 0.91 o

-3 9 4 1.64 3.28 0.44 o

-2 9 4 837.36 819.36 3.57 o

-1 9 4 104.26 102.88 1.11 o

0 9 4 189.67 183.47 1.71 o

-9 10 4 215.80 204.60 2.01 o

-8 10 4 24.22 30.12 0.80 o

-7 10 4 13.54 15.23 0.62 o

-6 10 4 355.97 352.74 2.33 o

-5 10 4 329.92 324.48 2.16 o

-4 10 4 34.68 37.78 0.86 o

-3 10 4 464.58 451.69 3.39 o

-2 10 4 776.12 768.14 3.74 o

-1 10 4 409.56 410.83 2.65 o

0 10 4 118.03 119.19 1.74 o

-10 11 4 1491.91 1503.23 7.55 o

-9 11 4 909.70 915.55 5.51 o

-8 11 4 3.22 3.31 0.53 o

-7 11 4 1727.37 1693.04 7.45 o

-6 11 4 980.15 993.28 4.88 o

-5 11 4 169.97 165.49 1.63 o

-4 11 4 744.17 728.80 4.05 o

-3 11 4 0.76 1.60 0.51 o

-2 11 4 189.60 191.36 1.98 o

-1 11 4 3.59 3.72 0.59 o

0 11 4 27.62 34.61 1.12 o

-11 12 4 36.66 41.43 4.81 o

-10 12 4 623.86 635.27 5.82 o

-9 12 4 109.07 113.80 1.76 o

-8 12 4 76.76 80.99 1.47 o

-7 12 4 32.23 33.99 0.96 o

-6 12 4 82.30 78.92 1.27 o

-5 12 4 308.79 316.32 2.66 o

-4 12 4 222.50 225.15 2.32 o

-3 12 4 215.38 225.17 2.33 o

-2 12 4 212.88 214.59 2.68 o

-1 12 4 25.20 28.42 3.88 o

-9 13 4 1.20 6.73 1.95 o

-8 13 4 192.66 215.66 3.67 o

-7 13 4 71.43 69.08 1.97 o

-6 13 4 467.26 468.74 6.23 o

-5 13 4 765.40 821.64 8.83 o

-4 13 4 127.87 127.98 3.70 o

0 1 5 47.41 45.87 0.48 o

-1 2 5 231.96 217.79 1.01 o

0 2 5 269.10 258.92 1.13 o

-2 3 5 1533.92 1540.63 4.35 o

-1 3 5 3586.77 3576.31 8.90 o

0 3 5 94.74 95.84 0.71 o

-3 4 5 621.33 644.38 2.28 o

-2 4 5 204.32 186.71 1.01 o

-1 4 5 92.99 73.45 0.65 o

0 4 5 177.15 163.54 1.04 o

-4 5 5 5.79 6.32 0.33 o

-3 5 5 2196.74 2122.21 6.56 o

-2 5 5 1042.18 1049.50 3.52 o

-1 5 5 12.37 10.24 0.44 o

0 5 5 556.33 538.99 2.31 o

-5 6 5 375.25 382.62 1.94 o

-4 6 5 792.96 804.31 3.24 o

-3 6 5 1063.68 1055.63 3.68 o

-2 6 5 180.19 185.06 1.20 o

-1 6 5 2974.58 2937.13 9.04 o

0 6 5 0.41 1.48 0.33 o

-6 7 5 116.97 105.07 1.11 o

-5 7 5 168.97 168.04 1.29 o

-4 7 5 68.23 63.50 0.81 o

-3 7 5 1148.51 1107.20 4.10 o

-2 7 5 471.39 466.34 2.35 o

-1 7 5 86.87 82.51 0.99 o

0 7 5 0.15 1.99 0.41 o

-7 8 5 4.26 5.06 0.46 o

-6 8 5 11.50 13.11 0.56 o

-5 8 5 32.04 30.34 0.72 o

-4 8 5 733.48 718.11 3.16 o

-3 8 5 19.20 22.61 0.65 o

-2 8 5 100.55 110.25 1.16 o

-1 8 5 160.48 161.10 1.55 o

0 8 5 0.88 1.17 0.41 o

-8 9 5 47.85 47.24 0.99 o

-7 9 5 0.22 0.21 0.43 o

-6 9 5 488.62 489.12 2.86 o

-5 9 5 479.90 484.25 2.82 o

-4 9 5 571.17 567.75 2.85 o

-3 9 5 1672.55 1648.37 6.46 o

-2 9 5 259.46 261.01 2.08 o

-1 9 5 165.75 162.76 1.54 o

0 9 5 252.44 258.13 2.07 o

-9 10 5 12.14 14.00 0.72 o

-8 10 5 234.58 242.92 2.07 o

-7 10 5 207.07 207.09 1.87 o

-6 10 5 132.10 138.98 1.48 o

-5 10 5 429.67 430.53 2.70 o

-4 10 5 4.85 6.02 0.53 o

-3 10 5 125.97 134.88 1.47 o

-2 10 5 50.44 51.42 1.04 o

-1 10 5 142.94 142.05 1.61 o

0 10 5 92.38 96.90 1.49 o

-10 11 5 101.95 106.92 1.69 o

-9 11 5 853.19 872.40 4.97 o

-8 11 5 9.51 10.50 0.68 o

-7 11 5 7.93 9.11 0.62 o

-6 11 5 731.07 741.52 4.07 o

-5 11 5 142.68 149.39 1.72 o

-4 11 5 120.77 120.68 1.68 o

-3 11 5 171.55 176.16 1.95 o

-2 11 5 1.39 1.65 0.54 o

-1 11 5 924.00 918.08 5.94 o

0 11 5 109.60 110.90 4.81 o

-9 12 5 122.56 129.48 6.66 o

-8 12 5 473.23 472.12 3.66 o

-7 12 5 109.53 117.36 1.61 o

-6 12 5 60.99 60.81 1.23 o

-5 12 5 420.66 428.73 3.51 o

-4 12 5 2.10 2.75 0.66 o

-3 12 5 163.23 147.50 4.05 o

0 0 6 10404.37 10162.01 67.89 o

0 1 6 443.19 432.48 1.89 o

-1 2 6 4754.20 4716.48 12.69 o

0 2 6 304.82 322.19 1.53 o

-2 3 6 259.85 248.98 1.36 o

-1 3 6 11.17 10.04 0.38 o

0 3 6 94.42 94.44 0.87 o

-3 4 6 2421.56 2353.24 7.61 o

-2 4 6 3060.93 2974.10 9.21 o

-1 4 6 58.46 62.69 0.86 o

0 4 6 1508.58 1483.41 4.95 o

-4 5 6 188.14 186.30 1.39 o

-3 5 6 10.98 9.08 0.45 o

-2 5 6 849.84 839.80 3.23 o

-1 5 6 395.55 404.22 1.98 o

0 5 6 1383.84 1365.48 4.99 o

-5 6 6 329.66 306.19 1.82 o

-4 6 6 370.98 369.12 2.03 o

-3 6 6 1064.43 1059.63 4.13 o

-2 6 6 44.59 38.71 0.72 o

-1 6 6 97.30 98.29 1.05 o

0 6 6 1138.94 1134.52 4.64 o

-6 7 6 25.28 25.01 0.73 o

-5 7 6 934.38 921.85 4.12 o

-4 7 6 1063.32 1085.82 4.71 o

-3 7 6 70.39 73.74 0.98 o

-2 7 6 49.55 45.26 0.88 o

-1 7 6 31.30 30.66 0.83 o

0 7 6 463.95 449.04 2.63 o

-7 8 6 43.11 46.94 0.97 o

-6 8 6 0.01 0.09 0.41 o

-5 8 6 1749.59 1726.91 6.93 o

-4 8 6 1.51 2.80 0.43 o

-3 8 6 658.29 648.17 3.31 o

-2 8 6 242.00 234.85 1.90 o

-1 8 6 695.56 691.31 3.75 o

0 8 6 2600.23 2633.17 9.67 o

-8 9 6 133.63 137.50 1.54 o

-7 9 6 11.48 13.95 0.73 o

-6 9 6 1989.71 1969.03 8.08 o

-5 9 6 65.85 63.70 1.10 o

-4 9 6 334.67 330.00 2.27 o

-3 9 6 1732.89 1714.83 7.03 o

-2 9 6 34.10 37.76 1.07 o

-1 9 6 479.01 477.11 3.19 o

0 9 6 414.46 417.60 2.88 o

-9 10 6 1.28 1.56 0.54 o

-8 10 6 687.41 690.68 4.20 o

-7 10 6 285.54 287.11 2.48 o

-6 10 6 0.33 0.63 0.48 o

-5 10 6 125.58 129.28 1.55 o

-4 10 6 415.56 419.41 2.96 o

-3 10 6 14.63 16.61 0.75 o

-2 10 6 54.53 55.63 1.13 o

-1 10 6 10.28 14.54 0.80 o

0 10 6 16.83 15.96 1.12 o

-9 11 6 27.40 28.00 1.53 o

-8 11 6 692.39 712.24 5.11 o

-7 11 6 4.59 5.95 0.61 o

-6 11 6 90.17 89.73 1.37 o

-5 11 6 89.93 88.64 1.53 o

-4 11 6 128.47 134.59 1.84 o

-3 11 6 202.42 211.81 2.97 o

-2 11 6 9.55 7.85 1.25 o

0 1 7 11.99 13.10 0.45 o

-1 2 7 1.94 2.17 0.34 o

0 2 7 5.47 7.41 0.40 o

-2 3 7 1229.67 1209.72 4.47 o

-1 3 7 1686.12 1674.84 6.11 o

0 3 7 69.52 67.42 0.92 o

-3 4 7 544.09 552.23 2.71 o

-2 4 7 46.81 46.07 0.84 o

-1 4 7 33.09 42.38 0.83 o

0 4 7 93.69 95.04 1.14 o

-4 5 7 65.67 66.26 1.03 o

-3 5 7 425.88 415.44 2.45 o

-2 5 7 779.74 771.50 3.64 o

-1 5 7 6.39 6.01 0.50 o

0 5 7 10.83 10.07 0.63 o

-5 6 7 279.81 281.61 2.10 o

-4 6 7 614.93 620.90 3.23 o

-3 6 7 412.49 399.28 2.44 o

-2 6 7 162.44 162.85 1.54 o

-1 6 7 1485.31 1447.91 6.26 o

0 6 7 102.63 106.25 1.32 o

-6 7 7 25.20 25.55 0.86 o

-5 7 7 127.92 123.68 1.46 o

-4 7 7 3.81 3.70 0.47 o

-3 7 7 1293.63 1246.69 5.60 o

-2 7 7 493.11 476.72 3.09 o

-1 7 7 32.28 34.86 0.93 o

0 7 7 62.18 59.21 1.22 o

-7 8 7 53.26 54.83 1.13 o

-6 8 7 25.62 26.66 0.91 o

-5 8 7 13.55 13.53 0.74 o

-4 8 7 174.19 177.39 1.77 o

-3 8 7 99.38 100.48 1.32 o

-2 8 7 4.01 5.18 0.57 o

-1 8 7 108.37 104.28 1.48 o

0 8 7 26.76 27.55 0.91 o

-8 9 7 45.39 44.07 1.25 o

-7 9 7 34.71 37.48 1.14 o

-6 9 7 94.45 97.47 1.54 o

-5 9 7 108.05 107.85 1.55 o

-4 9 7 283.06 286.04 2.49 o

-3 9 7 1026.03 1022.99 5.30 o

-2 9 7 179.25 187.88 1.98 o

-1 9 7 77.32 79.36 1.37 o

0 9 7 300.48 299.73 3.81 o

-8 10 7 143.59 158.46 6.47 o

-7 10 7 85.47 87.88 1.75 o

-6 10 7 207.75 212.63 2.30 o

-5 10 7 239.66 246.98 2.46 o

-4 10 7 1.43 1.76 0.55 o

-3 10 7 430.70 445.57 4.15 o

-2 10 7 34.49 37.64 1.88 o

0 0 8 7977.44 7792.82 60.12 o

0 1 8 134.15 141.32 1.19 o

-1 2 8 50.40 48.41 0.84 o

0 2 8 25.93 26.80 0.73 o

-2 3 8 796.12 791.37 3.89 o

-1 3 8 381.05 380.22 2.30 o

0 3 8 1878.21 1863.25 7.34 o

-3 4 8 87.46 88.01 1.28 o

-2 4 8 0.19 1.67 0.49 o

-1 4 8 32.79 35.18 0.94 o

0 4 8 97.97 95.90 1.28 o

-4 5 8 1388.70 1355.69 5.86 o

-3 5 8 329.10 330.88 2.42 o

-2 5 8 26.18 28.76 0.81 o

-1 5 8 578.55 568.72 3.55 o

0 5 8 299.91 289.02 2.29 o

-5 6 8 116.37 118.51 1.55 o

-4 6 8 1087.34 1069.48 4.99 o

-3 6 8 408.81 411.80 2.71 o

-2 6 8 1198.37 1197.13 5.82 o

-1 6 8 1437.08 1453.34 7.21 o

0 6 8 359.18 354.60 2.91 o

-6 7 8 956.94 943.76 5.37 o

-5 7 8 26.33 27.86 0.94 o

-4 7 8 95.23 103.07 1.47 o

-3 7 8 157.23 152.49 1.85 o

-2 7 8 435.69 441.63 3.34 o

-1 7 8 335.63 336.45 4.03 o

0 7 8 19.35 20.93 0.99 o

-7 8 8 1845.11 1888.25 14.42 o

-6 8 8 614.59 617.00 4.16 o

-5 8 8 249.13 238.92 2.40 o

-4 8 8 1895.83 1916.66 9.00 o

-3 8 8 31.11 29.49 1.09 o

-2 8 8 1.78 2.76 0.64 o

-1 8 8 72.94 79.89 2.24 o

0 8 8 375.76 390.22 8.37 o

-6 9 8 9.75 14.06 1.83 o

-5 9 8 65.92 66.28 3.52 o

-4 9 8 165.61 168.70 7.40 o

-3 9 8 4.97 4.44 2.59 o

0 1 9 9.57 11.61 0.78 o

-1 2 9 36.87 37.74 0.98 o

0 2 9 2.76 4.37 0.58 o

-2 3 9 593.25 586.65 3.48 o

-1 3 9 1473.79 1458.45 6.47 o

0 3 9 20.85 21.38 0.83 o

-3 4 9 183.62 186.84 1.89 o

-2 4 9 8.77 9.33 0.72 o

-1 4 9 174.49 184.61 1.89 o

0 4 9 27.67 31.91 1.02 o

-4 5 9 53.87 55.13 1.16 o

-3 5 9 335.74 342.05 2.59 o

-2 5 9 443.63 449.36 3.29 o

-1 5 9 19.21 20.60 0.86 o

0 5 9 0.03 1.43 0.57 o

-5 6 9 50.69 50.90 1.53 o

-4 6 9 697.02 710.06 4.24 o

-3 6 9 126.33 122.99 1.73 o

-2 6 9 24.11 26.76 1.02 o

-1 6 9 1240.65 1241.72 8.60 o

0 6 9 30.09 25.89 4.07 o

-5 7 9 109.56 116.56 3.54 o

-4 7 9 0.00 1.65 1.95 o

-3 7 9 550.96 566.28 8.40 o

-2 7 9 271.27 283.54 6.67 o

0 0 10 1627.17 1623.80 20.46 o

0 1 10 130.41 129.73 1.96 o

-1 2 10 1458.07 1492.87 9.52 o

0 2 10 107.37 104.29 2.24 o

-2 3 10 47.88 51.55 1.73 o

-1 3 10 0.92 1.21 0.93 o

0 3 10 1.61 1.51 0.95 o

-3 4 10 344.46 356.89 7.33 o

**Table 6d: FoFc for sample HNFCL10**

#

# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag

#

data\_hnf5cl510\_0m

\_shelx\_title ' HNF5CL510\_0m in P6(3)/m'

\_shelx\_refln\_list\_code 4

\_shelx\_F\_calc\_maximum 146.37

\_exptl\_crystal\_F\_000 508.00

\_reflns\_d\_resolution\_high 0.6509

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-y, x-y, z'

'-x+y, -x, z'

'-x, -y, z+1/2'

'y, -x+y, z+1/2'

'x-y, x, z+1/2'

'-x, -y, -z'

'y, -x+y, -z'

'x-y, x, -z'

'x, y, -z-1/2'

'-y, x-y, -z-1/2'

'-x+y, -x, -z-1/2'

\_cell\_length\_a 9.5084

\_cell\_length\_b 9.5084

\_cell\_length\_c 6.8293

\_cell\_angle\_alpha 90.000

\_cell\_angle\_beta 90.000

\_cell\_angle\_gamma 120.000

\_shelx\_F\_squared\_multiplier 1.000

loop\_

\_refln\_index\_h

\_refln\_index\_k

\_refln\_index\_l

\_refln\_F\_squared\_calc

\_refln\_F\_squared\_meas

\_refln\_F\_squared\_sigma

\_refln\_observed\_status

0 1 0 281.80 283.56 1.18 o

-1 2 0 49.11 51.79 0.42 o

0 2 0 260.60 272.16 1.23 o

-2 3 0 45.00 29.07 0.43 o

-1 3 0 2665.06 2584.16 8.68 o

0 3 0 21425.43 21542.40 78.70 o

-2 4 0 172.68 157.52 0.95 o

-1 4 0 1211.03 1262.40 4.55 o

0 4 0 724.14 687.69 2.58 o

-4 5 0 5358.69 5298.44 18.44 o

-3 5 0 2946.90 3076.64 10.21 o

-2 5 0 28.07 25.57 0.50 o

-1 5 0 6300.78 6404.71 21.65 o

0 5 0 218.20 193.81 1.17 o

-5 6 0 20.50 27.04 0.47 o

-4 6 0 4274.25 4375.72 14.44 o

-3 6 0 1465.06 1516.43 5.22 o

-2 6 0 114.79 107.05 0.81 o

-1 6 0 1859.31 1860.65 6.33 o

0 6 0 694.02 650.87 2.88 o

-6 7 0 1104.19 1034.89 4.41 o

-5 7 0 1539.48 1538.94 5.86 o

-4 7 0 475.80 472.87 2.28 o

-3 7 0 366.64 353.82 1.93 o

-2 7 0 5383.32 5358.20 18.26 o

-1 7 0 1473.91 1490.81 5.73 o

0 7 0 39.64 36.53 0.72 o

-7 8 0 4849.80 4922.84 18.46 o

-6 8 0 431.72 440.33 2.40 o

-5 8 0 1186.04 1202.55 5.07 o

-4 8 0 4727.98 4787.70 17.92 o

-3 8 0 140.47 140.80 1.29 o

-2 8 0 28.89 23.89 0.62 o

-1 8 0 767.75 811.97 4.17 o

0 8 0 2739.18 2727.74 11.38 o

-8 9 0 52.10 40.65 0.96 o

-7 9 0 609.93 615.54 3.94 o

-6 9 0 34.69 37.23 0.76 o

-5 9 0 139.53 133.61 1.34 o

-4 9 0 108.50 104.29 1.16 o

-3 9 0 1.21 2.68 0.39 o

-2 9 0 719.47 713.15 4.15 o

-1 9 0 189.86 182.78 1.80 o

0 9 0 528.94 507.06 3.21 o

-9 10 0 313.19 311.51 3.23 o

-8 10 0 377.95 388.13 3.61 o

-7 10 0 34.03 33.62 0.94 o

-6 10 0 403.56 394.96 2.89 o

-5 10 0 1703.41 1671.28 7.66 o

-4 10 0 97.24 96.94 1.25 o

-3 10 0 711.66 711.52 5.38 o

-2 10 0 1588.63 1594.66 7.84 o

-1 10 0 179.96 174.96 2.02 o

0 10 0 101.45 104.17 2.03 o

-10 11 0 2256.73 2238.14 14.16 o

-9 11 0 589.33 592.75 4.88 o

-8 11 0 391.69 394.75 3.72 o

-7 11 0 2391.84 2384.13 12.45 o

-6 11 0 1023.72 1035.62 6.41 o

-5 11 0 22.48 20.87 0.92 o

-4 11 0 1015.21 1011.42 5.96 o

-3 11 0 12.14 11.07 0.67 o

-2 11 0 148.29 138.84 1.96 o

-1 11 0 7.93 5.60 0.84 o

0 11 0 26.79 19.97 1.17 o

-11 12 0 2.60 3.66 0.78 o

-10 12 0 716.86 708.42 5.73 o

-9 12 0 344.90 343.06 3.60 o

-8 12 0 125.50 123.92 2.09 o

-7 12 0 23.26 22.56 1.06 o

-6 12 0 277.84 272.85 3.09 o

-5 12 0 455.16 473.37 4.27 o

-4 12 0 616.61 634.82 4.80 o

-3 12 0 802.73 808.06 6.62 o

-2 12 0 283.79 289.08 3.98 o

-1 12 0 154.41 147.39 3.30 o

0 12 0 1301.23 1314.80 10.80 o

-12 13 0 332.88 346.26 7.21 o

-11 13 0 4.14 5.92 0.88 o

-10 13 0 71.83 68.86 1.88 o

-9 13 0 8.94 12.09 1.05 o

-8 13 0 296.06 311.15 3.80 o

-7 13 0 582.10 577.96 4.99 o

-6 13 0 408.84 399.18 4.35 o

-5 13 0 1116.32 1158.11 10.83 o

-4 13 0 663.37 669.73 6.70 o

-3 13 0 345.52 341.83 4.52 o

-2 13 0 353.39 346.88 5.23 o

-9 14 0 222.23 219.01 4.00 o

-8 14 0 49.17 50.04 1.85 o

-7 14 0 130.76 132.20 3.12 o

-6 14 0 471.10 489.07 7.38 o

-5 14 0 237.56 232.74 5.97 o

0 1 1 179.11 187.19 0.76 o

-1 2 1 310.27 328.50 1.09 o

0 2 1 270.06 303.67 1.21 o

-2 3 1 4386.44 4417.92 10.78 o

-1 3 1 9658.93 9743.72 25.03 o

0 3 1 712.99 802.76 2.17 o

-3 4 1 1400.81 1433.68 3.85 o

-2 4 1 212.29 186.18 0.71 o

-1 4 1 220.06 274.73 0.97 o

0 4 1 111.98 95.30 0.52 o

-4 5 1 34.31 34.96 0.34 o

-3 5 1 3356.31 3378.12 8.36 o

-2 5 1 2978.49 3018.46 7.36 o

-1 5 1 36.33 38.63 0.35 o

0 5 1 943.08 1031.70 2.65 o

-5 6 1 679.35 703.12 2.11 o

-4 6 1 1485.38 1451.45 3.78 o

-3 6 1 1836.16 1783.35 4.60 o

-2 6 1 605.38 630.90 1.95 o

-1 6 1 5061.89 5185.50 12.34 o

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-6 7 1 332.81 314.08 1.31 o

-5 7 1 261.93 266.27 1.11 o

-4 7 1 83.95 96.75 0.64 o

-3 7 1 3135.06 3106.70 7.91 o

-2 7 1 1082.38 1064.20 3.06 o

-1 7 1 118.33 117.32 0.73 o

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-7 8 1 25.41 26.96 0.48 o

-6 8 1 38.61 29.05 0.48 o

-5 8 1 49.60 45.46 0.54 o

-4 8 1 1145.51 1124.06 3.40 o

-3 8 1 101.45 102.22 0.73 o

-2 8 1 62.88 66.22 0.64 o

-1 8 1 197.64 204.92 1.18 o

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-8 9 1 122.23 116.16 1.08 o

-7 9 1 14.03 16.24 0.44 o

-6 9 1 486.11 468.53 2.12 o

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-8 10 1 388.25 397.82 2.39 o

-7 10 1 242.94 232.11 1.55 o

-6 10 1 292.51 299.06 1.73 o

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-4 10 1 5.43 6.48 0.36 o

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-5 11 1 280.46 283.85 1.80 o

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-3 11 1 273.75 279.38 2.08 o

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-10 12 1 66.01 54.08 1.13 o

-9 12 1 190.96 198.18 2.07 o

-8 12 1 502.50 501.72 3.17 o

-7 12 1 145.28 155.01 1.51 o

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-2 12 1 338.42 324.85 2.74 o

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-9 14 1 931.17 956.98 8.59 o

-8 14 1 77.94 73.67 1.98 o

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-9 13 2 315.09 332.63 3.27 o

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-6 7 7 25.14 24.12 0.67 o

-5 7 7 126.59 125.18 1.31 o

-4 7 7 3.98 4.34 0.46 o

-3 7 7 1290.91 1239.48 5.15 o

-2 7 7 490.52 478.71 2.93 o

-1 7 7 32.10 33.77 0.89 o

0 7 7 62.28 60.83 0.98 o

-7 8 7 52.43 56.08 0.95 o

-6 8 7 25.50 25.03 0.76 o

-5 8 7 13.49 12.82 0.59 o

-4 8 7 173.56 173.24 1.64 o

-3 8 7 98.65 100.07 1.30 o

-2 8 7 3.93 5.00 0.49 o

-1 8 7 108.02 103.81 1.37 o

0 8 7 26.43 28.71 0.84 o

-8 9 7 45.04 45.54 0.95 o

-7 9 7 34.74 37.82 0.87 o

-6 9 7 93.73 99.48 1.30 o

-5 9 7 108.04 111.21 1.36 o

-4 9 7 280.76 279.58 2.25 o

-3 9 7 1019.99 999.54 5.11 o

-2 9 7 177.54 184.92 1.84 o

-1 9 7 77.06 74.48 1.21 o

0 9 7 299.02 303.80 3.88 o

-8 10 7 144.20 146.61 3.72 o

-7 10 7 84.61 88.76 1.60 o

-6 10 7 206.33 212.29 2.09 o

-5 10 7 238.54 241.30 2.22 o

-4 10 7 1.42 0.61 0.45 o

-3 10 7 427.20 439.75 4.88 o

-2 10 7 34.71 37.82 2.85 o

0 0 8 7943.66 7887.49 73.11 o

0 1 8 134.52 140.82 1.43 o

-1 2 8 50.37 47.95 0.88 o

0 2 8 25.72 26.31 0.70 o

-2 3 8 795.69 791.21 3.89 o

-1 3 8 381.30 380.69 2.43 o

0 3 8 1872.27 1885.84 7.70 o

-3 4 8 88.13 91.50 1.17 o

-2 4 8 0.19 1.17 0.35 o

-1 4 8 32.50 36.05 0.82 o

0 4 8 97.07 94.46 1.17 o

-4 5 8 1382.56 1367.67 6.37 o

-3 5 8 328.30 327.66 2.17 o

-2 5 8 26.05 29.00 0.83 o

-1 5 8 575.78 572.05 3.38 o

0 5 8 299.83 290.09 2.37 o

-5 6 8 115.07 114.94 1.35 o

-4 6 8 1084.42 1068.53 4.86 o

-3 6 8 409.83 405.93 2.78 o

-2 6 8 1196.05 1192.41 5.62 o

-1 6 8 1432.30 1450.85 6.34 o

0 6 8 357.77 354.13 2.65 o

-6 7 8 953.40 942.90 4.60 o

-5 7 8 26.18 29.99 0.81 o

-4 7 8 94.10 99.33 1.34 o

-3 7 8 156.60 150.04 1.68 o

-2 7 8 434.76 448.09 2.94 o

-1 7 8 334.07 341.92 2.55 o

0 7 8 19.36 21.73 0.83 o

-7 8 8 1839.77 1882.89 11.20 o

-6 8 8 611.77 615.48 3.47 o

-5 8 8 248.50 243.23 2.13 o

-4 8 8 1889.83 1928.48 8.59 o

-3 8 8 30.72 31.43 0.96 o

-2 8 8 1.75 2.24 0.46 o

-1 8 8 72.77 77.45 1.59 o

-7 9 8 275.88 277.58 8.80 o

-6 9 8 9.63 11.69 1.06 o

-5 9 8 65.43 66.48 2.84 o

0 1 9 9.34 10.02 0.58 o

-1 2 9 36.83 37.72 0.98 o

0 2 9 2.72 4.17 0.45 o

-2 3 9 587.49 586.02 3.94 o

-1 3 9 1468.06 1466.99 7.35 o

0 3 9 21.16 22.35 0.94 o

-3 4 9 183.00 188.26 2.12 o

-2 4 9 9.06 9.03 0.64 o

-1 4 9 174.54 184.48 2.17 o

0 4 9 27.25 30.77 1.08 o

-4 5 9 53.64 56.79 1.15 o

-3 5 9 334.25 342.55 2.95 o

-2 5 9 440.69 449.60 3.46 o

-1 5 9 19.00 19.96 0.88 o

0 5 9 0.03 0.97 0.46 o

-5 6 9 50.70 54.13 1.61 o

-4 6 9 694.65 714.99 5.12 o

-3 6 9 126.30 121.23 1.76 o

-2 6 9 24.36 26.25 0.95 o

-1 6 9 1231.82 1246.70 7.36 o

0 6 9 30.25 32.90 1.58 o

-5 7 9 107.81 111.49 5.47 o

-4 7 9 0.00 0.64 0.86 o

-3 7 9 549.58 550.22 7.64 o

-2 7 9 269.74 279.16 4.53 o

0 0 10 1620.07 1649.72 20.43 o

0 1 10 130.17 131.78 1.64 o

-1 2 10 1452.91 1494.22 8.07 o

0 2 10 107.22 108.92 1.87 o

-2 3 10 48.17 50.29 1.89 o

-1 3 10 0.98 0.91 0.81 o

0 3 10 1.56 1.64 1.02 o

-3 4 10 343.75 353.52 14.25 o

-2 4 10 1197.02 1240.00 16.30 o