|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pos. [°2θ] | Height [cts] | FWHM Left [°2θ] | d-spacing [Å] | Rel. Int. [%] |
| 26.1927 | 393.63 | 0.1440 | 3.39954 | 100.00 |
| 27.1923 | 195.55 | 0.1680 | 3.27680 | 49.68 |
| 29.4172 | 113.55 | 0.1902 | 3.03383 | 28.85 |
| 29.7896 | 70.72 | 0.2425 | 2.99674 | 17.97 |
| 30.0027 | 44.04 | 0.0900 | 2.97595 | 11.19 |
| 30.1679 | 33.93 | 0.0900 | 2.96003 | 8.62 |
| 31.7050 | 182.05 | 0.1440 | 2.81994 | 46.25 |
| 33.0745 | 202.23 | 0.2094 | 2.70624 | 51.38 |
| 36.0491 | 122.66 | 0.1940 | 2.48946 | 31.16 |
| 36.3438 | 53.98 | 0.0900 | 2.46995 | 13.71 |
| 37.2788 | 50.09 | 0.1920 | 2.41012 | 12.72 |
| 37.8469 | 173.75 | 0.1119 | 2.37523 | 44.14 |
| 38.3915 | 94.22 | 0.0900 | 2.34278 | 23.94 |
| 38.5444 | 102.53 | 0.1440 | 2.33384 | 26.05 |
| 39.3256 | 23.09 | 0.0511 | 2.28926 | 5.87 |
| 39.4501 | 32.06 | 0.0682 | 2.28232 | 8.15 |
| 39.8865 | 23.14 | 0.0900 | 2.25835 | 5.88 |
| 40.0280 | 20.55 | 0.0900 | 2.25069 | 5.22 |
| 40.3314 | 16.64 | 0.0477 | 2.23446 | 4.23 |
| 40.7116 | 17.48 | 0.0443 | 2.21446 | 4.44 |
| 41.1638 | 42.71 | 0.1440 | 2.19118 | 10.85 |
| 42.8640 | 82.33 | 0.0960 | 2.10812 | 20.91 |
| 43.5521 | 32.85 | 0.0900 | 2.07639 | 8.34 |
| 43.7543 | 34.36 | 0.0900 | 2.06726 | 8.73 |
| 45.4283 | 127.39 | 0.1200 | 1.99490 | 32.36 |
| 45.8201 | 266.16 | 0.1440 | 1.97875 | 67.62 |
| 47.5515 | 36.06 | 0.1440 | 1.91066 | 9.16 |
| 48.2668 | 119.21 | 0.2880 | 1.88401 | 30.29 |
| 50.1769 | 97.88 | 0.1982 | 1.81667 | 24.87 |
| 52.3879 | 101.92 | 0.1920 | 1.74508 | 25.89 |
| 52.9418 | 65.41 | 0.2191 | 1.72812 | 16.62 |
| 53.9154 | 11.24 | 0.2400 | 1.69919 | 2.86 |
| 56.4091 | 21.70 | 0.2880 | 1.62985 | 5.51 |
| 57.3785 | 18.21 | 0.0900 | 1.60459 | 4.63 |
| 58.2482 | 10.40 | 0.0900 | 1.58269 | 2.64 |
| 59.0466 | 14.99 | 0.2169 | 1.56318 | 3.81 |
| 59.3127 | 13.51 | 0.0900 | 1.55680 | 3.43 |
| 61.7937 | 15.70 | 0.2880 | 1.50011 | 3.99 |
| 63.2365 | 14.55 | 0.4800 | 1.46931 | 3.70 |
| 64.8030 | 16.68 | 0.0900 | 1.43753 | 4.24 |
| 66.1300 | 18.06 | 0.3823 | 1.41186 | 4.59 |
| 67.8487 | 14.03 | 0.0900 | 1.38022 | 3.56 |
|  |  |  |  |  |

Table 1: XRD peak positions inferred from Rietfeld refinement. Listed are peaks from the 0-3 cm increment of core CC-K04. HMC d104 peak positions are marked in red.