Supplementary Table 1. Carbon isotope and XRD data.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **δ13C‰** | **XRD results** | | | | | | | | |
| **2θ** | **d(002) (Å)** | **sd ±** | **FWHM (2θ)** | **Lc(002) (Å)** | **sd ±** | **GD** | **T(°C)** | **sd ±** |
| **012D-1** | -27.89 | 26.516 | 3.362 | 0.01 | 0.138 | 592 | 62 | 149 | 756 | 38 |
| **012D-2** | 26.491 | 3.365 | 0.01 | 0.138 | 592 | 62 | 147 | 752 | 38 |
| **012D-3** | 26.430 | 3.372 | 0.01 | 0.138 | 592 | 62 | 144 | 741 | 37 |
| **012D-4** | 26.586 | 3.353 | 0.005 | 0.138 | 592 | 62 | 153 | 768 | 38 |
| **014QZ-1** | - | 26.448 | 3.370 | 0.01 | 0.157 | 518 | 50 | 116 | 650 | 33 |
| **014QZ-2** | 26.546 | 3.358 | 0.005 | 0.217 | 377 | 39 | 81 | 538 | 27 |
| **014QZ-3** | 26.478 | 3.366 | 0.01 | 0.157 | 518 | 54 | 117 | 654 | 33 |
| **014QZ-4** | 26.514 | 3.362 | 0.01 | 0.177 | 461 | 48 | 101 | 602 | 30 |
| **014-1** | -25.70 | 26.519 | 3.361 | 0.01 | 0.197 | 415 | 43 | 89 | 564 | 28 |
| **014-2** | 26.504 | 3.363 | 0.01 | 0.157 | 519 | 54 | 118 | 658 | 33 |
| **014-3** | 26.629 | 3.348 | 0.005 | 0.177 | 461 | 48 | 105 | 615 | 31 |
| **014-4** | 26.555 | 3.357 | 0.005 | 0.177 | 461 | 48 | 102 | 606 | 30 |
| **015A-1** | -21.23 | 26.451 | 3.370 | 0.01 | 0.138 | 592 | 62 | 145 | 745 | 37 |
| **015A-2** | 26.507 | 3.363 | 0.01 | 0.138 | 592 | 62 | 148 | 754 | 38 |
| **015A-3** | 26.447 | 3.370 | 0.01 | 0.157 | 518 | 54 | 116 | 650 | 32 |
| **015A-4** | 26.555 | 3.357 | 0.005 | 0.157 | 519 | 54 | 120 | 665 | 33 |

Supplementary Table 2.Raman data (mean values and standard deviation std of the position, half width at half maximum (HWHM) obtained from the decomposition of three Raman spectra per analysis). R2 ratio and temperature estimates obtained by the IFORS method.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **D1 ±1350 cm−1** | | | |  | **D3 ±1500 cm−1** | | | |  | **D2 ±1610 cm−1** | | | |  | **G ±1580 cm−1** | | | |  | **R2** | **Std** | **T(°C)** | **Std** |
| **HWHM** | **Std** | **Center** | **Std** |  | **HWHM** | **Std** | **Center** | **Std** |  | **HWHM** | **Std** | **Center** | **Std** |  | **HWHM** | **Std** | **Center** | **Std** |  |
| **012Dg1p1(red)** | - | - | - | - |  | - | - | - | - |  | - | - | - | - |  | 7.94 | 0.42 | 1581.58 | 0.00 |  | 0.00 | 0.00 | 605 | 30 |
| **012Dg1p2(blue)** | 14.23 | 0.00 | 1360.38 | 0.00 |  | - | - | - | - |  | 5.61 | 0.01 | 1623.83 | 0.00 |  | 7.87 | 0.00 | 1581.58 | 0.00 |  | 0.07 | 0.00 | 594 | 30 |
| **012Dg1p3(green)** | 19.12 | 0.03 | 1357.90 | 0.00 |  | - | - | - | - |  | 4.13 | 0.00 | 1623.83 | 0.00 |  | 7.78 | 0.00 | 1581.58 | 0.00 |  | 0.07 | 0.00 | 598 | 30 |
| **012Dg2p1(red)** | 20.14 | 0.01 | 1355.41 | 0.00 |  | - | - | - | - |  | 6.38 | 0.01 | 1621.35 | 0.00 |  | 8.33 | 0.00 | 1581.58 | 0.00 |  | 0.12 | 0.00 | 586 | 29 |
| **012Dg2p2(blue)** | 20.87 | 0.03 | 1353.75 | 1.43 |  | 16.40 | 2.09 | 1503.70 | 1.43 |  | 6.12 | 0.03 | 1618.86 | 0.00 |  | 8.91 | 0.00 | 1581.58 | 0.00 |  | 0.07 | 0.00 | 588 | 29 |
| **012Dg2p3(green)** | - | - | - | - |  | - | - | - | - |  | - | - | - | - |  | 8.06 | 0.48 | 1581.58 | 0.00 |  | 0.00 | 0.00 | 600 | 30 |
| **012Dg3p1(red)** | 22.37 | 0.11 | 1357.90 | 0.00 |  | 13.58 | 0.28 | 1503.70 | 1.43 |  | 4.21 | 0.00 | 1623.83 | 0.00 |  | 7.90 | 0.00 | 1581.58 | 0.00 |  | 0.05 | 0.00 | 598 | 30 |
| **012Dg3p2(blue)** | 23.41 | 0.04 | 1357.90 | 0.00 |  | 24.47 | 0.10 | 1502.05 | 0.00 |  | 3.88 | 0.00 | 1623.83 | 0.00 |  | 8.08 | 0.00 | 1584.06 | 0.00 |  | 0.14 | 0.16 | 597 | 30 |
| **012Dg3p3(green)** | - | - | - | - |  | 26.16 | 0.03 | 1509.50 | 0.00 |  | 8.74 | 0.04 | 1606.43 | 0.00 |  | 7.67 | 0.00 | 1581.58 | 0.00 |  | 0.00 | 0.00 | 587 | 29 |
| **012Dg4p1(red)** | - | - | - | - |  | 4.95 | 0.58 | 1497.08 | 0.00 |  | - | - | - | - |  | 7.71 | 0.00 | 1581.58 | 0.00 |  | 0.00 | 0.00 | 606 | 30 |
| **012Dg4p2(blue)** | 15.91 | 0.03 | 1357.90 | 0.00 |  | 13.37 | 0.10 | 1499.56 | 0.00 |  | 6.73 | 0.01 | 1618.86 | 0.00 |  | 7.78 | 0.00 | 1579.09 | 0.00 |  | 0.13 | 0.00 | 585 | 29 |
| **012Dg4p3(green)** | 22.35 | 0.00 | 1352.92 | 0.00 |  | - | - | - | - |  | 17.98 | 0.24 | 1611.40 | 0.00 |  | 7.79 | 0.01 | 1581.58 | 0.00 |  | 0.12 | 0.00 | 587 | 29 |
| **012Dg5p1(red)** | 37.22 | 0.12 | 1340.50 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 7.85 | 0.00 | 1581.58 | 0.00 |  | 0.06 | 0.00 | 599 | 30 |
| **012Dg5p2(blue)** | 16.48 | 0.05 | 1355.41 | 0.00 |  | 16.12 | 0.37 | 1494.59 | 0.00 |  | 6.61 | 0.00 | 1613.89 | 0.00 |  | 8.00 | 0.00 | 1574.12 | 0.00 |  | 0.12 | 0.00 | 581 | 29 |
| **012Dg5p3(green)** | - | - | - | - |  | - | - | - | - |  | - | - | - | - |  | 8.89 | 0.00 | 1581.58 | 0.00 |  | 0.00 | 0.00 | 593 | 30 |
| **014QZg1p1(red)** | 21.92 | 0.00 | 1351.47 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.90 | 0.00 | 1583.28 | 0.00 |  | 0.22 | 0.00 | 567 | 28 |
| **014QZg1p2(blue)** | 21.65 | 0.00 | 1348.97 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.78 | 0.00 | 1580.79 | 0.00 |  | 0.05 | 0.00 | 591 | 30 |
| **014QZg1p3(green)** | 20.33 | 0.00 | 1351.47 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 9.58 | 0.01 | 1582.45 | 1.44 |  | 0.04 | 0.00 | 581 | 29 |
| **014QZg2p3(green)** | 21.02 | 0.00 | 1353.96 | 0.00 |  | - | - | - | - |  | 2.49 | 0.00 | 1623.17 | 0.00 |  | 8.12 | 0.00 | 1580.79 | 0.00 |  | 0.06 | 0.00 | 598 | 30 |
| **014QZg3p2(blue)** | 22.00 | 0.02 | 1346.48 | 0.00 |  | 17.55 | 0.20 | 1498.53 | 0.00 |  | 12.42 | 0.05 | 1610.70 | 0.00 |  | 8.17 | 0.01 | 1575.81 | 0.00 |  | 0.06 | 0.00 | 595 | 30 |
| **014QZg3p3(green)** | 20.54 | 0.02 | 1348.97 | 0.00 |  | - | - | - | - |  | 4.30 | 0.01 | 1625.66 | 0.00 |  | 8.46 | 0.00 | 1583.28 | 0.00 |  | 0.03 | 0.00 | 592 | 30 |
| **014QZg4p2(blue)** | 20.59 | 0.00 | 1348.97 | 0.00 |  | - | - | - | - |  | 9.82 | 9.00 | 1613.20 | 8.63 |  | 8.94 | 0.02 | 1578.30 | 0.00 |  | 0.08 | 0.00 | 581 | 29 |
| **014QZg4p3(green)** | - | - | - | - |  | - | - | - | - |  | - | - | - | - |  | 8.01 | 0.00 | 1580.79 | 0.00 |  | 0.00 | 0.00 | 576 | 29 |
| **014QZg5p2(blue)** | 19.95 | 0.09 | 1353.96 | 0.00 |  | 46.26 | 4.22 | 1497.70 | 1.44 |  | 6.63 | 0.15 | 1623.17 | 0.00 |  | 9.09 | 0.01 | 1583.28 | 0.00 |  | 0.14 | 0.00 | 575 | 29 |
| **014QZg5p3(green)** | 22.66 | 0.01 | 1351.47 | 0.00 |  | - | - | - | - |  | 5.01 | 0.04 | 1623.17 | 0.00 |  | 9.82 | 0.00 | 1583.28 | 0.00 |  | 0.06 | 0.00 | 578 | 29 |
| **014QZg6p1(red)** | 19.95 | 0.00 | 1364.88 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.51 | 0.00 | 1588.78 | 0.00 |  | 0.09 | 0.00 | 588 | 29 |
| **014QZg6p2(blue)** | 21.42 | 0.01 | 1360.73 | 0.00 |  | 17.07 | 0.18 | 1505.85 | 0.00 |  | - | - | - | - |  | 8.36 | 0.00 | 1588.78 | 0.00 |  | 0.04 | 0.00 | 593 | 30 |
| **014QZg6p3(green)** | 19.86 | 0.00 | 1360.73 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 9.32 | 0.00 | 1588.78 | 0.00 |  | 0.05 | 0.00 | 591 | 30 |
| **014g1p2(blue)** | 22.45 | 0.01 | 1347.95 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.82 | 0.00 | 1579.09 | 0.00 |  | 0.07 | 0.00 | 581 | 29 |
| **014g1p3(green)** | 24.88 | 0.02 | 1342.98 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 9.74 | 0.00 | 1571.64 | 0.00 |  | 0.12 | 0.00 | 570 | 29 |
| **014g2p1(red)** | 21.96 | 0.01 | 1338.01 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.22 | 0.00 | 1579.09 | 0.00 |  | 0.04 | 0.00 | 597 | 30 |
| **014g2p3(green)** | - | - | - | - |  | - | - | - | - |  | - | - | - | - |  | 8.59 | 0.00 | 1579.09 | 0.00 |  | 0.00 | 0.00 | 598 | 30 |
| **014g3p1(red)** | 53.17 | 18.04 | 1354.58 | 1.43 |  | 39.46 | 12.60 | 1502.05 | 0.00 |  | - | - | - | - |  | 8.00 | 0.00 | 1576.61 | 0.00 |  | 0.05 | 0.02 | 597 | 30 |
| **014g3p2(blue)** | 22.34 | 0.01 | 1335.53 | 0.00 |  | - | - | - | - |  | 21.77 | 0.14 | 1584.06 | 0.00 |  | 9.92 | 0.02 | 1559.21 | 0.00 |  | 0.10 | 0.00 | 564 | 28 |
| **014g4p1(red)** | 24.19 | 0.01 | 1340.50 | 0.00 |  | - | - | - | - |  | 15.63 | 0.01 | 1589.04 | 0.00 |  | 9.00 | 0.00 | 1564.18 | 0.00 |  | 0.04 | 0.00 | 589 | 29 |
| **014g4p2(blue)** | 25.50 | 0.13 | 1345.47 | 0.00 |  | 63.81 | 4.38 | 1499.56 | 0.00 |  | - | - | - | - |  | 10.83 | 0.00 | 1574.12 | 0.00 |  | 0.06 | 0.00 | 568 | 28 |
| **014g4p3(green)** | 18.65 | 0.18 | 1352.92 | 0.00 |  | - | - | - | - |  | 8.77 | 0.01 | 1616.37 | 0.00 |  | 8.17 | 0.00 | 1576.61 | 0.00 |  | 0.22 | 0.00 | 568 | 28 |
| **014g5p1(red)** | 22.85 | 0.02 | 1347.95 | 0.00 |  | 68.77 | 1.17 | 1502.05 | 0.00 |  | 16.15 | 0.02 | 1603.95 | 0.00 |  | 8.54 | 0.01 | 1579.09 | 0.00 |  | 0.14 | 0.00 | 568 | 28 |
| **014g5p2(blue)** | 49.64 | 0.99 | 1347.95 | 0.00 |  | 42.69 | 0.35 | 1507.02 | 2.49 |  | 26.45 | 0.69 | 1596.49 | 0.00 |  | 7.79 | 0.00 | 1571.64 | 0.00 |  | 0.05 | 0.00 | 597 | 30 |
| **014g5p3(green)** | 17.05 | 0.02 | 1345.47 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.06 | 0.00 | 1579.09 | 0.00 |  | 0.01 | 0.00 | 602 | 30 |
| **015Ag1p2(blue)** | 21.64 | 0.02 | 1356.45 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 7.98 | 0.01 | 1583.28 | 0.00 |  | 0.01 | 0.00 | 597 | 30 |
| **015Ag1p3(green)** | 22.68 | 0.01 | 1353.96 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.00 | 0.01 | 1580.79 | 0.00 |  | 0.27 | 0.00 | 576 | 29 |
| **015Ag2p1(red)** | - | - | - | - |  | 10.55 | 0.09 | 1503.52 | 0.00 |  | - | - | - | - |  | 8.05 | 0.00 | 1583.28 | 0.00 |  | 0.00 | 0.00 | 602 | 30 |
| **015Ag2p2(blue)** | 19.58 | 0.00 | 1358.94 | 0.00 |  | - | - | - | - |  | 4.68 | 0.00 | 1625.66 | 0.00 |  | 7.78 | 0.00 | 1583.28 | 0.00 |  | 0.04 | 0.00 | 602 | 30 |
| **015Ag2p3(green)** | 21.92 | 0.05 | 1356.45 | 0.00 |  | 12.36 | 0.72 | 1501.03 | 0.00 |  | 4.04 | 0.01 | 1625.66 | 0.00 |  | 8.22 | 0.00 | 1583.28 | 0.00 |  | 0.06 | 0.00 | 594 | 30 |
| **015Ag3p1(red)** | 20.19 | 0.16 | 1358.94 | 0.00 |  | 51.11 | 2.21 | 1517.23 | 1.76 |  | 5.70 | 0.24 | 1623.17 | 0.00 |  | 7.77 | 0.00 | 1583.28 | 0.00 |  | 0.13 | 0.01 | 591 | 30 |
| **015Ag3p2(blue)** | 11.63 | 0.10 | 1358.94 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 8.19 | 0.00 | 1583.28 | 0.00 |  | 0.10 | 0.00 | 590 | 30 |
| **015Ag4p1(red)** | 17.17 | 0.19 | 1360.61 | 1.44 |  | 11.92 | 1.64 | 1499.36 | 1.44 |  | 5.07 | 0.01 | 1625.66 | 0.00 |  | 8.91 | 0.00 | 1583.28 | 0.00 |  | 0.04 | 0.00 | 584 | 29 |
| **015Ag4p3(green)** | 19.31 | 0.02 | 1358.94 | 0.00 |  | 18.38 | 0.11 | 1503.52 | 0.00 |  | - | - | - | - |  | 7.97 | 0.00 | 1580.79 | 0.00 |  | 0.02 | 0.00 | 602 | 30 |
| **015Ag5p1(red)** | 22.61 | 0.00 | 1353.96 | 0.00 |  | - | - | - | - |  | 8.35 | 0.05 | 1620.67 | 0.00 |  | 8.39 | 0.01 | 1580.79 | 0.00 |  | 0.24 | 0.00 | 564 | 28 |
| **015Ag5p2(blue)** | 27.12 | 0.89 | 1351.47 | 0.00 |  | - | - | - | - |  | 11.61 | 5.48 | 1618.18 | 2.49 |  | 7.95 | 0.00 | 1580.79 | 0.00 |  | 0.07 | 0.01 | 597 | 30 |
| **015Ag6p2(blue)** | 20.88 | 0.00 | 1356.59 | 0.00 |  | - | - | - | - |  | - | - | - | - |  | 9.18 | 0.00 | 1580.49 | 0.00 |  | 0.05 | 0.00 | 592 | 30 |
| **015Ag6p3(green)** | 23.43 | 0.00 | 1352.44 | 0.00 |  | 24.24 | 0.03 | 1497.56 | 0.00 |  | 8.77 | 0.01 | 1613.66 | 0.00 |  | 8.91 | 0.00 | 1572.20 | 0.00 |  | 0.12 | 0.00 | 582 | 29 |

Supplementary Table 3.Mean values and standard deviation (std) for the XRD and Raman data. “n” shows the number of analysis.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **XRD** | | | | | | |  | **Raman** | | | | |
|  | **n** | **d(002) (Å)** | **std** | **GD** | **std** | **T(°C)** | **std** |  | **n** | **G HWHM (cm-1)** | **std** | **R2** | **std** |
| **012D** | 4 | 3.363 | 0.008 | 148.2 | 3.6 | 754 | 11 |  | 15 | 8.04 | 0.38 | 0.062 | 0.053 |
| **014QZ** | 4 | 3.364 | 0.005 | 103.5 | 16.9 | 611 | 54 |  | 13 | 8.77 | 0.57 | 0.071 | 0.055 |
| **014** | 4 | 3.357 | 0.007 | 103.4 | 12.1 | 611 | 39 |  | 12 | 8.81 | 0.92 | 0.075 | 0.062 |
| **015A** | 4 | 3.365 | 0.006 | 132.4 | 16.7 | 704 | 54 |  | 13 | 8.25 | 0.46 | 0.088 | 0.083 |