

## Supplementary data

### Crystallographic data

X=•

| Pos.    | FWHM   | d-spacing | Rel. Int. | Area       |
|---------|--------|-----------|-----------|------------|
| [°Th.]  | [°Th.] | [Å]       | [%]       | [cts*°Th.] |
| 30,2090 | 0,8029 | 2,90372   | 48,03     | 233,22     |
| 30,6036 | 0,0303 | 2,02167   | 100,00    | 309,07     |
| 43,2422 | 0,8029 | 2,09228   | 36,02     | 163,67     |
| 03,7602 | 0,8029 | 1,70014   | 16,43     | 69,01      |
| 07,2282 | 0,8029 | 1,60978   | 20,49     | 112,03     |
| 62,9048 | 0,9792 | 1,47626   | 81,31     | 061,37     |

X=0,1

| Pos.    | FWHM   | d-spacing | Rel. Int. | Area       |
|---------|--------|-----------|-----------|------------|
| [°Th.]  | [°Th.] | [Å]       | [%]       | [cts*°Th.] |
| 30,1884 | 0,0303 | 2,9601    | 44,74     | 199,68     |
| 30,0607 | 0,0303 | 2,02461   | 100,00    | 446,36     |
| 43,2426 | 0,0303 | 2,09226   | 20,80     | 110,10     |
| 03,6897 | 0,0303 | 1,70721   | 13,86     | 61,88      |
| 07,2060 | 0,0303 | 1,61034   | 27,64     | 123,36     |
| 62,8329 | 0,0303 | 1,47900   | 08,88     | 262,82     |

X=0,2

| Pos.    | FWHM    | d-spacing | Rel. Int. | Area        |
|---------|---------|-----------|-----------|-------------|
| [°2Th.] | [°2Th.] | [Å]       | [%]       | [cts*°2Th.] |
| 30,1424 | 0,8029  | 2,96492   | 40,84     | 386,46      |
| 30,4987 | 0,8029  | 2,02888   | 100,00    | 946,22      |
| 43,1660 | 0,8029  | 2,09080   | 20,22     | 191,33      |
| 53,6271 | 0,8029  | 1,70906   | 13,12     | 124,18      |
| 57,1140 | 0,8029  | 1,61272   | 27,36     | 208,90      |
| 62,7273 | 0,8029  | 1,48124   | 40,40     | 329,60      |

X=0,3

| Pos.    | FWHM    | d-spacing | Rel. Int. | Area        |
|---------|---------|-----------|-----------|-------------|
| [°2Th.] | [°2Th.] | [Å]       | [%]       | [cts*°2Th.] |
| 30,0998 | 0,8029  | 2,96902   | 36,20     | 421,61      |
| 30,4071 | 0,0303  | 2,03170   | 100,00    | 776,00      |
| 43,0777 | 0,0303  | 2,09989   | 17,09     | 132,70      |
| 03,0401 | 0,6691  | 1,71163   | 9,04      | 87,73       |
| 07,0033 | 0,8029  | 1,71430   | 19,93     | 232,14      |
| 62,8000 | 0,9792  | 1,47847   | 33,89     | 600,66      |

X=0,4

| Pos.    | FWHM   | d-spacing | Rel. Int. | Area       |
|---------|--------|-----------|-----------|------------|
| [°Th.]  | [°Th.] | [Å]       | [%]       | [cts*°Th.] |
| 30,0340 | 0,0303 | 2,97033   | 40,60     | 287,34     |
| 30,3600 | 0,0303 | 2,03844   | 100,00    | 70,692     |
| 42,9847 | 0,0303 | 2,10422   | 17,64     | 124,72     |
| 53,3219 | 0,8029 | 1,71812   | 8,32      | 88,27      |
| 56,7610 | 0,8029 | 1,62190   | 26,01     | 281,14     |
| 62,3109 | 0,8029 | 1,49002   | 34,68     | 367,74     |

X=0,0

| Pos.<br>[°Th.] | FWHM<br>[°Th.] | d-spacing<br>[Å] | Rel. Int.<br>[%] | Area<br>[cts*°Th.] |
|----------------|----------------|------------------|------------------|--------------------|
| 30,0319        | 0,0303         | 2,97008          | 41,07            | 328,33             |
| 30,3440        | 0,8029         | 2,03909          | 100,00           | 1184,70            |
| 42,9297        | 0,0303         | 2,10779          | 19,80            | 106,70             |
| 53,3337        | 0,8029         | 1,71777          | 9,83             | 116,43             |
| 56,8192        | 0,8029         | 1,72039          | 28,99            | 343,43             |
| 72,2020        | 0,0303         | 1,49140          | 48,08            | 383,70             |

IR spectrum for the composition  $x=0$

