**Text blocks for the publication of
powder X-ray diffraction data**

**Standard measurements conducted on Bruker D8**

Powder X-ray diffraction (PXRD) patterns of the pulverized samples were recorded at room temperature on a D8-A25-Advance diffractometer (Bruker, Karlsruhe, Germany) in Bragg-Brentano *θ-θ*-geometry (goniometer radius 280 mm) with Cu *K*α-radiation (λ = 154.0596 pm). A 12 µm Ni foil working as *K*β filter and a variable divergence slit were mounted at the primary beam side. A LYNXEYE detector with 192 channels was used at the secondary beam side. Experiments were carried out in a 2*θ* range of 7 to 120° with a step size of 0.013° and a total scan time of 1h.

**Standard measurements conducted on PANalytical X’Pert**

Powder X-ray diffraction (PXRD) patterns of the pulverized samples were recorded at room temperature on a X’Pert MPD diffractometer (PANalytical, Almelo, Netherlands) in Bragg-Brentano *θ-θ*-geometry (goniometer radius 280 mm) with Cu *K*α-radiation (λ = 154.0596 pm). A 12 µm Ni foil working as *K*β filter and a variable divergence slit were mounted at the primary beam side. A PIXcel1D detector was used at the secondary beam side. Experiments were carried out in a 2*θ* range of 7 to 120° with a step size of 0.013° and a total scan time of 1h.

*If data evaluation was conducted add:*

The recorded data was evaluated using the Bruker TOPAS 5.0 software [1], with the observed reflections being treated via single-line fits.

[1] Topas 5, Bruker AXS, Karlsruhe, Germany **2014**.

**High temperature measurements conducted on Bruker D8**

Powder X-ray diffraction (PXRD) patterns at elevated temperatures were recorded on a D8-A25-Advance diffractometer (Bruker, Karlsruhe, Germany) in Bragg-Brentano *θ-θ*-geometry (goniometer radius 280 mm) with Cu *K*α-radiation (λ = 154.0596 pm) using a XRK 900 / HTK 1200N (**Anton Paar GmbH,** Graz, Austria) reactor chamber. The samples were investigated in air / vacuum in the temperature range of 30 to 220 °C with heating rates of 10 or 50 K min–1, respectively. A 12 µm Ni foil working as *K*β filter and a variable divergence slit were mounted at the primary beam side. The secondary beam side was equipped with a LYNXEYE detector (192 channels). Diffraction patterns were recorded between 3 and 40° 2*θ* with a step size of 0.013° and a total scan time of 1h for each temperature. The thermal expansion of the reaction chamber and sample holder was determined using elemental Si (NIST Standard reference material 640f, *a* = 5.4311(1) nm). The obtained data were refined using the Bruker TOPAS 5.0 software package [1], keeping the lattice parameter of Si fixed while refining the height displacement. This was conducted for different temperatures from which a linear regression was determined. For the subsequent measurements, the *z*-height was modified by the previously determined values as a function of the temperature used.

*If data evaluation was conducted add:*

The recorded data was evaluated using the Bruker TOPAS 5.0 software [1], with the observed reflections being treated via single-line fits.

[1] Topas 5, Bruker AXS, Karlsruhe, Germany **2014**.

**Acknowledgments (choose the applicable one)**

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