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**Supporting information for article:**

**Beamline P02.1 at PETRA III for high-resolution and high-energy powder diffraction**

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**S1. Machine and undulator parameters****Table S1.A:** Selected machine parameters (complete list on [http://photon-science.desy.de/facilities/petra\\_iii/machine/parameters/index\\_eng.html](http://photon-science.desy.de/facilities/petra_iii/machine/parameters/index_eng.html))

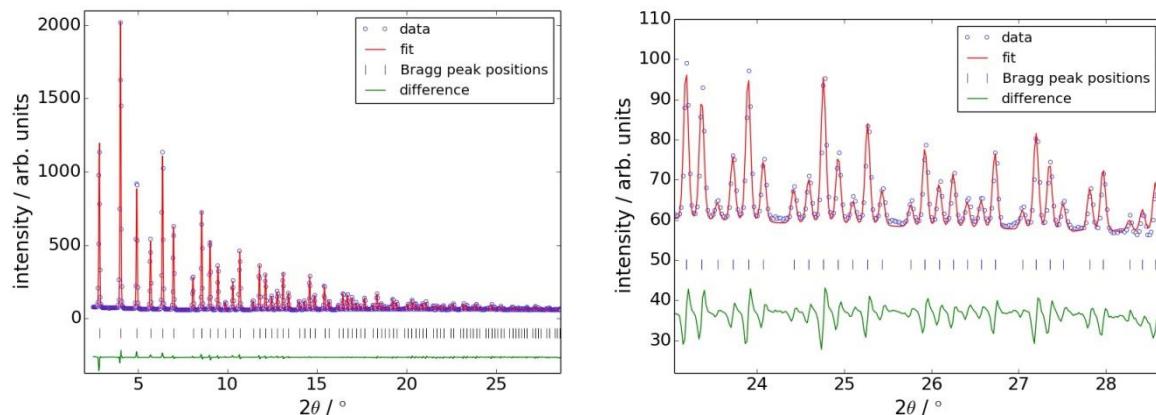
circumference	2304 m
energy	6.08 GeV
beam current	100 mA (top-up mode)
bunch number	960 / 40
RF frequency	500 MHz
horizontal emittance	1 nmrad
vertical emittance	10 pmrad
horizontal high- $\beta$ function (5m undulator)	20 m rad <sup>-1</sup>
vertical high- $\beta$ function (5m undulator)	2.4 m rad <sup>-1</sup>

**Table S1.B:** Selected undulator parameters (from Barthelmess *et al.* 2008 and calculated using the PETRA III Technical Design Report).

device	U23
type	planar, ex-vacuum
magnet material	Ni-Fe-B
device length	2 m
period length	23 mm
minimum gap	9.5 mm
gap @ 60 keV	~ 10 mm
peak magnetic field	0.61 T
total power	1.7 kW
on-axis power density	71 kW mrad <sup>-2</sup>
high- $\beta$ source size @ 60 keV, H × V (1 $\sigma$ )	127 × 5.0 $\mu\text{m}^2$
high- $\beta$ source divergence @ 60 keV, H × V (1 $\sigma$ )	8.2 × 2.3 $\mu\text{rad}^2$

## S2. Rietveld refinements for determination of instrumental resolution of the area detector

**Figure S2.A:** Exemplary Rietveld refinement plots and parameters for a PXRD measurement of LaB<sub>6</sub> filled into a capillary of 0.5 mm at a sample to detector distance of 510 mm. The refinement was carried out using the FullProf Suite (Rodriguez-Carvajal 2001), using Thompson-Cox-Hastings pseudo-Voigt peak shape and Chebychev polynomial background type with 5 coefficients. Left: full pattern; right: zoom into higher  $2\theta$  region.



### refined parameters:

<i>a</i>	4.154626
zero shift	-0.00324
scale	0.627 E-05
<i>B</i> <sub>iso</sub> (La)	0.318(1)
<i>B</i> <sub>iso</sub> (B)	0.277(8)
<i>U</i>	0.0356(6)
<i>V</i>	-0.0076(6)
<i>W</i>	0.0035(7)
<i>Y</i>	0.0114(9)

### agreement factors:

<i>R</i> <sub>p</sub>	6.26
<i>R</i> <sub>wp</sub>	6.08
<i>R</i> <sub>B</sub>	2.30
<i>R</i> <sub>F</sub>	2.81
$\chi^2$	0.0876

**Table S2:** Instrumental parameters from Rietveld refinement of data obtained in measurements of LaB<sub>6</sub> filled into capillaries of 0.57 mm (upper values in regular) and 1.0 mm (lower values in *italics*) diamenter, respectively. Rietveld refinements were carried out using the FullProf Suite (Rodriguez-Carvajal 2001), using Thompson-Cox-Hastings pseudo-Voigt peak shape and Chebychev polynomial background type with 5 coefficients..

sample to detector distance (SDD)	U	V	W	Y
385	0.0542(3) 0.0488(4)	-0.0123(4) -0.0088(9)	0.0061(4) 0.0098(4)	0.0114(9) 0.0057(0)
510	0.0356(6) 0.0417(5)	-0.0076(6) -0.0070(7)	0.0035(7) 0.0057(0)	0.0086(3) 0.0048(4)
760	0.0204(9) 0.0228(4)	-0.0037(8) -0.0037(1)	0.0016(4) 0.0025(8)	0.0057(4) 0.0038(5)
1260	0.0223(8) 0.0100(2)	-0.0026(2) -0.0011(6)	0.0006(4) 0.0009(3)	0.0035(2) 0.0027(2)
2760	0.0103(4) 0.0049(8)	-0.0008(3) -0.0005(3)	0.0001(4) 0.0002(2)	0.0017(5) 0.0015(6)

## References

Barthelmess, M., Englisch, U., Pflüger, J., Schöps, A., Skupin, J. & Tischer, M. (2008). *Proceedings of the 11th European Particle Accelerator Conference (EPAC08)*, 2320.

PETRA III Technical Design Report, DESY 2004-035, available on [http://petra3-project.desy.de/general/tdr/index\\_eng.html](http://petra3-project.desy.de/general/tdr/index_eng.html).

Rodriguez-Carvajal, J. (2001). *Commission on Powder Diffraction (IUCr) Newsletter*, **26**, 12-19.