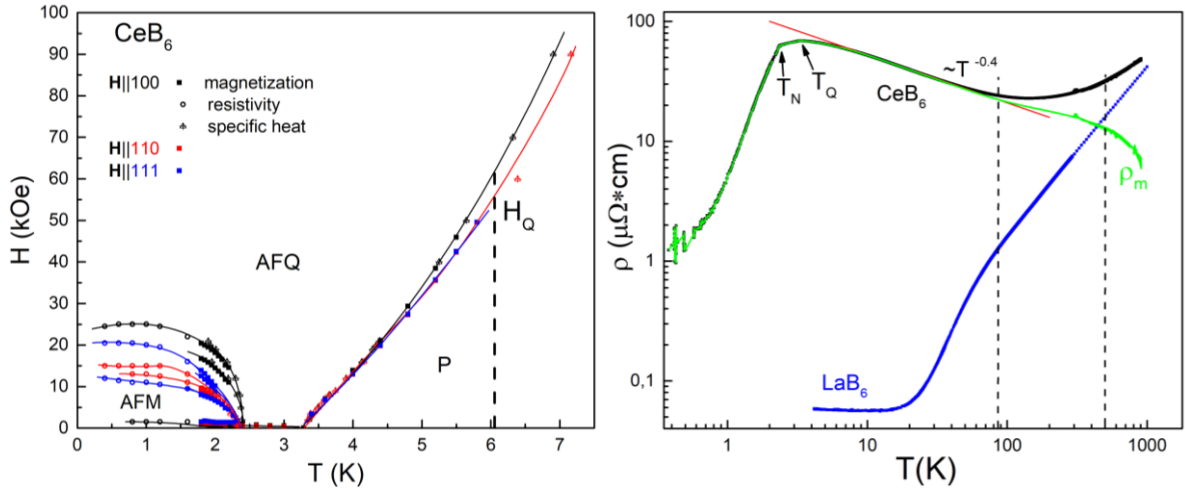
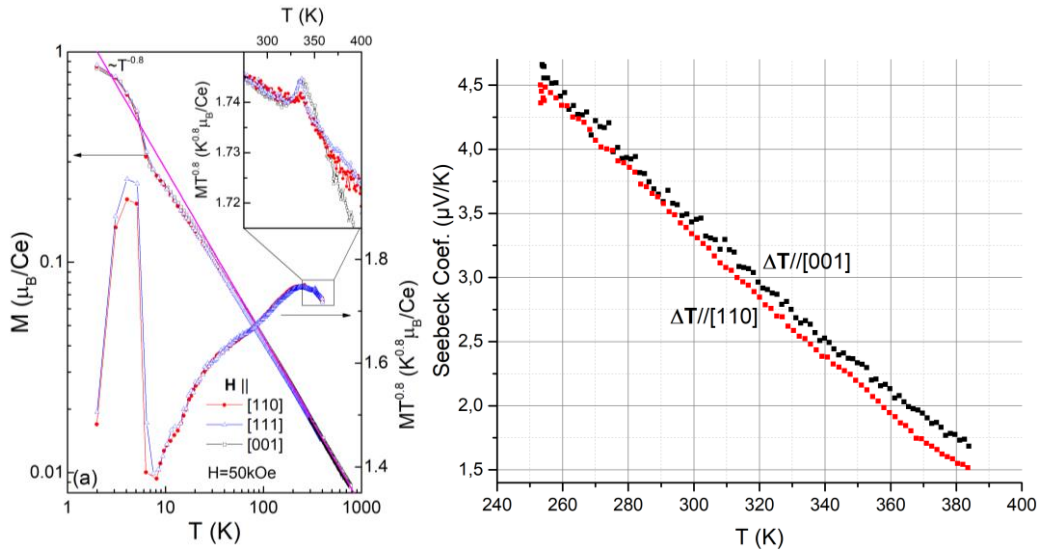


## Supplementary material to the article

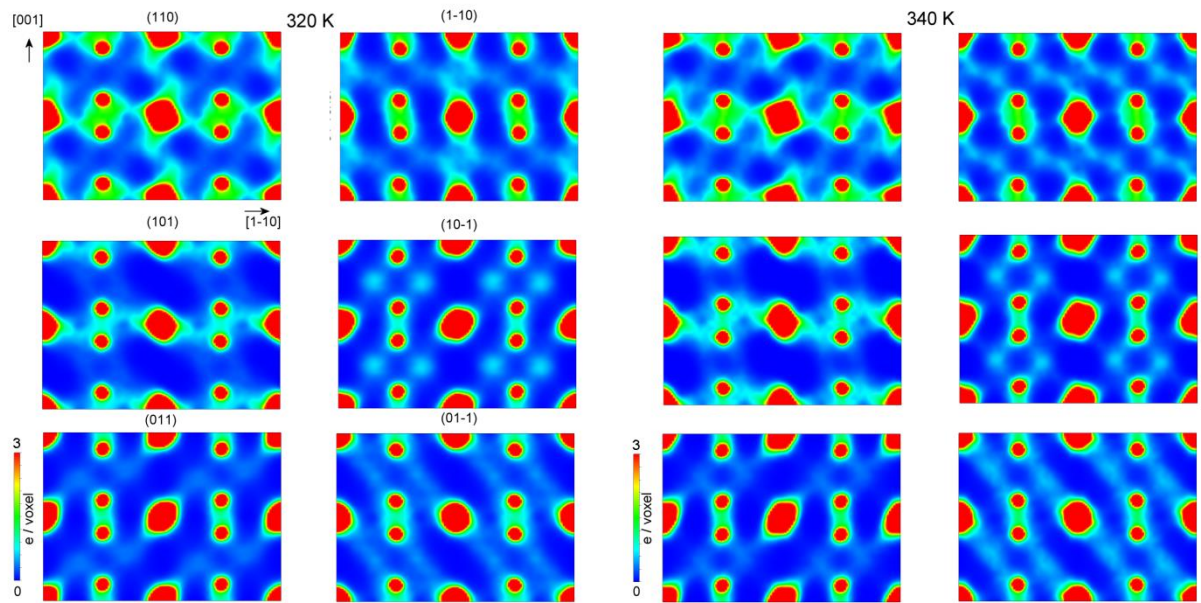
### “Electronic phase transition in the heavy fermions compound CeB<sub>6</sub>”



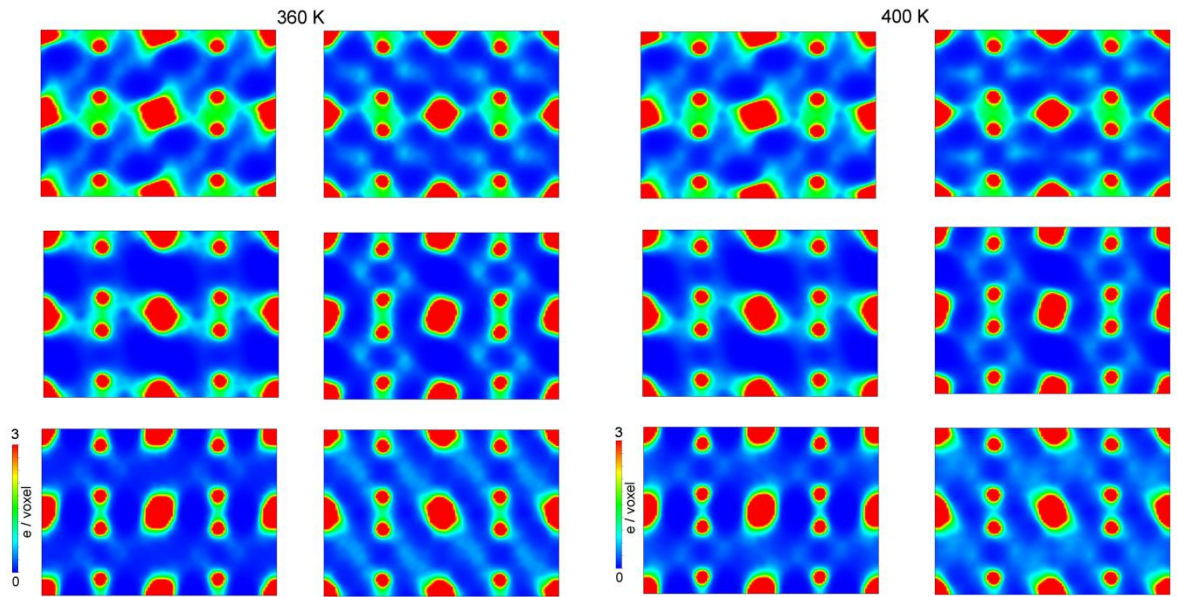
**Fig. S1.** (Left panel)  $H$ - $T$  phase diagram of CeB<sub>6</sub> for different directions of external magnetic field. Phase boundaries for  $\mathbf{H} \parallel [100]$ ,  $\mathbf{H} \parallel [110]$  and  $\mathbf{H} \parallel [111]$  are shown by black, red and blue lines, correspondingly. AFQ, AFM and P denote antiferroquadrupolar, antiferromagnetic and paramagnetic phases. (Right panel) Resistivity temperature dependences for CeB<sub>6</sub> and LaB<sub>6</sub> and magnetic contribution  $\rho_m(T)$  (green line) in CeB<sub>6</sub>. Red line demonstrates the power-law approximation  $\rho_m(T) \sim T^{-0.4}$ .  $T_N$  and  $T_Q$  denote the temperatures of AFQ and AFM magnetic phase transitions.



**Fig. S2.** (Left panel) Temperature dependences of magnetization  $M(T, H_0)$  measured in three CeB<sub>6</sub> crystals at  $H_0 = 50$  kOe in the principal directions  $\mathbf{H} \parallel [001]$ ,  $\mathbf{H} \parallel [110]$  and  $\mathbf{H} \parallel [111]$ , respectively (left axis) and the product  $M \cdot T^{0.8} = f(T)$  (right axis). Solid straight line demonstrates the exponential fit  $M \sim T^{-0.8}$ , and the inset shows a large-scale fragment of the dependences  $M \cdot T^{0.8} = f(T)$  in the temperature range 280–400 K. (Right panel) Temperature dependences of Seebeck coefficient for two directions  $\Delta T \parallel [001]$  and  $\Delta T \parallel [110]$  of the temperature gradient.



**Fig. S3.** MEM maps of the total ED distribution in the  $\{110\}$  planes of the  $\text{CeB}_6$  at the temperatures (left) 320 K and (right) 340 K. The calculations were carried out without restrictions on the  $Pm\bar{3}m$  symmetry. The planes pass through the metal atoms and two of the six B atoms forming the  $\text{B}_6$  cuboctahedron. ED peaks are cut at levels 3 e/voxel (red) and zero e/voxel (blue) to show in color subtle changes in the interstitial ED distribution.



**Fig. S4.** MEM maps of the total ED distribution in the  $\{110\}$  planes of the  $\text{CeB}_6$  at the temperature (left) 360 K and (right) 400 K. The calculations were carried out without restrictions on the  $Pm\bar{3}m$  symmetry. The planes pass through the metal atoms and two of the six B atoms forming the  $\text{B}_6$  cuboctahedron. ED peaks are cut at levels 3 e/voxel (red) and zero e/voxel (blue) to show in color subtle changes in the interstitial ED distribution.

**Table S1.** Crystallographic characteristics, details of X-ray diffraction experiments with CeB<sub>6</sub> single crystals

Chemical formula	CeB <sub>6</sub>			
<i>T</i> , K	320	340	360	400
Space group, <i>Z</i>	<i>Pm</i> $\bar{3}$ <i>m</i> , 1			
Lattice parameter <i>a</i> , Å	4.1404	4.14170	4.14270	4.14340
Radiation type; $\lambda$ , Å	AgK $\alpha$ ; 0.56087			
Maximum linear size of the sample, mm	0.258			
Diffractometer	XtaLAB Synergy-DW HyPix-Arc 150°			
Scan mode	$\omega$			
Absorption correction	polyhedron			
Absorption coefficient $\mu$ , MM <sup>-1</sup> ; <i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	8.325; 0.273, 0.676	8.317; 0.303, 0.636	8.311; 0.31, 0.638	8.307; 0.59, 1
$\theta$ <sub>max</sub> , deg	74.29	74.23	74.68	74.65
Limits of <i>h</i> ; <i>k</i> ; <i>l</i>	-14 ≤ <i>h</i> ≤ 12; -14 ≤ <i>k</i> ≤ 13; -14 ≤ <i>l</i> ≤ 14	-14 ≤ <i>h</i> ≤ 13; -14 ≤ <i>k</i> ≤ 14; -14 ≤ <i>l</i> ≤ 12	-14 ≤ <i>h</i> ≤ 13; -14 ≤ <i>k</i> ≤ 14; -14 ≤ <i>l</i> ≤ 12	-13 ≤ <i>h</i> ≤ 14; -14 ≤ <i>k</i> ≤ 14; -12 ≤ <i>l</i> ≤ 14
Number of reflection: observed <i>N</i> <sub>1</sub> ; with <i>I</i> > 3 $\sigma$ <i>I</i> ; independent <i>N</i> <sub>2</sub> ; <i>R</i> <sub>int</sub> , %	19982; 13770; 351; 6.19	19994; 12357; 351; 6.92	20046; 11579; 352; 5.65	20027; 10722; 354; 7.20
Number of refined parameters	6	6	6	6
Extinction method	Type 1, Lorentzian			
<i>R</i> <sub>1</sub> ( <i> F</i>  )/ <i>wR</i> <sub>2</sub> ( <i> F</i>  ), %	1.02/1.35	1.38/1.98	1.84/2.75	1.83/2.82
Goodness of fit <i>S</i>	1.04	1.09	1.17	1.18
$\Delta\rho$ <sub>min</sub> / $\Delta\rho$ <sub>max</sub> , e/Å <sup>3</sup>	-1.27/0.60	-1.66/0.73	-1.02/1.29	-2.05/1.49