Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2016

## **Supplementary Information for**

## "AIPd<sub>15</sub>B<sub>7</sub>: a new superconducting cage-compound with *anti*-Yb<sub>3</sub>Rh<sub>4</sub>Sn<sub>13</sub>-type of

## structure"

Qiang Zheng,<sup>a</sup> Walter Schnelle,<sup>a</sup> Yurii Prots,<sup>a</sup> Matej Bobnar,<sup>a</sup> Ulrich Burkhardt,<sup>a</sup> Andreas Leithe-Jasper<sup>a</sup> and Roman Gumeniuk,<sup>\*a,b</sup>

<sup>a</sup> Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden,

Germany

<sup>b</sup> Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23,

09596 Freiberg, Germany

\* *E-mail address: roman.gumeniuk@physik.tu-freiberg.de* 

Atoms		Distances	CN
Al	-6Pd2	2.730(1)	12
	-6Pd3	2.752(1)	
Pd1	-2B2	2.079(3)	14
	-2Pd3	2.774(1)	
	-2Pd2	2.782(1)	
	-2Pd2	2.857(1)	
	-2Pd2	2.976(1)	
	-2Pd3	3.012(1)	
	-2Pd3	3.214(1)	
Pd2	-1B3	2.139(6)	15
	-1B1	2.217(1)	
	-1B2	2.252(1)	
	-1Pd3	2.714(2)	
	-1Al	2.730(1)	
	-1Pd1	2.782(1)	
	-1Pd2	2.850(2)	
	-1Pd1	2.857(1)	
	-1Pd2	2.885(2)	
	-1Pd3	2.885(2)	
	-2Pd2	2.942(2)	
	-1Pd3	2.955(2)	
	-1Pd1	2.976(1)	
	-1Pd2	3.391(1)	
Pd3	-1B2	2.156(2)	14
	-1B3	2.157(5)	
	-1B3	2.28(2)	
	-1Pd2	2.714(2)	
	-1Al	2.752(1)	
	-1Pd1	2.774(2)	
	-2Pd3	2.789(2)	
	-1Pd2	2.885(1)	
	-2Pd3	2.921(2)	
	-1Pd2	2.955(2)	
	-1Pd1	3.012(1)	
	-1Pd1	3.214(1)	

Table S1. Interatomic distances (Å) in the AlPd $_{15}B_7$  structure

B1	-6Pd2	2.217(1)	6
B2	-2Pd1	2.079(3)	6
	-2Pd3	2.156(2)	
	-2Pd2	2.252(1)	
B3	-2Pd2	2.139(6)	6
	-2Pd3	2.157(5)	
	-2Pd3	2.28(2)	



**Figure S1.** X-ray diffraction pattern of powders of an as-cast AlPd<sub>15</sub>B<sub>7</sub> sample without stress annealing, showing broadening of all reflections, due to the ductility of the sample.



**Figure S2.** Microstructure of an as-cast AlPd<sub>15</sub>B<sub>7</sub> sample: (a) an image from optical microscope and (b) a BSE image in SEM, both revealing a very low amount of impurities in this sample; (c) EDXS mapping, where green and red contrasts belong to the AlPd<sub>15</sub>B<sub>7</sub> phase and impurities, respectively.

The content of impurities is less than 1 vol.%



Figure S3. Crystal structure of  $Yb_3Rh_4Sn_{13}$ . [Sn@Sn<sub>12</sub>] icosahedra – light gray; [Rh@Sn<sub>6</sub>] trigonal prisms – dark gray; [ $\Box$ @Yb<sub>2</sub>Sn<sub>4</sub>] octahedra – blue.



Figure S4. Coordination polyhedra in AlPd<sub>15</sub>B<sub>7</sub>



**Figure S5.** (a) Temperature dependence of  $c_{el}/T$  with the fit to  $c_{el} = \gamma_0 T + \gamma T_c A e^{\frac{-\Delta(0)}{k_B T}}$ ; (b)  $\gamma(H) - \gamma_0$  as a function of magnetic field  $\mu_0 H$ . The solid line shows a linear dependence of  $\gamma(H) - \gamma_0 vs \mu_0 H$ , indicating a typical *s*-wave gap for AlPd<sub>15</sub>B<sub>7</sub>.