Supporting Information

$Y_4Be_{33}Pt_{16}$ – a non-centrosymmetric cage superconductor with multi-centre bonding in the framework

Alfred Amon,[a,b] Eteri Svanidze,[a] Yurii Prots,[a] Michael Nicklas,[a] Ulrich Burkhardt,[a] Alim Ormeci,[a] Andreas Leithe-Jasper,*[a] and Yuri Grin [a]

Table S1. Anisotropic atomic displacement parameters for $Y_4Be_{33}Pt_{16}$

Atoms	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Y	0.58(3)	B_{11}	B_{11}	-0.06(2)	B_{12}	B_{12}
Pt1	0.53(1)	B_{11}	B_{11}	0.00(1)	B_{12}	B_{12}
Pt2	0.53(2)	0.51(2)	0.58(2)	0.01(2)	-0.01(2)	0.01(1)

Table S2. Interatomic distances in $Y_4Be_{33}Pt_{16}$ (in Å)

Y1 - 1Pt1 2.877(2) 3Pt2 3.044(2) 3Be4 3.15(3)

1Pt1 2.963(2) 3Be3 3.09(2) 3Pt2 3.171(2)

3Be2 3.032(15) 3Be4 3.15(3) 3Be1 3.666(1)

Pt1 - 3Be3 2.33(2) 3Be2 2.675(4) 3Pt2 2.8966(7)

3Be4 2.43(3) 1Y1 2.877(2) 1Y1 2.963(2)

Pt2 - 1Be1 2.3122(5) 2Be3 2.41(2) 1Be2 2.50(3) 1Pt1 2.8966(7)

1Be3 2.31(2) 1Be4 2.42(3) 1Be2 2.52(2) 1Y1 3.044(2)

1Be4 2.39(3) 1Be4 2.45(3) 1Pt2 2.8225(7) 1Y1 3.171(2)

Be1 - 4Be4 2.22(3) 4Pt2 2.3122(5) 4Y1 3.666(1)

Be2 - 2Be3 2.26(4) 2Pt2 2.50(3) 2Pt1 2.675(4)

2Be4 2.27(3) 2Pt2 2.52(2) 2Y1 3.032(15)

Be3 - 1Be4 2.20(3) 1Pt1 2.33(2) 2Pt2 2.41(2) 1Y1 3.09(2)

1Be2 2.26(4) 1Be3 2.34(3) 1Be4 2.48(3)

1Pt2 2.31(2) 1Be4 2.34(3) 2Be3 2.48(3)

Be4 - 1Be3 2.20(3) 1Be3 2.34(3) 1Pt1 2.43(3) 2Be4 3.14(4)

1Be1 2.22(3) 1Pt2 2.39(3) 1Pt2 2.45(3) 1Y1 3.15(3)

1Be2 2.27(3) 1Pt2 2.42(3) 1Be3 2.48(3) 1Y1 3.15(3)

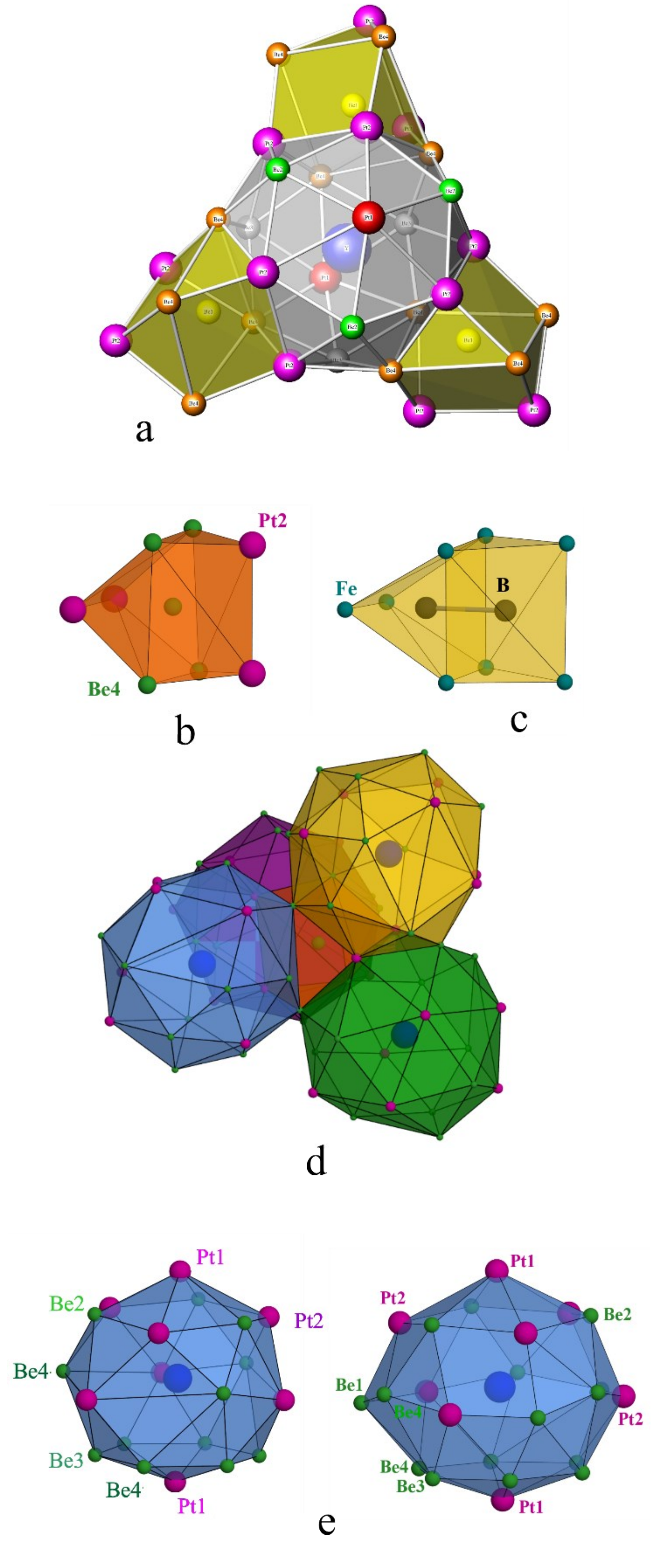

Figure S1. Crystal structure of $Y_4Be_{33}Pt_{16}$: (a) yttrium polyhedron with the adjacent bisdisphenoids of Be1; (b) coordination polyhedron of Be1; (c) the bisdisphenoid (B_2)@Fe8 in the crystal structure of $Nd_2Fe_{23}B_3$ (cf. panel b); (d) interconnection of the yttrium polyhedrons around the void at (⅜ 0 ¼) filled by Be1; coordination polyhedron of yttrium obtained from the interatomic distance analysis (left) and after involving the bonding information.

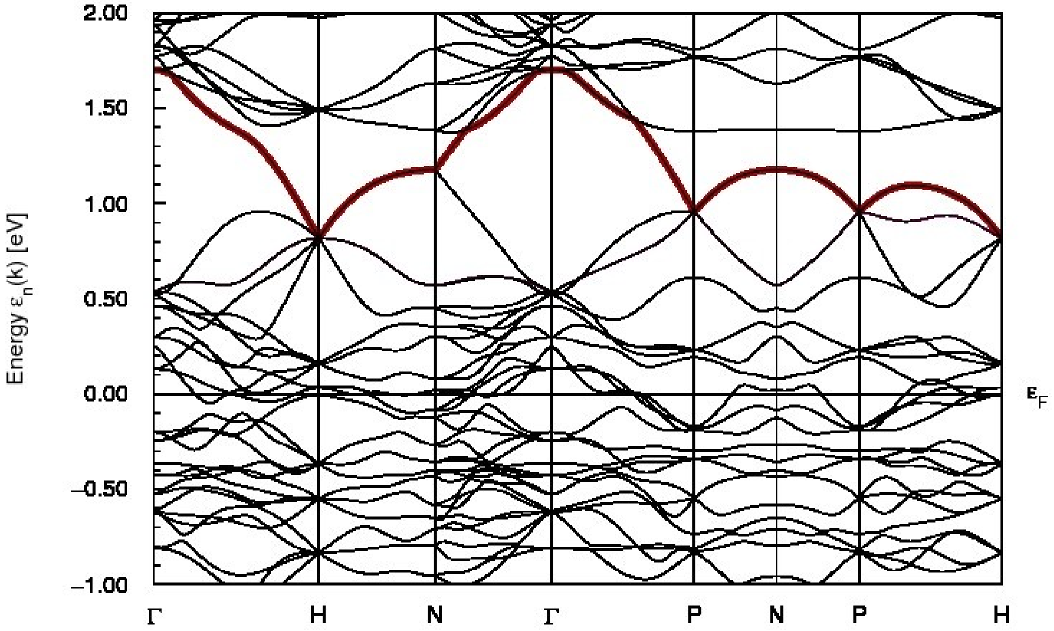

Figure S2. Electronic band structure computed for $Y_4Be_{33}Pt_{16}$. The Fermi energy E_F is at 0 eV. There are various flat bands in the small vicinity of the Fermi energy giving rise to a local maximum of the DOS (see main text, Fig. 5) at E_F. The pseudo gap features of the DOS (see main text, Fig. 5) between 1.3 and 1.4 eV stem from the band dispersing between 0.8 eV (at point H) and 1.7 eV (at point Γ). Y 4*d* orbitals provide the largest contribution to this band, and all the Pt and Be atoms also contribute through 5*d* and 2*p* orbitals, respectively.

Comment on the pseudogap formation:

Although the density of states (DOS) of $Y_4Be_{33}Pt_{16}$ and the complex intermetallic compound $Be_{21}Pt_5$ look similar, there are important differences regarding the pseudo gaps. As reported in our $Be_{21}Pt_5$ publication [1] the pseudo gap of the latter is located only 0.45 eV away from the Fermi level, and the pseudo gap is reached when 4 Be atoms per conventional cell are added. However, in this case no possible site in the crystal structure was found to accommodate such an additional Be species [1]. In the case of the title compound, the pseudo gap region is located further away from the Fermi level. The dip of the DOS around 0.9 eV corresponds to 12.2 electrons per formula unit (f.u.), and the relatively flat region (around 1.3 eV) just before the sharp increase corresponds to ~ 13.5 electrons per f.u. Neither of these numbers can be associated with an easily recognizable composition. The bands starting from about -1 eV and up to around 4 eV are mainly formed by hybridizations of Be 2p, Y 4d and Pt 5d. Since the first two states are largely empty (both in free atom and in the compound) the pseudo gap region, which may be considered as a boundary dividing the bands of "bonding" and "anti-bonding" combinations, is located at a high energy and also quite wide, not sharp as in $Be_{21}Pt_5$, for example.

[1] A. Amon et al., *Acc. Chem. Res.*, 2018, **51(2)**, 214-22.