Supporting Information

Cage compound $Sc_5Pt_{24}B_{12}$: a Pt-stuffed variant of filled skutterudite structure. Electronic and structural properties.

Leonid Salamakha[1,4,*], Oksana Sologub[1], Berthold Stöger[2], Herwig Michor[1], Ernst Bauer[1], Peter F. Rogl[3]

[1]Institute of Solid State Physics, TU Wien, A-1040 Vienna, Austria

[2]X-Ray Center, TU Wien, A-1060 Vienna, Austria

[3]Institute of Materials Chemistry, University of Vienna, A-1090 Vienna, Austria

[4]Department of Physics of Metals, L'viv National University, L'viv, Ukraine

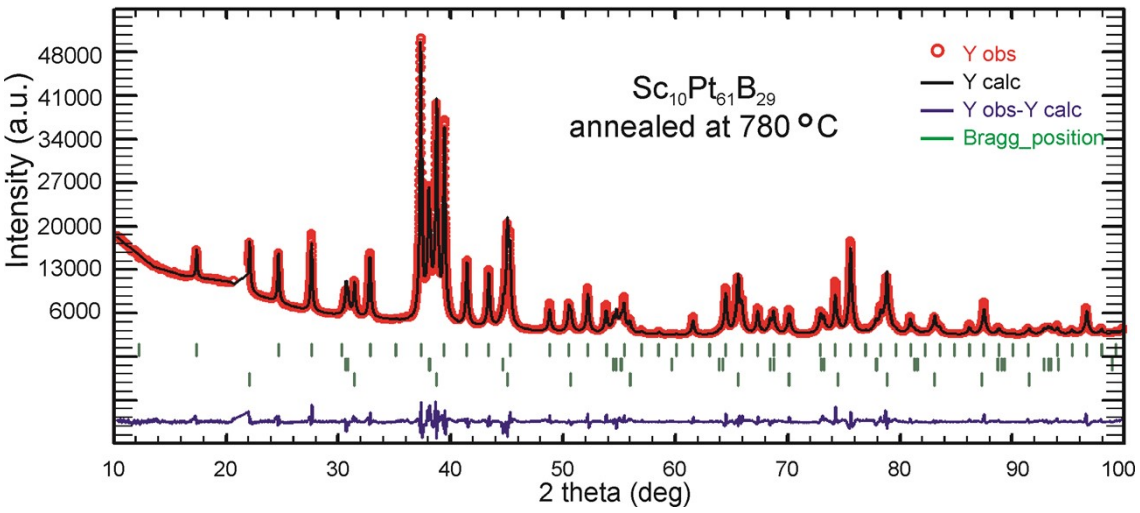

Figure S1. Powder X-ray diffraction pattern of alloy $Sc_{10}Pt_{61}B_{29}$ (in at.%) annealed at 780 ºC: upper row of *hkl* labels corresponds to $Sc_5Pt_{24}B_{12}$, space group *Im*-3, *a*=10.21112(9) Å; middle row stands for Pt_3B_2, space group *Cmcm*, *a*=3.3671(1) Å, *b*=5.7962(2) Å, *c*=4.0565(2) Å; lower row represents the phase $ScPt_3B_x$, space group *Pm*-3*m*, *a*=4.0235(4) Å. The excluded region contains a small peak from sample holder.

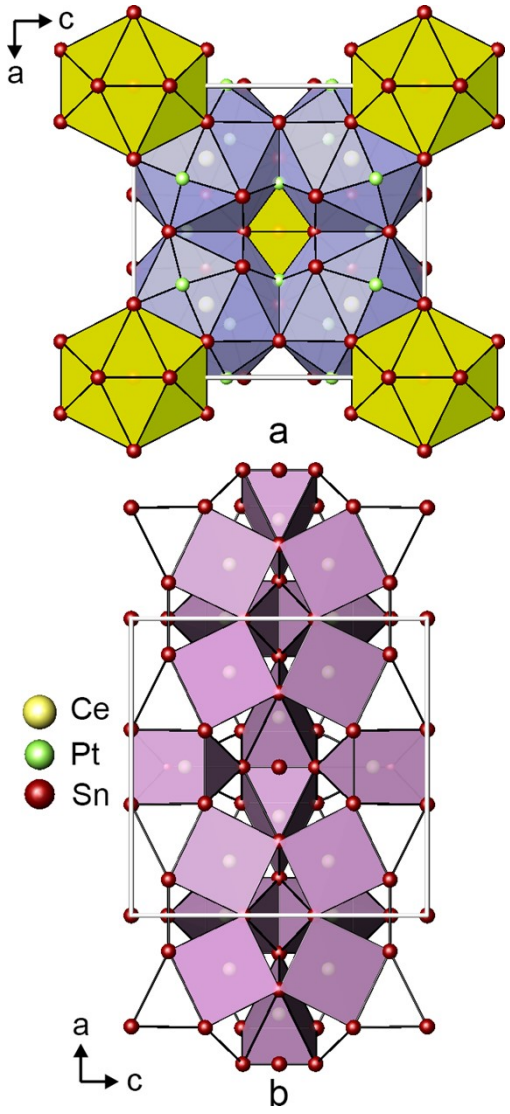

Figure S2. Polyhedral representation of $Ce_4Pt_{12}Sn_{25}$ structure showing [Sn_{12}] (gold) and [$Sn_{12}Pt_6$] (blue) cages capturing Sn and Ce, respectively (a). Linkage of [$PtSn_6$] trigonal prisms. For clarity, a half of the unit cell along *b* is shown (b).

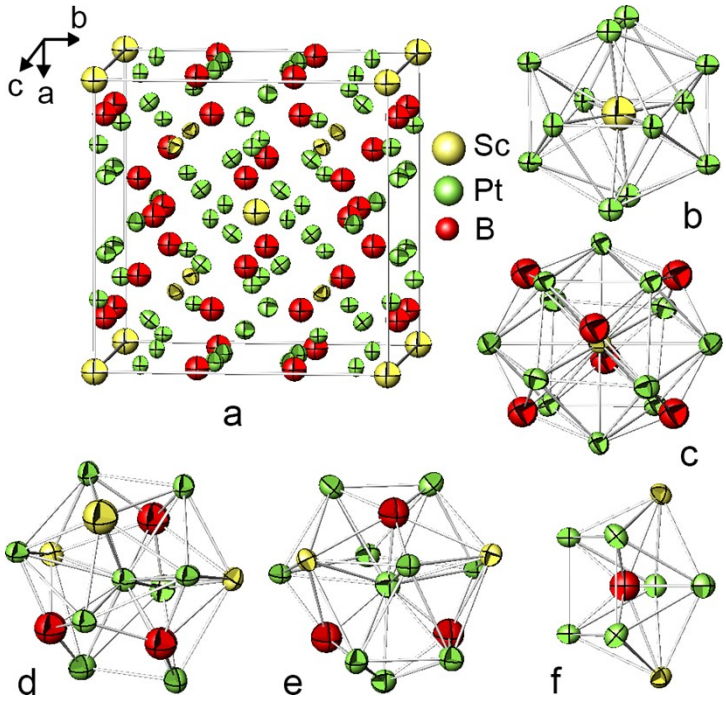

Figure S3. Ellipsoidal model of the $Sc_5Pt_{24}B_{12}$ crystal structure (a) and coordination polyhedra of atoms: Sc1 (b), Sc2 (c), Pt1 (d), Pt2 (e) and B1 (f). Thermal ellipsoids represent 99.99% probability level.

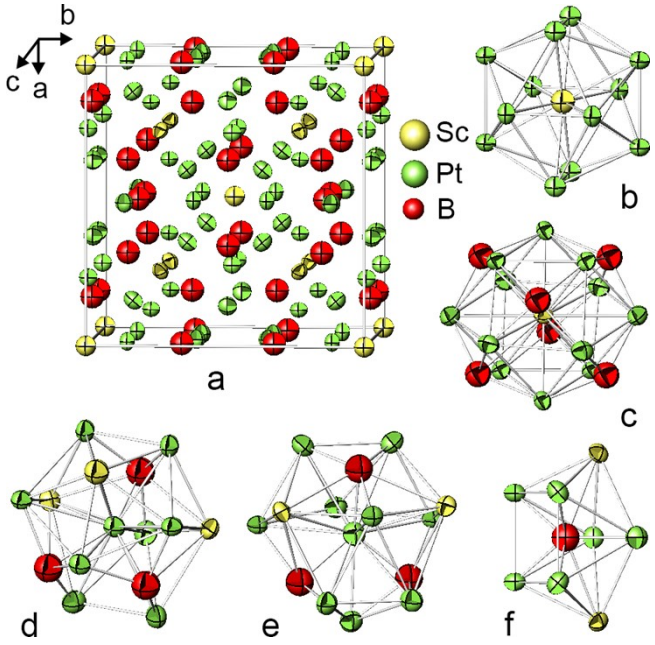

Figure S4. Ellipsoidal model of the $Sc_{4.9}Pt_{24}B_{12}$ crystal structure (a) and coordination polyhedra of atoms: Sc1 (b), Sc2 (c), Pt1 (d), Pt2 (e) and B1 (f). Thermal ellipsoids represent 99.99% probability level.

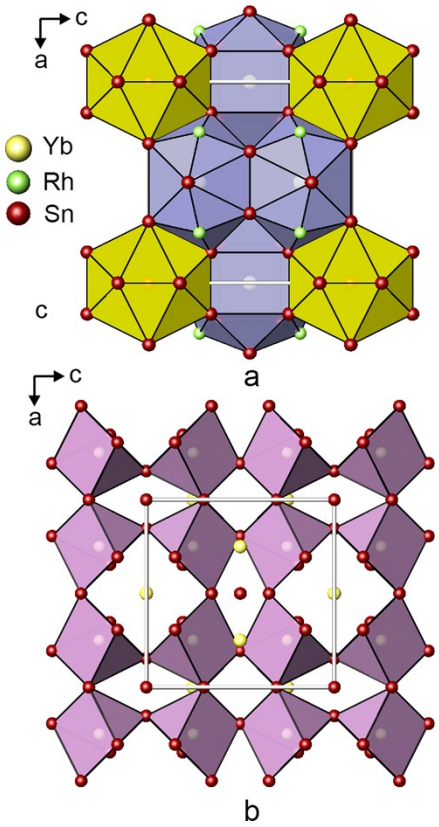

Figure S5. Polyhedral representation of the $Yb_3Rh_4Sn_{13}$ structure showing [Sn_{12}] (gold) and [$Sn_{12}Rh_4$] (blue) cages capturing Sn and Yb, respectively. (a). Linkage of [$RhSn_6$] trigonal prisms in $Yb_3Rh_4Sn_{13}$. For clarity, a half of the unit cell along *b* is shown (b).

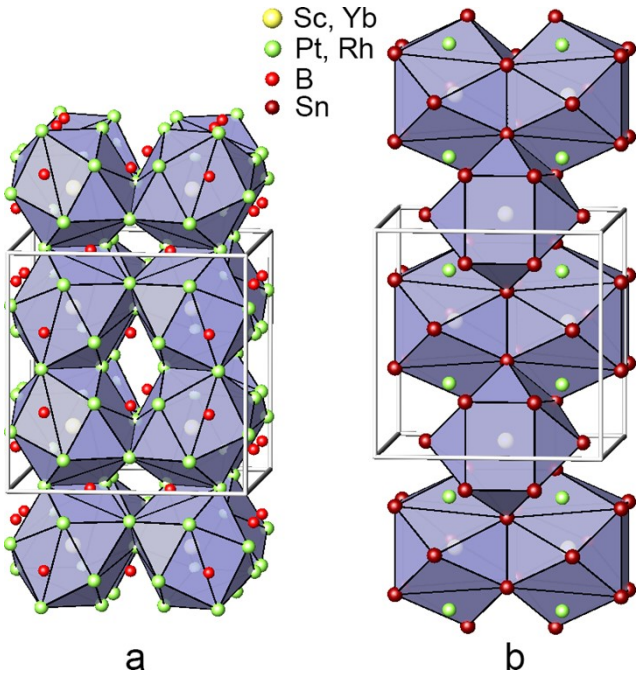

Figure S6. Arrangements of Sc-filled [Pt_{12}] and Yb-filled [Sn_{12}] cubooctahedra in $Sc_5Pt_{24}B_{12}$ (a) and $Yb_3Rh_4Sn_{13}$ (b) structures respectively.

Table S1. Refinement details, atomic coordinates and displacement parameters for $Sc_5Pt_{24}B_{12}$ at different levels of 2*a* site occupation.

Parameter	1.00 Sc1 in 2*a*	0.91 Sc1 in 2*a*
Formula from refinement	$Sc_5Pt_{24}B_{12}$	$Sc_{4.9}Pt_{24}B_{12}$
Composition (at.%)	$Sc_{12.2}Pt_{58.5}B_{29.3}$	$Sc_{12.0}Pt_{58.7}B_{29.3}$
GOF	1.146	1.165
Final R indices [I>2σ(I)]	R_1=0.0173 wR_2=0.0266	R_1=0.0173 wR_2=0.0254
R indices (all data)	R_1=0.0227 wR_2=0.0273	R_1=0.0227 wR_2=0.0261
Extinction (Zachariasen)	0.000147(8)	0.000148(8)
Sc1 in 2*a* (0,0,0); Oc. U_{11}[a]=U_{22}=U_{33}; U_{23}=U_{13}=U_{12}=0	1.00 0.0106(9)	0.91 0.0068(9)
Sc2 in 8*c* (¼,¼,¼); Oc. U_{11}=U_{22}=U_{33}; U_{23}=-U_{13}=-U_{12}	1.00 0.0046(4), 0.0007(4)	1.00 0.0046(4), 0.0007(4)
Pt1 in 24*g* (0,*y*,*z*); Oc. U_{11}, U_{22}, U_{33}, U_{13}, U_{23}=U_{12}=0	*y*=0.23486(3), *z*=0.13162(3); 1.00 0.0050(1), 0.0055(1), 0.0037(1), 0.0001(1)	*y*=0.23485(3), *z*=0.13162(2); 1.00 0.0050(1), 0.0055(1), 0.0037(1), 0.00004(8)
Pt2 in 24*g* (0,*y*,*z*); Oc. U_{11}, U_{22}, U_{33}, U_{13}, U_{23}=U_{12}=0	*y*=0.36478(3), *z*=0.37149(3); 1.00 0.0059(1), 0.0059(1), 0.0056(1), 0.0012(1)	*y*=0.36478(3), *z*=0.37149(3); 1.00 0.0059(1), 0.0059(1), 0.0056(1), 0.0012(1)
B1 in 24*g* (0,*y*,*z*); Oc. U_{iso}[b]	*y*=0.1522(9), *z*=0.3340(9); 1.00 0.009(1)	*y*=0.1522(8), *z*=0.3343(8); 1.00 0.009(1)
Residual density; max; min [el/Å^3]	1.789; -1.776	1.797; -1.759

[a,b]anisotropic (U_{ij}) and isotropic (U_{iso}) atomic displacement parameters are given in Å^2.

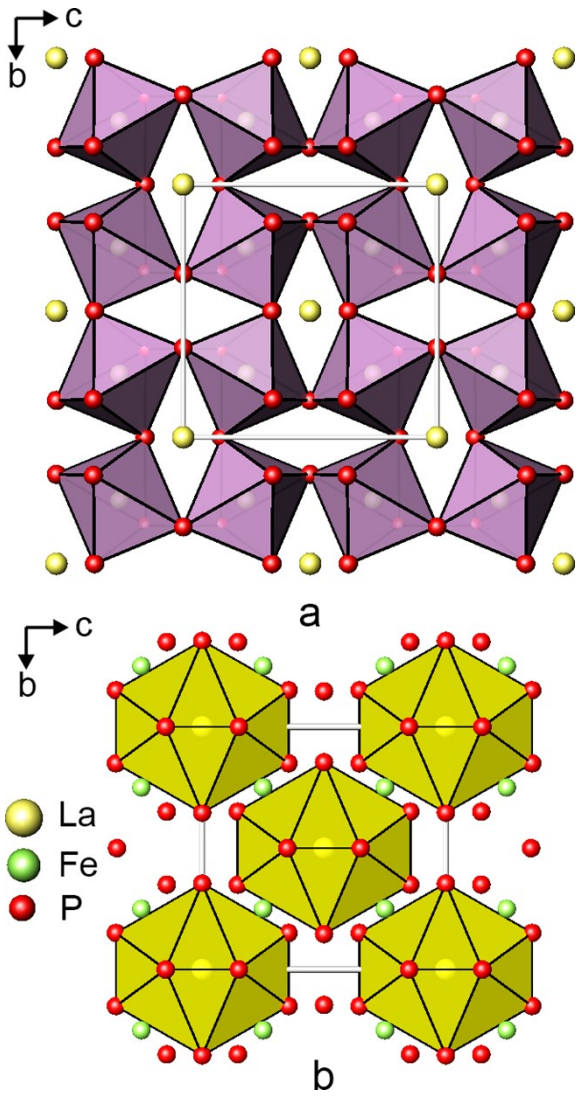

Figure S7. Arrangements of [FeP_6] octahedra (a) and P_{12} icosahedra around La atom (b) in the $LaFe_4P_{12}$ structure.

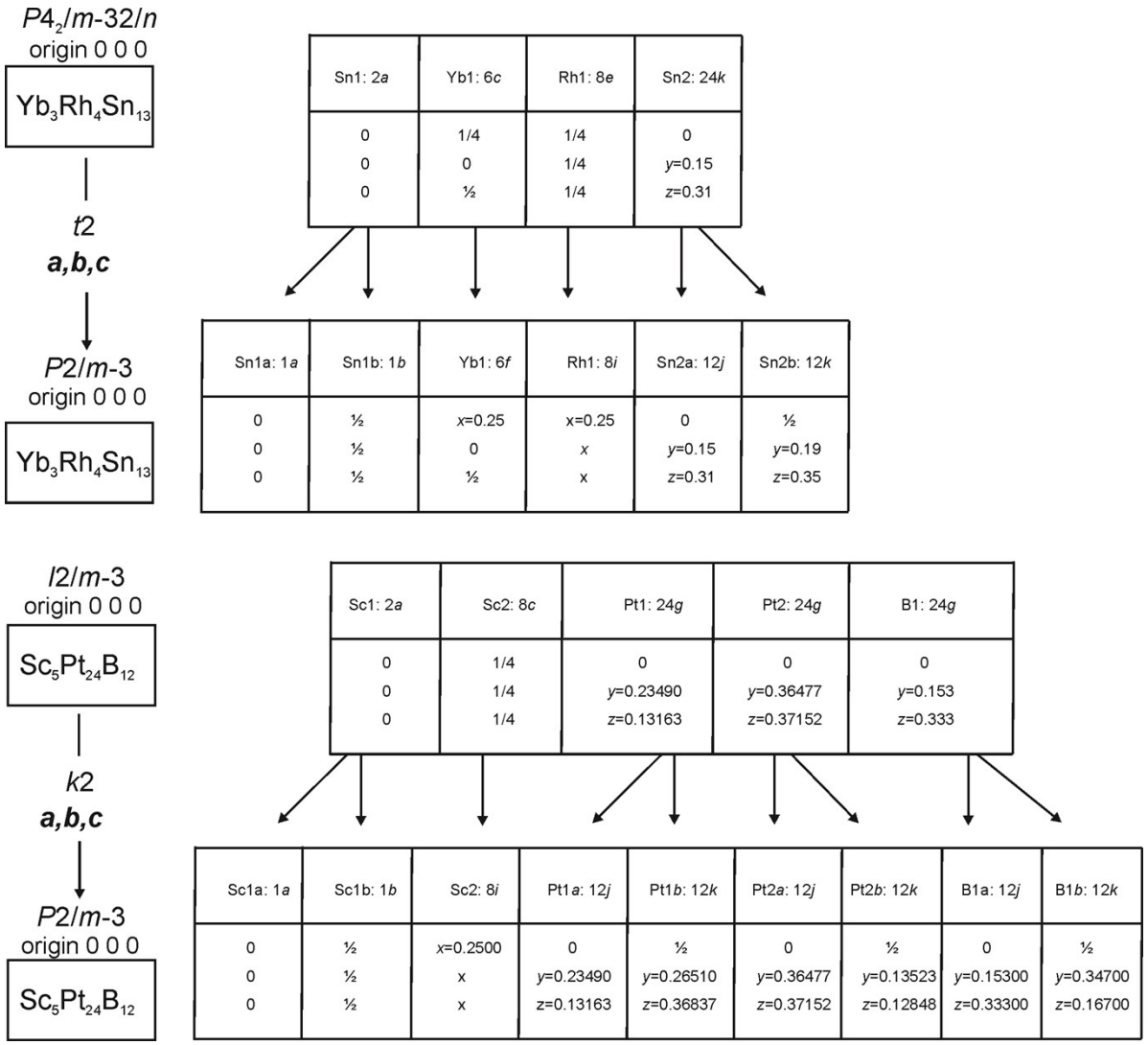

Figure S8. Group-subgroup relationships for the $Yb_3Rh_4Sn_{13}$ and $Sc_5Rh_{24}B_{12}$ structures.

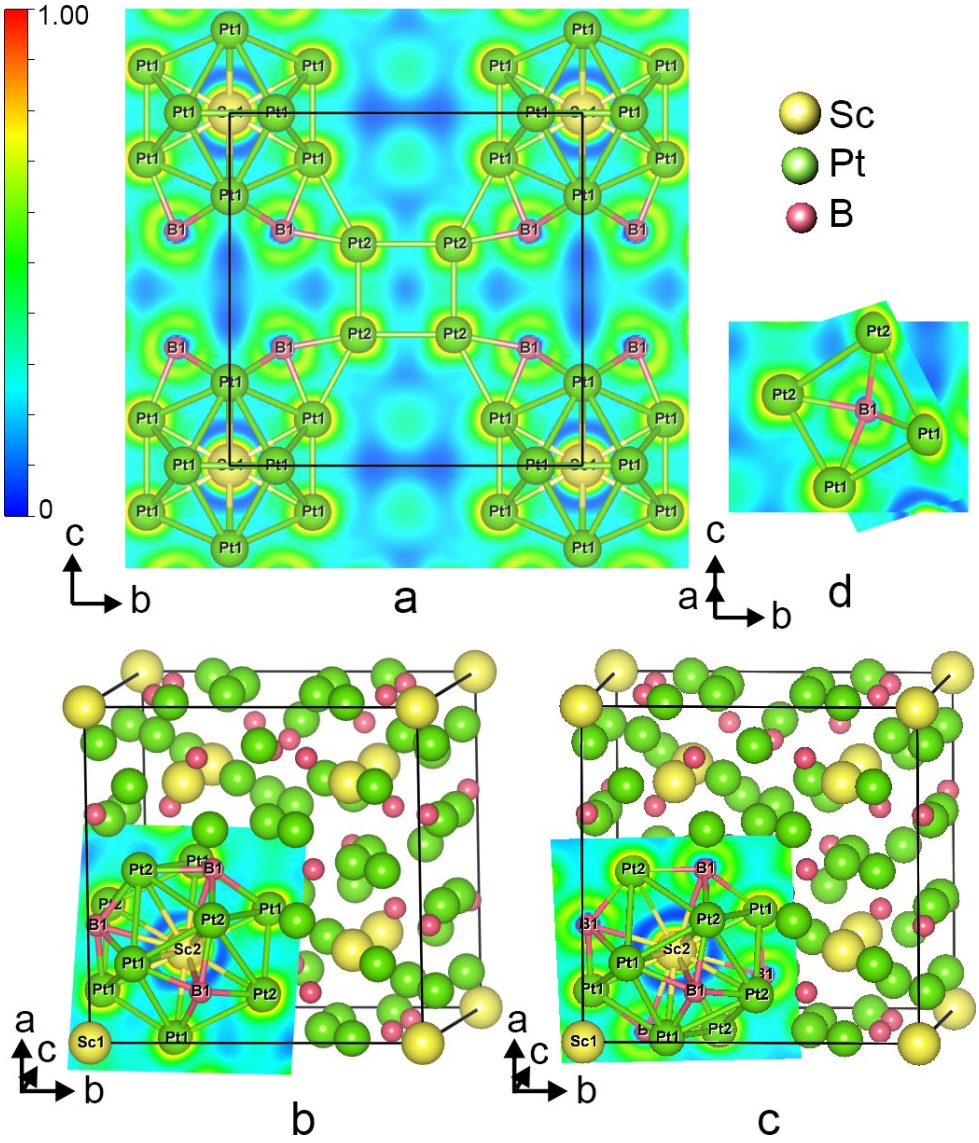

Figure S9. Distribution of electron localization function in $Sc_5Pt_{24}B_{12}$ in the plane (100) (a). Sections of calculated electron localization function in the planes within the $[Sc2Pt_{12}B_6]$ polyhedron containing the chemical bonds: Sc2-Pt1, Sc2-Pt2 and the bonds between platinum atoms (b); Sc2-B1, Pt1-B1 and Pt2-B1 (c). Sections of calculated electron localization function visualizing platinum-boron interactions in $[BPt_6]$ trigonal prism (d).