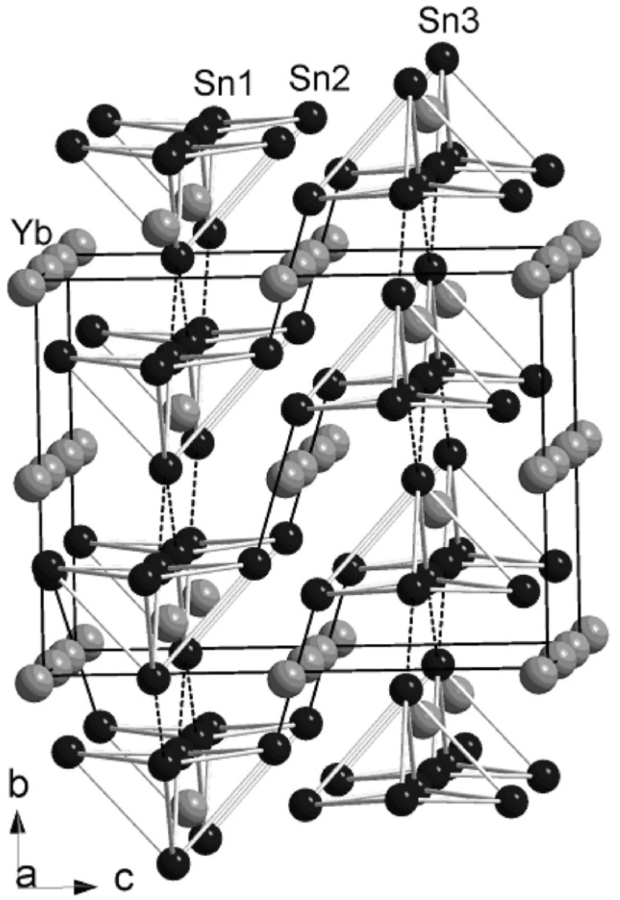
# Crystal structure of triytterbium pentastannide, $Sn_5Yb_3$

Ming-Hui Ge*,I and John D. Corbett II

I College of Chemical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, P. R. China
II Ames Laboratory, DOE and Department of Chemistry, Iowa State University, Ames 50010, U.S.A.

Received July 31, 2011, accepted and available on-line September 30, 2011, CSD no. 710073




**Abstract**
$Sn_5Yb_3$, orthorhombic, *Cmcm* (no. 63), $a = 10.193(2)$ Å, $b = 8.168(2)$ Å, $c = 10.375(2)$ Å, $V = 863.7$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.032$, $wR_{ref}(F^2) = 0.081$, $T = 293$ K.

**Source of material**

The compound was prepared from pure metals of ytterbium (Ames Laboratory, purity >99.9% total) and tin (Alfa Aesar, purity >99.9%), which were loaded into a tantalum tube already sealed at one end, subsequently arc-welded under an argon atmosphere, and finally sealed in an evacuated silica tube. All manipulations were performed in a nitrogen-filled glovebox with a moisture level below 0.1 ppm. Grey-black brittle crystals of $Yb_3Sn_5$ were obtained from an $Yb_2Sn_3$ composition and the sample was first heated to 1373 K and held for 5 h. The temperature was decreased to 973 K at a rate of 2 K/h and held there for 12 h, and then the temperature was decreased to 573 K at a rate of 3 K/h. The crystals are sensitive to air and moisture.

**Discussion**

Tin is very diverse in the formation of nominal Zintl phases and yields a variety of compounds containing isolated tin atoms, tin dimers, chains, networks, clusters and frameworks [1-6]. Several years ago, some isotypic $A_3Tt_5$ phases, namely $Ba_3Pb_5$, $Sr_3Sn_5$, $Ba_3Sn_5$, $Eu_3Sn_5$ and $RE_3Sn_5$ (RE = La-Pr) [7-9], were reported to crystallize with a novel $Pu_3Pd_5$-type structure. The existence of $Yb_3Sn_5$ was first reported in the paper of an updating phase diagram of the Yb-Sn system without crystal structure [10].
$Yb_3Sn_5$ crystallizes in a modified $Pu_3Pd_5$-type structure. Its substructures feature the novel [$Sn_5$] square pyramidal clusters. The polyanions have *mm* ($C_{2v}$) symmetry with 2-fold axes parallel to [100] and [010] axes. The tin clusters are slightly distorted square pyramids. The intra-cluster Sn—Sn distances range from 3.028 to 3.155 Å which are comparable to the values in $Sr_3Sn_5$, $Ba_3Sn_5$ and $Eu_3Sn_5$. The bond length $d$(Sn1—Sn3) = 3.049(1) Å is shorter than $d$(Sn2—Sn3) = 3.155(1) Å. The four tin atoms of the base in the pyramid are not located in a plane. The Sn—Sn distances in the base are all 3.028(1) Å. The pyramidal base is close to but not an ideal square plane in all this type of compounds. The bond angles ∠Sn1–Sn2–Sn1 and ∠Sn2–Sn1–Sn2 are 90.89(1)° and 88.69(1)°, respectively. From the figure one can see two types of longer intercluster distances, $d$(Sn2—Sn2) = 3.307 Å (base-to-base, thin solid lines) and $d$(Sn1—Sn3) = 3.515 Å (base-to-apex, dashed lines). They are 0.152 Å and 0.360 Å longer, respectively, than the largest intracluster distance. The former value is comparable to the corresponding value in metallic Zintl phase $La_3In_5$ [11], in which the short intercluster interaction was considered as bonding. The intervening Yb cations among the tin clusters make the structure dense and clearly influence the interactions between the tin clusters.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey-black grain, size 0.09 × 0.09 × 0.11 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 462.45 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART APEX CCD, $\omega$ |
| $2\theta_{max}$: | 56.52° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 2487, 567 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 552 |
| $N(param)_{refined}$: | 27 |
| Programs: | SHELXS-97, SHELXL-97 [12], DIAMOND [13] |

* Correspondence author (e-mail: mhge@bipt.edu.cn)

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Yb(1) | 4*c* | 0 | 0.1271(1) | ¼ | 0.0088(4) | 0.0078(4) | 0.0043(4) | 0 | 0 | 0 |
| Yb(2) | 8*e* | 0.29353(6) | 0 | 0 | 0.0095(4) | 0.0105(3) | 0.0079(4) | 0 | 0 | –0.0002(2) |
| Sn(1) | 8*g* | 0.71165(9) | 0.2835(1) | ¼ | 0.0077(5) | 0.0119(5) | 0.0063(5) | –0.0018(3) | 0 | 0 |
| Sn(2) | 8*f* | 0 | 0.8062(1) | 0.4540(1) | 0.0101(5) | 0.0101(5) | 0.0047(5) | 0 | 0 | –0.0010(3) |
| Sn(3) | 4*c* | 0 | 0.5197(2) | ¼ | 0.0098(6) | 0.0056(6) | 0.0057(7) | 0 | 0 | 0 |

*Acknowledgments.* This research was supported by the Ames Laboratory operated for DOE by Iowa State University (contract no. DE-AC02-07CH11358) and the fund for Young Scholars from Beijing Institute of Petrochemical Engineering.

## References

1. Corbett, J. D.: Polyanionic clusters and networks of the early *p*-element metals in the solid state: beyond the Zintl boundary. Angew. Chem., Int. Ed. **39** (2000) 670-690.
2. Leon-Escamilla, E. A.; Corbett, J. D.: Solid state compounds with tin-tin bonding. $Yb_{36}Sn_{23}$: a novel compound containing oligomeric tin anions. Inorg. Chem. **38** (1999) 738-743.
3. Dubois, F.; Schreyer, M.; Fässler, T. F.: $NaSn_2$: a novel binary Zintl phase with 2D polyanions of realgar-type units $[Sn_8]^{4-}$. Inorg. Chem. **44** (2005) 477-479.
4. Von Schnering, H.-G.; Kröner, R.; Baitinger, M.; Peters, K.; Nesper, R.; Grin, Y: Crystal structure of the defect clathrate $Cs_8Sn_{442}$. Z. Kristallogr. NCS **215** (2000) 205–206.
5. Hoffmann, S.; Fässler, T. F.: $SrSn_4$: a superconducting stannide with localized and delocalized bond character. Inorg. Chem. **42** (2003) 8748-8754.
6. Zhao, J.-T.; Corbett, J. D.: Zintl phases in alkali-metal-tin systems: $K_8Sn_{25}$ with condensed pentagonal dodecahedra of tin. Two $A_8Sn_{44}$ phases with a defect clathrate structure. Inorg. Chem. **33** (1994) 5721-5726.
7. Zürcher, F.; Nesper, R.; Hoffmann, S. and Fässler, T. F.: Novel arachno-type $X_5^{6-}$ Zintl anions in $Sr_3Sn_5$, $Ba_3Sn_5$, and $Ba_3Pb_5$ and charge influence on Zintl clusters. Z. Anorg. Allg. Chem. **627** (2001) 2211-2219.
8. Klem, M. T.; Vaughey, J. T.; Harp, J. G.; Corbett, J. D.: $A_3Tt_5$ phases $Sr_3Sn_5$, $Ba_3Pb_5$, and $La_3Sn_5$. Structure and bonding in a series of isotypic metallic compounds with increased electron count and their comparison with the nominal Zintl phase $La_3In_5$. Inorg. Chem. **40** (2001) 7020-7026.
9. Lei, X.-W.; Mao, J.-G.: Synthesis, crystal structure and band structure of $Eu_3Sn_5$ with arachno-type Zintl anions. Chinese J. Struct. Chem. **26** (2007) 1403-1408.
10. Manfrinetti, P.; Mazzone, D.; Palenzona, A.: An up-dating of the Yb-Sn phase diagram. J. Alloys Compounds **284** (1999) L1-L3.
11. Zhao, J.-T.; Corbett, J. D.: Square pyramidal clusters in $La_3In_5$ and $Y_3In_5$. $La_3In_5$ as a metallic Zintl phase. Inorg. Chem. **34** (1995) 378-383.
12. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.
13. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 2.1a. Crystal Impact, Bonn, Germany 1999.