The deprotonated dibenzoylethane (DBM) molecule is known to react with many metal ions to form chelate complexes. The C-bound H atoms were geometrically placed (C—H = 0.93–0.97 Å) and refined as riding with $U_{eq}(H) = 1.2U_{eq}(C)$. Owing to poor agreement, the (1 0 0) reflection was omitted from the final cycles of refinement.

**Experimental details**

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**Comment**

The deprotonated dibenzoylethane (DBM) molecule is known to react with many metal ions to form chelate complexes.
The molecular structure is shown in the figure (70% displacement ellipsoids) and shows the tin atom to be coordinated by four oxygen atoms, derived from two chelating ligands, as well as benzyl-C and chloride atoms. The benzyl-C and chloride atoms are mutually cis and trans to the Cl1 atom. The remaining Sn—O bond lengths are experimentally distinct with the shortest Sn—O1 bond [2.071(2) Å] having the O1 atom trans to the benzyl-C atom. The longest Sn—O4 bond [2.122(2) Å] sees the O4 atom trans to the Cl1 atom. The remaining Sn—O2 [2.108(2) Å] and Sn—O3 [2.102(2) Å] bonds are experimentally equivalent. These systematic variations follow the expected trends [11]. There is evidence that the disparity in the Sn—O bond lengths is due to the presence of a benzylidene(benzoylmethane)chloridoditin compound as the predominant product, where one chlorine and a benzyl group of the organotin precursor have been substituted by two DBM molecules.

The molecular structure is shown in the figure (70% displacement ellipsoids) and shows the tin atom to be coordinated by four oxygen atoms, derived from two chelating DBM anions, as well as benzyl-C and chloride atoms. The benzyl-C and chloride atoms are mutually cis and trans to the Cl1 atom. The remaining Sn—O bond lengths are experimentally distinct with the shortest Sn—O1 bond [2.071(2) Å] having the O1 atom trans to the benzyl-C atom. The longest Sn—O4 bond [2.122(2) Å] sees the O4 atom trans to the Cl1 atom. The remaining Sn—O2 [2.108(2) Å] and Sn—O3 [2.102(2) Å] bonds are experimentally equivalent. These systematic variations follow the expected trends [11]. There is evidence that the disparity in the Sn—O bond lengths is due to the presence of a benzylidene(benzoylmethane)chloridoditin compound as the predominant product, where one chlorine and a benzyl group of the organotin precursor have been substituted by two DBM molecules.

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The six-membered chelate rings are non-planar and are best described as having envelope conformations. Thus, for the O1-DBM ligand, the tin atom lies 0.547(3) Å out of the plane defined by the remaining five atoms of the six-membered ring, which have a r.m.s. deviation of 0.035 Å; the comparable values for the O3-DBM ligand are 0.343(4) and 0.030 Å, respectively. The dihedral angle between the planar regions of the chelate rings is 72.30(8)°, indicating an almost orthogonal relationship. Finally, the dihedral angles between the planar region of the O1-chelate ring and the pendant C4- and C10-phenyl rings are 26.73(16) and 31.74(14)°, respectively, and the dihedral angle between the outer rings is 30.51(14)°. The equivalent angles for the O3-chelate and the C19- and C25-rings are 31.24(9), 27.44(16) and 27.44(16)°, respectively.

In the crystal, supramolecular chains along the a axis are sustained by phenyl-C—H⋯O1 [C27—H27⋯O1; H27⋯O1 = 2.51 Å, C27⋯O1 = 3.428(4) Å with angle at H27 = 169° for symmetry operation (i) 1−x, −y, −z] and benzyl-phenyl-C—H⋯π(phenyl) [C36—H36⋯Cg(C10—C15); H36⋯Cg(C10—C15) = 2.63 Å, C36⋯Cg(C10—C15) = 3.503(4) Å and angle at H36 = 157°] interactions. The chains assemble into a three-dimensional architecture with no directional interactions between them.

According to a search of the Cambridge Structural Database [12], there are no examples of mixed organo/halotin(acetylacetonate)$_2$ structures related to the title structure in the crystallographic literature. However, there is a related diorganotin(III)$_2$ molecule, e.g. for $R=n$-Bu [9]. In the same way, there is also a related Sn(DBM)$_2$Cl$_2$ molecule [13]. In the former, the n-butyl groups are trans and in the latter, the chloride atoms are cis.

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References

1. Bruker. APEX2 and SAINT. Bruker AXS Inc., Madison, WI, USA (2008).
2. Sheldrick, G. M.: SADABS. University of Göttingen, Germany (1996).
3. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. A64 (2008) 112–122.
4. Sheldrick, G. M.: Crystal structure refinement with SHELXL. Acta Crystallogr. C71 (2015) 3–8.
5. Farrugia, L. J.: WinGX and ORTEP for Windows: an update. J. Appl. Crystallogr. 45 (2012) 849–854.
6. Sisido, K.; Takeda, Y.; Kinugawa, Z.: Direct synthesis of organotin compounds I. di- and tribenzyltin chlorides. J. Am. Chem. Soc. 83 (1961) 538–541.
7. Shimomatsu, T.; Tabushi, M.; Tarumoto, T.: Dibenzoylmethane as a chelating reagent in solvent extraction and spectroscopic determination. Bull. Inst. Chem. Res. Kyoto Univ. 40 (1963) 388–399.
8. Bancroft, G. M.; Davies, B. W.; Payne, N. C.; Sham, T. K.: Preparation and spectroscopic studies of five-co-ordinate β-diketonatotri(organo)tin compounds. Crystal structure of (1,3-diphenylpropane-1,3-dionato)-triphenyltin(IV). J. Chem. Soc. Dalton Trans. (1975) 973–978.
9. Poli, G.; Cheer, C. J.; Nelson, W. H.: The crystal and molecular structure of bis(1,3-diphenylpropane-1,3-dionato)-di-n-butyltin(IV). J. Organomet. Chem. 306 (1986) 347–354.
10. Thy, C. K.; Lo, K. M.; Ng, S. W.: Dichloridobis(1,3-phenylpropane-1,3-dionato-κ$^2$O,O)tin(IV) toluene hemisolvate. Acta Crystallogr. E66 (2010) m992.
11. Lee, S. M.; Lo, K. M.; Tiekink, E. R. T.: Crystal structure of chlorido-4-fluorobenzylbis[2-methylquinolin-8-olato-κ$^2$N,W,O]tin(IV), C$_{27}$H$_{29}$ClF$_{2}$O$_4$Sn. Z. Kristallogr. NCS 234 (2019) 823–825.
12. Groom, C. R.; Allen, F. H.: The cambridge structural database in retrospect and prospect. Angew. Chem. Int. Ed. 53 (2014) 662–671.
13. Searle, D.; Smith, P. J.; Bell, N. A.; March, L. A.; Nowell, I. W.; Donaldson, J. D.: Structural, infrared and Mössbauer studies of octahedral cis-dichlorobis(diketonate)tin(IV) complexes having anti-tumour activity. J. Organomet. Chem. 162 (1989) 143–149.