WZ13FMI

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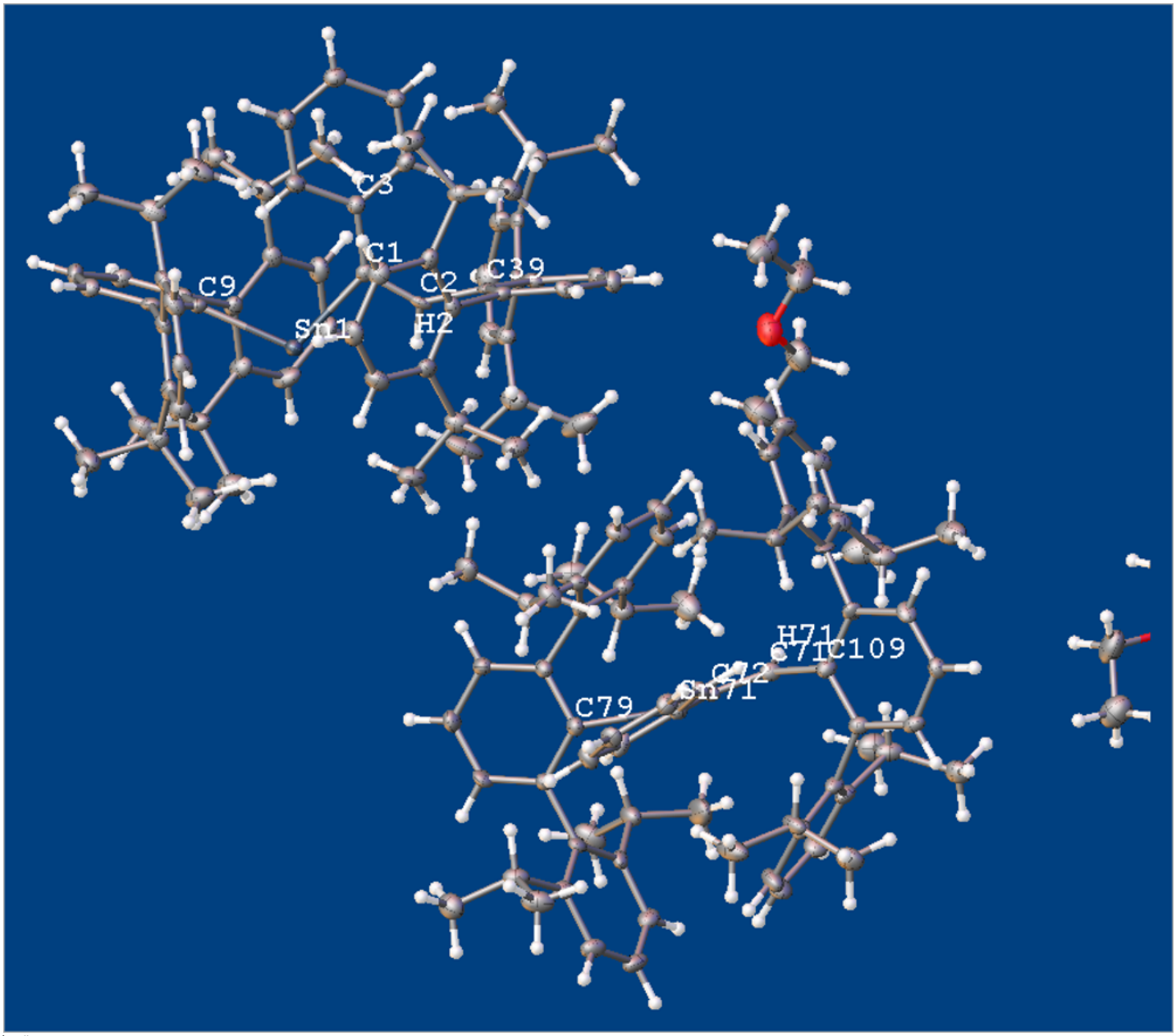

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Table 1 Crystal data and structure refinement for WZ13FMI.

Identification code	WZ13FMI
Empirical formula	$C_{72}H_{90}OSn$
Formula weight	1090.12
Temperature/K	90.15
Crystal system	triclinic
Space group	P-1
a/Å	17.8418(9)
b/Å	17.8598(9)
c/Å	19.2380(10)
α/°	88.9389(8)
β/°	81.5494(8)
γ/°	89.9199(8)
Volume/Å^3	6062.6(5)
Z	4
ϱ_{calc}g/cm^3	1.194
μ/mm^{-1}	0.464
F(000)	2320.0
Crystal size/mm^3	0.288 × 0.218 × 0.188
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.674 to 50.5
Index ranges	-21 ≤ h ≤ 21, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23

Reflections collected	43726
Independent reflections	21946 [R_{int} = 0.0589, R_{sigma} = 0.0826]
Data/restraints/parameters	21946/149/1434
Goodness-of-fit on F^2	1.136
Final R indexes [I>=2σ (I)]	R_1 = 0.0617, wR_2 = 0.1082
Final R indexes [all data]	R_1 = 0.0930, wR_2 = 0.1173
Largest diff. peak/hole / e $Å^{-3}$	0.68/-0.84

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for WZ13FMI. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sn1	2980.2(2)	2527.2(2)	10488.8(2)	18.71(9)
C2	2464(2)	2300(2)	9168(2)	16.3(10)
C1	2137(2)	2635(2)	9748(2)	16.0(10)
C3	1393.3(13)	3054.1(17)	9828.8(16)	18.1(10)
C4	874.6(16)	2927.4(16)	9370.8(13)	19.4(10)
C5	159.6(15)	3251.4(17)	9492.5(16)	19.0(11)
C6	-36.6(15)	3702(2)	10072.2(19)	22.6(11)
C7	482.1(19)	3828.7(19)	10530.3(16)	22.0(12)
C8	1197.1(17)	3504.8(18)	10408.6(15)	21.3(11)
Sn1B	2917(5)	2199(5)	9383(4)	23.9(13)
C1B	2560(30)	2930(40)	10730(30)	10(20)
C2B	2150(30)	2780(40)	10220(20)	16(2)
C3B	1410(20)	3130(40)	10090(30)	18(2)
C4B	960(30)	2750(30)	9680(40)	19(2)
C5B	220(30)	2990(40)	9650(40)	19(2)
C6B	-60(30)	3610(50)	10040(50)	22(2)
C7B	390(40)	3980(50)	10450(40)	22(2)
C8B	1120(40)	3740(40)	10480(20)	21(2)
C9	2493(2)	2942(2)	11538(2)	16.3(9)
C10	2609(2)	3635(2)	11848(2)	16.5(9)
C11	2378(2)	3715(2)	12564(2)	20.2(10)
C12	2047(3)	3125(2)	12980(2)	22.1(10)
C13	1962(2)	2438(2)	12679(2)	18.5(10)
C14	2193(2)	2346(2)	11969(2)	17.3(10)
C15	3043(2)	4266(2)	11423(2)	18.4(10)
C16	3837(2)	4204(2)	11253(2)	21.5(10)
C17	4241(3)	4786(3)	10873(2)	26.0(11)
C18	3874(3)	5424(3)	10692(2)	27.5(11)
C19	3100(3)	5499(3)	10880(2)	25.9(11)
C20	2668(3)	4926(2)	11249(2)	21.6(10)
C21	4275(3)	3567(2)	11540(2)	23.6(11)
C22	4958(3)	3298(3)	11028(3)	36.7(13)
C23	4527(3)	3789(3)	12234(3)	35.6(13)
C24	1822(3)	5051(3)	11472(3)	26.7(11)
C25	1441(3)	5412(3)	10882(3)	36.9(13)
C26	1669(3)	5530(3)	12135(3)	35.6(13)
C27	2176(2)	1585(2)	11630(2)	18.4(10)
C28	1536(2)	1344(2)	11353(2)	20.0(10)
C29	1554(3)	639(3)	11042(2)	26.7(11)
C30	2179(3)	176(3)	11023(3)	31.9(12)
C31	2803(3)	410(3)	11302(3)	30.7(12)
C32	2820(3)	1115(2)	11600(2)	23.6(11)
C33	824(2)	1814(2)	11416(2)	23.3(11)
C34	365(3)	1704(3)	10808(3)	31.6(12)
C35	330(3)	1635(3)	12118(3)	27.6(11)
C36	3517(3)	1344(3)	11916(3)	27.2(11)
C37	4264(3)	1097(3)	11479(3)	40.1(14)
C38	3461(3)	1023(3)	12675(3)	34.5(13)
C39	2334(2)	2285(2)	8420(2)	14.5(9)
C40	2571(2)	2912(2)	7984(2)	15.9(9)
C41	2557(2)	2869(2)	7266(2)	18.4(10)
C42	2333(3)	2225(2)	6968(2)	22.9(10)
C43	2107(2)	1605(2)	7392(2)	20.2(10)
C44	2109(2)	1629(2)	8120(2)	17.6(10)
C45	2873(2)	3599(2)	8300(2)	18.0(10)
C46	2429(2)	4246(2)	8419(2)	19.2(10)
C47	2712(3)	4835(2)	8769(2)	22.4(10)
C48	3422(3)	4797(3)	8978(2)	27.4(11)
C49	3868(3)	4170(3)	8837(2)	25.9(11)
C50	3606(2)	3570(2)	8494(2)	19.4(10)
C51	1664(2)	4324(2)	8164(2)	20.2(10)
C52	1086(3)	4778(3)	8656(3)	29.1(12)
C53	1747(3)	4688(3)	7427(2)	27.2(11)
C54	4130(3)	2903(3)	8292(2)	24.3(11)
C55	4730(3)	2775(3)	8772(3)	32.2(12)
C56	4500(3)	2980(3)	7532(3)	30.7(12)
C57	1904(2)	943(2)	8563(2)	16.0(9)
C58	2480(2)	486(2)	8772(2)	20.2(10)
C59	2276(3)	-147(2)	9188(2)	25.2(11)

Atom	*x*	*y*	*z*	U(eq)
C60	1529(3)	-331(3)	9400(2)	27.3(11)
C61	967(3)	105(2)	9187(2)	23.5(11)
C62	1133(2)	738(2)	8760(2)	16.5(9)
C63	3313(3)	643(3)	8497(3)	27.9(11)
C64	3834(3)	513(3)	9049(3)	48.1(16)
C65	3562(3)	167(3)	7858(3)	47.6(16)
C66	493(2)	1160(2)	8483(2)	20.2(10)
C67	-202(3)	1290(3)	9039(2)	27.0(11)
C68	257(3)	763(3)	7855(2)	25.2(11)
Sn71	7602.5(2)	1926.6(2)	5501.7(2)	16.81(11)
C71	7408(3)	2694(3)	4210(3)	17.7(11)
C72	7684(3)	2920(3)	4781(3)	15.5(12)
C73	8065(2)	3657.6(17)	4870(2)	16.2(13)
C74	7985(3)	4258(2)	4416(2)	16.7(13)
C75	8301(4)	4949(2)	4527(3)	21.3(15)
C76	8696(5)	5040(2)	5091(3)	22.0(18)
C77	8775(4)	4439(3)	5544(3)	23.4(18)
C78	8460(3)	3748(2)	5433.9(19)	20.9(15)
Sn72	7333.7(7)	2164.2(7)	4433.8(6)	20.5(3)
C71B	7844(11)	2268(12)	5803(11)	34(5)
C72B	7858(9)	2745(6)	5211(8)	18(4)
C73B	8096(8)	3555(5)	5212(6)	17(2)
C74B	7956(8)	4040(6)	4673(6)	16.7(14)
C75B	8196(13)	4781(7)	4664(10)	22(2)
C76B	8577(16)	5036(7)	5195(12)	22(2)
C77B	8717(13)	4551(8)	5734(10)	24(2)
C78B	8476(10)	3810(7)	5743(6)	21(2)
C79	7815(2)	2241(2)	6576(2)	19.0(10)
C80	8419(2)	2007(2)	6920(2)	17.8(10)
C81	8321(3)	1991(3)	7658(2)	24.1(11)
C82	7642(3)	2207(3)	8050(2)	26.3(11)
C83	7045(2)	2430(2)	7711(2)	21.2(10)
C84	7124(2)	2442(2)	6980(2)	18.9(10)
C85	9147(2)	1721(2)	6521(2)	18.4(10)
C86	9177(2)	981(2)	6263(2)	20.0(10)
C87	9861(3)	719(3)	5914(2)	24.1(11)
C88	10510(3)	1157(3)	5828(2)	27.2(11)
C89	10481(3)	1873(3)	6086(2)	25.9(11)
C90	9808(2)	2169(2)	6431(2)	19.4(10)
C91	8508(3)	446(3)	6417(2)	27.3(11)
C92	8398(3)	-36(3)	5789(3)	51.9(17)
C93	8613(3)	-54(3)	7048(3)	39.4(14)
C94	9811(3)	2955(2)	6728(2)	24.2(11)
C95	10278(3)	3512(3)	6216(3)	33.9(13)
C96	10122(3)	2947(3)	7435(3)	33.7(12)
C97	6476(2)	2617(2)	6583(2)	16.8(9)
C98	6322(2)	3367(2)	6395(2)	19.3(10)
C99	5761(2)	3490(3)	5970(2)	24.5(11)
C100	5370(3)	2907(3)	5737(3)	29.0(12)
C101	5507(3)	2178(3)	5931(3)	28.8(12)
C102	6061(2)	2018(3)	6355(2)	22.7(10)
C103	6715(3)	4016(2)	6684(2)	23.6(11)
C104	6805(3)	4709(3)	6194(2)	27.8(11)
C105	6294(3)	4236(3)	7407(2)	29.7(12)
C106	6147(3)	1217(2)	6621(2)	26.1(11)
C107	5995(3)	616(3)	6093(3)	45.3(15)
C108	5626(3)	1089(3)	7322(3)	36.6(13)
C109	7471(3)	2936(2)	3463(2)	20.0(10)
C110	6859(2)	3232(2)	3159(2)	17.3(10)
C111	6966(3)	3418(2)	2445(2)	20.2(10)
C112	7648(2)	3297(2)	2025(2)	18.9(10)
C113	8245(2)	2979(2)	2314(2)	20.7(10)
C114	8170(2)	2801(2)	3025(2)	18.1(10)
C115	6069(2)	3317(2)	3569(2)	18.2(10)
C116	5598(3)	2675(3)	3678(2)	24.5(11)
C117	4856(3)	2765(3)	4003(2)	26.3(11)
C118	4580(3)	3461(3)	4213(2)	27.9(11)
C119	5047(2)	4076(3)	4113(2)	23.9(11)
C120	5799(2)	4019(3)	3791(2)	20.8(10)
C121	5859(3)	1919(3)	3391(3)	28.9(12)
C122	5601(3)	1261(3)	3883(3)	52.1(17)
C123	5609(3)	1830(3)	2663(3)	39.0(14)

Atom	*x*	*y*	*z*	U(eq)
C124	6275(3)	4727(3)	3639(2)	22.5(10)
C125	6255(3)	5219(3)	4288(2)	31.2(12)
C126	6004(3)	5182(3)	3039(2)	26.7(11)
C127	8789(2)	2412(2)	3346(2)	20.1(10)
C128	9412(3)	2812(3)	3514(2)	23.8(11)
C129	9924(3)	2434(3)	3890(3)	30.6(12)
C130	9828(3)	1690(3)	4074(3)	36.8(13)
C131	9239(3)	1286(3)	3865(2)	28.9(12)
C132	8713(2)	1629(3)	3494(2)	21.3(10)
C133	9559(3)	3622(3)	3292(3)	28.1(12)
C134	9943(3)	4074(3)	3809(3)	41.6(15)
C135	10040(3)	3686(3)	2556(3)	33.4(12)
C136	8100(3)	1172(2)	3222(3)	25.5(11)
C137	7863(3)	471(3)	3672(3)	40.4(14)
C138	8355(3)	957(3)	2457(3)	30.3(12)
C141	8124(3)	2498(3)	140(3)	49.6(16)
C142	7297(3)	2416(3)	337(3)	50.3(16)
O142	7023(2)	1872.5(19)	-83.0(18)	34.8(9)
C143	6220(3)	1797(3)	40(3)	50.2(16)
C144	5986(3)	1211(3)	-432(3)	44.7(15)
C151	3739(3)	975(3)	5449(3)	54.0(17)
C152	3138(3)	1194(3)	5026(3)	40.5(14)
O152	2992(2)	1975(2)	5125.2(19)	44.0(10)
C153	2429(4)	2243(3)	4756(3)	55.2(17)
C154	2271(3)	3050(3)	4956(3)	45.4(15)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for WZ13FMI. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn1	15.17(17)	23.79(19)	17.65(18)	-2.53(14)	-3.72(13)	1.23(14)
C2	10(2)	15(2)	25(3)	3(2)	-8(2)	-1.9(19)
C1	15.1(19)	14.4(19)	18(2)	1.6(16)	-0.5(16)	-2.7(16)
C3	19(2)	16.2(19)	19(2)	-0.8(17)	-2.8(17)	0.0(16)
C4	20(2)	18(2)	19(2)	-2.3(17)	0.1(17)	-0.7(17)
C5	19(2)	16(2)	23(2)	0.3(17)	-4.8(17)	0.5(17)
C6	21(2)	21(2)	26(2)	2.0(18)	-2.0(18)	2.0(17)
C7	24(2)	21(2)	22(2)	-1.7(18)	-5.1(18)	1.7(17)
C8	19(2)	26(2)	19(2)	3.0(17)	-3.7(17)	3.1(18)
Sn1B	21(3)	25(3)	25(3)	-1(2)	-2(2)	2(2)
C9	11(2)	21(2)	17(2)	-1.3(19)	-1.5(18)	0.5(18)
C10	10(2)	16(2)	24(2)	-1.8(19)	-3.8(18)	2.3(17)
C11	19(2)	16(2)	26(3)	-4(2)	-5(2)	1.5(19)
C12	25(3)	26(3)	15(2)	-5(2)	-3(2)	2(2)
C13	17(2)	16(2)	22(2)	2.4(19)	-0.6(19)	-1.7(18)
C14	13(2)	16(2)	24(3)	-3.8(19)	-6.6(19)	0.7(18)
C15	21(2)	18(2)	17(2)	-1.8(18)	-7.6(19)	-4.3(19)
C16	22(3)	23(3)	20(2)	-6(2)	-4(2)	-4(2)
C17	23(3)	27(3)	28(3)	-1(2)	-2(2)	-5(2)
C18	35(3)	28(3)	20(3)	5(2)	-6(2)	-12(2)
C19	33(3)	21(3)	26(3)	1(2)	-13(2)	-3(2)
C20	25(3)	20(2)	23(3)	-2(2)	-11(2)	-2(2)
C21	22(3)	19(2)	30(3)	-2(2)	-1(2)	-5(2)
C22	25(3)	35(3)	49(4)	-8(3)	-1(2)	2(2)
C23	36(3)	36(3)	39(3)	-8(2)	-17(3)	9(2)
C24	28(3)	15(2)	40(3)	5(2)	-11(2)	-3(2)
C25	31(3)	26(3)	58(4)	8(3)	-22(3)	-2(2)
C26	23(3)	34(3)	50(4)	-6(3)	-4(2)	2(2)
C27	18(2)	18(2)	18(2)	-1.7(19)	0.3(19)	-4.3(19)
C28	22(2)	18(2)	20(2)	1.9(19)	-2.7(19)	-5.7(19)
C29	32(3)	23(3)	26(3)	-4(2)	-6(2)	-8(2)
C30	36(3)	24(3)	34(3)	-12(2)	0(2)	2(2)
C31	24(3)	23(3)	43(3)	-7(2)	3(2)	5(2)
C32	24(3)	16(2)	30(3)	-5(2)	-1(2)	-1(2)
C33	22(3)	16(2)	34(3)	0(2)	-11(2)	-5.7(19)
C34	28(3)	27(3)	43(3)	9(2)	-18(2)	-10(2)
C35	22(3)	23(3)	38(3)	-5(2)	-6(2)	0(2)
C36	19(3)	25(3)	39(3)	-10(2)	-7(2)	3(2)
C37	24(3)	46(3)	50(4)	-3(3)	-4(3)	1(3)
C38	28(3)	34(3)	44(3)	2(3)	-14(2)	-3(2)
C39	8(2)	18(2)	17(2)	-0.9(18)	-1.1(17)	5.5(17)
C40	12(2)	18(2)	17(2)	0.6(18)	-1.5(18)	1.9(18)
C41	18(2)	17(2)	21(2)	6.5(19)	-5.8(19)	-0.2(19)
C42	26(3)	23(3)	20(2)	-1(2)	-6(2)	1(2)
C43	20(2)	19(2)	23(3)	-4.4(19)	-6(2)	0.3(19)
C44	14(2)	17(2)	23(2)	1.1(19)	-6.1(19)	1.9(18)
C45	21(2)	18(2)	15(2)	1.2(18)	-2.8(19)	-4.9(19)
C46	21(2)	18(2)	18(2)	-0.7(19)	0.2(19)	-3.4(19)
C47	27(3)	13(2)	27(3)	0.7(19)	-3(2)	-2.8(19)
C48	30(3)	24(3)	29(3)	-4(2)	-6(2)	-8(2)
C49	20(3)	27(3)	32(3)	2(2)	-7(2)	-5(2)
C50	17(2)	23(2)	17(2)	1.6(19)	-0.6(19)	-2.5(19)
C51	16(2)	15(2)	29(3)	-0.2(19)	-1(2)	-2.0(18)
C52	25(3)	28(3)	34(3)	0(2)	-2(2)	2(2)
C53	26(3)	30(3)	27(3)	2(2)	-9(2)	0(2)
C54	21(3)	20(3)	32(3)	3(2)	-5(2)	-2(2)
C55	20(3)	35(3)	42(3)	3(2)	-6(2)	3(2)
C56	27(3)	28(3)	36(3)	3(2)	-2(2)	5(2)
C57	19(2)	16(2)	14(2)	-1.3(18)	-6.8(18)	-0.6(18)
C58	21(2)	17(2)	23(3)	-3.3(19)	-5(2)	0.7(19)
C59	30(3)	14(2)	32(3)	1(2)	-10(2)	2(2)
C60	38(3)	17(2)	28(3)	1(2)	-7(2)	-3(2)
C61	21(3)	20(2)	29(3)	-1(2)	-2(2)	-5(2)
C62	21(2)	15(2)	15(2)	-4.9(18)	-3.4(18)	-1.2(18)
C63	27(3)	16(2)	42(3)	-2(2)	-9(2)	-2(2)
C64	30(3)	49(4)	71(4)	19(3)	-28(3)	-4(3)
C65	27(3)	33(3)	77(5)	-19(3)	11(3)	-6(2)
C66	20(2)	16(2)	25(3)	0.1(19)	-3(2)	-2.1(19)
C67	23(3)	28(3)	30(3)	-4(2)	-3(2)	-4(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C68	23(3)	25(3)	30(3)	0(2)	-12(2)	1(2)
Sn71	22.4(2)	12.5(2)	16.4(2)	0.38(17)	-5.50(18)	0.78(17)
C71	18.2(19)	12.3(19)	22.0(19)	3.6(17)	-1.8(17)	-0.4(17)
C72	15(2)	15(2)	16(2)	0.3(19)	-3.4(19)	3.1(19)
C73	16(2)	17(2)	15(2)	1.5(19)	-1.1(18)	0.8(17)
C74	17(2)	18(2)	16(3)	1(2)	-6(2)	-2(2)
C75	25(4)	18(3)	20(4)	4(3)	-2(3)	3(3)
C76	19(4)	19(3)	27(4)	-4(2)	-2(3)	-8(2)
C77	25(3)	23(3)	24(5)	-2(3)	-10(3)	-3(3)
C78	33(3)	14(3)	14(4)	1(3)	3(4)	3(2)
Sn72	20.8(6)	20.6(7)	21.0(7)	-0.4(5)	-6.2(5)	-2.5(5)
C73B	17(3)	16(3)	17(3)	2(2)	-2(2)	1(2)
C74B	17(2)	18(3)	16(3)	1(2)	-6(2)	-1(2)
C75B	26(5)	20(4)	19(5)	5(4)	-1(4)	5(4)
C76B	20(5)	20(3)	27(4)	-5(3)	-2(4)	-7(3)
C77B	25(4)	22(4)	26(5)	0(4)	-9(4)	-1(4)
C78B	33(4)	15(4)	14(5)	1(4)	3(5)	2(3)
C79	20(2)	19(2)	19(2)	-4.1(19)	-4.6(19)	0.3(19)
C80	16(2)	20(2)	18(2)	-1.3(19)	-4.0(18)	0.5(19)
C81	22(3)	31(3)	23(3)	1(2)	-12(2)	7(2)
C82	27(3)	36(3)	17(2)	-3(2)	-7(2)	3(2)
C83	17(2)	24(3)	23(3)	-5(2)	-4.2(19)	2.8(19)
C84	20(2)	18(2)	20(2)	-4.4(19)	-5.8(19)	2.7(19)
C85	16(2)	24(2)	16(2)	0.5(19)	-7.1(18)	5.3(19)
C86	22(2)	24(3)	15(2)	-3.4(19)	-8.4(19)	8(2)
C87	26(3)	24(3)	22(3)	1(2)	-4(2)	11(2)
C88	22(3)	33(3)	24(3)	4(2)	3(2)	12(2)
C89	20(3)	29(3)	27(3)	6(2)	1(2)	2(2)
C90	20(2)	18(2)	21(2)	4.6(19)	-4.7(19)	5.6(19)
C91	24(3)	28(3)	32(3)	-10(2)	-11(2)	4(2)
C92	39(3)	66(4)	55(4)	-35(3)	-15(3)	-1(3)
C93	36(3)	31(3)	54(4)	6(3)	-17(3)	-9(2)
C94	18(2)	21(2)	34(3)	4(2)	-4(2)	2.5(19)
C95	24(3)	25(3)	52(4)	10(2)	-6(2)	-2(2)
C96	36(3)	27(3)	40(3)	-5(2)	-11(2)	0(2)
C97	11(2)	25(2)	14(2)	0.2(19)	-1.3(18)	-2.6(18)
C98	14(2)	24(3)	20(2)	1.5(19)	-2.8(19)	1.3(19)
C99	22(3)	24(3)	28(3)	6(2)	-8(2)	3(2)
C100	25(3)	31(3)	34(3)	2(2)	-16(2)	2(2)
C101	24(3)	29(3)	36(3)	-4(2)	-14(2)	-1(2)
C102	18(2)	26(3)	24(3)	-4(2)	-3(2)	4(2)
C103	24(3)	19(2)	30(3)	4(2)	-10(2)	-3(2)
C104	31(3)	24(3)	30(3)	4(2)	-10(2)	-4(2)
C105	27(3)	30(3)	32(3)	-6(2)	-7(2)	-7(2)
C106	25(3)	21(3)	34(3)	-2(2)	-8(2)	2(2)
C107	53(4)	27(3)	61(4)	-10(3)	-26(3)	6(3)
C108	29(3)	23(3)	57(4)	9(3)	-3(3)	-1(2)
C109	22(3)	19(2)	19(2)	0.9(19)	-2(2)	2.9(19)
C110	14(2)	20(2)	17(2)	2.8(19)	1.8(18)	-3.8(18)
C111	27(3)	13(2)	23(3)	0.5(19)	-10(2)	5.3(19)
C112	22(3)	18(2)	17(2)	1.6(19)	-4.9(19)	-1.4(19)
C113	16(2)	18(2)	27(3)	-3(2)	1(2)	-0.2(19)
C114	17(2)	15(2)	22(3)	0.7(19)	-2.5(19)	0.1(18)
C115	11(2)	26(3)	18(2)	1.7(19)	-2.0(18)	12.4(19)
C116	24(3)	27(3)	23(3)	6(2)	-8(2)	3(2)
C117	23(3)	30(3)	27(3)	9(2)	-6(2)	-3(2)
C118	19(3)	38(3)	26(3)	4(2)	0(2)	2(2)
C119	21(3)	27(3)	23(3)	-2(2)	-4(2)	6(2)
C120	21(2)	30(3)	12(2)	0.1(19)	-6.1(19)	7(2)
C121	26(3)	21(3)	41(3)	3(2)	-7(2)	5(2)
C122	46(4)	28(3)	78(5)	12(3)	3(3)	4(3)
C123	34(3)	26(3)	60(4)	-12(3)	-13(3)	7(2)
C124	19(2)	28(3)	21(3)	0(2)	-3.5(19)	4(2)
C125	32(3)	34(3)	28(3)	-11(2)	-3(2)	4(2)
C126	25(3)	27(3)	28(3)	0(2)	-2(2)	0(2)
C127	20(2)	23(3)	16(2)	0.9(19)	-2.5(19)	9(2)
C128	25(3)	25(3)	23(3)	-8(2)	-6(2)	9(2)
C129	34(3)	28(3)	35(3)	-10(2)	-20(2)	8(2)
C130	39(3)	38(3)	38(3)	-4(3)	-20(3)	16(3)
C131	34(3)	24(3)	30(3)	3(2)	-7(2)	10(2)
C132	21(2)	23(3)	18(2)	1(2)	1.2(19)	8(2)
C133	23(3)	24(3)	42(3)	-11(2)	-18(2)	5(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C134	28(3)	31(3)	71(4)	-18(3)	-22(3)	6(2)
C135	28(3)	30(3)	44(3)	-1(2)	-12(2)	-5(2)
C136	19(3)	19(2)	38(3)	8(2)	-2(2)	1(2)
C137	40(3)	31(3)	49(4)	11(3)	-3(3)	-5(3)
C138	27(3)	24(3)	41(3)	-5(2)	-9(2)	-3(2)
C141	50(4)	40(4)	55(4)	-7(3)	5(3)	-5(3)
C142	54(4)	51(4)	43(4)	-21(3)	6(3)	-7(3)
O142	38(2)	32(2)	33(2)	-5.5(16)	-1.0(17)	4.2(16)
C143	41(4)	51(4)	56(4)	-18(3)	3(3)	2(3)
C144	43(4)	44(4)	49(4)	-5(3)	-14(3)	10(3)
C151	49(4)	55(4)	62(4)	2(3)	-23(3)	3(3)
C152	49(4)	31(3)	44(3)	-8(3)	-14(3)	-6(3)
O152	58(3)	40(2)	37(2)	-4.7(18)	-15.3(19)	3.4(19)
C153	68(5)	57(4)	42(4)	-6(3)	-13(3)	25(3)
C154	50(4)	42(3)	43(4)	10(3)	-1(3)	11(3)

Table 4 Bond Lengths for WZ13FMI.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sn1	C1	2.225(4)	C72	C73	1.507(5)
Sn1	C9	2.217(4)	C73	C74	1.3900
C2	C1	1.332(6)	C73	C78	1.3900
C2	C39	1.492(6)	C74	C75	1.3900
C1	C3	1.512(5)	C75	C76	1.3900
C3	C4	1.3900	C76	C77	1.3900
C3	C8	1.3900	C77	C78	1.3900
C4	C5	1.3900	Sn72	C72B	2.158(14)
C5	C6	1.3900	Sn72	C109	2.285(5)
C6	C7	1.3900	C71B	C72B	1.41(2)
C7	C8	1.3900	C71B	C79	1.48(2)
Sn1B	C2B	2.22(2)	C72B	C73B	1.508(7)
Sn1B	C39	2.257(10)	C73B	C74B	1.3900
C1B	C2B	1.33(2)	C73B	C78B	1.3900
C1B	C9	1.54(5)	C74B	C75B	1.3900
C2B	C3B	1.513(17)	C75B	C76B	1.3900
C3B	C4B	1.3900	C76B	C77B	1.3900
C3B	C8B	1.3900	C77B	C78B	1.3900
C4B	C5B	1.3900	C79	C80	1.405(6)
C5B	C6B	1.3900	C79	C84	1.407(6)
C6B	C7B	1.3900	C80	C81	1.406(6)
C7B	C8B	1.3900	C80	C85	1.501(6)
C9	C10	1.411(6)	C81	C82	1.388(6)
C9	C14	1.396(6)	C82	C83	1.383(6)
C10	C11	1.389(6)	C83	C84	1.393(6)
C10	C15	1.524(6)	C84	C97	1.506(6)
C11	C12	1.390(6)	C85	C86	1.419(6)
C12	C13	1.384(6)	C85	C90	1.414(6)
C13	C14	1.380(6)	C86	C87	1.388(6)
C14	C27	1.519(6)	C86	C91	1.522(6)
C15	C16	1.411(6)	C87	C88	1.386(6)
C15	C20	1.413(6)	C88	C89	1.379(6)
C16	C17	1.398(6)	C89	C90	1.393(6)
C16	C21	1.519(6)	C90	C94	1.525(6)
C17	C18	1.379(6)	C91	C92	1.533(7)
C18	C19	1.381(7)	C91	C93	1.526(7)
C19	C20	1.399(6)	C94	C95	1.541(6)
C20	C24	1.526(6)	C94	C96	1.543(6)
C21	C22	1.533(6)	C97	C98	1.418(6)
C21	C23	1.531(6)	C97	C102	1.414(6)
C24	C25	1.538(6)	C98	C99	1.397(6)
C24	C26	1.539(7)	C98	C103	1.511(6)
C27	C28	1.403(6)	C99	C100	1.374(6)
C27	C32	1.417(6)	C100	C101	1.378(6)
C28	C29	1.401(6)	C101	C102	1.398(6)
C28	C33	1.513(6)	C102	C106	1.526(6)
C29	C30	1.385(7)	C103	C104	1.535(6)
C30	C31	1.374(7)	C103	C105	1.537(6)
C31	C32	1.394(6)	C106	C107	1.542(7)
C32	C36	1.521(6)	C106	C108	1.536(7)
C33	C34	1.540(6)	C109	C110	1.409(6)
C33	C35	1.529(6)	C109	C114	1.421(6)
C36	C37	1.537(6)	C110	C111	1.394(6)
C36	C38	1.549(7)	C110	C115	1.520(6)
C39	C40	1.413(6)	C111	C112	1.377(6)
C39	C44	1.402(6)	C112	C113	1.388(6)
C40	C41	1.388(6)	C113	C114	1.385(6)
C40	C45	1.515(6)	C114	C127	1.507(6)
C41	C42	1.379(6)	C115	C116	1.417(6)
C42	C43	1.388(6)	C115	C120	1.394(6)
C43	C44	1.402(6)	C116	C117	1.388(6)
C44	C57	1.494(6)	C116	C121	1.514(6)
C45	C46	1.404(6)	C117	C118	1.382(7)
C45	C50	1.413(6)	C118	C119	1.373(6)
C46	C47	1.393(6)	C119	C120	1.397(6)
C46	C51	1.522(6)	C120	C124	1.524(6)
C47	C48	1.386(6)	C121	C122	1.523(7)
C48	C49	1.381(6)	C121	C123	1.541(7)
C49	C50	1.386(6)	C124	C125	1.536(6)
C50	C54	1.533(6)	C124	C126	1.534(6)
C51	C52	1.534(6)	C127	C128	1.401(6)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C51	C53	1.536(6)	C127	C132	1.425(6)
C54	C55	1.528(6)	C128	C129	1.410(6)
C54	C56	1.517(6)	C128	C133	1.513(6)
C57	C58	1.411(6)	C129	C130	1.374(7)
C57	C62	1.419(6)	C130	C131	1.387(7)
C58	C59	1.390(6)	C131	C132	1.395(6)
C58	C63	1.526(6)	C132	C136	1.523(6)
C59	C60	1.375(6)	C133	C134	1.530(6)
C60	C61	1.373(6)	C133	C135	1.547(7)
C61	C62	1.391(6)	C136	C137	1.532(6)
C62	C66	1.523(6)	C136	C138	1.530(7)
C63	C64	1.526(7)	C141	C142	1.476(7)
C63	C65	1.518(7)	C142	O142	1.407(6)
C66	C67	1.534(6)	O142	C143	1.424(6)
C66	C68	1.523(6)	C143	C144	1.497(7)
Sn71	C72	2.223(5)	C151	C152	1.485(7)
Sn71	C79	2.237(4)	C152	O152	1.430(6)
C71	C72	1.337(8)	O152	C153	1.393(6)
C71	C109	1.481(7)	C153	C154	1.514(8)

Table 5 Bond Angles for WZ13FMI.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	Sn1	C1	110.22(15)	C71	C72	C73	126.8(5)
C1	C2	C39	135.5(4)	C73	C72	Sn71	127.4(3)
C2	C1	Sn1	104.3(3)	C74	C73	C72	120.3(3)
C2	C1	C3	125.9(4)	C74	C73	C78	120.0
C3	C1	Sn1	129.5(3)	C78	C73	C72	119.5(3)
C4	C3	C1	120.2(2)	C73	C74	C75	120.0
C4	C3	C8	120.0	C74	C75	C76	120.0
C8	C3	C1	119.4(2)	C77	C76	C75	120.0
C5	C4	C3	120.0	C76	C77	C78	120.0
C4	C5	C6	120.0	C77	C78	C73	120.0
C7	C6	C5	120.0	C72B	Sn72	C109	105.7(3)
C6	C7	C8	120.0	C72B	C71B	C79	144.6(18)
C7	C8	C3	120.0	C71B	C72B	Sn72	108.1(11)
C2B	Sn1B	C39	105.2(11)	C71B	C72B	C73B	122.5(13)
C2B	C1B	C9	142(6)	C73B	C72B	Sn72	128.7(7)
C1B	C2B	Sn1B	107(2)	C74B	C73B	C72B	120.1(4)
C1B	C2B	C3B	128(3)	C74B	C73B	C78B	120.0
C3B	C2B	Sn1B	122(2)	C78B	C73B	C72B	119.8(4)
C4B	C3B	C2B	119(2)	C73B	C74B	C75B	120.0
C4B	C3B	C8B	120.0	C74B	C75B	C76B	120.0
C8B	C3B	C2B	120(2)	C77B	C76B	C75B	120.0
C3B	C4B	C5B	120.0	C78B	C77B	C76B	120.0
C6B	C5B	C4B	120.0	C77B	C78B	C73B	120.0
C5B	C6B	C7B	120.0	C80	C79	Sn71	127.1(3)
C8B	C7B	C6B	120.0	C80	C79	C71B	124.1(8)
C7B	C8B	C3B	120.0	C80	C79	C84	119.2(4)
C10	C9	Sn1	129.2(3)	C84	C79	Sn71	109.1(3)
C10	C9	C1B	118(3)	C84	C79	C71B	116.8(8)
C14	C9	Sn1	110.0(3)	C79	C80	C81	119.1(4)
C14	C9	C1B	123(3)	C79	C80	C85	121.7(4)
C14	C9	C10	118.8(4)	C81	C80	C85	119.1(4)
C9	C10	C15	120.9(4)	C82	C81	C80	121.1(4)
C11	C10	C9	119.1(4)	C83	C82	C81	119.7(4)
C11	C10	C15	119.7(4)	C82	C83	C84	120.3(4)
C10	C11	C12	121.3(4)	C79	C84	C97	116.6(4)
C13	C12	C11	119.4(4)	C83	C84	C79	120.6(4)
C14	C13	C12	120.2(4)	C83	C84	C97	122.7(4)
C9	C14	C27	117.0(4)	C86	C85	C80	119.5(4)
C13	C14	C9	121.1(4)	C90	C85	C80	120.6(4)
C13	C14	C27	121.8(4)	C90	C85	C86	119.9(4)
C16	C15	C10	118.6(4)	C85	C86	C91	122.0(4)
C16	C15	C20	120.4(4)	C87	C86	C85	118.6(4)
C20	C15	C10	120.9(4)	C87	C86	C91	119.2(4)
C15	C16	C21	122.0(4)	C88	C87	C86	121.6(4)
C17	C16	C15	119.0(4)	C89	C88	C87	119.7(4)
C17	C16	C21	118.7(4)	C88	C89	C90	121.2(4)
C18	C17	C16	120.5(4)	C85	C90	C94	121.8(4)
C17	C18	C19	120.6(4)	C89	C90	C85	119.0(4)
C18	C19	C20	121.0(4)	C89	C90	C94	119.2(4)
C15	C20	C24	122.7(4)	C86	C91	C92	113.2(4)
C19	C20	C15	118.4(4)	C86	C91	C93	109.1(4)
C19	C20	C24	118.9(4)	C93	C91	C92	110.1(4)
C16	C21	C22	114.3(4)	C90	C94	C95	112.4(4)
C16	C21	C23	110.2(4)	C90	C94	C96	111.0(4)
C23	C21	C22	109.9(4)	C95	C94	C96	109.1(4)
C20	C24	C25	112.3(4)	C98	C97	C84	120.4(4)
C20	C24	C26	111.5(4)	C102	C97	C84	118.9(4)
C25	C24	C26	109.7(4)	C102	C97	C98	120.6(4)
C28	C27	C14	121.1(4)	C97	C98	C103	121.2(4)
C28	C27	C32	119.9(4)	C99	C98	C97	117.9(4)
C32	C27	C14	119.1(4)	C99	C98	C103	120.8(4)
C27	C28	C33	121.0(4)	C100	C99	C98	121.4(4)
C29	C28	C27	118.6(4)	C99	C100	C101	120.8(4)
C29	C28	C33	120.3(4)	C100	C101	C102	120.5(4)
C30	C29	C28	121.4(4)	C97	C102	C106	121.5(4)
C31	C30	C29	119.9(4)	C101	C102	C97	118.8(4)
C30	C31	C32	120.9(5)	C101	C102	C106	119.4(4)
C27	C32	C36	121.6(4)	C98	C103	C104	113.7(4)
C31	C32	C27	119.3(4)	C98	C103	C105	110.5(4)
C31	C32	C36	119.1(4)	C104	C103	C105	109.5(4)
C28	C33	C34	113.2(4)	C102	C106	C107	113.7(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C28	C33	C35	109.4(4)	C102	C106	C108	109.9(4)
C35	C33	C34	110.0(4)	C108	C106	C107	110.0(4)
C32	C36	C37	113.2(4)	C110	C109	C71	123.3(4)
C32	C36	C38	109.6(4)	C110	C109	Sn72	123.8(3)
C37	C36	C38	109.9(4)	C110	C109	C114	119.1(4)
C40	C39	C2	118.0(4)	C114	C109	C71	117.5(4)
C40	C39	Sn1B	113.3(4)	C114	C109	Sn72	111.0(3)
C44	C39	C2	121.5(4)	C109	C110	C115	122.8(4)
C44	C39	Sn1B	119.3(4)	C111	C110	C109	119.1(4)
C44	C39	C40	119.6(4)	C111	C110	C115	118.0(4)
C39	C40	C45	119.6(4)	C112	C111	C110	121.5(4)
C41	C40	C39	119.1(4)	C111	C112	C113	119.8(4)
C41	C40	C45	121.3(4)	C114	C113	C112	120.7(4)
C42	C41	C40	121.6(4)	C109	C114	C127	118.0(4)
C41	C42	C43	119.6(4)	C113	C114	C109	119.8(4)
C42	C43	C44	120.4(4)	C113	C114	C127	122.1(4)
C39	C44	C57	120.6(4)	C116	C115	C110	118.2(4)
C43	C44	C39	119.7(4)	C120	C115	C110	120.6(4)
C43	C44	C57	119.6(4)	C120	C115	C116	121.0(4)
C46	C45	C40	121.0(4)	C115	C116	C121	121.9(4)
C46	C45	C50	120.3(4)	C117	C116	C115	118.1(4)
C50	C45	C40	118.7(4)	C117	C116	C121	119.7(4)
C45	C46	C51	121.9(4)	C118	C117	C116	121.3(4)
C47	C46	C45	118.2(4)	C119	C118	C117	119.8(4)
C47	C46	C51	119.8(4)	C118	C119	C120	121.5(4)
C48	C47	C46	121.4(4)	C115	C120	C119	118.3(4)
C49	C48	C47	120.1(4)	C115	C120	C124	122.1(4)
C48	C49	C50	120.4(4)	C119	C120	C124	119.4(4)
C45	C50	C54	120.7(4)	C116	C121	C122	114.0(4)
C49	C50	C45	119.5(4)	C116	C121	C123	109.0(4)
C49	C50	C54	119.8(4)	C122	C121	C123	111.9(4)
C46	C51	C52	113.5(4)	C120	C124	C125	112.6(4)
C46	C51	C53	111.3(4)	C120	C124	C126	109.9(4)
C52	C51	C53	108.4(4)	C126	C124	C125	109.7(4)
C55	C54	C50	114.1(4)	C128	C127	C114	121.0(4)
C56	C54	C50	110.4(4)	C128	C127	C132	121.0(4)
C56	C54	C55	110.4(4)	C132	C127	C114	118.1(4)
C58	C57	C44	119.9(4)	C127	C128	C129	118.1(4)
C58	C57	C62	119.8(4)	C127	C128	C133	122.4(4)
C62	C57	C44	120.3(4)	C129	C128	C133	119.4(4)
C57	C58	C63	120.8(4)	C130	C129	C128	121.2(5)
C59	C58	C57	118.9(4)	C129	C130	C131	120.2(5)
C59	C58	C63	120.1(4)	C130	C131	C132	121.2(5)
C60	C59	C58	121.3(4)	C127	C132	C136	121.0(4)
C61	C60	C59	119.9(4)	C131	C132	C127	118.0(4)
C60	C61	C62	121.6(4)	C131	C132	C136	120.9(4)
C57	C62	C66	122.1(4)	C128	C133	C134	114.0(4)
C61	C62	C57	118.4(4)	C128	C133	C135	111.2(4)
C61	C62	C66	119.4(4)	C134	C133	C135	108.8(4)
C58	C63	C64	113.3(4)	C132	C136	C137	113.3(4)
C65	C63	C58	109.4(4)	C132	C136	C138	110.4(4)
C65	C63	C64	110.4(4)	C138	C136	C137	110.3(4)
C62	C66	C67	114.0(4)	O142	C142	C141	109.8(5)
C62	C66	C68	110.6(4)	C142	O142	C143	113.3(4)
C68	C66	C67	110.0(4)	O142	C143	C144	109.2(4)
C72	Sn71	C79	111.16(17)	O152	C152	C151	107.9(4)
C72	C71	C109	136.5(5)	C153	O152	C152	112.9(4)
C71	C72	Sn71	105.3(4)	O152	C153	C154	108.0(5)

Table 6 Torsion Angles for WZ13FMI.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Sn1	C1	C3	C4	-166.7(2)	Sn71	C79	C80	C81	-154.1(3)
Sn1	C1	C3	C8	6.4(4)	Sn71	C79	C80	C85	21.3(6)
Sn1	C9	C10	C11	-166.2(3)	Sn71	C79	C84	C83	159.4(3)
Sn1	C9	C10	C15	8.3(6)	Sn71	C79	C84	C97	-16.7(5)
Sn1	C9	C14	C13	169.9(3)	C71	C72	C73	C74	17.2(8)
Sn1	C9	C14	C27	-6.5(5)	C71	C72	C73	C78	-166.6(5)
C2	C1	C3	C4	20.3(5)	C71	C109	C110	C111	-177.6(4)
C2	C1	C3	C8	-166.6(4)	C71	C109	C110	C115	-1.1(7)
C2	C39	C40	C41	170.8(4)	C71	C109	C114	C113	176.5(4)
C2	C39	C40	C45	-5.8(6)	C71	C109	C114	C127	1.0(6)
C2	C39	C44	C43	-170.1(4)	C72	C71	C109	C110	-113.3(7)
C2	C39	C44	C57	7.1(6)	C72	C71	C109	C114	72.2(8)
C1	C2	C39	C40	76.5(7)	C72	C73	C74	C75	176.2(5)
C1	C2	C39	C44	-114.4(6)	C72	C73	C78	C77	-176.3(5)
C1	C3	C4	C5	173.0(3)	C73	C74	C75	C76	0.0
C1	C3	C8	C7	-173.0(3)	C74	C73	C78	C77	0.0
C3	C4	C5	C6	0.0	C74	C75	C76	C77	0.0
C4	C3	C8	C7	0.0	C75	C76	C77	C78	0.0
C4	C5	C6	C7	0.0	C76	C77	C78	C73	0.0
C5	C6	C7	C8	0.0	C78	C73	C74	C75	0.0
C6	C7	C8	C3	0.0	Sn72	C72B	C73B	C74B	2.7(19)
C8	C3	C4	C5	0.0	Sn72	C72B	C73B	C78B	-175.4(10)
Sn1B	C2B	C3B	C4B	40(8)	Sn72	C109	C110	C111	-153.2(3)
Sn1B	C2B	C3B	C8B	-151(5)	Sn72	C109	C110	C115	23.3(6)
Sn1B	C39	C40	C41	150.4(4)	Sn72	C109	C114	C113	155.3(3)
Sn1B	C39	C40	C45	-26.3(5)	Sn72	C109	C114	C127	-20.2(5)
Sn1B	C39	C44	C43	-148.2(4)	C71B	C72B	C73B	C74B	-167.0(15)
Sn1B	C39	C44	C57	29.0(6)	C71B	C72B	C73B	C78B	15(2)
C1B	C2B	C3B	C4B	-160(8)	C71B	C79	C80	C81	-178.8(11)
C1B	C2B	C3B	C8B	9(11)	C71B	C79	C80	C85	-3.4(12)
C1B	C9	C10	C11	164(2)	C71B	C79	C84	C83	179.8(10)
C1B	C9	C10	C15	-21(2)	C71B	C79	C84	C97	3.7(11)
C1B	C9	C14	C13	-163(2)	C72B	C71B	C79	C80	-111(3)
C1B	C9	C14	C27	21(2)	C72B	C71B	C79	C84	71(3)
C2B	C1B	C9	C10	-119(9)	C72B	C73B	C74B	C75B	-178.1(16)
C2B	C1B	C9	C14	49(10)	C72B	C73B	C78B	C77B	178.1(16)
C2B	C3B	C4B	C5B	169(7)	C73B	C74B	C75B	C76B	0.0
C2B	C3B	C8B	C7B	-169(7)	C74B	C73B	C78B	C77B	0.0
C3B	C4B	C5B	C6B	0.0	C74B	C75B	C76B	C77B	0.0
C4B	C3B	C8B	C7B	0.0	C75B	C76B	C77B	C78B	0.0
C4B	C5B	C6B	C7B	0.0	C76B	C77B	C78B	C73B	0.0
C5B	C6B	C7B	C8B	0.0	C78B	C73B	C74B	C75B	0.0
C6B	C7B	C8B	C3B	0.0	C79	C71B	C72B	Sn72	-151(2)
C8B	C3B	C4B	C5B	0.0	C79	C71B	C72B	C73B	21(4)
C9	C1B	C2B	Sn1B	-141(7)	C79	C80	C81	C82	-0.5(7)
C9	C1B	C2B	C3B	56(15)	C79	C80	C85	C86	-77.5(6)
C9	C10	C11	C12	1.0(6)	C79	C80	C85	C90	105.7(5)
C9	C10	C15	C16	-73.6(5)	C79	C84	C97	C98	-95.0(5)
C9	C10	C15	C20	111.2(5)	C79	C84	C97	C102	80.1(5)
C9	C14	C27	C28	-93.1(5)	C80	C79	C84	C83	1.7(7)
C9	C14	C27	C32	87.3(5)	C80	C79	C84	C97	-174.4(4)
C10	C9	C14	C13	4.4(6)	C80	C81	C82	C83	1.2(7)
C10	C9	C14	C27	-172.0(4)	C80	C85	C86	C87	-178.0(4)
C10	C11	C12	C13	1.5(7)	C80	C85	C86	C91	-4.0(6)
C10	C15	C16	C17	-179.0(4)	C80	C85	C90	C89	177.1(4)
C10	C15	C16	C21	-6.0(6)	C80	C85	C90	C94	-0.5(6)
C10	C15	C20	C19	177.7(4)	C81	C80	C85	C86	97.9(5)
C10	C15	C20	C24	0.2(6)	C81	C80	C85	C90	-78.9(5)
C11	C10	C15	C16	100.9(5)	C81	C82	C83	C84	-0.4(7)
C11	C10	C15	C20	-74.3(5)	C82	C83	C84	C79	-1.1(7)
C11	C12	C13	C14	-1.1(7)	C82	C83	C84	C97	174.7(4)
C12	C13	C14	C9	-1.9(6)	C83	C84	C97	C98	89.0(5)
C12	C13	C14	C27	174.3(4)	C83	C84	C97	C102	-95.9(5)
C13	C14	C27	C28	90.6(5)	C84	C79	C80	C81	-0.9(6)
C13	C14	C27	C32	-89.1(5)	C84	C79	C80	C85	174.5(4)
C14	C9	C10	C11	-3.9(6)	C84	C97	C98	C99	174.0(4)
C14	C9	C10	C15	170.7(4)	C84	C97	C98	C103	-10.0(6)
C14	C27	C28	C29	179.5(4)	C84	C97	C102	C101	-174.1(4)
C14	C27	C28	C33	-3.3(6)	C84	C97	C102	C106	12.4(6)
C14	C27	C32	C31	178.7(4)	C85	C80	C81	C82	-176.1(4)
C14	C27	C32	C36	1.7(6)	C85	C86	C87	C88	1.4(6)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C15	C10	C11	C12	-173.6(4)	C85	C86	C91	C92	140.9(5)
C15	C16	C17	C18	2.6(7)	C85	C86	C91	C93	-96.2(5)
C15	C16	C21	C22	145.2(4)	C85	C90	C94	C95	-139.5(4)
C15	C16	C21	C23	-90.5(5)	C85	C90	C94	C96	98.0(5)
C15	C20	C24	C25	-138.3(4)	C86	C85	C90	C89	0.3(6)
C15	C20	C24	C26	98.2(5)	C86	C85	C90	C94	-177.3(4)
C16	C15	C20	C19	2.6(6)	C86	C87	C88	C89	-0.6(7)
C16	C15	C20	C24	-174.9(4)	C87	C86	C91	C92	-45.1(6)
C16	C17	C18	C19	-0.2(7)	C87	C86	C91	C93	77.9(5)
C17	C16	C21	C22	-41.9(6)	C87	C88	C89	C90	-0.3(7)
C17	C16	C21	C23	82.5(5)	C88	C89	C90	C85	0.5(7)
C17	C18	C19	C20	-1.0(7)	C88	C89	C90	C94	178.1(4)
C18	C19	C20	C15	-0.2(7)	C89	C90	C94	C95	42.9(6)
C18	C19	C20	C24	177.4(4)	C89	C90	C94	C96	-79.6(5)
C19	C20	C24	C25	44.2(6)	C90	C85	C86	C87	-1.2(6)
C19	C20	C24	C26	-79.3(5)	C90	C85	C86	C91	172.9(4)
C20	C15	C16	C17	-3.8(6)	C91	C86	C87	C88	-172.9(4)
C20	C15	C16	C21	169.1(4)	C97	C98	C99	C100	-0.2(7)
C21	C16	C17	C18	-170.6(4)	C97	C98	C103	C104	151.4(4)
C27	C28	C29	C30	1.8(7)	C97	C98	C103	C105	-85.0(5)
C27	C28	C33	C34	150.5(4)	C97	C102	C106	C107	-151.4(4)
C27	C28	C33	C35	-86.5(5)	C97	C102	C106	C108	84.8(5)
C27	C32	C36	C37	-142.9(5)	C98	C97	C102	C101	1.0(6)
C27	C32	C36	C38	94.0(5)	C98	C97	C102	C106	-172.5(4)
C28	C27	C32	C31	-0.9(7)	C98	C99	C100	C101	1.6(7)
C28	C27	C32	C36	-178.0(4)	C99	C98	C103	C104	-32.6(6)
C28	C29	C30	C31	-1.1(7)	C99	C98	C103	C105	91.0(5)
C29	C28	C33	C34	-32.4(6)	C99	C100	C101	C102	-1.7(8)
C29	C28	C33	C35	90.6(5)	C100	C101	C102	C97	0.4(7)
C29	C30	C31	C32	-0.7(8)	C100	C101	C102	C106	174.0(4)
C30	C31	C32	C27	1.7(7)	C101	C102	C106	C107	35.1(6)
C30	C31	C32	C36	178.8(5)	C101	C102	C106	C108	-88.7(5)
C31	C32	C36	C37	40.0(6)	C102	C97	C98	C99	-1.1(6)
C31	C32	C36	C38	-83.1(5)	C102	C97	C98	C103	175.0(4)
C32	C27	C28	C29	-0.8(6)	C103	C98	C99	C100	-176.3(4)
C32	C27	C28	C33	176.3(4)	C109	C71	C72	Sn71	-158.4(6)
C33	C28	C29	C30	-175.4(4)	C109	C71	C72	C73	14.2(11)
C39	C2	C1	Sn1	-164.3(4)	C109	C110	C111	C112	2.3(6)
C39	C2	C1	C3	10.1(8)	C109	C110	C115	C116	-79.5(6)
C39	C40	C41	C42	-1.3(6)	C109	C110	C115	C120	104.5(5)
C39	C40	C45	C46	-104.1(5)	C109	C114	C127	C128	-104.2(5)
C39	C40	C45	C50	73.9(5)	C109	C114	C127	C132	74.1(5)
C39	C44	C57	C58	-78.1(5)	C110	C109	C114	C113	1.7(6)
C39	C44	C57	C62	103.5(5)	C110	C109	C114	C127	-173.8(4)
C40	C39	C44	C43	-1.1(6)	C110	C111	C112	C113	0.2(7)
C40	C39	C44	C57	176.0(4)	C110	C115	C116	C117	-174.9(4)
C40	C41	C42	C43	0.7(7)	C110	C115	C116	C121	-0.9(6)
C40	C45	C46	C47	174.3(4)	C110	C115	C120	C119	174.7(4)
C40	C45	C46	C51	-7.1(6)	C110	C115	C120	C124	-0.2(6)
C40	C45	C50	C49	-174.6(4)	C111	C110	C115	C116	97.0(5)
C40	C45	C50	C54	8.9(6)	C111	C110	C115	C120	-78.9(5)
C41	C40	C45	C46	79.4(5)	C111	C112	C113	C114	-1.8(6)
C41	C40	C45	C50	-102.7(5)	C112	C113	C114	C109	0.8(6)
C41	C42	C43	C44	-0.3(7)	C112	C113	C114	C127	176.0(4)
C42	C43	C44	C39	0.5(6)	C113	C114	C127	C128	80.5(6)
C42	C43	C44	C57	-176.6(4)	C113	C114	C127	C132	-101.3(5)
C43	C44	C57	C58	99.0(5)	C114	C109	C110	C111	-3.2(6)
C43	C44	C57	C62	-79.3(5)	C114	C109	C110	C115	173.4(4)
C44	C39	C40	C41	1.5(6)	C114	C127	C128	C129	172.5(4)
C44	C39	C40	C45	-175.2(4)	C114	C127	C128	C133	-8.9(7)
C44	C57	C58	C59	179.6(4)	C114	C127	C132	C131	-172.7(4)
C44	C57	C58	C63	-5.6(6)	C114	C127	C132	C136	10.4(6)
C44	C57	C62	C61	-178.5(4)	C115	C110	C111	C112	-174.4(4)
C44	C57	C62	C66	5.3(6)	C115	C116	C117	C118	0.2(7)
C45	C40	C41	C42	175.3(4)	C115	C116	C121	C122	141.8(5)
C45	C46	C47	C48	1.7(7)	C115	C116	C121	C123	-92.5(5)
C45	C46	C51	C52	146.2(4)	C115	C120	C124	C125	-133.8(4)
C45	C46	C51	C53	-91.2(5)	C115	C120	C124	C126	103.6(5)
C45	C50	C54	C55	-155.5(4)	C116	C115	C120	C119	-1.2(6)
C45	C50	C54	C56	79.5(5)	C116	C115	C120	C124	-176.0(4)
C46	C45	C50	C49	3.4(6)	C116	C117	C118	C119	-1.2(7)
C46	C45	C50	C54	-173.1(4)	C117	C116	C121	C122	-44.3(6)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C46	C47	C48	C49	0.5(7)	C117	C116	C121	C123	81.5(5)
C47	C46	C51	C52	-35.3(6)	C117	C118	C119	C120	1.0(7)
C47	C46	C51	C53	87.3(5)	C118	C119	C120	C115	0.1(7)
C47	C48	C49	C50	-0.8(7)	C118	C119	C120	C124	175.1(4)
C48	C49	C50	C45	-1.1(7)	C119	C120	C124	C125	51.4(5)
C48	C49	C50	C54	175.4(4)	C119	C120	C124	C126	-71.2(5)
C49	C50	C54	C55	28.1(6)	C120	C115	C116	C117	1.0(6)
C49	C50	C54	C56	-97.0(5)	C120	C115	C116	C121	175.1(4)
C50	C45	C46	C47	-3.6(6)	C121	C116	C117	C118	-174.0(4)
C50	C45	C46	C51	174.9(4)	C127	C128	C129	C130	1.5(7)
C51	C46	C47	C48	-176.9(4)	C127	C128	C133	C134	148.2(4)
C57	C58	C59	C60	-0.3(7)	C127	C128	C133	C135	-88.3(5)
C57	C58	C63	C64	141.6(5)	C127	C132	C136	C137	-154.0(4)
C57	C58	C63	C65	-94.7(5)	C127	C132	C136	C138	81.7(5)
C57	C62	C66	C67	-138.7(4)	C128	C127	C132	C131	5.5(6)
C57	C62	C66	C68	96.7(5)	C128	C127	C132	C136	-171.3(4)
C58	C57	C62	C61	3.1(6)	C128	C129	C130	C131	2.8(8)
C58	C57	C62	C66	-173.0(4)	C129	C128	C133	C134	-33.2(6)
C58	C59	C60	C61	1.4(7)	C129	C128	C133	C135	90.2(5)
C59	C58	C63	C64	-43.6(6)	C129	C130	C131	C132	-2.9(8)
C59	C58	C63	C65	80.1(6)	C130	C131	C132	C127	-1.2(7)
C59	C60	C61	C62	-0.3(7)	C130	C131	C132	C136	175.7(4)
C60	C61	C62	C57	-2.0(7)	C131	C132	C136	C137	29.2(6)
C60	C61	C62	C66	174.3(4)	C131	C132	C136	C138	-95.1(5)
C61	C62	C66	C67	45.2(5)	C132	C127	C128	C129	-5.7(7)
C61	C62	C66	C68	-79.4(5)	C132	C127	C128	C133	172.9(4)
C62	C57	C58	C59	-2.0(6)	C133	C128	C129	C130	-177.2(5)
C62	C57	C58	C63	172.8(4)	C141	C142	O142	C143	-175.8(5)
C63	C58	C59	C60	-175.2(4)	C142	O142	C143	C144	179.8(5)
Sn71	C72	C73	C74	-171.9(3)	C151	C152	O152	C153	-179.5(5)
Sn71	C72	C73	C78	4.4(6)	C152	O152	C153	C154	174.5(5)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for WZ13FMI.

Atom	*x*	*y*	*z*	U(eq)
H2	2881.14	1997.44	9251.47	20
H4	1008.69	2619.41	8974.54	23
H5	-194.94	3164.82	9179.4	23
H6	-525.29	3923.49	10155.41	27
H7	348	4136.75	10926.55	26
H8	1551.64	3591.35	10721.69	26
H1B	3053.06	3075.53	10530.32	9
H4B	1152.31	2332.79	9414.33	23
H5B	-87.12	2739.7	9369.17	23
H6B	-566.43	3774.52	10018.72	27
H7B	193.69	4402.42	10713.44	27
H8B	1433.13	3995.52	10758.6	25
H11	2447.02	4182.92	12773.27	24
H12	1881.16	3192.08	13467.22	27
H13	1744.88	2029.63	12961.4	22
H17	4772.77	4741.25	10739.29	31
H18	4155.18	5816.25	10434.64	33
H19	2857.78	5945.8	10757.58	31
H21	3919.15	3133.28	11642.93	28
H22A	4800.67	3197.24	10571.84	55
H22B	5160.05	2838.08	11215.96	55
H22C	5351.53	3685.83	10969.57	55
H23A	4869.36	4221.21	12152.83	53
H23B	4792.04	3368.12	12423.2	53
H23C	4082.44	3921.25	12571.64	53
H24	1580.92	4550.19	11588.69	32
H25A	1609.49	5933.31	10806.8	55
H25B	889.7	5398.13	11014.64	55
H25C	1582.23	5134.99	10446.95	55
H26A	1869.91	5274.32	12522.78	53
H26B	1121.69	5602.46	12261.98	53
H26C	1917.58	6017.69	12040.83	53
H29	1128.43	476.43	10840.64	32
H30	2177.07	-302.99	10816.45	38
H31	3228.18	87.93	11292.74	37
H33	975.95	2352.78	11415.21	28
H34A	711.22	1683.96	10363.21	47
H34B	13.41	2124.01	10789.39	47
H34C	77.8	1235.11	10883.18	47
H35A	208.84	1099.09	12147.49	41
H35B	-140.56	1925.06	12152.2	41
H35C	603.87	1765.71	12504.58	41
H36	3521.11	1903.02	11939.99	33
H37A	4295.86	549.39	11488.49	60
H37B	4691.44	1307.38	11678.4	60
H37C	4282.05	1277.44	10992.95	60
H38A	3016.59	1234.1	12965.59	52
H38B	3919.18	1153.91	12870.67	52
H38C	3411.16	476.55	12668.2	52
H41	2706.01	3292.6	6973.44	22
H42	2333.64	2206.72	6474.52	27
H43	1949.64	1162.31	7188.1	24
H47	2412.96	5271.14	8865.15	27
H48	3602.77	5203.79	9219.14	33
H49	4356.75	4148.95	8976.79	31
H51	1451.87	3809.66	8133.97	24
H52A	1093.66	4611.11	9142.99	44
H52B	578.8	4701.59	8532.08	44
H52C	1217.83	5310.7	8606.54	44
H53A	1947.97	5196.43	7443.23	41
H53B	1250.59	4708.36	7266.92	41
H53C	2095.61	4390.17	7100.34	41
H54	3804.55	2443.85	8329.42	29
H55A	5014.47	2317.99	8635.49	48
H55B	4483.08	2722.24	9260.49	48
H55C	5078.08	3203.09	8728.97	48
H56A	4106.68	3007.82	7226.22	46
H56B	4824.07	2545.3	7408.12	46
H56C	4806.84	3437.56	7471.28	46

Atom	*x*	*y*	*z*	U(eq)
H59	2661.45	-457.94	9328.35	30
H60	1401.24	-759.45	9692.82	33
H61	452.69	-28.91	9334.87	28
H63	3358.69	1180.65	8342.22	34
H64A	3831.35	-19.51	9180.99	72
H64B	3653.54	807.72	9465.71	72
H64C	4350.13	668.54	8856.7	72
H65A	4102.38	249.04	7694.78	71
H65B	3269.94	308.44	7482.13	71
H65C	3473.23	-362.6	7984.55	71
H66	694.08	1663.01	8313.02	24
H67A	-577.8	1587	8831.03	41
H67B	-48.55	1559.27	9434.33	41
H67C	-424.85	806.33	9206.95	41
H68A	695.27	722.9	7485.28	38
H68B	-143.97	1049.79	7675.14	38
H68C	69.13	260.36	8000.94	38
H71	7089.25	2268.31	4308.71	21
H74	7714.95	4195.84	4030.93	20
H75	8246.22	5359.13	4216.86	26
H76	8911.41	5511.89	5166.28	26
H77	9045.33	4501.36	5929.78	28
H78	8514.07	3338.07	5743.86	25
H71B	7861.19	1766.86	5644.7	40
H74B	7695.74	3865.79	4310.26	20
H75B	8100.69	5112.36	4295.46	26
H76B	8741.26	5542.06	5188.55	27
H77B	8976.89	4725.19	6096.45	29
H78B	8571.94	3478.61	6111.26	25
H81	8726.99	1829.19	7893.44	29
H82	7587.93	2201.85	8548.59	32
H83	6578.28	2575.29	7978.28	25
H87	9885.15	228.02	5730.71	29
H88	10973.49	963.95	5591.68	33
H89	10928.19	2169.32	6027.44	31
H91	8039.11	750.03	6545.78	33
H92A	8381.92	286.96	5374.03	78
H92B	7921.71	-315.69	5895.98	78
H92C	8821.14	-388.62	5694.21	78
H93A	9089.84	-330.17	6945.89	59
H93B	8189.83	-408.17	7142.33	59
H93C	8625.82	257.02	7460.68	59
H94	9276.09	3137.78	6813.21	29
H95A	10817.19	3390.02	6183.42	51
H95B	10191.25	4022.01	6389.23	51
H95C	10120.88	3477.84	5750.32	51
H96A	9806.11	2619.89	7772.26	51
H96B	10113.11	3456.77	7616.73	51
H96C	10643.81	2760.71	7364.76	51
H99	5648.35	3988.87	5839.5	29
H100	5000.96	3006.63	5438.17	35
H101	5221.43	1782.17	5775.32	35
H103	7233.71	3845.99	6751.03	28
H10A	6996.74	4555.33	5713.91	42
H10B	7163.18	5058.65	6353.84	42
H10C	6312.3	4954.11	6200.5	42
H10D	5776.72	4391.47	7359.27	44
H10E	6561.1	4650.6	7589.73	44
H10F	6275.91	3804.85	7731.6	44
H106	6681.75	1154.54	6711.23	31
H10G	5469.82	656.17	6003.14	68
H10H	6078.97	117.84	6288.96	68
H10I	6339.85	692.89	5651.79	68
H10J	5764.26	1437.31	7670.49	55
H10K	5681.89	573.24	7488.73	55
H10L	5098.42	1176.12	7255.33	55
H111	6559.55	3634.34	2243.12	24
H112	7709.21	3429.82	1539.83	23
H113	8710.77	2883.07	2021.06	25
H117	4532.79	2340.65	4081.32	32
H118	4067.77	3513.84	4426.65	33
H119	4854.63	4550.75	4266.27	29

Atom	*x*	*y*	*z*	U(eq)
H121	6425.13	1922.37	3318.97	35
H12A	5743.64	1351.65	4347.33	78
H12B	5844.12	801.49	3693.02	78
H12C	5049.42	1208.15	3925.86	78
H12D	5056.97	1878.58	2706.19	59
H12E	5761.6	1335.79	2480.02	59
H12F	5849.72	2219.58	2340.19	59
H124	6812.57	4575.3	3483.77	27
H12G	5739.79	5408.11	4426.1	47
H12H	6604.38	5641.76	4176.35	47
H12I	6408.21	4921.08	4676.4	47
H12J	6046.31	4875.95	2617.73	40
H12K	6317.99	5631.71	2939.53	40
H12L	5474.18	5327.99	3177.71	40
H129	10342.77	2699.17	4017.58	37
H130	10166.98	1451.28	4344.87	44
H131	9193.02	765.99	3977.31	35
H133	9057.2	3861.01	3260.19	34
H13A	9661.93	4009.64	4283.48	62
H13B	9949.07	4605.73	3671.19	62
H13C	10464.07	3897.56	3802.6	62
H13D	10526.29	3432.04	2563.92	50
H13E	10129.99	4214.8	2427.76	50
H13F	9768.78	3449.73	2209.92	50
H136	7643.22	1497.94	3232.49	31
H13G	8288.77	119.69	3639.72	61
H13H	7432.32	232.22	3502.33	61
H13I	7717.1	613.7	4163.09	61
H13J	8460.4	1412.41	2166.95	45
H13K	7952.78	670.28	2287.52	45
H13L	8815.11	651.91	2426.99	45
H	8374.26	2029.22	245.41	74
HA	8306.29	2904.46	406.9	74
HB	8241.43	2614.77	-364.26	74
HC	7178.49	2263.12	838.81	60
HD	7045.63	2901.25	272.21	60
HE	5980.14	2281.06	-55.14	60
HF	6050.64	1651.1	537.26	60
HG	6124.87	1373.58	-923.57	67
HH	5436.21	1136.8	-330.71	67
HI	6243.36	739.16	-351.55	67
HJ	4206.51	1249.15	5274.09	81
HK	3833.24	435.25	5407.56	81
HL	3575.21	1094.32	5942.6	81
HM	3307.87	1095.96	4523.03	49
HN	2671.75	900.64	5182.38	49
HO	1962.67	1938.73	4875.74	66
HP	2599.21	2211.44	4243.57	66
HQ	2128.49	3078.16	5467.03	68
HR	1855	3241.64	4723.09	68
HS	2726.39	3352.04	4809.09	68

Table 8 Atomic Occupancy for WZ13FMI.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Sn1	0.96	C2	0.96	H2	0.96
C1	0.96	C3	0.96	C4	0.96
H4	0.96	C5	0.96	H5	0.96
C6	0.96	H6	0.96	C7	0.96
H7	0.96	C8	0.96	H8	0.96
Sn1B	0.04	C1B	0.04	H1B	0.04
C2B	0.04	C3B	0.04	C4B	0.04
H4B	0.04	C5B	0.04	H5B	0.04
C6B	0.04	H6B	0.04	C7B	0.04
H7B	0.04	C8B	0.04	H8B	0.04
Sn71	0.74	C71	0.74	H71	0.74
C72	0.74	C73	0.74	C74	0.74
H74	0.74	C75	0.74	H75	0.74
C76	0.74	H76	0.74	C77	0.74
H77	0.74	C78	0.74	H78	0.74
Sn72	0.26	C71B	0.26	H71B	0.26
C72B	0.26	C73B	0.26	C74B	0.26
H74B	0.26	C75B	0.26	H75B	0.26
C76B	0.26	H76B	0.26	C77B	0.26
H77B	0.26	C78B	0.26	H78B	0.26

Experimental

Single crystals of $C_{72}H_{90}OSn$ **[WZ13FMI]** were **[]**. A suitable crystal was selected and **[]** on a **Bruker APEX-II CCD** diffractometer. The crystal was kept at 90.15 K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [WZ13FMI]

Crystal Data for $C_{72}H_{90}OSn$ (M =1090.12 g/mol): triclinic, space group P-1 (no. 2), a = 17.8418(9) Å, b = 17.8598(9) Å, c = 19.2380(10) Å, α = 88.9389(8)°, β = 81.5494(8)°, γ = 89.9199(8)°, V = 6062.6(5) Å^3, Z = 4, T = 90.15 K, μ(MoKα) = 0.464 mm^{-1}, *Dcalc* = 1.194 g/cm^3, 43726 reflections measured (3.674° ≤ 2Θ ≤ 50.5°), 21946 unique (R_{int} = 0.0589, R_{sigma} = 0.0826) which were used in all calculations. The final R_1 was 0.0617 (I > 2σ(I)) and wR_2 was 0.1173 (all data).

Refinement model description

Number of restraints - 149, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Restrained distances
 H8B-H24
 1.95 with sigma of 0.01
 C72-C73 = C72B-C73B
 1.5 with sigma of 0.01
 C72-C74 ≈ C72-C78 ≈ C72B-C74B ≈ C72B-C78B
 with sigma of 0.01
3. Uiso/Uaniso restraints and constraints
Sn71 ≈ Sn72: within 2A with sigma of 0.002 and sigma for terminal atoms of
0.004 within 2A
Sn1 ≈ Sn1B: within 5A with sigma of 0.003 and sigma for terminal atoms of
0.003 within 5A
C1 ≈ C2B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C3 ≈ C3B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C4 ≈ C4B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C5 ≈ C5B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C6 ≈ C6B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C7 ≈ C7B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C8 ≈ C8B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
Sn72 ≈ C71: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C73 ≈ C73B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C74 ≈ C74B: within 2A with sigma of 0.001 and sigma for terminal atoms of
0.002 within 2A
C75 ≈ C75B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C76 ≈ C76B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C77 ≈ C77B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
C78 ≈ C78B: within 2A with sigma of 0.003 and sigma for terminal atoms of
0.006 within 2A
Uanis(C71) ≈ Ueq, Uanis(C72) ≈ Ueq, Uanis(C73) ≈ Ueq, Uanis(C73B)
≈ Ueq, Uanis(C74B) ≈ Ueq: with sigma of 0.003 and sigma for terminal
atoms of 0.006
4. Same fragment restrains
{Sn1, C2, C1, C3, C4, C5, C6, C7, C8} sigma for 1-2: 0.02, 1-3: 0.04
as in
{Sn1B, C1B, C2B, C3B, C4B, C5B, C6B, C7B, C8B}
```

5. Others
 Fixed Sof: Sn1(0.96) C2(0.96) H2(0.96) C1(0.96) C3(0.96) C4(0.96) H4(0.96)
 C5(0.96) H5(0.96) C6(0.96) H6(0.96) C7(0.96) H7(0.96) C8(0.96) H8(0.96)
 Sn1B(0.04) C1B(0.04) H1B(0.04) C2B(0.04) C3B(0.04) C4B(0.04) H4B(0.04)
 C5B(0.04) H5B(0.04) C6B(0.04) H6B(0.04) C7B(0.04) H7B(0.04) C8B(0.04)
 H8B(0.04) Sn71(0.74) C71(0.74) H71(0.74) C72(0.74) C73(0.74) C74(0.74)
 H74(0.74) C75(0.74) H75(0.74) C76(0.74) H76(0.74) C77(0.74) H77(0.74)
 C78(0.74) H78(0.74) Sn72(0.26) C71B(0.26) H71B(0.26) C72B(0.26) C73B(0.26)
 C74B(0.26) H74B(0.26) C75B(0.26) H75B(0.26) C76B(0.26) H76B(0.26) C77B(0.26)
 H77B(0.26) C78B(0.26) H78B(0.26)
6.a Ternary CH refined with riding coordinates:
 C21(H21), C24(H24), C33(H33), C36(H36), C51(H51), C54(H54), C63(H63),
 C66(H66), C91(H91), C94(H94), C103(H103), C106(H106), C121(H121), C124(H124),
 C133(H133), C136(H136)
6.b Secondary CH2 refined with riding coordinates:
 C142(HC,HD), C143(HE,HF), C152(HM,HN), C153(HO,HP)
6.c Aromatic/amide H refined with riding coordinates:
 C2(H2), C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C1B(H1B), C4B(H4B), C5B(H5B),
 C6B(H6B), C7B(H7B), C8B(H8B), C11(H11), C12(H12), C13(H13), C17(H17), C18(H18),
  C19(H19), C29(H29), C30(H30), C31(H31), C41(H41), C42(H42), C43(H43),
 C47(H47), C48(H48), C49(H49), C59(H59), C60(H60), C61(H61), C71(H71), C74(H74),
  C75(H75), C76(H76), C77(H77), C78(H78), C71B(H71B), C74B(H74B), C75B(H75B),
 C76B(H76B), C77B(H77B), C78B(H78B), C81(H81), C82(H82), C83(H83), C87(H87),
 C88(H88), C89(H89), C99(H99), C100(H100), C101(H101), C111(H111), C112(H112),
 C113(H113), C117(H117), C118(H118), C119(H119), C129(H129), C130(H130),
 C131(H131)
6.d Fitted hexagon refined as free rotating group:
 C3(C4,C5,C6,C7,C8), C3B(C4B,C5B,C6B,C7B,C8B), C73(C74,C75,C76,C77,C78),
 C73B(C74B,C75B,C76B,C77B,C78B)
6.e Idealised Me refined as rotating group:
 C22(H22A,H22B,H22C), C23(H23A,H23B,H23C), C25(H25A,H25B,H25C), C26(H26A,H26B,
 H26C), C34(H34A,H34B,H34C), C35(H35A,H35B,H35C), C37(H37A,H37B,H37C), C38(H38A,
 H38B,H38C), C52(H52A,H52B,H52C), C53(H53A,H53B,H53C), C55(H55A,H55B,H55C),
 C56(H56A,H56B,H56C), C64(H64A,H64B,H64C), C65(H65A,H65B,H65C), C67(H67A,H67B,
 H67C), C68(H68A,H68B,H68C), C92(H92A,H92B,H92C), C93(H93A,H93B,H93C), C95(H95A,
 H95B,H95C), C96(H96A,H96B,H96C), C104(H10A,H10B,H10C), C105(H10D,H10E,H10F),
 C107(H10G,H10H,H10I), C108(H10J,H10K,H10L), C122(H12A,H12B,H12C), C123(H12D,
 H12E,H12F), C125(H12G,H12H,H12I), C126(H12J,H12K,H12L), C134(H13A,H13B,H13C),
 C135(H13D,H13E,H13F), C137(H13G,H13H,H13I), C138(H13J,H13K,H13L), C141(H,HA,
 HB), C144(HG,HH,HI), C151(HJ,HK,HL), C154(HQ,HR,HS)