WZ14FMI

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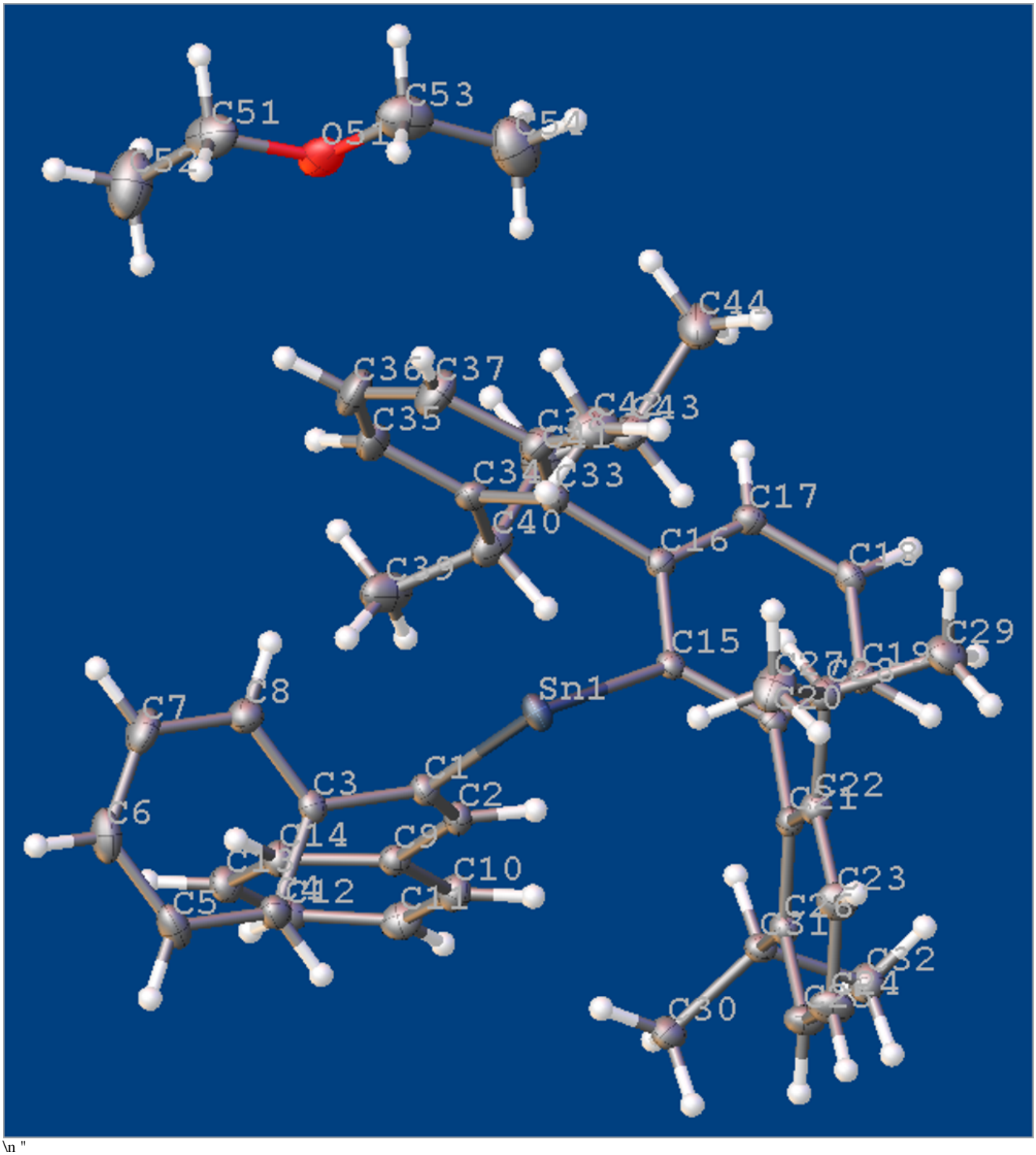

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Table 1 Crystal data and structure refinement for WZ14FMI.

Identification code	WZ14FMI
Empirical formula	$C_{46}H_{53}O_{0.5}Sn$
Formula weight	732.57
Temperature/K	90.15
Crystal system	triclinic
Space group	P-1
a/Å	9.6825(11)
b/Å	11.7854(13)
c/Å	18.190(2)
α/°	90.3576(17)
β/°	100.7821(17)

γ/°	107.7753(15)
Volume/Å^3	1937.2(4)
Z	2
ϱ_{calc}g/cm^3	1.256
μ/mm^{-1}	0.691
F(000)	766.0
Crystal size/mm^3	0.381 × 0.331 × 0.266
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.424 to 61.496
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -26 ≤ l ≤ 26
Reflections collected	23310
Independent reflections	11955 [R_{int} = 0.0183, R_{sigma} = 0.0273]
Data/restraints/parameters	11955/9/459
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0252, wR_2 = 0.0613
Final R indexes [all data]	R_1 = 0.0289, wR_2 = 0.0632
Largest diff. peak/hole / e Å^{-3}	0.54/-0.27

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for WZ14FMI. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sn1	7083.0(2)	3576.3(2)	7180.3(2)	17.54(3)
C15	5304.5(13)	2422.1(10)	7686.9(7)	13.8(2)
C20	5531.5(13)	1523.0(10)	8151.3(7)	13.6(2)
C19	4325.7(14)	689.3(11)	8362.5(7)	15.6(2)
C18	2896.8(14)	731.4(11)	8101.9(7)	16.7(2)
C17	2654.5(14)	1599.2(11)	7621.2(7)	16.9(2)
C16	3853.8(14)	2440.9(11)	7410.5(7)	14.9(2)
C21	7047.7(13)	1396.9(10)	8375.3(7)	13.9(2)
C26	7935.5(14)	1839.1(11)	9087.8(7)	15.5(2)
C25	9317.6(14)	1661.0(13)	9278.3(8)	20.8(3)
C24	9808.9(15)	1047.3(14)	8786.2(8)	24.2(3)
C23	8936.7(15)	611.7(13)	8083.2(8)	21.4(3)
C22	7558.2(14)	784.4(11)	7864.0(7)	16.7(2)
C31	7411.4(14)	2460.8(11)	9663.6(7)	15.8(2)
C30	8566.9(16)	3646.0(12)	9988.5(8)	22.4(3)
C32	7004.9(16)	1633.9(13)	10292.4(8)	22.0(3)
C28	6610.8(16)	266.7(12)	7099.3(7)	20.5(2)
C29	5754.9(18)	-1055.4(13)	7126.0(9)	28.2(3)
C27	7518(2)	453.0(15)	6476.5(8)	31.0(3)
C33	3648.1(14)	3321.4(11)	6836.6(7)	16.6(2)
C38	3798.3(16)	3081.2(13)	6095.6(8)	22.0(3)
C37	3738(2)	3938.6(15)	5573.8(9)	31.6(3)
C36	3497.5(19)	4990.2(15)	5768.6(9)	31.6(3)
C35	3299.6(16)	5199.7(13)	6481.9(9)	25.2(3)
C34	3365.0(14)	4379.3(12)	7027.9(8)	19.5(2)
C43	3853.7(18)	1862.5(13)	5840.4(8)	25.8(3)
C44	2267(2)	1016.4(15)	5578.8(9)	33.1(3)
C42	4770(2)	1905.5(16)	5236.9(9)	32.8(3)
C40	3077.8(18)	4617.3(14)	7798.6(8)	27.0(3)
C41	1424(2)	4116.2(16)	7810.4(12)	40.5(4)
C39	3627(2)	5946.7(15)	8060.2(10)	36.4(4)
C1	7544.0(14)	5234.8(11)	7874.3(7)	16.4(2)
C2	7045.6(14)	5251.3(11)	8518.2(7)	16.7(2)
C9	7099.4(14)	6260.3(11)	9021.1(7)	16.2(2)
C14	7459.8(15)	7453.6(12)	8833.3(7)	19.0(2)
C13	7276.7(15)	8326.3(12)	9289.0(8)	20.5(2)
C12	6764.0(15)	8039.4(12)	9948.7(8)	20.6(3)
C11	6454.4(16)	6873.7(13)	10159.5(8)	22.9(3)
C10	6609.2(15)	5994.5(12)	9698.1(8)	20.4(2)
C3	8452.4(14)	6282.6(11)	7547.2(7)	15.2(2)
C8	7868.7(16)	6683.0(12)	6874.7(8)	21.3(3)
C7	8746.2(19)	7624.5(13)	6546.7(8)	28.1(3)
C6	10221.5(18)	8162.9(13)	6871.1(9)	28.8(3)
C5	10822.1(16)	7751.8(12)	7528.3(9)	25.0(3)
C4	9950.8(15)	6824.4(11)	7865.0(8)	19.7(2)
O51	217(3)	5108(4)	5086(3)	29.2(8)
C51	640(4)	6066(3)	4623.8(19)	37.1(8)
C52	921(5)	7233(4)	5061(3)	49.8(12)
C53	-61(4)	3970(3)	4747(2)	38.4(8)
C54	-491(5)	3058(4)	5315(3)	46.3(10)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for WZ14FMI. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka*b*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn1	18.33(5)	13.28(4)	20.14(5)	-1.72(3)	8.28(3)	1.05(3)
C15	14.5(5)	12.6(5)	13.0(5)	-1.1(4)	2.3(4)	2.6(4)
C20	14.4(5)	12.7(5)	12.7(5)	-1.7(4)	1.9(4)	3.2(4)
C19	19.1(6)	13.8(5)	13.8(5)	1.0(4)	4.2(4)	4.3(4)
C18	16.1(5)	14.7(5)	19.0(6)	0.1(4)	6.7(4)	2.5(4)
C17	13.9(5)	17.6(6)	18.7(6)	-0.7(4)	2.4(4)	4.9(4)
C16	16.4(5)	13.3(5)	15.2(5)	-0.2(4)	3.0(4)	5.1(4)
C21	14.0(5)	13.0(5)	14.8(5)	2.1(4)	3.6(4)	4.0(4)
C26	15.4(5)	14.5(5)	16.1(5)	1.0(4)	4.3(4)	3.4(4)
C25	15.2(6)	25.6(6)	19.7(6)	-2.6(5)	0.4(5)	5.6(5)
C24	14.7(6)	32.1(7)	26.7(7)	-2.9(6)	3.1(5)	9.3(5)
C23	18.2(6)	25.9(7)	22.6(6)	-1.4(5)	7.6(5)	8.5(5)
C22	18.7(6)	17.2(6)	15.0(5)	1.2(4)	4.3(4)	5.9(5)
C31	16.1(5)	16.1(5)	14.5(5)	-1.3(4)	1.6(4)	5.1(4)
C30	25.0(7)	17.4(6)	21.5(6)	-2.8(5)	-1.1(5)	5.1(5)
C32	25.8(7)	22.1(6)	19.3(6)	2.1(5)	8.2(5)	6.8(5)
C28	26.2(7)	20.9(6)	16.0(6)	-2.2(5)	1.7(5)	11.3(5)
C29	29.5(7)	23.7(7)	27.4(7)	-5.6(6)	1.8(6)	5.2(6)
C27	48.4(10)	30.5(8)	18.7(6)	0.1(6)	10.4(6)	16.6(7)
C33	14.5(5)	15.3(5)	18.7(6)	3.2(4)	1.5(4)	3.9(4)
C38	24.9(6)	22.8(6)	19.1(6)	4.4(5)	3.1(5)	9.3(5)
C37	42.7(9)	34.7(8)	23.5(7)	11.0(6)	9.3(6)	19.4(7)
C36	36.5(8)	29.7(8)	33.3(8)	16.9(6)	8.7(7)	15.9(7)
C35	23.3(7)	19.7(6)	33.1(8)	6.1(5)	1.3(6)	9.7(5)
C34	15.5(5)	19.1(6)	22.7(6)	1.7(5)	-0.8(5)	6.4(5)
C43	37.5(8)	25.3(7)	15.6(6)	0.5(5)	1.3(5)	13.7(6)
C44	44.8(9)	28.0(8)	23.4(7)	0.8(6)	5.3(7)	7.8(7)
C42	38.2(9)	39.5(9)	23.0(7)	-5.4(6)	3.7(6)	17.1(7)
C40	34.8(8)	26.4(7)	25.6(7)	0.2(6)	3.0(6)	19.5(6)
C41	46.7(10)	29.1(8)	56.5(11)	3.0(8)	28.4(9)	16.5(8)
C39	38.1(9)	33.9(8)	39.4(9)	-10.5(7)	-6.3(7)	22.9(7)
C1	16.7(5)	13.7(5)	17.9(6)	0.1(4)	3.2(4)	3.4(4)
C2	18.0(6)	13.2(5)	19.1(6)	2.5(4)	4.6(4)	4.3(4)
C9	15.9(5)	16.6(5)	16.2(5)	0.7(4)	2.9(4)	5.6(4)
C14	22.6(6)	17.3(6)	17.4(6)	0.9(4)	5.4(5)	5.7(5)
C13	23.0(6)	17.2(6)	21.2(6)	-0.8(5)	4.3(5)	6.1(5)
C12	19.7(6)	23.8(6)	19.1(6)	-4.6(5)	2.5(5)	8.8(5)
C11	24.4(7)	29.6(7)	17.0(6)	1.6(5)	6.7(5)	10.0(6)
C10	21.6(6)	20.9(6)	20.2(6)	4.4(5)	6.8(5)	7.2(5)
C3	17.5(5)	12.1(5)	16.4(5)	-0.8(4)	5.4(4)	3.9(4)
C8	23.7(6)	20.9(6)	18.3(6)	0.8(5)	2.2(5)	6.8(5)
C7	42.2(9)	24.5(7)	20.9(7)	8.4(5)	10.1(6)	12.8(6)
C6	37.3(8)	17.9(6)	35.9(8)	6.9(6)	21.8(7)	6.5(6)
C5	20.1(6)	16.4(6)	38.6(8)	0.0(5)	10.4(6)	3.0(5)
C4	19.0(6)	15.1(5)	23.8(6)	0.5(5)	2.3(5)	4.6(5)
O51	16(2)	40.3(19)	35(3)	10.3(16)	8.1(17)	11.6(17)
C51	30.5(16)	53(2)	28.7(16)	9.8(15)	10.4(13)	11.1(15)
C52	75(4)	39(2)	48(3)	12(2)	32(2)	25(2)
C53	32.3(17)	47(2)	39.9(19)	-6.7(15)	4.7(14)	19.2(15)
C54	48(2)	34(2)	60(3)	-3(2)	18(2)	13.1(18)

Table 4 Bond Lengths for WZ14FMI.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sn1	C15	2.2009(12)	C36	C35	1.378(2)
Sn1	C1	2.1999(13)	C35	C34	1.3967(19)
C15	C20	1.4030(16)	C34	C40	1.520(2)
C15	C16	1.4076(17)	C43	C44	1.538(2)
C20	C19	1.3957(17)	C43	C42	1.527(2)
C20	C21	1.5012(17)	C40	C41	1.532(2)
C19	C18	1.3922(18)	C40	C39	1.533(2)
C18	C17	1.3951(18)	C1	C2	1.3497(17)
C17	C16	1.3955(17)	C1	C3	1.4814(17)
C16	C33	1.5060(17)	C2	C9	1.4779(18)
C21	C26	1.4112(17)	C9	C14	1.4026(18)
C21	C22	1.4183(17)	C9	C10	1.4045(18)
C26	C25	1.3978(18)	C14	C13	1.3900(18)
C26	C31	1.5190(17)	C13	C12	1.3879(19)
C25	C24	1.3827(19)	C12	C11	1.386(2)
C24	C23	1.391(2)	C11	C10	1.3899(19)
C23	C22	1.3963(18)	C3	C8	1.3964(18)
C22	C28	1.5229(18)	C3	C4	1.4010(18)
C31	C30	1.5297(18)	C8	C7	1.390(2)
C31	C32	1.5365(18)	C7	C6	1.385(2)
C28	C29	1.531(2)	C6	C5	1.386(2)
C28	C27	1.536(2)	C5	C4	1.3857(19)
C33	C38	1.4184(19)	O51	C51	1.418(6)
C33	C34	1.4105(18)	O51	C53	1.400(5)
C38	C37	1.397(2)	C51	C52	1.509(5)
C38	C43	1.526(2)	C53	C54	1.516(5)
C37	C36	1.384(2)			

Table 5 Bond Angles for WZ14FMI.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Sn1	C15	98.57(5)	C37	C38	C43	119.72(13)
C20	C15	Sn1	121.71(9)	C36	C37	C38	120.83(15)
C20	C15	C16	119.54(11)	C35	C36	C37	120.16(14)
C16	C15	Sn1	117.48(8)	C36	C35	C34	121.40(14)
C15	C20	C21	120.34(10)	C33	C34	C40	121.54(12)
C19	C20	C15	119.82(11)	C35	C34	C33	118.54(13)
C19	C20	C21	119.68(11)	C35	C34	C40	119.89(12)
C18	C19	C20	120.29(11)	C38	C43	C44	109.35(13)
C19	C18	C17	120.35(11)	C38	C43	C42	114.08(13)
C18	C17	C16	119.78(12)	C42	C43	C44	110.96(13)
C15	C16	C33	117.67(11)	C34	C40	C41	110.69(13)
C17	C16	C15	120.17(11)	C34	C40	C39	113.16(14)
C17	C16	C33	121.95(11)	C41	C40	C39	108.95(13)
C26	C21	C20	121.17(11)	C2	C1	Sn1	122.34(9)
C26	C21	C22	120.22(11)	C2	C1	C3	126.03(11)
C22	C21	C20	118.58(11)	C3	C1	Sn1	111.63(8)
C21	C26	C31	122.03(11)	C1	C2	C9	130.92(12)
C25	C26	C21	118.87(11)	C14	C9	C2	124.26(11)
C25	C26	C31	119.06(11)	C14	C9	C10	117.58(12)
C24	C25	C26	121.09(12)	C10	C9	C2	117.81(11)
C25	C24	C23	120.14(13)	C13	C14	C9	120.77(12)
C24	C23	C22	120.78(12)	C12	C13	C14	120.64(13)
C21	C22	C28	121.54(11)	C11	C12	C13	119.53(12)
C23	C22	C21	118.88(12)	C12	C11	C10	119.96(13)
C23	C22	C28	119.52(11)	C11	C10	C9	121.46(13)
C26	C31	C30	111.88(11)	C8	C3	C1	120.48(12)
C26	C31	C32	110.24(10)	C8	C3	C4	118.33(12)
C30	C31	C32	110.61(11)	C4	C3	C1	120.92(11)
C22	C28	C29	110.90(11)	C7	C8	C3	120.46(13)
C22	C28	C27	112.44(12)	C6	C7	C8	120.65(14)
C29	C28	C27	111.09(12)	C7	C6	C5	119.35(13)
C38	C33	C16	118.09(11)	C4	C5	C6	120.42(14)
C34	C33	C16	121.60(12)	C5	C4	C3	120.76(13)
C34	C33	C38	120.26(12)	C53	O51	C51	115.1(5)
C33	C38	C43	121.21(12)	O51	C51	C52	109.5(3)
C37	C38	C33	118.72(13)	O51	C53	C54	108.2(4)

Table 6 Torsion Angles for WZ14FMI.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Sn1	C15	C20	C19	-169.67(9)	C23	C22	C28	C29	81.96(16)
Sn1	C15	C20	C21	5.75(15)	C23	C22	C28	C27	-43.10(17)
Sn1	C15	C16	C17	169.86(9)	C22	C21	C26	C25	-0.08(18)
Sn1	C15	C16	C33	-4.96(14)	C22	C21	C26	C31	-177.76(11)
Sn1	C1	C2	C9	-173.17(10)	C31	C26	C25	C24	176.76(13)
Sn1	C1	C3	C8	67.82(13)	C33	C38	C37	C36	-1.6(2)
Sn1	C1	C3	C4	-106.20(12)	C33	C38	C43	C44	85.23(16)
C15	C20	C19	C18	1.32(18)	C33	C38	C43	C42	-149.87(13)
C15	C20	C21	C26	100.78(14)	C33	C34	C40	C41	-89.23(16)
C15	C20	C21	C22	-81.34(15)	C33	C34	C40	C39	148.14(13)
C15	C16	C33	C38	73.88(15)	C38	C33	C34	C35	-2.65(19)
C15	C16	C33	C34	-103.93(14)	C38	C33	C34	C40	175.09(13)
C20	C15	C16	C17	2.53(18)	C38	C37	C36	C35	-0.7(3)
C20	C15	C16	C33	-172.29(11)	C37	C38	C43	C44	-87.97(17)
C20	C19	C18	C17	0.66(19)	C37	C38	C43	C42	36.9(2)
C20	C21	C26	C25	177.76(11)	C37	C36	C35	C34	1.3(2)
C20	C21	C26	C31	0.07(18)	C36	C35	C34	C33	0.3(2)
C20	C21	C22	C23	-176.84(12)	C36	C35	C34	C40	-177.46(14)
C20	C21	C22	C28	0.42(17)	C35	C34	C40	C41	88.48(16)
C19	C20	C21	C26	-83.78(15)	C35	C34	C40	C39	-34.16(18)
C19	C20	C21	C22	94.09(14)	C34	C33	C38	C37	3.3(2)
C19	C18	C17	C16	-1.03(19)	C34	C33	C38	C43	-169.97(13)
C18	C17	C16	C15	-0.57(18)	C43	C38	C37	C36	171.73(15)
C18	C17	C16	C33	174.02(12)	C1	C2	C9	C14	13.1(2)
C17	C16	C33	C38	-100.84(15)	C1	C2	C9	C10	-173.91(14)
C17	C16	C33	C34	81.35(16)	C1	C3	C8	C7	-176.45(13)
C16	C15	C20	C19	-2.90(17)	C1	C3	C4	C5	175.54(12)
C16	C15	C20	C21	172.53(11)	C2	C1	C3	C8	-112.63(15)
C16	C33	C38	C37	-174.54(13)	C2	C1	C3	C4	73.35(18)
C16	C33	C38	C43	12.19(19)	C2	C9	C14	C13	170.45(12)
C16	C33	C34	C35	175.12(12)	C2	C9	C10	C11	-172.14(12)
C16	C33	C34	C40	-7.14(19)	C9	C14	C13	C12	1.4(2)
C21	C20	C19	C18	-174.14(11)	C14	C9	C10	C11	1.3(2)
C21	C26	C25	C24	-1.0(2)	C14	C13	C12	C11	1.0(2)
C21	C26	C31	C30	-130.59(12)	C13	C12	C11	C10	-2.2(2)
C21	C26	C31	C32	105.89(13)	C12	C11	C10	C9	1.0(2)
C21	C22	C28	C29	-95.29(15)	C10	C9	C14	C13	-2.58(19)
C21	C22	C28	C27	139.65(13)	C3	C1	C2	C9	7.3(2)
C26	C21	C22	C23	1.05(18)	C3	C8	C7	C6	1.5(2)
C26	C21	C22	C28	178.32(12)	C8	C3	C4	C5	1.39(19)
C26	C25	C24	C23	1.1(2)	C8	C7	C6	C5	0.2(2)
C25	C26	C31	C30	51.74(16)	C7	C6	C5	C4	-1.1(2)
C25	C26	C31	C32	-71.79(15)	C6	C5	C4	C3	0.3(2)
C25	C24	C23	C22	-0.1(2)	C4	C3	C8	C7	-2.3(2)
C24	C23	C22	C21	-1.0(2)	C51	O51	C53	C54	179.8(2)
C24	C23	C22	C28	-178.30(13)	C53	O51	C51	C52	-179.30(18)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for WZ14FMI.

Atom	*x*	*y*	*z*	U(eq)
H19	4480.79	90.55	8685.42	19
H18	2082.38	166.23	8252.25	20
H17	1676.48	1617.07	7438.01	20
H25	9929.41	1966.67	9753.63	25
H24	10744.17	922.81	8928.59	29
H23	9283.04	191.85	7748.31	26
H31	6498.27	2635.27	9406.72	19
H30A	9464.47	3495.06	10255.56	34
H30B	8170.34	4038.41	10337.57	34
H30C	8806.12	4163.82	9580.55	34
H32A	6254.43	884.79	10074.85	33
H32B	6611.31	2025.35	10643.39	33
H32C	7889.59	1464.25	10559.86	33
H28	5866.65	701.6	6972.44	25
H29A	6454.36	-1509.21	7248.08	42
H29B	5112.5	-1357.67	6636.43	42
H29C	5149.9	-1145.52	7510.76	42
H27A	8103.06	1296.78	6491.92	47
H27B	6847.3	217.86	5987.53	47
H27C	8182.14	-36.89	6552.7	47
H37	3862.53	3798.08	5079.26	38
H36	3469.21	5568.86	5409.57	38
H35	3114.71	5917.32	6604.9	30
H43	4322.49	1527.64	6288.09	31
H44A	1727.16	950.3	5989.73	50
H44B	2300.22	225.64	5430.65	50
H44C	1764.06	1334.21	5149.5	50
H42A	4270.54	2134.23	4768.53	49
H42B	4876.12	1116.49	5154.39	49
H42C	5750.54	2493.51	5400.42	49
H40	3614.62	4193.61	8166.55	32
H41A	872.95	4516.61	7451.84	61
H41B	1265.51	4255.16	8315.42	61
H41C	1076.76	3256.52	7671.67	61
H39A	4637.09	6304.26	7977.52	55
H39B	3620.7	6033.69	8595.62	55
H39C	2975.4	6351.79	7774.8	55
H2	6581.68	4484.53	8674.56	20
H14	7833.4	7667.85	8389.44	23
H13	7504.76	9126.99	9147.47	25
H12	6626.21	8637.44	10253.64	25
H11	6136.6	6676.17	10619.08	28
H10	6378.33	5196.06	9843.88	24
H8	6864.69	6309.16	6639.71	26
H7	8329.84	7901.57	6095.56	34
H6	10816.01	8807.56	6645.4	35
H5	11837.47	8108.16	7749.28	30
H4	10374.42	6552.88	8316.48	24
H51A	-155.44	5976.95	4176.89	45
H51B	1547.53	6056.85	4451.21	45
H52A	1213.85	7895.62	4740.96	75
H52B	17.22	7241.69	5226.13	75
H52C	1716.08	7321.41	5499.79	75
H53A	834.52	3912.01	4581.85	46
H53B	-873.29	3818.51	4301.7	46
H54A	-689.97	2253.99	5087.86	70
H54B	321.39	3212.26	5752.59	70
H54C	-1380.49	3119.09	5473.42	70

Table 8 Atomic Occupancy for WZ14FMI.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O51	0.5	C51	0.5	H51A	0.5
H51B	0.5	C52	0.5	H52A	0.5
H52B	0.5	H52C	0.5	C53	0.5
H53A	0.5	H53B	0.5	C54	0.5
H54A	0.5	H54B	0.5	H54C	0.5

Experimental

Single crystals of $C_{46}H_{53}O_{0.5}Sn$ **[WZ14FMI]** 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 [WZ14FMI]

Crystal Data for $C_{46}H_{53}O_{0.5}Sn$ (M =732.57 g/mol): triclinic, space group P-1 (no. 2), a = 9.6825(11) Å, b = 11.7854(13) Å, c = 18.190(2) Å, α = 90.3576(17)°, β = 100.7821(17)°, γ = 107.7753(15)°, V = 1937.2(4) Å^3, Z = 2, T = 90.15 K, μ(MoKα) = 0.691 mm^{-1}, *Dcalc* = 1.256 g/cm^3, 23310 reflections measured (4.424° ≤ 2Θ ≤ 61.496°), 11955 unique (R_{int} = 0.0183, R_{sigma} = 0.0273) which were used in all calculations. The final R_1 was 0.0252 (I > 2σ(I)) and wR_2 was 0.0632 (all data).

Refinement model description

Number of restraints - 9, 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
 O51-C51 = O51-C53
 1.45 with sigma of 0.01
 C51-C52 = C53-C54
 1.5 with sigma of 0.01
 C51-C53
 2.4 with sigma of 0.01
 O51-C52 = O51-C54
 2.45 with sigma of 0.01
3. Restrained planarity
 O51, C51, C52, C53, C54
 with sigma of 0.01
4. Others
 Fixed Sof: O51(0.5) C51(0.5) H51A(0.5) H51B(0.5) C52(0.5) H52A(0.5) H52B(0.5)
 H52C(0.5) C53(0.5) H53A(0.5) H53B(0.5) C54(0.5) H54A(0.5) H54B(0.5) H54C(0.5)
5.a Ternary CH refined with riding coordinates:
 C31(H31), C28(H28), C43(H43), C40(H40)
5.b Secondary CH2 refined with riding coordinates:
 C51(H51A,H51B), C53(H53A,H53B)
5.c Me refined with riding coordinates:
 C52(H52A,H52B,H52C), C54(H54A,H54B,H54C)
5.d Aromatic/amide H refined with riding coordinates:
 C19(H19), C18(H18), C17(H17), C25(H25), C24(H24), C23(H23), C37(H37),
 C36(H36), C35(H35), C2(H2), C14(H14), C13(H13), C12(H12), C11(H11), C10(H10),
 C8(H8), C7(H7), C6(H6), C5(H5), C4(H4)
5.e Idealised Me refined as rotating group:
 C30(H30A,H30B,H30C), C32(H32A,H32B,H32C), C29(H29A,H29B,H29C), C27(H27A,H27B,
 H27C), C44(H44A,H44B,H44C), C42(H42A,H42B,H42C), C41(H41A,H41B,H41C), C39(H39A,
 H39B,H39C)
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