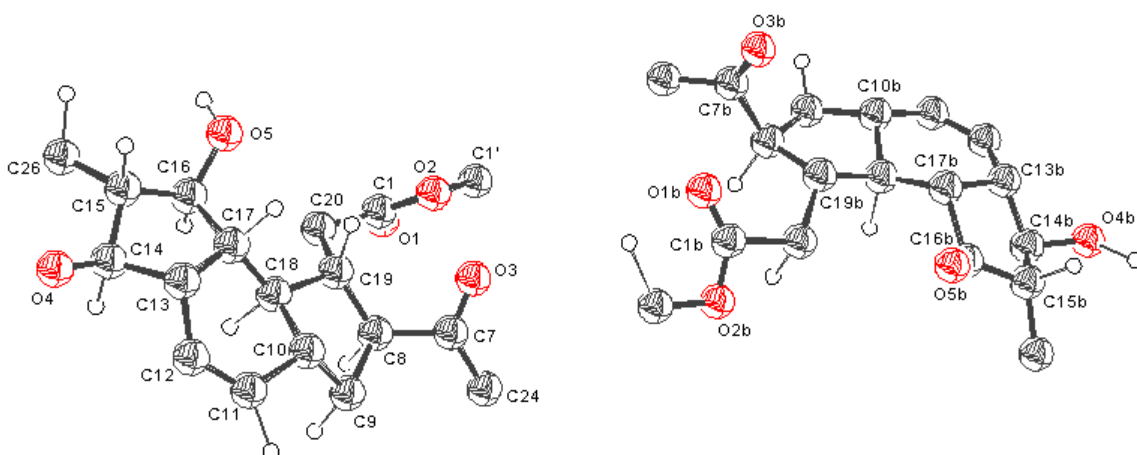


Verbindung (8*S*)-237



[2-Acetyl-6-(*tert*-butyldimethylsilanyloxy)-8-(*tert*-butyldiphenylsilanyloxy)-7-methyl-1,2,3,3a,5a,6,7,8,8a,8b-decahydro-as-indacen-1-yl]-essigsäuremethylester

(In der Abbildung wurde die Hexacyclinsäure-Nummerierung verwendet)

Crystal Data and structure refinement	
Empirical formula	C ₁₈ H ₂₆ O ₅
Formula weight	322.4
Unit-cell contents	C ₇₂ H ₁₀₄ O ₂₀
Unit-cell weight	1289.6
Temperature (K)	293
Wavelength (Å)	0.71069
Crystal System	Monoclinic
Space group	P 1 2 ₁ 1
Unit-cell dimensions (Å)	a = 14.653, α = 90° b = 5.201, β = 91° c = 22.709, γ = 90°
Volume (Å ³)	1730.52
Calculated density (g·cm ⁻³)	1.237
F (000)	695.9
Crystal description	needle
Crystal colour	colourless
Crystal size	0.015 x 0.14 x 0.70 mm ³
Max. 2-θ	46.51
Limiting indices	-16 ≤ h ≤ 16, -5 ≤ k ≤ 5, -24 ≤ l ≤ 25
Unique reflections	4928
R	0.0816

Bond lengths [pm]			
C1'-O2	140.3	C1'b-O2b	147.3
C1-O1	121.9	C1b-O1b	112.8
C1-O2	137.0	C1b-O2b	126.7
C1-C20	151.0	C1b-C20b	166.5
C7-O3	116.0	C7b-O3b	124.9
C7-C24	140.6	C7b-C24b	143.6
C7-C8	150.0	C7b-C8b	156.4
C8-C19	149.7	C8b-C19b	157.3
C8-C9	163.2	C8b-C9b	153.1
C9-C10	148.2	C9b-C10b	147.4
C10-C18	148.8	C10b-C18b	157.0
C10-C11	158.2	C10b-C11b	157.7
C11-C12	131.1	C11b-C12b	126.2
C12-C13	146.8	C12b-C13b	150.3
C13-C17	146.9	C13b-C17b	160.4
C13-C14	152.4	C13b-C14b	146.4
C14-O4	141.4	C14b-O4b	140.1
C14-C15	147.2	C14b-C15b	151.0
C15-C16	151.7	C15b-C16b	140.6
C15-C26	156.0	C15b-C26b	147.1
C16-O5	140.6	C16b-O5b	142.3
C16-C17	151.6	C16b-C17b	161.0
C17-C18	152.7	C17b-C18b	144.2
C18-C19	154.0	C18b-C19b	149.3
C19-C20	150.6	C19b-C20b	149.3
H8-C8	148.2	H8b-C8b	118.3
H14-C14	127.7	H15b-C15b	121.4
H15-C15	115.6	H16b-C16b	123.0
H16-C16	136.7	H17b-C17b	125.1
H17-C17	115.1	H18b-C18b	139.9
H18-C18	126.9	H9b ₂ -C9b	104.6
H9 ₁ -C9	116.2	H20b ₁ -C20b	134.9
H26 ₁ -C26	122.0		

Bond angles [°]			
O1-C1-O2	122.1	O1b-C1b-O2b	137.3
O1-C1-C20	123.1	O1b-C1b-C20b	118.0
O2-C1-C20	114.2	O2b-C1b-C20b	104.7
O3-C7-C24	124.3	O3b-C7b-C24b	122.8
O3-C7-C8	113.9	O3b-C7b-C8b	121.7
C24-C7-C8	117.6	C24b-C7b-C8b	114.5
C19-C8-C7	119.9	C19b-C8b-C7b	112.5
C19-C8-C9	105.7	C19b-C8b-C9b	104.9
C7-C8-C9	108.3	C7b-C8b-C9b	105.6
C10-C9-C8	99.4	C10b-C9b-C8b	107.3
C9-C10-C18	109.1	C9b-C10b-C18b	104.8
C9-C10-C11	116.3	C9b-C10b-C11b	124.9
C18-C10-C11	108.8	C18b-C10b-C11b	108.8
C12-C11-C10	120.1	C12b-C11b-C10b	120.4
C11-C12-C13	123.1	C11b-C12b-C13b	129.6
C12-C13-C17	117.9	C12b-C13b-C17b	111.3
C12-C13-C14	113.6	C12b-C13b-C14b	117.1
C17-C13-C14	105.8	C17b-C13b-C14b	107.0
O4-C14-C15	114.5	O4b-C14b-C15b	114.7
O4-C14-C13	111.8	O4b-C14b-C13b	107.9
C15-C14-C13	99.5	C15b-C14b-C13b	105.0
C14-C15-C16	102.5	C14b-C15b-C16b	100.2
C14-C15-C26	112.5	C14b-C15b-C26b	119.7
C16-C15-C26	113.4	C16b-C15b-C26b	114.1
O5-C16-C17	108.2	O5b-C16b-C17b	106.8
O5-C16-C15	110.9	O5b-C16b-C15b	120.6
C17-C16-C15	101.3	C17b-C16b-C15b	114.4
C13-C17-C16	106.6	C13b-C17b-C16b	94.9
C13-C17-C18	113.8	C13b-C17b-C18b	115.2
C16-C17-C18	112.4	C16b-C17b-C18b	120.0
C10-C18-C17	112.2	C10b-C18b-C17b	115.0
C10-C18-C19	98.9	C10b-C18b-C19b	102.6
C17-C18-C19	123.5	C17b-C18b-C19b	123.4
C8-C19-C20	115.4	C8b-C19b-C20b	114.3
C8-C19-C18	106.9	C8b-C19b-C18b	106.3
C20-C19-C18	114.8	C20b-C19b-C18b	112.8
C19-C20-C1	111.4	C19b-C20b-C1b	112.8
C1-O2-C1'	97.1	C1b-O2b-C1'b	108.5