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Supporting information for article:

Two crystallographic forms and the absolute structure of 5α,14α-androstane

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S1. Crystallographic Tables for Pure Form I

Table 1. Crystal data and structure refinement for Form I.

Identification code	Form_I	
Empirical formula	C19 H32	
Formula weight	260.44	
Temperature	90(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.44170(10) Å	α= 90°.
	b = 9.88310(10) Å	β= 92.7420(10)°.
	c = 43.0002(6) Å	γ = 90°.
Volume	3158.92(7) $Å^3$	
Z	8	
Density (calculated)	1.095 Mg/m^3	
Absorption coefficient	0.438 mm^{-1}	
F(000)	1168	
Crystal size	0.198 x 0.126 x 0.060 mm^3	
Theta range for data collection	2.057 to 75.478°.	
Index ranges	-9<=h<=9, -12<=k<=12, -53<=l<=52	
Reflections collected	64068	
Independent reflections	15656 [R(int) = 0.0254]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.776	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15656 / 1 / 695	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1289	
R indices (all data)	R1 = 0.0461, wR2 = 0.1328	
Absolute structure parameter	0.0(5)	
Extinction coefficient	0.0006(2)	
Largest diff. peak and hole	0.307 and -0.214 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Form I. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	11169(6)	7345(5)	8155(1)	20(1)
C(2)	10973(7)	6982(5)	8498(1)	24(1)
C(3)	9395(7)	7729(5)	8637(1)	24(1)
C(4)	7657(6)	7537(5)	8438(1)	20(1)
C(5)	7907(6)	7925(4)	8097(1)	19(1)
C(6)	6148(6)	7860(5)	7903(1)	22(1)
C(7)	6392(6)	8372(5)	7572(1)	22(1)
C(8)	7892(6)	7616(4)	7415(1)	19(1)
C(9)	9663(6)	7669(4)	7616(1)	15(1)
C(10)	9444(6)	7113(4)	7952(1)	17(1)
C(11)	11224(6)	7024(5)	7449(1)	22(1)
C(12)	11436(7)	7589(5)	7119(1)	24(1)
C(13)	9694(7)	7482(4)	6922(1)	21(1)
C(14)	8203(6)	8208(4)	7094(1)	19(1)
C(15)	6621(7)	8284(5)	6853(1)	25(1)
C(16)	7565(7)	8521(6)	6542(1)	30(1)
C(17)	9618(7)	8274(5)	6615(1)	26(1)
C(18)	9012(6)	5583(4)	7940(1)	19(1)
C(19)	9256(7)	5987(5)	6850(1)	26(1)
C(20)	-4513(7)	1102(5)	4453(1)	22(1)
C(21)	-5006(7)	855(5)	4105(1)	24(1)
C(22)	-3414(8)	1077(5)	3904(1)	28(1)
C(23)	-1775(6)	237(5)	4019(1)	23(1)
C(24)	-1336(6)	495(4)	4365(1)	18(1)
C(25)	415(6)	-272(5)	4474(1)	21(1)
C(26)	941(6)	99(5)	4810(1)	20(1)
C(27)	-562(6)	-78(4)	5032(1)	16(1)
C(28)	-2312(6)	683(4)	4912(1)	16(1)
C(29)	-2888(6)	234(4)	4575(1)	16(1)
C(30)	-3775(6)	624(5)	5148(1)	18(1)
C(31)	-3120(6)	1099(5)	5476(1)	20(1)

C(32)	-1497(6)	298(4)	5595(1)	18(1)
C(33)	-19(6)	438(4)	5357(1)	18(1)
C(34)	1657(6)	-134(5)	5526(1)	21(1)
C(35)	1483(7)	313(5)	5869(1)	26(1)
C(36)	-472(6)	850(5)	5889(1)	21(1)
C(37)	-3478(6)	-1268(4)	4573(1)	20(1)
C(38)	-2011(7)	-1177(5)	5657(1)	24(1)
C(39)	6365(7)	2470(5)	6954(1)	23(1)
C(40)	6407(7)	2810(5)	6605(1)	27(1)
C(41)	4873(7)	2112(5)	6415(1)	26(1)
C(42)	3050(7)	2402(5)	6551(1)	24(1)
C(43)	3076(6)	2015(4)	6896(1)	19(1)
C(44)	1207(6)	2148(5)	7026(1)	22(1)
C(45)	1205(6)	1657(4)	7362(1)	19(1)
C(46)	2643(6)	2353(4)	7571(1)	15(1)
C(47)	4521(6)	2211(5)	7432(1)	18(1)
C(48)	4528(6)	2775(4)	7095(1)	18(1)
C(49)	6021(6)	2773(5)	7654(1)	25(1)
C(50)	5977(6)	2212(5)	7987(1)	25(1)
C(51)	4145(7)	2424(4)	8119(1)	21(1)
C(52)	2699(6)	1756(4)	7900(1)	18(1)
C(53)	1014(7)	1757(5)	8085(1)	23(1)
C(54)	1721(8)	1563(5)	8427(1)	30(1)
C(55)	3794(7)	1669(5)	8423(1)	26(1)
C(56)	4224(7)	4317(4)	7090(1)	23(1)
C(57)	3797(7)	3943(5)	8172(1)	24(1)
C(58)	786(6)	8877(5)	10534(1)	18(1)
C(59)	479(7)	9126(5)	10880(1)	23(1)
C(60)	2197(7)	8904(5)	11082(1)	24(1)
C(61)	3743(7)	9760(5)	10969(1)	24(1)
C(62)	4028(6)	9511(4)	10623(1)	18(1)
C(63)	5643(6)	10279(5)	10512(1)	19(1)
C(64)	6062(7)	9901(5)	10179(1)	21(1)
C(65)	4423(6)	10070(4)	9955(1)	15(1)
C(66)	2773(6)	9320(4)	10076(1)	17(1)
C(67)	2305(6)	9766(4)	10410(1)	15(1)

C(68)	1146(6)	9374(5)	9837(1)	18(1)
C(69)	1616(6)	8900(5)	9510(1)	19(1)
C(70)	3187(6)	9688(4)	9391(1)	16(1)
C(71)	4774(6)	9547(4)	9631(1)	16(1)
C(72)	6400(6)	10101(5)	9464(1)	18(1)
C(73)	6032(7)	9640(5)	9123(1)	24(1)
C(74)	4042(7)	9122(4)	9100(1)	21(1)
C(75)	1725(6)	11254(4)	10412(1)	19(1)
C(76)	2670(7)	11172(4)	9327(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for Form I.

C(1)-C(2)	1.532(6)	C(12)-H(12B)	0.9900
C(1)-C(10)	1.534(6)	C(13)-C(17)	1.534(6)
C(1)-H(1A)	0.9900	C(13)-C(14)	1.541(6)
C(1)-H(1B)	0.9900	C(13)-C(19)	1.541(6)
C(2)-C(3)	1.532(6)	C(14)-C(15)	1.533(6)
C(2)-H(2A)	0.9900	C(14)-H(14)	1.0000
C(2)-H(2B)	0.9900	C(15)-C(16)	1.556(6)
C(3)-C(4)	1.527(6)	C(15)-H(15A)	0.9900
C(3)-H(3A)	0.9900	C(15)-H(15B)	0.9900
C(3)-H(3B)	0.9900	C(16)-C(17)	1.564(7)
C(4)-C(5)	1.536(5)	C(16)-H(16A)	0.9900
C(4)-H(4A)	0.9900	C(16)-H(16B)	0.9900
C(4)-H(4B)	0.9900	C(17)-H(17A)	0.9900
C(5)-C(6)	1.519(6)	C(17)-H(17B)	0.9900
C(5)-C(10)	1.551(6)	C(18)-H(18A)	0.9800
C(5)-H(5)	1.0000	C(18)-H(18B)	0.9800
C(6)-C(7)	1.529(5)	C(18)-H(18C)	0.9800
C(6)-H(6A)	0.9900	C(19)-H(19A)	0.9800
C(6)-H(6B)	0.9900	C(19)-H(19B)	0.9800
C(7)-C(8)	1.529(6)	C(19)-H(19C)	0.9800
C(7)-H(7A)	0.9900	C(20)-C(21)	1.540(6)
C(7)-H(7B)	0.9900	C(20)-C(29)	1.554(6)
C(8)-C(14)	1.523(5)	C(20)-H(20A)	0.9900
C(8)-C(9)	1.544(5)	C(20)-H(20B)	0.9900
C(8)-H(8)	1.0000	C(21)-C(22)	1.517(7)
C(9)-C(11)	1.534(6)	C(21)-H(21A)	0.9900
C(9)-C(10)	1.561(5)	C(21)-H(21B)	0.9900
C(9)-H(9)	1.0000	C(22)-C(23)	1.538(7)
C(10)-C(18)	1.547(6)	C(22)-H(22A)	0.9900
C(11)-C(12)	1.543(6)	C(22)-H(22B)	0.9900
C(11)-H(11A)	0.9900	C(23)-C(24)	1.526(5)
C(11)-H(11B)	0.9900	C(23)-H(23A)	0.9900
C(12)-C(13)	1.517(6)	C(23)-H(23B)	0.9900
C(12)-H(12A)	0.9900	C(24)-C(29)	1.523(6)

C(24)-C(25)	1.560(6)	C(37)-H(37C)	0.9800
C(24)-H(24)	1.0000	C(38)-H(38A)	0.9800
C(25)-C(26)	1.523(6)	C(38)-H(38B)	0.9800
C(25)-H(25A)	0.9900	C(38)-H(38C)	0.9800
C(25)-H(25B)	0.9900	C(39)-C(40)	1.538(6)
C(26)-C(27)	1.513(6)	C(39)-C(48)	1.552(6)
C(26)-H(26A)	0.9900	C(39)-H(39A)	0.9900
C(26)-H(26B)	0.9900	C(39)-H(39B)	0.9900
C(27)-C(33)	1.525(5)	C(40)-C(41)	1.535(7)
C(27)-C(28)	1.569(6)	C(40)-H(40A)	0.9900
C(27)-H(27)	1.0000	C(40)-H(40B)	0.9900
C(28)-C(30)	1.524(5)	C(41)-C(42)	1.531(6)
C(28)-C(29)	1.555(5)	C(41)-H(41A)	0.9900
C(28)-H(28)	1.0000	C(41)-H(41B)	0.9900
C(29)-C(37)	1.548(6)	C(42)-C(43)	1.531(5)
C(30)-C(31)	1.544(5)	C(42)-H(42A)	0.9900
C(30)-H(30A)	0.9900	C(42)-H(42B)	0.9900
C(30)-H(30B)	0.9900	C(43)-C(44)	1.530(6)
C(31)-C(32)	1.513(6)	C(43)-C(48)	1.540(6)
C(31)-H(31A)	0.9900	C(43)-H(43)	1.0000
C(31)-H(31B)	0.9900	C(44)-C(45)	1.524(5)
C(32)-C(38)	1.534(6)	C(44)-H(44A)	0.9900
C(32)-C(36)	1.544(6)	C(44)-H(44B)	0.9900
C(32)-C(33)	1.544(6)	C(45)-C(46)	1.529(6)
C(33)-C(34)	1.521(6)	C(45)-H(45A)	0.9900
C(33)-H(33)	1.0000	C(45)-H(45B)	0.9900
C(34)-C(35)	1.552(6)	C(46)-C(52)	1.528(5)
C(34)-H(34A)	0.9900	C(46)-C(47)	1.553(6)
C(34)-H(34B)	0.9900	C(46)-H(46)	1.0000
C(35)-C(36)	1.555(6)	C(47)-C(49)	1.536(6)
C(35)-H(35A)	0.9900	C(47)-C(48)	1.552(5)
C(35)-H(35B)	0.9900	C(47)-H(47)	1.0000
C(36)-H(36A)	0.9900	C(48)-C(56)	1.541(6)
C(36)-H(36B)	0.9900	C(49)-C(50)	1.539(6)
C(37)-H(37A)	0.9800	C(49)-H(49A)	0.9900
C(37)-H(37B)	0.9800	C(49)-H(49B)	0.9900

C(50)-C(51)	1.516(7)	C(62)-C(67)	1.560(6)
C(50)-H(50A)	0.9900	C(62)-H(62)	1.0000
C(50)-H(50B)	0.9900	C(63)-C(64)	1.527(5)
C(51)-C(55)	1.539(6)	C(63)-H(63A)	0.9900
C(51)-C(57)	1.542(6)	C(63)-H(63B)	0.9900
C(51)-C(52)	1.545(6)	C(64)-C(65)	1.526(6)
C(52)-C(53)	1.517(6)	C(64)-H(64A)	0.9900
C(52)-H(52)	1.0000	C(64)-H(64B)	0.9900
C(53)-C(54)	1.551(6)	C(65)-C(71)	1.520(5)
C(53)-H(53A)	0.9900	C(65)-C(66)	1.545(6)
C(53)-H(53B)	0.9900	C(65)-H(65)	1.0000
C(54)-C(55)	1.547(7)	C(66)-C(68)	1.550(6)
C(54)-H(54A)	0.9900	C(66)-C(67)	1.561(5)
C(54)-H(54B)	0.9900	C(66)-H(66)	1.0000
C(55)-H(55A)	0.9900	C(67)-C(75)	1.533(6)
C(55)-H(55B)	0.9900	C(68)-C(69)	1.539(5)
C(56)-H(56A)	0.9800	C(68)-H(68A)	0.9900
C(56)-H(56B)	0.9800	C(68)-H(68B)	0.9900
C(56)-H(56C)	0.9800	C(69)-C(70)	1.515(6)
C(57)-H(57A)	0.9800	C(69)-H(69A)	0.9900
C(57)-H(57B)	0.9800	C(69)-H(69B)	0.9900
C(57)-H(57C)	0.9800	C(70)-C(74)	1.534(6)
C(58)-C(59)	1.533(5)	C(70)-C(76)	1.538(6)
C(58)-C(67)	1.546(6)	C(70)-C(71)	1.538(6)
C(58)-H(58A)	0.9900	C(71)-C(72)	1.539(6)
C(58)-H(58B)	0.9900	C(71)-H(71)	1.0000
C(59)-C(60)	1.526(6)	C(72)-C(73)	1.548(5)
C(59)-H(59A)	0.9900	C(72)-H(72A)	0.9900
C(59)-H(59B)	0.9900	C(72)-H(72B)	0.9900
C(60)-C(61)	1.525(7)	C(73)-C(74)	1.565(7)
C(60)-H(60A)	0.9900	C(73)-H(73A)	0.9900
C(60)-H(60B)	0.9900	C(73)-H(73B)	0.9900
C(61)-C(62)	1.532(5)	C(74)-H(74A)	0.9900
C(61)-H(61A)	0.9900	C(74)-H(74B)	0.9900
C(61)-H(61B)	0.9900	C(75)-H(75A)	0.9800
C(62)-C(63)	1.518(6)	C(75)-H(75B)	0.9800

C(75)-H(75C)	0.9800	C(76)-H(76B)	0.9800
C(76)-H(76A)	0.9800	C(76)-H(76C)	0.9800

C(2)-C(1)-C(10)	113.3(4)	C(5)-C(6)-H(6B)	109.4
C(2)-C(1)-H(1A)	108.9	C(7)-C(6)-H(6B)	109.4
C(10)-C(1)-H(1A)	108.9	H(6A)-C(6)-H(6B)	108.0
C(2)-C(1)-H(1B)	108.9	C(6)-C(7)-C(8)	111.9(4)
C(10)-C(1)-H(1B)	108.9	C(6)-C(7)-H(7A)	109.2
H(1A)-C(1)-H(1B)	107.7	C(8)-C(7)-H(7A)	109.2
C(3)-C(2)-C(1)	111.8(4)	C(6)-C(7)-H(7B)	109.2
C(3)-C(2)-H(2A)	109.2	C(8)-C(7)-H(7B)	109.2
C(1)-C(2)-H(2A)	109.2	H(7A)-C(7)-H(7B)	107.9
C(3)-C(2)-H(2B)	109.2	C(14)-C(8)-C(7)	111.0(4)
C(1)-C(2)-H(2B)	109.2	C(14)-C(8)-C(9)	109.4(4)
H(2A)-C(2)-H(2B)	107.9	C(7)-C(8)-C(9)	110.8(3)
C(4)-C(3)-C(2)	111.5(3)	C(14)-C(8)-H(8)	108.5
C(4)-C(3)-H(3A)	109.3	C(7)-C(8)-H(8)	108.5
C(2)-C(3)-H(3A)	109.3	C(9)-C(8)-H(8)	108.5
C(4)-C(3)-H(3B)	109.3	C(11)-C(9)-C(8)	111.6(3)
C(2)-C(3)-H(3B)	109.3	C(11)-C(9)-C(10)	113.7(3)
H(3A)-C(3)-H(3B)	108.0	C(8)-C(9)-C(10)	112.6(3)
C(3)-C(4)-C(5)	111.4(4)	C(11)-C(9)-H(9)	106.1
C(3)-C(4)-H(4A)	109.4	C(8)-C(9)-H(9)	106.1
C(5)-C(4)-H(4A)	109.4	C(10)-C(9)-H(9)	106.1
C(3)-C(4)-H(4B)	109.4	C(1)-C(10)-C(18)	109.4(3)
C(5)-C(4)-H(4B)	109.4	C(1)-C(10)-C(5)	107.9(3)
H(4A)-C(4)-H(4B)	108.0	C(18)-C(10)-C(5)	111.3(4)
C(6)-C(5)-C(4)	111.9(4)	C(1)-C(10)-C(9)	110.6(4)
C(6)-C(5)-C(10)	113.0(3)	C(18)-C(10)-C(9)	110.1(3)
C(4)-C(5)-C(10)	112.3(3)	C(5)-C(10)-C(9)	107.5(3)
C(6)-C(5)-H(5)	106.4	C(9)-C(11)-C(12)	113.2(4)
C(4)-C(5)-H(5)	106.4	C(9)-C(11)-H(11A)	108.9
C(10)-C(5)-H(5)	106.4	C(12)-C(11)-H(11A)	108.9
C(5)-C(6)-C(7)	111.0(4)	C(9)-C(11)-H(11B)	108.9
C(5)-C(6)-H(6A)	109.4	C(12)-C(11)-H(11B)	108.9
C(7)-C(6)-H(6A)	109.4	H(11A)-C(11)-H(11B)	107.7

C(13)-C(12)-C(11)	111.5(4)	C(10)-C(18)-H(18A)	109.5
C(13)-C(12)-H(12A)	109.3	C(10)-C(18)-H(18B)	109.5
C(11)-C(12)-H(12A)	109.3	H(18A)-C(18)-H(18B)	109.5
C(13)-C(12)-H(12B)	109.3	C(10)-C(18)-H(18C)	109.5
C(11)-C(12)-H(12B)	109.3	H(18A)-C(18)-H(18C)	109.5
H(12A)-C(12)-H(12B)	108.0	H(18B)-C(18)-H(18C)	109.5
C(12)-C(13)-C(17)	116.1(4)	C(13)-C(19)-H(19A)	109.5
C(12)-C(13)-C(14)	108.4(3)	C(13)-C(19)-H(19B)	109.5
C(17)-C(13)-C(14)	100.4(4)	H(19A)-C(19)-H(19B)	109.5
C(12)-C(13)-C(19)	110.2(4)	C(13)-C(19)-H(19C)	109.5
C(17)-C(13)-C(19)	108.6(4)	H(19A)-C(19)-H(19C)	109.5
C(14)-C(13)-C(19)	113.0(4)	H(19B)-C(19)-H(19C)	109.5
C(8)-C(14)-C(15)	119.1(4)	C(21)-C(20)-C(29)	112.8(4)
C(8)-C(14)-C(13)	113.6(4)	C(21)-C(20)-H(20A)	109.0
C(15)-C(14)-C(13)	104.1(3)	C(29)-C(20)-H(20A)	109.0
C(8)-C(14)-H(14)	106.4	C(21)-C(20)-H(20B)	109.0
C(15)-C(14)-H(14)	106.4	C(29)-C(20)-H(20B)	109.0
C(13)-C(14)-H(14)	106.4	H(20A)-C(20)-H(20B)	107.8
C(14)-C(15)-C(16)	103.0(4)	C(22)-C(21)-C(20)	112.0(4)
C(14)-C(15)-H(15A)	111.2	C(22)-C(21)-H(21A)	109.2
C(16)-C(15)-H(15A)	111.2	C(20)-C(21)-H(21A)	109.2
C(14)-C(15)-H(15B)	111.2	C(22)-C(21)-H(21B)	109.2
C(16)-C(15)-H(15B)	111.2	C(20)-C(21)-H(21B)	109.2
H(15A)-C(15)-H(15B)	109.1	H(21A)-C(21)-H(21B)	107.9
C(15)-C(16)-C(17)	106.4(4)	C(21)-C(22)-C(23)	111.5(4)
C(15)-C(16)-H(16A)	110.4	C(21)-C(22)-H(22A)	109.3
C(17)-C(16)-H(16A)	110.4	C(23)-C(22)-H(22A)	109.3
C(15)-C(16)-H(16B)	110.4	C(21)-C(22)-H(22B)	109.3
C(17)-C(16)-H(16B)	110.4	C(23)-C(22)-H(22B)	109.3
H(16A)-C(16)-H(16B)	108.6	H(22A)-C(22)-H(22B)	108.0
C(13)-C(17)-C(16)	104.3(4)	C(24)-C(23)-C(22)	110.7(4)
C(13)-C(17)-H(17A)	110.9	C(24)-C(23)-H(23A)	109.5
C(16)-C(17)-H(17A)	110.9	C(22)-C(23)-H(23A)	109.5
C(13)-C(17)-H(17B)	110.9	C(24)-C(23)-H(23B)	109.5
C(16)-C(17)-H(17B)	110.9	C(22)-C(23)-H(23B)	109.5
H(17A)-C(17)-H(17B)	108.9	H(23A)-C(23)-H(23B)	108.1

C(29)-C(24)-C(23)	114.7(4)	C(28)-C(30)-C(31)	113.1(3)
C(29)-C(24)-C(25)	112.6(3)	C(28)-C(30)-H(30A)	109.0
C(23)-C(24)-C(25)	110.5(4)	C(31)-C(30)-H(30A)	109.0
C(29)-C(24)-H(24)	106.1	C(28)-C(30)-H(30B)	109.0
C(23)-C(24)-H(24)	106.1	C(31)-C(30)-H(30B)	109.0
C(25)-C(24)-H(24)	106.1	H(30A)-C(30)-H(30B)	107.8
C(26)-C(25)-C(24)	110.0(3)	C(32)-C(31)-C(30)	111.2(4)
C(26)-C(25)-H(25A)	109.7	C(32)-C(31)-H(31A)	109.4
C(24)-C(25)-H(25A)	109.7	C(30)-C(31)-H(31A)	109.4
C(26)-C(25)-H(25B)	109.7	C(32)-C(31)-H(31B)	109.4
C(24)-C(25)-H(25B)	109.7	C(30)-C(31)-H(31B)	109.4
H(25A)-C(25)-H(25B)	108.2	H(31A)-C(31)-H(31B)	108.0
C(27)-C(26)-C(25)	113.9(4)	C(31)-C(32)-C(38)	110.8(4)
C(27)-C(26)-H(26A)	108.8	C(31)-C(32)-C(36)	116.5(4)
C(25)-C(26)-H(26A)	108.8	C(38)-C(32)-C(36)	108.1(3)
C(27)-C(26)-H(26B)	108.8	C(31)-C(32)-C(33)	108.2(3)
C(25)-C(26)-H(26B)	108.8	C(38)-C(32)-C(33)	113.1(4)
H(26A)-C(26)-H(26B)	107.7	C(36)-C(32)-C(33)	99.8(3)
C(26)-C(27)-C(33)	111.5(4)	C(34)-C(33)-C(27)	119.2(4)
C(26)-C(27)-C(28)	111.4(3)	C(34)-C(33)-C(32)	104.1(3)
C(33)-C(27)-C(28)	108.6(3)	C(27)-C(33)-C(32)	114.3(4)
C(26)-C(27)-H(27)	108.4	C(34)-C(33)-H(33)	106.1
C(33)-C(27)-H(27)	108.4	C(27)-C(33)-H(33)	106.1
C(28)-C(27)-H(27)	108.4	C(32)-C(33)-H(33)	106.1
C(30)-C(28)-C(29)	115.7(4)	C(33)-C(34)-C(35)	104.1(4)
C(30)-C(28)-C(27)	111.9(3)	C(33)-C(34)-H(34A)	110.9
C(29)-C(28)-C(27)	110.8(3)	C(35)-C(34)-H(34A)	110.9
C(30)-C(28)-H(28)	105.9	C(33)-C(34)-H(34B)	110.9
C(29)-C(28)-H(28)	105.9	C(35)-C(34)-H(34B)	110.9
C(27)-C(28)-H(28)	105.9	H(34A)-C(34)-H(34B)	108.9
C(24)-C(29)-C(37)	112.4(3)	C(34)-C(35)-C(36)	105.7(3)
C(24)-C(29)-C(20)	107.7(3)	C(34)-C(35)-H(35A)	110.6
C(37)-C(29)-C(20)	108.1(4)	C(36)-C(35)-H(35A)	110.6
C(24)-C(29)-C(28)	108.8(3)	C(34)-C(35)-H(35B)	110.6
C(37)-C(29)-C(28)	110.2(3)	C(36)-C(35)-H(35B)	110.6
C(20)-C(29)-C(28)	109.5(3)	H(35A)-C(35)-H(35B)	108.7

C(32)-C(36)-C(35)	105.1(3)	C(41)-C(42)-C(43)	110.7(4)
C(32)-C(36)-H(36A)	110.7	C(41)-C(42)-H(42A)	109.5
C(35)-C(36)-H(36A)	110.7	C(43)-C(42)-H(42A)	109.5
C(32)-C(36)-H(36B)	110.7	C(41)-C(42)-H(42B)	109.5
C(35)-C(36)-H(36B)	110.7	C(43)-C(42)-H(42B)	109.5
H(36A)-C(36)-H(36B)	108.8	H(42A)-C(42)-H(42B)	108.1
C(29)-C(37)-H(37A)	109.5	C(44)-C(43)-C(42)	111.2(4)
C(29)-C(37)-H(37B)	109.5	C(44)-C(43)-C(48)	112.4(3)
H(37A)-C(37)-H(37B)	109.5	C(42)-C(43)-C(48)	113.1(4)
C(29)-C(37)-H(37C)	109.5	C(44)-C(43)-H(43)	106.5
H(37A)-C(37)-H(37C)	109.5	C(42)-C(43)-H(43)	106.5
H(37B)-C(37)-H(37C)	109.5	C(48)-C(43)-H(43)	106.5
C(32)-C(38)-H(38A)	109.5	C(45)-C(44)-C(43)	111.1(4)
C(32)-C(38)-H(38B)	109.5	C(45)-C(44)-H(44A)	109.4
H(38A)-C(38)-H(38B)	109.5	C(43)-C(44)-H(44A)	109.4
C(32)-C(38)-H(38C)	109.5	C(45)-C(44)-H(44B)	109.4
H(38A)-C(38)-H(38C)	109.5	C(43)-C(44)-H(44B)	109.4
H(38B)-C(38)-H(38C)	109.5	H(44A)-C(44)-H(44B)	108.0
C(40)-C(39)-C(48)	113.5(4)	C(44)-C(45)-C(46)	112.5(4)
C(40)-C(39)-H(39A)	108.9	C(44)-C(45)-H(45A)	109.1
C(48)-C(39)-H(39A)	108.9	C(46)-C(45)-H(45A)	109.1
C(40)-C(39)-H(39B)	108.9	C(44)-C(45)-H(45B)	109.1
C(48)-C(39)-H(39B)	108.9	C(46)-C(45)-H(45B)	109.1
H(39A)-C(39)-H(39B)	107.7	H(45A)-C(45)-H(45B)	107.8
C(41)-C(40)-C(39)	111.8(4)	C(52)-C(46)-C(45)	111.0(4)
C(41)-C(40)-H(40A)	109.3	C(52)-C(46)-C(47)	109.6(3)
C(39)-C(40)-H(40A)	109.3	C(45)-C(46)-C(47)	110.5(3)
C(41)-C(40)-H(40B)	109.3	C(52)-C(46)-H(46)	108.6
C(39)-C(40)-H(40B)	109.3	C(45)-C(46)-H(46)	108.6
H(40A)-C(40)-H(40B)	107.9	C(47)-C(46)-H(46)	108.6
C(42)-C(41)-C(40)	111.3(4)	C(49)-C(47)-C(48)	114.5(4)
C(42)-C(41)-H(41A)	109.4	C(49)-C(47)-C(46)	111.6(3)
C(40)-C(41)-H(41A)	109.4	C(48)-C(47)-C(46)	111.8(3)
C(42)-C(41)-H(41B)	109.4	C(49)-C(47)-H(47)	106.1
C(40)-C(41)-H(41B)	109.4	C(48)-C(47)-H(47)	106.1
H(41A)-C(41)-H(41B)	108.0	C(46)-C(47)-H(47)	106.1

C(43)-C(48)-C(56)	112.1(4)	C(55)-C(54)-C(53)	105.9(4)
C(43)-C(48)-C(47)	108.1(3)	C(55)-C(54)-H(54A)	110.6
C(56)-C(48)-C(47)	111.2(3)	C(53)-C(54)-H(54A)	110.6
C(43)-C(48)-C(39)	107.2(3)	C(55)-C(54)-H(54B)	110.6
C(56)-C(48)-C(39)	108.5(4)	C(53)-C(54)-H(54B)	110.6
C(47)-C(48)-C(39)	109.8(4)	H(54A)-C(54)-H(54B)	108.7
C(47)-C(49)-C(50)	113.6(4)	C(51)-C(55)-C(54)	104.6(4)
C(47)-C(49)-H(49A)	108.8	C(51)-C(55)-H(55A)	110.8
C(50)-C(49)-H(49A)	108.8	C(54)-C(55)-H(55A)	110.8
C(47)-C(49)-H(49B)	108.8	C(51)-C(55)-H(55B)	110.8
C(50)-C(49)-H(49B)	108.8	C(54)-C(55)-H(55B)	110.8
H(49A)-C(49)-H(49B)	107.7	H(55A)-C(55)-H(55B)	108.9
C(51)-C(50)-C(49)	111.0(4)	C(48)-C(56)-H(56A)	109.5
C(51)-C(50)-H(50A)	109.4	C(48)-C(56)-H(56B)	109.5
C(49)-C(50)-H(50A)	109.4	H(56A)-C(56)-H(56B)	109.5
C(51)-C(50)-H(50B)	109.4	C(48)-C(56)-H(56C)	109.5
C(49)-C(50)-H(50B)	109.4	H(56A)-C(56)-H(56C)	109.5
H(50A)-C(50)-H(50B)	108.0	H(56B)-C(56)-H(56C)	109.5
C(50)-C(51)-C(55)	116.3(4)	C(51)-C(57)-H(57A)	109.5
C(50)-C(51)-C(57)	110.5(4)	C(51)-C(57)-H(57B)	109.5
C(55)-C(51)-C(57)	108.1(4)	H(57A)-C(57)-H(57B)	109.5
C(50)-C(51)-C(52)	109.0(3)	C(51)-C(57)-H(57C)	109.5
C(55)-C(51)-C(52)	99.8(4)	H(57A)-C(57)-H(57C)	109.5
C(57)-C(51)-C(52)	112.9(4)	H(57B)-C(57)-H(57C)	109.5
C(53)-C(52)-C(46)	119.8(4)	C(59)-C(58)-C(67)	112.8(4)
C(53)-C(52)-C(51)	104.4(3)	C(59)-C(58)-H(58A)	109.0
C(46)-C(52)-C(51)	112.7(4)	C(67)-C(58)-H(58A)	109.0
C(53)-C(52)-H(52)	106.3	C(59)-C(58)-H(58B)	109.0
C(46)-C(52)-H(52)	106.3	C(67)-C(58)-H(58B)	109.0
C(51)-C(52)-H(52)	106.3	H(58A)-C(58)-H(58B)	107.8
C(52)-C(53)-C(54)	104.3(4)	C(60)-C(59)-C(58)	111.6(4)
C(52)-C(53)-H(53A)	110.9	C(60)-C(59)-H(59A)	109.3
C(54)-C(53)-H(53A)	110.9	C(58)-C(59)-H(59A)	109.3
C(52)-C(53)-H(53B)	110.9	C(60)-C(59)-H(59B)	109.3
C(54)-C(53)-H(53B)	110.9	C(58)-C(59)-H(59B)	109.3
H(53A)-C(53)-H(53B)	108.9	H(59A)-C(59)-H(59B)	108.0

C(61)-C(60)-C(59)	111.4(4)	C(65)-C(66)-C(68)	111.7(3)
C(61)-C(60)-H(60A)	109.4	C(65)-C(66)-C(67)	113.0(3)
C(59)-C(60)-H(60A)	109.4	C(68)-C(66)-C(67)	113.5(4)
C(61)-C(60)-H(60B)	109.4	C(65)-C(66)-H(66)	106.0
C(59)-C(60)-H(60B)	109.4	C(68)-C(66)-H(66)	106.0
H(60A)-C(60)-H(60B)	108.0	C(67)-C(66)-H(66)	106.0
C(60)-C(61)-C(62)	111.1(4)	C(75)-C(67)-C(58)	109.5(4)
C(60)-C(61)-H(61A)	109.4	C(75)-C(67)-C(62)	112.1(3)
C(62)-C(61)-H(61A)	109.4	C(58)-C(67)-C(62)	107.5(3)
C(60)-C(61)-H(61B)	109.4	C(75)-C(67)-C(66)	110.5(3)
C(62)-C(61)-H(61B)	109.4	C(58)-C(67)-C(66)	110.8(3)
H(61A)-C(61)-H(61B)	108.0	C(62)-C(67)-C(66)	106.4(3)
C(63)-C(62)-C(61)	112.0(4)	C(69)-C(68)-C(66)	112.9(4)
C(63)-C(62)-C(67)	112.0(3)	C(69)-C(68)-H(68A)	109.0
C(61)-C(62)-C(67)	113.3(4)	C(66)-C(68)-H(68A)	109.0
C(63)-C(62)-H(62)	106.3	C(69)-C(68)-H(68B)	109.0
C(61)-C(62)-H(62)	106.3	C(66)-C(68)-H(68B)	109.0
C(67)-C(62)-H(62)	106.3	H(68A)-C(68)-H(68B)	107.8
C(62)-C(63)-C(64)	112.0(4)	C(70)-C(69)-C(68)	111.5(3)
C(62)-C(63)-H(63A)	109.2	C(70)-C(69)-H(69A)	109.3
C(64)-C(63)-H(63A)	109.2	C(68)-C(69)-H(69A)	109.3
C(62)-C(63)-H(63B)	109.2	C(70)-C(69)-H(69B)	109.3
C(64)-C(63)-H(63B)	109.2	C(68)-C(69)-H(69B)	109.3
H(63A)-C(63)-H(63B)	107.9	H(69A)-C(69)-H(69B)	108.0
C(65)-C(64)-C(63)	111.8(4)	C(69)-C(70)-C(74)	116.4(4)
C(65)-C(64)-H(64A)	109.2	C(69)-C(70)-C(76)	111.2(4)
C(63)-C(64)-H(64A)	109.2	C(74)-C(70)-C(76)	108.2(3)
C(65)-C(64)-H(64B)	109.2	C(69)-C(70)-C(71)	107.8(3)
C(63)-C(64)-H(64B)	109.2	C(74)-C(70)-C(71)	100.3(3)
H(64A)-C(64)-H(64B)	107.9	C(76)-C(70)-C(71)	112.6(3)
C(71)-C(65)-C(64)	111.9(4)	C(65)-C(71)-C(70)	115.1(4)
C(71)-C(65)-C(66)	108.6(3)	C(65)-C(71)-C(72)	118.8(4)
C(64)-C(65)-C(66)	111.1(3)	C(70)-C(71)-C(72)	104.4(3)
C(71)-C(65)-H(65)	108.4	C(65)-C(71)-H(71)	105.8
C(64)-C(65)-H(65)	108.4	C(70)-C(71)-H(71)	105.8
C(66)-C(65)-H(65)	108.4	C(72)-C(71)-H(71)	105.8

C(71)-C(72)-C(73)	103.4(3)	C(70)-C(74)-H(74B)	110.7
C(71)-C(72)-H(72A)	111.1	C(73)-C(74)-H(74B)	110.7
C(73)-C(72)-H(72A)	111.1	H(74A)-C(74)-H(74B)	108.8
C(71)-C(72)-H(72B)	111.1	C(67)-C(75)-H(75A)	109.5
C(73)-C(72)-H(72B)	111.1	C(67)-C(75)-H(75B)	109.5
H(72A)-C(72)-H(72B)	109.1	H(75A)-C(75)-H(75B)	109.5
C(72)-C(73)-C(74)	106.2(3)	C(67)-C(75)-H(75C)	109.5
C(72)-C(73)-H(73A)	110.5	H(75A)-C(75)-H(75C)	109.5
C(74)-C(73)-H(73A)	110.5	H(75B)-C(75)-H(75C)	109.5
C(72)-C(73)-H(73B)	110.5	C(70)-C(76)-H(76A)	109.5
C(74)-C(73)-H(73B)	110.5	C(70)-C(76)-H(76B)	109.5
H(73A)-C(73)-H(73B)	108.7	H(76A)-C(76)-H(76B)	109.5
C(70)-C(74)-C(73)	105.0(3)	C(70)-C(76)-H(76C)	109.5
C(70)-C(74)-H(74A)	110.7	H(76A)-C(76)-H(76C)	109.5
C(73)-C(74)-H(74A)	110.7	H(76B)-C(76)-H(76C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for Form I. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(2)	22(2)	24(2)	-2(2)	2(2)	-2(2)
C(2)	21(2)	28(2)	23(2)	-1(2)	-3(2)	1(2)
C(3)	29(3)	24(2)	20(2)	-2(2)	2(2)	-1(2)
C(4)	16(2)	20(2)	24(2)	-2(2)	5(2)	1(2)
C(5)	16(2)	16(2)	24(2)	-1(2)	3(2)	-1(2)
C(6)	16(2)	24(2)	27(2)	2(2)	4(2)	1(2)
C(7)	16(2)	27(2)	23(2)	2(2)	2(2)	4(2)
C(8)	20(2)	15(2)	21(2)	0(2)	1(2)	0(2)
C(9)	8(2)	15(2)	23(2)	-3(2)	3(2)	-3(2)
C(10)	17(2)	15(2)	21(2)	0(2)	1(2)	2(2)
C(11)	17(2)	24(2)	24(2)	0(2)	2(2)	5(2)
C(12)	22(2)	21(2)	29(2)	-1(2)	11(2)	2(2)
C(13)	25(2)	17(2)	21(2)	-1(2)	5(2)	-1(2)
C(14)	20(2)	16(2)	21(2)	-1(2)	2(2)	-3(2)
C(15)	26(3)	25(2)	23(2)	2(2)	0(2)	1(2)
C(16)	24(3)	39(3)	27(2)	5(2)	2(2)	4(2)
C(17)	30(3)	25(2)	25(2)	2(2)	5(2)	1(2)
C(18)	15(2)	16(2)	24(2)	-1(2)	0(2)	2(2)
C(19)	29(3)	19(2)	28(2)	-5(2)	4(2)	0(2)
C(20)	22(2)	18(2)	25(2)	-2(2)	2(2)	1(2)
C(21)	17(2)	25(2)	29(2)	0(2)	-1(2)	3(2)
C(22)	34(3)	30(2)	20(2)	2(2)	-1(2)	3(2)
C(23)	18(2)	26(2)	24(2)	-1(2)	5(2)	2(2)
C(24)	13(2)	16(2)	24(2)	-1(2)	4(2)	-3(2)
C(25)	15(2)	22(2)	25(2)	-4(2)	5(2)	1(2)
C(26)	9(2)	23(2)	28(2)	-1(2)	4(2)	-1(2)
C(27)	10(2)	18(2)	21(2)	-1(2)	2(2)	1(2)
C(28)	11(2)	15(2)	21(2)	0(2)	2(2)	2(2)
C(29)	9(2)	13(2)	24(2)	0(2)	1(2)	-2(2)
C(30)	7(2)	22(2)	25(2)	-2(2)	4(2)	-1(2)
C(31)	18(2)	20(2)	22(2)	-2(2)	5(2)	-1(2)

C(32)	16(2)	15(2)	23(2)	0(2)	5(2)	-5(2)
C(33)	18(2)	14(2)	24(2)	-1(2)	6(2)	-4(2)
C(34)	12(2)	25(2)	26(2)	2(2)	0(2)	0(2)
C(35)	18(2)	36(3)	22(2)	1(2)	0(2)	0(2)
C(36)	17(2)	23(2)	21(2)	-1(2)	1(2)	-3(2)
C(37)	19(2)	17(2)	23(2)	-1(2)	0(2)	-4(2)
C(38)	24(3)	21(2)	27(2)	1(2)	7(2)	-4(2)
C(39)	21(2)	23(2)	25(2)	-1(2)	-1(2)	-1(2)
C(40)	21(2)	35(3)	25(2)	1(2)	6(2)	-3(2)
C(41)	27(3)	32(3)	20(2)	-3(2)	4(2)	2(2)
C(42)	22(2)	31(3)	20(2)	-2(2)	1(2)	1(2)
C(43)	18(2)	16(2)	21(2)	-2(2)	0(2)	4(2)
C(44)	20(2)	22(2)	25(2)	-2(2)	-1(2)	1(2)
C(45)	5(2)	23(2)	27(2)	-3(2)	1(2)	1(2)
C(46)	9(2)	16(2)	20(2)	-1(2)	3(2)	3(2)
C(47)	15(2)	20(2)	20(2)	-3(2)	1(2)	1(2)
C(48)	13(2)	19(2)	21(2)	0(2)	2(2)	1(2)
C(49)	12(2)	37(3)	25(2)	-6(2)	-1(2)	-6(2)
C(50)	16(2)	35(3)	23(2)	-2(2)	-5(2)	2(2)
C(51)	27(3)	18(2)	18(2)	0(2)	-1(2)	4(2)
C(52)	15(2)	14(2)	24(2)	1(2)	1(2)	1(2)
C(53)	22(2)	20(2)	27(2)	1(2)	4(2)	0(2)
C(54)	37(3)	29(3)	24(2)	3(2)	4(2)	-6(2)
C(55)	27(3)	27(3)	23(2)	4(2)	1(2)	4(2)
C(56)	22(2)	19(2)	27(2)	-2(2)	3(2)	-1(2)
C(57)	26(2)	22(2)	24(2)	-4(2)	1(2)	-1(2)
C(58)	16(2)	17(2)	22(2)	0(2)	0(2)	-1(2)
C(59)	23(3)	21(2)	23(2)	2(2)	-1(2)	-1(2)
C(60)	22(2)	30(2)	20(2)	3(2)	2(2)	0(2)
C(61)	30(3)	25(2)	17(2)	1(2)	-3(2)	-3(2)
C(62)	18(2)	14(2)	22(2)	-1(2)	0(2)	4(2)
C(63)	11(2)	24(2)	21(2)	-1(2)	-5(2)	1(2)
C(64)	23(2)	18(2)	21(2)	0(2)	-3(2)	0(2)
C(65)	13(2)	14(2)	18(2)	-2(2)	0(2)	0(2)
C(66)	23(2)	12(2)	16(2)	0(1)	-1(2)	0(2)
C(67)	11(2)	14(2)	20(2)	1(2)	-1(2)	-1(2)

C(68)	8(2)	22(2)	23(2)	-1(2)	1(2)	-2(2)
C(69)	18(2)	20(2)	19(2)	-3(2)	-1(2)	-4(2)
C(70)	14(2)	17(2)	18(2)	0(2)	1(2)	0(2)
C(71)	12(2)	16(2)	20(2)	-1(2)	1(2)	2(2)
C(72)	8(2)	23(2)	23(2)	0(2)	3(2)	0(2)
C(73)	22(2)	31(3)	21(2)	3(2)	4(2)	3(2)
C(74)	27(3)	17(2)	19(2)	0(2)	0(2)	4(2)
C(75)	22(2)	15(2)	20(2)	-1(2)	2(2)	6(2)
C(76)	27(3)	17(2)	22(2)	3(2)	2(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Form I.

	x	y	z	U(eq)
H(1A)	12149	6795	8072	24
H(1B)	11520	8309	8140	24
H(2A)	10785	5994	8517	29
H(2B)	12098	7217	8618	29
H(3A)	9222	7387	8850	29
H(3B)	9678	8706	8652	29
H(4A)	6697	8103	8523	24
H(4B)	7274	6579	8449	24
H(5)	8291	8895	8098	22
H(6A)	5231	8418	8003	27
H(6B)	5711	6914	7895	27
H(7A)	6680	9350	7580	26
H(7B)	5249	8258	7448	26
H(8)	7525	6647	7388	22
H(9)	9971	8650	7641	18
H(11A)	11027	6035	7436	26
H(11B)	12356	7179	7575	26
H(12A)	11809	8549	7133	28
H(12B)	12392	7080	7017	28
H(14)	8625	9158	7130	22
H(15A)	5807	9044	6898	30
H(15B)	5925	7430	6846	30
H(16A)	7353	9457	6467	36
H(16B)	7095	7884	6380	36
H(17A)	10147	7741	6447	32
H(17B)	10274	9142	6638	32
H(18A)	10029	5092	7857	28
H(18B)	7933	5431	7805	28
H(18C)	8799	5256	8150	28
H(19A)	10241	5581	6739	38

H(19B)	8138	5931	6721	38
H(19C)	9109	5498	7046	38
H(20A)	-5568	890	4576	26
H(20B)	-4222	2071	4484	26
H(21A)	-5446	-85	4077	29
H(21B)	-5993	1474	4037	29
H(22A)	-3090	2049	3906	34
H(22B)	-3755	822	3686	34
H(23A)	-2031	-736	3986	27
H(23B)	-724	480	3898	27
H(24)	-1053	1481	4384	21
H(25A)	214	-1260	4458	25
H(25B)	1402	-28	4338	25
H(26A)	1973	-470	4883	24
H(26B)	1343	1054	4817	24
H(27)	-843	-1065	5046	19
H(28)	-1969	1659	4897	19
H(30A)	-4218	-318	5161	22
H(30B)	-4797	1198	5073	22
H(31A)	-2805	2072	5469	24
H(31B)	-4103	990	5621	24
H(33)	201	1431	5334	22
H(34A)	2760	243	5439	25
H(34B)	1688	-1133	5509	25
H(35A)	2365	1034	5925	31
H(35B)	1697	-462	6012	31
H(36A)	-1017	514	6080	25
H(36B)	-489	1851	5891	25
H(37A)	-3685	-1573	4358	30
H(37B)	-4591	-1361	4684	30
H(37C)	-2531	-1820	4676	30
H(38A)	-3010	-1201	5797	35
H(38B)	-973	-1654	5754	35
H(38C)	-2377	-1618	5460	35
H(39A)	7314	2998	7068	28
H(39B)	6648	1499	6983	28

H(40A)	6305	3802	6577	33
H(40B)	7574	2520	6526	33
H(41A)	4860	2436	6197	31
H(41B)	5086	1123	6414	31
H(42A)	2101	1880	6435	29
H(42B)	2763	3376	6528	29
H(43)	3398	1034	6908	22
H(44A)	823	3107	7016	27
H(44B)	334	1610	6897	27
H(45A)	1414	667	7367	22
H(45B)	8	1830	7445	22
H(46)	2341	3336	7585	18
H(47)	4752	1218	7415	22
H(49A)	5913	3771	7661	30
H(49B)	7200	2554	7569	30
H(50A)	6261	1234	7986	30
H(50B)	6905	2673	8121	30
H(52)	3062	788	7879	21
H(53A)	201	1008	8018	28
H(53B)	358	2625	8059	28
H(54A)	1235	2274	8562	36
H(54B)	1360	668	8506	36
H(55A)	4285	2180	8606	31
H(55B)	4350	758	8424	31
H(56A)	5229	4767	7204	34
H(56B)	3100	4530	7189	34
H(56C)	4151	4636	6874	34
H(57A)	3774	4419	7972	36
H(57B)	4758	4316	8310	36
H(57C)	2638	4059	8268	36
H(58A)	-345	9064	10411	22
H(58B)	1092	7912	10504	22
H(59A)	53	10065	10907	27
H(59B)	-468	8505	10948	27
H(60A)	1973	9143	11300	29
H(60B)	2535	7936	11076	29

H(61A)	4860	9535	11093	29
H(61B)	3477	10730	11002	29
H(62)	4318	8527	10603	21
H(63A)	6704	10079	10652	22
H(63B)	5403	11262	10523	22
H(64A)	7050	10481	10109	25
H(64B)	6474	8950	10174	25
H(65)	4128	11056	9939	18
H(66)	3127	8346	10092	20
H(68A)	171	8796	9913	21
H(68B)	689	10314	9824	21
H(69A)	1922	7925	9517	23
H(69B)	555	9017	9365	23
H(71)	4989	8553	9655	19
H(72A)	7539	9712	9552	22
H(72B)	6462	11100	9478	22
H(73A)	6869	8907	9069	29
H(73B)	6187	10406	8978	29
H(74A)	3406	9461	8908	25
H(74B)	4004	8121	9100	25
H(75A)	2615	11804	10309	29
H(75B)	1637	11562	10627	29
H(75C)	550	11348	10301	29
H(76A)	1596	11207	9186	33
H(76B)	3667	11635	9230	33
H(76C)	2419	11620	9523	33

Table 6. Torsion angles [°] for Form I.

C(10)-C(1)-C(2)-C(3)	-54.9(5)
C(1)-C(2)-C(3)-C(4)	52.3(5)
C(2)-C(3)-C(4)-C(5)	-53.5(5)
C(3)-C(4)-C(5)-C(6)	-174.8(4)
C(3)-C(4)-C(5)-C(10)	56.9(5)
C(4)-C(5)-C(6)-C(7)	174.8(4)
C(10)-C(5)-C(6)-C(7)	-57.3(5)
C(5)-C(6)-C(7)-C(8)	54.9(5)
C(6)-C(7)-C(8)-C(14)	-176.0(4)
C(6)-C(7)-C(8)-C(9)	-54.2(5)
C(14)-C(8)-C(9)-C(11)	-52.2(5)
C(7)-C(8)-C(9)-C(11)	-175.0(4)
C(14)-C(8)-C(9)-C(10)	178.5(3)
C(7)-C(8)-C(9)-C(10)	55.7(5)
C(2)-C(1)-C(10)-C(18)	-65.6(5)
C(2)-C(1)-C(10)-C(5)	55.6(5)
C(2)-C(1)-C(10)-C(9)	173.0(4)
C(6)-C(5)-C(10)-C(1)	175.8(4)
C(4)-C(5)-C(10)-C(1)	-56.5(5)
C(6)-C(5)-C(10)-C(18)	-64.1(5)
C(4)-C(5)-C(10)-C(18)	63.6(5)
C(6)-C(5)-C(10)-C(9)	56.5(5)
C(4)-C(5)-C(10)-C(9)	-175.8(3)
C(11)-C(9)-C(10)-C(1)	58.7(5)
C(8)-C(9)-C(10)-C(1)	-173.1(3)
C(11)-C(9)-C(10)-C(18)	-62.3(5)
C(8)-C(9)-C(10)-C(18)	65.8(5)
C(11)-C(9)-C(10)-C(5)	176.3(4)
C(8)-C(9)-C(10)-C(5)	-55.5(4)
C(8)-C(9)-C(11)-C(12)	51.8(5)
C(10)-C(9)-C(11)-C(12)	-179.6(4)
C(9)-C(11)-C(12)-C(13)	-54.2(5)
C(11)-C(12)-C(13)-C(17)	167.6(4)
C(11)-C(12)-C(13)-C(14)	55.6(5)

C(11)-C(12)-C(13)-C(19)	-68.5(5)
C(7)-C(8)-C(14)-C(15)	-56.5(5)
C(9)-C(8)-C(14)-C(15)	-179.1(4)
C(7)-C(8)-C(14)-C(13)	-179.7(4)
C(9)-C(8)-C(14)-C(13)	57.7(5)
C(12)-C(13)-C(14)-C(8)	-59.6(5)
C(17)-C(13)-C(14)-C(8)	178.3(4)
C(19)-C(13)-C(14)-C(8)	62.9(5)
C(12)-C(13)-C(14)-C(15)	169.4(4)
C(17)-C(13)-C(14)-C(15)	47.2(4)
C(19)-C(13)-C(14)-C(15)	-68.2(4)
C(8)-C(14)-C(15)-C(16)	-163.9(4)
C(13)-C(14)-C(15)-C(16)	-36.1(4)
C(14)-C(15)-C(16)-C(17)	11.2(5)
C(12)-C(13)-C(17)-C(16)	-155.5(4)
C(14)-C(13)-C(17)-C(16)	-39.0(4)
C(19)-C(13)-C(17)-C(16)	79.7(5)
C(15)-C(16)-C(17)-C(13)	17.7(5)
C(29)-C(20)-C(21)-C(22)	-55.3(5)
C(20)-C(21)-C(22)-C(23)	53.5(5)
C(21)-C(22)-C(23)-C(24)	-53.0(5)
C(22)-C(23)-C(24)-C(29)	55.9(5)
C(22)-C(23)-C(24)-C(25)	-175.6(4)
C(29)-C(24)-C(25)-C(26)	-55.8(5)
C(23)-C(24)-C(25)-C(26)	174.6(4)
C(24)-C(25)-C(26)-C(27)	52.4(5)
C(25)-C(26)-C(27)-C(33)	-174.4(4)
C(25)-C(26)-C(27)-C(28)	-52.8(5)
C(26)-C(27)-C(28)-C(30)	-174.6(4)
C(33)-C(27)-C(28)-C(30)	-51.3(5)
C(26)-C(27)-C(28)-C(29)	54.6(5)
C(33)-C(27)-C(28)-C(29)	177.9(3)
C(23)-C(24)-C(29)-C(37)	63.7(5)
C(25)-C(24)-C(29)-C(37)	-63.8(4)
C(23)-C(24)-C(29)-C(20)	-55.3(5)
C(25)-C(24)-C(29)-C(20)	177.2(3)

C(23)-C(24)-C(29)-C(28)	-174.0(3)
C(25)-C(24)-C(29)-C(28)	58.6(5)
C(21)-C(20)-C(29)-C(24)	54.1(5)
C(21)-C(20)-C(29)-C(37)	-67.6(5)
C(21)-C(20)-C(29)-C(28)	172.3(4)
C(30)-C(28)-C(29)-C(24)	174.1(3)
C(27)-C(28)-C(29)-C(24)	-57.1(4)
C(30)-C(28)-C(29)-C(37)	-62.2(5)
C(27)-C(28)-C(29)-C(37)	66.5(4)
C(30)-C(28)-C(29)-C(20)	56.6(5)
C(27)-C(28)-C(29)-C(20)	-174.7(3)
C(29)-C(28)-C(30)-C(31)	-179.3(4)
C(27)-C(28)-C(30)-C(31)	52.5(5)
C(28)-C(30)-C(31)-C(32)	-55.9(5)
C(30)-C(31)-C(32)-C(38)	-67.9(4)
C(30)-C(31)-C(32)-C(36)	168.0(4)
C(30)-C(31)-C(32)-C(33)	56.6(5)
C(26)-C(27)-C(33)-C(34)	-56.3(5)
C(28)-C(27)-C(33)-C(34)	-179.6(4)
C(26)-C(27)-C(33)-C(32)	179.6(4)
C(28)-C(27)-C(33)-C(32)	56.4(5)
C(31)-C(32)-C(33)-C(34)	168.4(4)
C(38)-C(32)-C(33)-C(34)	-68.5(4)
C(36)-C(32)-C(33)-C(34)	46.1(4)
C(31)-C(32)-C(33)-C(27)	-59.8(5)
C(38)-C(32)-C(33)-C(27)	63.3(5)
C(36)-C(32)-C(33)-C(27)	177.9(4)
C(27)-C(33)-C(34)-C(35)	-165.1(4)
C(32)-C(33)-C(34)-C(35)	-36.2(4)
C(33)-C(34)-C(35)-C(36)	11.7(5)
C(31)-C(32)-C(36)-C(35)	-154.2(4)
C(38)-C(32)-C(36)-C(35)	80.3(4)
C(33)-C(32)-C(36)-C(35)	-38.1(4)
C(34)-C(35)-C(36)-C(32)	16.9(5)
C(48)-C(39)-C(40)-C(41)	-54.1(5)
C(39)-C(40)-C(41)-C(42)	52.6(6)

C(40)-C(41)-C(42)-C(43)	-54.5(5)
C(41)-C(42)-C(43)-C(44)	-173.6(4)
C(41)-C(42)-C(43)-C(48)	58.8(5)
C(42)-C(43)-C(44)-C(45)	175.5(4)
C(48)-C(43)-C(44)-C(45)	-56.5(5)
C(43)-C(44)-C(45)-C(46)	53.9(5)
C(44)-C(45)-C(46)-C(52)	-175.5(4)
C(44)-C(45)-C(46)-C(47)	-53.7(5)
C(52)-C(46)-C(47)-C(49)	-51.5(5)
C(45)-C(46)-C(47)-C(49)	-174.1(4)
C(52)-C(46)-C(47)-C(48)	178.8(3)
C(45)-C(46)-C(47)-C(48)	56.2(5)
C(44)-C(43)-C(48)-C(56)	-65.3(5)
C(42)-C(43)-C(48)-C(56)	61.7(5)
C(44)-C(43)-C(48)-C(47)	57.5(5)
C(42)-C(43)-C(48)-C(47)	-175.4(4)
C(44)-C(43)-C(48)-C(39)	175.8(3)
C(42)-C(43)-C(48)-C(39)	-57.1(5)
C(49)-C(47)-C(48)-C(43)	174.5(4)
C(46)-C(47)-C(48)-C(43)	-57.3(5)
C(49)-C(47)-C(48)-C(56)	-62.1(5)
C(46)-C(47)-C(48)-C(56)	66.1(5)
C(49)-C(47)-C(48)-C(39)	57.9(5)
C(46)-C(47)-C(48)-C(39)	-173.9(3)
C(40)-C(39)-C(48)-C(43)	54.7(5)
C(40)-C(39)-C(48)-C(56)	-66.5(5)
C(40)-C(39)-C(48)-C(47)	171.8(4)
C(48)-C(47)-C(49)-C(50)	179.4(4)
C(46)-C(47)-C(49)-C(50)	51.1(5)
C(47)-C(49)-C(50)-C(51)	-54.1(5)
C(49)-C(50)-C(51)-C(55)	168.3(4)
C(49)-C(50)-C(51)-C(57)	-68.0(5)
C(49)-C(50)-C(51)-C(52)	56.6(5)
C(45)-C(46)-C(52)-C(53)	-57.0(5)
C(47)-C(46)-C(52)-C(53)	-179.3(4)
C(45)-C(46)-C(52)-C(51)	179.6(3)

C(47)-C(46)-C(52)-C(51)	57.3(5)
C(50)-C(51)-C(52)-C(53)	168.1(4)
C(55)-C(51)-C(52)-C(53)	45.8(4)
C(57)-C(51)-C(52)-C(53)	-68.7(4)
C(50)-C(51)-C(52)-C(46)	-60.3(5)
C(55)-C(51)-C(52)-C(46)	177.4(4)
C(57)-C(51)-C(52)-C(46)	62.9(5)
C(46)-C(52)-C(53)-C(54)	-160.9(4)
C(51)-C(52)-C(53)-C(54)	-33.5(5)
C(52)-C(53)-C(54)-C(55)	7.9(5)
C(50)-C(51)-C(55)-C(54)	-156.9(4)
C(57)-C(51)-C(55)-C(54)	78.1(5)
C(52)-C(51)-C(55)-C(54)	-40.0(5)
C(53)-C(54)-C(55)-C(51)	20.5(5)
C(67)-C(58)-C(59)-C(60)	-56.6(5)
C(58)-C(59)-C(60)-C(61)	54.6(5)
C(59)-C(60)-C(61)-C(62)	-54.1(5)
C(60)-C(61)-C(62)-C(63)	-176.0(4)
C(60)-C(61)-C(62)-C(67)	56.1(5)
C(61)-C(62)-C(63)-C(64)	173.2(4)
C(67)-C(62)-C(63)-C(64)	-58.3(5)
C(62)-C(63)-C(64)-C(65)	54.0(5)
C(63)-C(64)-C(65)-C(71)	-173.6(4)
C(63)-C(64)-C(65)-C(66)	-52.0(5)
C(71)-C(65)-C(66)-C(68)	-51.5(4)
C(64)-C(65)-C(66)-C(68)	-174.9(3)
C(71)-C(65)-C(66)-C(67)	179.2(3)
C(64)-C(65)-C(66)-C(67)	55.7(5)
C(59)-C(58)-C(67)-C(75)	-66.8(5)
C(59)-C(58)-C(67)-C(62)	55.2(5)
C(59)-C(58)-C(67)-C(66)	171.0(4)
C(63)-C(62)-C(67)-C(75)	-62.8(4)
C(61)-C(62)-C(67)-C(75)	65.0(5)
C(63)-C(62)-C(67)-C(58)	176.8(3)
C(61)-C(62)-C(67)-C(58)	-55.3(5)
C(63)-C(62)-C(67)-C(66)	58.1(4)

C(61)-C(62)-C(67)-C(66)	-174.1(4)
C(65)-C(66)-C(67)-C(75)	64.8(5)
C(68)-C(66)-C(67)-C(75)	-63.7(5)
C(65)-C(66)-C(67)-C(58)	-173.7(3)
C(68)-C(66)-C(67)-C(58)	57.9(5)
C(65)-C(66)-C(67)-C(62)	-57.1(4)
C(68)-C(66)-C(67)-C(62)	174.4(3)
C(65)-C(66)-C(68)-C(69)	52.3(5)
C(67)-C(66)-C(68)-C(69)	-178.6(4)
C(66)-C(68)-C(69)-C(70)	-55.0(5)
C(68)-C(69)-C(70)-C(74)	167.5(4)
C(68)-C(69)-C(70)-C(76)	-68.0(4)
C(68)-C(69)-C(70)-C(71)	55.9(4)
C(64)-C(65)-C(71)-C(70)	-179.7(3)
C(66)-C(65)-C(71)-C(70)	57.4(5)
C(64)-C(65)-C(71)-C(72)	-54.8(5)
C(66)-C(65)-C(71)-C(72)	-177.8(4)
C(69)-C(70)-C(71)-C(65)	-59.8(5)
C(74)-C(70)-C(71)-C(65)	178.0(4)
C(76)-C(70)-C(71)-C(65)	63.2(5)
C(69)-C(70)-C(71)-C(72)	168.2(3)
C(74)-C(70)-C(71)-C(72)	46.0(4)
C(76)-C(70)-C(71)-C(72)	-68.8(4)
C(65)-C(71)-C(72)-C(73)	-165.8(4)
C(70)-C(71)-C(72)-C(73)	-35.9(4)
C(71)-C(72)-C(73)-C(74)	11.6(5)
C(69)-C(70)-C(74)-C(73)	-153.7(4)
C(76)-C(70)-C(74)-C(73)	80.3(4)
C(71)-C(70)-C(74)-C(73)	-37.8(4)
C(72)-C(73)-C(74)-C(70)	16.6(4)

S2. Crystallographic Tables for Form II with Impurity

Table 1. Crystal data and structure refinement for Form II w/Impurity.

Identification code	Form_II_impure
Empirical formula	C57 H94 O
Formula weight	795.32

Temperature	90(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.16990(10) Å	α= 90°.
	b = 22.1480(3) Å	β= 90°.
	c = 29.8734(5) Å	γ = 90°.
Volume	4743.86(12) $Å^3$	
Z	4	
Density (calculated)	1.114 Mg/m^3	
Absorption coefficient	0.463 mm^{-1}	
F(000)	1776	
Crystal size	0.190 x 0.060 x 0.030 mm^3	
Theta range for data collection	2.483 to 75.097°.	
Index ranges	-8<=h<=7, -26<=k<=27, -36<=l<=34	
Reflections collected	59898	
Independent reflections	9113 [R(int) = 0.0592]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.757	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9113 / 0 / 539	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1106	
R indices (all data)	R1 = 0.0478, wR2 = 0.1122	
Absolute structure parameter	0.0(2)	
Extinction coefficient	0.00062(10)	
Largest diff. peak and hole	0.237 and -0.342 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Form II w/Impurity. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3096(3)	6977(1)	4626(1)	26(1)
C(2)	3441(4)	6310(1)	4728(1)	30(1)
C(3)	1641(4)	5981(1)	4847(1)	33(1)
C(4)	181(4)	6071(1)	4481(1)	30(1)
C(5)	-148(3)	6741(1)	4378(1)	25(1)
C(6)	-1690(3)	6835(1)	4033(1)	27(1)
C(7)	-2144(4)	7505(1)	3973(1)	26(1)
C(8)	-416(3)	7888(1)	3874(1)	22(1)
C(9)	1160(3)	7764(1)	4216(1)	22(1)
C(10)	1666(3)	7079(1)	4247(1)	24(1)
C(11)	2840(3)	8183(1)	4139(1)	26(1)
C(12)	2300(3)	8858(1)	4133(1)	26(1)
C(13)	777(3)	8978(1)	3787(1)	25(1)
C(14)	-884(3)	8561(1)	3885(1)	24(1)
C(15)	-2436(4)	8805(1)	3585(1)	28(1)
C(16)	-2110(4)	9497(1)	3589(1)	34(1)
C(17)	-189(4)	9597(1)	3815(1)	30(1)
C(18)	2495(4)	6851(1)	3804(1)	27(1)
C(19)	1557(4)	8900(1)	3310(1)	32(1)
C(20)	4793(3)	8214(1)	2489(1)	23(1)
C(21)	4442(4)	8829(1)	2267(1)	27(1)
C(22)	6247(4)	9186(1)	2213(1)	29(1)
C(23)	7706(4)	8818(1)	1964(1)	27(1)
C(24)	8057(3)	8210(1)	2194(1)	22(1)
C(25)	9643(3)	7853(1)	1981(1)	25(1)
C(26)	10082(3)	7288(1)	2254(1)	26(1)
C(27)	8361(3)	6889(1)	2318(1)	21(1)
C(28)	6737(3)	7258(1)	2527(1)	20(1)
C(29)	6253(3)	7827(1)	2243(1)	20(1)
C(30)	5042(3)	6856(1)	2635(1)	23(1)
C(31)	5544(3)	6296(1)	2914(1)	24(1)

C(32)	7077(3)	5931(1)	2689(1)	24(1)
C(33)	8774(3)	6346(1)	2615(1)	24(1)
C(34)	10338(4)	5906(1)	2487(1)	35(1)
C(35)	9958(4)	5353(1)	2793(1)	45(1)
C(36)	7968(4)	5438(1)	2971(1)	26(1)
C(36A)	7968(4)	5438(1)	2971(1)	26(1)
C(37)	5469(3)	7643(1)	1782(1)	24(1)
C(38)	6357(4)	5640(1)	2253(1)	29(1)
C(39)	13496(4)	3373(1)	5375(1)	32(1)
C(40)	14440(4)	3144(1)	5796(1)	34(1)
C(41)	14359(4)	3607(1)	6171(1)	33(1)
C(42)	12337(4)	3788(1)	6265(1)	30(1)
C(43)	11377(3)	4017(1)	5841(1)	23(1)
C(44)	9406(4)	4246(1)	5929(1)	26(1)
C(45)	8606(4)	4551(1)	5513(1)	25(1)
C(46)	8689(4)	4148(1)	5098(1)	23(1)
C(47)	10676(3)	3892(1)	5028(1)	25(1)
C(48)	11434(3)	3561(1)	5448(1)	25(1)
C(49)	10793(4)	3521(2)	4594(1)	38(1)
C(50)	10134(4)	3876(2)	4180(1)	42(1)
C(51)	8163(4)	4119(1)	4249(1)	32(1)
C(52)	8128(4)	4498(1)	4679(1)	25(1)
C(53)	6238(4)	4823(1)	4660(1)	31(1)
C(54)	6004(4)	4968(1)	4155(1)	37(1)
C(55)	7472(4)	4586(1)	3914(1)	36(1)
C(55A)	7472(4)	4586(1)	3914(1)	36(1)
C(56)	10282(4)	2989(1)	5549(1)	31(1)
C(57)	6750(5)	3600(1)	4251(1)	41(1)
O(1)	6982(6)	5160(2)	3288(1)	44(1)
O(2)	7997(6)	4697(2)	3518(2)	45(1)

Table 3. Bond lengths [Å] and angles [°] for Form II w/Impurity.

C(1)-C(2)	1.530(4)	C(12)-H(12B)	0.9900
C(1)-C(10)	1.543(3)	C(13)-C(14)	1.536(3)
C(1)-H(1A)	0.9900	C(13)-C(17)	1.538(3)
C(1)-H(1B)	0.9900	C(13)-C(19)	1.539(4)
C(2)-C(3)	1.524(4)	C(14)-C(15)	1.526(3)
C(2)-H(2A)	0.9900	C(14)-H(14)	1.0000
C(2)-H(2B)	0.9900	C(15)-C(16)	1.551(4)
C(3)-C(4)	1.526(4)	C(15)-H(15A)	0.9900
C(3)-H(3A)	0.9900	C(15)-H(15B)	0.9900
C(3)-H(3B)	0.9900	C(16)-C(17)	1.550(4)
C(4)-C(5)	1.535(4)	C(16)-H(16A)	0.9900
C(4)-H(4A)	0.9900	C(16)-H(16B)	0.9900
C(4)-H(4B)	0.9900	C(17)-H(17A)	0.9900
C(5)-C(6)	1.527(3)	C(17)-H(17B)	0.9900
C(5)-C(10)	1.551(3)	C(18)-H(18A)	0.9800
C(5)-H(5)	1.0000	C(18)-H(18B)	0.9800
C(6)-C(7)	1.530(4)	C(18)-H(18C)	0.9800
C(6)-H(6A)	0.9900	C(19)-H(19A)	0.9800
C(6)-H(6B)	0.9900	C(19)-H(19B)	0.9800
C(7)-C(8)	1.530(3)	C(19)-H(19C)	0.9800
C(7)-H(7A)	0.9900	C(20)-C(21)	1.537(3)
C(7)-H(7B)	0.9900	C(20)-C(29)	1.540(3)
C(8)-C(14)	1.528(3)	C(20)-H(20A)	0.9900
C(8)-C(9)	1.548(3)	C(20)-H(20B)	0.9900
C(8)-H(8)	1.0000	C(21)-C(22)	1.525(4)
C(9)-C(11)	1.538(3)	C(21)-H(21A)	0.9900
C(9)-C(10)	1.563(3)	C(21)-H(21B)	0.9900
C(9)-H(9)	1.0000	C(22)-C(23)	1.521(4)
C(10)-C(18)	1.538(4)	C(22)-H(22A)	0.9900
C(11)-C(12)	1.544(4)	C(22)-H(22B)	0.9900
C(11)-H(11A)	0.9900	C(23)-C(24)	1.532(3)
C(11)-H(11B)	0.9900	C(23)-H(23A)	0.9900
C(12)-C(13)	1.527(4)	C(23)-H(23B)	0.9900
C(12)-H(12A)	0.9900	C(24)-C(25)	1.524(3)

C(24)-C(29)	1.553(3)	C(36A)-O(1)	1.335(5)
C(24)-H(24)	1.0000	C(37)-H(37A)	0.9800
C(25)-C(26)	1.527(4)	C(37)-H(37B)	0.9800
C(25)-H(25A)	0.9900	C(37)-H(37C)	0.9800
C(25)-H(25B)	0.9900	C(38)-H(38A)	0.9800
C(26)-C(27)	1.529(3)	C(38)-H(38B)	0.9800
C(26)-H(26A)	0.9900	C(38)-H(38C)	0.9800
C(26)-H(26B)	0.9900	C(39)-C(40)	1.516(4)
C(27)-C(33)	1.523(3)	C(39)-C(48)	1.551(3)
C(27)-C(28)	1.553(3)	C(39)-H(39A)	0.9900
C(27)-H(27)	1.0000	C(39)-H(39B)	0.9900
C(28)-C(30)	1.541(3)	C(40)-C(41)	1.520(4)
C(28)-C(29)	1.558(3)	C(40)-H(40A)	0.9900
C(28)-H(28)	1.0000	C(40)-H(40B)	0.9900
C(29)-C(37)	1.541(3)	C(41)-C(42)	1.530(4)
C(30)-C(31)	1.538(3)	C(41)-H(41A)	0.9900
C(30)-H(30A)	0.9900	C(41)-H(41B)	0.9900
C(30)-H(30B)	0.9900	C(42)-C(43)	1.528(3)
C(31)-C(32)	1.521(4)	C(42)-H(42A)	0.9900
C(31)-H(31A)	0.9900	C(42)-H(42B)	0.9900
C(31)-H(31B)	0.9900	C(43)-C(44)	1.525(3)
C(32)-C(36A)	1.520(3)	C(43)-C(48)	1.549(3)
C(32)-C(36)	1.520(3)	C(43)-H(43)	1.0000
C(32)-C(33)	1.540(3)	C(44)-C(45)	1.527(3)
C(32)-C(38)	1.543(4)	C(44)-H(44A)	0.9900
C(33)-C(34)	1.534(4)	C(44)-H(44B)	0.9900
C(33)-H(33)	1.0000	C(45)-C(46)	1.528(3)
C(34)-C(35)	1.551(4)	C(45)-H(45A)	0.9900
C(34)-H(34A)	0.9900	C(45)-H(45B)	0.9900
C(34)-H(34B)	0.9900	C(46)-C(52)	1.525(3)
C(35)-C(36A)	1.534(4)	C(46)-C(47)	1.548(3)
C(35)-C(36)	1.534(4)	C(46)-H(46)	1.0000
C(35)-H(35A)	0.9900	C(47)-C(49)	1.537(4)
C(35)-H(35B)	0.9900	C(47)-C(48)	1.552(4)
C(36)-H(36A)	0.9900	C(47)-H(47)	1.0000
C(36)-H(36B)	0.9900	C(48)-C(56)	1.541(3)

C(49)-C(50)	1.540(4)	C(53)-H(53B)	0.9900
C(49)-H(49A)	0.9900	C(54)-C(55A)	1.528(4)
C(49)-H(49B)	0.9900	C(54)-C(55)	1.528(4)
C(50)-C(51)	1.526(4)	C(54)-H(54A)	0.9900
C(50)-H(50A)	0.9900	C(54)-H(54B)	0.9900
C(50)-H(50B)	0.9900	C(55)-H(55A)	0.9900
C(51)-C(55A)	1.523(4)	C(55)-H(55B)	0.9900
C(51)-C(55)	1.523(4)	C(55A)-O(2)	1.267(5)
C(51)-C(57)	1.532(4)	C(56)-H(56A)	0.9800
C(51)-C(52)	1.535(4)	C(56)-H(56B)	0.9800
C(52)-C(53)	1.536(4)	C(56)-H(56C)	0.9800
C(52)-H(52)	1.0000	C(57)-H(57A)	0.9800
C(53)-C(54)	1.553(4)	C(57)-H(57B)	0.9800
C(53)-H(53A)	0.9900	C(57)-H(57C)	0.9800

C(2)-C(1)-C(10)	113.2(2)	C(3)-C(4)-H(4B)	109.2
C(2)-C(1)-H(1A)	108.9	C(5)-C(4)-H(4B)	109.2
C(10)-C(1)-H(1A)	108.9	H(4A)-C(4)-H(4B)	107.9
C(2)-C(1)-H(1B)	108.9	C(6)-C(5)-C(4)	112.3(2)
C(10)-C(1)-H(1B)	108.9	C(6)-C(5)-C(10)	111.8(2)
H(1A)-C(1)-H(1B)	107.7	C(4)-C(5)-C(10)	112.9(2)
C(3)-C(2)-C(1)	111.8(2)	C(6)-C(5)-H(5)	106.4
C(3)-C(2)-H(2A)	109.3	C(4)-C(5)-H(5)	106.4
C(1)-C(2)-H(2A)	109.3	C(10)-C(5)-H(5)	106.4
C(3)-C(2)-H(2B)	109.3	C(5)-C(6)-C(7)	111.4(2)
C(1)-C(2)-H(2B)	109.3	C(5)-C(6)-H(6A)	109.3
H(2A)-C(2)-H(2B)	107.9	C(7)-C(6)-H(6A)	109.3
C(2)-C(3)-C(4)	110.6(2)	C(5)-C(6)-H(6B)	109.3
C(2)-C(3)-H(3A)	109.5	C(7)-C(6)-H(6B)	109.3
C(4)-C(3)-H(3A)	109.5	H(6A)-C(6)-H(6B)	108.0
C(2)-C(3)-H(3B)	109.5	C(8)-C(7)-C(6)	112.8(2)
C(4)-C(3)-H(3B)	109.5	C(8)-C(7)-H(7A)	109.0
H(3A)-C(3)-H(3B)	108.1	C(6)-C(7)-H(7A)	109.0
C(3)-C(4)-C(5)	112.0(2)	C(8)-C(7)-H(7B)	109.0
C(3)-C(4)-H(4A)	109.2	C(6)-C(7)-H(7B)	109.0
C(5)-C(4)-H(4A)	109.2	H(7A)-C(7)-H(7B)	107.8

C(14)-C(8)-C(7)	111.0(2)	C(15)-C(14)-C(8)	119.6(2)
C(14)-C(8)-C(9)	108.62(19)	C(15)-C(14)-C(13)	103.9(2)
C(7)-C(8)-C(9)	111.5(2)	C(8)-C(14)-C(13)	114.4(2)
C(14)-C(8)-H(8)	108.6	C(15)-C(14)-H(14)	106.0
C(7)-C(8)-H(8)	108.6	C(8)-C(14)-H(14)	106.0
C(9)-C(8)-H(8)	108.6	C(13)-C(14)-H(14)	106.0
C(11)-C(9)-C(8)	111.5(2)	C(14)-C(15)-C(16)	103.7(2)
C(11)-C(9)-C(10)	114.4(2)	C(14)-C(15)-H(15A)	111.0
C(8)-C(9)-C(10)	112.38(19)	C(16)-C(15)-H(15A)	111.0
C(11)-C(9)-H(9)	105.9	C(14)-C(15)-H(15B)	111.0
C(8)-C(9)-H(9)	105.9	C(16)-C(15)-H(15B)	111.0
C(10)-C(9)-H(9)	105.9	H(15A)-C(15)-H(15B)	109.0
C(18)-C(10)-C(1)	109.1(2)	C(17)-C(16)-C(15)	106.1(2)
C(18)-C(10)-C(5)	112.5(2)	C(17)-C(16)-H(16A)	110.5
C(1)-C(10)-C(5)	107.6(2)	C(15)-C(16)-H(16A)	110.5
C(18)-C(10)-C(9)	110.9(2)	C(17)-C(16)-H(16B)	110.5
C(1)-C(10)-C(9)	109.9(2)	C(15)-C(16)-H(16B)	110.5
C(5)-C(10)-C(9)	106.8(2)	H(16A)-C(16)-H(16B)	108.7
C(9)-C(11)-C(12)	112.9(2)	C(13)-C(17)-C(16)	104.4(2)
C(9)-C(11)-H(11A)	109.0	C(13)-C(17)-H(17A)	110.9
C(12)-C(11)-H(11A)	109.0	C(16)-C(17)-H(17A)	110.9
C(9)-C(11)-H(11B)	109.0	C(13)-C(17)-H(17B)	110.9
C(12)-C(11)-H(11B)	109.0	C(16)-C(17)-H(17B)	110.9
H(11A)-C(11)-H(11B)	107.8	H(17A)-C(17)-H(17B)	108.9
C(13)-C(12)-C(11)	110.9(2)	C(10)-C(18)-H(18A)	109.5
C(13)-C(12)-H(12A)	109.5	C(10)-C(18)-H(18B)	109.5
C(11)-C(12)-H(12A)	109.5	H(18A)-C(18)-H(18B)	109.5
C(13)-C(12)-H(12B)	109.5	C(10)-C(18)-H(18C)	109.5
C(11)-C(12)-H(12B)	109.5	H(18A)-C(18)-H(18C)	109.5
H(12A)-C(12)-H(12B)	108.1	H(18B)-C(18)-H(18C)	109.5
C(12)-C(13)-C(14)	108.7(2)	C(13)-C(19)-H(19A)	109.5
C(12)-C(13)-C(17)	116.1(2)	C(13)-C(19)-H(19B)	109.5
C(14)-C(13)-C(17)	100.2(2)	H(19A)-C(19)-H(19B)	109.5
C(12)-C(13)-C(19)	110.3(2)	C(13)-C(19)-H(19C)	109.5
C(14)-C(13)-C(19)	113.0(2)	H(19A)-C(19)-H(19C)	109.5
C(17)-C(13)-C(19)	108.3(2)	H(19B)-C(19)-H(19C)	109.5

C(21)-C(20)-C(29)	113.4(2)	C(25)-C(26)-C(27)	112.0(2)
C(21)-C(20)-H(20A)	108.9	C(25)-C(26)-H(26A)	109.2
C(29)-C(20)-H(20A)	108.9	C(27)-C(26)-H(26A)	109.2
C(21)-C(20)-H(20B)	108.9	C(25)-C(26)-H(26B)	109.2
C(29)-C(20)-H(20B)	108.9	C(27)-C(26)-H(26B)	109.2
H(20A)-C(20)-H(20B)	107.7	H(26A)-C(26)-H(26B)	107.9
C(22)-C(21)-C(20)	111.5(2)	C(33)-C(27)-C(26)	111.9(2)
C(22)-C(21)-H(21A)	109.3	C(33)-C(27)-C(28)	109.15(19)
C(20)-C(21)-H(21A)	109.3	C(26)-C(27)-C(28)	110.58(19)
C(22)-C(21)-H(21B)	109.3	C(33)-C(27)-H(27)	108.4
C(20)-C(21)-H(21B)	109.3	C(26)-C(27)-H(27)	108.4
H(21A)-C(21)-H(21B)	108.0	C(28)-C(27)-H(27)	108.4
C(23)-C(22)-C(21)	110.9(2)	C(30)-C(28)-C(27)	111.80(19)
C(23)-C(22)-H(22A)	109.5	C(30)-C(28)-C(29)	113.94(19)
C(21)-C(22)-H(22A)	109.5	C(27)-C(28)-C(29)	111.96(19)
C(23)-C(22)-H(22B)	109.5	C(30)-C(28)-H(28)	106.2
C(21)-C(22)-H(22B)	109.5	C(27)-C(28)-H(28)	106.2
H(22A)-C(22)-H(22B)	108.0	C(29)-C(28)-H(28)	106.2
C(22)-C(23)-C(24)	111.4(2)	C(20)-C(29)-C(37)	109.07(19)
C(22)-C(23)-H(23A)	109.3	C(20)-C(29)-C(24)	107.87(19)
C(24)-C(23)-H(23A)	109.3	C(37)-C(29)-C(24)	111.4(2)
C(22)-C(23)-H(23B)	109.3	C(20)-C(29)-C(28)	109.88(19)
C(24)-C(23)-H(23B)	109.3	C(37)-C(29)-C(28)	110.71(19)
H(23A)-C(23)-H(23B)	108.0	C(24)-C(29)-C(28)	107.83(19)
C(25)-C(24)-C(23)	113.0(2)	C(31)-C(30)-C(28)	113.3(2)
C(25)-C(24)-C(29)	112.2(2)	C(31)-C(30)-H(30A)	108.9
C(23)-C(24)-C(29)	112.6(2)	C(28)-C(30)-H(30A)	108.9
C(25)-C(24)-H(24)	106.2	C(31)-C(30)-H(30B)	108.9
C(23)-C(24)-H(24)	106.2	C(28)-C(30)-H(30B)	108.9
C(29)-C(24)-H(24)	106.2	H(30A)-C(30)-H(30B)	107.7
C(24)-C(25)-C(26)	110.8(2)	C(32)-C(31)-C(30)	111.0(2)
C(24)-C(25)-H(25A)	109.5	C(32)-C(31)-H(31A)	109.4
C(26)-C(25)-H(25A)	109.5	C(30)-C(31)-H(31A)	109.4
C(24)-C(25)-H(25B)	109.5	C(32)-C(31)-H(31B)	109.4
C(26)-C(25)-H(25B)	109.5	C(30)-C(31)-H(31B)	109.4
H(25A)-C(25)-H(25B)	108.1	H(31A)-C(31)-H(31B)	108.0

C(36A)-C(32)-C(31)	116.1(2)	C(32)-C(36A)-C(35)	106.7(2)
C(36)-C(32)-C(31)	116.1(2)	C(29)-C(37)-H(37A)	109.5
C(36A)-C(32)-C(33)	100.2(2)	C(29)-C(37)-H(37B)	109.5
C(36)-C(32)-C(33)	100.2(2)	H(37A)-C(37)-H(37B)	109.5
C(31)-C(32)-C(33)	108.5(2)	C(29)-C(37)-H(37C)	109.5
C(36A)-C(32)-C(38)	107.9(2)	H(37A)-C(37)-H(37C)	109.5
C(36)-C(32)-C(38)	107.9(2)	H(37B)-C(37)-H(37C)	109.5
C(31)-C(32)-C(38)	110.7(2)	C(32)-C(38)-H(38A)	109.5
C(33)-C(32)-C(38)	113.1(2)	C(32)-C(38)-H(38B)	109.5
C(27)-C(33)-C(34)	120.0(2)	H(38A)-C(38)-H(38B)	109.5
C(27)-C(33)-C(32)	113.6(2)	C(32)-C(38)-H(38C)	109.5
C(34)-C(33)-C(32)	103.5(2)	H(38A)-C(38)-H(38C)	109.5
C(27)-C(33)-H(33)	106.3	H(38B)-C(38)-H(38C)	109.5
C(34)-C(33)-H(33)	106.3	C(40)-C(39)-C(48)	113.5(2)
C(32)-C(33)-H(33)	106.3	C(40)-C(39)-H(39A)	108.9
C(33)-C(34)-C(35)	103.1(2)	C(48)-C(39)-H(39A)	108.9
C(33)-C(34)-H(34A)	111.1	C(40)-C(39)-H(39B)	108.9
C(35)-C(34)-H(34A)	111.1	C(48)-C(39)-H(39B)	108.9
C(33)-C(34)-H(34B)	111.1	H(39A)-C(39)-H(39B)	107.7
C(35)-C(34)-H(34B)	111.1	C(39)-C(40)-C(41)	111.5(2)
H(34A)-C(34)-H(34B)	109.1	C(39)-C(40)-H(40A)	109.3
C(36A)-C(35)-C(34)	105.6(2)	C(41)-C(40)-H(40A)	109.3
C(36)-C(35)-C(34)	105.6(2)	C(39)-C(40)-H(40B)	109.3
C(36)-C(35)-H(35A)	110.6	C(41)-C(40)-H(40B)	109.3
C(34)-C(35)-H(35A)	110.6	H(40A)-C(40)-H(40B)	108.0
C(36)-C(35)-H(35B)	110.6	C(40)-C(41)-C(42)	110.4(2)
C(34)-C(35)-H(35B)	110.6	C(40)-C(41)-H(41A)	109.6
H(35A)-C(35)-H(35B)	108.7	C(42)-C(41)-H(41A)	109.6
C(32)-C(36)-C(35)	106.7(2)	C(40)-C(41)-H(41B)	109.6
C(32)-C(36)-H(36A)	110.4	C(42)-C(41)-H(41B)	109.6
C(35)-C(36)-H(36A)	110.4	H(41A)-C(41)-H(41B)	108.1
C(32)-C(36)-H(36B)	110.4	C(43)-C(42)-C(41)	111.2(2)
C(35)-C(36)-H(36B)	110.4	C(43)-C(42)-H(42A)	109.4
H(36A)-C(36)-H(36B)	108.6	C(41)-C(42)-H(42A)	109.4
O(1)-C(36A)-C(32)	120.2(3)	C(43)-C(42)-H(42B)	109.4
O(1)-C(36A)-C(35)	133.0(3)	C(41)-C(42)-H(42B)	109.4

H(42A)-C(42)-H(42B)	108.0	C(39)-C(48)-C(47)	110.3(2)
C(44)-C(43)-C(42)	112.6(2)	C(47)-C(49)-C(50)	112.7(2)
C(44)-C(43)-C(48)	111.9(2)	C(47)-C(49)-H(49A)	109.0
C(42)-C(43)-C(48)	113.6(2)	C(50)-C(49)-H(49A)	109.0
C(44)-C(43)-H(43)	106.0	C(47)-C(49)-H(49B)	109.0
C(42)-C(43)-H(43)	106.0	C(50)-C(49)-H(49B)	109.0
C(48)-C(43)-H(43)	106.0	H(49A)-C(49)-H(49B)	107.8
C(43)-C(44)-C(45)	110.7(2)	C(51)-C(50)-C(49)	110.8(2)
C(43)-C(44)-H(44A)	109.5	C(51)-C(50)-H(50A)	109.5
C(45)-C(44)-H(44A)	109.5	C(49)-C(50)-H(50A)	109.5
C(43)-C(44)-H(44B)	109.5	C(51)-C(50)-H(50B)	109.5
C(45)-C(44)-H(44B)	109.5	C(49)-C(50)-H(50B)	109.5
H(44A)-C(44)-H(44B)	108.1	H(50A)-C(50)-H(50B)	108.1
C(44)-C(45)-C(46)	112.8(2)	C(55A)-C(51)-C(50)	116.9(3)
C(44)-C(45)-H(45A)	109.0	C(55)-C(51)-C(50)	116.9(3)
C(46)-C(45)-H(45A)	109.0	C(55A)-C(51)-C(57)	107.3(2)
C(44)-C(45)-H(45B)	109.0	C(55)-C(51)-C(57)	107.3(2)
C(46)-C(45)-H(45B)	109.0	C(50)-C(51)-C(57)	110.4(3)
H(45A)-C(45)-H(45B)	107.8	C(55A)-C(51)-C(52)	99.9(2)
C(52)-C(46)-C(45)	111.1(2)	C(55)-C(51)-C(52)	99.9(2)
C(52)-C(46)-C(47)	108.5(2)	C(50)-C(51)-C(52)	108.7(2)
C(45)-C(46)-C(47)	111.1(2)	C(57)-C(51)-C(52)	113.3(2)
C(52)-C(46)-H(46)	108.7	C(46)-C(52)-C(51)	113.9(2)
C(45)-C(46)-H(46)	108.7	C(46)-C(52)-C(53)	120.1(2)
C(47)-C(46)-H(46)	108.7	C(51)-C(52)-C(53)	103.9(2)
C(49)-C(47)-C(46)	111.2(2)	C(46)-C(52)-H(52)	106.0
C(49)-C(47)-C(48)	114.1(2)	C(51)-C(52)-H(52)	106.0
C(46)-C(47)-C(48)	112.7(2)	C(53)-C(52)-H(52)	106.0
C(49)-C(47)-H(47)	106.1	C(52)-C(53)-C(54)	103.2(2)
C(46)-C(47)-H(47)	106.1	C(52)-C(53)-H(53A)	111.1
C(48)-C(47)-H(47)	106.1	C(54)-C(53)-H(53A)	111.1
C(56)-C(48)-C(43)	111.9(2)	C(52)-C(53)-H(53B)	111.1
C(56)-C(48)-C(39)	108.6(2)	C(54)-C(53)-H(53B)	111.1
C(43)-C(48)-C(39)	107.8(2)	H(53A)-C(53)-H(53B)	109.1
C(56)-C(48)-C(47)	111.1(2)	C(55A)-C(54)-C(53)	105.6(2)
C(43)-C(48)-C(47)	107.13(19)	C(55)-C(54)-C(53)	105.6(2)

C(55)-C(54)-H(54A)	110.6	C(51)-C(55A)-C(54)	107.0(2)
C(53)-C(54)-H(54A)	110.6	C(48)-C(56)-H(56A)	109.5
C(55)-C(54)-H(54B)	110.6	C(48)-C(56)-H(56B)	109.5
C(53)-C(54)-H(54B)	110.6	H(56A)-C(56)-H(56B)	109.5
H(54A)-C(54)-H(54B)	108.8	C(48)-C(56)-H(56C)	109.5
C(51)-C(55)-C(54)	107.0(2)	H(56A)-C(56)-H(56C)	109.5
C(51)-C(55)-H(55A)	110.3	H(56B)-C(56)-H(56C)	109.5
C(54)-C(55)-H(55A)	110.3	C(51)-C(57)-H(57A)	109.5
C(51)-C(55)-H(55B)	110.3	C(51)-C(57)-H(57B)	109.5
C(54)-C(55)-H(55B)	110.3	H(57A)-C(57)-H(57B)	109.5
H(55A)-C(55)-H(55B)	108.6	C(51)-C(57)-H(57C)	109.5
O(2)-C(55A)-C(51)	130.5(3)	H(57A)-C(57)-H(57C)	109.5
O(2)-C(55A)-C(54)	122.4(3)	H(57B)-C(57)-H(57C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Form II w/Impurity. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	27(1)	29(1)	-2(1)	-1(1)	0(1)
C(2)	27(1)	31(1)	33(1)	-1(1)	-4(1)	2(1)
C(3)	34(2)	28(1)	36(2)	7(1)	-2(1)	0(1)
C(4)	26(1)	27(1)	39(2)	1(1)	0(1)	-4(1)
C(5)	20(1)	27(1)	27(1)	-1(1)	1(1)	-4(1)
C(6)	19(1)	29(1)	32(1)	-1(1)	-1(1)	-5(1)
C(7)	19(1)	30(1)	30(1)	0(1)	-1(1)	-1(1)
C(8)	18(1)	25(1)	24(1)	-1(1)	1(1)	-2(1)
C(9)	18(1)	25(1)	23(1)	-3(1)	1(1)	-1(1)
C(10)	18(1)	28(1)	25(1)	-2(1)	-1(1)	-4(1)
C(11)	16(1)	26(1)	37(1)	0(1)	0(1)	-1(1)
C(12)	20(1)	25(1)	34(1)	-1(1)	0(1)	-1(1)
C(13)	23(1)	23(1)	29(1)	-2(1)	2(1)	-2(1)
C(14)	20(1)	29(1)	22(1)	-3(1)	1(1)	-1(1)
C(15)	23(1)	31(1)	30(1)	0(1)	-3(1)	2(1)
C(16)	30(2)	31(2)	41(2)	-3(1)	-7(1)	3(1)
C(17)	29(1)	24(1)	36(1)	-3(1)	-1(1)	1(1)
C(18)	23(1)	29(1)	30(1)	-2(1)	0(1)	2(1)
C(19)	31(1)	32(1)	33(1)	2(1)	5(1)	-1(1)
C(20)	19(1)	24(1)	26(1)	-1(1)	2(1)	0(1)
C(21)	26(1)	24(1)	30(1)	0(1)	3(1)	3(1)
C(22)	29(1)	21(1)	36(1)	1(1)	2(1)	0(1)
C(23)	25(1)	23(1)	32(1)	0(1)	3(1)	-3(1)
C(24)	19(1)	23(1)	25(1)	-2(1)	1(1)	-3(1)
C(25)	20(1)	26(1)	30(1)	2(1)	5(1)	-4(1)
C(26)	17(1)	27(1)	33(1)	1(1)	1(1)	0(1)
C(27)	15(1)	23(1)	25(1)	0(1)	1(1)	-1(1)
C(28)	17(1)	22(1)	21(1)	0(1)	-1(1)	-2(1)
C(29)	16(1)	22(1)	22(1)	-1(1)	0(1)	0(1)
C(30)	16(1)	25(1)	28(1)	5(1)	1(1)	-1(1)
C(31)	20(1)	26(1)	27(1)	5(1)	1(1)	-1(1)

C(32)	22(1)	23(1)	27(1)	4(1)	0(1)	0(1)
C(33)	18(1)	26(1)	29(1)	1(1)	-2(1)	0(1)
C(34)	21(1)	32(2)	52(2)	4(1)	3(1)	3(1)
C(35)	28(2)	31(2)	77(2)	13(2)	2(2)	6(1)
C(36)	28(1)	23(1)	28(1)	2(1)	-2(1)	0(1)
C(36A)	28(1)	23(1)	28(1)	2(1)	-2(1)	0(1)
C(37)	22(1)	24(1)	25(1)	1(1)	-2(1)	-3(1)
C(38)	30(1)	25(1)	33(1)	1(1)	-1(1)	-1(1)
C(39)	22(1)	36(2)	39(2)	-3(1)	4(1)	5(1)
C(40)	20(1)	34(2)	49(2)	4(1)	-2(1)	4(1)
C(41)	23(1)	35(2)	40(2)	9(1)	-6(1)	-3(1)
C(42)	26(1)	32(1)	30(1)	6(1)	-3(1)	-3(1)
C(43)	19(1)	24(1)	27(1)	3(1)	2(1)	-1(1)
C(44)	25(1)	31(1)	22(1)	2(1)	2(1)	3(1)
C(45)	24(1)	28(1)	24(1)	1(1)	2(1)	6(1)
C(46)	21(1)	23(1)	25(1)	1(1)	2(1)	-2(1)
C(47)	23(1)	25(1)	26(1)	-2(1)	3(1)	-2(1)
C(48)	19(1)	23(1)	33(1)	-1(1)	2(1)	-1(1)
C(49)	34(2)	46(2)	34(2)	-13(1)	-1(1)	11(1)
C(50)	41(2)	58(2)	26(1)	-13(1)	0(1)	8(2)
C(51)	34(2)	34(1)	27(1)	-2(1)	-4(1)	-3(1)
C(52)	27(1)	23(1)	25(1)	1(1)	1(1)	-4(1)
C(53)	33(1)	27(1)	33(1)	2(1)	-5(1)	1(1)
C(54)	36(2)	41(2)	35(2)	10(1)	-10(1)	-3(1)
C(55)	45(2)	39(2)	25(1)	5(1)	-7(1)	-12(1)
C(55A)	45(2)	39(2)	25(1)	5(1)	-7(1)	-12(1)
C(56)	24(1)	23(1)	46(2)	3(1)	-6(1)	-3(1)
C(57)	47(2)	31(2)	45(2)	-6(1)	-16(1)	-5(1)
O(1)	48(3)	41(2)	42(2)	5(2)	-6(2)	0(2)
O(2)	48(3)	43(2)	43(2)	3(2)	-2(2)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Form II w/Impurity.

	x	y	z	U(eq)
H(1A)	4292	7169	4541	31
H(1B)	2643	7179	4901	31
H(2A)	4014	6115	4463	36
H(2B)	4329	6276	4980	36
H(3A)	1154	6137	5135	39
H(3B)	1899	5545	4884	39
H(4A)	-1009	5884	4577	36
H(4B)	597	5863	4205	36
H(5)	-598	6929	4662	30
H(6A)	-2826	6618	4130	32
H(6B)	-1291	6664	3742	32
H(7A)	-3044	7551	3724	32
H(7B)	-2746	7658	4249	32
H(8)	50	7783	3568	27
H(9)	642	7877	4515	27
H(11A)	3434	8078	3850	32
H(11B)	3769	8115	4379	32
H(12A)	1850	8979	4433	32
H(12B)	3412	9104	4061	32
H(14)	-1275	8651	4199	28
H(15A)	-3679	8703	3708	34
H(15B)	-2334	8641	3278	34
H(16A)	-2102	9658	3279	41
H(16B)	-3107	9703	3760	41
H(17A)	540	9908	3654	36
H(17B)	-343	9724	4130	36
H(18A)	2645	6412	3817	41
H(18B)	3712	7041	3754	41
H(18C)	1654	6956	3557	41
H(19A)	1958	8481	3267	48

H(19B)	2623	9171	3268	48
H(19C)	584	8999	3091	48
H(20A)	3603	7988	2502	28
H(20B)	5219	8281	2801	28
H(21A)	3868	8766	1969	32
H(21B)	3555	9064	2452	32
H(22A)	5992	9563	2046	34
H(22B)	6733	9298	2512	34
H(23A)	8887	9048	1951	32
H(23B)	7278	8746	1654	32
H(24)	8472	8306	2506	27
H(25A)	10769	8111	1963	30
H(25B)	9288	7736	1673	30
H(26A)	10571	7409	2551	31
H(26B)	11064	7053	2099	31
H(27)	7953	6739	2018	25
H(28)	7207	7412	2821	24
H(30A)	4109	7098	2801	28
H(30B)	4460	6724	2351	28
H(31A)	5966	6424	3215	29
H(31B)	4423	6040	2951	29
H(33)	9110	6512	2916	29
H(34A)	11581	6082	2549	42
H(34B)	10265	5793	2167	42
H(35A)	10056	4973	2620	54
H(35B)	10863	5339	3043	54
H(36A)	7252	5057	2943	31
H(36B)	7995	5558	3290	31
H(37A)	4223	7468	1820	35
H(37B)	6296	7344	1644	35
H(37C)	5390	8000	1589	35
H(38A)	7358	5402	2115	44
H(38B)	5959	5957	2045	44
H(38C)	5298	5376	2321	44
H(39A)	13545	3054	5144	39
H(39B)	14199	3725	5261	39

H(40A)	15760	3048	5729	41
H(40B)	13821	2767	5895	41
H(41A)	15086	3969	6084	39
H(41B)	14923	3436	6445	39
H(42A)	11647	3435	6383	35
H(42B)	12312	4108	6496	35
H(43)	12112	4376	5740	28
H(44A)	9429	4538	6180	31
H(44B)	8597	3904	6017	31
H(45A)	9310	4927	5453	30
H(45B)	7291	4663	5571	30
H(46)	7804	3804	5139	28
H(47)	11507	4250	4982	30
H(49A)	10017	3153	4627	46
H(49B)	12099	3390	4547	46
H(50A)	10997	4216	4124	50
H(50B)	10156	3609	3914	50
H(52)	9097	4818	4639	30
H(53A)	6258	5198	4841	37
H(53B)	5221	4559	4769	37
H(54A)	4736	4859	4051	45
H(54B)	6214	5403	4097	45
H(55A)	6918	4385	3650	44
H(55B)	8517	4844	3812	44
H(56A)	10485	2690	5313	47
H(56B)	8955	3094	5563	47
H(56C)	10673	2820	5838	47
H(57A)	5493	3763	4295	61
H(57B)	7049	3320	4495	61
H(57C)	6805	3385	3965	61

Table 6. Torsion angles [°] for Form II w/Impurity.

C(10)-C(1)-C(2)-C(3)	-56.7(3)
C(1)-C(2)-C(3)-C(4)	54.1(3)
C(2)-C(3)-C(4)-C(5)	-53.9(3)
C(3)-C(4)-C(5)-C(6)	-176.6(2)
C(3)-C(4)-C(5)-C(10)	56.0(3)
C(4)-C(5)-C(6)-C(7)	173.7(2)
C(10)-C(5)-C(6)-C(7)	-58.2(3)
C(5)-C(6)-C(7)-C(8)	52.6(3)
C(6)-C(7)-C(8)-C(14)	-171.7(2)
C(6)-C(7)-C(8)-C(9)	-50.5(3)
C(14)-C(8)-C(9)-C(11)	-53.0(3)
C(7)-C(8)-C(9)-C(11)	-175.6(2)
C(14)-C(8)-C(9)-C(10)	177.0(2)
C(7)-C(8)-C(9)-C(10)	54.4(3)
C(2)-C(1)-C(10)-C(18)	-67.1(3)
C(2)-C(1)-C(10)-C(5)	55.2(3)
C(2)-C(1)-C(10)-C(9)	171.1(2)
C(6)-C(5)-C(10)-C(18)	-62.2(3)
C(4)-C(5)-C(10)-C(18)	65.5(3)
C(6)-C(5)-C(10)-C(1)	177.6(2)
C(4)-C(5)-C(10)-C(1)	-54.7(3)
C(6)-C(5)-C(10)-C(9)	59.7(3)
C(4)-C(5)-C(10)-C(9)	-172.6(2)
C(11)-C(9)-C(10)-C(18)	-63.4(3)
C(8)-C(9)-C(10)-C(18)	65.0(3)
C(11)-C(9)-C(10)-C(1)	57.3(3)
C(8)-C(9)-C(10)-C(1)	-174.3(2)
C(11)-C(9)-C(10)-C(5)	173.7(2)
C(8)-C(9)-C(10)-C(5)	-57.8(3)
C(8)-C(9)-C(11)-C(12)	53.9(3)
C(10)-C(9)-C(11)-C(12)	-177.2(2)
C(9)-C(11)-C(12)-C(13)	-55.1(3)
C(11)-C(12)-C(13)-C(14)	55.2(3)
C(11)-C(12)-C(13)-C(17)	167.2(2)

C(11)-C(12)-C(13)-C(19)	-69.1(3)
C(7)-C(8)-C(14)-C(15)	-55.7(3)
C(9)-C(8)-C(14)-C(15)	-178.6(2)
C(7)-C(8)-C(14)-C(13)	-179.8(2)
C(9)-C(8)-C(14)-C(13)	57.3(3)
C(12)-C(13)-C(14)-C(15)	169.0(2)
C(17)-C(13)-C(14)-C(15)	46.7(2)
C(19)-C(13)-C(14)-C(15)	-68.2(3)
C(12)-C(13)-C(14)-C(8)	-58.9(3)
C(17)-C(13)-C(14)-C(8)	178.9(2)
C(19)-C(13)-C(14)-C(8)	63.9(3)
C(8)-C(14)-C(15)-C(16)	-164.5(2)
C(13)-C(14)-C(15)-C(16)	-35.5(3)
C(14)-C(15)-C(16)-C(17)	10.3(3)
C(12)-C(13)-C(17)-C(16)	-156.3(2)
C(14)-C(13)-C(17)-C(16)	-39.4(3)
C(19)-C(13)-C(17)-C(16)	79.0(3)
C(15)-C(16)-C(17)-C(13)	18.4(3)
C(29)-C(20)-C(21)-C(22)	-55.4(3)
C(20)-C(21)-C(22)-C(23)	54.2(3)
C(21)-C(22)-C(23)-C(24)	-55.4(3)
C(22)-C(23)-C(24)-C(25)	-174.5(2)
C(22)-C(23)-C(24)-C(29)	57.2(3)
C(23)-C(24)-C(25)-C(26)	173.5(2)
C(29)-C(24)-C(25)-C(26)	-58.0(3)
C(24)-C(25)-C(26)-C(27)	55.7(3)
C(25)-C(26)-C(27)-C(33)	-176.4(2)
C(25)-C(26)-C(27)-C(28)	-54.5(3)
C(33)-C(27)-C(28)-C(30)	-51.4(3)
C(26)-C(27)-C(28)-C(30)	-174.88(19)
C(33)-C(27)-C(28)-C(29)	179.34(19)
C(26)-C(27)-C(28)-C(29)	55.9(3)
C(21)-C(20)-C(29)-C(37)	-66.9(3)
C(21)-C(20)-C(29)-C(24)	54.3(3)
C(21)-C(20)-C(29)-C(28)	171.6(2)
C(25)-C(24)-C(29)-C(20)	176.21(19)

C(23)-C(24)-C(29)-C(20)	-55.1(3)
C(25)-C(24)-C(29)-C(37)	-64.1(3)
C(23)-C(24)-C(29)-C(37)	64.6(3)
C(25)-C(24)-C(29)-C(28)	57.6(3)
C(23)-C(24)-C(29)-C(28)	-173.67(19)
C(30)-C(28)-C(29)-C(20)	58.2(3)
C(27)-C(28)-C(29)-C(20)	-173.71(19)
C(30)-C(28)-C(29)-C(37)	-62.3(3)
C(27)-C(28)-C(29)-C(37)	65.8(2)
C(30)-C(28)-C(29)-C(24)	175.51(19)
C(27)-C(28)-C(29)-C(24)	-56.4(2)
C(27)-C(28)-C(30)-C(31)	51.6(3)
C(29)-C(28)-C(30)-C(31)	179.8(2)
C(28)-C(30)-C(31)-C(32)	-54.6(3)
C(30)-C(31)-C(32)-C(36A)	168.4(2)
C(30)-C(31)-C(32)-C(36)	168.4(2)
C(30)-C(31)-C(32)-C(33)	56.6(3)
C(30)-C(31)-C(32)-C(38)	-68.1(3)
C(26)-C(27)-C(33)-C(34)	-56.8(3)
C(28)-C(27)-C(33)-C(34)	-179.5(2)
C(26)-C(27)-C(33)-C(32)	-180.0(2)
C(28)-C(27)-C(33)-C(32)	57.3(3)
C(36A)-C(32)-C(33)-C(27)	177.5(2)
C(36)-C(32)-C(33)-C(27)	177.5(2)
C(31)-C(32)-C(33)-C(27)	-60.3(3)
C(38)-C(32)-C(33)-C(27)	62.9(3)
C(36A)-C(32)-C(33)-C(34)	45.7(2)
C(36)-C(32)-C(33)-C(34)	45.7(2)
C(31)-C(32)-C(33)-C(34)	167.9(2)
C(38)-C(32)-C(33)-C(34)	-68.8(3)
C(27)-C(33)-C(34)-C(35)	-165.8(2)
C(32)-C(33)-C(34)-C(35)	-37.9(3)
C(33)-C(34)-C(35)-C(36A)	15.0(3)
C(33)-C(34)-C(35)-C(36)	15.0(3)
C(31)-C(32)-C(36)-C(35)	-152.7(2)
C(33)-C(32)-C(36)-C(35)	-36.1(3)

C(38)-C(32)-C(36)-C(35)	82.3(3)
C(34)-C(35)-C(36)-C(32)	13.5(3)
C(31)-C(32)-C(36A)-O(1)	29.7(4)
C(33)-C(32)-C(36A)-O(1)	146.3(3)
C(38)-C(32)-C(36A)-O(1)	-95.3(3)
C(31)-C(32)-C(36A)-C(35)	-152.7(2)
C(33)-C(32)-C(36A)-C(35)	-36.1(3)
C(38)-C(32)-C(36A)-C(35)	82.3(3)
C(34)-C(35)-C(36A)-O(1)	-169.4(4)
C(34)-C(35)-C(36A)-C(32)	13.5(3)
C(48)-C(39)-C(40)-C(41)	-56.8(3)
C(39)-C(40)-C(41)-C(42)	56.1(3)
C(40)-C(41)-C(42)-C(43)	-55.5(3)
C(41)-C(42)-C(43)-C(44)	-175.6(2)
C(41)-C(42)-C(43)-C(48)	55.9(3)
C(42)-C(43)-C(44)-C(45)	172.0(2)
C(48)-C(43)-C(44)-C(45)	-58.7(3)
C(43)-C(44)-C(45)-C(46)	53.8(3)
C(44)-C(45)-C(46)-C(52)	-172.2(2)
C(44)-C(45)-C(46)-C(47)	-51.4(3)
C(52)-C(46)-C(47)-C(49)	-54.0(3)
C(45)-C(46)-C(47)-C(49)	-176.3(2)
C(52)-C(46)-C(47)-C(48)	176.4(2)
C(45)-C(46)-C(47)-C(48)	54.1(3)
C(44)-C(43)-C(48)-C(56)	-62.6(3)
C(42)-C(43)-C(48)-C(56)	66.2(3)
C(44)-C(43)-C(48)-C(39)	178.1(2)
C(42)-C(43)-C(48)-C(39)	-53.1(3)
C(44)-C(43)-C(48)-C(47)	59.4(3)
C(42)-C(43)-C(48)-C(47)	-171.8(2)
C(40)-C(39)-C(48)-C(56)	-67.9(3)
C(40)-C(39)-C(48)-C(43)	53.4(3)
C(40)-C(39)-C(48)-C(47)	170.1(2)
C(49)-C(47)-C(48)-C(56)	-62.6(3)
C(46)-C(47)-C(48)-C(56)	65.4(3)
C(49)-C(47)-C(48)-C(43)	174.9(2)

C(46)-C(47)-C(48)-C(43)	-57.0(3)
C(49)-C(47)-C(48)-C(39)	57.9(3)
C(46)-C(47)-C(48)-C(39)	-174.1(2)
C(46)-C(47)-C(49)-C(50)	54.5(3)
C(48)-C(47)-C(49)-C(50)	-176.7(2)
C(47)-C(49)-C(50)-C(51)	-55.3(3)
C(49)-C(50)-C(51)-C(55A)	167.6(3)
C(49)-C(50)-C(51)-C(55)	167.6(3)
C(49)-C(50)-C(51)-C(57)	-69.4(3)
C(49)-C(50)-C(51)-C(52)	55.5(3)
C(45)-C(46)-C(52)-C(51)	-179.5(2)
C(47)-C(46)-C(52)-C(51)	58.2(3)
C(45)-C(46)-C(52)-C(53)	-55.4(3)
C(47)-C(46)-C(52)-C(53)	-177.8(2)
C(55A)-C(51)-C(52)-C(46)	177.7(2)
C(55)-C(51)-C(52)-C(46)	177.7(2)
C(50)-C(51)-C(52)-C(46)	-59.3(3)
C(57)-C(51)-C(52)-C(46)	63.9(3)
C(55A)-C(51)-C(52)-C(53)	45.3(3)
C(55)-C(51)-C(52)-C(53)	45.3(3)
C(50)-C(51)-C(52)-C(53)	168.3(2)
C(57)-C(51)-C(52)-C(53)	-68.5(3)
C(46)-C(52)-C(53)-C(54)	-165.8(2)
C(51)-C(52)-C(53)-C(54)	-37.1(3)
C(52)-C(53)-C(54)-C(55A)	13.9(3)
C(52)-C(53)-C(54)-C(55)	13.9(3)
C(50)-C(51)-C(55)-C(54)	-153.6(2)
C(57)-C(51)-C(55)-C(54)	81.8(3)
C(52)-C(51)-C(55)-C(54)	-36.6(3)
C(53)-C(54)-C(55)-C(51)	14.4(3)
C(50)-C(51)-C(55A)-O(2)	22.5(5)
C(57)-C(51)-C(55A)-O(2)	-102.1(4)
C(52)-C(51)-C(55A)-O(2)	139.5(4)
C(50)-C(51)-C(55A)-C(54)	-153.6(2)
C(57)-C(51)-C(55A)-C(54)	81.8(3)
C(52)-C(51)-C(55A)-C(54)	-36.6(3)

C(53)-C(54)-C(55A)-O(2)	-162.0(3)
C(53)-C(54)-C(55A)-C(51)	14.4(3)

Symmetry transformations used to generate equivalent atoms:

S3. Crystallographic Tables for Pure Form II

Table 1. Crystal data and structure refinement for Pure Form II.

Identification code	Form_II	
Empirical formula	C19 H32	
Formula weight	260.44	
Temperature	90(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.14650(10) Å	α= 90°.
	b = 22.20640(10) Å	β= 90°.
	c = 30.06790(10) Å	γ = 90°.
Volume	4771.72(7) $Å^3$	
Z	12	
Density (calculated)	1.088 Mg/m^3	
Absorption coefficient	0.435 mm^{-1}	
F(000)	1752	
Crystal size	0.190 x 0.060 x 0.030 mm^3	
Theta range for data collection	2.474 to 75.289°.	
Index ranges	-8<=h<=8, -27<=k<=27, -36<=l<=37	
Reflections collected	116227	
Independent reflections	9535 [R(int) = 0.0299]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.798	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9535 / 0 / 521	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0797	
R indices (all data)	R1 = 0.0305, wR2 = 0.0799	
Absolute structure parameter	-0.16(12)	
Extinction coefficient	0.00036(8)	
Largest diff. peak and hole	0.292 and -0.142 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Pure Form II. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3130(2)	6973(1)	4633(1)	21(1)
C(2)	3486(2)	6308(1)	4734(1)	25(1)
C(3)	1679(2)	5975(1)	4841(1)	28(1)
C(4)	237(2)	6060(1)	4470(1)	26(1)
C(5)	-98(2)	6727(1)	4369(1)	20(1)
C(6)	-1628(2)	6821(1)	4022(1)	22(1)
C(7)	-2082(2)	7488(1)	3963(1)	21(1)
C(8)	-350(2)	7875(1)	3871(1)	17(1)
C(9)	1214(2)	7753(1)	4216(1)	17(1)
C(10)	1724(2)	7073(1)	4249(1)	18(1)
C(11)	2896(2)	8176(1)	4145(1)	21(1)
C(12)	2347(2)	8844(1)	4135(1)	21(1)
C(13)	839(2)	8964(1)	3786(1)	20(1)
C(14)	-832(2)	8546(1)	3880(1)	18(1)
C(15)	-2369(2)	8786(1)	3574(1)	23(1)
C(16)	-2051(3)	9477(1)	3578(1)	29(1)
C(17)	-132(2)	9581(1)	3808(1)	25(1)
C(18)	2589(2)	6847(1)	3811(1)	22(1)
C(19)	1650(2)	8886(1)	3315(1)	26(1)
C(20)	4800(2)	8216(1)	2486(1)	16(1)
C(21)	4433(2)	8824(1)	2262(1)	20(1)
C(22)	6235(2)	9185(1)	2201(1)	23(1)
C(23)	7712(2)	8816(1)	1955(1)	20(1)
C(24)	8068(2)	8211(1)	2186(1)	16(1)
C(25)	9655(2)	7855(1)	1972(1)	19(1)
C(26)	10103(2)	7291(1)	2242(1)	19(1)
C(27)	8379(2)	6894(1)	2309(1)	15(1)
C(28)	6762(2)	7262(1)	2520(1)	14(1)
C(29)	6259(2)	7828(1)	2238(1)	13(1)
C(30)	5066(2)	6860(1)	2632(1)	17(1)
C(31)	5588(2)	6301(1)	2908(1)	18(1)

C(32)	7117(2)	5934(1)	2677(1)	17(1)
C(33)	8808(2)	6350(1)	2600(1)	17(1)
C(34)	10371(2)	5915(1)	2463(1)	25(1)
C(35)	9982(2)	5343(1)	2747(1)	28(1)
C(36)	8028(2)	5440(1)	2962(1)	22(1)
C(37)	5454(2)	7643(1)	1782(1)	17(1)
C(38)	6365(2)	5649(1)	2246(1)	22(1)
C(39)	13354(2)	3336(1)	5388(1)	22(1)
C(40)	14330(2)	3119(1)	5811(1)	25(1)
C(41)	14338(2)	3610(1)	6167(1)	25(1)
C(42)	12345(2)	3821(1)	6264(1)	20(1)
C(43)	11379(2)	4040(1)	5840(1)	15(1)
C(44)	9436(2)	4300(1)	5929(1)	17(1)
C(45)	8642(2)	4592(1)	5510(1)	18(1)
C(46)	8629(2)	4162(1)	5112(1)	15(1)
C(47)	10576(2)	3870(1)	5039(1)	16(1)
C(48)	11331(2)	3557(1)	5465(1)	16(1)
C(49)	10594(2)	3466(1)	4623(1)	23(1)
C(50)	9925(3)	3801(1)	4204(1)	27(1)
C(51)	7995(2)	4077(1)	4274(1)	24(1)
C(52)	8074(2)	4489(1)	4685(1)	18(1)
C(53)	6228(2)	4842(1)	4667(1)	24(1)
C(54)	5900(3)	4932(1)	4158(1)	33(1)
C(55)	7370(3)	4534(1)	3921(1)	32(1)
C(56)	10103(2)	3014(1)	5592(1)	19(1)
C(57)	6499(3)	3583(1)	4311(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for Pure Form II.

C(1)-C(2)	1.530(2)	C(12)-H(12B)	0.9900
C(1)-C(10)	1.546(2)	C(13)-C(17)	1.536(2)
C(1)-H(1A)	0.9900	C(13)-C(14)	1.539(2)
C(1)-H(1B)	0.9900	C(13)-C(19)	1.540(2)
C(2)-C(3)	1.523(2)	C(14)-C(15)	1.527(2)
C(2)-H(2A)	0.9900	C(14)-H(14)	1.0000
C(2)-H(2B)	0.9900	C(15)-C(16)	1.553(2)
C(3)-C(4)	1.531(2)	C(15)-H(15A)	0.9900
C(3)-H(3A)	0.9900	C(15)-H(15B)	0.9900
C(3)-H(3B)	0.9900	C(16)-C(17)	1.553(2)
C(4)-C(5)	1.531(2)	C(16)-H(16A)	0.9900
C(4)-H(4A)	0.9900	C(16)-H(16B)	0.9900
C(4)-H(4B)	0.9900	C(17)-H(17A)	0.9900
C(5)-C(6)	1.525(2)	C(17)-H(17B)	0.9900
C(5)-C(10)	1.554(2)	C(18)-H(18A)	0.9800
C(5)-H(5)	1.0000	C(18)-H(18B)	0.9800
C(6)-C(7)	1.527(2)	C(18)-H(18C)	0.9800
C(6)-H(6A)	0.9900	C(19)-H(19A)	0.9800
C(6)-H(6B)	0.9900	C(19)-H(19B)	0.9800
C(7)-C(8)	1.532(2)	C(19)-H(19C)	0.9800
C(7)-H(7A)	0.9900	C(20)-C(21)	1.5319(19)
C(7)-H(7B)	0.9900	C(20)-C(29)	1.5440(19)
C(8)-C(14)	1.5289(19)	C(20)-H(20A)	0.9900
C(8)-C(9)	1.550(2)	C(20)-H(20B)	0.9900
C(8)-H(8)	1.0000	C(21)-C(22)	1.528(2)
C(9)-C(11)	1.539(2)	C(21)-H(21A)	0.9900
C(9)-C(10)	1.557(2)	C(21)-H(21B)	0.9900
C(9)-H(9)	1.0000	C(22)-C(23)	1.527(2)
C(10)-C(18)	1.540(2)	C(22)-H(22A)	0.9900
C(11)-C(12)	1.536(2)	C(22)-H(22B)	0.9900
C(11)-H(11A)	0.9900	C(23)-C(24)	1.5348(19)
C(11)-H(11B)	0.9900	C(23)-H(23A)	0.9900
C(12)-C(13)	1.527(2)	C(23)-H(23B)	0.9900
C(12)-H(12A)	0.9900	C(24)-C(25)	1.526(2)

C(24)-C(29)	1.5543(18)	C(37)-H(37C)	0.9800
C(24)-H(24)	1.0000	C(38)-H(38A)	0.9800
C(25)-C(26)	1.5286(19)	C(38)-H(38B)	0.9800
C(25)-H(25A)	0.9900	C(38)-H(38C)	0.9800
C(25)-H(25B)	0.9900	C(39)-C(40)	1.528(2)
C(26)-C(27)	1.5280(19)	C(39)-C(48)	1.5446(19)
C(26)-H(26A)	0.9900	C(39)-H(39A)	0.9900
C(26)-H(26B)	0.9900	C(39)-H(39B)	0.9900
C(27)-C(33)	1.5229(18)	C(40)-C(41)	1.528(2)
C(27)-C(28)	1.5507(18)	C(40)-H(40A)	0.9900
C(27)-H(27)	1.0000	C(40)-H(40B)	0.9900
C(28)-C(30)	1.5421(19)	C(41)-C(42)	1.527(2)
C(28)-C(29)	1.5591(18)	C(41)-H(41A)	0.9900
C(28)-H(28)	1.0000	C(41)-H(41B)	0.9900
C(29)-C(37)	1.5430(18)	C(42)-C(43)	1.5298(19)
C(30)-C(31)	1.5385(18)	C(42)-H(42A)	0.9900
C(30)-H(30A)	0.9900	C(42)-H(42B)	0.9900
C(30)-H(30B)	0.9900	C(43)-C(44)	1.5274(19)
C(31)-C(32)	1.529(2)	C(43)-C(48)	1.5568(19)
C(31)-H(31A)	0.9900	C(43)-H(43)	1.0000
C(31)-H(31B)	0.9900	C(44)-C(45)	1.5282(19)
C(32)-C(36)	1.5344(19)	C(44)-H(44A)	0.9900
C(32)-C(38)	1.539(2)	C(44)-H(44B)	0.9900
C(32)-C(33)	1.5394(19)	C(45)-C(46)	1.5294(18)
C(33)-C(34)	1.533(2)	C(45)-H(45A)	0.9900
C(33)-H(33)	1.0000	C(45)-H(45B)	0.9900
C(34)-C(35)	1.555(2)	C(46)-C(52)	1.5270(18)
C(34)-H(34A)	0.9900	C(46)-C(47)	1.5503(19)
C(34)-H(34B)	0.9900	C(46)-H(46)	1.0000
C(35)-C(36)	1.553(2)	C(47)-C(49)	1.5404(19)
C(35)-H(35A)	0.9900	C(47)-C(48)	1.5535(18)
C(35)-H(35B)	0.9900	C(47)-H(47)	1.0000
C(36)-H(36A)	0.9900	C(48)-C(56)	1.5395(19)
C(36)-H(36B)	0.9900	C(49)-C(50)	1.538(2)
C(37)-H(37A)	0.9800	C(49)-H(49A)	0.9900
C(37)-H(37B)	0.9800	C(49)-H(49B)	0.9900

C(50)-C(51)	1.524(2)	C(54)-C(55)	1.547(3)
C(50)-H(50A)	0.9900	C(54)-H(54A)	0.9900
C(50)-H(50B)	0.9900	C(54)-H(54B)	0.9900
C(51)-C(55)	1.533(2)	C(55)-H(55A)	0.9900
C(51)-C(57)	1.537(2)	C(55)-H(55B)	0.9900
C(51)-C(52)	1.539(2)	C(56)-H(56A)	0.9800
C(52)-C(53)	1.536(2)	C(56)-H(56B)	0.9800
C(52)-H(52)	1.0000	C(56)-H(56C)	0.9800
C(53)-C(54)	1.561(2)	C(57)-H(57A)	0.9800
C(53)-H(53A)	0.9900	C(57)-H(57B)	0.9800
C(53)-H(53B)	0.9900	C(57)-H(57C)	0.9800

C(2)-C(1)-C(10)	113.28(12)	C(6)-C(5)-C(4)	112.36(12)
C(2)-C(1)-H(1A)	108.9	C(6)-C(5)-C(10)	111.96(12)
C(10)-C(1)-H(1A)	108.9	C(4)-C(5)-C(10)	113.21(13)
C(2)-C(1)-H(1B)	108.9	C(6)-C(5)-H(5)	106.2
C(10)-C(1)-H(1B)	108.9	C(4)-C(5)-H(5)	106.2
H(1A)-C(1)-H(1B)	107.7	C(10)-C(5)-H(5)	106.2
C(3)-C(2)-C(1)	111.72(13)	C(5)-C(6)-C(7)	111.45(12)
C(3)-C(2)-H(2A)	109.3	C(5)-C(6)-H(6A)	109.3
C(1)-C(2)-H(2A)	109.3	C(7)-C(6)-H(6A)	109.3
C(3)-C(2)-H(2B)	109.3	C(5)-C(6)-H(6B)	109.3
C(1)-C(2)-H(2B)	109.3	C(7)-C(6)-H(6B)	109.3
H(2A)-C(2)-H(2B)	107.9	H(6A)-C(6)-H(6B)	108.0
C(2)-C(3)-C(4)	110.87(13)	C(6)-C(7)-C(8)	113.15(12)
C(2)-C(3)-H(3A)	109.5	C(6)-C(7)-H(7A)	108.9
C(4)-C(3)-H(3A)	109.5	C(8)-C(7)-H(7A)	108.9
C(2)-C(3)-H(3B)	109.5	C(6)-C(7)-H(7B)	108.9
C(4)-C(3)-H(3B)	109.5	C(8)-C(7)-H(7B)	108.9
H(3A)-C(3)-H(3B)	108.1	H(7A)-C(7)-H(7B)	107.8
C(5)-C(4)-C(3)	111.65(13)	C(14)-C(8)-C(7)	111.15(12)
C(5)-C(4)-H(4A)	109.3	C(14)-C(8)-C(9)	108.66(11)
C(3)-C(4)-H(4A)	109.3	C(7)-C(8)-C(9)	111.31(12)
C(5)-C(4)-H(4B)	109.3	C(14)-C(8)-H(8)	108.5
C(3)-C(4)-H(4B)	109.3	C(7)-C(8)-H(8)	108.5
H(4A)-C(4)-H(4B)	108.0	C(9)-C(8)-H(8)	108.5

C(11)-C(9)-C(8)	111.37(12)	C(14)-C(15)-C(16)	103.63(12)
C(11)-C(9)-C(10)	114.64(12)	C(14)-C(15)-H(15A)	111.0
C(8)-C(9)-C(10)	112.40(11)	C(16)-C(15)-H(15A)	111.0
C(11)-C(9)-H(9)	105.9	C(14)-C(15)-H(15B)	111.0
C(8)-C(9)-H(9)	105.9	C(16)-C(15)-H(15B)	111.0
C(10)-C(9)-H(9)	105.9	H(15A)-C(15)-H(15B)	109.0
C(18)-C(10)-C(1)	109.31(12)	C(15)-C(16)-C(17)	106.16(13)
C(18)-C(10)-C(5)	111.92(12)	C(15)-C(16)-H(16A)	110.5
C(1)-C(10)-C(5)	107.49(12)	C(17)-C(16)-H(16A)	110.5
C(18)-C(10)-C(9)	110.75(12)	C(15)-C(16)-H(16B)	110.5
C(1)-C(10)-C(9)	109.88(11)	C(17)-C(16)-H(16B)	110.5
C(5)-C(10)-C(9)	107.42(11)	H(16A)-C(16)-H(16B)	108.7
C(12)-C(11)-C(9)	113.04(12)	C(13)-C(17)-C(16)	104.35(12)
C(12)-C(11)-H(11A)	109.0	C(13)-C(17)-H(17A)	110.9
C(9)-C(11)-H(11A)	109.0	C(16)-C(17)-H(17A)	110.9
C(12)-C(11)-H(11B)	109.0	C(13)-C(17)-H(17B)	110.9
C(9)-C(11)-H(11B)	109.0	C(16)-C(17)-H(17B)	110.9
H(11A)-C(11)-H(11B)	107.8	H(17A)-C(17)-H(17B)	108.9
C(13)-C(12)-C(11)	111.28(12)	C(10)-C(18)-H(18A)	109.5
C(13)-C(12)-H(12A)	109.4	C(10)-C(18)-H(18B)	109.5
C(11)-C(12)-H(12A)	109.4	H(18A)-C(18)-H(18B)	109.5
C(13)-C(12)-H(12B)	109.4	C(10)-C(18)-H(18C)	109.5
C(11)-C(12)-H(12B)	109.4	H(18A)-C(18)-H(18C)	109.5
H(12A)-C(12)-H(12B)	108.0	H(18B)-C(18)-H(18C)	109.5
C(12)-C(13)-C(17)	116.41(12)	C(13)-C(19)-H(19A)	109.5
C(12)-C(13)-C(14)	108.43(12)	C(13)-C(19)-H(19B)	109.5
C(17)-C(13)-C(14)	100.34(12)	H(19A)-C(19)-H(19B)	109.5
C(12)-C(13)-C(19)	110.29(13)	C(13)-C(19)-H(19C)	109.5
C(17)-C(13)-C(19)	108.07(12)	H(19A)-C(19)-H(19C)	109.5
C(14)-C(13)-C(19)	113.08(12)	H(19B)-C(19)-H(19C)	109.5
C(15)-C(14)-C(8)	119.39(12)	C(21)-C(20)-C(29)	113.26(11)
C(15)-C(14)-C(13)	103.74(12)	C(21)-C(20)-H(20A)	108.9
C(8)-C(14)-C(13)	114.22(12)	C(29)-C(20)-H(20A)	108.9
C(15)-C(14)-H(14)	106.2	C(21)-C(20)-H(20B)	108.9
C(8)-C(14)-H(14)	106.2	C(29)-C(20)-H(20B)	108.9
C(13)-C(14)-H(14)	106.2	H(20A)-C(20)-H(20B)	107.7

C(22)-C(21)-C(20)	111.77(12)	C(33)-C(27)-C(26)	111.76(11)
C(22)-C(21)-H(21A)	109.3	C(33)-C(27)-C(28)	109.48(11)
C(20)-C(21)-H(21A)	109.3	C(26)-C(27)-C(28)	110.57(11)
C(22)-C(21)-H(21B)	109.3	C(33)-C(27)-H(27)	108.3
C(20)-C(21)-H(21B)	109.3	C(26)-C(27)-H(27)	108.3
H(21A)-C(21)-H(21B)	107.9	C(28)-C(27)-H(27)	108.3
C(23)-C(22)-C(21)	111.05(12)	C(30)-C(28)-C(27)	111.74(11)
C(23)-C(22)-H(22A)	109.4	C(30)-C(28)-C(29)	113.89(11)
C(21)-C(22)-H(22A)	109.4	C(27)-C(28)-C(29)	111.99(11)
C(23)-C(22)-H(22B)	109.4	C(30)-C(28)-H(28)	106.2
C(21)-C(22)-H(22B)	109.4	C(27)-C(28)-H(28)	106.2
H(22A)-C(22)-H(22B)	108.0	C(29)-C(28)-H(28)	106.2
C(22)-C(23)-C(24)	111.38(12)	C(37)-C(29)-C(20)	109.03(11)
C(22)-C(23)-H(23A)	109.4	C(37)-C(29)-C(24)	111.55(11)
C(24)-C(23)-H(23A)	109.4	C(20)-C(29)-C(24)	107.76(11)
C(22)-C(23)-H(23B)	109.4	C(37)-C(29)-C(28)	110.75(11)
C(24)-C(23)-H(23B)	109.4	C(20)-C(29)-C(28)	110.03(11)
H(23A)-C(23)-H(23B)	108.0	C(24)-C(29)-C(28)	107.67(11)
C(25)-C(24)-C(23)	112.62(11)	C(31)-C(30)-C(28)	113.25(12)
C(25)-C(24)-C(29)	112.18(11)	C(31)-C(30)-H(30A)	108.9
C(23)-C(24)-C(29)	112.70(11)	C(28)-C(30)-H(30A)	108.9
C(25)-C(24)-H(24)	106.2	C(31)-C(30)-H(30B)	108.9
C(23)-C(24)-H(24)	106.2	C(28)-C(30)-H(30B)	108.9
C(29)-C(24)-H(24)	106.2	H(30A)-C(30)-H(30B)	107.7
C(24)-C(25)-C(26)	110.80(11)	C(32)-C(31)-C(30)	111.11(11)
C(24)-C(25)-H(25A)	109.5	C(32)-C(31)-H(31A)	109.4
C(26)-C(25)-H(25A)	109.5	C(30)-C(31)-H(31A)	109.4
C(24)-C(25)-H(25B)	109.5	C(32)-C(31)-H(31B)	109.4
C(26)-C(25)-H(25B)	109.5	C(30)-C(31)-H(31B)	109.4
H(25A)-C(25)-H(25B)	108.1	H(31A)-C(31)-H(31B)	108.0
C(27)-C(26)-C(25)	111.96(12)	C(31)-C(32)-C(36)	115.59(12)
C(27)-C(26)-H(26A)	109.2	C(31)-C(32)-C(38)	110.55(12)
C(25)-C(26)-H(26A)	109.2	C(36)-C(32)-C(38)	108.94(12)
C(27)-C(26)-H(26B)	109.2	C(31)-C(32)-C(33)	108.01(11)
C(25)-C(26)-H(26B)	109.2	C(36)-C(32)-C(33)	100.32(11)
H(26A)-C(26)-H(26B)	107.9	C(38)-C(32)-C(33)	113.15(12)

C(27)-C(33)-C(34)	119.52(12)	C(40)-C(39)-C(48)	113.68(12)
C(27)-C(33)-C(32)	113.90(11)	C(40)-C(39)-H(39A)	108.8
C(34)-C(33)-C(32)	103.54(11)	C(48)-C(39)-H(39A)	108.8
C(27)-C(33)-H(33)	106.3	C(40)-C(39)-H(39B)	108.8
C(34)-C(33)-H(33)	106.3	C(48)-C(39)-H(39B)	108.8
C(32)-C(33)-H(33)	106.3	H(39A)-C(39)-H(39B)	107.7
C(33)-C(34)-C(35)	103.71(12)	C(41)-C(40)-C(39)	111.08(12)
C(33)-C(34)-H(34A)	111.0	C(41)-C(40)-H(40A)	109.4
C(35)-C(34)-H(34A)	111.0	C(39)-C(40)-H(40A)	109.4
C(33)-C(34)-H(34B)	111.0	C(41)-C(40)-H(40B)	109.4
C(35)-C(34)-H(34B)	111.0	C(39)-C(40)-H(40B)	109.4
H(34A)-C(34)-H(34B)	109.0	H(40A)-C(40)-H(40B)	108.0
C(36)-C(35)-C(34)	105.94(12)	C(42)-C(41)-C(40)	110.44(12)
C(36)-C(35)-H(35A)	110.5	C(42)-C(41)-H(41A)	109.6
C(34)-C(35)-H(35A)	110.5	C(40)-C(41)-H(41A)	109.6
C(36)-C(35)-H(35B)	110.5	C(42)-C(41)-H(41B)	109.6
C(34)-C(35)-H(35B)	110.5	C(40)-C(41)-H(41B)	109.6
H(35A)-C(35)-H(35B)	108.7	H(41A)-C(41)-H(41B)	108.1
C(32)-C(36)-C(35)	104.50(12)	C(41)-C(42)-C(43)	111.00(12)
C(32)-C(36)-H(36A)	110.9	C(41)-C(42)-H(42A)	109.4
C(35)-C(36)-H(36A)	110.9	C(43)-C(42)-H(42A)	109.4
C(32)-C(36)-H(36B)	110.9	C(41)-C(42)-H(42B)	109.4
C(35)-C(36)-H(36B)	110.9	C(43)-C(42)-H(42B)	109.4
H(36A)-C(36)-H(36B)	108.9	H(42A)-C(42)-H(42B)	108.0
C(29)-C(37)-H(37A)	109.5	C(44)-C(43)-C(42)	112.60(11)
C(29)-C(37)-H(37B)	109.5	C(44)-C(43)-C(48)	111.59(11)
H(37A)-C(37)-H(37B)	109.5	C(42)-C(43)-C(48)	113.18(11)
C(29)-C(37)-H(37C)	109.5	C(44)-C(43)-H(43)	106.3
H(37A)-C(37)-H(37C)	109.5	C(42)-C(43)-H(43)	106.3
H(37B)-C(37)-H(37C)	109.5	C(48)-C(43)-H(43)	106.3
C(32)-C(38)-H(38A)	109.5	C(43)-C(44)-C(45)	110.64(11)
C(32)-C(38)-H(38B)	109.5	C(43)-C(44)-H(44A)	109.5
H(38A)-C(38)-H(38B)	109.5	C(45)-C(44)-H(44A)	109.5
C(32)-C(38)-H(38C)	109.5	C(43)-C(44)-H(44B)	109.5
H(38A)-C(38)-H(38C)	109.5	C(45)-C(44)-H(44B)	109.5
H(38B)-C(38)-H(38C)	109.5	H(44A)-C(44)-H(44B)	108.1

C(44)-C(45)-C(46)	112.54(11)	C(50)-C(51)-C(55)	115.79(14)
C(44)-C(45)-H(45A)	109.1	C(50)-C(51)-C(57)	110.60(13)
C(46)-C(45)-H(45A)	109.1	C(55)-C(51)-C(57)	108.77(14)
C(44)-C(45)-H(45B)	109.1	C(50)-C(51)-C(52)	108.40(13)
C(46)-C(45)-H(45B)	109.1	C(55)-C(51)-C(52)	100.01(12)
H(45A)-C(45)-H(45B)	107.8	C(57)-C(51)-C(52)	112.96(13)
C(52)-C(46)-C(45)	111.27(11)	C(46)-C(52)-C(53)	119.71(13)
C(52)-C(46)-C(47)	108.25(11)	C(46)-C(52)-C(51)	113.85(11)
C(45)-C(46)-C(47)	111.49(11)	C(53)-C(52)-C(51)	104.07(12)
C(52)-C(46)-H(46)	108.6	C(46)-C(52)-H(52)	106.1
C(45)-C(46)-H(46)	108.6	C(53)-C(52)-H(52)	106.1
C(47)-C(46)-H(46)	108.6	C(51)-C(52)-H(52)	106.1
C(49)-C(47)-C(46)	111.46(12)	C(52)-C(53)-C(54)	103.25(13)
C(49)-C(47)-C(48)	114.02(11)	C(52)-C(53)-H(53A)	111.1
C(46)-C(47)-C(48)	112.51(11)	C(54)-C(53)-H(53A)	111.1
C(49)-C(47)-H(47)	106.1	C(52)-C(53)-H(53B)	111.1
C(46)-C(47)-H(47)	106.1	C(54)-C(53)-H(53B)	111.1
C(48)-C(47)-H(47)	106.1	H(53A)-C(53)-H(53B)	109.1
C(56)-C(48)-C(39)	108.76(11)	C(55)-C(54)-C(53)	106.03(13)
C(56)-C(48)-C(47)	110.87(12)	C(55)-C(54)-H(54A)	110.5
C(39)-C(48)-C(47)	110.08(12)	C(53)-C(54)-H(54A)	110.5
C(56)-C(48)-C(43)	111.91(11)	C(55)-C(54)-H(54B)	110.5
C(39)-C(48)-C(43)	107.94(11)	C(53)-C(54)-H(54B)	110.5
C(47)-C(48)-C(43)	107.22(10)	H(54A)-C(54)-H(54B)	108.7
C(50)-C(49)-C(47)	112.45(12)	C(51)-C(55)-C(54)	104.93(13)
C(50)-C(49)-H(49A)	109.1	C(51)-C(55)-H(55A)	110.8
C(47)-C(49)-H(49A)	109.1	C(54)-C(55)-H(55A)	110.8
C(50)-C(49)-H(49B)	109.1	C(51)-C(55)-H(55B)	110.8
C(47)-C(49)-H(49B)	109.1	C(54)-C(55)-H(55B)	110.8
H(49A)-C(49)-H(49B)	107.8	H(55A)-C(55)-H(55B)	108.8
C(51)-C(50)-C(49)	111.33(13)	C(48)-C(56)-H(56A)	109.5
C(51)-C(50)-H(50A)	109.4	C(48)-C(56)-H(56B)	109.5
C(49)-C(50)-H(50A)	109.4	H(56A)-C(56)-H(56B)	109.5
C(51)-C(50)-H(50B)	109.4	C(48)-C(56)-H(56C)	109.5
C(49)-C(50)-H(50B)	109.4	H(56A)-C(56)-H(56C)	109.5
H(50A)-C(50)-H(50B)	108.0	H(56B)-C(56)-H(56C)	109.5

C(51)-C(57)-H(57A)	109.5
C(51)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(51)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Pure Form II. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	20(1)	21(1)	22(1)	-1(1)	-2(1)	0(1)
C(2)	26(1)	23(1)	27(1)	1(1)	-4(1)	3(1)
C(3)	33(1)	20(1)	31(1)	7(1)	0(1)	1(1)
C(4)	23(1)	19(1)	36(1)	2(1)	0(1)	-4(1)
C(5)	18(1)	20(1)	22(1)	0(1)	1(1)	-3(1)
C(6)	17(1)	20(1)	31(1)	-2(1)	-1(1)	-5(1)
C(7)	16(1)	22(1)	25(1)	0(1)	-2(1)	-4(1)
C(8)	14(1)	17(1)	19(1)	-3(1)	1(1)	-1(1)
C(9)	16(1)	19(1)	18(1)	-2(1)	1(1)	-2(1)
C(10)	15(1)	18(1)	19(1)	-1(1)	1(1)	-2(1)
C(11)	14(1)	19(1)	30(1)	-1(1)	-1(1)	-1(1)
C(12)	18(1)	17(1)	28(1)	-1(1)	-1(1)	-3(1)
C(13)	20(1)	17(1)	22(1)	-2(1)	1(1)	-1(1)
C(14)	17(1)	19(1)	19(1)	-2(1)	0(1)	-1(1)
C(15)	20(1)	23(1)	26(1)	-1(1)	-3(1)	0(1)
C(16)	29(1)	22(1)	36(1)	0(1)	-9(1)	4(1)
C(17)	25(1)	17(1)	31(1)	-2(1)	-2(1)	1(1)
C(18)	20(1)	21(1)	24(1)	-3(1)	2(1)	1(1)
C(19)	27(1)	27(1)	25(1)	1(1)	6(1)	-3(1)
C(20)	15(1)	16(1)	18(1)	1(1)	2(1)	1(1)
C(21)	19(1)	17(1)	25(1)	1(1)	3(1)	4(1)
C(22)	23(1)	15(1)	30(1)	1(1)	2(1)	1(1)
C(23)	19(1)	14(1)	26(1)	2(1)	3(1)	-2(1)
C(24)	14(1)	15(1)	18(1)	1(1)	1(1)	-2(1)
C(25)	14(1)	18(1)	24(1)	4(1)	4(1)	-2(1)
C(26)	12(1)	18(1)	26(1)	4(1)	2(1)	0(1)
C(27)	12(1)	16(1)	17(1)	2(1)	1(1)	-1(1)
C(28)	14(1)	15(1)	13(1)	1(1)	-1(1)	-1(1)
C(29)	12(1)	14(1)	14(1)	1(1)	1(1)	0(1)
C(30)	13(1)	18(1)	20(1)	4(1)	2(1)	0(1)
C(31)	16(1)	19(1)	18(1)	5(1)	3(1)	-2(1)

C(32)	17(1)	16(1)	18(1)	3(1)	-1(1)	-2(1)
C(33)	13(1)	17(1)	20(1)	3(1)	-1(1)	0(1)
C(34)	17(1)	20(1)	37(1)	8(1)	4(1)	3(1)
C(35)	25(1)	21(1)	38(1)	9(1)	2(1)	5(1)
C(36)	24(1)	18(1)	24(1)	6(1)	-2(1)	-1(1)
C(37)	17(1)	17(1)	16(1)	1(1)	-2(1)	-2(1)
C(38)	27(1)	19(1)	21(1)	0(1)	-2(1)	-4(1)
C(39)	18(1)	21(1)	27(1)	0(1)	4(1)	4(1)
C(40)	16(1)	23(1)	36(1)	4(1)	-1(1)	5(1)
C(41)	18(1)	24(1)	32(1)	4(1)	-7(1)	-1(1)
C(42)	19(1)	21(1)	20(1)	2(1)	-4(1)	-1(1)
C(43)	15(1)	14(1)	16(1)	1(1)	0(1)	-1(1)
C(44)	18(1)	20(1)	14(1)	-2(1)	1(1)	2(1)
C(45)	18(1)	17(1)	18(1)	-1(1)	0(1)	4(1)
C(46)	17(1)	14(1)	15(1)	1(1)	0(1)	-1(1)
C(47)	20(1)	14(1)	15(1)	0(1)	2(1)	-1(1)
C(48)	15(1)	14(1)	18(1)	0(1)	1(1)	-1(1)
C(49)	31(1)	19(1)	18(1)	-3(1)	3(1)	4(1)
C(50)	44(1)	22(1)	14(1)	-2(1)	3(1)	0(1)
C(51)	38(1)	17(1)	16(1)	2(1)	-5(1)	-4(1)
C(52)	24(1)	13(1)	17(1)	1(1)	-2(1)	-2(1)
C(53)	27(1)	21(1)	26(1)	4(1)	-8(1)	1(1)
C(54)	46(1)	25(1)	28(1)	6(1)	-17(1)	0(1)
C(55)	54(1)	23(1)	19(1)	5(1)	-11(1)	-3(1)
C(56)	21(1)	15(1)	23(1)	4(1)	-2(1)	-3(1)
C(57)	44(1)	19(1)	27(1)	1(1)	-13(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Pure Form II.

	x	y	z	U(eq)
H(1A)	4332	7167	4555	25
H(1B)	2647	7171	4904	25
H(2A)	4091	6116	4473	30
H(2B)	4353	6274	4989	30
H(3A)	1160	6128	5125	33
H(3B)	1946	5540	4879	33
H(4A)	683	5855	4197	31
H(4B)	-959	5870	4560	31
H(5)	-574	6910	4651	24
H(6A)	-2771	6604	4116	27
H(6B)	-1214	6651	3734	27
H(7A)	-2704	7638	4236	25
H(7B)	-2973	7534	3713	25
H(8)	137	7772	3568	20
H(9)	673	7865	4511	21
H(11A)	3812	8110	4387	25
H(11B)	3516	8071	3861	25
H(12A)	1877	8965	4432	25
H(12B)	3465	9090	4067	25
H(14)	-1245	8636	4190	22
H(15A)	-3624	8683	3691	28
H(15B)	-2239	8621	3270	28
H(16A)	-3062	9682	3745	35
H(16B)	-2030	9637	3271	35
H(17A)	606	9890	3649	30
H(17B)	-304	9710	4121	30
H(18A)	2766	6410	3826	32
H(18B)	3801	7044	3764	32
H(18C)	1750	6945	3563	32
H(19A)	2047	8468	3273	39

H(19B)	2728	9154	3277	39
H(19C)	690	8987	3094	39
H(20A)	3609	7990	2504	19
H(20B)	5243	8287	2793	19
H(21A)	3847	8756	1968	24
H(21B)	3546	9060	2445	24
H(22A)	5962	9556	2031	27
H(22B)	6727	9305	2496	27
H(23A)	8895	9047	1941	24
H(23B)	7288	8743	1646	24
H(24)	8493	8309	2495	19
H(25A)	10785	8112	1952	23
H(25B)	9291	7738	1666	23
H(26A)	11084	7056	2087	23
H(26B)	10604	7411	2536	23
H(27)	7958	6746	2011	18
H(28)	7247	7416	2810	17
H(30A)	4140	7101	2800	20
H(30B)	4467	6729	2352	20
H(31A)	6032	6428	3205	21
H(31B)	4464	6046	2949	21
H(33)	9166	6512	2899	20
H(34A)	11618	6085	2532	30
H(34B)	10306	5822	2142	30
H(35A)	9979	4979	2558	34
H(35B)	10951	5295	2980	34
H(36A)	7281	5065	2952	26
H(36B)	8151	5572	3275	26
H(37A)	4206	7469	1822	25
H(37B)	6279	7344	1643	25
H(37C)	5366	7998	1589	25
H(38A)	7347	5403	2109	33
H(38B)	5987	5968	2040	33
H(38C)	5283	5395	2315	33
H(39A)	13331	3002	5170	26
H(39B)	14094	3668	5257	26

H(40A)	13676	2759	5927	30
H(40B)	15634	3003	5740	30
H(41A)	14914	3452	6442	30
H(41B)	15097	3956	6063	30
H(42A)	12379	4151	6485	24
H(42B)	11620	3484	6394	24
H(43)	12155	4380	5724	18
H(44A)	9515	4604	6170	21
H(44B)	8588	3975	6030	21
H(45A)	9399	4951	5435	21
H(45B)	7347	4728	5569	21
H(46)	7698	3836	5171	18
H(47)	11456	4209	4976	19
H(49A)	11881	3316	4573	27
H(49B)	9775	3114	4675	27
H(50A)	10830	4123	4129	32
H(50B)	9878	3517	3951	32
H(52)	9090	4788	4626	22
H(53A)	6345	5234	4821	29
H(53B)	5194	4610	4803	29
H(54A)	4618	4806	4075	39
H(54B)	6068	5360	4075	39
H(55A)	6812	4327	3662	38
H(55B)	8443	4780	3819	38
H(56A)	10202	2704	5361	29
H(56B)	8797	3144	5619	29
H(56C)	10528	2848	5877	29
H(57A)	5262	3768	4342	45
H(57B)	6757	3333	4573	45
H(57C)	6524	3331	4044	45

Table 6. Torsion angles [°] for Pure Form II.

C(10)-C(1)-C(2)-C(3)	-56.62(18)
C(1)-C(2)-C(3)-C(4)	54.22(18)
C(2)-C(3)-C(4)-C(5)	-53.98(18)
C(3)-C(4)-C(5)-C(6)	-176.07(13)
C(3)-C(4)-C(5)-C(10)	55.88(17)
C(4)-C(5)-C(6)-C(7)	173.97(13)
C(10)-C(5)-C(6)-C(7)	-57.32(17)
C(5)-C(6)-C(7)-C(8)	52.42(17)
C(6)-C(7)-C(8)-C(14)	-171.88(12)
C(6)-C(7)-C(8)-C(9)	-50.60(16)
C(14)-C(8)-C(9)-C(11)	-52.96(15)
C(7)-C(8)-C(9)-C(11)	-175.68(12)
C(14)-C(8)-C(9)-C(10)	176.82(11)
C(7)-C(8)-C(9)-C(10)	54.11(15)
C(2)-C(1)-C(10)-C(18)	-66.77(16)
C(2)-C(1)-C(10)-C(5)	54.90(16)
C(2)-C(1)-C(10)-C(9)	171.50(12)
C(6)-C(5)-C(10)-C(18)	-62.88(16)
C(4)-C(5)-C(10)-C(18)	65.38(16)
C(6)-C(5)-C(10)-C(1)	177.09(12)
C(4)-C(5)-C(10)-C(1)	-54.65(15)
C(6)-C(5)-C(10)-C(9)	58.89(15)
C(4)-C(5)-C(10)-C(9)	-172.85(12)
C(11)-C(9)-C(10)-C(18)	-63.32(16)
C(8)-C(9)-C(10)-C(18)	65.20(15)
C(11)-C(9)-C(10)-C(1)	57.55(16)
C(8)-C(9)-C(10)-C(1)	-173.93(12)
C(11)-C(9)-C(10)-C(5)	174.19(12)
C(8)-C(9)-C(10)-C(5)	-57.29(15)
C(8)-C(9)-C(11)-C(12)	53.58(16)
C(10)-C(9)-C(11)-C(12)	-177.39(12)
C(9)-C(11)-C(12)-C(13)	-55.03(17)
C(11)-C(12)-C(13)-C(17)	167.40(13)
C(11)-C(12)-C(13)-C(14)	55.27(16)

C(11)-C(12)-C(13)-C(19)	-69.04(16)
C(7)-C(8)-C(14)-C(15)	-56.08(17)
C(9)-C(8)-C(14)-C(15)	-178.89(13)
C(7)-C(8)-C(14)-C(13)	-179.60(12)
C(9)-C(8)-C(14)-C(13)	57.58(15)
C(12)-C(13)-C(14)-C(15)	169.46(12)
C(17)-C(13)-C(14)-C(15)	46.96(14)
C(19)-C(13)-C(14)-C(15)	-67.90(15)
C(12)-C(13)-C(14)-C(8)	-58.93(15)
C(17)-C(13)-C(14)-C(8)	178.57(12)
C(19)-C(13)-C(14)-C(8)	63.70(16)
C(8)-C(14)-C(15)-C(16)	-164.31(13)
C(13)-C(14)-C(15)-C(16)	-35.81(15)
C(14)-C(15)-C(16)-C(17)	10.78(17)
C(12)-C(13)-C(17)-C(16)	-156.05(14)
C(14)-C(13)-C(17)-C(16)	-39.35(15)
C(19)-C(13)-C(17)-C(16)	79.25(15)
C(15)-C(16)-C(17)-C(13)	18.08(17)
C(29)-C(20)-C(21)-C(22)	-55.67(16)
C(20)-C(21)-C(22)-C(23)	53.82(17)
C(21)-C(22)-C(23)-C(24)	-54.47(17)
C(22)-C(23)-C(24)-C(25)	-175.05(12)
C(22)-C(23)-C(24)-C(29)	56.80(16)
C(23)-C(24)-C(25)-C(26)	173.76(12)
C(29)-C(24)-C(25)-C(26)	-57.82(15)
C(24)-C(25)-C(26)-C(27)	55.59(16)
C(25)-C(26)-C(27)-C(33)	-176.90(12)
C(25)-C(26)-C(27)-C(28)	-54.66(15)
C(33)-C(27)-C(28)-C(30)	-51.06(15)
C(26)-C(27)-C(28)-C(30)	-174.63(11)
C(33)-C(27)-C(28)-C(29)	179.79(11)
C(26)-C(27)-C(28)-C(29)	56.23(15)
C(21)-C(20)-C(29)-C(37)	-66.37(15)
C(21)-C(20)-C(29)-C(24)	54.86(15)
C(21)-C(20)-C(29)-C(28)	171.98(11)
C(25)-C(24)-C(29)-C(37)	-64.15(15)

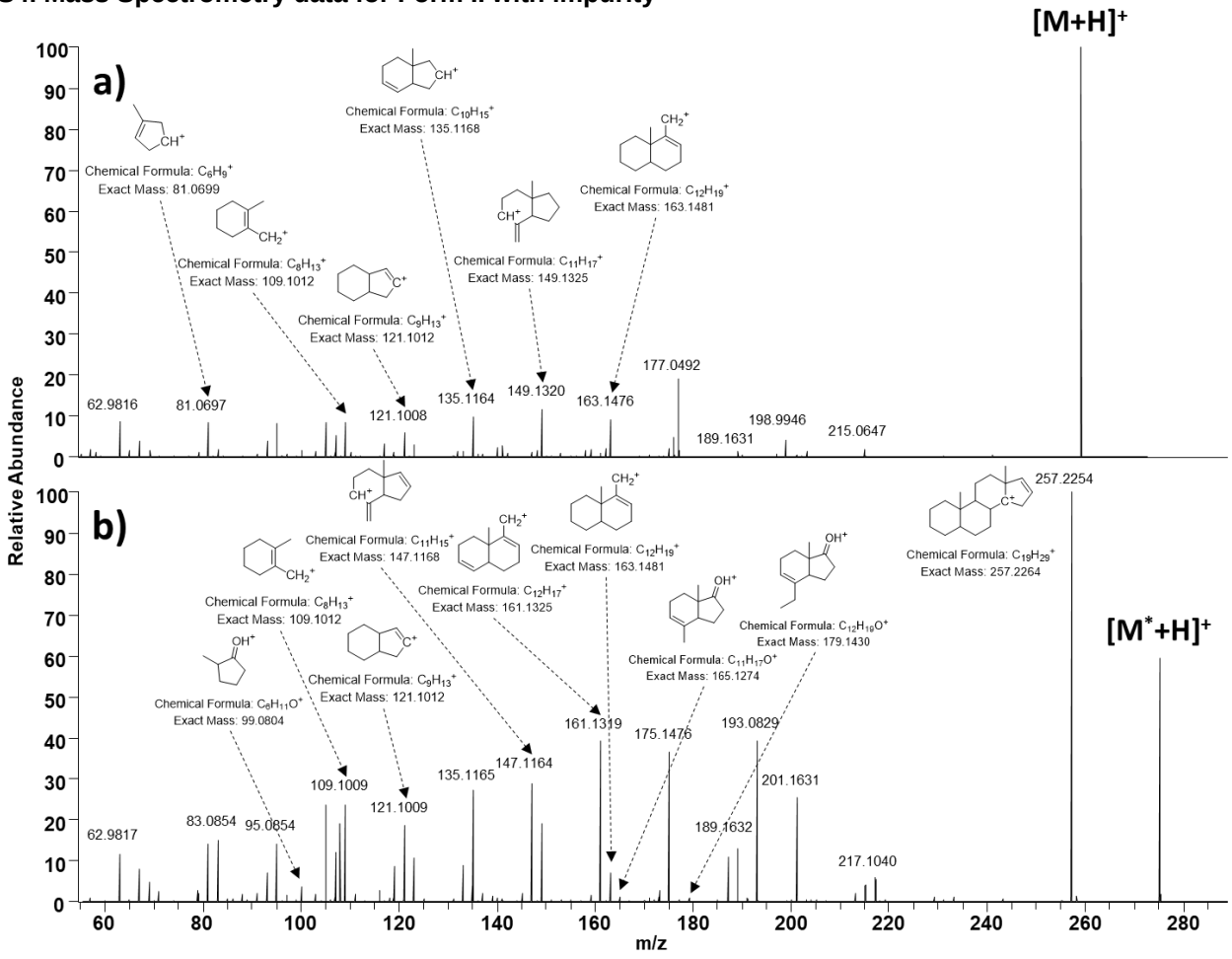
C(23)-C(24)-C(29)-C(37)	64.23(15)
C(25)-C(24)-C(29)-C(20)	176.21(11)
C(23)-C(24)-C(29)-C(20)	-55.41(14)
C(25)-C(24)-C(29)-C(28)	57.56(14)
C(23)-C(24)-C(29)-C(28)	-174.06(11)
C(30)-C(28)-C(29)-C(37)	-62.42(14)
C(27)-C(28)-C(29)-C(37)	65.59(14)
C(30)-C(28)-C(29)-C(20)	58.20(14)
C(27)-C(28)-C(29)-C(20)	-173.80(11)
C(30)-C(28)-C(29)-C(24)	175.38(11)
C(27)-C(28)-C(29)-C(24)	-56.61(14)
C(27)-C(28)-C(30)-C(31)	51.40(15)
C(29)-C(28)-C(30)-C(31)	179.54(11)
C(28)-C(30)-C(31)-C(32)	-54.78(16)
C(30)-C(31)-C(32)-C(36)	168.07(12)
C(30)-C(31)-C(32)-C(38)	-67.60(15)
C(30)-C(31)-C(32)-C(33)	56.69(15)
C(26)-C(27)-C(33)-C(34)	-56.81(17)
C(28)-C(27)-C(33)-C(34)	-179.67(12)
C(26)-C(27)-C(33)-C(32)	-179.85(11)
C(28)-C(27)-C(33)-C(32)	57.30(15)
C(31)-C(32)-C(33)-C(27)	-60.18(15)
C(36)-C(32)-C(33)-C(27)	178.42(12)
C(38)-C(32)-C(33)-C(27)	62.53(16)
C(31)-C(32)-C(33)-C(34)	168.44(11)
C(36)-C(32)-C(33)-C(34)	47.04(14)
C(38)-C(32)-C(33)-C(34)	-68.85(15)
C(27)-C(33)-C(34)-C(35)	-163.47(13)
C(32)-C(33)-C(34)-C(35)	-35.51(16)
C(33)-C(34)-C(35)-C(36)	10.22(17)
C(31)-C(32)-C(36)-C(35)	-155.81(13)
C(38)-C(32)-C(36)-C(35)	79.03(15)
C(33)-C(32)-C(36)-C(35)	-39.98(14)
C(34)-C(35)-C(36)-C(32)	18.76(16)
C(48)-C(39)-C(40)-C(41)	-56.35(17)
C(39)-C(40)-C(41)-C(42)	56.13(17)

C(40)-C(41)-C(42)-C(43)	-56.52(16)
C(41)-C(42)-C(43)-C(44)	-175.54(12)
C(41)-C(42)-C(43)-C(48)	56.75(16)
C(42)-C(43)-C(44)-C(45)	172.12(12)
C(48)-C(43)-C(44)-C(45)	-59.33(15)
C(43)-C(44)-C(45)-C(46)	54.40(16)
C(44)-C(45)-C(46)-C(52)	-172.49(12)
C(44)-C(45)-C(46)-C(47)	-51.53(15)
C(52)-C(46)-C(47)-C(49)	-53.94(14)
C(45)-C(46)-C(47)-C(49)	-176.65(11)
C(52)-C(46)-C(47)-C(48)	176.55(11)
C(45)-C(46)-C(47)-C(48)	53.84(14)
C(40)-C(39)-C(48)-C(56)	-68.22(15)
C(40)-C(39)-C(48)-C(47)	170.12(12)
C(40)-C(39)-C(48)-C(43)	53.40(15)
C(49)-C(47)-C(48)-C(56)	-62.46(16)
C(46)-C(47)-C(48)-C(56)	65.73(14)
C(49)-C(47)-C(48)-C(39)	57.93(16)
C(46)-C(47)-C(48)-C(39)	-173.88(11)
C(49)-C(47)-C(48)-C(43)	175.10(12)
C(46)-C(47)-C(48)-C(43)	-56.71(14)
C(44)-C(43)-C(48)-C(56)	-62.14(15)
C(42)-C(43)-C(48)-C(56)	66.10(15)
C(44)-C(43)-C(48)-C(39)	178.21(11)
C(42)-C(43)-C(48)-C(39)	-53.55(15)
C(44)-C(43)-C(48)-C(47)	59.65(14)
C(42)-C(43)-C(48)-C(47)	-172.11(12)
C(46)-C(47)-C(49)-C(50)	54.01(17)
C(48)-C(47)-C(49)-C(50)	-177.28(13)
C(47)-C(49)-C(50)-C(51)	-55.13(18)
C(49)-C(50)-C(51)-C(55)	167.09(13)
C(49)-C(50)-C(51)-C(57)	-68.62(16)
C(49)-C(50)-C(51)-C(52)	55.73(16)
C(45)-C(46)-C(52)-C(53)	-54.84(17)
C(47)-C(46)-C(52)-C(53)	-177.68(12)
C(45)-C(46)-C(52)-C(51)	-178.77(13)

C(47)-C(46)-C(52)-C(51)	58.39(16)
C(50)-C(51)-C(52)-C(46)	-59.64(16)
C(55)-C(51)-C(52)-C(46)	178.74(14)
C(57)-C(51)-C(52)-C(46)	63.29(18)
C(50)-C(51)-C(52)-C(53)	168.33(12)
C(55)-C(51)-C(52)-C(53)	46.71(16)
C(57)-C(51)-C(52)-C(53)	-68.74(16)
C(46)-C(52)-C(53)-C(54)	-163.51(13)
C(51)-C(52)-C(53)-C(54)	-34.98(15)
C(52)-C(53)-C(54)-C(55)	9.59(17)
C(50)-C(51)-C(55)-C(54)	-156.18(14)
C(57)-C(51)-C(55)-C(54)	78.58(16)
C(52)-C(51)-C(55)-C(54)	-40.00(17)
C(53)-C(54)-C(55)-C(51)	19.21(18)

Symmetry transformations used to generate equivalent atoms:

S4. Mass Spectrometry data for Form II with impurity



Supplemental Figure S4.1: Collisional fragmentation spectra of **a)** protonated 5α-14α-androstane at *m/z* 259.2421 (Δ*m/z* = 0.39 ppm, labeled as $[M+H]^+$) and **b)** protonated 5α-14α-androstan-17-one at *m/z* 275.2373 (Δ*m/z* = 1.45 ppm, labeled as $[M^*+H]^+$). Select fragment ions are identified with chemical formulae and theoretical exact mass values. A complete list of identified fragment ions and associated mass errors are given in **Supplemental Table S4.1 and S4.2**.

Supplemental Table S4.1: Identified fragment ions for the protonated 5α-14α-androstane (*m/z* 259.2421) via collisional activation.

Experimental *m/z*	Theoretical *m/z*	Molecular Formula	Δ*m/z* (ppm)
203.1787	203.1794	$C_{15}H_{23}^{+}$	-3.45
163.1476	163.1481	$C_{12}H_{19}^{+}$	-3.06
149.1320	149.1325	$C_{11}H_{17}^{+}$	-3.35
135.1164	135.1168	$C_{10}H_{15}^{+}$	-2.96
121.1008	121.1012	$C_{9}H_{13}^{+}$	-3.30
109.1009	109.1012	$C_{8}H_{13}^{+}$	-2.75
95.0853	95.0855	$C_{7}H_{11}^{+}$	-2.10
81.0697	81.0699	$C_{6}H_{9}^{+}$	-2.47

Supplemental Table S4.2: Identified fragment ions for the protonated 5α-14α-androstan-17-one (*m/z* 275.2373) via collisional activation.

Experimental *m/z*	Theoretical *m/z*	Molecular Formula	Δ*m/z* (ppm)
257.2254	257.2264	$C_{19}H_{29}^{+}$	-3.89
179.1426	179.1430	$C_{12}H_{19}O^{+}$	-2.23
165.1270	165.1274	$C_{11}H_{17}O^{+}$	-2.42
163.1477	163.1481	$C_{12}H_{19}^{+}$	-2.45
161.1319	161.1325	$C_{12}H_{17}^{+}$	-3.72
151.1113	151.1117	$C_{10}H_{15}O^{+}$	-2.65
147.1164	147.1168	$C_{11}H_{15}^{+}$	-2.72
135.1165	135.1168	$C_{10}H_{15}^{+}$	-2.22
121.1009	121.1012	$C_{9}H_{13}^{+}$	-2.48
109.1009	109.1012	$C_{8}H_{13}^{+}$	-2.75
99.0803	99.0804	$C_{6}H_{11}O^{+}$	-1.01
95.0854	95.0855	$C_{7}H_{11}^{+}$	-1.05