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Supporting Information

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Investigations on the Polymorphism of Triamcinolonacetonide

by

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- Crystal structure analysis of form **I**

- Crystal structure analysis of form **II**

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- Powder pattern of crystallized and micronized batches of sterilized triamcinolone acetonide

- Powder pattern of crystallized and micronized batches of sterilized triamcinolone acetonide

- Experimental powder pattern of the residue obtained by stirring crystalline suspensions of triamcinoloneacetonide in acetone and ethanol and calculated powder pattern for form **I** and **II**

- Experimental powder pattern of the residue obtained at 250°C in the DSC measurement and calculated powder pattern for the tetragonal form **II**

- Experimental powder pattern of crystal suspensions stirred in ethanol, after adding some drops of water and calculated powder pattern for the trigonal form **I**

- Experimental powder pattern of form I evacuated at 50°C and 10 mbar and calculated pattern for the tetragonal form II.

- Results of the thermomicroscopic investigations

Table 1. Crystal data and structure refinement for triamcinolonacetonide-hydrate (form **I**).

Identification code	hpp1ctt	
Empirical formula	$C_{24}H_{31.82}FO_{6.41}$	
Formula weight	441.87	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	trigonal	
Space group	R3	
Unit cell dimensions	a = 17.6840(9) Å	α= 90°.
	b = 17.6840(9) Å	β= 90°.
	c = 18.1428(9) Å	γ = 120°.
Volume	4913.6(4) $Å^3$	
Z	9	
Density (calculated)	1.344 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	2125	
Crystal size	0.5 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.61 to 28.01°.	
Index ranges	-23<=h<=19, -23<=k<=23, -18<=l<=23	
Reflections collected	9159	
Independent reflections	2628 [R(int) = 0.0299]	
Completeness to theta = 28.01°	99.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2628 / 1 / 289	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0807	
R indices (all data)	R1 = 0.0336, wR2 = 0.0822	
Absolute structure parameter	0.3(6)	
Extinction coefficient	0.0055(8)	
Largest diff. peak and hole	0.224 and -0.201 $e.Å^{-3}$	

Comments:
All non-hydrogen atoms were refined anisotropic. The C-H hydrogen atoms were positioned with idealized geometry and refind using a riding model. The O-H-hydrogen atom were located in difference map but were positioned with idealized geometry allowed to rotate but not tip. The absolute structure cannot be determined. Therefore, friedel opposites were merged in the refinement. The water positions are not fully occupied. Therefore, the s.o.f. was refined.

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

	x	y	z	U(eq)
O(1)	10714(1)	2418(1)	5323(1)	26(1)
O(2)	6572(1)	-1161(1)	6115(1)	26(1)
O(3)	4974(1)	327(1)	5007(1)	18(1)
O(4)	5089(1)	1419(1)	5732(1)	27(1)
O(5)	3329(1)	-990(1)	6223(1)	26(1)
O(6)	2763(1)	-2219(1)	5198(1)	37(1)
C(1)	10007(1)	1870(1)	5590(1)	18(1)
C(2)	9501(1)	999(1)	5270(1)	19(1)
C(3)	8731(1)	409(1)	5553(1)	17(1)
C(4)	8322(1)	564(1)	6219(1)	13(1)
C(5)	7405(1)	436(1)	5998(1)	13(1)
C(6)	6764(1)	-452(1)	5634(1)	16(1)
C(7)	5910(1)	-497(1)	5388(1)	15(1)
C(8)	5480(1)	-250(1)	6002(1)	14(1)
C(9)	4760(1)	-45(1)	5728(1)	15(1)
C(10)	4854(1)	710(1)	6233(1)	19(1)
C(11)	5625(1)	948(1)	6746(1)	19(1)
C(12)	6160(1)	660(1)	6287(1)	14(1)
C(13)	6978(1)	699(1)	6610(1)	14(1)
C(14)	7602(1)	1619(1)	6905(1)	17(1)
C(15)	8475(1)	1716(1)	7152(1)	19(1)
C(16)	8868(1)	1484(1)	6523(1)	15(1)
C(17)	9647(1)	2057(1)	6239(1)	18(1)
C(18)	8272(1)	-78(1)	6828(1)	20(1)
C(19)	5098(1)	-942(1)	6615(1)	20(1)
C(20)	4886(1)	1088(1)	5000(1)	21(1)
C(21)	5569(2)	1744(2)	4481(1)	33(1)
C(22)	3960(1)	849(2)	4794(1)	28(1)
C(23)	3841(1)	-841(1)	5725(1)	18(1)
C(24)	3574(1)	-1461(2)	5078(1)	32(1)
F(1)	7607(1)	1043(1)	5409(1)	16(1)
O(10)	6667	3333	6445(9)	163(10)
O(11)	3333	-3333	5752(6)	76(4)

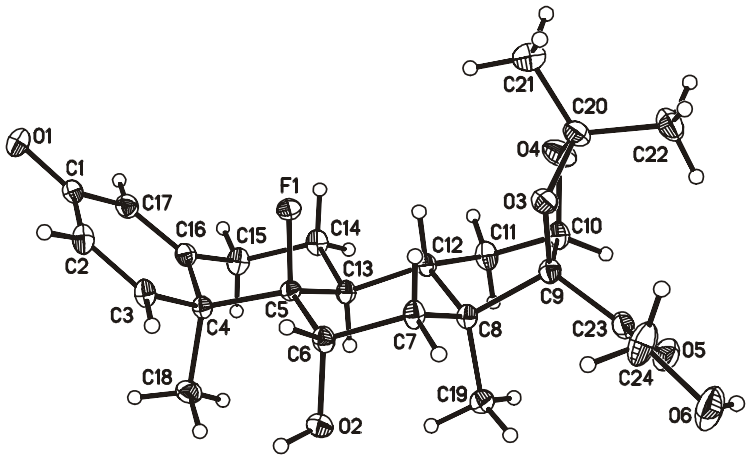


Table 3. Bond lengths [Å] and angles [°].

O(1)-C(1)	1.236(2)	C(6)-C(7)	1.538(2)
O(2)-C(6)	1.421(2)	C(7)-C(8)	1.530(2)
O(3)-C(9)	1.428(2)	C(8)-C(19)	1.538(2)
O(3)-C(20)	1.430(2)	C(8)-C(12)	1.539(2)
O(4)-C(20)	1.423(2)	C(8)-C(9)	1.568(2)
O(4)-C(10)	1.431(2)	C(9)-C(23)	1.527(2)
O(5)-C(23)	1.212(2)	C(9)-C(10)	1.558(2)
O(6)-C(24)	1.407(3)	C(10)-C(11)	1.526(2)
C(1)-C(17)	1.452(3)	C(11)-C(12)	1.525(2)
C(1)-C(2)	1.460(3)	C(12)-C(13)	1.530(2)
C(2)-C(3)	1.337(2)	C(13)-C(14)	1.534(2)
C(3)-C(4)	1.503(2)	C(14)-C(15)	1.534(2)
C(4)-C(16)	1.520(2)	C(15)-C(16)	1.496(2)
C(4)-C(18)	1.554(2)	C(16)-C(17)	1.340(2)
C(4)-C(5)	1.573(2)	C(20)-C(21)	1.513(3)
C(5)-F(1)	1.427(2)	C(20)-C(22)	1.519(3)
C(5)-C(13)	1.540(2)	C(23)-C(24)	1.511(3)
C(5)-C(6)	1.552(2)		
C(9)-O(3)-C(20)	108.29(13)		
C(20)-O(4)-C(10)	109.21(14)	C(23)-C(9)-C(10)	113.65(14)
O(1)-C(1)-C(17)	121.74(17)	O(3)-C(9)-C(8)	109.71(14)
O(1)-C(1)-C(2)	121.10(18)	C(23)-C(9)-C(8)	113.63(14)
C(17)-C(1)-C(2)	117.15(15)	C(10)-C(9)-C(8)	105.14(14)
C(3)-C(2)-C(1)	121.16(17)	O(4)-C(10)-C(11)	108.49(15)
C(2)-C(3)-C(4)	124.22(16)	O(4)-C(10)-C(9)	103.76(14)
C(3)-C(4)-C(16)	112.36(14)	C(11)-C(10)-C(9)	106.98(14)
C(3)-C(4)-C(18)	107.14(14)	C(12)-C(11)-C(10)	101.14(14)
C(16)-C(4)-C(18)	107.33(14)	C(11)-C(12)-C(13)	120.39(14)
C(3)-C(4)-C(5)	108.87(14)	C(11)-C(12)-C(8)	103.99(13)
C(16)-C(4)-C(5)	107.71(13)	C(13)-C(12)-C(8)	113.72(13)
C(18)-C(4)-C(5)	113.51(13)	C(12)-C(13)-C(14)	110.07(14)
F(1)-C(5)-C(13)	106.74(13)	C(12)-C(13)-C(5)	107.79(13)
F(1)-C(5)-C(6)	103.02(13)	C(14)-C(13)-C(5)	111.73(13)
C(13)-C(5)-C(6)	113.03(13)	C(15)-C(14)-C(13)	111.79(14)
F(1)-C(5)-C(4)	103.40(12)	C(16)-C(15)-C(14)	108.97(14)
C(13)-C(5)-C(4)	113.43(13)	C(17)-C(16)-C(15)	121.87(16)
C(6)-C(5)-C(4)	115.68(13)	C(17)-C(16)-C(4)	122.24(16)
O(2)-C(6)-C(7)	109.74(14)	C(15)-C(16)-C(4)	115.88(15)
O(2)-C(6)-C(5)	111.31(14)	C(16)-C(17)-C(1)	122.74(17)
C(7)-C(6)-C(5)	112.18(13)	O(4)-C(20)-O(3)	104.74(14)
C(8)-C(7)-C(6)	112.89(14)	O(4)-C(20)-C(21)	108.94(17)
C(7)-C(8)-C(19)	112.41(14)	O(3)-C(20)-C(21)	107.83(16)
C(7)-C(8)-C(12)	107.67(13)	O(4)-C(20)-C(22)	111.10(17)
C(19)-C(8)-C(12)	113.07(14)	O(3)-C(20)-C(22)	110.47(16)
C(7)-C(8)-C(9)	114.40(14)	C(21)-C(20)-C(22)	113.35(17)
C(19)-C(8)-C(9)	109.18(14)	O(5)-C(23)-C(24)	119.50(18)
C(12)-C(8)-C(9)	99.49(13)	O(5)-C(23)-C(9)	122.17(18)
O(3)-C(9)-C(23)	109.59(14)	C(24)-C(23)-C(9)	118.33(16)
O(3)-C(9)-C(10)	104.67(14)	O(6)-C(24)-C(23)	111.80(19)

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	16(1)	25(1)	34(1)	7(1)	7(1)	8(1)
O(2)	20(1)	15(1)	45(1)	6(1)	2(1)	10(1)
O(3)	20(1)	21(1)	15(1)	2(1)	2(1)	13(1)
O(4)	39(1)	22(1)	26(1)	-3(1)	-6(1)	20(1)
O(5)	18(1)	31(1)	27(1)	3(1)	5(1)	10(1)
O(6)	17(1)	30(1)	53(1)	-12(1)	-5(1)	4(1)
C(1)	13(1)	19(1)	22(1)	4(1)	-1(1)	9(1)
C(2)	15(1)	25(1)	17(1)	-2(1)	0(1)	12(1)
C(3)	13(1)	20(1)	19(1)	-3(1)	-2(1)	9(1)
C(4)	12(1)	14(1)	15(1)	-1(1)	-1(1)	7(1)
C(5)	12(1)	13(1)	13(1)	2(1)	1(1)	6(1)
C(6)	15(1)	15(1)	20(1)	-4(1)	-1(1)	9(1)
C(7)	13(1)	17(1)	17(1)	-6(1)	-3(1)	8(1)
C(8)	12(1)	15(1)	15(1)	-2(1)	-1(1)	7(1)
C(9)	14(1)	18(1)	13(1)	0(1)	0(1)	9(1)
C(10)	17(1)	23(1)	20(1)	-2(1)	2(1)	12(1)
C(11)	19(1)	24(1)	17(1)	-6(1)	-1(1)	14(1)
C(12)	13(1)	15(1)	13(1)	-2(1)	-1(1)	8(1)
C(13)	12(1)	15(1)	13(1)	-2(1)	-1(1)	7(1)
C(14)	16(1)	19(1)	17(1)	-5(1)	-2(1)	9(1)
C(15)	17(1)	21(1)	17(1)	-6(1)	-3(1)	8(1)
C(16)	14(1)	17(1)	13(1)	-1(1)	-4(1)	8(1)
C(17)	15(1)	17(1)	22(1)	-1(1)	-3(1)	8(1)
C(18)	20(1)	19(1)	22(1)	4(1)	-4(1)	10(1)
C(19)	17(1)	21(1)	22(1)	5(1)	1(1)	8(1)
C(20)	23(1)	22(1)	23(1)	3(1)	-1(1)	15(1)
C(21)	29(1)	28(1)	39(1)	12(1)	5(1)	13(1)
C(22)	26(1)	42(1)	25(1)	6(1)	2(1)	24(1)
C(23)	15(1)	23(1)	19(1)	2(1)	-1(1)	11(1)
C(24)	18(1)	34(1)	33(1)	-11(1)	-4(1)	4(1)
F(1)	17(1)	18(1)	14(1)	4(1)	2(1)	9(1)
O(10)	185(12)	185(12)	119(13)	0	0	92(6)
O(11)	56(4)	56(4)	116(9)	0	0	28(2)

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

	x	y	z	U(eq)
H(1O2)	6828	-1416	5918	39
H(1O6)	2508	-2059	5514	55
H(2)	9724	849	4852	22
H(3)	8422	-144	5318	20
H(6)	7054	-519	5186	19
H(7A)	6035	-98	4965	18
H(7B)	5496	-1098	5219	18
H(10)	4305	551	6509	23
H(11A)	5956	1583	6848	23
H(11B)	5434	624	7217	23
H(12)	6361	1050	5845	16
H(13)	6803	271	7024	16
H(14A)	7709	2052	6514	21
H(14B)	7325	1741	7327	21
H(15A)	8876	2325	7309	23
H(15B)	8381	1326	7576	23
H(17)	9979	2609	6472	21
H(18A)	8006	4	7273	30
H(18B)	8862	38	6943	30
H(18C)	7916	-680	6652	30
H(19A)	4666	-1504	6403	30
H(19B)	4818	-764	6987	30
H(19C)	5569	-1000	6844	30
H(21A)	5438	1517	3976	49
H(21B)	6146	1843	4625	49
H(21C)	5566	2296	4507	49
H(22A)	3838	627	4287	42
H(22B)	3898	1369	4829	42
H(22C)	3547	399	5131	42
H(24A)	3539	-1162	4630	39
H(24B)	4025	-1628	4994	39

Table 1. Crystal data and structure refinement for triamcinolonacetonide (form **II**).

Identification code	form2	
Empirical formula	$C_{24}H_{31}FO_6$	
Formula weight	434.49	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	tetragonal	
Space group	$P4_12_12$	
Unit cell dimensions	a = 9.1692(4) Å	α= 90°.
	b = 9.1692(4) Å	β= 90°.
	c = 49.946(4) Å	γ = 90°.
Volume	4199.1(4) $Å^3$	
Z	8	
Density (calculated)	1.375 Mg/m^3	
Absorption coefficient	0.103 mm^{-1}	
F(000)	1856	
Crystal size	0.25 x 0.25 x 0.08 mm^3	
Theta range for data collection	2.26 to 25.62°.	
Index ranges	-11<=h<=10, -11<=k<=11, -50<=l<=60	
Reflections collected	24250	
Independent reflections	2418 [R(int) = 0.1099]	
Completeness to theta = 25.62°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2418 / 0 / 287	
Goodness-of-fit on F^2	0.834	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0641	
R indices (all data)	R1 = 0.0647, wR2 = 0.0698	
Absolute structure parameter	0.4(11)	
Extinction coefficient	0.0116(7)	
Largest diff. peak and hole	0.153 and -0.146 $e.Å^{-3}$	

Comments:
All non-hydrogen atoms were refined anisotropic. The C-H hydrogen atoms were positioned with idealized geometry and refind using a riding model. The O-H-hydrogen atom were located in difference map but were positioned with idealized geometry allowed to rotate but not tip. The absolute structure cannot be determined. Therefore, friedel opposites were merged in the refinement.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for form2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	12046(2)	-281(2)	622(1)	40(1)
O(2)	10774(2)	7066(2)	446(1)	37(1)
O(3)	5984(2)	7238(2)	1017(1)	32(1)
O(4)	4098(2)	6155(2)	804(1)	42(1)
O(5)	5403(2)	10182(2)	575(1)	46(1)
O(6)	6139(4)	11777(2)	994(1)	76(1)
C(1)	11706(3)	950(3)	538(1)	33(1)
C(2)	12430(3)	2284(3)	633(1)	34(1)
C(3)	11966(3)	3597(3)	559(1)	34(1)
C(4)	10722(3)	3867(3)	369(1)	30(1)
C(5)	9512(3)	4794(3)	516(1)	28(1)
C(6)	10044(3)	6241(3)	648(1)	31(1)
C(7)	8802(3)	7108(3)	783(1)	30(1)
C(8)	7452(3)	7295(3)	604(1)	29(1)
C(9)	6038(3)	7829(3)	751(1)	30(1)
C(10)	4764(3)	7052(3)	601(1)	34(1)
C(11)	5450(3)	6035(3)	393(1)	35(1)
C(12)	6963(3)	5772(3)	512(1)	30(1)
C(13)	8113(3)	4967(3)	347(1)	30(1)
C(14)	7546(3)	3494(3)	249(1)	35(1)
C(15)	8705(3)	2624(3)	99(1)	38(1)
C(16)	10014(3)	2460(3)	274(1)	31(1)
C(17)	10532(3)	1154(3)	346(1)	33(1)
C(18)	11365(3)	4631(3)	119(1)	39(1)
C(19)	7759(3)	8332(3)	369(1)	35(1)
C(20)	4540(3)	6681(3)	1060(1)	36(1)
C(21)	4651(3)	5415(4)	1251(1)	52(1)
C(22)	3502(3)	7859(4)	1156(1)	44(1)
C(23)	5871(3)	9491(3)	763(1)	37(1)
C(24)	6383(4)	10265(3)	1010(1)	50(1)
F(1)	9113(2)	3919(2)	741(1)	33(1)

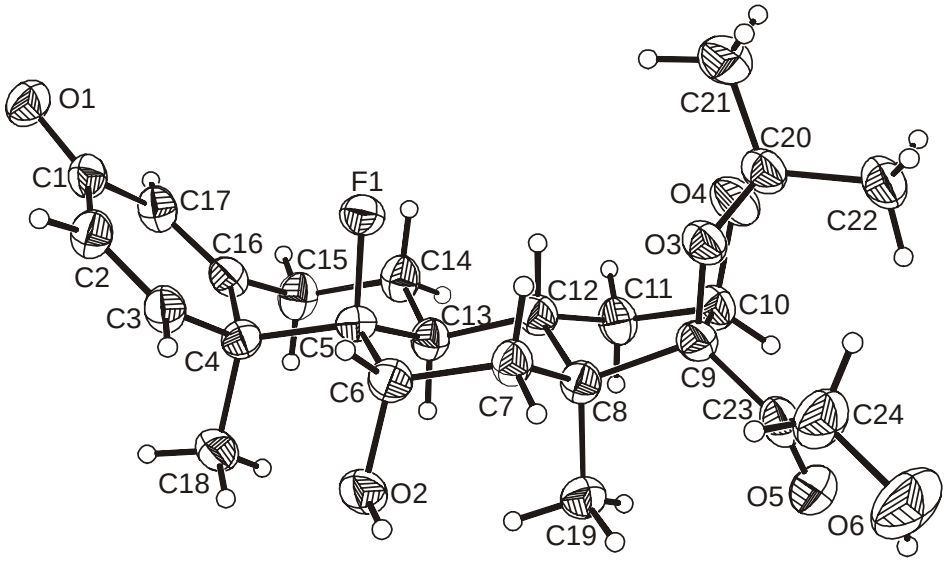

O1
C1
C17
C2
C3
C4
C16
C15
F1
C14
C5
C6
C13
C12
C11
C10
C9
C7
C8
C18
O2
C19
C21
C20
O4
O3
C22
C23
C24
O5
O6

Table 3. Bond lengths [Å] and angles [°] for form2.

O(1)-C(1)	1.243(3)	C(6)-C(7)	1.543(4)
O(2)-C(6)	1.428(3)	C(7)-C(8)	1.536(4)
O(3)-C(9)	1.435(3)	C(8)-C(12)	1.538(4)
O(3)-C(20)	1.436(3)	C(8)-C(19)	1.538(4)
O(4)-C(20)	1.429(4)	C(8)-C(9)	1.568(4)
O(4)-C(10)	1.440(3)	C(9)-C(23)	1.533(4)
O(5)-C(23)	1.212(3)	C(9)-C(10)	1.560(4)
O(6)-C(24)	1.406(3)	C(10)-C(11)	1.529(4)
C(1)-C(17)	1.454(4)	C(11)-C(12)	1.528(4)
C(1)-C(2)	1.469(4)	C(12)-C(13)	1.528(4)
C(2)-C(3)	1.329(4)	C(13)-C(14)	1.527(4)
C(3)-C(4)	1.503(4)	C(14)-C(15)	1.527(4)
C(4)-C(16)	1.520(4)	C(15)-C(16)	1.494(4)
C(4)-C(18)	1.550(4)	C(16)-C(17)	1.338(4)
C(4)-C(5)	1.577(4)	C(20)-C(21)	1.505(4)
C(5)-F(1)	1.430(3)	C(20)-C(22)	1.516(4)
C(5)-C(13)	1.544(4)	C(23)-C(24)	1.499(4)
C(5)-C(6)	1.559(4)		
		O(3)-C(9)-C(10)	104.2(2)
C(9)-O(3)-C(20)	107.9(2)	C(23)-C(9)-C(10)	113.5(2)
C(20)-O(4)-C(10)	108.6(2)	O(3)-C(9)-C(8)	110.1(2)
O(1)-C(1)-C(17)	121.5(3)	C(23)-C(9)-C(8)	114.3(2)
O(1)-C(1)-C(2)	122.4(3)	C(10)-C(9)-C(8)	104.6(2)
C(17)-C(1)-C(2)	116.1(3)	O(4)-C(10)-C(11)	107.6(2)
C(3)-C(2)-C(1)	121.3(3)	O(4)-C(10)-C(9)	103.9(2)
C(2)-C(3)-C(4)	124.6(3)	C(11)-C(10)-C(9)	107.2(2)
C(3)-C(4)-C(16)	112.4(2)	C(12)-C(11)-C(10)	102.0(2)
C(3)-C(4)-C(18)	107.1(2)	C(11)-C(12)-C(13)	119.6(2)
C(16)-C(4)-C(18)	107.1(2)	C(11)-C(12)-C(8)	103.7(2)
C(3)-C(4)-C(5)	109.3(2)	C(13)-C(12)-C(8)	113.5(2)
C(16)-C(4)-C(5)	107.6(2)	C(14)-C(13)-C(12)	111.4(2)
C(18)-C(4)-C(5)	113.4(2)	C(14)-C(13)-C(5)	111.5(2)
F(1)-C(5)-C(13)	105.9(2)	C(12)-C(13)-C(5)	109.1(2)
F(1)-C(5)-C(6)	103.0(2)	C(13)-C(14)-C(15)	112.5(2)
C(13)-C(5)-C(6)	113.8(2)	C(16)-C(15)-C(14)	108.8(2)
F(1)-C(5)-C(4)	104.0(2)	C(17)-C(16)-C(15)	122.2(3)
C(13)-C(5)-C(4)	112.7(2)	C(17)-C(16)-C(4)	121.6(3)
C(6)-C(5)-C(4)	115.8(2)	C(15)-C(16)-C(4)	116.2(2)
O(2)-C(6)-C(7)	112.5(2)	C(16)-C(17)-C(1)	123.7(3)
O(2)-C(6)-C(5)	107.3(2)	O(4)-C(20)-O(3)	104.2(2)
C(7)-C(6)-C(5)	113.1(2)	O(4)-C(20)-C(21)	109.1(2)
C(8)-C(7)-C(6)	113.4(2)	O(3)-C(20)-C(21)	108.0(2)
C(7)-C(8)-C(12)	107.9(2)	O(4)-C(20)-C(22)	110.2(2)
C(7)-C(8)-C(19)	111.5(2)	O(3)-C(20)-C(22)	111.9(2)
C(12)-C(8)-C(19)	112.7(2)	C(21)-C(20)-C(22)	113.1(3)
C(7)-C(8)-C(9)	115.5(2)	O(5)-C(23)-C(24)	120.1(3)
C(12)-C(8)-C(9)	100.5(2)	O(5)-C(23)-C(9)	121.7(3)
C(19)-C(8)-C(9)	108.4(2)	C(24)-C(23)-C(9)	118.1(3)
O(3)-C(9)-C(23)	109.7(2)	O(6)-C(24)-C(23)	111.8(3)

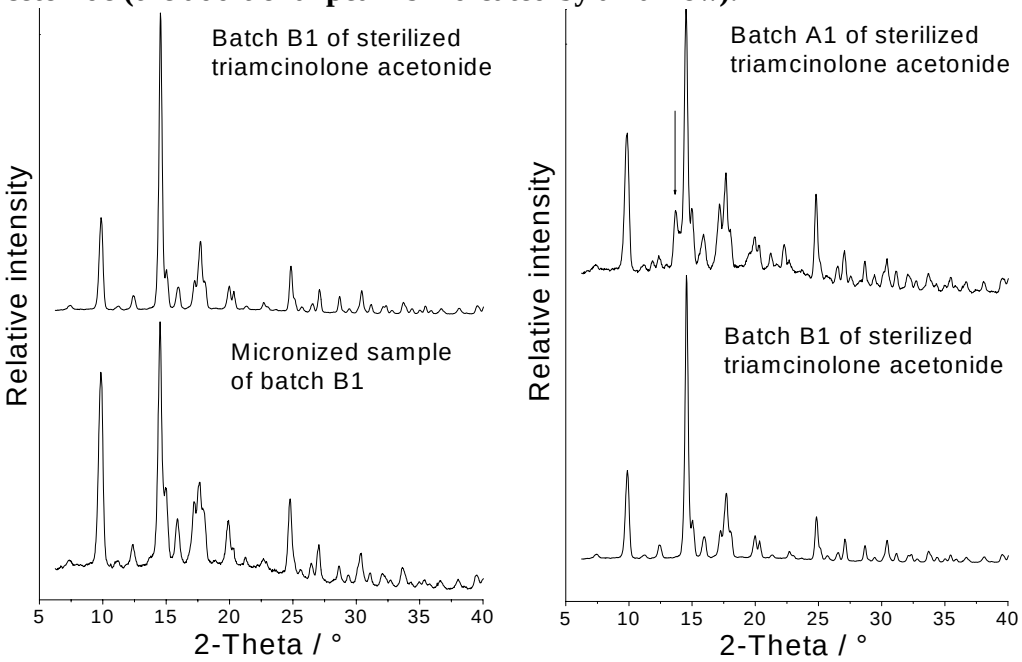
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	41(1)	28(1)	50(1)	2(1)	0(1)	3(1)
O(2)	33(1)	30(1)	48(1)	-3(1)	7(1)	-8(1)
O(3)	25(1)	39(1)	34(1)	2(1)	3(1)	-1(1)
O(4)	33(1)	48(1)	43(1)	-7(1)	6(1)	-12(1)
O(5)	44(1)	40(1)	53(2)	9(1)	2(1)	9(1)
O(6)	113(2)	33(1)	82(2)	-13(1)	-2(2)	2(1)
C(1)	32(2)	29(2)	37(2)	-1(2)	7(1)	4(1)
C(2)	30(2)	31(2)	42(2)	-3(1)	-2(1)	2(1)
C(3)	28(2)	29(2)	45(2)	-5(1)	3(2)	-2(1)
C(4)	29(2)	23(2)	37(2)	-1(1)	2(1)	-1(1)
C(5)	28(2)	25(2)	30(2)	5(1)	2(1)	0(1)
C(6)	29(2)	30(2)	35(2)	0(1)	1(1)	-2(1)
C(7)	26(2)	27(2)	38(2)	-4(1)	1(1)	0(1)
C(8)	25(2)	28(2)	35(2)	-1(1)	-1(1)	-2(1)
C(9)	26(2)	32(2)	31(2)	3(1)	1(1)	-1(1)
C(10)	26(2)	38(2)	39(2)	0(2)	2(1)	0(1)
C(11)	27(2)	40(2)	38(2)	-6(2)	-2(1)	2(1)
C(12)	26(2)	31(2)	33(2)	-1(1)	0(1)	-1(1)
C(13)	27(2)	30(2)	33(2)	-2(1)	-2(1)	1(1)
C(14)	29(2)	35(2)	42(2)	-5(2)	-5(2)	1(1)
C(15)	35(2)	33(2)	45(2)	-8(2)	-6(2)	2(1)
C(16)	29(2)	30(2)	33(2)	-3(1)	5(1)	-4(1)
C(17)	27(2)	31(2)	41(2)	-8(1)	1(1)	-4(1)
C(18)	38(2)	35(2)	45(2)	0(2)	15(2)	1(1)
C(19)	36(2)	29(2)	40(2)	1(1)	1(2)	-2(1)
C(20)	27(2)	42(2)	38(2)	2(2)	5(1)	-3(1)
C(21)	40(2)	55(2)	60(2)	14(2)	12(2)	-2(2)
C(22)	33(2)	55(2)	43(2)	1(2)	8(2)	6(2)
C(23)	25(2)	42(2)	43(2)	-4(2)	6(2)	1(1)
C(24)	59(2)	32(2)	60(2)	-9(2)	0(2)	0(2)
F(1)	31(1)	33(1)	35(1)	5(1)	1(1)	-3(1)

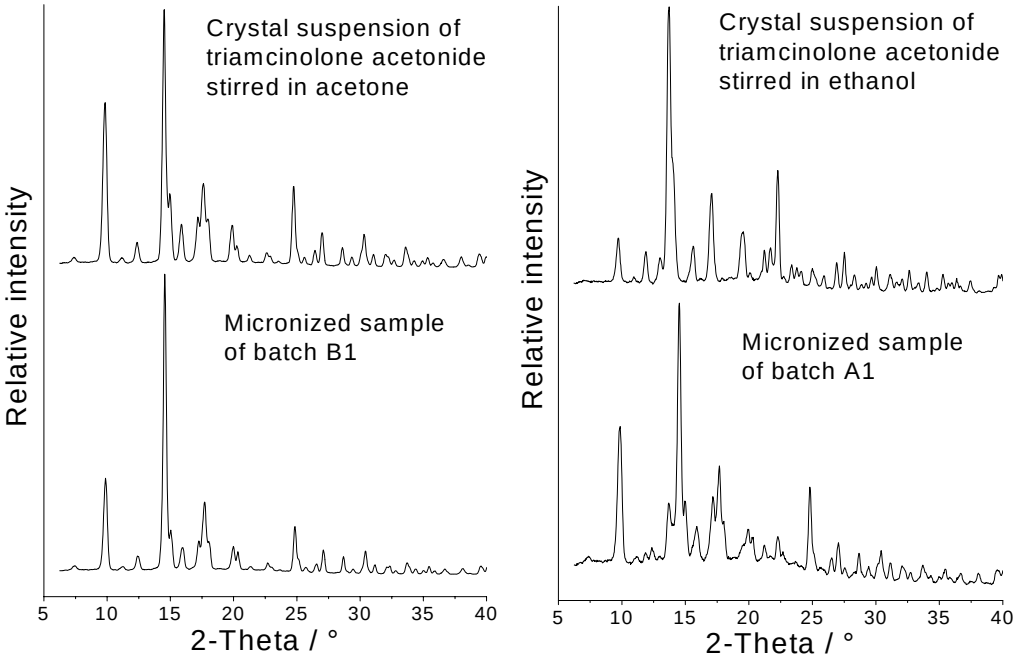
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3).

	x	y	z	U(eq)
H(1O2)	11111	7834	513	56
H(1O6)	5887	11998	838	114
H(2)	13247	2207	749	41
H(3)	12454	4422	631	40
H(6)	10775	5985	789	38
H(7A)	8511	6600	949	37
H(7B)	9173	8084	833	37
H(10)	4061	7757	519	41
H(11A)	4894	5114	377	42
H(11B)	5511	6508	216	42
H(12)	6814	5183	678	36
H(13)	8351	5576	186	36
H(14A)	6699	3654	130	42
H(14B)	7207	2919	405	42
H(15A)	8318	1651	50	45
H(15B)	8976	3138	-68	45
H(17)	10110	311	267	40
H(18A)	10572	5049	12	59
H(18B)	11901	3918	11	59
H(18C)	12029	5410	175	59
H(19A)	6873	8444	261	52
H(19B)	8540	7926	257	52
H(19C)	8060	9286	438	52
H(21A)	5034	5757	1423	77
H(21B)	5309	4678	1177	77
H(21C)	3683	4987	1278	77
H(22A)	3853	8259	1326	66
H(22B)	2529	7440	1182	66
H(22C)	3453	8639	1022	66
H(24A)	5863	9868	1167	60
H(24B)	7439	10082	1035	60

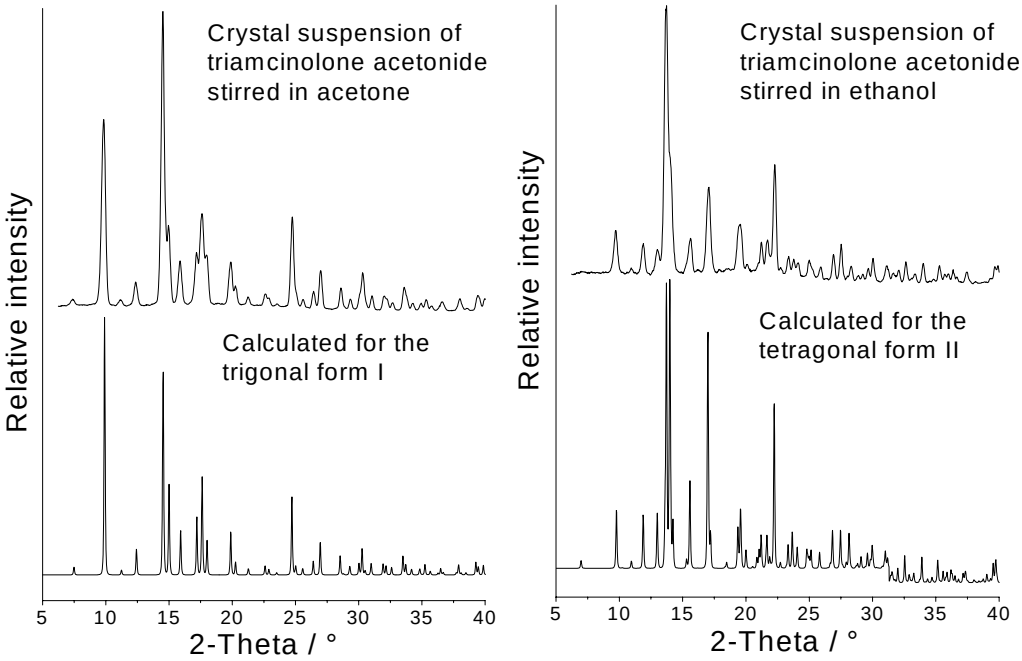
Powder pattern of crystallized and micronized batches of sterilized triamcinolone acetonide (the additional peak is indicated by an arrow).



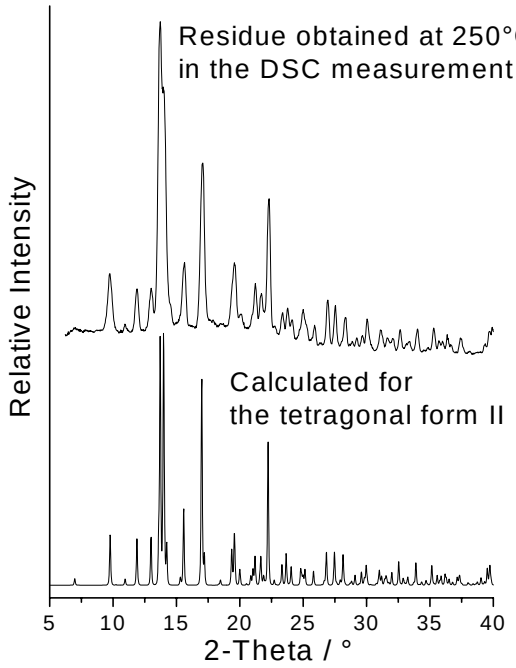
Powder pattern of crystallized and micronized batches of sterilized triamcinolone acetonide (the additional peak is indicated by an arrow).



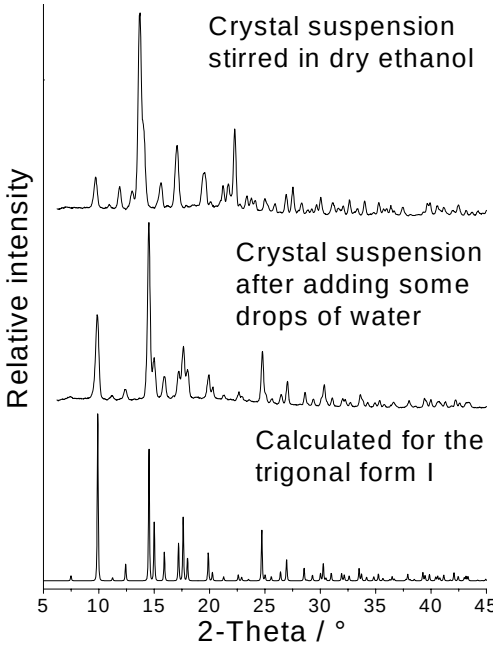
Experimental powder pattern of the residue obtained by stirring crystalline suspensions of triamcinoloneacetonide in acetone and ethanol and calculated powder pattern for form I and II.



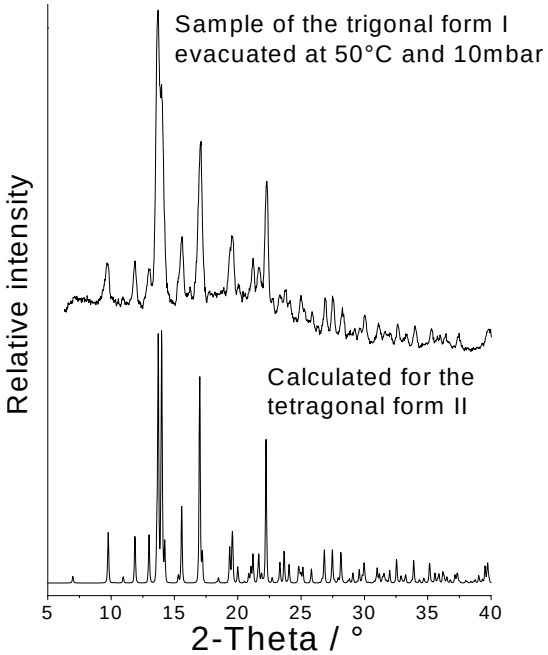
Experimental powder pattern of the residue obtained at 250°C in the DSC measurement and calculated powder pattern for the tetragonal form II.



Experimental powder pattern of crystal suspensions stirred in ethanol, after adding some drops of water and calculated powder pattern for the trigonal form I.



Experimental powder pattern of form I evacuated at 50°C and 10 mbar and calculated pattern for the tetragonal form II.



Results of the thermomicroscopic investigations