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125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800 825 850 875

Crystal data for mo_compound 9_0m: C₂₇H₄₂O₅Si, M = 474.69, a = 15.4436(16)Å, b = 12.5510(13) Å, c = 14.2702(15) Å, $a = 90^{\circ}$, $\beta = 93.048(2)^{\circ}$, $\gamma = 90^{\circ}$, V = 2762.1(5) Å³, T = 100(2) K, space group P21/c, Z = 4, μ (MoK α) = 0.117 mm⁻¹, 29302 reflections measured, 7944 independent reflections ($R_{int} = 0.0453$). The final R_I values were 0.0441 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1100 ($I > 2\sigma(I)$). The final R_I values were 0.0663 (all data). The final $wR(F^2)$ values were 0.1216 (all data). The goodness of fit on F^2 was 1.049.

View of a molecule of compound 9 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

View of the pack drawing of compound 9. Hydrogen-bonds are shown as dashed lines.

	Identification code	mo_compound 9_0m	
	Empirical formula	C27 H42 O5 Si	
	Formula weight	474.69	
	Temperature	100(2) K	
	Wavelength	0.71073 Å	
	Crystal system	Monoclinic	
	Space group	P21/c	
	Unit cell dimensions	a = 15.4436(16) Å	α= 90°.
		b = 12.5510(13) Å	β=
93.(048(2)°.		
		c = 14.2702(15) Å	$\gamma = 90^{\circ}$.
	Volume	2762.1(5) Å ³	
	Z	4	
	Density (calculated)	1.142 Mg/m ³	
	Absorption coefficient	0.117 mm ⁻¹	
	F(000)	1032	
	Crystal size	0.720 x 0.340 x 0.180 mm ³	
	Theta range for data collection	1.320 to 30.739°.	
	Index ranges	-21<=h<=21, -18<=k<=16, -20)<=l<=19
	Reflections collected	29302	
	Independent reflections	7944 [R(int) = 0.0453]	
	Completeness to theta = 25.242°	99.8 %	
	Absorption correction	Semi-empirical from equivalen	its
	Refinement method	Full-matrix least-squares on F ²	
	Data / restraints / parameters	7944 / 0 / 306	
	Goodness-of-fit on F ²	1.049	
	Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.1100	
	R indices (all data)	R1 = 0.0663, wR2 = 0.1216	

Table 1. Crystal data and structure refinement for mo_compound 9_0m.

Extinction coefficient

n/a

Largest diff. peak and hole

0.475 and -0.230 e.Å $^{\text{-3}}$

	х	У	Z	U(eq)	
Si(1)	4257(1)	2361(1)	2185(1)	23(1)	
O(1)	1414(1)	5686(1)	1285(1)	23(1)	
O(2)	3328(1)	2193(1)	1585(1)	22(1)	
O(3)	-515(1)	1284(1)	1555(1)	26(1)	
O(4)	1985(1)	4746(1)	2508(1)	23(1)	
O(5)	1778(1)	3425(1)	-887(1)	32(1)	
C(1)	2900(1)	5920(2)	828(1)	41(1)	
C(2)	2164(1)	6381(1)	1348(1)	31(1)	
C(3)	1416(1)	4882(1)	1913(1)	17(1)	
C(4)	642(1)	4162(1)	1731(1)	15(1)	
C(5)	779(1)	3512(1)	818(1)	15(1)	
C(6)	1671(1)	2971(1)	765(1)	16(1)	
C(7)	1816(1)	1880(1)	1249(1)	16(1)	
C(8)	2547(1)	1908(1)	2010(1)	19(1)	
C(9)	5056(1)	2552(1)	1249(1)	31(1)	
C(10)	4797(1)	3535(2)	658(1)	46(1)	
C(11)	5975(1)	2714(2)	1689(1)	55(1)	
C(12)	5047(1)	1566(2)	612(1)	48(1)	
C(13)	4501(1)	1155(2)	2906(1)	46(1)	
C(14)	2012(1)	1125(1)	457(1)	16(1)	
C(15)	2049(1)	1629(1)	-369(1)	19(1)	

for mo_compound 9_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

 $(Å^2 x \ 10^3)$

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters

C(16)	1841(1)	2752(1)	-269(1)	20(1)
C(17)	27(1)	2706(1)	621(1)	18(1)
C(18)	-325(1)	2219(1)	1496(1)	18(1)
C(19)	-423(1)	2996(1)	2299(1)	17(1)
C(20)	-903(1)	3976(1)	1921(1)	19(1)
C(21)	-1755(1)	4092(1)	1852(1)	24(1)
C(22)	-230(1)	4776(1)	1621(1)	19(1)
C(23)	490(1)	3428(1)	2570(1)	16(1)
C(24)	2095(1)	-51(1)	629(1)	22(1)
C(25)	2611(1)	-619(1)	-107(1)	38(1)
C(26)	1178(1)	-519(1)	656(1)	26(1)
C(27)	4189(1)	3540(2)	2969(1)	39(1)

Si(1)-O(2)	1.6452(10)
Si(1)-C(13)	1.8581(18)
Si(1)-C(27)	1.8607(17)
Si(1)-C(9)	1.8813(15)
O(1)-C(3)	1.3503(15)
O(1)-C(2)	1.4496(16)
O(2)-C(8)	1.4248(14)
O(3)-C(18)	1.2127(16)
O(4)-C(3)	1.2018(15)
O(5)-C(16)	1.2221(16)
C(1)-C(2)	1.506(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5095(17)
C(4)-C(23)	1.5386(16)
C(4)-C(22)	1.5519(17)
C(4)-C(5)	1.5605(16)
C(5)-C(6)	1.5417(17)
C(5)-C(17)	1.5547(17)
C(5)-H(5)	1.0000
C(6)-C(16)	1.5370(16)
C(6)-C(7)	1.5447(17)
C(6)-H(6)	1.0000
C(7)-C(14)	1.5177(16)

Table 3. Bond lengths [Å] and angles [°] for mo_compound 9_0m.

C(7)-C(8)	1.5244(17)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(11)	1.535(2)
C(9)-C(12)	1.535(2)
C(9)-C(10)	1.535(2)
С(10)-Н(10А)	0.9800
С(10)-Н(10В)	0.9800
С(10)-Н(10С)	0.9800
С(11)-Н(11А)	0.9800
С(11)-Н(11В)	0.9800
С(11)-Н(11С)	0.9800
С(12)-Н(12А)	0.9800
С(12)-Н(12В)	0.9800
С(12)-Н(12С)	0.9800
С(13)-Н(13А)	0.9800
С(13)-Н(13В)	0.9800
С(13)-Н(13С)	0.9800
C(14)-C(15)	1.3421(17)
C(14)-C(24)	1.4995(17)
C(15)-C(16)	1.4552(18)
С(15)-Н(15)	0.9500
C(17)-C(18)	1.5181(17)
С(17)-Н(17А)	0.9900
С(17)-Н(17В)	0.9900
C(18)-C(19)	1.5184(17)
C(19)-C(20)	1.5208(18)
C(19)-C(23)	1.5401(17)

C(19)-H(19)	1.0000
C(20)-C(21)	1.3217(18)
C(20)-C(22)	1.5232(17)
C(21)-H(21A)	0.9500
C(21)-H(21B)	0.9500
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.5286(19)
C(24)-C(26)	1.5357(19)
C(24)-H(24)	1.0000
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
O(2)-Si(1)-C(13)	109.25(7)
O(2)-Si(1)-C(27)	109.88(7)
C(13)-Si(1)-C(27)	109.33(9)
O(2)-Si(1)-C(9)	103.53(6)
C(13)-Si(1)-C(9)	112.02(8)
C(27)-Si(1)-C(9)	112.66(8)
C(3)-O(1)-C(2)	115.74(11)

C(8)-O(2)-Si(1)	123.01(8)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-C(2)-C(1)	111.05(13)
O(1)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2A)	109.4
O(1)-C(2)-H(2B)	109.4
C(1)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
O(4)-C(3)-O(1)	123.50(11)
O(4)-C(3)-C(4)	125.38(11)
O(1)-C(3)-C(4)	111.05(10)
C(3)-C(4)-C(23)	112.15(10)
C(3)-C(4)-C(22)	113.28(10)
C(23)-C(4)-C(22)	101.97(9)
C(3)-C(4)-C(5)	108.39(9)
C(23)-C(4)-C(5)	111.68(10)
C(22)-C(4)-C(5)	109.30(10)
C(6)-C(5)-C(17)	111.44(10)
C(6)-C(5)-C(4)	115.61(10)
C(17)-C(5)-C(4)	111.03(9)
C(6)-C(5)-H(5)	106.0
С(17)-С(5)-Н(5)	106.0
C(4)-C(5)-H(5)	106.0
C(16)-C(6)-C(5)	108.91(10)

C(16)-C(6)-C(7)	104.07(9)
C(5)-C(6)-C(7)	118.52(9)
C(16)-C(6)-H(6)	108.3
C(5)-C(6)-H(6)	108.3
C(7)-C(6)-H(6)	108.3
C(14)-C(7)-C(8)	112.11(10)
C(14)-C(7)-C(6)	104.50(9)
C(8)-C(7)-C(6)	112.45(10)
С(14)-С(7)-Н(7)	109.2
С(8)-С(7)-Н(7)	109.2
С(6)-С(7)-Н(7)	109.2
O(2)-C(8)-C(7)	108.25(9)
O(2)-C(8)-H(8A)	110.0
C(7)-C(8)-H(8A)	110.0
O(2)-C(8)-H(8B)	110.0
C(7)-C(8)-H(8B)	110.0
H(8A)-C(8)-H(8B)	108.4
C(11)-C(9)-C(12)	109.15(14)
C(11)-C(9)-C(10)	109.09(15)
C(12)-C(9)-C(10)	109.13(14)
C(11)-C(9)-Si(1)	110.76(11)
C(12)-C(9)-Si(1)	109.35(11)
C(10)-C(9)-Si(1)	109.33(10)
С(9)-С(10)-Н(10А)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
С(9)-С(10)-Н(10С)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(24)	126.87(11)
C(15)-C(14)-C(7)	112.31(11)
C(24)-C(14)-C(7)	120.73(10)
C(14)-C(15)-C(16)	110.51(11)
С(14)-С(15)-Н(15)	124.7
С(16)-С(15)-Н(15)	124.7
O(5)-C(16)-C(15)	127.46(11)
O(5)-C(16)-C(6)	124.01(11)
C(15)-C(16)-C(6)	108.49(10)
C(18)-C(17)-C(5)	114.18(10)
С(18)-С(17)-Н(17А)	108.7

C(5)-C(17)-H(17A)	108.7
С(18)-С(17)-Н(17В)	108.7
С(5)-С(17)-Н(17В)	108.7
H(17A)-C(17)-H(17B)	107.6
O(3)-C(18)-C(17)	123.03(12)
O(3)-C(18)-C(19)	122.36(11)
C(17)-C(18)-C(19)	114.62(11)
C(18)-C(19)-C(20)	108.54(10)
C(18)-C(19)-C(23)	106.82(9)
C(20)-C(19)-C(23)	103.11(10)
С(18)-С(19)-Н(19)	112.6
С(20)-С(19)-Н(19)	112.6
С(23)-С(19)-Н(19)	112.6
C(21)-C(20)-C(19)	125.47(12)
C(21)-C(20)-C(22)	126.77(12)
C(19)-C(20)-C(22)	107.75(10)
C(20)-C(21)-H(21A)	120.0
C(20)-C(21)-H(21B)	120.0
H(21A)-C(21)-H(21B)	120.0
C(20)-C(22)-C(4)	104.30(10)
C(20)-C(22)-H(22A)	110.9
C(4)-C(22)-H(22A)	110.9
C(20)-C(22)-H(22B)	110.9
C(4)-C(22)-H(22B)	110.9
H(22A)-C(22)-H(22B)	108.9
C(4)-C(23)-C(19)	101.06(9)
C(4)-C(23)-H(23A)	111.6
С(19)-С(23)-Н(23А)	111.6
C(4)-C(23)-H(23B)	111.6

C(19)-C(23)-H(23B)	111.6
H(23A)-C(23)-H(23B)	109.4
C(14)-C(24)-C(25)	112.95(11)
C(14)-C(24)-C(26)	108.06(11)
C(25)-C(24)-C(26)	110.70(12)
C(14)-C(24)-H(24)	108.3
C(25)-C(24)-H(24)	108.3
C(26)-C(24)-H(24)	108.3
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(1)-C(27)-H(27A)	109.5
Si(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Si(1)	18(1)	34(1)	17(1)	-1(1)	-2(1)	2(1)
O(1)	19(1)	18(1)	31(1)	7(1)	1(1)	-2(1)
O(2)	16(1)	34(1)	16(1)	1(1)	2(1)	-1(1)
O(3)	28(1)	19(1)	30(1)	-1(1)	2(1)	-6(1)
O(4)	22(1)	25(1)	21(1)	-2(1)	-2(1)	-2(1)
O(5)	51(1)	23(1)	22(1)	6(1)	16(1)	6(1)
C(1)	26(1)	53(1)	44(1)	4(1)	11(1)	-7(1)
C(2)	23(1)	20(1)	49(1)	6(1)	5(1)	-6(1)
C(3)	18(1)	15(1)	18(1)	-2(1)	4(1)	2(1)
C(4)	16(1)	15(1)	15(1)	0(1)	0(1)	1(1)
C(5)	17(1)	16(1)	12(1)	1(1)	1(1)	-1(1)
C(6)	17(1)	15(1)	15(1)	0(1)	4(1)	-1(1)
C(7)	15(1)	16(1)	16(1)	0(1)	4(1)	1(1)
C(8)	19(1)	24(1)	15(1)	1(1)	2(1)	-1(1)
C(9)	16(1)	53(1)	25(1)	-4(1)	1(1)	0(1)
C(10)	37(1)	65(1)	36(1)	12(1)	11(1)	-6(1)
C(11)	19(1)	105(2)	42(1)	-6(1)	1(1)	-6(1)
C(12)	35(1)	71(1)	38(1)	-17(1)	10(1)	9(1)
C(13)	43(1)	54(1)	39(1)	14(1)	-8(1)	11(1)
C(14)	13(1)	17(1)	19(1)	-1(1)	1(1)	1(1)
C(15)	20(1)	19(1)	17(1)	-3(1)	4(1)	1(1)
C(16)	22(1)	20(1)	17(1)	0(1)	7(1)	-1(1)

Table 4. Anisotropic displacement parameters $(Å^2x \ 10^3)$ for mo_compound 9_0m. The anisotropic

displacement factor exponent takes the form: $-2\pi^2$ [h² a^{*2}U¹¹ + ... + 2 h k a^{*} b^{*} U¹²]

C(17)	18(1)	21(1)	16(1)	-1(1)	0(1)	-1(1)
C(18)	14(1)	21(1)	20(1)	1(1)	-2(1)	-1(1)
C(19)	17(1)	20(1)	16(1)	2(1)	3(1)	0(1)
C(20)	19(1)	20(1)	17(1)	-2(1)	2(1)	0(1)
C(21)	18(1)	26(1)	28(1)	1(1)	2(1)	1(1)
C(22)	17(1)	18(1)	21(1)	2(1)	1(1)	2(1)
C(23)	18(1)	18(1)	14(1)	0(1)	1(1)	0(1)
C(24)	26(1)	18(1)	23(1)	1(1)	2(1)	3(1)
C(25)	46(1)	22(1)	49(1)	1(1)	20(1)	11(1)
C(26)	32(1)	18(1)	28(1)	-1(1)	3(1)	-4(1)
C(27)	36(1)	50(1)	30(1)	-15(1)	3(1)	-6(1)

			·····	
-	x	у	Z	U(eq)
H(1A)	3108	5266	1142	61
H(1B)	3375	6438	822	61
H(1C)	2698	5754	182	61
H(2A)	2353	6484	2016	37
H(2B)	2005	7087	1081	37
H(5)	737	4038	292	18
H(6)	2125	3475	1023	19
H(7)	1268	1651	1533	19
H(8A)	2414	2437	2497	23
H(8B)	2611	1200	2313	23
H(10A)	5199	3618	154	69
H(10B)	4822	4170	1057	69
H(10C)	4206	3442	385	69
H(11A)	6150	2082	2056	83
H(11B)	5984	3339	2101	83
H(11C)	6380	2823	1191	83
H(12A)	5446	1676	110	72
H(12B)	4459	1453	338	72
H(12C)	5229	940	983	72
H(13A)	4068	1080	3379	68
H(13B)	5079	1224	3219	68

Table 5. Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å²x 10³) for mo_compound 9_0m.

H(13C)	4486	524	2500	68
H(15)	2192	1298	-940	23
H(17A)	-452	3074	264	22
H(17B)	235	2126	220	22
H(19)	-707	2667	2843	21
H(21A)	-2120	3534	2047	29
H(21B)	-2003	4733	1606	29
H(22A)	-220	5414	2029	22
H(22B)	-351	5000	962	22
H(23A)	499	3832	3167	20
H(23B)	924	2849	2622	20
H(24)	2399	-161	1258	26
H(25A)	2306	-550	-724	58
H(25B)	2670	-1375	56	58
H(25C)	3187	-296	-126	58
H(26A)	856	-140	1127	39
H(26B)	1216	-1277	820	39
H(26C)	876	-440	38	39
H(27A)	3980	4156	2601	58
H(27B)	4765	3695	3258	58
H(27C)	3787	3388	3460	58

Table 6. Torsion angles [°] for mo_compound 9_0m.

C(13)-Si(1)-O(2)-C(8)	53.74(12)
C(27)-Si(1)-O(2)-C(8)	-66.20(12)
C(9)-Si(1)-O(2)-C(8)	173.25(10)
C(3)-O(1)-C(2)-C(1)	83.71(15)
C(2)-O(1)-C(3)-O(4)	1.70(17)
C(2)-O(1)-C(3)-C(4)	-175.43(10)
O(4)-C(3)-C(4)-C(23)	18.23(16)
O(1)-C(3)-C(4)-C(23)	-164.70(9)
O(4)-C(3)-C(4)-C(22)	132.99(12)
O(1)-C(3)-C(4)-C(22)	-49.94(13)
O(4)-C(3)-C(4)-C(5)	-105.52(13)
O(1)-C(3)-C(4)-C(5)	71.54(12)
C(3)-C(4)-C(5)-C(6)	48.61(13)
C(23)-C(4)-C(5)-C(6)	-75.42(12)
C(22)-C(4)-C(5)-C(6)	172.51(10)
C(3)-C(4)-C(5)-C(17)	176.82(10)
C(23)-C(4)-C(5)-C(17)	52.78(13)
C(22)-C(4)-C(5)-C(17)	-59.28(12)
C(17)-C(5)-C(6)-C(16)	73.86(12)
C(4)-C(5)-C(6)-C(16)	-158.14(10)
C(17)-C(5)-C(6)-C(7)	-44.73(14)
C(4)-C(5)-C(6)-C(7)	83.27(13)
C(16)-C(6)-C(7)-C(14)	-2.59(12)
C(5)-C(6)-C(7)-C(14)	118.49(11)
C(16)-C(6)-C(7)-C(8)	119.24(11)
C(5)-C(6)-C(7)-C(8)	-119.67(11)
Si(1)-O(2)-C(8)-C(7)	177.13(8)

C(14)-C(7)-C(8)-O(2)	56.50(13)
C(6)-C(7)-C(8)-O(2)	-60.90(12)
O(2)-Si(1)-C(9)-C(11)	-179.49(13)
C(13)-Si(1)-C(9)-C(11)	-61.91(16)
C(27)-Si(1)-C(9)-C(11)	61.86(16)
O(2)-Si(1)-C(9)-C(12)	-59.16(12)
C(13)-Si(1)-C(9)-C(12)	58.42(14)
C(27)-Si(1)-C(9)-C(12)	-177.81(12)
O(2)-Si(1)-C(9)-C(10)	60.27(12)
C(13)-Si(1)-C(9)-C(10)	177.86(12)
C(27)-Si(1)-C(9)-C(10)	-58.38(13)
C(8)-C(7)-C(14)-C(15)	-118.36(12)
C(6)-C(7)-C(14)-C(15)	3.70(14)
C(8)-C(7)-C(14)-C(24)	64.78(14)
C(6)-C(7)-C(14)-C(24)	-173.16(11)
C(24)-C(14)-C(15)-C(16)	173.41(12)
C(7)-C(14)-C(15)-C(16)	-3.21(15)
C(14)-C(15)-C(16)-O(5)	-176.52(14)
C(14)-C(15)-C(16)-C(6)	1.35(15)
C(5)-C(6)-C(16)-O(5)	51.60(17)
C(7)-C(6)-C(16)-O(5)	178.91(13)
C(5)-C(6)-C(16)-C(15)	-126.35(11)
C(7)-C(6)-C(16)-C(15)	0.95(13)
C(6)-C(5)-C(17)-C(18)	94.96(12)
C(4)-C(5)-C(17)-C(18)	-35.46(14)
C(5)-C(17)-C(18)-O(3)	-138.67(13)
C(5)-C(17)-C(18)-C(19)	41.36(15)
O(3)-C(18)-C(19)-C(20)	-130.61(13)
C(17)-C(18)-C(19)-C(20)	49.36(14)

O(3)-C(18)-C(19)-C(23)	118.83(13)
C(17)-C(18)-C(19)-C(23)	-61.20(13)
C(18)-C(19)-C(20)-C(21)	87.62(15)
C(23)-C(19)-C(20)-C(21)	-159.34(13)
C(18)-C(19)-C(20)-C(22)	-91.13(12)
C(23)-C(19)-C(20)-C(22)	21.91(12)
C(21)-C(20)-C(22)-C(4)	-172.13(13)
C(19)-C(20)-C(22)-C(4)	6.60(13)
C(3)-C(4)-C(22)-C(20)	-153.24(10)
C(23)-C(4)-C(22)-C(20)	-32.53(12)
C(5)-C(4)-C(22)-C(20)	85.79(11)
C(3)-C(4)-C(23)-C(19)	167.43(9)
C(22)-C(4)-C(23)-C(19)	45.93(11)
C(5)-C(4)-C(23)-C(19)	-70.68(11)
C(18)-C(19)-C(23)-C(4)	72.44(11)
C(20)-C(19)-C(23)-C(4)	-41.86(11)
C(15)-C(14)-C(24)-C(25)	25.3(2)
C(7)-C(14)-C(24)-C(25)	-158.35(12)
C(15)-C(14)-C(24)-C(26)	-97.52(15)
C(7)-C(14)-C(24)-C(26)	78.85(14)

Symmetry transformations used to generate equivalent atoms:

D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)
С(15)-Н(15)О(4)#1	0.95	2.58	3.4825(15)	159.1
C(15)-H(15)O(4)#1	0.95	2.58	3.4825(15)	159.1
C(15)-H(15)O(4)#1	0.95	2.58	3.4825(15)	159.1
C(15)-H(15)O(4)#1	0.95	2.58	3.4825(15)	159.1

Table 7. Hydrogen bonds for mo_compound 9_0m [Å and °].

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z-1/2