Table 1. Crystal data and structure refinement for $C_{16}H_{11}Cl_3OS_3$.

Identification code	mm7raba2	
Empirical formula	C16 H11 Cl3 O S3	
Formula weight	421.78	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Aba2	
Unit cell dimensions	a = 24.646(5) Å	α= 90°.
	b = 10.612(2) Å	β= 90°.
	c = 13.602(3) Å	γ = 90°.
Volume	3557.6(12) $Å^3$	
Z	8	
Density (calculated)	1.575 Mg/m^3	
Absorption coefficient	0.867 mm^{-1}	
F(000)	1712	
Crystal size	0.35 x 0.26 x 0.04 mm^3	
Theta range for data collection	1.65 to 28.28°.	
Index ranges	-32<=h<=28, -14<=k<=14, -18<=l<=15	
Reflections collected	12941	
Independent reflections	4067 [R(int) = 0.0660]	
Completeness to theta = 28.28°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9662 and 0.7513	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4067 / 747 / 408	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0749, wR2 = 0.2001	
R indices (all data)	R1 = 0.1175, wR2 = 0.2329	
Absolute structure parameter	0.3(3)	
Largest diff. peak and hole	0.787 and -0.342 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{16}H_{11}Cl_3OS_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	5993(2)	10007(7)	8131(17)	44(3)
S(1)	5321(3)	8260(6)	9322(3)	33(1)
C(2)	5529(4)	8802(9)	8184(9)	29(4)
C(3)	5286(7)	8174(18)	7440(7)	31(4)
C(4)	4918(8)	7220(19)	7783(8)	27(4)
C(5)	4900(6)	7171(14)	8779(9)	29(4)
Cl(2)	3202(2)	4982(6)	10830(5)	59(2)
S(2)	3876(2)	6658(5)	9578(5)	40(1)
C(6)	3814(4)	5360(9)	10330(6)	42(4)
C(7)	4290(6)	4746(14)	10447(13)	50(1)
C(8)	4726(5)	5325(16)	9917(14)	26(3)
C(9)	4559(4)	6361(13)	9420(10)	27(3)
Cl(3)	3145(3)	5876(6)	5868(6)	73(2)
S(3)	4221(3)	4602(5)	6087(5)	35(1)
C(10)	3791(3)	5848(10)	6310(6)	41(4)
C(11)	4022(6)	6763(12)	6859(11)	30(3)
C(12)	4570(6)	6463(13)	7116(13)	26(3)
C(13)	4729(4)	5324(14)	6748(11)	39(5)
Cl(1D)	6003(4)	9971(10)	8300(20)	74(4)
S(1D)	5353(3)	8246(7)	7174(4)	42(1)
C(2D)	5537(4)	8782(10)	8311(9)	41(5)
C(3D)	5277(8)	8164(18)	9051(8)	40(4)
C(4D)	4915(9)	7218(19)	8679(10)	36(4)
C(5D)	4918(6)	7166(14)	7685(9)	27(3)
Cl(2D)	3214(2)	5111(9)	5633(6)	87(2)
S(2D)	3910(2)	6697(6)	6890(7)	49(2)
C(6D)	3828(4)	5381(9)	6166(6)	41(4)
C(7D)	4288(6)	4682(12)	6104(12)	41(5)
C(8D)	4726(5)	5220(14)	6659(14)	31(4)
C(9D)	4572(5)	6306(13)	7114(10)	35(4)
Cl(3D)	3144(3)	5783(11)	10574(6)	109(3)

S(3D)	4204(3)	4601(6)	10369(6)	50(1)
C(10D)	3785(3)	5838(11)	10097(6)	45(3)
C(11D)	4028(6)	6715(13)	9524(12)	40(1)
C(12D)	4581(6)	6371(15)	9294(14)	33(4)
C(13D)	4725(4)	5252(14)	9705(11)	26(3)
O(1T)	2186(6)	3098(18)	8137(14)	105(5)
C(2T)	2585(9)	3480(30)	7499(19)	129(7)
C(3T)	3148(7)	3130(30)	7874(16)	121(8)
C(4T)	3038(6)	2720(30)	8934(16)	107(7)
C(5T)	2424(7)	2820(30)	9028(15)	99(6)
O(1TD)	3023(7)	3814(18)	8491(16)	136(7)
C(2TD)	2947(10)	2500(20)	8490(20)	119(7)
C(3TD)	2475(10)	2200(20)	7780(20)	129(8)
C(4TD)	2129(8)	3390(20)	7890(20)	111(8)
C(5TD)	2487(9)	4200(20)	8562(19)	121(7)

Table 3. Bond lengths [Å] and angles [°] for $C_{16}H_{11}Cl_3OS_3$.

Cl(1)-C(2)	1.718(7)
S(1)-C(5)	1.719(10)
S(1)-C(2)	1.729(10)
C(2)-C(3)	1.351(10)
C(3)-C(4)	1.436(12)
C(4)-C(5)	1.357(8)
C(4)-C(12)	1.485(9)
C(5)-C(9)	1.486(9)
Cl(2)-C(6)	1.705(8)
S(2)-C(6)	1.722(8)
S(2)-C(9)	1.726(10)
C(6)-C(7)	1.350(10)
C(7)-C(8)	1.432(13)
C(8)-C(9)	1.355(9)
C(8)-C(8)#1	1.52(2)
Cl(3)-C(10)	1.701(8)
S(3)-C(13)	1.722(10)
S(3)-C(10)	1.722(8)
C(10)-C(11)	1.351(10)
C(11)-C(12)	1.431(13)
C(12)-C(13)	1.365(9)
C(13)-C(13)#1	1.50(2)
Cl(1D)-C(2D)	1.706(8)
S(1D)-C(2D)	1.709(10)
S(1D)-C(5D)	1.716(10)
C(2D)-C(3D)	1.361(10)
C(3D)-C(4D)	1.437(13)
C(4D)-C(5D)	1.353(9)
C(4D)-C(12D)	1.478(9)
C(5D)-C(9D)	1.471(9)
Cl(2D)-C(6D)	1.703(8)
S(2D)-C(9D)	1.712(10)
S(2D)-C(6D)	1.721(9)
C(6D)-C(7D)	1.358(10)

C(7D)-C(8D)	1.434(13)
C(8D)-C(9D)	1.362(9)
C(8D)-C(8D)#1	1.43(2)
Cl(3D)-C(10D)	1.709(8)
S(3D)-C(10D)	1.711(9)
S(3D)-C(13D)	1.714(10)
C(10D)-C(11D)	1.354(10)
C(11D)-C(12D)	1.444(13)
C(12D)-C(13D)	1.359(9)
C(13D)-C(13D)#1	1.46(2)
O(1T)-C(2T)	1.372(19)
O(1T)-C(5T)	1.380(18)
C(2T)-C(3T)	1.524(15)
C(3T)-C(4T)	1.532(15)
C(4T)-C(5T)	1.521(15)
O(1TD)-C(5TD)	1.386(19)
O(1TD)-C(2TD)	1.405(19)
C(2TD)-C(3TD)	1.550(16)
C(3TD)-C(4TD)	1.534(16)
C(4TD)-C(5TD)	1.527(15)

C(5)-S(1)-C(2)	91.0(4)
C(3)-C(2)-Cl(1)	129.2(12)
C(3)-C(2)-S(1)	112.0(6)
Cl(1)-C(2)-S(1)	118.8(10)
C(2)-C(3)-C(4)	112.6(8)
C(5)-C(4)-C(3)	111.9(7)
C(5)-C(4)-C(12)	124.8(13)
C(3)-C(4)-C(12)	123.1(12)
C(4)-C(5)-C(9)	128.8(11)
C(4)-C(5)-S(1)	112.5(6)
C(9)-C(5)-S(1)	118.6(9)
C(6)-S(2)-C(9)	90.7(4)
C(7)-C(6)-Cl(2)	127.4(10)
C(7)-C(6)-S(2)	112.4(7)
Cl(2)-C(6)-S(2)	120.2(7)

C(6)-C(7)-C(8)	112.6(8)
C(9)-C(8)-C(7)	111.8(8)
C(9)-C(8)-C(8)#1	129.7(15)
C(7)-C(8)-C(8)#1	118.3(14)
C(8)-C(9)-C(5)	126.2(13)
C(8)-C(9)-S(2)	112.5(7)
C(5)-C(9)-S(2)	121.3(11)
C(13)-S(3)-C(10)	90.8(4)
C(11)-C(10)-Cl(3)	125.3(9)
C(11)-C(10)-S(3)	112.9(7)
Cl(3)-C(10)-S(3)	121.8(7)
C(10)-C(11)-C(12)	111.9(8)
C(13)-C(12)-C(11)	112.2(7)
C(13)-C(12)-C(4)	122.5(15)
C(11)-C(12)-C(4)	125.0(14)
C(12)-C(13)-C(13)#1	131.3(14)
C(12)-C(13)-S(3)	112.2(7)
C(13)#1-C(13)-S(3)	116.3(12)
C(2D)-S(1D)-C(5D)	91.2(4)
C(3D)-C(2D)-Cl(1D)	132.6(14)
C(3D)-C(2D)-S(1D)	112.6(7)
Cl(1D)-C(2D)-S(1D)	114.8(13)
C(2D)-C(3D)-C(4D)	111.6(8)
C(5D)-C(4D)-C(3D)	112.1(8)
C(5D)-C(4D)-C(12D)	123.0(15)
C(3D)-C(4D)-C(12D)	124.9(13)
C(4D)-C(5D)-C(9D)	123.3(12)
C(4D)-C(5D)-S(1D)	112.4(7)
C(9D)-C(5D)-S(1D)	124.2(10)
C(9D)-S(2D)-C(6D)	90.9(4)
C(7D)-C(6D)-Cl(2D)	128.7(10)
C(7D)-C(6D)-S(2D)	112.4(7)
Cl(2D)-C(6D)-S(2D)	118.9(8)
C(6D)-C(7D)-C(8D)	112.2(8)
C(9D)-C(8D)-C(8D)#1	122.6(16)
C(9D)-C(8D)-C(7D)	111.6(8)

C(8D)#1-C(8D)-C(7D)	125.4(13)
C(8D)-C(9D)-C(5D)	127.2(14)
C(8D)-C(9D)-S(2D)	112.9(7)
C(5D)-C(9D)-S(2D)	119.8(12)
C(10D)-S(3D)-C(13D)	91.6(5)
C(11D)-C(10D)-Cl(3D)	130.6(10)
C(11D)-C(10D)-S(3D)	112.6(7)
Cl(3D)-C(10D)-S(3D)	116.7(8)
C(10D)-C(11D)-C(12D)	111.6(8)
C(13D)-C(12D)-C(11D)	112.2(8)
C(13D)-C(12D)-C(4D)	128.2(16)
C(11D)-C(12D)-C(4D)	119.6(14)
C(12D)-C(13D)-C(13D)#1	124.3(15)
C(12D)-C(13D)-S(3D)	111.9(7)
C(13D)#1-C(13D)-S(3D)	123.2(12)
C(2T)-O(1T)-C(5T)	108.3(14)
O(1T)-C(2T)-C(3T)	111.6(11)
C(2T)-C(3T)-C(4T)	103.0(8)
C(5T)-C(4T)-C(3T)	103.5(8)
O(1T)-C(5T)-C(4T)	111.4(10)
C(5TD)-O(1TD)-C(2TD)	99.6(17)
O(1TD)-C(2TD)-C(3TD)	107.7(12)
C(4TD)-C(3TD)-C(2TD)	100.5(9)
C(5TD)-C(4TD)-C(3TD)	101.8(9)
O(1TD)-C(5TD)-C(4TD)	110.1(11)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{16}H_{11}Cl_3OS_3$. 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}
Cl(1)	33(2)	26(3)	71(8)	5(2)	-8(3)	-9(2)
S(1)	38(2)	36(3)	24(2)	-4(2)	-2(2)	-10(2)
C(2)	35(9)	21(8)	30(6)	-2(6)	-2(6)	-5(6)
C(3)	38(8)	32(8)	21(6)	2(6)	16(7)	-13(6)
C(4)	24(8)	29(8)	29(6)	7(6)	3(6)	-14(7)
C(5)	37(8)	32(8)	20(6)	-1(5)	8(6)	0(6)
Cl(2)	39(3)	71(4)	66(4)	8(3)	13(2)	-14(2)
S(2)	33(2)	51(2)	36(2)	-3(2)	3(2)	-9(2)
C(6)	48(6)	43(9)	36(9)	-1(6)	13(7)	-23(6)
C(7)	58(3)	51(2)	41(2)	8(2)	8(2)	-20(2)
C(8)	39(3)	27(4)	12(7)	-8(4)	-6(3)	-14(3)
C(9)	34(6)	31(7)	16(7)	-6(5)	4(5)	-8(5)
Cl(3)	46(3)	70(4)	104(6)	-12(4)	-30(3)	-5(3)
S(3)	42(2)	35(2)	28(3)	4(2)	-11(2)	-16(2)
C(10)	39(7)	42(8)	42(9)	-3(7)	-19(7)	-10(5)
C(11)	33(7)	37(6)	20(7)	8(5)	-1(6)	-17(5)
C(12)	32(6)	17(5)	30(8)	14(5)	-10(6)	-4(5)
C(13)	41(8)	42(9)	35(10)	-4(8)	-17(8)	-5(7)
Cl(1D)	88(6)	49(5)	85(10)	4(4)	9(5)	-29(4)
S(1D)	49(3)	40(3)	38(3)	1(2)	7(2)	-8(2)
C(2D)	45(12)	40(11)	40(8)	-15(6)	8(6)	-5(8)
C(3D)	43(10)	40(9)	38(7)	-16(7)	15(8)	-1(6)
C(4D)	44(8)	28(8)	35(6)	7(6)	3(6)	4(7)
C(5D)	25(7)	32(8)	26(6)	4(6)	6(6)	9(6)
Cl(2D)	36(3)	150(8)	75(5)	10(6)	-14(3)	-18(4)
S(2D)	27(2)	53(4)	67(4)	4(3)	4(2)	12(2)
C(6D)	34(6)	52(10)	37(9)	4(7)	5(6)	-3(6)
C(7D)	33(7)	40(10)	51(12)	-1(8)	13(7)	-4(6)
C(8D)	39(7)	27(7)	26(9)	7(6)	7(7)	2(6)
C(9D)	32(6)	38(8)	36(9)	1(7)	4(7)	4(5)
Cl(3D)	46(3)	183(9)	97(7)	-11(7)	44(4)	-11(5)

S(3D)	58(3)	51(2)	41(2)	8(2)	8(2)	-20(2)
C(10D)	36(6)	72(10)	26(8)	-13(7)	6(6)	-13(6)
C(11D)	33(2)	51(2)	36(2)	-3(2)	3(2)	-9(2)
C(12D)	32(6)	35(8)	32(8)	-2(6)	5(6)	-3(5)
C(13D)	39(3)	27(4)	12(7)	-8(4)	-6(3)	-14(3)
O(1T)	59(6)	146(12)	110(11)	25(11)	-58(7)	4(7)
C(2T)	118(12)	147(16)	121(12)	75(12)	-37(10)	5(13)
C(3T)	84(9)	138(17)	142(16)	90(13)	16(10)	2(12)
C(4T)	48(7)	149(16)	124(14)	80(13)	-18(9)	-3(11)
C(5T)	51(8)	155(16)	92(11)	27(12)	-2(8)	28(11)
O(1TD)	97(9)	166(13)	147(17)	-11(12)	-55(11)	-20(9)
C(2TD)	70(10)	155(12)	132(18)	25(14)	-38(10)	24(10)
C(3TD)	97(13)	128(13)	161(18)	-23(13)	-49(12)	4(10)
C(4TD)	72(10)	128(15)	133(18)	11(14)	-46(11)	9(9)
C(5TD)	113(11)	119(12)	131(16)	-6(11)	-43(11)	15(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{16}H_{11}Cl_3OS_3$.

	x	y	z	U(eq)
H(3A)	5350	8343	6771	37
H(7A)	4330	4018	10835	60
H(11A)	3845	7508	7049	36
H(3DA)	5329	8335	9723	48
H(7DA)	4317	3932	5740	50
H(11B)	3859	7456	9304	48
H(2TA)	2563	4399	7414	154
H(2TB)	2526	3090	6856	154
H(3TA)	3393	3862	7855	146
H(3TB)	3305	2448	7486	146
H(4TA)	3160	1849	9042	128
H(4TB)	3220	3273	9405	128
H(5TA)	2279	2017	9274	119
H(5TB)	2334	3476	9506	119
H(2TC)	2859	2207	9154	143
H(2TD)	3280	2078	8274	143
H(3TC)	2603	2099	7099	154
H(3TD)	2276	1444	7977	154
H(4TC)	2065	3806	7261	133
H(4TD)	1780	3204	8206	133
H(5TC)	2457	5086	8369	145
H(5TD)	2363	4121	9244	145

Table 6. Torsion angles [°] for $C_{16}H_{11}Cl_3OS_3$.

C(5)-S(1)-C(2)-C(3)	0.0(2)
C(5)-S(1)-C(2)-Cl(1)	179.97(13)
Cl(1)-C(2)-C(3)-C(4)	179.97(19)
S(1)-C(2)-C(3)-C(4)	0.0(3)
C(2)-C(3)-C(4)-C(5)	0.1(4)
C(2)-C(3)-C(4)-C(12)	175(2)
C(3)-C(4)-C(5)-C(9)	177.3(13)
C(12)-C(4)-C(5)-C(9)	2.2(15)
C(3)-C(4)-C(5)-S(1)	-0.1(4)
C(12)-C(4)-C(5)-S(1)	-175(2)
C(2)-S(1)-C(5)-C(4)	0.1(3)
C(2)-S(1)-C(5)-C(9)	-177.6(12)
C(9)-S(2)-C(6)-C(7)	0.0(2)
C(9)-S(2)-C(6)-Cl(2)	179.96(13)
Cl(2)-C(6)-C(7)-C(8)	180.0(2)
S(2)-C(6)-C(7)-C(8)	-0.1(3)
C(6)-C(7)-C(8)-C(9)	0.1(5)
C(6)-C(7)-C(8)-C(8)#1	-175.2(13)
C(7)-C(8)-C(9)-C(5)	-178.6(11)
C(8)#1-C(8)-C(9)-C(5)	-3.9(15)
C(7)-C(8)-C(9)-S(2)	-0.1(4)
C(8)#1-C(8)-C(9)-S(2)	174.6(16)
C(4)-C(5)-C(9)-C(8)	103.7(9)
S(1)-C(5)-C(9)-C(8)	-79.0(12)
C(4)-C(5)-C(9)-S(2)	-74.7(12)
S(1)-C(5)-C(9)-S(2)	102.7(12)
C(6)-S(2)-C(9)-C(8)	0.1(3)
C(6)-S(2)-C(9)-C(5)	178.6(10)
C(13)-S(3)-C(10)-C(11)	0.0(2)
C(13)-S(3)-C(10)-Cl(3)	179.98(13)
Cl(3)-C(10)-C(11)-C(12)	-179.9(2)
S(3)-C(10)-C(11)-C(12)	0.1(3)
C(10)-C(11)-C(12)-C(13)	-0.1(5)
C(10)-C(11)-C(12)-C(4)	-174.4(16)

C(5)-C(4)-C(12)-C(13)	-92.9(16)
C(3)-C(4)-C(12)-C(13)	92.5(14)
C(5)-C(4)-C(12)-C(11)	80.8(17)
C(3)-C(4)-C(12)-C(11)	-93.8(13)
C(11)-C(12)-C(13)-C(13)#1	173.9(8)
C(4)-C(12)-C(13)-C(13)#1	-11.7(15)
C(11)-C(12)-C(13)-S(3)	0.1(4)
C(4)-C(12)-C(13)-S(3)	174.6(16)
C(10)-S(3)-C(13)-C(12)	0.0(3)
C(10)-S(3)-C(13)-C(13)#1	-174.8(8)
C(5D)-S(1D)-C(2D)-C(3D)	0.0(2)
C(5D)-S(1D)-C(2D)-Cl(1D)	179.96(12)
Cl(1D)-C(2D)-C(3D)-C(4D)	179.97(18)
S(1D)-C(2D)-C(3D)-C(4D)	0.0(3)
C(2D)-C(3D)-C(4D)-C(5D)	0.1(4)
C(2D)-C(3D)-C(4D)-C(12D)	179(2)
C(3D)-C(4D)-C(5D)-C(9D)	-178.1(13)
C(12D)-C(4D)-C(5D)-C(9D)	3.0(15)
C(3D)-C(4D)-C(5D)-S(1D)	-0.1(4)
C(12D)-C(4D)-C(5D)-S(1D)	-179.0(19)
C(2D)-S(1D)-C(5D)-C(4D)	0.1(3)
C(2D)-S(1D)-C(5D)-C(9D)	178.1(13)
C(9D)-S(2D)-C(6D)-C(7D)	0.0(2)
C(9D)-S(2D)-C(6D)-Cl(2D)	-179.96(13)
Cl(2D)-C(6D)-C(7D)-C(8D)	179.96(19)
S(2D)-C(6D)-C(7D)-C(8D)	0.0(3)
C(6D)-C(7D)-C(8D)-C(9D)	0.0(5)
C(6D)-C(7D)-C(8D)-C(8D)#1	-173.2(14)
C(8D)#1-C(8D)-C(9D)-C(5D)	-1.8(13)
C(7D)-C(8D)-C(9D)-C(5D)	-175.2(12)
C(8D)#1-C(8D)-C(9D)-S(2D)	173.4(12)
C(7D)-C(8D)-C(9D)-S(2D)	0.0(4)
C(4D)-C(5D)-C(9D)-C(8D)	-103.8(9)
S(1D)-C(5D)-C(9D)-C(8D)	78.4(15)
C(4D)-C(5D)-C(9D)-S(2D)	81.2(11)
S(1D)-C(5D)-C(9D)-S(2D)	-96.5(14)

C(6D)-S(2D)-C(9D)-C(8D)	0.0(3)
C(6D)-S(2D)-C(9D)-C(5D)	175.6(11)
C(13D)-S(3D)-C(10D)-C(11D)	0.0(2)
C(13D)-S(3D)-C(10D)-Cl(3D)	-179.97(12)
Cl(3D)-C(10D)-C(11D)-C(12D)	179.96(18)
S(3D)-C(10D)-C(11D)-C(12D)	0.0(3)
C(10D)-C(11D)-C(12D)-C(13D)	0.0(4)
C(10D)-C(11D)-C(12D)-C(4D)	-179.6(17)
C(5D)-C(4D)-C(12D)-C(13D)	93.2(17)
C(3D)-C(4D)-C(12D)-C(13D)	-85.4(18)
C(5D)-C(4D)-C(12D)-C(11D)	-87.2(15)
C(3D)-C(4D)-C(12D)-C(11D)	94.1(13)
C(11D)-C(12D)-C(13D)-C(13D)#1	-171.7(9)
C(4D)-C(12D)-C(13D)-C(13D)#1	7.8(17)
C(11D)-C(12D)-C(13D)-S(3D)	0.0(4)
C(4D)-C(12D)-C(13D)-S(3D)	179.6(19)
C(10D)-S(3D)-C(13D)-C(12D)	0.0(3)
C(10D)-S(3D)-C(13D)-C(13D)#1	171.8(10)
C(5T)-O(1T)-C(2T)-C(3T)	16(4)
O(1T)-C(2T)-C(3T)-C(4T)	-11(4)
C(2T)-C(3T)-C(4T)-C(5T)	2(3)
C(2T)-O(1T)-C(5T)-C(4T)	-14(4)
C(3T)-C(4T)-C(5T)-O(1T)	7(4)
C(5TD)-O(1TD)-C(2TD)-C(3TD)	45(3)
O(1TD)-C(2TD)-C(3TD)-C(4TD)	-31(3)
C(2TD)-C(3TD)-C(4TD)-C(5TD)	5(3)
C(2TD)-O(1TD)-C(5TD)-C(4TD)	-42(3)
C(3TD)-C(4TD)-C(5TD)-O(1TD)	22(3)

Symmetry transformations used to generate equivalent atoms:

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