JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(30), 7659-7660, DOI:10.1021/ja980435a

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Cl(1)	0.3167(3)	0.1393(2)	0.43821(9)	7.44(5)
Cl(2)	0.1625(3)	0.1223(2)	0.69077(10)	7.54(5)
O(1)	0.2480(8)	-0.1903(4)	0.4537(2)	7.7(1)
C(1)	0.3112(10)	-0.0993(5)	0.4876(3)	4.8(1)
C(2)	0.4799(9)	-0.0047(5)	0.4577(3)	4.4(1)
C(3)	0.652(1)	0.0265(6)	0.5127(3)	5.3(1)
C(4)	0.5614(10)	0.0610(5)	0.5844(3)	5.1(1)
C(5)	0.4152(8)	-0.0467(5)	0.6131(3)	4.1(1)
C(6)	0.2266(9)	-0.0718(5)	0.5607(3)	4.7(1)
C(7)	0.583(1)	-0.0490(7)	0.3887(3)	7.2(2)
C(8)	0.3322(10)	-0.0253(5)	0.6890(3)	4.7(1)
C(9)	0.521(1)	-0.0058(7)	0.7403(3)	7.2(2)
C(10)	0.171(1)	-0.1336(6)	0.7145(3)	6.3(2)
H(1)	0.7459	-0.0473	0.5180	6.3056
H(2)	0.7377	0.0979	0.4962	6.3056
H(3)	0.6820	0.0750	0.6160	6.0820
H(4)	0.4758	0.1383	0.5806	6.0820
H(5)	0.5039	-0.1230	0.6139	4.8790
H(6)	0.1333	0.0027	0.5591	5.6862
H(7)	0.1428	-0.1445	0.5765	5.6862
H(8)	0.4691	-0.0680	0.3555	8.7024
H(9)	0.6703	-0.1247	0.3968	8.7024
H(10)	0.6760	0.0180	0.3705	8.7024
H(11)	0.6147	-0.0803	0.7399	8.6375

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(12)	0.6049	0.0684	0.7269	8.6375
H(13)	0.4629	0.0065	0.7865	8.6375
H(14)	0.1098	-0.1102	0.7591	7.5950
H(15)	0.0539	-0.1437	0.6811	7.5950
H(16)	0.2499	-0.2131	0.7189	7.5950

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.127(2)	0.067(1)	0.088(1)	0.030(1)	0.002(1)	0.0185(8)
Cl(2)	0.105(1)	0.084(1)	0.098(1)	0.023(1)	0.020(1)	-0.0145(9)
O(1)	0.134(5)	0.079(3)	0.080(3)	-0.042(3)	-0.011(3)	-0.020(2)
C(1)	0.065(3)	0.058(4)	0.059(3)	0.001(3)	-0.012(3)	-0.002(3)
C(2)	0.067(4)	0.045(3)	0.056(3)	0.007(3)	-0.001(3)	0.002(2)
C(3)	0.059(3)	0.070(4)	0.071(4)	-0.014(3)	0.008(3)	0.002(3)
C(4)	0.061(4)	0.071(4)	0.061(3)	-0.019(3)	0.000(3)	-0.008(3)
C(5)	0.051(3)	0.050(3)	0.054(3)	0.002(3)	-0.007(2)	-0.003(2)
C(6)	0.060(4)	0.060(3)	0.060(3)	-0.016(3)	-0.007(3)	0.000(3)
C(7)	0.121(6)	0.087(5)	0.067(4)	0.013(5)	0.014(4)	-0.007(4)
C(8)	0.066(3)	0.055(3)	0.059(3)	-0.001(3)	0.002(3)	-0.005(3)
C(9)	0.097(5)	0.120(6)	0.056(4)	0.000(5)	-0.016(3)	-0.007(4)
C(10)	0.118(6)	0.066(4)	0.056(3)	-0.018(4)	0.019(3)	0.003(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Cl(1)	C(2)	1.815(5)	Cl(2)	C(8)	1.830(6)
O(1)	C(1)	1.197(6)	C(1)	C(2)	1.514(7)
C(1)	C(6)	1.500(7)	C(2)	C(3)	1.503(8)
C(2)	C(7)	1.515(8)	C(3)	C(4)	1.503(8)
C(4)	C(5)	1.515(7)	C(5)	C(6)	1.527(7)
C(5)	C(8)	1.534(7)	C(8)	C(9)	1.507(9)
C(8)	C(10)	1.554(8)			

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.95	C(3)	H(2)	0.95
C(4)	H(3)	0.95	C(4)	H(4)	0.95
C(5)	H(5)	0.95	C(6)	H(6)	0.95
C(6)	H(7)	0.95	C(7)	H(8)	0.95
C(7)	H(9)	0.95	C(7)	H(10)	0.95
C(9)	H(11)	0.95	C(9)	H(12)	0.95
C(9)	H(13)	0.95	C(10)	H(14)	0.95
C(10)	H(15)	0.95	C(10)	H(16)	0.95

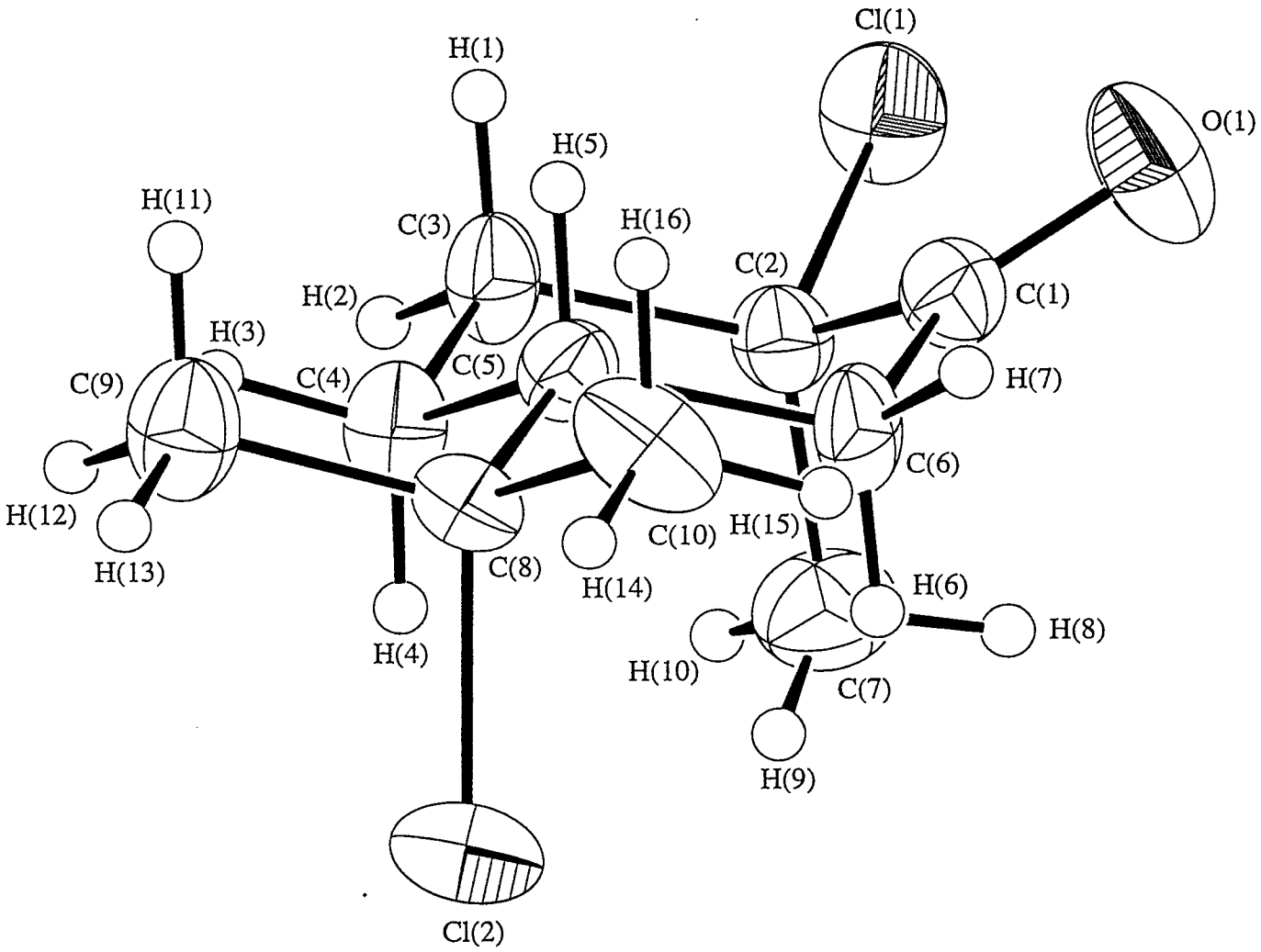
Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	C(1)	C(2)	121.1(5)	O(1)	C(1)	C(6)	122.2(5)
C(2)	C(1)	C(6)	116.7(4)	Cl(1)	C(2)	C(1)	103.9(4)
Cl(1)	C(2)	C(3)	109.7(4)	Cl(1)	C(2)	C(7)	107.0(4)
C(1)	C(2)	C(3)	109.9(4)	C(1)	C(2)	C(7)	113.7(5)
C(3)	C(2)	C(7)	112.2(5)	C(2)	C(3)	C(4)	115.1(5)
C(3)	C(4)	C(5)	111.1(5)	C(4)	C(5)	C(6)	108.7(4)
C(4)	C(5)	C(8)	114.8(4)	C(6)	C(5)	C(8)	113.0(4)
C(1)	C(6)	C(5)	112.3(4)	Cl(2)	C(8)	C(5)	108.5(3)
Cl(2)	C(8)	C(9)	107.3(4)	Cl(2)	C(8)	C(10)	104.1(4)
C(5)	C(8)	C(9)	112.1(5)	C(5)	C(8)	C(10)	112.9(4)
C(9)	C(8)	C(10)	111.4(5)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	108.0	C(2)	C(3)	H(2)	108.0
C(4)	C(3)	H(1)	108.0	C(4)	C(3)	H(2)	108.0
H(1)	C(3)	H(2)	109.5	C(3)	C(4)	H(3)	109.0
C(3)	C(4)	H(4)	109.1	C(5)	C(4)	H(3)	109.1
C(5)	C(4)	H(4)	109.1	H(3)	C(4)	H(4)	109.5
C(4)	C(5)	H(5)	106.6	C(6)	C(5)	H(5)	106.6
C(8)	C(5)	H(5)	106.6	C(1)	C(6)	H(6)	108.8
C(1)	C(6)	H(7)	108.8	C(5)	C(6)	H(6)	108.8
C(5)	C(6)	H(7)	108.8	H(6)	C(6)	H(7)	109.4
C(2)	C(7)	H(8)	109.5	C(2)	C(7)	H(9)	109.5
C(2)	C(7)	H(10)	109.5	H(8)	C(7)	H(9)	109.5
H(8)	C(7)	H(10)	109.5	H(9)	C(7)	H(10)	109.5
C(8)	C(9)	H(11)	109.5	C(8)	C(9)	H(12)	109.5
C(8)	C(9)	H(13)	109.4	H(11)	C(9)	H(12)	109.5
H(11)	C(9)	H(13)	109.5	H(12)	C(9)	H(13)	109.5
C(8)	C(10)	H(14)	109.5	C(8)	C(10)	H(15)	109.5
C(8)	C(10)	H(16)	109.5	H(14)	C(10)	H(15)	109.5
H(14)	C(10)	H(16)	109.5	H(15)	C(10)	H(16)	109.5

X-ray Analysis of Ketone 8



Crystal data. $[C_{10}H_{16}OCl_2]$; $M_r = 223.14$, orthorhombic, space group $P2_12_12_1$ (No.19), $a = 8.937(2)$ Å, $b = 9.485(2)$ Å, $c = 13.385(3)$ Å, $V = 1614.2(6)$ Å^3, $Z = 4$, $D_c = 1.463$ g cm^{-3}, μ(Mo-Kα) = 8.54 cm^{-1}, $F(000) = 660$, $T = 301$ K. A yellow crystal of dimensions 0.20 × 0.10 × 0.45 mm in a glass capillary was used for data collection at 28°C on a MAR diffractometer with a 300 mm image plate detector using graphite monochromatized Mo-Kα radiation ($\lambda = 0.71073$ Å). Data collection was made with 3° oscillation (60 images) at 100 mm distance and 220 s exposure. The images were interpreted and intensities integrated using program *DENZO* [1]. 1428 unique reflections were obtained from a total of 12985 measured reflections ($R_{int} = 0.047$). 1046 reflections with $I > 3\ \sigma(I)$ were considered observed and used in the structural analysis. These reflections were in the range h : 0 to 11; k : 0 to 11; and l : 0 to 16 with $2\theta_{max} = 56.1°$. The space group was uniquely determined based on systematic absences and the structure was solved by direct methods (*SIR92* [2]) and expanded by Fourier method and refinement by full-matrix least-squares using the software package *TeXsan* [3] on a Silicon Graphics Indy computer. One crystallographic asymmetric unit consists of one formula unit. In the least-squares refinement, all 13 non-H atoms were refined anisotropically and 16 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms, were not refined. Convergence for 118 variable parameters by least-squares refinement on F with $w = 4\,F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.045\,F_o^2)^2]$ for 1046 reflections with $I > 3\ \sigma(I)$ was reached at $R = 0.056$ and $wR = 0.085$ with a goodness-of-fit of 2.37. $(\Delta / \sigma)_{max} = 0.01$. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.37 and 0.39 e Å^{-3} respectively. The *ORTEP* [4] drawing of the complex molecule shows thermal ellipsoids at the 50 % probability level and the numbering scheme. Tables of atomic coordinates, thermal parameters, bond lengths and angles are attached.

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Cl(1)	0.2852(1)	0.5014(2)	0.39656(9)	5.84(3)
Cl(2)	0.6313(1)	0.5062(2)	0.84118(8)	6.12(3)
O(1)	0.4600(5)	0.2763(4)	0.4757(3)	7.0(1)
C(1)	0.4583(7)	0.3716(6)	0.5336(4)	4.3(1)
C(2)	0.3616(4)	0.5000(6)	0.5216(3)	4.02(8)
C(3)	0.4594(7)	0.6310(5)	0.5328(4)	4.6(1)
C(4)	0.5478(7)	0.6324(6)	0.6286(4)	4.7(2)
C(5)	0.6484(4)	0.5025(5)	0.6375(3)	3.69(8)
C(6)	0.5540(7)	0.3696(5)	0.6264(4)	4.6(2)
C(7)	0.2306(6)	0.494(1)	0.5926(5)	6.6(1)
C(8)	0.7487(5)	0.5026(6)	0.7305(3)	3.96(8)
C(9)	0.8464(7)	0.6318(6)	0.7362(5)	5.6(2)
C(10)	0.8435(7)	0.3708(7)	0.7368(5)	5.9(2)
H(1)	0.5274	0.6344	0.4783	5.5062
H(2)	0.3968	0.7119	0.5314	5.5062
H(3)	0.6084	0.7146	0.6301	5.6798
H(4)	0.4803	0.6338	0.6834	5.6798
H(5)	0.7137	0.5048	0.5815	4.4237
H(6)	0.4906	0.3614	0.6831	5.5080
H(7)	0.6188	0.2904	0.6233	5.5080
H(8)	0.1727	0.4125	0.5792	7.9201
H(9)	0.2663	0.4909	0.6594	7.9201
H(10)	0.1704	0.5759	0.5839	7.9201
H(11)	0.9150	0.6315	0.6820	6.7235

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(12)	0.7858	0.7139	0.7327	6.7235
H(13)	0.9002	0.6315	0.7974	6.7235
H(14)	0.8968	0.3704	0.7981	7.0973
H(15)	0.7807	0.2901	0.7334	7.0973
H(16)	0.9122	0.3693	0.6827	7.0973

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.0806(8)	0.0745(8)	0.0667(7)	-0.003(1)	-0.0269(5)	0.0053(8)
Cl(2)	0.0809(8)	0.103(1)	0.0482(6)	0.010(1)	0.0102(5)	-0.005(1)
O(1)	0.121(3)	0.068(2)	0.077(3)	0.020(2)	-0.038(3)	-0.022(2)
C(1)	0.060(3)	0.055(3)	0.050(4)	-0.008(3)	-0.004(3)	-0.003(2)
C(2)	0.050(2)	0.055(2)	0.048(2)	-0.008(3)	-0.006(2)	-0.007(3)
C(3)	0.072(4)	0.038(2)	0.064(4)	-0.003(3)	-0.017(4)	0.003(2)
C(4)	0.063(4)	0.048(3)	0.069(5)	-0.003(3)	-0.014(4)	0.002(2)
C(5)	0.048(2)	0.046(2)	0.046(2)	-0.003(3)	-0.002(1)	0.003(3)
C(6)	0.085(5)	0.029(2)	0.061(4)	0.000(3)	-0.016(4)	0.004(2)
C(7)	0.064(3)	0.099(4)	0.088(4)	-0.002(5)	0.017(3)	-0.002(4)
C(8)	0.051(2)	0.055(2)	0.045(2)	0.007(3)	0.002(2)	-0.008(3)
C(9)	0.072(5)	0.064(3)	0.076(5)	-0.012(3)	-0.024(4)	0.000(3)
C(10)	0.066(4)	0.090(4)	0.069(5)	0.033(3)	-0.017(4)	-0.018(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Cl(1)	C(2)	1.808(4)	Cl(2)	C(8)	1.815(4)
O(1)	C(1)	1.191(6)	C(1)	C(2)	1.502(7)
C(1)	C(6)	1.508(7)	C(2)	C(3)	1.526(7)
C(2)	C(7)	1.508(6)	C(3)	C(4)	1.505(7)
C(4)	C(5)	1.530(7)	C(5)	C(6)	1.524(7)
C(5)	C(8)	1.534(5)	C(8)	C(9)	1.507(8)
C(8)	C(10)	1.512(7)			

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.95	C(3)	H(2)	0.95
C(4)	H(3)	0.95	C(4)	H(4)	0.95
C(5)	H(5)	0.95	C(6)	H(6)	0.95
C(6)	H(7)	0.95	C(7)	H(8)	0.95
C(7)	H(9)	0.95	C(7)	H(10)	0.95
C(9)	H(11)	0.95	C(9)	H(12)	0.95
C(9)	H(13)	0.95	C(10)	H(14)	0.95
C(10)	H(15)	0.95	C(10)	H(16)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	C(1)	C(2)	123.6(5)	O(1)	C(1)	C(6)	121.3(5)
C(2)	C(1)	C(6)	115.1(4)	Cl(1)	C(2)	C(1)	108.8(3)
Cl(1)	C(2)	C(3)	107.5(4)	Cl(1)	C(2)	C(7)	106.9(3)
C(1)	C(2)	C(3)	108.7(3)	C(1)	C(2)	C(7)	110.5(5)
C(3)	C(2)	C(7)	114.3(5)	C(2)	C(3)	C(4)	113.0(4)
C(3)	C(4)	C(5)	111.6(4)	C(4)	C(5)	C(6)	109.4(3)
C(4)	C(5)	C(8)	114.0(4)	C(6)	C(5)	C(8)	113.8(4)
C(1)	C(6)	C(5)	112.6(4)	Cl(2)	C(8)	C(5)	109.0(3)
Cl(2)	C(8)	C(9)	106.2(4)	Cl(2)	C(8)	C(10)	107.1(4)
C(5)	C(8)	C(9)	112.3(4)	C(5)	C(8)	C(10)	111.8(4)
C(9)	C(8)	C(10)	110.2(4)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	108.6	C(2)	C(3)	H(2)	108.6
C(4)	C(3)	H(1)	108.5	C(4)	C(3)	H(2)	108.6
H(1)	C(3)	H(2)	109.4	C(3)	C(4)	H(3)	109.0
C(3)	C(4)	H(4)	108.9	C(5)	C(4)	H(3)	108.9
C(5)	C(4)	H(4)	108.9	H(3)	C(4)	H(4)	109.5
C(4)	C(5)	H(5)	106.3	C(6)	C(5)	H(5)	106.4
C(8)	C(5)	H(5)	106.4	C(1)	C(6)	H(6)	108.7
C(1)	C(6)	H(7)	108.7	C(5)	C(6)	H(6)	108.7
C(5)	C(6)	H(7)	108.7	H(6)	C(6)	H(7)	109.5
C(2)	C(7)	H(8)	109.5	C(2)	C(7)	H(9)	109.5
C(2)	C(7)	H(10)	109.5	H(8)	C(7)	H(9)	109.5
H(8)	C(7)	H(10)	109.5	H(9)	C(7)	H(10)	109.5
C(8)	C(9)	H(11)	109.5	C(8)	C(9)	H(12)	109.5
C(8)	C(9)	H(13)	109.5	H(11)	C(9)	H(12)	109.5
H(11)	C(9)	H(13)	109.4	H(12)	C(9)	H(13)	109.5
C(8)	C(10)	H(14)	109.5	C(8)	C(10)	H(15)	109.5
C(8)	C(10)	H(16)	109.5	H(14)	C(10)	H(15)	109.5
H(14)	C(10)	H(16)	109.5	H(15)	C(10)	H(16)	109.5

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cl(1)	C(2)	C(1)	O(1)	-12.3(7)	Cl(1)	C(2)	C(1)	C(6)	168.5(4)
Cl(1)	C(2)	C(3)	C(4)	-171.7(4)	Cl(2)	C(8)	C(5)	C(4)	60.7(5)
Cl(2)	C(8)	C(5)	C(6)	-65.7(5)	O(1)	C(1)	C(2)	C(3)	-129.1(6)
O(1)	C(1)	C(2)	C(7)	104.8(6)	O(1)	C(1)	C(6)	C(5)	127.9(6)
C(1)	C(2)	C(3)	C(4)	-54.1(5)	C(1)	C(6)	C(5)	C(4)	52.1(5)
C(1)	C(6)	C(5)	C(8)	-179.2(4)	C(2)	C(1)	C(6)	C(5)	-52.9(6)
C(2)	C(3)	C(4)	C(5)	57.9(6)	C(3)	C(2)	C(1)	C(6)	51.7(5)
C(3)	C(4)	C(5)	C(6)	-55.0(5)	C(3)	C(4)	C(5)	C(8)	176.4(4)
C(4)	C(3)	C(2)	C(7)	69.8(6)	C(4)	C(5)	C(8)	C(9)	-56.7(5)
C(4)	C(5)	C(8)	C(10)	178.9(4)	C(6)	C(1)	C(2)	C(7)	-74.4(5)
C(6)	C(5)	C(8)	C(9)	176.9(4)	C(6)	C(5)	C(8)	C(10)	52.5(5)

O(13M)-Mn(10)-Mn(4)	133.45(15)
O(11)-Mn(10)-Mn(4)	42.73(13)
O(14M)-Mn(10)-Mn(4)	135.37(14)
O(12)-Mn(10)-Mn(4)	42.74(12)
O(2D)-Mn(10)-Mn(4)	81.80(14)
O(2)-Mn(10)-Mn(4)	91.57(11)
O(13M)-Mn(10)-Mn(11)	84.31(14)
O(11)-Mn(10)-Mn(11)	85.94(13)
O(14M)-Mn(10)-Mn(11)	125.44(14)
O(12)-Mn(10)-Mn(11)	37.91(12)
O(2D)-Mn(10)-Mn(11)	131.54(14)
O(2)-Mn(10)-Mn(11)	40.16(11)
Mn(4)-Mn(10)-Mn(11)	64.59(3)
O(13M)-Mn(10)-Mn(3)	135.72(14)
O(11)-Mn(10)-Mn(3)	35.42(12)
O(14M)-Mn(10)-Mn(3)	84.06(14)
O(12)-Mn(10)-Mn(3)	82.46(12)
O(2D)-Mn(10)-Mn(3)	127.68(14)
O(2)-Mn(10)-Mn(3)	51.37(10)
Mn(4)-Mn(10)-Mn(3)	60.49(3)
Mn(11)-Mn(10)-Mn(3)	64.32(3)
O(13M)-Mn(10)-Mn(9)	90.28(14)
O(11)-Mn(10)-Mn(9)	86.55(13)
O(14M)-Mn(10)-Mn(9)	37.00(13)
O(12)-Mn(10)-Mn(9)	125.82(12)
O(2D)-Mn(10)-Mn(9)	139.70(14)
O(2)-Mn(10)-Mn(9)	48.50(11)
Mn(4)-Mn(10)-Mn(9)	120.71(4)
Mn(11)-Mn(10)-Mn(9)	88.61(4)
Mn(3)-Mn(10)-Mn(9)	60.25(3)
O(12)-Mn(11)-O(14)	96.5(2)
O(12)-Mn(11)-O(4)	165.9(2)
O(14)-Mn(11)-O(4)	88.7(2)
O(12)-Mn(11)-O(2)	88.8(2)
O(14)-Mn(11)-O(2)	164.5(2)
O(4)-Mn(11)-O(2)	82.9(2)
O(12)-Mn(11)-O(6)	107.6(2)
O(14)-Mn(11)-O(6)	101.8(2)
O(4)-Mn(11)-O(6)	83.9(2)
O(2)-Mn(11)-O(6)	90.2(2)
O(12)-Mn(11)-Mn(8)	128.92(13)
O(14)-Mn(11)-Mn(8)	129.71(12)
O(4)-Mn(11)-Mn(8)	42.05(12)
O(2)-Mn(11)-Mn(8)	40.87(12)
O(6)-Mn(11)-Mn(8)	85.40(12)
O(12)-Mn(11)-Mn(16)	145.61(13)
O(14)-Mn(11)-Mn(16)	92.61(12)
O(4)-Mn(11)-Mn(16)	46.44(12)
O(2)-Mn(11)-Mn(16)	91.04(13)
O(6)-Mn(11)-Mn(16)	37.97(11)
Mn(8)-Mn(11)-Mn(16)	63.18(3)
O(12)-Mn(11)-Mn(10)	38.80(13)
O(14)-Mn(11)-Mn(10)	134.79(12)
O(4)-Mn(11)-Mn(10)	132.83(13)
O(2)-Mn(11)-Mn(10)	50.30(12)
O(6)-Mn(11)-Mn(10)	99.87(12)
Mn(8)-Mn(11)-Mn(10)	91.05(4)
Mn(16)-Mn(11)-Mn(10)	127.33(4)
O(12)-Mn(11)-Mn(12)	133.85(13)
O(14)-Mn(11)-Mn(12)	37.86(12)
O(4)-Mn(11)-Mn(12)	51.03(12)
O(2)-Mn(11)-Mn(12)	133.11(12)
O(6)-Mn(11)-Mn(12)	92.70(12)
Mn(8)-Mn(11)-Mn(12)	92.76(4)