Table 3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Cl(1)	C(6)	1.729(2)	Cl(2)	C(6)	1.733(2)
C(3)	C(1)	1.422(2)	C(3)	C(2)	1.530(2)
C(3)	C(5)	1.496(2)	C(3)	C(4)	1.501(2)
C(1)	C(2)	1.499(2)	C(1)	C(6)	1.299(2)
C(2)	C(7)	1.509(2)	C(2)	C(17)	1.517(2)
C(15)	C(7)	1.436(2)	C(15)	C(16)	1.418(2)
C(15)	C(14)	1.414(2)	C(5)	C(4)	1.528(2)
C(5)	C(20)	1.531(2)	C(5)	C(21)	1.504(3)
C(7)	C(8)	1.365(2)	C(4)	C(18)	1.507(2)
C(4)	C(19)	1.510(3)	C(16)	C(10)	1.426(2)
C(16)	C(11)	1.403(2)	C(10)	C(9)	1.345(3)
C(14)	C(13)	1.367(2)	C(8)	C(9)	1.418(3)
C(11)	C(12)	1.361(3)	C(13)	C(12)	1.407(2)

Table 4. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(10)	H(3)	1.036(3)	C(14)	H(7)	0.947(2)
C(17)	H(8)	0.946(2)	C(17)	H(9)	1.043(3)
C(17)	H(10)	0.982(3)	C(8)	H(1)	0.951(3)
C(11)	H(4)	1.051(3)	C(13)	H(6)	0.974(3)
C(9)	H(2)	1.017(3)	C(18)	H(11)	0.944(3)
C(18)	H(12)	0.992(3)	C(18)	H(13)	1.066(3)
C(19)	H(14)	0.969(2)	C(19)	H(15)	0.954(3)
C(19)	H(16)	0.950(3)	C(12)	H(5)	0.995(3)
C(20)	H(17)	1.041(3)	C(20)	H(18)	0.885(2)
C(20)	H(19)	1.150(4)	C(21)	H(20)	0.980(3)
C(21)	H(21)	0.943(3)	C(21)	H(22)	1.056(3)

Table 5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(3)	C(2)	60.9(1)	C(1)	C(3)	C(5)	135.4(2)
C(2)	C(3)	C(5)	140.1(2)	C(1)	C(3)	C(4)	135.8(2)
C(2)	C(3)	C(4)	140.0(2)	C(5)	C(3)	C(4)	61.3(1)
C(3)	C(1)	C(2)	63.1(1)	C(3)	C(1)	C(6)	152.5(2)
C(2)	C(1)	C(6)	143.1(2)	C(3)	C(2)	C(1)	56.0(1)
C(3)	C(2)	C(7)	118.9(2)	C(1)	C(2)	C(7)	118.1(1)
C(3)	C(2)	C(17)	119.3(2)	C(1)	C(2)	C(17)	113.5(2)
C(7)	C(2)	C(17)	116.8(1)	C(7)	C(15)	C(16)	119.4(2)
C(7)	C(15)	C(14)	123.3(2)	C(16)	C(15)	C(14)	117.2(2)
C(3)	C(5)	C(4)	59.5(1)	C(3)	C(5)	C(20)	115.7(2)
C(4)	C(5)	C(20)	118.9(2)	C(3)	C(5)	C(21)	120.2(1)
C(4)	C(5)	C(21)	120.5(2)	C(20)	C(5)	C(21)	112.5(2)
C(2)	C(7)	C(15)	121.3(1)	C(2)	C(7)	C(8)	120.2(2)
C(15)	C(7)	C(8)	118.4(2)	C(3)	C(4)	C(5)	59.2(1)
C(3)	C(4)	C(18)	118.5(1)	C(5)	C(4)	C(18)	118.9(2)
C(3)	C(4)	C(19)	117.8(2)	C(5)	C(4)	C(19)	120.3(2)
C(18)	C(4)	C(19)	112.4(2)	C(15)	C(16)	C(10)	119.3(2)
C(15)	C(16)	C(11)	120.3(2)	C(10)	C(16)	C(11)	120.4(2)
C(16)	C(10)	C(9)	120.4(2)	C(15)	C(14)	C(13)	121.2(2)
Cl(1)	C(6)	Cl(2)	112.3(1)	Cl(1)	C(6)	C(1)	125.1(1)
Cl(2)	C(6)	C(1)	122.6(1)	C(7)	C(8)	C(9)	122.1(2)
C(16)	C(11)	C(12)	121.0(2)	C(14)	C(13)	C(12)	120.8(2)
C(10)	C(9)	C(8)	120.3(2)	C(11)	C(12)	C(13)	119.4(2)

Table 6. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(16)	C(10)	H(3)	117.2(2)	C(9)	C(10)	H(3)	122.4(2)
C(15)	C(14)	H(7)	121.4(2)	C(13)	C(14)	H(7)	117.4(2)
C(2)	C(17)	H(8)	111.7(2)	C(2)	C(17)	H(9)	110.8(2)
H(8)	C(17)	H(9)	108.6(2)	C(2)	C(17)	H(10)	116.1(2)
H(8)	C(17)	H(10)	108.6(3)	H(9)	C(17)	H(10)	100.2(2)
C(7)	C(8)	H(1)	121.3(2)	C(9)	C(8)	H(1)	116.6(2)
C(16)	C(11)	H(4)	119.9(2)	C(12)	C(11)	H(4)	119.1(2)
C(14)	C(13)	H(6)	116.3(2)	C(12)	C(13)	H(6)	122.7(2)
C(10)	C(9)	H(2)	121.9(2)	C(8)	C(9)	H(2)	117.7(2)
C(4)	C(18)	H(11)	115.9(2)	C(4)	C(18)	H(12)	110.7(2)
H(11)	C(18)	H(12)	102.9(2)	C(4)	C(18)	H(13)	105.9(2)
H(11)	C(18)	H(13)	108.9(2)	H(12)	C(18)	H(13)	112.7(2)
C(4)	C(19)	H(14)	111.3(2)	C(4)	C(19)	H(15)	114.3(2)
H(14)	C(19)	H(15)	109.7(3)	C(4)	C(19)	H(16)	113.2(2)
H(14)	C(19)	H(16)	104.6(3)	H(15)	C(19)	H(16)	102.9(3)
C(11)	C(12)	H(5)	121.6(2)	C(13)	C(12)	H(5)	118.9(2)
C(5)	C(20)	H(17)	112.6(2)	C(5)	C(20)	H(18)	109.5(2)
H(17)	C(20)	H(18)	107.2(3)	C(5)	C(20)	H(19)	111.0(2)
H(17)	C(20)	H(19)	104.0(2)	H(18)	C(20)	H(19)	112.4(3)
C(5)	C(21)	H(20)	114.7(2)	C(5)	C(21)	H(21)	111.8(2)
H(20)	C(21)	H(21)	107.6(3)	C(5)	C(21)	H(22)	108.9(2)
H(20)	C(21)	H(22)	111.2(3)	H(21)	C(21)	H(22)	101.9(2)

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(2)	C(3)	C(1)	C(2)	0.0(1)	C(2)	C(3)	C(1)	C(6)	165.4(5)
C(5)	C(3)	C(1)	C(2)	133.2(3)	C(5)	C(3)	C(1)	C(6)	-61.4(6)
C(4)	C(3)	C(1)	C(2)	-133.2(3)	C(4)	C(3)	C(1)	C(6)	32.1(7)
C(1)	C(3)	C(2)	C(1)	0.0(1)	C(1)	C(3)	C(2)	C(7)	106.0(2)
C(1)	C(3)	C(2)	C(17)	-99.9(2)	C(5)	C(3)	C(2)	C(1)	-127.2(4)
C(5)	C(3)	C(2)	C(7)	-21.1(4)	C(5)	C(3)	C(2)	C(17)	132.9(3)
C(4)	C(3)	C(2)	C(1)	127.8(4)	C(4)	C(3)	C(2)	C(7)	-126.2(3)
C(4)	C(3)	C(2)	C(17)	27.9(4)	C(1)	C(3)	C(5)	C(4)	127.5(3)
C(1)	C(3)	C(5)	C(20)	17.8(4)	C(1)	C(3)	C(5)	C(21)	-122.7(3)
C(2)	C(3)	C(5)	C(4)	-134.9(3)	C(2)	C(3)	C(5)	C(20)	115.3(3)
C(2)	C(3)	C(5)	C(21)	-25.2(4)	C(4)	C(3)	C(5)	C(4)	0.0(1)
C(4)	C(3)	C(5)	C(20)	-109.8(2)	C(4)	C(3)	C(5)	C(21)	109.8(3)
C(1)	C(3)	C(4)	C(5)	-127.0(3)	C(1)	C(3)	C(4)	C(18)	124.5(3)
C(1)	C(3)	C(4)	C(19)	-16.5(4)	C(2)	C(3)	C(4)	C(5)	135.0(3)
C(2)	C(3)	C(4)	C(18)	26.5(4)	C(2)	C(3)	C(4)	C(19)	-114.5(3)
C(5)	C(3)	C(4)	C(5)	0.0(1)	C(5)	C(3)	C(4)	C(18)	-108.5(3)
C(5)	C(3)	C(4)	C(19)	110.5(3)	C(3)	C(1)	C(2)	C(3)	0.0(1)
C(3)	C(1)	C(2)	C(7)	-107.5(2)	C(3)	C(1)	C(2)	C(17)	110.5(2)
C(6)	C(1)	C(2)	C(3)	-168.8(4)	C(6)	C(1)	C(2)	C(7)	83.7(4)
C(6)	C(1)	C(2)	C(17)	-58.3(5)	C(3)	C(1)	C(6)	Cl(1)	12.7(6)
C(3)	C(1)	C(6)	Cl(2)	-167.3(3)	C(2)	C(1)	C(6)	Cl(1)	170.6(2)
C(2)	C(1)	C(6)	Cl(2)	-9.4(4)	C(3)	C(2)	C(7)	C(15)	94.1(3)
C(3)	C(2)	C(7)	C(8)	-88.3(3)	C(1)	C(2)	C(7)	C(15)	158.7(2)
C(1)	C(2)	C(7)	C(8)	-23.8(3)	C(17)	C(2)	C(7)	C(15)	-60.6(3)
C(17)	C(2)	C(7)	C(8)	117.0(3)	C(16)	C(15)	C(7)	C(2)	175.0(2)
C(16)	C(15)	C(7)	C(8)	-2.6(3)	C(14)	C(15)	C(7)	C(2)	-5.0(4)
C(14)	C(15)	C(7)	C(8)	177.4(2)	C(7)	C(15)	C(16)	C(10)	2.3(3)
C(7)	C(15)	C(16)	C(11)	-177.3(2)	C(14)	C(15)	C(16)	C(10)	-177.8(2)
C(14)	C(15)	C(16)	C(11)	2.7(3)	C(7)	C(15)	C(14)	C(13)	177.2(2)
C(16)	C(15)	C(14)	C(13)	-2.8(4)	C(3)	C(5)	C(4)	C(3)	0.0(1)
C(3)	C(5)	C(4)	C(18)	107.7(3)	C(3)	C(5)	C(4)	C(19)	-106.3(3)
C(20)	C(5)	C(4)	C(3)	104.5(3)	C(20)	C(5)	C(4)	C(18)	-147.8(3)
C(20)	C(5)	C(4)	C(19)	-1.8(4)	C(21)	C(5)	C(4)	C(3)	-109.4(3)
C(21)	C(5)	C(4)	C(18)	-1.6(4)	C(21)	C(5)	C(4)	C(19)	144.3(3)
C(2)	C(7)	C(8)	C(9)	-176.4(2)	C(15)	C(7)	C(8)	C(9)	1.2(3)
C(15)	C(16)	C(10)	C(9)	-0.5(4)	C(11)	C(16)	C(10)	C(9)	179.0(2)
C(15)	C(16)	C(11)	C(12)	-0.3(4)	C(10)	C(16)	C(11)	C(12)	-179.9(2)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle
C(16)	C(10)	C(9)	C(8)	-0.9(4)
C(7)	C(8)	C(9)	C(10)	0.6(4)
C(14)	C(13)	C(12)	C(11)	2.0(4)
C(15)	C(14)	C(13)	C(12)	0.5(4)
C(16)	C(11)	C(12)	C(13)	-2.0(4)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
CL(1)	CL(2)	2.875(1)	(1)	CL(1)	C(1)	2.695(2)	(1)
CL(1)	C(6)	1.729(2)	(1)	CL(2)	C(1)	2.668(2)	(1)
CL(2)	C(2)	3.482(2)	(1)	CL(2)	C(6)	1.733(2)	(1)
CL(2)	C(9)	3.466(2)	(1,1,0,1)	C(3)	C(1)	1.422(2)	(1)
C(3)	C(2)	1.530(2)	(1)	C(3)	C(15)	3.536(2)	(1)
C(3)	C(5)	1.496(2)	(1)	C(3)	C(7)	2.617(2)	(1)
C(3)	C(4)	1.501(2)	(1)	C(3)	C(17)	2.629(2)	(1)
C(3)	C(6)	2.644(3)	(1)	C(3)	C(8)	3.421(2)	(1)
C(3)	C(18)	2.584(2)	(1)	C(3)	C(19)	2.579(2)	(1)
C(3)	C(20)	2.563(2)	(1)	C(3)	C(21)	2.601(3)	(1)
C(1)	C(2)	1.499(2)	(1)	C(1)	C(5)	2.700(2)	(1)
C(1)	C(7)	2.579(2)	(1)	C(1)	C(4)	2.708(2)	(1)
C(1)	C(17)	2.521(2)	(1)	C(1)	C(6)	1.299(2)	(1)
C(1)	C(8)	2.949(2)	(1)	C(1)	C(19)	3.260(2)	(1)
C(1)	C(20)	3.216(3)	(1)	C(2)	C(15)	2.567(2)	(1)
C(2)	C(5)	2.844(2)	(1)	C(2)	C(7)	1.509(2)	(1)
C(2)	C(4)	2.848(2)	(1)	C(2)	C(14)	3.001(2)	(1)
C(2)	C(17)	1.517(2)	(1)	C(2)	C(6)	2.655(2)	(1)
C(2)	C(8)	2.492(2)	(1)	C(2)	C(18)	3.448(2)	(1)
C(2)	C(21)	3.476(3)	(1)	C(15)	C(7)	1.436(2)	(1)
C(15)	C(16)	1.418(2)	(1)	C(15)	C(10)	2.454(2)	(1)
C(15)	C(14)	1.414(2)	(1)	C(15)	C(17)	3.216(3)	(1)
C(15)	C(8)	2.406(2)	(1)	C(15)	C(11)	2.447(2)	(1)
C(15)	C(13)	2.423(2)	(1)	C(15)	C(9)	2.801(2)	(1)
C(15)	C(12)	2.820(3)	(1)	C(5)	C(7)	3.450(2)	(1)
C(5)	C(4)	1.528(2)	(1)	C(5)	C(18)	2.614(3)	(1)
C(5)	C(19)	2.636(3)	(1)	C(5)	C(20)	1.531(2)	(1)
C(5)	C(21)	1.504(3)	(1)	C(7)	C(16)	2.464(2)	(1)
C(7)	C(10)	2.821(2)	(1)	C(7)	C(14)	2.509(2)	(1)
C(7)	C(17)	2.577(3)	(1)	C(7)	C(6)	3.564(2)	(1)
C(7)	C(8)	1.365(2)	(1)	C(7)	C(9)	2.434(2)	(1)
C(7)	C(21)	3.571(2)	(1)	C(4)	C(17)	3.483(2)	(1)
C(4)	C(18)	1.507(2)	(1)	C(4)	C(19)	1.510(3)	(1)
C(4)	C(20)	2.633(3)	(1)	C(4)	C(21)	2.632(3)	(1)
C(16)	C(10)	1.426(2)	(1)	C(16)	C(14)	2.418(2)	(1)
C(16)	C(8)	2.783(2)	(1)	C(16)	C(11)	1.403(2)	(1)
C(16)	C(13)	2.774(3)	(1)	C(16)	C(9)	2.405(3)	(1)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(16)	C(12)	2.406(3)	(1)	C(10)	C(8)	2.397(3)	(1)
C(10)	C(11)	2.455(3)	(1)	C(10)	C(9)	1.345(3)	(1)
C(14)	C(17)	3.237(3)	(1)	C(14)	C(11)	2.774(2)	(1)
C(14)	C(13)	1.367(2)	(1)	C(14)	C(12)	2.411(3)	(1)
C(17)	C(6)	3.357(2)	(1)	C(17)	C(8)	3.600(3)	(1)
C(6)	C(8)	3.537(3)	(1)	C(8)	C(9)	1.418(3)	(1)
C(11)	C(13)	2.389(3)	(1)	C(11)	C(12)	1.361(3)	(1)
C(13)	C(12)	1.407(2)	(1)	C(18)	C(19)	2.508(3)	(1)
C(18)	C(21)	3.020(3)	(1)	C(19)	C(20)	3.030(3)	(1)
C(20)	C(20)	3.503(4)	(2,1,1)	C(20)	C(21)	2.523(3)	(1)

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z
(2) -X,Y,-Z+1/2

L: Lattice translation.
(1) 0, 0, 0
(2) 1/2, 1/2, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
CL(1)	H(13)	3.13(1)	(-2,1,0,1,-1)	CL(1)	H(15)	2.901(7)	(1)
CL(1)	H(15)	3.055(7)	(2,1,1)	CL(1)	H(22)	3.52(1)	(-2,1,0,1,-1)
CL(1)	H(18)	3.27(1)	(1,1,0,1)	CL(1)	H(19)	2.900(7)	(1)
CL(2)	H(1)	2.993(7)	(1)	CL(2)	H(6)	3.25(3)	(-2,1,0,1,-1)
CL(2)	H(2)	3.50(1)	(1,1,0,1)	CL(2)	H(12)	3.29(2)	(-2,1,0,2,-1)
CL(2)	H(20)	3.35(2)	(-2,1,0,1,-1)	CL(2)	H(21)	3.57(2)	(1,1,0,1)
CL(2)	H(9)	3.289(9)	(1)	C(3)	H(1)	3.43(1)	(1)
C(3)	H(7)	3.261(9)	(1)	C(3)	H(11)	2.738(7)	(1)
C(3)	H(12)	3.002(7)	(1)	C(3)	H(13)	3.393(9)	(1)
C(3)	H(14)	3.36(1)	(1)	C(3)	H(15)	2.693(7)	(1)
C(3)	H(16)	3.034(9)	(1)	C(3)	H(20)	2.760(8)	(1)
C(3)	H(21)	3.049(9)	(1)	C(3)	H(22)	3.435(9)	(1)
C(3)	H(17)	3.418(9)	(1)	C(3)	H(18)	2.931(9)	(1)
C(3)	H(19)	2.711(7)	(1)	C(3)	H(8)	2.673(7)	(1)
C(3)	H(9)	3.405(9)	(1)	C(3)	H(10)	3.258(9)	(1)
C(1)	H(1)	2.625(7)	(1)	C(1)	H(15)	3.016(9)	(1)
C(1)	H(16)	3.52(1)	(1)	C(1)	H(21)	3.41(1)	(1,1,0,1)
C(1)	H(18)	3.40(1)	(1)	C(1)	H(19)	2.977(8)	(1)
C(1)	H(8)	2.661(8)	(1)	C(1)	H(9)	2.879(8)	(1)
C(1)	H(10)	3.40(1)	(1)	C(2)	H(1)	2.664(7)	(1)
C(2)	H(7)	2.705(7)	(1)	C(2)	H(11)	3.289(9)	(1)
C(2)	H(20)	3.310(9)	(1)	C(2)	H(8)	2.064(6)	(1)
C(2)	H(9)	2.125(6)	(1)	C(2)	H(10)	2.140(6)	(1)
C(15)	H(1)	3.281(9)	(1)	C(15)	H(7)	2.072(5)	(1)
C(15)	H(6)	3.277(9)	(1)	C(15)	H(5)	3.34(1)	(2,2)
C(15)	H(4)	3.397(8)	(1)	C(15)	H(4)	2.761(8)	(2,2)
C(15)	H(3)	3.37(1)	(1)	C(15)	H(20)	3.14(1)	(1)
C(15)	H(21)	3.531(9)	(1)	C(15)	H(9)	3.49(1)	(1,1,0,-1)
C(15)	H(10)	2.976(8)	(1)	C(5)	H(11)	2.787(8)	(1)
C(5)	H(12)	3.41(1)	(1)	C(5)	H(13)	2.998(8)	(1)
C(5)	H(14)	3.039(9)	(1)	C(5)	H(14)	3.218(9)	(-1,1,1,1,1)
C(5)	H(15)	2.816(8)	(1)	C(5)	H(16)	3.42(1)	(1)
C(5)	H(20)	2.111(6)	(1)	C(5)	H(21)	2.051(6)	(1)
C(5)	H(22)	2.099(6)	(1)	C(5)	H(17)	2.156(6)	(1)
C(5)	H(18)	2.008(6)	(1)	C(5)	H(19)	2.220(6)	(1)
C(7)	H(1)	2.028(5)	(1)	C(7)	H(7)	2.725(7)	(1)
C(7)	H(5)	3.47(2)	(2,2)	C(7)	H(4)	3.58(1)	(2,2)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(7)	H(2)	3.326(9)	(1)	C(7)	H(20)	3.35(1)	(1)
C(7)	H(21)	3.46(1)	(1)	C(7)	H(8)	3.378(9)	(1)
C(7)	H(9)	2.894(8)	(1)	C(7)	H(10)	2.798(8)	(1)
C(4)	H(11)	2.099(6)	(1)	C(4)	H(12)	2.076(6)	(1)
C(4)	H(13)	2.071(5)	(1)	C(4)	H(14)	2.069(5)	(1)
C(4)	H(14)	3.233(5)	(-1,1,1,1,1)	C(4)	H(15)	2.093(6)	(1)
C(4)	H(16)	2.077(6)	(1)	C(4)	H(20)	2.816(8)	(1)
C(4)	H(21)	3.41(1)	(1)	C(4)	H(22)	3.073(9)	(1)
C(4)	H(17)	3.095(9)	(1)	C(4)	H(18)	3.33(1)	(1)
C(4)	H(19)	2.772(8)	(1)	C(4)	H(8)	3.171(8)	(1)
C(16)	H(7)	3.288(9)	(1)	C(16)	H(5)	3.31(1)	(1)
C(16)	H(5)	3.03(1)	(2,2)	C(16)	H(4)	2.131(5)	(1)
C(16)	H(4)	2.869(5)	(2,2)	C(16)	H(3)	2.111(6)	(1)
C(16)	H(2)	3.341(9)	(1)	C(16)	H(9)	2.94(1)	(1,1,0,-1)
C(10)	H(1)	3.226(9)	(1)	C(10)	H(5)	2.91(1)	(2,2)
C(10)	H(4)	2.668(8)	(1)	C(10)	H(3)	1.036(3)	(1)
C(10)	H(3)	3.369(3)	(-1,2)	C(10)	H(2)	2.071(6)	(1)
C(10)	H(9)	3.42(2)	(1,1,0,-1)	C(14)	H(1)	3.32(1)	(-2,1,0,1)
C(14)	H(7)	0.947(2)	(1)	C(14)	H(6)	2.000(6)	(1)
C(14)	H(5)	3.297(9)	(1)	C(14)	H(4)	2.80(1)	(2,2)
C(14)	H(2)	3.09(1)	(-2,1,0,1)	C(14)	H(11)	3.25(1)	(1)
C(14)	H(20)	2.784(7)	(1)	C(14)	H(10)	2.693(8)	(1)
C(17)	H(7)	2.768(8)	(1)	C(17)	H(2)	3.30(2)	(-2,1,0,1)
C(17)	H(11)	3.45(1)	(1)	C(17)	H(12)	3.38(1)	(1)
C(17)	H(21)	3.38(1)	(1,1,0,1)	C(17)	H(8)	0.946(2)	(1)
C(17)	H(9)	1.043(3)	(1)	C(17)	H(10)	0.982(3)	(1)
C(6)	H(1)	2.892(8)	(1)	C(6)	H(11)	3.41(1)	(-2,1,0,1,-1)
C(6)	H(13)	3.44(2)	(-2,1,0,1,-1)	C(6)	H(15)	3.28(1)	(1)
C(6)	H(21)	3.16(2)	(1,1,0,1)	C(6)	H(19)	3.274(9)	(1)
C(6)	H(8)	3.40(1)	(1)	C(6)	H(9)	3.38(1)	(1)
C(8)	H(1)	0.951(3)	(1)	C(8)	H(7)	3.28(1)	(-2,1,0,1,-1)
C(8)	H(6)	3.00(2)	(-2,1,0,1,-1)	C(8)	H(5)	3.34(2)	(2,2)
C(8)	H(3)	3.354(9)	(1)	C(8)	H(2)	2.094(6)	(1)
C(8)	H(11)	3.33(2)	(-2,1,0,1,-1)	C(11)	H(6)	3.283(9)	(1)
C(11)	H(5)	2.064(6)	(1)	C(11)	H(4)	1.051(3)	(1)
C(11)	H(4)	2.982(3)	(2,2)	C(11)	H(3)	2.626(7)	(1)
C(11)	H(9)	2.85(2)	(1,1,0,-1)	C(11)	H(10)	3.54(1)	(1,1,0,-1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(13)	H(1)	3.32(2)	(-2,1,0,1)	C(13)	H(7)	1.989(6)	(1)
C(13)	H(6)	0.974(3)	(1)	C(13)	H(5)	2.079(6)	(1)
C(13)	H(4)	3.34(1)	(1)	C(13)	H(4)	2.91(1)	(2,2)
C(13)	H(3)	3.59(1)	(2,2)	C(13)	H(2)	3.34(2)	(-2,1,0,1)
C(13)	H(20)	3.58(1)	(1)	C(9)	H(1)	2.030(6)	(1)
C(9)	H(7)	3.24(1)	(-2,1,0,1,-1)	C(9)	H(6)	3.15(2)	(-2,1,0,1,-1)
C(9)	H(5)	3.07(2)	(2,2)	C(9)	H(3)	2.092(6)	(1)
C(9)	H(3)	3.322(6)	(-1,2)	C(9)	H(2)	1.017(3)	(1)
C(9)	H(10)	3.40(1)	(-2,1,0,1,-1)	C(18)	H(1)	3.30(2)	(-2,1,0,1)
C(18)	H(7)	3.208(9)	(1)	C(18)	H(11)	0.944(3)	(1)
C(18)	H(12)	0.992(3)	(1)	C(18)	H(13)	1.066(3)	(1)
C(18)	H(14)	2.757(8)	(1)	C(18)	H(14)	3.575(8)	(-1,1,1,1,1)
C(18)	H(15)	3.35(1)	(1)	C(18)	H(16)	2.701(9)	(1)
C(18)	H(20)	2.766(9)	(1)	C(18)	H(22)	3.32(1)	(1)
C(18)	H(17)	3.58(1)	(-1,1,1,1,1)	C(18)	H(18)	3.50(1)	(-2,1,0,1)
C(18)	H(8)	3.24(1)	(1)	C(19)	H(11)	3.36(1)	(1)
C(19)	H(12)	2.712(9)	(1)	C(19)	H(13)	2.724(9)	(1)
C(19)	H(13)	3.514(9)	(-1,1,1,1,1)	C(19)	H(14)	0.969(2)	(1)
C(19)	H(14)	3.213(2)	(-1,1,1,1,1)	C(19)	H(15)	0.954(3)	(1)
C(19)	H(16)	0.950(3)	(1)	C(19)	H(22)	3.26(1)	(1,1,0,1)
C(19)	H(22)	3.59(1)	(-1,1,1,1,1)	C(19)	H(17)	3.30(1)	(1)
C(19)	H(17)	3.27(1)	(-1,1,1,1,1)	C(19)	H(19)	2.641(8)	(1)
C(12)	H(7)	3.250(9)	(1)	C(12)	H(6)	2.099(6)	(1)
C(12)	H(5)	0.995(3)	(1)	C(12)	H(4)	2.085(6)	(1)
C(12)	H(4)	2.993(6)	(2,2)	C(12)	H(9)	3.30(2)	(1,1,0,-1)
C(12)	H(10)	3.47(1)	(1,1,0,-1)	C(20)	H(13)	3.54(1)	(-1,1,1,1,1)
C(20)	H(13)	3.45(1)	(-2,1,0,1,-1)	C(20)	H(14)	3.28(1)	(1)
C(20)	H(14)	3.21(1)	(-1,1,1,1,1)	C(20)	H(15)	2.789(9)	(1)
C(20)	H(20)	3.40(1)	(1)	C(20)	H(21)	2.670(8)	(1)
C(20)	H(22)	2.750(9)	(1)	C(20)	H(17)	1.041(3)	(1)
C(20)	H(17)	3.234(3)	(2,1,1)	C(20)	H(18)	0.885(2)	(1)
C(20)	H(18)	3.474(2)	(2,1,1)	C(20)	H(19)	1.150(4)	(1)
C(20)	H(19)	3.089(4)	(2,1,1)	C(21)	H(7)	3.364(9)	(1)
C(21)	H(11)	2.776(9)	(1)	C(21)	H(13)	3.24(1)	(1)
C(21)	H(14)	3.52(1)	(-1,1,1,1,1)	C(21)	H(16)	3.29(1)	(1,1,0,-1)
C(21)	H(20)	0.980(3)	(1)	C(21)	H(21)	0.943(3)	(1)
C(21)	H(22)	1.056(3)	(1)	C(21)	H(17)	2.823(8)	(1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

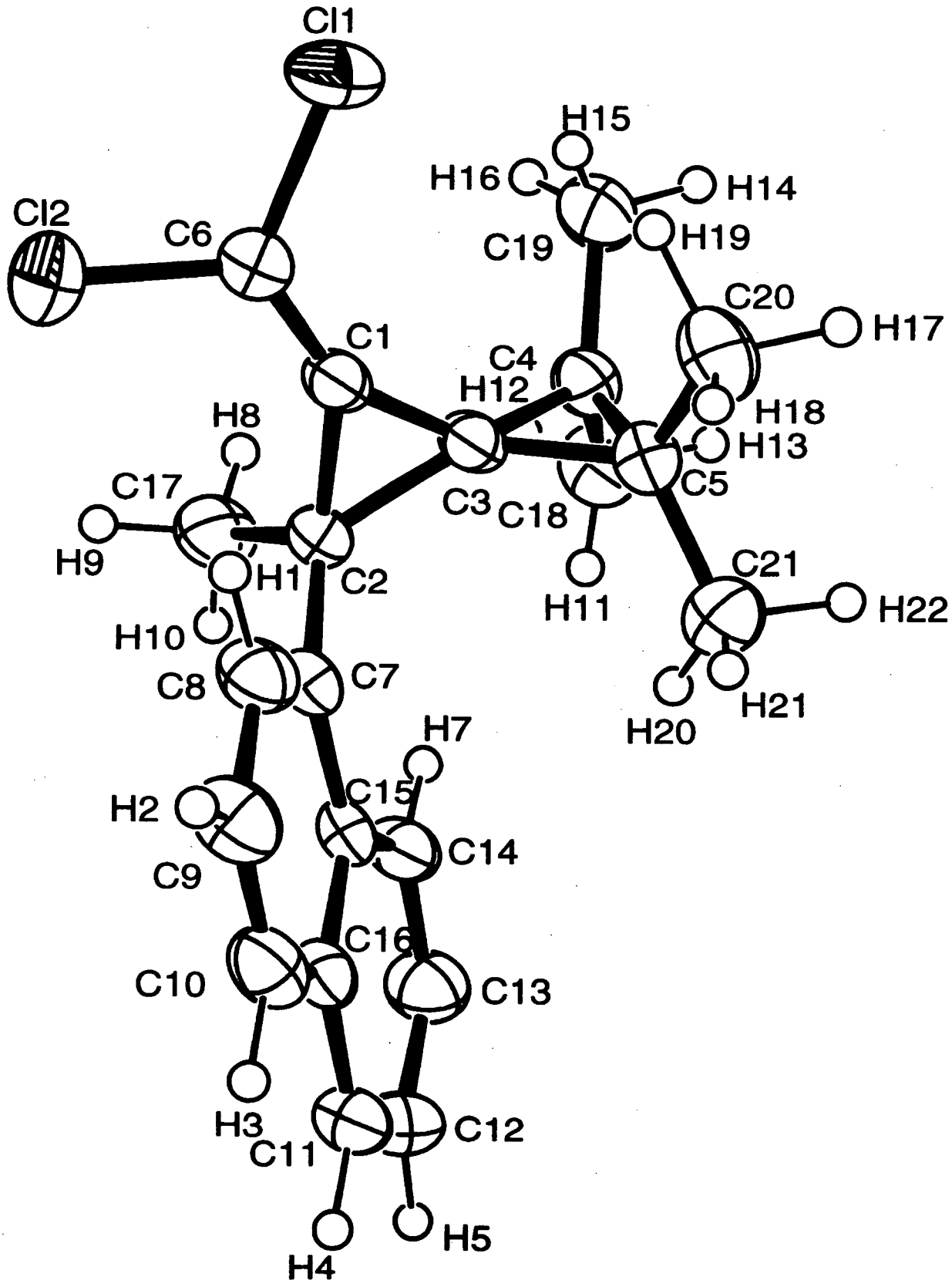
atom	atom	distance	ADC	atom	atom	distance	ADC
C(21)	H(18)	2.656(9)	(1)	C(21)	H(19)	3.52(1)	(1)
C(21)	H(8)	3.16(1)	(1,1,0,-1)				

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z
(2) -X,Y,-Z+1/2

L: Lattice translation.
(1) 0, 0, 0
(2) 1/2, 1/2, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.



ORTEP Drawing of **3g**

X-ray Structure Report of **4**

Experimental

Data Collection

A colorless block crystal of $C_{34}H_{32}$ having approximate dimensions of 0.20 x 0.20 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 ° oscillations that were exposed for 60 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a =	11.8779(9) Å	α =	90.122(1)°
b =	12.792(1) Å	β =	98.129(5)°
c =	8.8346(5) Å	γ =	84.297(2)°

V = 1322.2(2) Å^3

For Z = 2 and F.W. = 440.63, the calculated density is 1.11 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of 23 ± 1°C to a maximum 2θ value of 55.0°. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0° in 5.0° step, at χ=45.0° and φ = 0.0°. The exposure rate was 330.0 [sec./°]. A second sweep was performed using ω scans from 0.0 to 160.0° in 5.0° step, at χ=45.0° and φ = 180.0°. The exposure rate was 330.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 11777 reflections that were collected, 5791 were unique (R_{int} = 0.025); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.6 cm^{-1}. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction[1] was applied (coefficient = 966.799988).

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[4] on F was based on 3462 observed reflections ($I > 1.70\sigma(I)$) and 339 variable parameters and converged (largest parameter shift was 0.95 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.100$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.193$$

The standard deviation of an observation of unit weight[5] was 1.05. A Sheldrick weighting scheme was used. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.49 and -0.40 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf" were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10,11] crystallographic software package.

References

(1) Larson, A.C. (1970), Crystallographic Computing, 291-294. F.R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where w = Least Squares weights.

(5) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

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(10) CrystalStructure 3.00: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2002).

(11) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{34}H_{32}$
Formula Weight	440.63
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.20 X 0.20 X 0.10 mm
Crystal System	triclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 60.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.8779(9) Å b = 12.792(1) Å c = 8.8346(5) Å α = 90.122(1) ° β = 98.129(5) ° γ = 84.297(2) ° V = 1322.2(2) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.107 g/cm^3
F_{000}	472.00
μ(MoKα)	0.62 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0°
Exposure Rate	330.0 sec./°
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 160.0°
Exposure Rate	330.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 11777 Unique: 5791 (R_{int} = 0.025)
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 9.66800e+002)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1 / [0.030Fo^2 + 1.000σ^2(Fo) + 0.000]
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>1.70σ(I))	3462
No. Variables	339
Reflection/Parameter Ratio	10.21
Residuals: R (I>2.00σ(I))	0.100
Residuals: Rw (I>1.70σ(I))	0.193
Goodness of Fit Indicator	1.05
Max Shift/Error in Final Cycle	0.95
Maximum peak in Final Diff. Map	0.49 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.40 e$^-$/Å^3

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

atom	x	y	z	B_{eq}
C(3)	0.3297(3)	0.2485(3)	1.0229(5)	4.10(9)
C(7)	0.0542(3)	0.3472(3)	1.2010(5)	3.90(8)
C(6)	0.1716(3)	0.3563(3)	1.1658(4)	3.55(8)
C(13)	0.2280(3)	0.4512(3)	1.2281(5)	3.71(8)
C(19)	0.1663(4)	0.1671(4)	0.8600(5)	4.7(1)
C(2)	0.2322(3)	0.1777(3)	1.0167(5)	3.86(9)
C(1)	0.2291(3)	0.2856(3)	1.0876(5)	3.59(8)
C(5)	0.3937(4)	0.2881(4)	0.9007(6)	5.1(1)
C(25)	0.2421(4)	0.0877(3)	1.1292(5)	4.31(9)
C(8)	0.0004(4)	0.4250(4)	1.2859(6)	5.2(1)
C(12)	-0.0069(4)	0.2622(4)	1.1509(6)	4.8(1)
C(14)	0.2171(5)	0.5450(3)	1.1460(6)	5.1(1)
C(4)	0.4583(4)	0.2435(3)	1.0528(7)	5.2(1)
C(18)	0.2913(4)	0.4452(4)	1.3717(5)	4.9(1)
C(26)	0.1668(4)	0.0102(4)	1.1109(7)	5.4(1)
C(11)	-0.1156(4)	0.2539(5)	1.1889(7)	6.3(1)
C(30)	0.3236(5)	0.0800(4)	1.2568(7)	5.9(1)
C(16)	0.3348(5)	0.6232(5)	1.3487(8)	6.5(2)
C(15)	0.2700(6)	0.6315(4)	1.2069(8)	6.5(2)
C(17)	0.3450(4)	0.5315(5)	1.4314(7)	5.9(1)
C(20)	0.0925(5)	0.2487(5)	0.7920(6)	6.4(1)
C(34)	0.3825(5)	0.4043(4)	0.8689(8)	7.0(2)
C(9)	-0.1078(4)	0.4163(5)	1.3228(6)	6.4(1)
C(31)	0.5105(4)	0.3166(5)	1.1698(8)	6.9(1)
C(27)	0.1735(6)	-0.0703(4)	1.2159(9)	7.1(2)
C(24)	0.1825(5)	0.0742(5)	0.7772(7)	6.6(2)
C(29)	0.3319(6)	-0.0014(5)	1.3625(8)	7.0(2)
C(10)	-0.1649(4)	0.3295(6)	1.2766(7)	6.9(2)
C(28)	0.2561(7)	-0.0772(5)	1.3393(9)	7.7(2)
C(33)	0.4039(6)	0.2215(5)	0.7591(8)	8.2(2)
C(32)	0.5301(5)	0.1374(5)	1.049(1)	8.3(2)
C(22)	0.062(1)	0.143(1)	0.5631(9)	11.8(3)
C(23)	0.1293(8)	0.0648(9)	0.635(1)	9.6(3)
C(21)	0.0390(8)	0.2386(7)	0.6407(8)	10.2(3)
H(10)	0.2984(4)	0.3821(4)	1.4303(5)	5.9(1)
H(9)	0.3889(4)	0.5271(5)	1.5303(7)	7.1(2)
H(8)	0.3720(5)	0.6816(5)	1.3897(8)	8.1(2)

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

atom	x	y	z	B_{eq}
H(7)	0.2626(6)	0.6953(4)	1.1499(8)	8.1(2)
H(6)	0.1722(5)	0.5510(3)	1.0479(6)	6.2(1)
H(20)	0.3748(5)	0.1327(4)	1.2744(7)	7.1(2)
H(19)	0.3893(6)	-0.0055(5)	1.4493(8)	8.3(2)
H(18)	0.2624(7)	-0.1344(5)	1.4095(9)	9.4(2)
H(17)	0.1202(6)	-0.1214(4)	1.2029(9)	8.9(2)
H(16)	0.1089(4)	0.0131(4)	1.0246(7)	6.7(2)
H(15)	0.2323(5)	0.0166(5)	0.8229(7)	8.3(2)
H(14)	0.1396(8)	0.0002(9)	0.583(1)	12.2(3)
H(13)	0.028(1)	0.137(1)	0.4598(9)	15.0(5)
H(12)	-0.0115(8)	0.2952(7)	0.5937(8)	12.2(3)
H(11)	0.0787(5)	0.3115(5)	0.8469(6)	7.8(2)
H(1)	0.0390(4)	0.4844(4)	1.3191(6)	6.2(1)
H(2)	-0.1429(4)	0.4702(5)	1.3797(6)	7.6(2)
H(3)	-0.2383(4)	0.3232(6)	1.3047(7)	8.3(2)
H(4)	-0.1555(4)	0.1954(5)	1.1549(7)	7.6(2)
H(5)	0.0264(4)	0.2095(4)	1.0904(6)	5.9(1)
H(21)	0.5328(4)	0.2804(5)	1.2648(8)	8.2(2)
H(22)	0.5756(4)	0.3419(5)	1.1365(8)	8.2(2)
H(23)	0.4556(4)	0.3741(5)	1.1821(8)	8.2(2)
H(30)	0.4140(5)	0.4407(4)	0.9563(8)	8.7(2)
H(31)	0.4213(5)	0.4179(4)	0.7852(8)	8.7(2)
H(32)	0.3036(5)	0.4277(4)	0.8438(8)	8.7(2)
H(24)	0.4818(5)	0.0826(5)	1.050(1)	10.1(3)
H(25)	0.5653(5)	0.1328(5)	0.959(1)	10.1(3)
H(26)	0.5873(5)	0.1307(5)	1.136(1)	10.1(3)
H(27)	0.3522(6)	0.1691(5)	0.7544(8)	10.6(3)
H(28)	0.3856(6)	0.2653(5)	0.6706(8)	10.6(3)
H(29)	0.4797(6)	0.1889(5)	0.7636(8)	10.6(3)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(3)	0.046(2)	0.033(2)	0.081(3)	-0.014(2)	0.018(2)	-0.010(2)
C(7)	0.034(2)	0.054(2)	0.057(2)	0.000(2)	0.002(2)	0.004(2)
C(6)	0.039(2)	0.039(2)	0.054(2)	-0.003(1)	0.000(2)	-0.003(1)
C(13)	0.040(2)	0.041(2)	0.061(2)	-0.002(1)	0.010(2)	-0.010(2)
C(19)	0.066(3)	0.063(3)	0.058(3)	-0.033(2)	0.019(2)	-0.011(2)
C(2)	0.044(2)	0.039(2)	0.069(2)	-0.015(2)	0.015(2)	-0.012(2)
C(1)	0.039(2)	0.035(2)	0.064(2)	-0.011(1)	0.006(2)	-0.006(2)
C(5)	0.053(2)	0.051(2)	0.099(4)	-0.017(2)	0.034(2)	-0.009(2)
C(25)	0.050(2)	0.036(2)	0.080(3)	-0.006(2)	0.016(2)	-0.005(2)
C(8)	0.049(2)	0.077(3)	0.069(3)	0.006(2)	0.007(2)	-0.014(2)
C(12)	0.043(2)	0.064(3)	0.078(3)	-0.010(2)	0.012(2)	-0.001(2)
C(14)	0.081(3)	0.042(2)	0.072(3)	-0.008(2)	0.009(2)	-0.002(2)
C(4)	0.042(2)	0.043(2)	0.115(4)	-0.009(2)	0.016(2)	-0.006(2)
C(18)	0.053(2)	0.065(3)	0.068(3)	-0.009(2)	0.006(2)	-0.008(2)
C(26)	0.069(3)	0.045(2)	0.097(4)	-0.017(2)	0.024(3)	-0.009(2)
C(11)	0.048(3)	0.095(4)	0.098(4)	-0.019(2)	0.013(2)	0.003(3)
C(30)	0.067(3)	0.070(3)	0.087(3)	-0.013(2)	0.006(3)	0.006(3)
C(16)	0.073(3)	0.069(3)	0.115(5)	-0.032(3)	0.032(3)	-0.038(3)
C(15)	0.102(4)	0.044(3)	0.109(4)	-0.020(3)	0.032(4)	-0.009(3)
C(17)	0.054(3)	0.087(4)	0.084(3)	-0.018(3)	0.008(2)	-0.029(3)
C(20)	0.103(4)	0.080(4)	0.064(3)	-0.044(3)	-0.002(3)	0.012(3)
C(34)	0.077(4)	0.065(3)	0.133(5)	-0.013(3)	0.044(4)	0.010(3)
C(9)	0.041(2)	0.121(5)	0.078(3)	0.009(3)	0.012(2)	-0.017(3)
C(31)	0.045(3)	0.083(4)	0.131(5)	-0.021(2)	0.002(3)	-0.021(3)
C(27)	0.106(5)	0.044(3)	0.131(6)	-0.020(3)	0.045(4)	0.002(3)
C(24)	0.088(4)	0.087(4)	0.088(4)	-0.041(3)	0.032(3)	-0.041(3)
C(29)	0.087(4)	0.080(4)	0.097(4)	0.007(3)	0.010(3)	0.017(3)
C(10)	0.038(2)	0.134(6)	0.091(4)	-0.006(3)	0.013(2)	0.001(4)
C(28)	0.127(6)	0.052(3)	0.120(5)	0.010(3)	0.051(5)	0.019(3)
C(33)	0.107(5)	0.103(5)	0.125(5)	-0.046(4)	0.074(4)	-0.039(4)
C(32)	0.067(4)	0.059(3)	0.193(8)	0.012(3)	0.044(4)	-0.001(4)
C(22)	0.22(1)	0.20(1)	0.056(4)	-0.141(9)	0.025(5)	-0.028(5)
C(23)	0.152(8)	0.151(8)	0.083(5)	-0.083(6)	0.043(5)	-0.053(5)
C(21)	0.157(8)	0.136(7)	0.093(5)	-0.081(6)	-0.036(5)	0.053(5)

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 (Å)

atom	atom	distance	atom	atom	distance
C(3)	C(2)	1.535(5)	C(3)	C(1)	1.435(5)
C(3)	C(5)	1.520(6)	C(3)	C(4)	1.507(6)
C(7)	C(6)	1.487(5)	C(7)	C(8)	1.402(6)
C(7)	C(12)	1.402(7)	C(6)	C(13)	1.509(5)
C(6)	C(1)	1.330(5)	C(13)	C(14)	1.389(6)
C(13)	C(18)	1.378(6)	C(19)	C(2)	1.504(6)
C(19)	C(20)	1.376(8)	C(19)	C(24)	1.406(7)
C(2)	C(1)	1.514(5)	C(2)	C(25)	1.508(6)
C(5)	C(4)	1.530(8)	C(5)	C(34)	1.503(7)
C(5)	C(33)	1.525(8)	C(25)	C(26)	1.394(6)
C(25)	C(30)	1.375(7)	C(8)	C(9)	1.386(7)
C(12)	C(11)	1.393(6)	C(14)	C(15)	1.397(7)
C(4)	C(31)	1.503(7)	C(4)	C(32)	1.533(7)
C(18)	C(17)	1.396(7)	C(26)	C(27)	1.376(8)
C(11)	C(10)	1.376(8)	C(30)	C(29)	1.387(8)
C(16)	C(15)	1.373(9)	C(16)	C(17)	1.370(9)
C(20)	C(21)	1.408(9)	C(9)	C(10)	1.389(9)
C(27)	C(28)	1.36(1)	C(24)	C(23)	1.33(1)
C(29)	C(28)	1.38(1)	C(22)	C(23)	1.32(1)
C(22)	C(21)	1.42(1)			

Table 4. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(8)	H(1)	0.950(7)	C(12)	H(5)	0.950(7)
C(14)	H(6)	0.950(7)	C(18)	H(10)	0.950(7)
C(26)	H(16)	0.950(7)	C(11)	H(4)	0.950(8)
C(30)	H(20)	0.950(8)	C(16)	H(8)	0.950(8)
C(15)	H(7)	0.950(8)	C(17)	H(9)	0.950(7)
C(20)	H(11)	0.950(8)	C(34)	H(30)	0.950(9)
C(34)	H(31)	0.95(1)	C(34)	H(32)	0.950(8)
C(9)	H(2)	0.950(8)	C(31)	H(21)	0.950(9)
C(31)	H(22)	0.950(8)	C(31)	H(23)	0.950(8)
C(27)	H(17)	0.950(9)	C(24)	H(15)	0.950(8)
C(29)	H(19)	0.950(9)	C(10)	H(3)	0.950(8)
C(28)	H(18)	0.950(9)	C(33)	H(27)	0.95(1)
C(33)	H(28)	0.95(1)	C(33)	H(29)	0.950(9)
C(32)	H(24)	0.950(9)	C(32)	H(25)	0.95(1)
C(32)	H(26)	0.95(1)	C(22)	H(13)	0.95(1)
C(23)	H(14)	0.95(1)	C(21)	H(12)	0.95(1)

Table 5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	C(1)	61.2(2)	C(2)	C(3)	C(5)	132.6(4)
C(1)	C(3)	C(5)	135.4(4)	C(2)	C(3)	C(4)	141.1(4)
C(1)	C(3)	C(4)	142.0(4)	C(5)	C(3)	C(4)	60.7(3)
C(6)	C(7)	C(8)	120.3(4)	C(6)	C(7)	C(12)	122.0(4)
C(8)	C(7)	C(12)	117.7(4)	C(7)	C(6)	C(13)	116.5(3)
C(7)	C(6)	C(1)	124.2(3)	C(13)	C(6)	C(1)	119.3(3)
C(6)	C(13)	C(14)	122.1(4)	C(6)	C(13)	C(18)	119.1(4)
C(14)	C(13)	C(18)	118.8(4)	C(2)	C(19)	C(20)	121.2(4)
C(2)	C(19)	C(24)	120.3(5)	C(20)	C(19)	C(24)	118.5(5)
C(3)	C(2)	C(19)	114.5(3)	C(3)	C(2)	C(1)	56.2(2)
C(19)	C(2)	C(1)	118.0(4)	C(3)	C(2)	C(25)	119.5(4)
C(19)	C(2)	C(25)	118.8(3)	C(1)	C(2)	C(25)	114.8(3)
C(3)	C(1)	C(6)	151.1(4)	C(3)	C(1)	C(2)	62.7(3)
C(6)	C(1)	C(2)	146.0(3)	C(3)	C(5)	C(4)	59.2(3)
C(3)	C(5)	C(34)	118.1(4)	C(4)	C(5)	C(34)	120.1(5)
C(3)	C(5)	C(33)	118.5(4)	C(4)	C(5)	C(33)	117.0(5)
C(34)	C(5)	C(33)	113.6(5)	C(2)	C(25)	C(26)	121.5(4)
C(2)	C(25)	C(30)	121.5(4)	C(26)	C(25)	C(30)	117.0(4)
C(7)	C(8)	C(9)	121.0(5)	C(7)	C(12)	C(11)	121.0(5)
C(13)	C(14)	C(15)	120.8(5)	C(3)	C(4)	C(5)	60.0(3)
C(3)	C(4)	C(31)	117.7(4)	C(5)	C(4)	C(31)	119.6(4)
C(3)	C(4)	C(32)	119.7(4)	C(5)	C(4)	C(32)	117.3(5)
C(31)	C(4)	C(32)	112.9(5)	C(13)	C(18)	C(17)	120.2(5)
C(25)	C(26)	C(27)	121.5(6)	C(12)	C(11)	C(10)	120.2(5)
C(25)	C(30)	C(29)	121.9(5)	C(15)	C(16)	C(17)	120.2(5)
C(14)	C(15)	C(16)	119.6(5)	C(18)	C(17)	C(16)	120.5(5)
C(19)	C(20)	C(21)	119.5(7)	C(8)	C(9)	C(10)	120.3(5)
C(26)	C(27)	C(28)	120.3(6)	C(19)	C(24)	C(23)	121.4(8)
C(30)	C(29)	C(28)	119.3(6)	C(11)	C(10)	C(9)	119.8(5)
C(27)	C(28)	C(29)	120.0(6)	C(23)	C(22)	C(21)	119.8(7)
C(24)	C(23)	C(22)	122.0(8)	C(20)	C(21)	C(22)	118.7(8)

Table 6. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	C(8)	H(1)	119.6(6)	C(9)	C(8)	H(1)	119.5(6)
C(7)	C(12)	H(5)	119.5(5)	C(11)	C(12)	H(5)	119.5(6)
C(13)	C(14)	H(6)	119.9(6)	C(15)	C(14)	H(6)	119.4(6)
C(13)	C(18)	H(10)	119.9(6)	C(17)	C(18)	H(10)	119.8(6)
C(25)	C(26)	H(16)	119.5(6)	C(27)	C(26)	H(16)	118.9(7)
C(12)	C(11)	H(4)	120.0(7)	C(10)	C(11)	H(4)	119.9(7)
C(25)	C(30)	H(20)	119.2(6)	C(29)	C(30)	H(20)	118.9(7)
C(15)	C(16)	H(8)	119.8(7)	C(17)	C(16)	H(8)	120.1(7)
C(14)	C(15)	H(7)	120.4(7)	C(16)	C(15)	H(7)	120.1(7)
C(18)	C(17)	H(9)	120.1(6)	C(16)	C(17)	H(9)	119.5(7)
C(19)	C(20)	H(11)	119.8(7)	C(21)	C(20)	H(11)	120.7(8)
C(5)	C(34)	H(30)	110.5(7)	C(5)	C(34)	H(31)	109.6(7)
H(30)	C(34)	H(31)	109.5(8)	C(5)	C(34)	H(32)	108.3(7)
H(30)	C(34)	H(32)	109.5(8)	H(31)	C(34)	H(32)	109.5(8)
C(8)	C(9)	H(2)	119.6(7)	C(10)	C(9)	H(2)	120.1(7)
C(4)	C(31)	H(21)	109.8(7)	C(4)	C(31)	H(22)	109.7(7)
H(21)	C(31)	H(22)	109.5(8)	C(4)	C(31)	H(23)	109.0(7)
H(21)	C(31)	H(23)	109.5(8)	H(22)	C(31)	H(23)	109.5(8)
C(26)	C(27)	H(17)	120.4(8)	C(28)	C(27)	H(17)	119.3(8)
C(19)	C(24)	H(15)	119.7(7)	C(23)	C(24)	H(15)	118.9(9)
C(30)	C(29)	H(19)	120.5(8)	C(28)	C(29)	H(19)	120.3(8)
C(11)	C(10)	H(3)	120.4(7)	C(9)	C(10)	H(3)	119.8(7)
C(27)	C(28)	H(18)	120.1(9)	C(29)	C(28)	H(18)	119.9(9)
C(5)	C(33)	H(27)	109.5(8)	C(5)	C(33)	H(28)	109.1(8)
H(27)	C(33)	H(28)	109.5(9)	C(5)	C(33)	H(29)	109.8(8)
H(27)	C(33)	H(29)	109.5(9)	H(28)	C(33)	H(29)	109.5(9)
C(4)	C(32)	H(24)	109.1(7)	C(4)	C(32)	H(25)	109.9(7)
H(24)	C(32)	H(25)	109.5(9)	C(4)	C(32)	H(26)	109.4(7)
H(24)	C(32)	H(26)	109.5(9)	H(25)	C(32)	H(26)	109.5(9)
C(23)	C(22)	H(13)	121.4(1)	C(21)	C(22)	H(13)	118.8(1)
C(24)	C(23)	H(14)	119.7(1)	C(22)	C(23)	H(14)	118.3(1)
C(20)	C(21)	H(12)	119.4(1)	C(22)	C(21)	H(12)	121.9(1)

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	C(3)	C(2)	C(19)	108.3(6)	C(1)	C(3)	C(2)	C(1)	0.0(3)
C(1)	C(3)	C(2)	C(25)	-101.6(6)	C(5)	C(3)	C(2)	C(19)	-18.4(1)
C(5)	C(3)	C(2)	C(1)	-126.7(9)	C(5)	C(3)	C(2)	C(25)	131.7(7)
C(4)	C(3)	C(2)	C(19)	-113.1(9)	C(4)	C(3)	C(2)	C(1)	138.6(1)
C(4)	C(3)	C(2)	C(25)	37.0(1)	C(2)	C(3)	C(1)	C(6)	173.9(1)
C(2)	C(3)	C(1)	C(2)	0.0(3)	C(5)	C(3)	C(1)	C(6)	-63.2(2)
C(5)	C(3)	C(1)	C(2)	122.8(9)	C(4)	C(3)	C(1)	C(6)	36.3(2)
C(4)	C(3)	C(1)	C(2)	-137.6(1)	C(2)	C(3)	C(5)	C(4)	-134.2(7)
C(2)	C(3)	C(5)	C(34)	115.6(8)	C(2)	C(3)	C(5)	C(33)	-28.0(1)
C(1)	C(3)	C(5)	C(4)	135.8(8)	C(1)	C(3)	C(5)	C(34)	25.7(1)
C(1)	C(3)	C(5)	C(33)	-118.0(8)	C(4)	C(3)	C(5)	C(4)	0.0(4)
C(4)	C(3)	C(5)	C(34)	-110.2(7)	C(4)	C(3)	C(5)	C(33)	106.2(8)
C(2)	C(3)	C(4)	C(5)	122.8(9)	C(2)	C(3)	C(4)	C(31)	-127.2(8)
C(2)	C(3)	C(4)	C(32)	16.4(1)	C(1)	C(3)	C(4)	C(5)	-127.4(9)
C(1)	C(3)	C(4)	C(31)	-17.4(1)	C(1)	C(3)	C(4)	C(32)	126.2(8)
C(5)	C(3)	C(4)	C(5)	0.0(4)	C(5)	C(3)	C(4)	C(31)	110.0(7)
C(5)	C(3)	C(4)	C(32)	-106.4(8)	C(8)	C(7)	C(6)	C(13)	1.0(9)
C(8)	C(7)	C(6)	C(1)	179.2(6)	C(12)	C(7)	C(6)	C(13)	-179.3(6)
C(12)	C(7)	C(6)	C(1)	-1.1(1)	C(6)	C(7)	C(8)	C(9)	-178.3(6)
C(12)	C(7)	C(8)	C(9)	2.0(1)	C(6)	C(7)	C(12)	C(11)	178.2(6)
C(8)	C(7)	C(12)	C(11)	-2.1(1)	C(7)	C(6)	C(13)	C(14)	-89.9(7)
C(7)	C(6)	C(13)	C(18)	89.3(7)	C(1)	C(6)	C(13)	C(14)	91.8(7)
C(1)	C(6)	C(13)	C(18)	-89.0(7)	C(7)	C(6)	C(1)	C(3)	-178.9(7)
C(7)	C(6)	C(1)	C(2)	-8.6(1)	C(13)	C(6)	C(1)	C(3)	-0.7(1)
C(13)	C(6)	C(1)	C(2)	169.6(6)	C(6)	C(13)	C(14)	C(15)	179.8(6)
C(18)	C(13)	C(14)	C(15)	0.6(1)	C(6)	C(13)	C(18)	C(17)	179.5(5)
C(14)	C(13)	C(18)	C(17)	-1.3(1)	C(20)	C(19)	C(2)	C(3)	-72.4(9)
C(20)	C(19)	C(2)	C(1)	-9.2(1)	C(20)	C(19)	C(2)	C(25)	137.4(7)
C(24)	C(19)	C(2)	C(3)	105.1(8)	C(24)	C(19)	C(2)	C(1)	168.3(7)
C(24)	C(19)	C(2)	C(25)	-45.2(1)	C(2)	C(19)	C(20)	C(21)	175.2(7)
C(24)	C(19)	C(20)	C(21)	-2.3(1)	C(2)	C(19)	C(24)	C(23)	-176.7(8)
C(20)	C(19)	C(24)	C(23)	0.8(1)	C(3)	C(2)	C(1)	C(3)	0.0(3)
C(3)	C(2)	C(1)	C(6)	-174.8(1)	C(19)	C(2)	C(1)	C(3)	-102.1(6)
C(19)	C(2)	C(1)	C(6)	83.2(1)	C(25)	C(2)	C(1)	C(3)	110.1(6)
C(25)	C(2)	C(1)	C(6)	-64.7(1)	C(3)	C(2)	C(25)	C(26)	-168.0(6)
C(3)	C(2)	C(25)	C(30)	14.0(9)	C(19)	C(2)	C(25)	C(26)	-19.3(9)
C(19)	C(2)	C(25)	C(30)	162.8(6)	C(1)	C(2)	C(25)	C(26)	128.3(6)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle
C(1)	C(2)	C(25)	C(30)	-49.7(8)
C(3)	C(5)	C(4)	C(31)	-106.8(7)
C(34)	C(5)	C(4)	C(3)	106.7(9)
C(34)	C(5)	C(4)	C(32)	-143.1(8)
C(33)	C(5)	C(4)	C(31)	144.6(8)
C(2)	C(25)	C(26)	C(27)	-178.0(6)
C(2)	C(25)	C(30)	C(29)	178.7(6)
C(7)	C(8)	C(9)	C(10)	0.3(1)
C(13)	C(14)	C(15)	C(16)	0.9(1)
C(25)	C(26)	C(27)	C(28)	-1.4(1)
C(25)	C(30)	C(29)	C(28)	-0.0(1)
C(15)	C(16)	C(17)	C(18)	1.0(1)
C(8)	C(9)	C(10)	C(11)	-2.5(1)
C(19)	C(24)	C(23)	C(22)	2.6(2)
C(21)	C(22)	C(23)	C(24)	-4.2(2)

atom	atom	atom	atom	angle
C(3)	C(5)	C(4)	C(3)	0.0(3)
C(3)	C(5)	C(4)	C(32)	110.2(7)
C(34)	C(5)	C(4)	C(31)	-0.1(1)
C(33)	C(5)	C(4)	C(3)	-108.6(9)
C(33)	C(5)	C(4)	C(32)	1.6(1)
C(30)	C(25)	C(26)	C(27)	0.0(1)
C(26)	C(25)	C(30)	C(29)	0.6(1)
C(7)	C(12)	C(11)	C(10)	0.0(1)
C(13)	C(18)	C(17)	C(16)	0.5(1)
C(12)	C(11)	C(10)	C(9)	2.3(1)
C(17)	C(16)	C(15)	C(14)	-1.8(1)
C(19)	C(20)	C(21)	C(22)	0.7(1)
C(26)	C(27)	C(28)	C(29)	2.0(1)
C(30)	C(29)	C(28)	C(27)	-1.3(1)
C(23)	C(22)	C(21)	C(20)	2.5(2)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
C(3)	C(6)	2.678(5)	(1)	C(3)	C(13)	3.383(5)	(1)
C(3)	C(19)	2.555(6)	(1)	C(3)	C(2)	1.535(5)	(1)
C(3)	C(1)	1.435(5)	(1)	C(3)	C(5)	1.520(6)	(1)
C(3)	C(25)	2.628(5)	(1)	C(3)	C(4)	1.507(6)	(1)
C(3)	C(30)	3.002(7)	(1)	C(3)	C(20)	3.237(7)	(1)
C(3)	C(34)	2.592(6)	(1)	C(3)	C(31)	2.576(6)	(1)
C(3)	C(24)	3.525(6)	(1)	C(3)	C(33)	2.616(7)	(1)
C(3)	C(32)	2.629(7)	(1)	C(7)	C(6)	1.487(5)	(1)
C(7)	C(13)	2.548(5)	(1)	C(7)	C(2)	3.445(5)	(1)
C(7)	C(1)	2.490(5)	(1)	C(7)	C(8)	1.402(6)	(1)
C(7)	C(12)	1.402(7)	(1)	C(7)	C(14)	3.409(6)	(1)
C(7)	C(18)	3.357(6)	(1)	C(7)	C(11)	2.433(7)	(1)
C(7)	C(9)	2.426(6)	(1)	C(7)	C(10)	2.807(6)	(1)
C(6)	C(13)	1.509(5)	(1)	C(6)	C(2)	2.720(5)	(1)
C(6)	C(1)	1.330(5)	(1)	C(6)	C(25)	3.481(5)	(1)
C(6)	C(8)	2.507(5)	(1)	C(6)	C(12)	2.527(6)	(1)
C(6)	C(14)	2.537(6)	(1)	C(6)	C(18)	2.491(6)	(1)
C(13)	C(1)	2.452(5)	(1)	C(13)	C(8)	2.872(6)	(1)
C(13)	C(14)	1.389(6)	(1)	C(13)	C(18)	1.378(6)	(1)
C(13)	C(16)	2.784(7)	(1)	C(13)	C(15)	2.422(6)	(1)
C(13)	C(17)	2.405(6)	(1)	C(19)	C(2)	1.504(6)	(1)
C(19)	C(1)	2.586(6)	(1)	C(19)	C(5)	3.221(6)	(1)
C(19)	C(25)	2.593(7)	(1)	C(19)	C(26)	2.992(7)	(1)
C(19)	C(20)	1.376(8)	(1)	C(19)	C(24)	1.406(7)	(1)
C(19)	C(33)	3.217(7)	(1)	C(19)	C(22)	2.77(1)	(1)
C(19)	C(23)	2.389(8)	(1)	C(19)	C(21)	2.404(8)	(1)
C(2)	C(1)	1.514(5)	(1)	C(2)	C(5)	2.797(5)	(1)
C(2)	C(25)	1.508(6)	(1)	C(2)	C(12)	3.313(6)	(1)
C(2)	C(4)	2.869(6)	(1)	C(2)	C(26)	2.532(6)	(1)
C(2)	C(30)	2.516(7)	(1)	C(2)	C(20)	2.510(7)	(1)
C(2)	C(24)	2.524(6)	(1)	C(2)	C(33)	3.346(6)	(1)
C(2)	C(32)	3.496(7)	(1)	C(1)	C(5)	2.734(6)	(1)
C(1)	C(25)	2.546(5)	(1)	C(1)	C(12)	2.978(5)	(1)
C(1)	C(14)	3.349(6)	(1)	C(1)	C(4)	2.782(5)	(1)
C(1)	C(18)	3.281(6)	(1)	C(1)	C(30)	3.060(7)	(1)
C(1)	C(20)	2.937(7)	(1)	C(1)	C(34)	3.305(6)	(1)
C(1)	C(31)	3.382(6)	(1)	C(5)	C(4)	1.530(8)	(1)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(5)	C(34)	1.503(7)	(1)	C(5)	C(31)	2.622(8)	(1)
C(5)	C(33)	1.525(8)	(1)	C(5)	C(32)	2.617(8)	(1)
C(25)	C(12)	3.552(6)	(1)	C(25)	C(4)	3.541(6)	(1)
C(25)	C(26)	1.394(6)	(1)	C(25)	C(30)	1.375(7)	(1)
C(25)	C(27)	2.417(6)	(1)	C(25)	C(24)	3.098(8)	(1)
C(25)	C(29)	2.415(8)	(1)	C(25)	C(28)	2.790(7)	(1)
C(8)	C(12)	2.400(7)	(1)	C(8)	C(14)	3.492(7)	(1)
C(8)	C(18)	3.466(7)	(1)	C(8)	C(11)	2.772(8)	(1)
C(8)	C(9)	1.386(7)	(1)	C(8)	C(10)	2.406(8)	(1)
C(12)	C(11)	1.393(6)	(1)	C(12)	C(20)	3.535(7)	(1)
C(12)	C(9)	2.768(7)	(1)	C(12)	C(10)	2.401(7)	(1)
C(14)	C(18)	2.382(7)	(1)	C(14)	C(16)	2.393(8)	(1)
C(14)	C(15)	1.397(7)	(1)	C(14)	C(17)	2.751(8)	(1)
C(4)	C(30)	3.418(7)	(1)	C(4)	C(34)	2.629(8)	(1)
C(4)	C(31)	1.503(7)	(1)	C(4)	C(33)	2.605(9)	(1)
C(4)	C(32)	1.533(7)	(1)	C(18)	C(16)	2.401(7)	(1)
C(18)	C(15)	2.767(8)	(1)	C(18)	C(17)	1.396(7)	(1)
C(26)	C(30)	2.361(8)	(1)	C(26)	C(27)	1.376(8)	(1)
C(26)	C(24)	3.097(8)	(1)	C(26)	C(29)	2.742(9)	(1)
C(26)	C(28)	2.37(1)	(1)	C(11)	C(9)	2.393(9)	(1)
C(11)	C(10)	1.376(8)	(1)	C(30)	C(27)	2.739(8)	(1)
C(30)	C(29)	1.387(8)	(1)	C(30)	C(28)	2.390(8)	(1)
C(30)	C(32)	3.400(9)	(1)	C(16)	C(15)	1.373(9)	(1)
C(16)	C(17)	1.370(9)	(1)	C(15)	C(17)	2.377(9)	(1)
C(20)	C(24)	2.390(9)	(1)	C(20)	C(22)	2.43(1)	(1)
C(20)	C(23)	2.76(1)	(1)	C(20)	C(21)	1.408(9)	(1)
C(34)	C(31)	3.03(1)	(1)	C(34)	C(33)	2.534(8)	(1)
C(9)	C(10)	1.389(9)	(1)	C(31)	C(32)	2.531(8)	(1)
C(27)	C(29)	2.37(1)	(1)	C(27)	C(28)	1.36(1)	(1)
C(24)	C(33)	3.405(8)	(1)	C(24)	C(22)	2.32(1)	(1)
C(24)	C(23)	1.33(1)	(1)	C(24)	C(21)	2.74(1)	(1)
C(29)	C(28)	1.38(1)	(1)	C(28)	C(23)	3.60(1)	(1,1,0,0,1)
C(33)	C(32)	2.93(1)	(1)	C(22)	C(23)	1.32(1)	(1)
C(22)	C(21)	1.42(1)	(1)	C(23)	C(21)	2.37(2)	(1)

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z

L: Lattice translation.
(1) 0, 0, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
C(3)	H(20)	2.63(2)	(1)	C(3)	H(11)	3.19(3)	(1)
C(3)	H(21)	3.05(3)	(1)	C(3)	H(22)	3.29(3)	(1)
C(3)	H(23)	2.58(2)	(1)	C(3)	H(30)	2.84(2)	(1)
C(3)	H(31)	3.38(3)	(1)	C(3)	H(32)	2.75(2)	(1)
C(3)	H(24)	2.63(2)	(1)	C(3)	H(25)	3.15(3)	(1)
C(3)	H(26)	3.29(3)	(1)	C(3)	H(27)	2.62(2)	(1)
C(3)	H(28)	3.29(3)	(1)	C(3)	H(29)	3.14(3)	(1)
C(7)	H(10)	3.36(3)	(1)	C(7)	H(6)	3.44(3)	(1)
C(7)	H(6)	3.38(3)	(-1,1,0,1,2)	C(7)	H(13)	3.60(7)	(1,1,0,0,1)
C(7)	H(11)	3.21(2)	(1)	C(7)	H(1)	2.04(1)	(1)
C(7)	H(2)	3.28(3)	(1)	C(7)	H(4)	3.29(3)	(1)
C(7)	H(5)	2.04(1)	(1)	C(6)	H(10)	2.63(2)	(1)
C(6)	H(6)	2.70(2)	(1)	C(6)	H(20)	3.59(3)	(1)
C(6)	H(11)	2.95(2)	(1)	C(6)	H(1)	2.66(2)	(1)
C(6)	H(5)	2.69(2)	(1)	C(6)	H(23)	3.39(2)	(1)
C(6)	H(32)	3.60(4)	(1)	C(13)	H(10)	2.03(1)	(1)
C(13)	H(9)	3.26(3)	(1)	C(13)	H(7)	3.28(2)	(1)
C(13)	H(6)	2.04(1)	(1)	C(13)	H(1)	2.49(2)	(1)
C(13)	H(23)	2.87(2)	(1)	C(13)	H(30)	3.48(4)	(1)
C(19)	H(17)	3.48(4)	(-1,1,0,0,2)	C(19)	H(16)	2.65(2)	(1)
C(19)	H(15)	2.05(2)	(1)	C(19)	H(14)	3.25(4)	(1)
C(19)	H(12)	3.26(4)	(1)	C(19)	H(11)	2.02(2)	(1)
C(19)	H(5)	2.82(3)	(1)	C(19)	H(27)	2.52(2)	(1)
C(2)	H(20)	2.67(3)	(1)	C(2)	H(16)	2.69(2)	(1)
C(2)	H(15)	2.68(2)	(1)	C(2)	H(11)	2.67(2)	(1)
C(2)	H(5)	2.61(2)	(1)	C(2)	H(24)	3.06(2)	(1)
C(2)	H(27)	2.88(3)	(1)	C(1)	H(10)	3.29(2)	(1)
C(1)	H(6)	3.40(2)	(1)	C(1)	H(20)	2.84(2)	(1)
C(1)	H(11)	2.58(2)	(1)	C(1)	H(5)	2.69(2)	(1)
C(1)	H(23)	3.03(2)	(1)	C(1)	H(30)	3.42(3)	(1)
C(1)	H(32)	3.10(3)	(1)	C(5)	H(21)	3.40(4)	(1)
C(5)	H(22)	2.91(3)	(1)	C(5)	H(23)	2.75(2)	(1)
C(5)	H(30)	2.04(2)	(1)	C(5)	H(31)	2.03(2)	(1)
C(5)	H(32)	2.02(1)	(1)	C(5)	H(24)	2.97(2)	(1)
C(5)	H(25)	2.69(2)	(1)	C(5)	H(26)	3.38(4)	(1)
C(5)	H(27)	2.05(2)	(1)	C(5)	H(28)	2.04(2)	(1)
C(5)	H(29)	2.05(2)	(1)	C(25)	H(20)	2.02(2)	(1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(25)	H(19)	3.27(3)	(1)	C(25)	H(17)	3.27(3)	(1)
C(25)	H(16)	2.04(2)	(1)	C(25)	H(15)	2.84(2)	(1)
C(25)	H(5)	2.84(2)	(1)	C(25)	H(24)	3.02(3)	(1)
C(8)	H(10)	3.58(3)	(1)	C(8)	H(6)	3.34(3)	(-1,1,0,1,2)
C(8)	H(12)	3.22(6)	(1,1,0,0,1)	C(8)	H(11)	3.56(4)	(-1,1,0,1,2)
C(8)	H(1)	0.950(7)	(1)	C(8)	H(2)	2.03(2)	(1)
C(8)	H(2)	3.52(2)	(-1,1,0,1,3)	C(8)	H(3)	3.26(3)	(1)
C(8)	H(5)	3.26(2)	(1)	C(12)	H(6)	3.28(4)	(-1,1,0,1,2)
C(12)	H(16)	3.58(3)	(1)	C(12)	H(13)	3.12(6)	(1,1,0,0,1)
C(12)	H(11)	3.09(3)	(1)	C(12)	H(1)	3.26(2)	(1)
C(12)	H(3)	3.26(3)	(1)	C(12)	H(4)	2.04(2)	(1)
C(12)	H(5)	0.950(7)	(1)	C(14)	H(10)	3.24(3)	(1)
C(14)	H(8)	3.25(3)	(1)	C(14)	H(7)	2.05(1)	(1)
C(14)	H(6)	0.950(7)	(1)	C(14)	H(1)	2.94(3)	(1)
C(14)	H(23)	3.38(3)	(1)	C(14)	H(30)	3.25(3)	(1)
C(14)	H(32)	3.30(3)	(1)	C(4)	H(20)	2.77(2)	(1)
C(4)	H(21)	2.03(2)	(1)	C(4)	H(22)	2.03(2)	(1)
C(4)	H(23)	2.02(2)	(1)	C(4)	H(30)	2.64(2)	(1)
C(4)	H(31)	3.21(3)	(1)	C(4)	H(32)	3.25(3)	(1)
C(4)	H(24)	2.05(1)	(1)	C(4)	H(25)	2.06(2)	(1)
C(4)	H(26)	2.05(2)	(1)	C(4)	H(27)	2.96(3)	(1)
C(4)	H(28)	3.37(3)	(1)	C(4)	H(29)	2.69(3)	(1)
C(18)	H(10)	0.950(7)	(1)	C(18)	H(9)	2.04(2)	(1)
C(18)	H(8)	3.26(3)	(1)	C(18)	H(6)	3.24(3)	(1)
C(18)	H(1)	2.96(2)	(1)	C(18)	H(2)	3.13(3)	(-1,1,0,1,3)
C(18)	H(23)	2.83(3)	(1)	C(18)	H(28)	3.49(7)	(1,1,0,0,1)
C(26)	H(20)	3.22(3)	(1)	C(26)	H(18)	3.23(3)	(1)
C(26)	H(17)	2.03(2)	(1)	C(26)	H(16)	0.950(7)	(1)
C(26)	H(16)	3.365(7)	(-1,1,0,0,2)	C(26)	H(15)	2.77(3)	(1)
C(26)	H(4)	3.52(4)	(-1,1,0,0,2)	C(26)	H(5)	2.90(2)	(1)
C(11)	H(7)	3.28(8)	(-1,1,0,1,2)	C(11)	H(6)	3.22(5)	(-1,1,0,1,2)
C(11)	H(13)	3.04(9)	(1,1,0,0,1)	C(11)	H(2)	3.25(3)	(1)
C(11)	H(3)	2.03(2)	(1)	C(11)	H(4)	0.950(8)	(1)
C(11)	H(5)	2.04(2)	(1)	C(30)	H(20)	0.950(8)	(1)
C(30)	H(19)	2.04(2)	(1)	C(30)	H(18)	3.25(3)	(1)
C(30)	H(16)	3.22(3)	(1)	C(30)	H(24)	2.80(3)	(1)
C(30)	H(25)	3.57(6)	(-1,1,1,0,2)	C(30)	H(26)	3.57(4)	(1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(16)	H(10)	3.25(3)	(1)	C(16)	H(9)	2.02(2)	(1)
C(16)	H(8)	0.950(8)	(1)	C(16)	H(7)	2.02(2)	(1)
C(16)	H(6)	3.25(3)	(1)	C(16)	H(18)	3.20(9)	(1,1,0,1)
C(16)	H(3)	3.46(8)	(-1,1,0,1,3)	C(16)	H(31)	3.28(6)	(-1,1,1,1,2)
C(15)	H(9)	3.23(3)	(1)	C(15)	H(8)	2.02(2)	(1)
C(15)	H(7)	0.950(8)	(1)	C(15)	H(6)	2.04(2)	(1)
C(15)	H(18)	3.48(8)	(1,1,0,1)	C(15)	H(17)	3.47(8)	(1,1,0,1)
C(17)	H(10)	2.04(2)	(1)	C(17)	H(9)	0.950(7)	(1)
C(17)	H(9)	3.145(7)	(-1,1,1,1,3)	C(17)	H(8)	2.02(2)	(1)
C(17)	H(7)	3.23(3)	(1)	C(17)	H(2)	3.11(4)	(-1,1,0,1,3)
C(17)	H(3)	3.29(8)	(-1,1,0,1,3)	C(17)	H(23)	3.30(3)	(1)
C(17)	H(31)	3.41(6)	(1,1,0,0,1)	C(20)	H(17)	3.15(6)	(-1,1,0,0,2)
C(20)	H(15)	3.25(3)	(1)	C(20)	H(13)	3.29(4)	(1)
C(20)	H(12)	2.05(2)	(1)	C(20)	H(11)	0.950(8)	(1)
C(20)	H(5)	2.91(2)	(1)	C(20)	H(32)	3.54(3)	(1)
C(20)	H(27)	3.21(3)	(1)	C(34)	H(9)	3.40(6)	(1,1,0,0,-1)
C(34)	H(6)	3.53(4)	(1)	C(34)	H(2)	3.6(2)	(-1,1,0,1,2)
C(34)	H(22)	3.10(4)	(1)	C(34)	H(22)	3.33(4)	(-1,1,1,1,2)
C(34)	H(23)	2.80(3)	(1)	C(34)	H(30)	0.950(9)	(1)
C(34)	H(30)	3.470(9)	(-1,1,1,1,2)	C(34)	H(31)	0.95(1)	(1)
C(34)	H(32)	0.950(8)	(1)	C(34)	H(27)	3.21(3)	(1)
C(34)	H(28)	2.50(2)	(1)	C(34)	H(29)	3.08(3)	(1)
C(9)	H(6)	3.27(6)	(-1,1,0,1,2)	C(9)	H(12)	2.88(8)	(1,1,0,0,1)
C(9)	H(1)	2.03(2)	(1)	C(9)	H(1)	3.43(2)	(-1,1,0,1,3)
C(9)	H(2)	0.950(8)	(1)	C(9)	H(3)	2.04(2)	(1)
C(9)	H(4)	3.25(3)	(1)	C(9)	H(32)	3.1(1)	(-1,1,0,1,2)
C(31)	H(9)	3.46(5)	(-1,1,1,1,3)	C(31)	H(20)	3.19(3)	(1)
C(31)	H(3)	3.06(9)	(1,1,1)	C(31)	H(21)	0.950(9)	(1)
C(31)	H(22)	0.950(8)	(1)	C(31)	H(23)	0.950(8)	(1)
C(31)	H(30)	2.54(2)	(1)	C(31)	H(30)	3.54(2)	(-1,1,1,1,2)
C(31)	H(31)	3.58(4)	(-1,1,1,1,2)	C(31)	H(24)	3.21(3)	(1)
C(31)	H(25)	3.07(3)	(1)	C(31)	H(26)	2.49(2)	(1)
C(27)	H(7)	3.16(8)	(1,1,0,-1)	C(27)	H(19)	3.23(4)	(1)
C(27)	H(18)	2.01(2)	(1)	C(27)	H(17)	0.950(9)	(1)
C(27)	H(16)	2.02(2)	(1)	C(27)	H(14)	3.43(7)	(1,1,0,0,1)
C(24)	H(16)	2.62(2)	(1)	C(24)	H(15)	0.950(8)	(1)
C(24)	H(14)	1.98(2)	(1)	C(24)	H(13)	3.18(4)	(1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

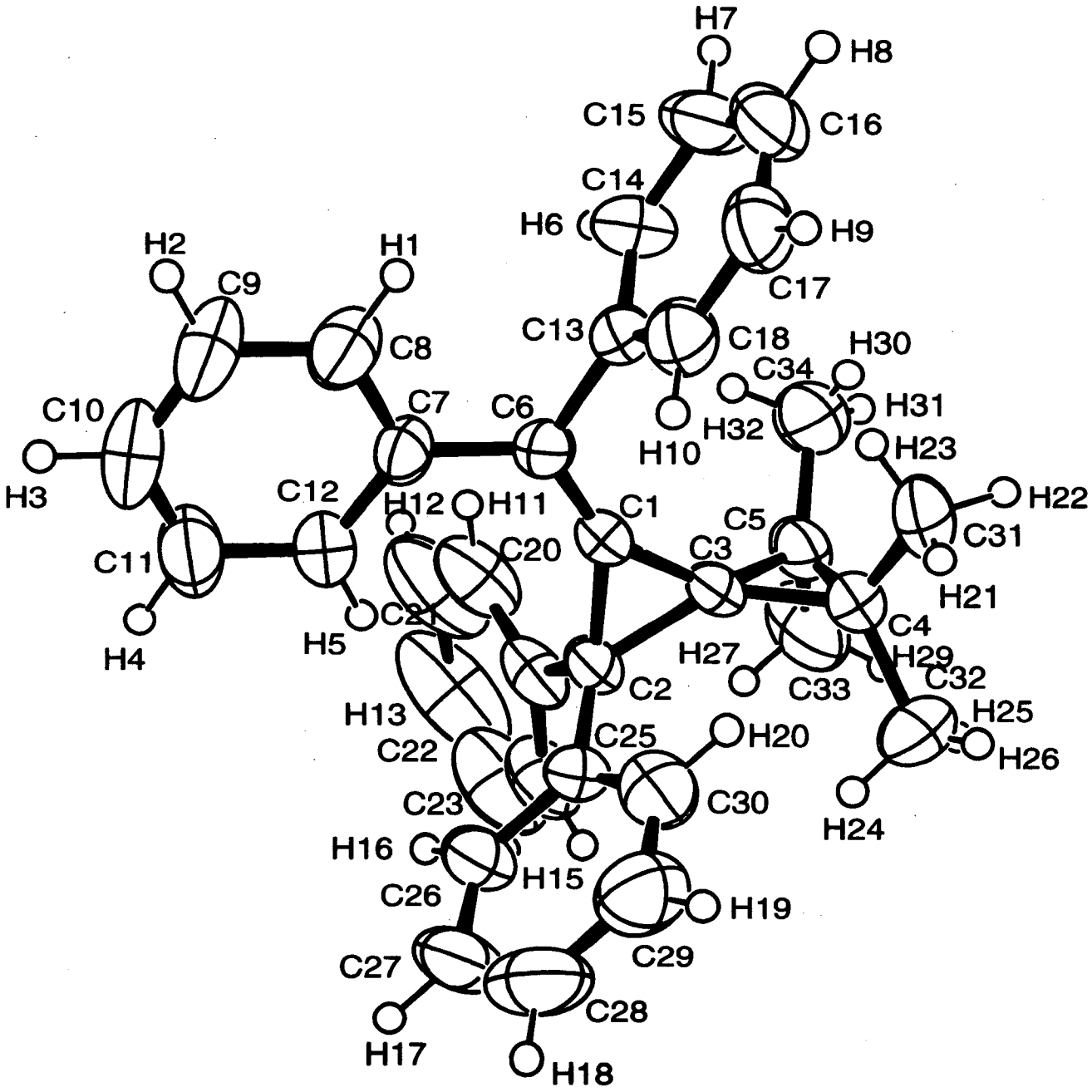
atom	atom	distance	ADC	atom	atom	distance	ADC
C(24)	H(11)	3.25(3)	(1)	C(24)	H(4)	3.56(8)	(-1,1,0,0,2)
C(24)	H(26)	3.60(9)	(-1,1,1,0,2)	C(24)	H(27)	2.49(3)	(1)
C(29)	H(20)	2.02(2)	(1)	C(29)	H(19)	0.950(9)	(1)
C(29)	H(19)	3.498(9)	(-1,1,1,0,3)	C(29)	H(18)	2.03(2)	(1)
C(29)	H(17)	3.23(4)	(1)	C(29)	H(14)	3.2(1)	(1,1,0,0,1)
C(29)	H(25)	3.60(7)	(-1,1,1,0,2)	C(29)	H(29)	3.41(8)	(-1,1,1,0,2)
C(10)	H(6)	3.24(6)	(-1,1,0,1,2)	C(10)	H(13)	3.4(1)	(1,1,0,0,1)
C(10)	H(12)	3.12(8)	(1,1,0,0,1)	C(10)	H(1)	3.26(3)	(1)
C(10)	H(2)	2.04(2)	(1)	C(10)	H(3)	0.950(8)	(1)
C(10)	H(4)	2.02(2)	(1)	C(10)	H(5)	3.25(3)	(1)
C(10)	H(22)	3.14(9)	(1,1,-1)	C(10)	H(32)	3.5(1)	(-1,1,0,1,2)
C(28)	H(8)	3.26(9)	(1,1,0,-1)	C(28)	H(7)	3.35(8)	(1,1,0,-1)
C(28)	H(20)	3.24(3)	(1)	C(28)	H(19)	2.04(2)	(1)
C(28)	H(18)	0.950(9)	(1)	C(28)	H(17)	2.00(2)	(1)
C(28)	H(16)	3.22(4)	(1)	C(28)	H(14)	2.85(9)	(1,1,0,0,1)
C(28)	H(29)	3.6(1)	(-1,1,1,0,2)	C(33)	H(10)	3.56(7)	(1,1,0,0,-1)
C(33)	H(8)	3.46(9)	(-1,1,1,1,2)	C(33)	H(15)	3.57(4)	(1)
C(33)	H(30)	3.30(3)	(1)	C(33)	H(31)	2.55(2)	(1)
C(33)	H(32)	2.92(3)	(1)	C(33)	H(24)	3.11(3)	(1)
C(33)	H(25)	2.59(3)	(1)	C(33)	H(27)	0.95(1)	(1)
C(33)	H(28)	0.95(1)	(1)	C(33)	H(29)	0.950(9)	(1)
C(32)	H(20)	2.90(3)	(1)	C(32)	H(15)	3.34(5)	(-1,1,1,0,2)
C(32)	H(21)	2.64(3)	(1)	C(32)	H(22)	2.81(2)	(1)
C(32)	H(23)	3.33(3)	(1)	C(32)	H(24)	0.950(9)	(1)
C(32)	H(24)	2.957(9)	(-1,1,1,0,2)	C(32)	H(25)	0.95(1)	(1)
C(32)	H(26)	0.95(1)	(1)	C(32)	H(27)	3.11(4)	(1)
C(32)	H(29)	2.58(3)	(1)	C(22)	H(17)	3.23(8)	(-1,1,0,0,2)
C(22)	H(15)	3.17(4)	(1)	C(22)	H(14)	1.96(3)	(1)
C(22)	H(14)	3.28(3)	(-1,1,0,0,1)	C(22)	H(13)	0.95(1)	(1)
C(22)	H(12)	2.09(3)	(1)	C(22)	H(11)	3.30(4)	(1)
C(23)	H(17)	3.48(7)	(-1,1,0,0,2)	C(23)	H(16)	3.55(4)	(1)
C(23)	H(15)	1.98(2)	(1)	C(23)	H(14)	0.95(1)	(1)
C(23)	H(13)	1.99(3)	(1)	C(23)	H(13)	3.37(3)	(-1,1,0,0,1)
C(23)	H(12)	3.24(4)	(1)	C(23)	H(27)	3.13(4)	(1)
C(21)	H(17)	3.01(8)	(-1,1,0,0,2)	C(21)	H(14)	3.23(4)	(1)
C(21)	H(13)	2.06(3)	(1)	C(21)	H(12)	0.95(1)	(1)
C(21)	H(11)	2.06(2)	(1)				

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z

L: Lattice translation.
(1) 0, 0, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.



ORTEP Drawing of **4**