C(63)	-	C(73)	2.72	0.09	2	2	-1	0	0	0.50640	0.41680	0.72320
C(67)	-	C(73)	2.61	0.09	2	2	-1	0	0	0.50640	0.41680	0.72320
C(73)	-	C(76)	3.19	0.09	2	1	0	0	-1	1.04030	-0.03050	0.12630
C(73)	-	H(63)	2.43	0.09	2	2	0	0	-1	0.94190	0.11230	0.03870
C(73)	-	H(67A)	2.80	0.09	2	2	0	0	-1	1.06680	0.13550	0.42650
C(73)	-	H(67B)	1.78	0.08	2	2	0	0	-1	1.06060	0.13470	0.28790
C(73)	-	H(67C)	2.98	0.09	2	2	0	0	-1	1.13390	0.12750	0.36180
C(90)	-	H(51)	3.11	0.01	1	1	0	0	1	0.62530	0.18710	1.10460
C(90)	-	H(55)	3.09	0.02	1	1	0	0	1	0.77070	0.11780	1.03190

---

ns is the symmetry operator number - (* denotes inversion indicator)

np is the lattice point number

Ta,Tb & Tc are unit cell translations. The symmetry operations are:

1 + X, + Y, + Z

2 + X, - Y, 1/2 + Z

GEOMETRY TABLES :ATPH-crotonaldehyde complex (ATPH-6)

FRACTIONAL ATOMIC COORDINATES & U(iso)

Atom	x/a	y/b	z/c	U(iso)
Al(1)	0.27700(5)	0.33000	0.69060(5)	0.0618(3)
O(2)	0.2788(1)	0.31180(8)	0.5359(1)	0.0603(7)
O(3)	0.3335(1)	0.40750(7)	0.7216(1)	0.0568(7)
O(4)	0.1344(1)	0.31600(8)	0.7361(2)	0.0679(8)
O(5)	0.3855(2)	0.2719(1)	0.7788(2)	0.083(1)
C(4)	0.4483(2)	0.4364(1)	0.7466(2)	0.055(1)
C(6)	0.2789(2)	0.2631(1)	0.4511(2)	0.051(1)
C(8)	0.4947(2)	0.4738(1)	0.6517(2)	0.065(1)
C(9)	0.3465(2)	0.3993(1)	0.9928(2)	0.066(1)

C(10)	0.5203(2)	0.4297(1)	0.8665(2)	0.058(1)
C(11)	0.4714(2)	0.3945(1)	0.9712(2)	0.060(1)
C(12)	0.5085(2)	0.2398(1)	0.5246(2)	0.056(1)
C(13)	0.0016(2)	0.3549(1)	0.8817(2)	0.068(1)
C(14)	0.4187(3)	0.4862(1)	0.5280(3)	0.072(1)
C(15)	0.0544(2)	0.2926(1)	0.3675(2)	0.061(1)
C(16)	0.0609(2)	0.3030(1)	0.8273(2)	0.059(1)
C(17)	0.3823(2)	0.1754(1)	0.3549(2)	0.067(1)
C(18)	-0.0627(2)	0.2637(2)	0.3724(3)	0.079(2)
C(19)	0.3015(3)	0.3652(2)	1.0898(3)	0.081(2)
C(20)	0.3876(2)	0.2252(1)	0.4433(2)	0.055(1)
C(21)	0.6408(2)	0.4567(1)	0.8856(3)	0.069(1)
C(22)	0.6619(2)	0.3175(1)	0.6257(2)	0.073(1)
C(23)	0.5854(2)	0.1884(1)	0.5755(2)	0.067(1)
C(24)	0.2727(3)	0.1618(1)	0.2731(3)	0.076(1)
C(25)	0.1688(2)	0.2007(1)	0.2792(2)	0.072(1)
C(26)	0.1681(2)	0.2512(1)	0.3669(2)	0.059(1)
C(27)	0.0433(2)	0.2374(1)	0.8634(2)	0.061(1)
C(28)	0.7000(2)	0.2023(2)	0.6514(3)	0.081(2)
C(29)	0.5488(2)	0.3041(1)	0.5483(2)	0.062(1)
C(30)	0.1005(2)	0.1810(1)	0.8039(3)	0.068(1)
C(31)	0.4026(3)	0.2372(2)	0.8648(4)	0.102(2)
C(32)	0.6173(3)	0.4993(1)	0.6769(3)	0.081(2)
C(33)	0.1518(3)	0.1283(2)	0.8753(4)	0.092(2)
C(34)	0.7350(3)	0.2654(2)	0.6765(3)	0.081(2)
C(35)	0.1015(3)	0.1777(1)	0.6719(3)	0.074(1)
C(36)	0.4911(3)	0.1920(2)	0.9122(3)	0.087(2)
C(37)	-0.0710(2)	0.3398(2)	0.9789(3)	0.089(2)
C(38)	0.5530(2)	0.3552(1)	1.0567(3)	0.078(1)
C(39)	0.0594(3)	0.3603(2)	0.3539(3)	0.078(2)
C(40)	0.6895(2)	0.4909(1)	0.7924(3)	0.079(1)
C(41)	0.0156(2)	0.4232(2)	0.8423(3)	0.083(2)
C(42)	-0.0317(3)	0.2259(2)	0.9587(3)	0.089(2)

C(43)	0.4752(4)	0.4794(2)	0.4167(3)	0.099(2)
C(44)	-0.0021(3)	0.4407(2)	0.7115(5)	0.104(2)
C(45)	0.3841(3)	0.3271(2)	1.1712(3)	0.090(2)
C(46)	-0.0880(3)	0.2760(2)	1.0151(3)	0.101(2)
C(47)	0.5077(3)	0.3225(2)	1.1537(3)	0.089(2)
C(48)	0.1575(3)	0.1240(2)	0.6178(4)	0.100(2)
C(49)	-0.1717(3)	0.3004(2)	0.3644(3)	0.094(2)
C(50)	0.2963(3)	0.5082(1)	0.5175(3)	0.083(2)
C(51)	-0.0505(3)	0.3969(2)	0.3441(3)	0.099(2)
C(52)	0.2896(6)	0.5157(2)	0.2917(3)	0.123(3)
C(53)	0.2066(4)	0.0732(2)	0.6917(5)	0.118(2)
C(54)	-0.1647(3)	0.3669(3)	0.3491(3)	0.108(2)
C(55)	0.2302(4)	0.5239(2)	0.4000(4)	0.107(2)
C(56)	0.2044(4)	0.0747(2)	0.8203(5)	0.113(2)
C(57)	0.4076(5)	0.4940(2)	0.3000(4)	0.117(3)
C(58)	0.5921(5)	0.1058(3)	1.0590(5)	0.145(3)
C(59)	0.0099(4)	0.5041(2)	0.6777(7)	0.162(4)
C(60)	0.0411(3)	0.4732(2)	0.9295(5)	0.125(2)
C(61)	0.0338(6)	0.5534(3)	0.760(1)	0.212(6)
C(62)	0.4980(5)	0.1573(2)	1.0077(6)	0.155(3)
C(63)	0.0505(5)	0.5375(3)	0.887(1)	0.212(5)
H(9)	0.293(2)	0.435(1)	0.950(2)	0.046(7)
H(17)	0.458(2)	0.148(1)	0.346(2)	0.039(6)
H(18)	-0.062(2)	0.214(1)	0.378(2)	0.035(6)
H(19)	0.213(3)	0.367(1)	1.112(3)	0.063(8)
H(21)	0.691(3)	0.451(1)	0.966(3)	0.08(1)
H(22)	0.679(3)	0.368(2)	0.640(3)	0.061(8)
H(23)	0.567(2)	0.140(1)	0.557(2)	0.033(6)
H(24)	0.280(2)	0.127(1)	0.212(3)	0.049(7)
H(25)	0.093(3)	0.193(2)	0.222(3)	0.073(9)
H(28)	0.733(3)	0.157(2)	0.684(3)	0.067(9)
H(29)	0.493(3)	0.345(1)	0.505(3)	0.060(8)
H(31)	0.317(7)	0.244(3)	0.924(6)	0.21(3)

H(32)	0.652(2)	0.523(1)	0.618(2)	0.029(6)
H(33)	0.145(4)	0.131(2)	0.964(5)	0.11(2)
H(34)	0.800(3)	0.274(2)	0.738(3)	0.08(1)
H(35)	0.059(2)	0.213(1)	0.616(3)	0.050(7)
H(36)	0.591(3)	0.200(1)	0.906(3)	0.29(4)
H(37)	-0.124(3)	0.382(1)	1.021(3)	0.061(8)
H(38)	0.640(2)	0.349(1)	1.035(2)	0.029(5)
H(39)	0.137(3)	0.383(1)	0.347(3)	0.052(7)
H(40)	0.774(3)	0.516(1)	0.818(3)	0.063(8)
H(42)	-0.038(3)	0.181(2)	0.983(3)	0.07(1)
H(43)	0.567(3)	0.466(2)	0.432(3)	0.14(2)
H(44)	-0.024(3)	0.407(2)	0.665(3)	0.06(1)
H(45)	0.349(3)	0.299(1)	1.233(3)	0.064(9)
H(46)	-0.154(4)	0.265(2)	1.081(4)	0.13(1)
H(47)	0.56530	0.29660	1.20820	0.16(2)
H(48)	0.16410	0.12400	0.52740	0.70(8)
H(49)	-0.254(3)	0.275(1)	0.380(3)	0.053(7)
H(50)	0.25990	0.51380	0.60300	0.11(1)
H(51)	-0.036(3)	0.448(2)	0.331(3)	0.09(1)
H(52)	0.24620	0.52490	0.20630	0.07(1)
H(53)	0.24470	0.03550	0.65320	0.10(1)
H(54)	-0.237(4)	0.394(2)	0.337(3)	0.09(1)
H(55)	0.134(3)	0.533(1)	0.405(3)	0.071(9)
H(56)	0.23360	0.03890	0.87220	0.10(1)
H(57)	0.44600	0.48840	0.22220	0.28(4)
H(58A)	0.59810	0.07840	1.13300	0.22(3)
H(58B)	0.67030	0.12940	1.06950	0.20(3)
H(58C)	0.59240	0.07490	0.99100	0.6(1)
H(59)	-0.00590	0.50870	0.58720	0.08(1)
H(60)	0.05040	0.46450	1.02180	0.13(2)
H(61)	0.03240	0.59800	0.71860	0.17(2)
H(62)	0.42920	0.16360	1.05560	0.9(9)
H(63)	0.07360	0.57620	0.93530	0.25(3)

Temperature factor of the form: exp[-2pi^2U], U=U(iso)

or 1/3 SUM(i)SUM(j){U(ij)*astar(i).astar(j).a(i).a(j).cos(ij)}

ANISOTROPIC THERMAL PARAMETERS

Atom	U11	U22	U33	U12	U13	U23
Al(1)	0.0616(3)	0.0647(3)	0.0581(3)	-.0027(3)	0.0095(2)	-.0017(3)
O(2)	0.0590(7)	0.072(1)	0.0483(8)	0.0074(7)	0.0043(5)	-.0096(7)
O(3)	0.0588(7)	0.0578(8)	0.0526(9)	-.0098(6)	0.0065(6)	0.0025(7)
O(4)	0.0663(8)	0.063(1)	0.075(1)	-.0084(7)	0.0272(7)	-.0026(8)
O(5)	0.090(1)	0.079(1)	0.077(1)	0.0105(9)	-.0011(9)	0.013(1)
C(4)	0.052(1)	0.051(1)	0.062(1)	-.0083(8)	0.0113(9)	-.005(1)
C(6)	0.056(1)	0.049(1)	0.048(1)	-.0041(8)	0.0093(8)	-.0027(9)
C(8)	0.067(1)	0.055(1)	0.073(2)	-.006(1)	0.023(1)	-.003(1)
C(9)	0.064(1)	0.080(2)	0.053(1)	0.004(1)	0.010(1)	-.006(1)
C(10)	0.053(1)	0.055(1)	0.063(1)	-.0035(9)	0.0048(9)	-.009(1)
C(11)	0.057(1)	0.067(1)	0.053(1)	-.0038(9)	0.0000(9)	-.006(1)
C(12)	0.054(1)	0.060(1)	0.052(1)	0.0010(9)	0.0124(8)	-.004(1)
C(13)	0.051(1)	0.090(2)	0.061(1)	0.002(1)	0.004(1)	-.014(1)
C(14)	0.093(2)	0.051(1)	0.072(2)	-.014(1)	0.023(1)	0.001(1)
C(15)	0.053(1)	0.080(2)	0.047(1)	-.001(1)	0.0009(9)	-.005(1)
C(16)	0.0461(9)	0.082(2)	0.048(1)	-.008(1)	0.0030(8)	-.001(1)
C(17)	0.072(1)	0.062(1)	0.066(2)	0.009(1)	0.005(1)	-.007(1)
C(18)	0.066(1)	0.102(2)	0.067(2)	-.006(1)	0.003(1)	0.003(2)
C(19)	0.072(2)	0.107(2)	0.064(2)	-.004(1)	0.013(1)	0.005(1)
C(20)	0.059(1)	0.055(1)	0.050(1)	0.0007(9)	0.0067(8)	-.001(1)
C(21)	0.054(1)	0.065(1)	0.086(2)	-.007(1)	0.004(1)	-.008(1)
C(22)	0.058(1)	0.078(2)	0.082(2)	-.003(1)	0.005(1)	-.011(1)
C(23)	0.068(1)	0.067(2)	0.066(2)	0.011(1)	0.001(1)	-.006(1)
C(24)	0.087(2)	0.064(2)	0.073(2)	0.011(1)	-.007(1)	-.020(1)
C(25)	0.077(2)	0.068(1)	0.066(2)	-.007(1)	-.006(1)	-.009(1)

C(26)	0.058(1)	0.059(1)	0.059(1)	-.0009(9)	0.0030(9)	0.002(1)
C(27)	0.050(1)	0.083(2)	0.050(1)	-.007(1)	0.0038(9)	0.008(1)
C(28)	0.069(1)	0.086(2)	0.084(2)	0.014(1)	-.008(1)	0.000(2)
C(29)	0.054(1)	0.067(1)	0.064(1)	0.005(1)	0.0128(9)	-.007(1)
C(30)	0.065(1)	0.064(1)	0.074(2)	-.011(1)	0.007(1)	0.012(1)
C(31)	0.091(2)	0.090(2)	0.119(3)	-.009(2)	-.014(2)	0.030(2)
C(32)	0.079(2)	0.058(1)	0.109(2)	-.014(1)	0.041(2)	0.001(1)
C(33)	0.090(2)	0.087(2)	0.097(3)	0.001(1)	0.006(2)	0.025(2)
C(34)	0.067(1)	0.094(2)	0.080(2)	0.006(1)	-.008(1)	-.007(2)
C(35)	0.084(2)	0.061(2)	0.077(2)	-.010(1)	0.006(1)	0.004(1)
C(36)	0.095(2)	0.079(2)	0.082(2)	0.014(1)	0.001(1)	0.021(2)
C(37)	0.066(1)	0.135(3)	0.065(2)	0.021(2)	0.009(1)	-.010(2)
C(38)	0.069(1)	0.085(2)	0.075(2)	-.001(1)	-.007(1)	0.001(1)
C(39)	0.072(2)	0.083(2)	0.077(2)	0.008(1)	0.002(1)	-.007(1)
C(40)	0.056(1)	0.072(2)	0.106(2)	-.013(1)	0.009(1)	0.001(2)
C(41)	0.050(1)	0.080(2)	0.118(3)	0.008(1)	0.010(1)	-.025(2)
C(42)	0.073(2)	0.117(3)	0.074(2)	0.003(2)	0.009(1)	0.034(2)
C(43)	0.138(3)	0.081(2)	0.079(2)	-.015(2)	0.037(2)	-.002(2)
C(44)	0.086(2)	0.080(2)	0.149(4)	0.019(2)	0.051(2)	0.017(3)
C(45)	0.102(2)	0.103(2)	0.062(2)	-.011(2)	0.009(1)	0.014(2)
C(46)	0.084(2)	0.155(3)	0.066(2)	0.025(2)	0.027(1)	0.027(2)
C(47)	0.091(2)	0.102(2)	0.069(2)	0.001(2)	-.010(1)	0.016(2)
C(48)	0.130(3)	0.063(2)	0.107(3)	-.007(2)	0.022(2)	-.010(2)
C(49)	0.058(2)	0.143(3)	0.081(2)	0.005(2)	0.007(1)	-.007(2)
C(50)	0.093(2)	0.078(2)	0.074(2)	-.015(1)	0.004(1)	0.017(1)
C(51)	0.093(2)	0.092(2)	0.109(3)	0.029(2)	0.005(2)	-.009(2)
C(52)	0.201(5)	0.096(3)	0.066(2)	-.044(3)	-.011(3)	0.024(2)
C(53)	0.142(3)	0.067(2)	0.144(4)	0.007(2)	0.026(3)	-.007(2)
C(54)	0.073(2)	0.152(4)	0.095(3)	0.034(2)	0.001(2)	-.020(2)
C(55)	0.117(3)	0.093(2)	0.105(3)	-.019(2)	-.013(2)	0.025(2)
C(56)	0.140(3)	0.067(2)	0.130(3)	0.015(2)	0.010(2)	0.024(2)
C(57)	0.169(4)	0.093(3)	0.087(3)	-.012(2)	0.018(3)	0.006(2)
C(58)	0.141(4)	0.131(3)	0.156(4)	0.042(3)	-.014(3)	0.059(3)

C(59)	0.136(3)	0.083(3)	0.275(8)	0.038(2)	0.112(4)	0.057(4)
C(60)	0.077(2)	0.109(3)	0.185(5)	0.017(2)	0.006(2)	-.061(3)
C(61)	0.104(4)	0.073(3)	0.46(2)	0.019(3)	0.110(7)	0.027(6)
C(62)	0.137(3)	0.134(3)	0.186(5)	-.004(3)	-.034(3)	0.073(3)
C(63)	0.077(3)	0.085(4)	0.47(1)	0.008(2)	0.029(5)	-.105(6)

T=exp[-2pi**2(U11.h**2.astar**2+U22.k**2.bstar**2+ U33.l**2.cstar**2 +2U12.h.k.astar.bstar +2U13.h.l.astar.cstar+2U23.k.l.bstar.cstar)]

INTRAMOLECULAR BOND LENGTHS

Bond length limits based on covalent radii

Al(1) - O(2)	1.692(2)	Al(1) - O(3)	1.706(2)
Al(1) - O(4)	1.688(2)	Al(1) - O(5)	1.829(2)
O(2) - C(6)	1.341(3)	O(3) - C(4)	1.358(3)
O(4) - C(16)	1.356(3)	O(5) - C(31)	1.152(5)
C(4) - C(8)	1.408(4)	C(4) - C(10)	1.409(4)
C(6) - C(20)	1.409(3)	C(6) - C(26)	1.412(3)
C(8) - C(14)	1.477(4)	C(8) - C(32)	1.406(4)
C(9) - C(11)	1.392(3)	C(9) - C(19)	1.384(4)
C(10) - C(11)	1.479(4)	C(10) - C(21)	1.394(3)
C(11) - C(38)	1.423(4)	C(12) - C(20)	1.491(3)
C(12) - C(23)	1.396(4)	C(12) - C(29)	1.390(4)
C(13) - C(16)	1.397(4)	C(13) - C(37)	1.410(4)
C(13) - C(41)	1.465(5)	C(14) - C(43)	1.408(5)
C(14) - C(50)	1.377(4)	C(15) - C(18)	1.394(4)
C(15) - C(26)	1.483(4)	C(15) - C(39)	1.387(5)
C(16) - C(27)	1.409(4)	C(17) - C(20)	1.379(4)
C(17) - C(24)	1.395(4)	C(18) - C(49)	1.380(5)
C(19) - C(45)	1.391(5)	C(21) - C(40)	1.371(4)
C(22) - C(29)	1.400(4)	C(22) - C(34)	1.385(5)
C(23) - C(28)	1.407(4)	C(24) - C(25)	1.375(4)

C(25) - C(26)	1.390(4)	C(27) - C(30)	1.482(4)
C(27) - C(42)	1.396(4)	C(28) - C(34)	1.354(5)
C(30) - C(33)	1.386(5)	C(30) - C(35)	1.410(4)
C(31) - C(36)	1.369(5)	C(32) - C(40)	1.375(5)
C(33) - C(56)	1.392(6)	C(35) - C(48)	1.406(5)
C(36) - C(62)	1.233(7)	C(37) - C(46)	1.373(6)
C(38) - C(47)	1.371(4)	C(39) - C(51)	1.386(5)
C(41) - C(44)	1.427(7)	C(41) - C(60)	1.380(6)
C(42) - C(46)	1.364(6)	C(43) - C(57)	1.386(6)
C(44) - C(59)	1.350(7)	C(45) - C(47)	1.366(5)
C(48) - C(53)	1.362(6)	C(49) - C(54)	1.366(8)
C(50) - C(55)	1.392(6)	C(51) - C(54)	1.376(6)
C(52) - C(55)	1.400(7)	C(52) - C(57)	1.332(9)
C(53) - C(56)	1.374(8)	C(58) - C(62)	1.506(8)
C(59) - C(61)	1.34(2)	C(60) - C(63)	1.392(9)
C(61) - C(63)	1.38(2)	C(9) - H(9)	1.00(3)
C(17) - H(17)	1.00(3)	C(18) - H(18)	1.01(3)
C(19) - H(19)	1.02(3)	C(21) - H(21)	0.96(3)
C(22) - H(22)	1.06(4)	C(23) - H(23)	1.03(3)
C(24) - H(24)	0.98(3)	C(25) - H(25)	0.96(4)
C(28) - H(28)	1.04(4)	C(29) - H(29)	1.10(3)
C(31) - H(31)	1.19(7)	C(32) - H(32)	0.91(3)
C(33) - H(33)	0.96(5)	C(34) - H(34)	0.91(4)
C(35) - H(35)	1.00(3)	C(36) - H(36)	1.09(4)
C(37) - H(37)	1.16(3)	C(38) - H(38)	1.00(3)
C(39) - H(39)	0.96(3)	C(40) - H(40)	1.04(3)
C(42) - H(42)	0.95(4)	C(43) - H(43)	1.02(4)
C(44) - H(44)	0.85(4)	C(45) - H(45)	0.99(4)
C(46) - H(46)	1.09(5)	C(47) - H(47)	0.949(3)
C(48) - H(48)	0.975(4)	C(49) - H(49)	1.05(3)
C(50) - H(50)	1.044(3)	C(51) - H(51)	1.06(4)
C(52) - H(52)	0.984(5)	C(53) - H(53)	0.984(4)
C(54) - H(54)	0.94(4)	C(55) - H(55)	1.06(4)

C(56) - H(56)	0.943(4)	C(57) - H(57)	0.980(5)
C(58) - H(58A)	0.961(6)	C(58) - H(58B)	0.960(6)
C(58) - H(58C)	0.960(6)	C(59) - H(59)	0.961(8)
C(60) - H(60)	0.991(6)	C(61) - H(61)	1.010(9)
C(62) - H(62)	0.960(6)	C(63) - H(63)	0.955(8)

INTRAMOLECULAR BOND ANGLES

Bond length limits based on covalent radii

O(2) - Al(1) - O(3)	110.0(1)	O(2) - Al(1) - O(4)	111.7(1)		
O(2) - Al(1) - O(5)	105.7(1)	O(3) - Al(1) - O(4)	114.3(1)		
O(3) - Al(1) - O(5)	108.2(1)	O(4) - Al(1) - O(5)	106.4(1)		
Al(1) - O(2) - C(6)	145.0(2)	Al(1) - O(3) - C(4)	136.7(2)		
Al(1) - O(4) - C(16)	150.8(2)	Al(1) - O(5) - C(31)	145.9(3)		
O(3) - C(4) - C(8)	119.4(2)	O(3) - C(4) - C(10)	120.6(2)		
C(8) - C(4) - C(10)	120.0(2)	O(2) - C(6) - C(20)	121.2(2)		
O(2) - C(6) - C(26)	118.6(2)	C(20) - C(6) - C(26)	120.1(2)		
C(4) - C(8) - C(14)	121.8(3)	C(4) - C(8) - C(32)	118.2(3)		
C(14) - C(8) - C(32)	119.9(3)	C(11) - C(9) - C(19)	121.8(3)		
C(4) - C(10) - C(11)	121.6(2)	C(4) - C(10) - C(21)	118.7(3)		
C(11) - C(10) - C(21)	119.7(3)	C(9) - C(11) - C(10)	122.4(2)		
C(9) - C(11) - C(38)	117.2(3)	C(10) - C(11) - C(38)	120.4(2)		
C(20) - C(12) - C(23)	120.0(3)	C(20) - C(12) - C(29)	121.2(2)		
C(23) - C(12) - C(29)	118.7(2)	C(16) - C(13) - C(37)	117.8(3)		
C(16) - C(13) - C(41)	121.9(3)	C(37) - C(13) - C(41)	120.3(3)		
C(8) - C(14) - C(43)	119.1(3)	C(8) - C(14) - C(50)	122.4(3)		
C(43) - C(14) - C(50)	118.4(3)	C(18) - C(15) - C(26)	120.4(3)		
C(18) - C(15) - C(39)	118.1(3)	C(26) - C(15) - C(39)	121.4(3)		
O(4) - C(16) - C(13)	119.3(3)	O(4) - C(16) - C(27)	119.5(2)		
C(13) - C(16) - C(27)	121.2(2)	C(20) - C(17) - C(24)	121.8(3)		
C(15) - C(18) - C(49)	122.0(4)	C(9) - C(19) - C(45)	119.3(3)		

C(6) -	C(20) - C(12)	121.3(2)	C(6) -	C(20) - C(17)	118.9(2)
C(12) -	C(20) - C(17)	119.8(2)	C(10) -	C(21) - C(40)	121.9(3)
C(29) -	C(22) - C(34)	118.8(3)	C(12) -	C(23) - C(28)	119.9(3)
C(17) -	C(24) - C(25)	118.5(3)	C(24) -	C(25) - C(26)	122.3(3)
C(6) -	C(26) - C(15)	121.5(3)	C(6) -	C(26) - C(25)	118.4(2)
C(15) -	C(26) - C(25)	120.0(2)	C(16) -	C(27) - C(30)	122.6(2)
C(16) -	C(27) - C(42)	117.9(3)	C(30) -	C(27) - C(42)	119.5(3)
C(23) -	C(28) - C(34)	120.1(3)	C(12) -	C(29) - C(22)	121.0(3)
C(27) -	C(30) - C(33)	121.4(3)	C(27) -	C(30) - C(35)	121.5(3)
C(33) -	C(30) - C(35)	117.1(3)	O(5) -	C(31) - C(36)	137.3(4)
C(8) -	C(32) - C(40)	121.8(3)	C(30) -	C(33) - C(56)	121.9(4)
C(22) -	C(34) - C(28)	121.4(3)	C(30) -	C(35) - C(48)	120.4(3)
C(31) -	C(36) - C(62)	130.7(4)	C(13) -	C(37) - C(46)	121.3(4)
C(11) -	C(38) - C(47)	120.4(3)	C(15) -	C(39) - C(51)	119.8(3)
C(21) -	C(40) - C(32)	119.2(3)	C(13) -	C(41) - C(44)	120.7(3)
C(13) -	C(41) - C(60)	121.6(4)	C(44) -	C(41) - C(60)	117.6(4)
C(27) -	C(42) - C(46)	121.8(4)	C(14) -	C(43) - C(57)	120.2(4)
C(41) -	C(44) - C(59)	119.6(5)	C(19) -	C(45) - C(47)	120.2(3)
C(37) -	C(46) - C(42)	120.0(3)	C(38) -	C(47) - C(45)	121.1(3)
C(35) -	C(48) - C(53)	120.4(4)	C(18) -	C(49) - C(54)	118.9(4)
C(14) -	C(50) - C(55)	120.9(3)	C(39) -	C(51) - C(54)	120.7(4)
C(55) -	C(52) - C(57)	121.1(4)	C(48) -	C(53) - C(56)	120.2(4)
C(49) -	C(54) - C(51)	120.5(4)	C(50) -	C(55) - C(52)	118.8(4)
C(33) -	C(56) - C(53)	119.9(4)	C(43) -	C(57) - C(52)	120.7(5)
C(44) -	C(59) - C(61)	123.9(8)	C(41) -	C(60) - C(63)	119.4(7)
C(59) -	C(61) - C(63)	117.3(7)	C(36) -	C(62) - C(58)	131.5(5)
C(60) -	C(63) - C(61)	122.2(8)	C(11) -	C(9) - H(9)	118.7(15)
C(19) -	C(9) - H(9)	118.2(15)	C(20) -	C(17) - H(17)	120.7(14)
C(24) -	C(17) - H(17)	117.5(14)	C(15) -	C(18) - H(18)	115.1(13)
C(49) -	C(18) - H(18)	122.9(13)	C(9) -	C(19) - H(19)	126.4(17)
C(45) -	C(19) - H(19)	114.2(17)	C(10) -	C(21) - H(21)	119.1(17)
C(40) -	C(21) - H(21)	119.0(17)	C(29) -	C(22) - H(22)	113.0(16)
C(34) -	C(22) - H(22)	128.1(16)	C(12) -	C(23) - H(23)	124.2(13)

C(28) - C(23) - H(23)	115.7(13) C(17) - C(24) - H(24)	115.4(15)
C(25) - C(24) - H(24)	125.9(15) C(24) - C(25) - H(25)	120.1(21)
C(26) - C(25) - H(25)	117.6(21) C(23) - C(28) - H(28)	104.2(17)
C(34) - C(28) - H(28)	135.2(18) C(12) - C(29) - H(29)	120.2(15)
C(22) - C(29) - H(29)	118.9(15) O(5) - C(31) - H(31)	107.3(33)
C(36) - C(31) - H(31)	115.4(33) C(8) - C(32) - H(32)	121.6(15)
C(40) - C(32) - H(32)	116.6(15) C(30) - C(33) - H(33)	114.8(27)
C(56) - C(33) - H(33)	123.3(27) C(22) - C(34) - H(34)	118.0(21)
C(28) - C(34) - H(34)	119.9(21) C(30) - C(35) - H(35)	120.1(17)
C(48) - C(35) - H(35)	119.5(17) C(31) - C(36) - H(36)	121.3(16)
C(62) - C(36) - H(36)	100.3(17) C(13) - C(37) - H(37)	118.1(15)
C(46) - C(37) - H(37)	120.3(15) C(11) - C(38) - H(38)	116.0(13)
C(47) - C(38) - H(38)	123.1(13) C(15) - C(39) - H(39)	121.7(17)
C(51) - C(39) - H(39)	118.4(17) C(21) - C(40) - H(40)	117.5(16)
C(32) - C(40) - H(40)	122.5(16) C(27) - C(42) - H(42)	115.3(19)
C(46) - C(42) - H(42)	122.9(20) C(14) - C(43) - H(43)	114.0(20)
C(57) - C(43) - H(43)	125.8(20) C(41) - C(44) - H(44)	111.3(23)
C(59) - C(44) - H(44)	128.9(24) C(19) - C(45) - H(45)	118.3(17)
C(47) - C(45) - H(45)	120.9(17) C(37) - C(46) - H(46)	119.5(24)
C(42) - C(46) - H(46)	120.2(24) C(38) - C(47) - H(47)	117.6(3)
C(45) - C(47) - H(47)	121.3(3) C(35) - C(48) - H(48)	119.7(4)
C(53) - C(48) - H(48)	119.9(4) C(18) - C(49) - H(49)	116.7(15)
C(54) - C(49) - H(49)	124.1(15) C(14) - C(50) - H(50)	115.3(3)
C(55) - C(50) - H(50)	123.7(4) C(39) - C(51) - H(51)	113.3(20)
C(54) - C(51) - H(51)	125.9(20) C(55) - C(52) - H(52)	121.9(6)
C(57) - C(52) - H(52)	117.0(5) C(48) - C(53) - H(53)	120.0(5)
C(56) - C(53) - H(53)	119.7(5) C(49) - C(54) - H(54)	122.2(23)
C(51) - C(54) - H(54)	117.2(24) C(50) - C(55) - H(55)	112.5(18)
C(52) - C(55) - H(55)	127.9(18) C(33) - C(56) - H(56)	118.7(5)
C(53) - C(56) - H(56)	121.3(4) C(43) - C(57) - H(57)	120.4(5)
C(52) - C(57) - H(57)	119.0(5) C(62) - C(58) - H(58A)	132.1(6)
C(62) - C(58) - H(58B)	103.1(5) C(62) - C(58) - H(58C)	104.5(5)
H(58A) - C(58) - H(58B)	103.4(6) H(58A) - C(58) - H(58C)	103.5(5)

H(58B) - C(58) - H(58C)	109.0(6)	C(44) - C(59) - H(59)	110.5(6)		
C(61) - C(59) - H(59)	125.5(7)	C(41) - C(60) - H(60)	121.4(5)		
C(63) - C(60) - H(60)	119.2(7)	C(59) - C(61) - H(61)	113.1(12)		
C(63) - C(61) - H(61)	129.5(10)	C(36) - C(62) - H(62)	113.3(5)		
C(58) - C(62) - H(62)	115.2(6)	C(60) - C(63) - H(63)	128.7(11)		
C(61) - C(63) - H(63)	108.9(8)				

INTRAMOLECULAR TORSION ANGLES

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Bond length limits based on covalent radii

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O(2) - Al(1) - O(3) - C(4)	-82.0(2)	O(3) - Al(1) - O(2) - C(6)	158.6(3)		
O(4) - Al(1) - O(2) - C(6)	-73.3(3)	O(2) - Al(1) - O(4) - C(16)	156.4(4)		
O(5) - Al(1) - O(2) - C(6)	42.0(3)	O(2) - Al(1) - O(5) - C(31)	-137.2(5)		
O(4) - Al(1) - O(3) - C(4)	151.3(3)	O(3) - Al(1) - O(4) - C(16)	-77.9(3)		
O(5) - Al(1) - O(3) - C(4)	33.0(2)	O(3) - Al(1) - O(5) - C(31)	105.1(5)		
O(5) - Al(1) - O(4) - C(16)	41.5(3)	O(4) - Al(1) - O(5) - C(31)	-18.2(5)		
Al(1) - O(2) - C(6) - C(20)	-74.5(3)	Al(1) - O(2) - C(6) - C(26)	107.0(3)		
Al(1) - O(3) - C(4) - C(8)	104.9(3)	Al(1) - O(3) - C(4) - C(10)	-75.6(3)		
Al(1) - O(4) - C(16) - C(13)	95.9(4)	Al(1) - O(4) - C(16) - C(27)	-85.6(4)		
Al(1) - O(5) - C(31) - C(36)	173.9(8)	O(3) - C(4) - C(8) - C(14)	4.0(2)		
O(3) - C(4) - C(8) - C(32)	-175.6(4)	O(3) - C(4) - C(10) - C(11)	-3.5(2)		
O(3) - C(4) - C(10) - C(21)	176.0(4)	C(8) - C(4) - C(10) - C(11)	175.9(4)		
C(10) - C(4) - C(8) - C(14)	-175.4(4)	C(8) - C(4) - C(10) - C(21)	-4.5(3)		
C(10) - C(4) - C(8) - C(32)	5.0(3)	O(2) - C(6) - C(20) - C(12)	-3.0(2)		
O(2) - C(6) - C(20) - C(17)	179.6(4)	O(2) - C(6) - C(26) - C(15)	2.2(2)		
O(2) - C(6) - C(26) - C(25)	180.0(4)	C(26) - C(6) - C(20) - C(12)	175.5(4)		
C(20) - C(6) - C(26) - C(15)	-176.4(4)	C(26) - C(6) - C(20) - C(17)	-1.9(3)		
C(20) - C(6) - C(26) - C(25)	1.4(3)	C(4) - C(8) - C(14) - C(43)	-135.3(4)		
C(4) - C(8) - C(14) - C(50)	48.8(3)	C(4) - C(8) - C(32) - C(40)	-2.8(3)		

C(14) - C(8) - C(32) - C(40)	177.6(5)	C(32) - C(8) - C(14) - C(43)	44.3(3)
C(32) - C(8) - C(14) - C(50)	-131.6(4)	C(19) - C(9) - C(11) - C(10)	178.9(4)
C(19) - C(9) - C(11) - C(38)	-2.7(3)	C(11) - C(9) - C(19) - C(45)	2.6(3)
C(4) - C(10) - C(11) - C(9)	-38.7(3)	C(4) - C(10) - C(11) - C(38)	143.0(4)
C(4) - C(10) - C(21) - C(40)	1.8(3)	C(21) - C(10) - C(11) - C(9)	141.8(4)
C(21) - C(10) - C(11) - C(38)	-36.6(3)	C(11) - C(10) - C(21) - C(40)	-178.7(4)
C(9) - C(11) - C(38) - C(47)	1.6(3)	C(10) - C(11) - C(38) - C(47)	-179.9(4)
C(23) - C(12) - C(20) - C(6)	141.3(4)	C(23) - C(12) - C(20) - C(17)	-41.3(3)
C(20) - C(12) - C(23) - C(28)	179.5(4)	C(29) - C(12) - C(20) - C(6)	-40.6(3)
C(29) - C(12) - C(20) - C(17)	136.8(4)	C(20) - C(12) - C(29) - C(22)	179.4(4)
C(23) - C(12) - C(29) - C(22)	-2.5(3)	C(29) - C(12) - C(23) - C(28)	1.3(3)
C(37) - C(13) - C(16) - O(4)	-178.1(4)	C(37) - C(13) - C(16) - C(27)	3.4(3)
C(16) - C(13) - C(37) - C(46)	-3.0(3)	C(41) - C(13) - C(16) - O(4)	0.5(3)
C(41) - C(13) - C(16) - C(27)	-178.0(4)	C(16) - C(13) - C(41) - C(44)	49.1(4)
C(16) - C(13) - C(41) - C(60)	-133.6(5)	C(37) - C(13) - C(41) - C(44)	-132.3(5)
C(41) - C(13) - C(37) - C(46)	178.3(5)	C(37) - C(13) - C(41) - C(60)	45.0(4)
C(8) - C(14) - C(43) - C(57)	-176.7(5)	C(8) - C(14) - C(50) - C(55)	175.4(5)
C(43) - C(14) - C(50) - C(55)	-0.5(4)	C(50) - C(14) - C(43) - C(57)	-0.7(4)
C(18) - C(15) - C(26) - C(6)	-129.8(4)	C(18) - C(15) - C(26) - C(25)	52.5(3)
C(26) - C(15) - C(18) - C(49)	-175.5(5)	C(39) - C(15) - C(18) - C(49)	-0.1(3)
C(18) - C(15) - C(39) - C(51)	-0.8(3)	C(39) - C(15) - C(26) - C(6)	55.0(3)
C(39) - C(15) - C(26) - C(25)	-122.7(4)	C(26) - C(15) - C(39) - C(51)	174.5(5)
O(4) - C(16) - C(27) - C(30)	-1.1(2)	O(4) - C(16) - C(27) - C(42)	179.2(4)
C(13) - C(16) - C(27) - C(30)	177.4(4)	C(13) - C(16) - C(27) - C(42)	-2.3(3)
C(24) - C(17) - C(20) - C(6)	0.2(3)	C(24) - C(17) - C(20) - C(12)	-177.2(4)
C(20) - C(17) - C(24) - C(25)	1.9(3)	C(15) - C(18) - C(49) - C(54)	1.1(4)
C(9) - C(19) - C(45) - C(47)	-1.3(3)	C(10) - C(21) - C(40) - C(32)	0.5(3)
C(34) - C(22) - C(29) - C(12)	1.4(3)	C(29) - C(22) - C(34) - C(28)	0.9(3)
C(12) - C(23) - C(28) - C(34)	0.9(3)	C(17) - C(24) - C(25) - C(26)	-2.5(3)
C(24) - C(25) - C(26) - C(6)	0.8(3)	C(24) - C(25) - C(26) - C(15)	178.7(4)
C(16) - C(27) - C(30) - C(33)	139.2(4)	C(16) - C(27) - C(30) - C(35)	-42.8(3)
C(16) - C(27) - C(42) - C(46)	0.7(3)	C(42) - C(27) - C(30) - C(33)	-41.1(3)
C(42) - C(27) - C(30) - C(35)	136.9(4)	C(30) - C(27) - C(42) - C(46)	-179.0(5)

C(23) - C(28) - C(34) - C(22)	-2.0(3)	C(27) - C(30) - C(33) - C(56)	179.2(5)
C(27) - C(30) - C(35) - C(48)	179.3(4)	C(33) - C(30) - C(35) - C(48)	-2.6(3)
C(35) - C(30) - C(33) - C(56)	1.2(4)	O(5) - C(31) - C(36) - C(62)	-179.9(8)
C(8) - C(32) - C(40) - C(21)	0.0(3)	C(30) - C(33) - C(56) - C(53)	0.1(4)
C(30) - C(35) - C(48) - C(53)	2.8(4)	C(31) - C(36) - C(62) - C(58)	177.7(9)
C(13) - C(37) - C(46) - C(42)	1.5(4)	C(11) - C(38) - C(47) - C(45)	-0.4(3)
C(15) - C(39) - C(51) - C(54)	0.7(4)	C(13) - C(41) - C(44) - C(59)	179.2(6)
C(13) - C(41) - C(60) - C(63)	-178.5(7)	C(60) - C(41) - C(44) - C(59)	1.8(5)
C(44) - C(41) - C(60) - C(63)	-1.1(5)	C(27) - C(42) - C(46) - C(37)	-0.4(4)
C(14) - C(43) - C(57) - C(52)	1.2(4)	C(41) - C(44) - C(59) - C(61)	-2.3(7)
C(19) - C(45) - C(47) - C(38)	0.2(3)	C(35) - C(48) - C(53) - C(56)	-1.5(4)
C(18) - C(49) - C(54) - C(51)	-1.2(4)	C(14) - C(50) - C(55) - C(52)	1.3(4)
C(39) - C(51) - C(54) - C(49)	0.3(4)	C(55) - C(52) - C(57) - C(43)	-0.5(5)
C(57) - C(52) - C(55) - C(50)	-0.7(5)	C(48) - C(53) - C(56) - C(33)	0.0(4)
C(44) - C(59) - C(61) - C(63)	1.9(7)	C(41) - C(60) - C(63) - C(61)	0.7(7)
C(59) - C(61) - C(63) - C(60)	-1.1(7)	Al(1) - O(5) - C(31) - H(31)	-4.9(35)
C(4) - C(8) - C(32) - H(32)	178.2(18)	C(14) - C(8) - C(32) - H(32)	-1.4(18)
C(11) - C(9) - C(19) - H(19)	178.9(21)	H(9) - C(9) - C(11) - C(10)	-14.5(17)
H(9) - C(9) - C(11) - C(38)	163.9(18)	H(9) - C(9) - C(19) - C(45)	-164.1(18)
H(9) - C(9) - C(19) - H(19)	12.2(27)	C(4) - C(10) - C(21) - H(21)	-178.2(20)
C(11) - C(10) - C(21) - H(21)	1.3(19)	C(9) - C(11) - C(38) - H(38)	174.1(14)
C(10) - C(11) - C(38) - H(38)	-7.5(14)	C(20) - C(12) - C(23) - H(23)	3.6(16)
C(20) - C(12) - C(29) - H(29)	-1.6(17)	C(29) - C(12) - C(23) - H(23)	-174.6(16)
C(23) - C(12) - C(29) - H(29)	176.5(18)	C(16) - C(13) - C(37) - H(37)	-177.1(17)
C(41) - C(13) - C(37) - H(37)	4.2(17)	C(8) - C(14) - C(43) - H(43)	0.0(22)
C(8) - C(14) - C(50) - H(50)	-2.2(3)	C(50) - C(14) - C(43) - H(43)	176.0(22)
C(43) - C(14) - C(50) - H(50)	-178.1(5)	C(26) - C(15) - C(18) - H(18)	1.9(16)
C(39) - C(15) - C(18) - H(18)	177.3(16)	C(18) - C(15) - C(39) - H(39)	-177.9(20)
C(26) - C(15) - C(39) - H(39)	-2.6(20)	C(20) - C(17) - C(24) - H(24)	177.5(18)
H(17) - C(17) - C(20) - C(6)	179.3(17)	H(17) - C(17) - C(20) - C(12)	1.8(16)
H(17) - C(17) - C(24) - C(25)	-177.2(16)	H(17) - C(17) - C(24) - H(24)	-1.6(24)
C(15) - C(18) - C(49) - H(49)	-173.1(18)	H(18) - C(18) - C(49) - C(54)	-176.1(18)
H(18) - C(18) - C(49) - H(49)	9.7(24)	C(9) - C(19) - C(45) - H(45)	-172.4(21)

H(19) - C(19) - C(45) - C(47)	-178.1(19)	H(19) - C(19) - C(45) - H(45)	10.8(27)
C(10) - C(21) - C(40) - H(40)	170.7(19)	H(21) - C(21) - C(40) - C(32)	-179.5(20)
H(21) - C(21) - C(40) - H(40)	-9.3(26)	C(34) - C(22) - C(29) - H(29)	-177.6(17)
C(29) - C(22) - C(34) - H(34)	-168.9(25)	H(22) - C(22) - C(29) - C(12)	-176.8(18)
H(22) - C(22) - C(29) - H(29)	4.2(24)	H(22) - C(22) - C(34) - C(28)	178.8(21)
H(22) - C(22) - C(34) - H(34)	9.0(32)	C(12) - C(23) - C(28) - H(28)	174.5(18)
H(23) - C(23) - C(28) - C(34)	177.1(15)	H(23) - C(23) - C(28) - H(28)	-9.3(23)
C(17) - C(24) - C(25) - H(25)	178.4(24)	H(24) - C(24) - C(25) - C(26)	-177.5(20)
H(24) - C(24) - C(25) - H(25)	3.3(31)	H(25) - C(25) - C(26) - C(6)	-180.0(24)
H(25) - C(25) - C(26) - C(15)	-2.2(23)	C(16) - C(27) - C(42) - H(42)	-177.4(22)
C(30) - C(27) - C(42) - H(42)	2.9(22)	C(23) - C(28) - C(34) - H(34)	167.6(26)
H(28) - C(28) - C(34) - C(22)	-173.1(25)	H(28) - C(28) - C(34) - H(34)	-3.6(35)
C(27) - C(30) - C(33) - H(33)	1.8(30)	C(27) - C(30) - C(35) - H(35)	-3.3(19)
C(35) - C(30) - C(33) - H(33)	-176.3(30)	C(33) - C(30) - C(35) - H(35)	174.7(19)
O(5) - C(31) - C(36) - H(36)	37.1(20)	H(31) - C(31) - C(36) - C(62)	-1.2(37)
H(31) - C(31) - C(36) - H(36)	-144.2(42)	C(8) - C(32) - C(40) - H(40)	-169.6(20)
H(32) - C(32) - C(40) - C(21)	179.1(17)	H(32) - C(32) - C(40) - H(40)	9.5(26)
C(30) - C(33) - C(56) - H(56)	-176.3(7)	H(33) - C(33) - C(56) - C(53)	177.4(33)
H(33) - C(33) - C(56) - H(56)	0.9(33)	C(30) - C(35) - C(48) - H(48)	-174.8(5)
H(35) - C(35) - C(48) - C(53)	-174.5(19)	H(35) - C(35) - C(48) - H(48)	7.9(19)
C(31) - C(36) - C(62) - H(62)	0.1(4)	H(36) - C(36) - C(62) - C(58)	-33.8(18)
H(36) - C(36) - C(62) - H(62)	148.6(18)	C(13) - C(37) - C(46) - H(46)	-171.9(28)
H(37) - C(37) - C(46) - C(42)	175.5(18)	H(37) - C(37) - C(46) - H(46)	2.1(32)
C(11) - C(38) - C(47) - H(47)	179.6(5)	H(38) - C(38) - C(47) - C(45)	-172.3(16)
H(38) - C(38) - C(47) - H(47)	7.7(15)	C(15) - C(39) - C(51) - H(51)	-177.8(23)
H(39) - C(39) - C(51) - C(54)	178.0(20)	H(39) - C(39) - C(51) - H(51)	-0.5(29)
C(13) - C(41) - C(44) - H(44)	2.8(24)	C(13) - C(41) - C(60) - H(60)	-0.3(4)
C(60) - C(41) - C(44) - H(44)	-174.6(25)	C(44) - C(41) - C(60) - H(60)	177.1(7)
C(27) - C(42) - C(46) - H(46)	173.0(28)	H(42) - C(42) - C(46) - C(37)	177.6(24)
H(42) - C(42) - C(46) - H(46)	-9.1(36)	C(14) - C(43) - C(57) - H(57)	-178.6(7)
H(43) - C(43) - C(57) - C(52)	-175.1(25)	H(43) - C(43) - C(57) - H(57)	5.1(25)
C(41) - C(44) - C(59) - H(59)	-179.0(8)	H(44) - C(44) - C(59) - C(61)	173.4(30)
H(44) - C(44) - C(59) - H(59)	-3.3(29)	C(19) - C(45) - C(47) - H(47)	-179.8(5)

H(45) - C(45) - C(47) - C(38)	171.1(21)	H(45) - C(45) - C(47) - H(47)	-8.9(21)
C(35) - C(48) - C(53) - H(53)	179.2(7)	H(48) - C(48) - C(53) - C(56)	176.1(7)
H(48) - C(48) - C(53) - H(53)	-3.2(4)	C(18) - C(49) - C(54) - H(54)	175.0(28)
H(49) - C(49) - C(54) - C(51)	172.6(19)	H(49) - C(49) - C(54) - H(54)	-11.2(32)
C(14) - C(50) - C(55) - H(55)	171.2(20)	H(50) - C(50) - C(55) - C(52)	178.6(6)
H(50) - C(50) - C(55) - H(55)	-11.4(19)	C(39) - C(51) - C(54) - H(54)	-176.1(26)
H(51) - C(51) - C(54) - C(49)	178.6(26)	H(51) - C(51) - C(54) - H(54)	2.2(36)
C(57) - C(52) - C(55) - H(55)	-169.0(24)	C(55) - C(52) - C(57) - H(57)	179.4(8)
H(52) - C(52) - C(55) - C(50)	178.3(7)	H(52) - C(52) - C(55) - H(55)	10.0(23)
H(52) - C(52) - C(57) - C(43)	-179.5(8)	H(52) - C(52) - C(57) - H(57)	0.3(5)
C(48) - C(53) - C(56) - H(56)	176.4(7)	H(53) - C(53) - C(56) - C(33)	179.3(7)
H(53) - C(53) - C(56) - H(56)	-4.4(5)	H(58A) - C(58) - C(62) - C(36)	-179.7(11)
H(58A) - C(58) - C(62) - H(62)	-2.1(6)	H(58B) - C(58) - C(62) - C(36)	58.2(7)
H(58B) - C(58) - C(62) - H(62)	-124.2(7)	H(58C) - C(58) - C(62) - C(36)	-55.7(6)
H(58C) - C(58) - C(62) - H(62)	121.8(7)	C(44) - C(59) - C(61) - H(61)	-175.1(12)
H(59) - C(59) - C(61) - C(63)	178.1(13)	H(59) - C(59) - C(61) - H(61)	1.1(7)
C(41) - C(60) - C(63) - H(63)	-174.9(12)	H(60) - C(60) - C(63) - C(61)	-177.5(11)
H(60) - C(60) - C(63) - H(63)	6.9(8)	C(59) - C(61) - C(63) - H(63)	175.3(12)
H(61) - C(61) - C(63) - C(60)	175.4(16)	H(61) - C(61) - C(63) - H(63)	-8.2(10)

INTERMOLECULAR NON-BONDED DISTANCES

Non-bonded distance limits based on Van der Waal's radii

Atom(1)	Atom(2)	dist	e.s.d.	ns	np	Ta Tb Tc	x(2)	y(2)	z(2)
C(6)	C(45)	3.571	0.004	1	1	0 0 -1	0.38410	0.32710	0.17120
C(6)	H(45)	2.63	0.03	1	1	0 0 -1	0.34880	0.29860	0.23330
C(9)	C(57)	3.780	0.005	1	1	0 0 1	0.40760	0.49400	1.30000
C(9)	H(57)	3.116	0.002	1	1	0 0 1	0.44600	0.48840	1.22220
C(10)	C(58)	3.895	0.006	2	1	1 0 2	0.40790	0.60580	0.94100

C(13)	-	C(34)	3.823	0.004	1	1	-1	0	0	-0.26500	0.26540	0.67650
C(13)	-	H(34)	2.97	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(15)	-	C(46)	3.877	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(16)	-	C(34)	3.727	0.003	1	1	-1	0	0	-0.26500	0.26540	0.67650
C(16)	-	H(34)	2.89	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(17)	-	C(32)	3.599	0.004	2	1	1	-1	1	0.38270	-0.00070	0.32310
C(17)	-	C(45)	3.656	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(17)	-	H(32)	3.14	0.02	2	1	1	-1	1	0.34750	0.02280	0.38220
C(17)	-	H(45)	2.82	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(18)	-	C(46)	3.789	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(18)	-	H(46)	3.13	0.05	1	1	0	0	-1	-0.15450	0.26540	0.08140
C(19)	-	C(52)	3.754	0.005	1	1	0	0	1	0.28960	0.51570	1.29170
C(19)	-	C(57)	3.536	0.005	1	1	0	0	1	0.40760	0.49400	1.30000
C(19)	-	H(57)	3.177	0.003	1	1	0	0	1	0.44600	0.48840	1.22220
C(20)	-	C(45)	3.561	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(20)	-	H(45)	2.68	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(21)	-	C(37)	3.922	0.004	1	1	1	0	0	0.92900	0.33980	0.97890
C(21)	-	H(37)	3.13	0.03	1	1	1	0	0	0.87580	0.38220	1.02100
C(22)	-	C(49)	3.518	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(22)	-	C(54)	3.822	0.004	1	1	1	0	0	0.83530	0.36690	0.34910
C(22)	-	H(49)	3.01	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(23)	-	C(52)	3.955	0.005	2	1	1	-1	1	0.71040	0.01570	0.70830
C(23)	-	C(55)	3.878	0.004	2	1	1	-1	1	0.76980	0.02390	0.60000
C(24)	-	C(32)	3.527	0.004	2	1	1	-1	1	0.38270	-0.00070	0.32310
C(24)	-	C(40)	3.580	0.004	2	1	1	-1	1	0.31050	-0.00910	0.20760
C(24)	-	C(45)	3.776	0.005	1	1	0	0	-1	0.38410	0.32710	0.17120
C(24)	-	C(61)	3.935	0.007	2	1	0	-1	1	-0.03380	0.05340	0.23960
C(24)	-	C(62)	3.956	0.006	1	1	0	0	-1	0.49800	0.15730	0.00770
C(24)	-	H(32)	3.12	0.02	2	1	1	-1	1	0.34750	0.02280	0.38220
C(24)	-	H(40)	3.14	0.03	2	1	1	-1	1	0.22600	0.01580	0.18240
C(24)	-	H(45)	2.95	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(24)	-	H(62)	3.036	0.003	1	1	0	0	-1	0.42920	0.16360	0.05560
C(25)	-	C(42)	3.822	0.004	1	1	0	0	-1	-0.03170	0.22590	-0.04130

C(25)	-	C(45)	3.738	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(25)	-	C(46)	3.975	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(25)	-	C(61)	3.693	0.007	2	1	0	-1	1	-0.03380	0.05340	0.23960
C(25)	-	H(45)	2.86	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(25)	-	H(61)	3.006	0.003	2	1	0	-1	1	-0.03240	0.09800	0.28140
C(26)	-	C(45)	3.657	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(26)	-	H(45)	2.73	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(27)	-	C(34)	3.671	0.003	1	1	-1	0	0	-0.26500	0.26540	0.67650
C(27)	-	H(34)	2.87	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(28)	-	C(52)	3.844	0.005	2	1	1	-1	1	0.71040	0.01570	0.70830
C(28)	-	C(55)	3.760	0.005	2	1	1	-1	1	0.76980	0.02390	0.60000
C(29)	-	C(49)	3.793	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(29)	-	H(49)	3.01	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(32)	-	H(17)	3.13	0.02	2	1	1	0	1	0.54180	0.64800	0.65360
C(32)	-	H(24)	3.00	0.03	2	1	1	0	1	0.72020	0.62670	0.78850
C(33)	-	C(63)	3.998	0.010	2	1	0	-1	2	-0.05050	0.03750	1.11290
C(34)	-	C(37)	3.902	0.004	1	1	1	0	0	0.92900	0.33980	0.97890
C(34)	-	C(42)	3.736	0.004	1	1	1	0	0	0.96830	0.22590	0.95870
C(34)	-	C(46)	3.854	0.004	1	1	1	0	0	0.91200	0.27600	1.01510
C(34)	-	C(49)	3.667	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(34)	-	H(49)	3.19	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(37)	-	H(34)	3.06	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(40)	-	C(41)	3.730	0.003	1	1	1	0	0	1.01560	0.42320	0.84230
C(40)	-	C(44)	3.671	0.004	1	1	1	0	0	0.99790	0.44070	0.71150
C(40)	-	C(59)	3.806	0.006	1	1	1	0	0	1.00990	0.50410	0.67770
C(40)	-	C(60)	3.876	0.004	1	1	1	0	0	1.04110	0.47320	0.92950
C(40)	-	C(61)	3.962	0.007	1	1	1	0	0	1.03380	0.55340	0.76040
C(40)	-	C(63)	3.983	0.006	1	1	1	0	0	1.05050	0.53750	0.88710
C(40)	-	H(24)	2.78	0.03	2	1	1	0	1	0.72020	0.62670	0.78850
C(41)	-	H(40)	3.19	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(42)	-	H(25)	3.02	0.03	1	1	0	0	1	0.09300	0.19310	1.22250
C(42)	-	H(34)	2.94	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(44)	-	H(40)	3.18	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760

C(45)	- C(57)	3.658	0.006	1	1	0	0	1	0.40760	0.49400	1.30000
C(46)	- C(49)	3.974	0.004	1	1	0	0	1	-0.17170	0.30040	1.36440
C(46)	- H(34)	3.04	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(47)	- C(49)	3.875	0.004	1	1	1	0	1	0.82830	0.30040	1.36440
C(47)	- C(54)	3.944	0.005	1	1	1	0	1	0.83530	0.36690	1.34910
C(49)	- H(46)	3.13	0.05	1	1	0	0	-1	-0.15450	0.26540	0.08140
C(49)	- H(47)	3.080	0.003	1	1	-1	0	-1	-0.43470	0.29660	0.20820
C(50)	- H(23)	3.20	0.02	2	1	1	0	1	0.43280	0.63960	0.44300
C(51)	- C(53)	3.955	0.005	2	1	0	0	1	-0.20660	0.57320	0.30830
C(52)	- H(28)	2.89	0.03	2	1	1	0	1	0.26690	0.65670	0.31640
C(53)	- H(51)	3.13	0.04	2	1	0	-1	1	0.03600	-0.05240	0.66940
C(55)	- H(23)	3.19	0.02	2	1	1	0	1	0.43280	0.63960	0.44300
C(55)	- H(28)	2.89	0.03	2	1	1	0	1	0.26690	0.65670	0.31640
C(59)	- H(40)	3.11	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(60)	- H(40)	3.08	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(61)	- H(25)	3.17	0.04	2	1	0	0	1	-0.09300	0.69310	0.77750
C(61)	- H(40)	3.03	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(63)	- H(40)	2.99	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
H(24)	- H(40)	2.34	0.04	2	1	1	-1	1	0.22600	0.01580	0.18240
H(42)	- H(63)	2.36	0.03	2	1	0	-1	2	-0.07360	0.07620	1.06470
C(6)	- C(45)	3.571	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(6)	- H(45)	2.63	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(9)	- C(57)	3.780	0.005	1	1	0	0	1	0.40760	0.49400	1.30000
C(9)	- H(57)	3.116	0.002	1	1	0	0	1	0.44600	0.48840	1.22220
C(10)	- C(58)	3.895	0.006	2	1	1	0	2	0.40790	0.60580	0.94100
C(13)	- C(34)	3.823	0.004	1	1	-1	0	0	-0.26500	0.26540	0.67650
C(13)	- H(34)	2.97	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(15)	- C(46)	3.877	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(16)	- C(34)	3.727	0.003	1	1	-1	0	0	-0.26500	0.26540	0.67650
C(16)	- H(34)	2.89	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(17)	- C(32)	3.599	0.004	2	1	1	-1	1	0.38270	-0.00070	0.32310
C(17)	- C(45)	3.656	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(17)	- H(32)	3.14	0.02	2	1	1	-1	1	0.34750	0.02280	0.38220

C(17)	-	H(45)	2.82	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(18)	-	C(46)	3.789	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(18)	-	H(46)	3.13	0.05	1	1	0	0	-1	-0.15450	0.26540	0.08140
C(19)	-	C(52)	3.754	0.005	1	1	0	0	1	0.28960	0.51570	1.29170
C(19)	-	C(57)	3.536	0.005	1	1	0	0	1	0.40760	0.49400	1.30000
C(19)	-	H(57)	3.177	0.003	1	1	0	0	1	0.44600	0.48840	1.22220
C(20)	-	C(45)	3.561	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(20)	-	H(45)	2.68	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(21)	-	C(37)	3.922	0.004	1	1	1	0	0	0.92900	0.33980	0.97890
C(21)	-	H(37)	3.13	0.03	1	1	1	0	0	0.87580	0.38220	1.02100
C(22)	-	C(49)	3.518	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(22)	-	C(54)	3.822	0.004	1	1	1	0	0	0.83530	0.36690	0.34910
C(22)	-	H(49)	3.01	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(23)	-	C(52)	3.955	0.005	2	1	1	-1	1	0.71040	0.01570	0.70830
C(23)	-	C(55)	3.878	0.004	2	1	1	-1	1	0.76980	0.02390	0.60000
C(24)	-	C(32)	3.527	0.004	2	1	1	-1	1	0.38270	-0.00070	0.32310
C(24)	-	C(40)	3.580	0.004	2	1	1	-1	1	0.31050	-0.00910	0.20760
C(24)	-	C(45)	3.776	0.005	1	1	0	0	-1	0.38410	0.32710	0.17120
C(24)	-	C(61)	3.935	0.007	2	1	0	-1	1	-0.03380	0.05340	0.23960
C(24)	-	C(62)	3.956	0.006	1	1	0	0	-1	0.49800	0.15730	0.00770
C(24)	-	H(32)	3.12	0.02	2	1	1	-1	1	0.34750	0.02280	0.38220
C(24)	-	H(40)	3.14	0.03	2	1	1	-1	1	0.22600	0.01580	0.18240
C(24)	-	H(45)	2.95	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(24)	-	H(62)	3.036	0.003	1	1	0	0	-1	0.42920	0.16360	0.05560
C(25)	-	C(42)	3.822	0.004	1	1	0	0	-1	-0.03170	0.22590	-0.04130
C(25)	-	C(45)	3.738	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(25)	-	C(46)	3.975	0.004	1	1	0	0	-1	-0.08800	0.27600	0.01510
C(25)	-	C(61)	3.693	0.007	2	1	0	-1	1	-0.03380	0.05340	0.23960
C(25)	-	H(45)	2.86	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(25)	-	H(61)	3.006	0.003	2	1	0	-1	1	-0.03240	0.09800	0.28140
C(26)	-	C(45)	3.657	0.004	1	1	0	0	-1	0.38410	0.32710	0.17120
C(26)	-	H(45)	2.73	0.03	1	1	0	0	-1	0.34880	0.29860	0.23330
C(27)	-	C(34)	3.671	0.003	1	1	-1	0	0	-0.26500	0.26540	0.67650

C(27)	- H(34)	2.87	0.03	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(28)	- C(52)	3.844	0.005	2	1	1	-1	1	0.71040	0.01570	0.70830
C(28)	- C(55)	3.760	0.005	2	1	1	-1	1	0.76980	0.02390	0.60000
C(29)	- C(49)	3.793	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(29)	- H(49)	3.01	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(32)	- H(17)	3.13	0.02	2	1	1	0	1	0.54180	0.64800	0.65360
C(32)	- H(24)	3.00	0.03	2	1	1	0	1	0.72020	0.62670	0.78850
C(33)	- C(63)	3.998	0.010	2	1	0	-1	2	-0.05050	0.03750	1.11290
C(34)	- C(37)	3.902	0.004	1	1	1	0	0	0.92900	0.33980	0.97890
C(34)	- C(42)	3.736	0.004	1	1	1	0	0	0.96830	0.22590	0.95870
C(34)	- C(46)	3.854	0.004	1	1	1	0	0	0.91200	0.27600	1.01510
C(34)	- C(49)	3.667	0.004	1	1	1	0	0	0.82830	0.30040	0.36440
C(34)	- H(49)	3.19	0.03	1	1	1	0	0	0.74610	0.27530	0.37950
C(37)	- H(34)	3.06	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(40)	- C(41)	3.730	0.003	1	1	1	0	0	1.01560	0.42320	0.84230
C(40)	- C(44)	3.671	0.004	1	1	1	0	0	0.99790	0.44070	0.71150
C(40)	- C(59)	3.806	0.006	1	1	1	0	0	1.00990	0.50410	0.67770
C(40)	- C(60)	3.876	0.004	1	1	1	0	0	1.04110	0.47320	0.92950
C(40)	- C(61)	3.962	0.007	1	1	1	0	0	1.03380	0.55340	0.76040
C(40)	- C(63)	3.983	0.006	1	1	1	0	0	1.05050	0.53750	0.88710
C(40)	- H(24)	2.78	0.03	2	1	1	0	1	0.72020	0.62670	0.78850
C(41)	- H(40)	3.19	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(42)	- H(25)	3.02	0.03	1	1	0	0	1	0.09300	0.19310	1.22250
C(42)	- H(34)	2.94	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(44)	- H(40)	3.18	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(45)	- C(57)	3.658	0.006	1	1	0	0	1	0.40760	0.49400	1.30000
C(46)	- C(49)	3.974	0.004	1	1	0	0	1	-0.17170	0.30040	1.36440
C(46)	- H(34)	3.04	0.04	1	1	-1	0	0	-0.20000	0.27430	0.73750
C(47)	- C(49)	3.875	0.004	1	1	1	0	1	0.82830	0.30040	1.36440
C(47)	- C(54)	3.944	0.005	1	1	1	0	1	0.83530	0.36690	1.34910
C(49)	- H(46)	3.13	0.05	1	1	0	0	-1	-0.15450	0.26540	0.08140
C(49)	- H(47)	3.080	0.003	1	1	-1	0	-1	-0.43470	0.29660	0.20820
C(50)	- H(23)	3.20	0.02	2	1	1	0	1	0.43280	0.63960	0.44300

C(51)	-	C(53)	3.955	0.005	2	1	0	0	1	-0.20660	0.57320	0.30830
C(52)	-	H(28)	2.89	0.03	2	1	1	0	1	0.26690	0.65670	0.31640
C(53)	-	H(51)	3.13	0.04	2	1	0	-1	1	0.03600	-0.05240	0.66940
C(55)	-	H(23)	3.19	0.02	2	1	1	0	1	0.43280	0.63960	0.44300
C(55)	-	H(28)	2.89	0.03	2	1	1	0	1	0.26690	0.65670	0.31640
C(59)	-	H(40)	3.11	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(60)	-	H(40)	3.08	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(61)	-	H(25)	3.17	0.04	2	1	0	0	1	-0.09300	0.69310	0.77750
C(61)	-	H(40)	3.03	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
C(63)	-	H(40)	2.99	0.03	1	1	-1	0	0	-0.22600	0.51580	0.81760
H(24)	-	H(40)	2.34	0.04	2	1	1	-1	1	0.22600	0.01580	0.18240
H(42)	-	H(63)	2.36	0.03	2	1	0	-1	2	-0.07360	0.07620	1.06470

---

ns is the symmetry operator number - (* denotes inversion indicator)

np is the lattice point number

Ta.Tb & Tc are unit cell translations. The symmetry operations are:

1 + X, + Y, + Z

2 - X, 1/2 + Y, - Z

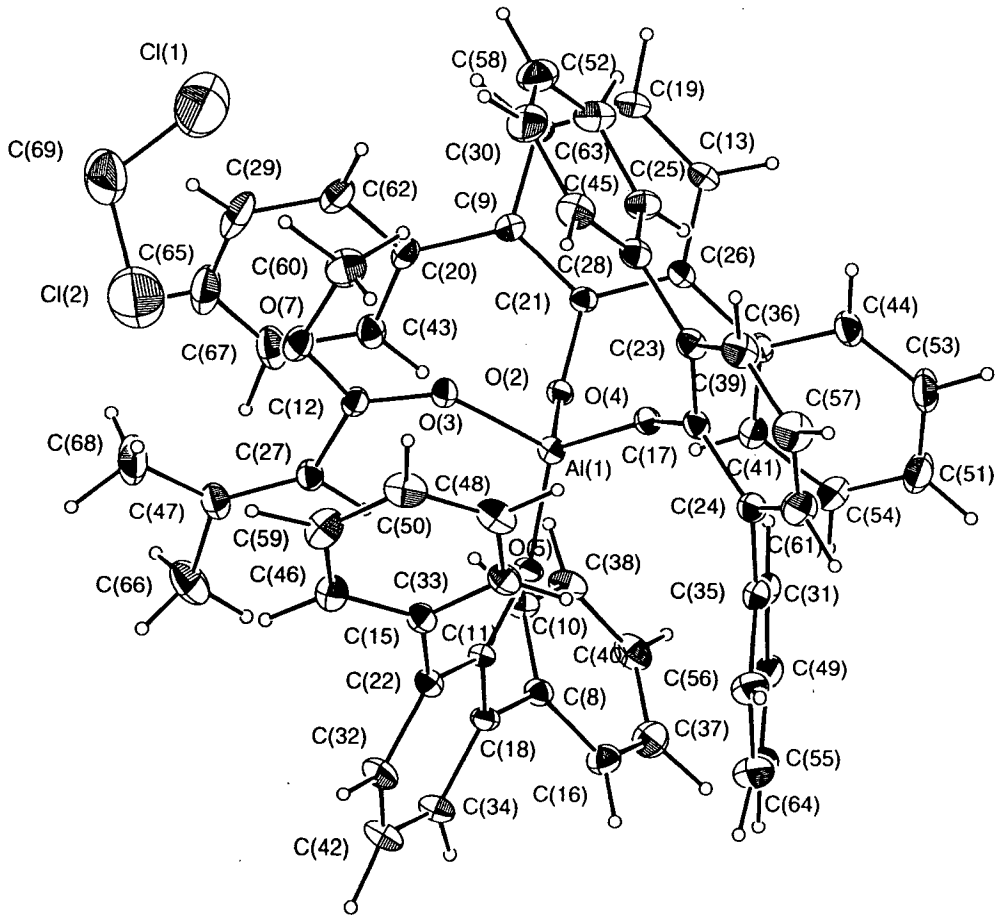

Figure I. ORTEP Representation of the ATPH-1 Complex

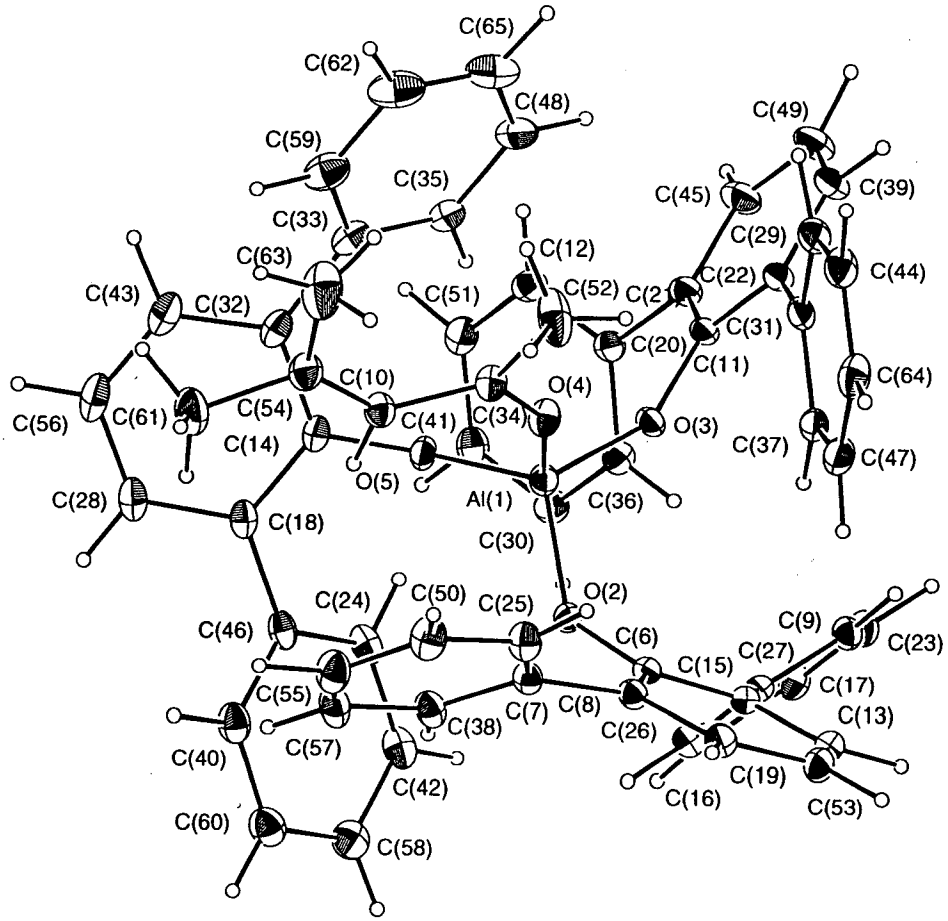

Figure II. ORTEP Representation of the ATPH-2 Complex

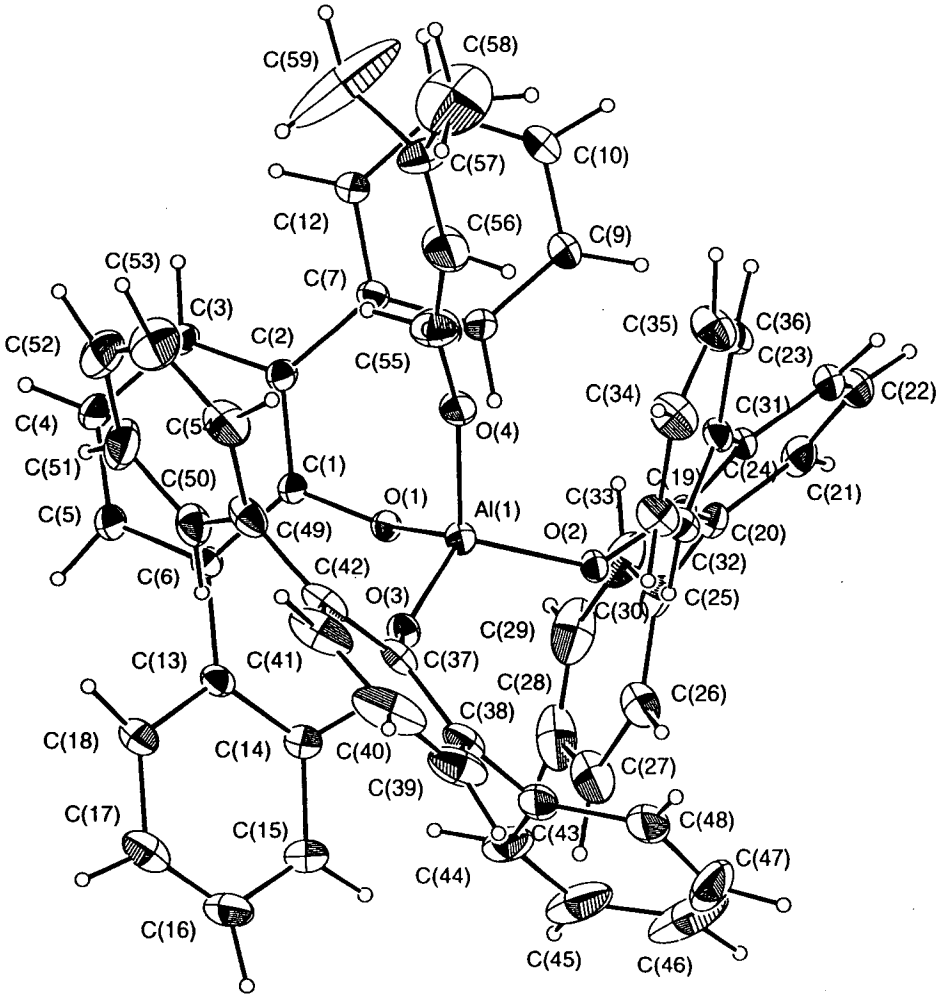

Figure III. ORTEP Representation of the ATPH-3 Complex

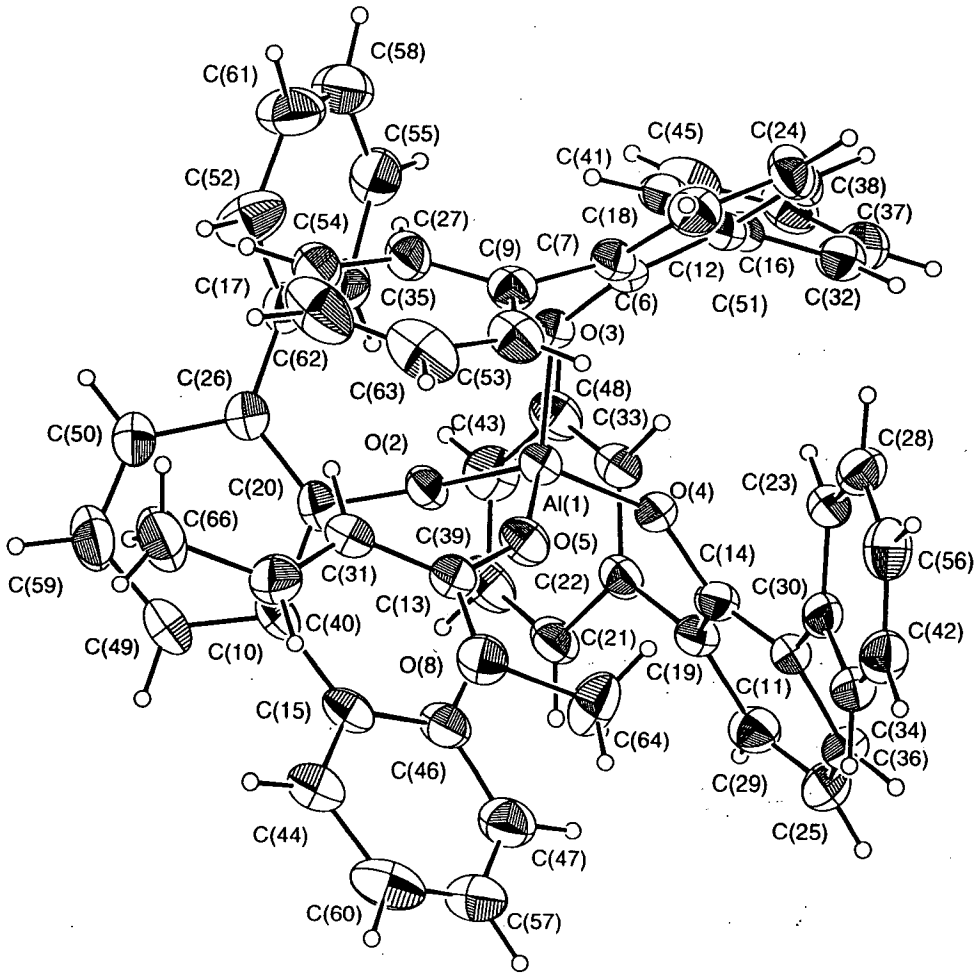

Figure IV. ORTEP Representation of the ATPH-4 Complex

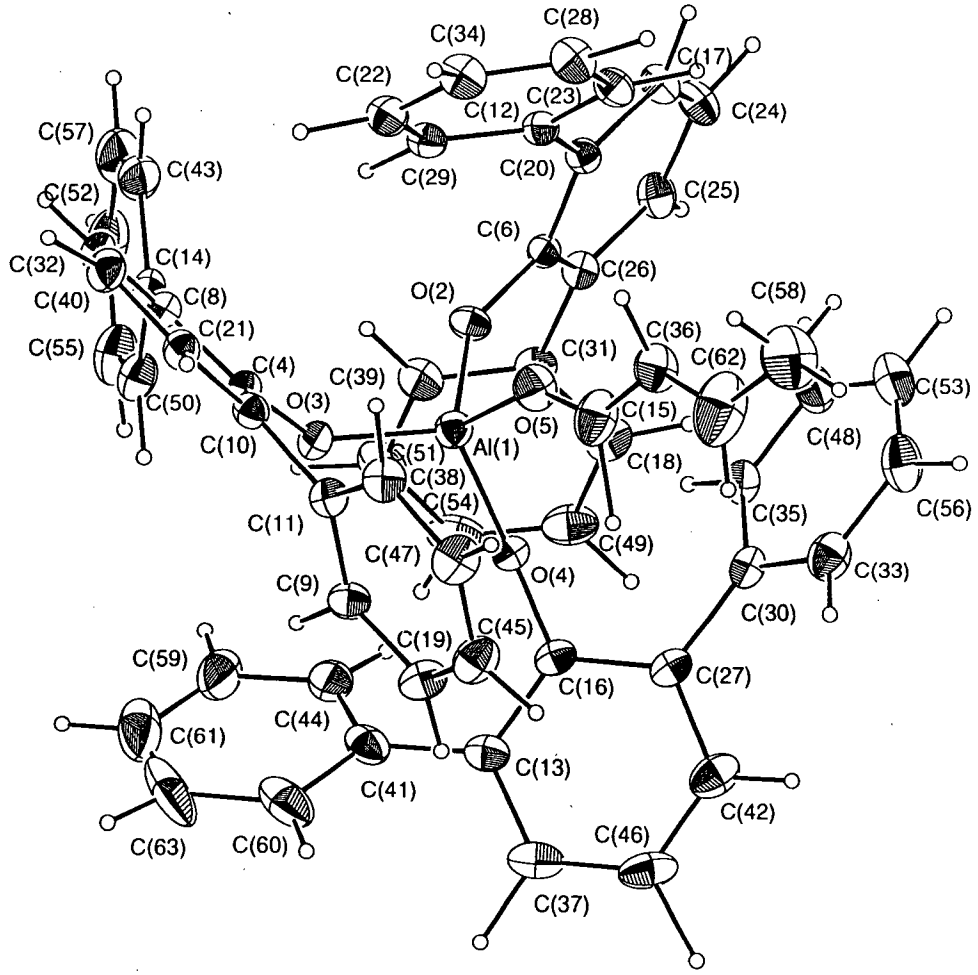

Figure V. ORTEP Representation of the ATPH-6 Complex

Crystal and molecular structure of ATPH-mecrotonate complex
(ATPH-1 Complex)

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Abstract

We present the crystal and molecular structure of ATPH-mecrotonate Complex.

Comment

The study of the titled structure was undertaken to establish its three dimensional structure. Geometries are tabulated below. All Diagrams and calculations were performed using maXus (MacScience, Japan).

Experimental

Compound atph mecrotonate

Crystal data

$C_{60}H_{49}O_5Al$
$M_r = 877.00$
Monoclinic
$P2_1/c$
$a = 10.3370\ (4)$ Å
$b = 20.2030\ (8)$ Å
$c = 24.869\ (1)$ Å
$\beta = 96.515\ (3)°$
$V = 5213.0\ (3)$ Å^3
$Z = 4$
$D_x = 1.117$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from all reflections
$\theta = 1$–$27°$
$\mu = 0.086$ mm^{-1}
$T = 298$ K
Prism
0.35 × 0.2 × 0.15 mm
Colourless
Crystal source: Local laboratory

Data collection

Absorption correction:	$\theta_{max} = 26.84°$
none	$h = 0 \rightarrow 13$
11476 measured reflections	$k = 0 \rightarrow 26$
11171 independent reflections	$l = -32 \rightarrow 32$
7828 observed reflections	

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} = 0.3549$
$R = 0.068$	$\Delta\rho_{max} = 0.64$ e Å^{-3}
$wR = 0.064$	$\Delta\rho_{min} = -0.68$ e Å^{-3}
$S = 1.537$	Extinction correction: Larson
7828 reflections	Extinction coefficient: 0.058953
819 parameters	Atomic scattering factors from
Only coordinates of H atoms refined	*D.* Waasmaier&*A.* Kirfel,*Acta*
Unit	*Cryst.*1995,*A*51, 416-431

Data collection: DIP Image plate. Data reduction: maXus. Program(s) used to solve structure: maXus. Program(s) used to refine structure: maXus. Molecular graphics: maXus. Software used to prepare material for publication: maXus.

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* atph mecrotonate

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Cl1	0.28860 (9)	0.11070 (4)	0.12920 (3)	0.3216 (5)
Cl2	0.2617 (2)	0.0430 (1)	0.22440 (7)	0.274 (1)
Al1	0.8018 (2)	0.2407 (1)	0.39340 (8)	0.049 (1)
O2	0.9592 (2)	0.2352 (1)	0.37650 (8)	0.044 (1)
O3	0.7084 (2)	0.1865 (1)	0.34420 (8)	0.050 (1)
O4	0.7410 (5)	0.3180 (1)	0.3816 (1)	0.049 (3)
O5	0.7979 (3)	0.2088 (1)	0.4562 (1)	0.048 (2)
O7	0.6192 (3)	0.1032 (2)	0.2956 (1)	0.072 (2)

C9	1.0225 (4)	0.2153 (2)	0.2884 (1)	0.048 (2)
C10	1.0699 (3)	0.1665 (2)	0.4979 (1)	0.056 (2)
C11	0.7641 (3)	0.1692 (2)	0.4955 (1)	0.044 (2)
C12	0.6907 (4)	0.1256 (2)	0.3386 (1)	0.052 (2)
C13	1.1238 (4)	0.3429 (2)	0.2878 (2)	0.059 (3)
C15	0.5331 (3)	0.1612 (2)	0.4496 (1)	0.052 (2)
C16	1.0566 (4)	0.2031 (2)	0.5882 (1)	0.064 (2)
C17	0.6451 (3)	0.3632 (2)	0.3803 (1)	0.051 (2)
C18	0.8593 (3)	0.1512 (2)	0.5379 (1)	0.049 (2)
C19	1.1246 (4)	0.3034 (2)	0.2424 (1)	0.066 (2)
C20	0.9877 (3)	0.1441 (2)	0.2891 (1)	0.055 (2)
C21	1.0158 (3)	0.2571 (2)	0.3334 (1)	0.042 (2)
C22	0.6355 (3)	0.1449 (2)	0.4944 (1)	0.051 (2)
C23	0.5744 (3)	0.3793 (2)	0.3303 (1)	0.056 (2)
C24	0.6139 (4)	0.3936 (2)	0.4285 (1)	0.061 (2)
C25	0.7272 (4)	0.3457 (2)	0.2638 (2)	0.066 (2)
C26	1.0707 (3)	0.3210 (2)	0.3341 (1)	0.046 (2)
C27	0.7445 (4)	0.0781 (2)	0.3785 (2)	0.057 (2)
C28	0.6022 (3)	0.3494 (2)	0.2787 (1)	0.056 (2)
C29	0.8955 (6)	0.0460 (3)	0.2439 (3)	0.110 (4)
C30	1.0763 (4)	0.2401 (2)	0.2429 (1)	0.060 (2)
C31	0.8164 (5)	0.3682 (2)	0.4915 (2)	0.070 (2)
C32	0.6064 (4)	0.1022 (2)	0.5357 (2)	0.070 (2)
C33	0.5062 (4)	0.2265 (2)	0.4345 (2)	0.061 (2)
C34	0.8236 (4)	0.1101 (2)	0.5788 (2)	0.067 (2)
C35	0.6830 (5)	0.3763 (2)	0.4824 (2)	0.068 (2)
C36	1.0828 (3)	0.3644 (2)	0.3824 (1)	0.051 (2)
C37	1.1851 (5)	0.2221 (2)	0.5928 (2)	0.080 (3)
C38	1.2006 (4)	0.1843 (2)	0.5027 (2)	0.069 (2)
C39	0.4710 (4)	0.4246 (2)	0.3298 (2)	0.077 (3)
C40	1.2584 (4)	0.2129 (2)	0.5501 (2)	0.077 (3)

C42	0.6994 (4)	0.0847 (2)	0.5776 (2)	0.078 (3)
C43	1.0372 (4)	0.1040 (2)	0.3316 (2)	0.062 (2)
C44	1.0517 (5)	0.4314 (2)	0.3777 (2)	0.071 (2)
C45	0.5017 (5)	0.3265 (2)	0.2415 (2)	0.077 (3)
C46	0.4636 (4)	0.1109 (2)	0.4214 (2)	0.067 (2)
C47	0.7208 (4)	0.0130 (2)	0.3816 (2)	0.074 (2)
C48	0.4122 (4)	0.2410 (3)	0.3914 (2)	0.075 (3)
C49	0.8775 (6)	0.3501 (2)	0.5420 (2)	0.089 (3)
C50	0.3476 (4)	0.1904 (3)	0.3623 (2)	0.084 (3)
C51	1.1370 (6)	0.4500 (3)	0.4700 (3)	0.097 (4)
C52	0.7515 (5)	0.3215 (3)	0.2133 (2)	0.086 (3)
C53	1.0778 (6)	0.4733 (2)	0.4213 (3)	0.095 (3)
C54	1.1660 (5)	0.3842 (3)	0.4755 (2)	0.083 (3)
C55	0.8041 (9)	0.3415 (3)	0.5847 (2)	0.111 (5)
C56	0.6101 (6)	0.3683 (3)	0.5261 (2)	0.093 (4)
C57	0.4388 (5)	0.4542 (3)	0.3761 (2)	0.093 (3)
C58	0.6506 (6)	0.3003 (3)	0.1773 (2)	0.093 (4)
C59	0.3721 (4)	0.1258 (3)	0.3776 (2)	0.083 (3)
C60	0.5677 (8)	0.1526 (4)	0.2554 (3)	0.098 (4)
C61	0.5105 (5)	0.4390 (2)	0.4246 (2)	0.085 (3)
C62	0.9146 (5)	0.1141 (3)	0.2451 (2)	0.081 (3)
C63	0.5254 (6)	0.3020 (3)	0.1912 (2)	0.095 (4)
C64	0.6731 (9)	0.3519 (3)	0.5770 (2)	0.117 (5)
C65	0.9512 (7)	0.0071 (3)	0.2856 (3)	0.114 (4)
C66	0.7873 (8)	−0.0242 (3)	0.4291 (3)	0.111 (4)
C67	1.0218 (5)	0.0357 (2)	0.3295 (3)	0.092 (3)
C68	0.627 (1)	−0.0264 (3)	0.3429 (4)	0.120 (5)
C69	0.2590 (9)	0.0391 (4)	0.1562 (4)	0.182 (7)
H10	1.034 (3)	0.144 (2)	0.465 (1)	0.047 (9)
H13	1.163 (3)	0.387 (2)	0.290 (1)	0.036 (9)
H16	1.006 (4)	0.208 (2)	0.618 (1)	0.03 (1)

H25	0.796 (4)	0.362 (2)	0.287 (2)	0.06 (1)
H27	0.804 (4)	0.104 (2)	0.408 (2)	0.05 (1)
H29	0.835 (4)	0.027 (2)	0.218 (2)	0.09 (1)
H30	1.083 (3)	0.205 (2)	0.211 (1)	0.05 (1)
H31	0.875 (4)	0.371 (2)	0.460 (1)	0.04 (1)
H32	0.511 (4)	0.086 (2)	0.535 (2)	0.05 (1)
H33	0.545 (4)	0.261 (2)	0.454 (2)	0.03 (1)
H34	0.893 (4)	0.105 (2)	0.610 (2)	0.04 (1)
H37	1.219 (4)	0.250 (2)	0.627 (2)	0.07 (1)
H38	1.248 (4)	0.174 (2)	0.472 (1)	0.06 (1)
H39	0.429 (4)	0.434 (2)	0.297 (2)	0.04 (1)
H40	1.352 (4)	0.227 (2)	0.552 (2)	0.07 (1)
H41	1.157 (4)	0.296 (2)	0.437 (2)	0.02 (1)
H42	0.675 (4)	0.055 (2)	0.611 (2)	0.06 (1)
H43	1.088 (5)	0.127 (3)	0.363 (2)	0.03 (2)
H44	1.025 (4)	0.445 (2)	0.345 (2)	0.05 (1)
H45	0.420 (4)	0.326 (2)	0.252 (2)	0.05 (1)
H46	0.489 (4)	0.059 (2)	0.431 (2)	0.07 (1)
H48	0.399 (4)	0.289 (2)	0.381 (2)	0.05 (1)
H49	0.974 (4)	0.345 (2)	0.547 (2)	0.06 (1)
H50	0.286 (4)	0.206 (2)	0.331 (2)	0.07 (1)
H51	1.140 (4)	0.480 (2)	0.501 (2)	0.09 (1)
H52	0.851 (5)	0.330 (3)	0.203 (2)	0.09 (2)
H53	1.055 (5)	0.521 (3)	0.417 (2)	0.09 (2)
H54	1.215 (4)	0.368 (2)	0.509 (2)	0.05 (1)
H55	0.851 (5)	0.326 (2)	0.622 (2)	0.10 (2)
H56	0.520 (5)	0.385 (2)	0.524 (2)	0.10 (1)
H57	0.357 (5)	0.488 (2)	0.373 (2)	0.07 (2)
H58	0.671 (5)	0.282 (2)	0.142 (2)	0.07 (2)
H59	0.323 (5)	0.085 (3)	0.357 (2)	0.05 (2)
H60A	0.516 (5)	0.124 (2)	0.220 (2)	0.19 (2)

H60C	0.512 (8)	0.172 (4)	0.269 (3)	0.10 (3)
H61	0.493 (7)	0.458 (4)	0.458 (3)	0.06 (3)
H62	0.873 (5)	0.142 (3)	0.218 (2)	0.04 (2)
H63	0.456 (5)	0.285 (3)	0.167 (2)	0.10 (2)
H64	0.623 (6)	0.339 (3)	0.605 (2)	0.10 (2)
H65	0.942 (6)	−0.051 (3)	0.285 (2)	0.10 (2)
H66A	0.858 (8)	0.001 (4)	0.459 (3)	0.10 (3)
H66B	0.864 (7)	−0.053 (4)	0.416 (3)	0.16 (4)
H66C	0.73 (1)	−0.056 (5)	0.444 (4)	0.14 (6)
H67	1.060 (8)	0.005 (4)	0.363 (3)	0.09 (3)
H68A	0.668 (7)	−0.039 (4)	0.319 (3)	0.12 (3)
H68B	0.530 (6)	−0.009 (3)	0.328 (2)	0.28 (3)
H68C	0.616 (5)	−0.073 (3)	0.362 (2)	0.17 (2)

Table 2. *Geometric parameters* (Å, °) *for* atph mecrotonate

Cl1—C69	1.638 (9)	C15—C22	1.484 (5)
Cl2—C69	1.69 (1)	C15—C33	1.391 (6)
Al1—O2	1.730 (4)	C15—C46	1.388 (6)
Al1—O3	1.833 (3)	C16—C37	1.375 (7)
Al1—O4	1.697 (4)	C17—C23	1.407 (5)
Al1—O5	1.694 (4)	C17—C24	1.416 (5)
O2—C21	1.352 (4)	C18—C34	1.395 (6)
O3—C12	1.249 (5)	C19—C30	1.373 (7)
O4—C17	1.346 (6)	C20—C43	1.383 (6)
O5—C11	1.340 (5)	C20—C62	1.396 (6)
O7—C12	1.310 (5)	C21—C26	1.410 (5)
O7—C60	1.469 (8)	C22—C32	1.400 (6)
C8—C10	1.387 (5)	C23—C28	1.476 (5)
C8—C16	1.398 (5)	C23—C39	1.406 (6)
C8—C18	1.485 (5)	C24—C35	1.487 (6)
C9—C20	1.483 (6)	C24—C61	1.403 (7)
C9—C21	1.410 (5)	C25—C28	1.386 (6)
C9—C30	1.408 (5)	C25—C52	1.397 (6)
C10—C38	1.390 (6)	C26—C36	1.481 (5)
C11—C18	1.406 (5)	C27—C47	1.342 (6)
C11—C22	1.414 (5)	C28—C45	1.390 (6)
C12—C27	1.446 (6)	C29—C62	1.390 (9)
C13—C19	1.383 (6)	C29—C65	1.37 (1)
C13—C26	1.402 (5)	C31—C35	1.382 (8)

C32—C42	1.381 (6)	C37—H37	1.05 (5)
C33—C48	1.394 (6)	C38—H38	0.98 (4)
C34—C42	1.380 (7)	C39—H39	0.90 (4)
C35—C56	1.400 (7)	C40—H40	1.01 (5)
C36—C41	1.388 (6)	C41—H41	0.93 (5)
C36—C44	1.393 (6)	C42—H42	1.07 (4)
C37—C40	1.385 (7)	C43—H43	1.02 (6)
C38—C40	1.386 (7)	C44—H44	0.89 (4)
C39—C57	1.372 (8)	C45—H45	0.91 (5)
C41—C54	1.390 (7)	C46—H46	1.10 (4)
C43—C67	1.389 (6)	C48—H48	1.00 (5)
C44—C53	1.378 (8)	C49—H49	1.00 (5)
C45—C63	1.393 (7)	C50—H50	1.01 (5)
C46—C59	1.392 (7)	C51—H51	0.97 (5)
C47—C66	1.500 (9)	C52—H52	1.10 (6)
C47—C68	1.51 (1)	C53—H53	0.99 (6)
C48—C50	1.380 (8)	C54—H54	0.98 (5)
C49—C55	1.384 (9)	C55—H55	1.05 (5)
C50—C59	1.375 (9)	C56—H56	0.99 (5)
C51—C53	1.376 (9)	C57—H57	1.08 (5)
C51—C54	1.366 (8)	C58—H58	0.99 (5)
C52—C58	1.364 (8)	C59—H59	1.07 (6)
C55—C64	1.36 (2)	C60—H60A	1.14 (5)
C56—C64	1.396 (9)	C60—H60B	1.07 (6)
C57—C61	1.377 (8)	C60—H60C	0.80 (8)
C58—C63	1.38 (1)	C61—H61	0.95 (7)
C65—C67	1.37 (1)	C62—H62	0.94 (6)
C10—H10	0.97 (4)	C63—H63	0.95 (6)
C13—H13	0.99 (4)	C64—H64	0.95 (6)
C16—H16	0.97 (4)	C65—H65	1.17 (6)
C19—H19	1.00 (4)	C66—H66A	1.11 (8)
C25—H25	0.92 (4)	C66—H66B	1.06 (8)
C27—H27	1.04 (4)	C66—H66C	0.99 (12)
C29—H29	0.94 (4)	C67—H67	1.09 (8)
C30—H30	1.08 (4)	C68—H68A	0.82 (7)
C31—H31	1.05 (4)	C68—H68B	1.09 (7)
C32—H32	1.04 (5)	C68—H68C	1.07 (6)
C33—H33	0.93 (5)		

O2—Al1—O4	110.9 (3)	O2—C21—C26	120.0 (3)
O2—Al1—O5	108.7 (2)	C9—C21—C26	120.2 (3)
O3—Al1—O4	106.1 (2)	C11—C22—C15	121.7 (3)
O3—Al1—O5	108.8 (2)	C11—C22—C32	118.6 (4)
O4—Al1—O5	117.6 (2)	C15—C22—C32	119.6 (4)
Al1—O2—C21	132.5 (3)	C17—C23—C28	122.7 (4)
Al1—O3—C12	136.2 (3)	C17—C23—C39	118.4 (4)
Al1—O4—C17	152.4 (4)	C28—C23—C39	118.8 (4)
Al1—O5—C11	159.2 (3)	C17—C24—C35	121.9 (4)
C12—O7—C60	116.6 (4)	C17—C24—C61	118.0 (4)
C10—C8—C16	117.7 (4)	C35—C24—C61	120.0 (4)
C10—C8—C18	122.1 (3)	C28—C25—C52	121.8 (4)
C16—C8—C18	120.1 (3)	C13—C26—C21	118.3 (3)
C20—C9—C21	122.5 (3)	C13—C26—C36	118.3 (3)
C20—C9—C30	118.2 (4)	C21—C26—C36	123.3 (3)
C21—C9—C30	119.0 (4)	C12—C27—C47	129.2 (4)
C8—C10—C38	121.2 (3)	C23—C28—C25	122.3 (4)
O5—C11—C18	118.9 (4)	C23—C28—C45	120.7 (4)
O5—C11—C22	121.0 (3)	C25—C28—C45	117.0 (4)
C18—C11—C22	120.1 (3)	C62—C29—C65	120.2 (6)
O3—C12—O7	119.6 (4)	C9—C30—C19	121.0 (4)
O3—C12—C27	122.5 (4)	C35—C31—C49	121.5 (5)
O7—C12—C27	117.9 (4)	C22—C32—C42	121.5 (4)
C19—C13—C26	121.8 (4)	C15—C33—C48	120.5 (4)
C22—C15—C33	121.1 (4)	C18—C34—C42	121.9 (4)
C22—C15—C46	120.1 (4)	C24—C35—C31	122.9 (4)
C33—C15—C46	118.8 (4)	C24—C35—C56	118.7 (5)
C8—C16—C37	121.4 (4)	C31—C35—C56	118.3 (5)
O4—C17—C23	119.0 (3)	C26—C36—C41	120.7 (4)
O4—C17—C24	120.8 (3)	C26—C36—C44	120.6 (4)
C23—C17—C24	120.2 (4)	C41—C36—C44	118.3 (4)
C8—C18—C11	122.2 (3)	C16—C37—C40	120.4 (5)
C8—C18—C34	119.1 (3)	C10—C38—C40	120.1 (4)
C11—C18—C34	118.7 (4)	C23—C39—C57	122.2 (5)
C13—C19—C30	119.6 (4)	C37—C40—C38	119.2 (5)
C9—C20—C43	120.5 (4)	C36—C41—C54	120.3 (4)
C9—C20—C62	121.5 (4)	C32—C42—C34	119.2 (4)
C43—C20—C62	117.7 (4)	C20—C43—C67	121.5 (5)

C28—C45—C63	121.5 (5)	C19—C30—H30	123.2 (19)
C15—C46—C59	120.3 (5)	C35—C31—H31	121.5 (21)
C27—C47—C66	117.8 (5)	C49—C31—H31	116.8 (21)
C27—C47—C68	126.0 (5)	C22—C32—H32	117.8 (23)
C66—C47—C68	116.2 (5)	C42—C32—H32	120.7 (23)
C33—C48—C50	120.1 (5)	C15—C33—H33	120.9 (28)
C31—C49—C55	119.6 (7)	C48—C33—H33	118.4 (28)
C48—C50—C59	119.7 (5)	C18—C34—H34	114.2 (23)
C53—C51—C54	119.4 (6)	C42—C34—H34	123.7 (22)
C25—C52—C58	119.9 (5)	C16—C37—H37	116.8 (24)
C44—C53—C51	120.7 (5)	C40—C37—H37	122.3 (24)
C41—C54—C51	120.7 (5)	C10—C38—H38	116.4 (22)
C49—C55—C64	119.7 (6)	C40—C38—H38	123.4 (22)
C35—C56—C64	119.6 (7)	C23—C39—H39	115.5 (27)
C39—C57—C61	118.7 (5)	C57—C39—H39	122.3 (27)
C52—C58—C63	119.8 (5)	C37—C40—H40	123.0 (24)
C46—C59—C50	120.6 (5)	C38—C40—H40	117.8 (24)
C24—C61—C57	122.4 (5)	C36—C41—H41	120.6 (25)
C20—C62—C29	120.6 (5)	C54—C41—H41	119.1 (25)
C45—C63—C58	120.0 (6)	C32—C42—H42	121.1 (22)
C55—C64—C56	121.2 (7)	C34—C42—H42	119.5 (22)
C29—C65—C67	120.0 (6)	C20—C43—H43	115.9 (32)
C43—C67—C65	119.8 (6)	C67—C43—H43	122.6 (32)
Cl1—C69—Cl2	112.7 (5)	C36—C44—H44	115.4 (26)
C8—C10—H10	120.8 (20)	C53—C44—H44	123.6 (26)
C38—C10—H10	117.8 (20)	C28—C45—H45	117.8 (29)
C19—C13—H13	122.8 (18)	C63—C45—H45	120.6 (29)
C26—C13—H13	115.3 (18)	C15—C46—H46	119.2 (21)
C8—C16—H16	118.3 (22)	C59—C46—H46	120.3 (21)
C37—C16—H16	120.3 (22)	C33—C48—H48	117.3 (25)
C13—C19—H19	122.8 (22)	C50—C48—H48	122.5 (25)
C30—C19—H19	117.5 (22)	C31—C49—H49	119.5 (25)
C28—C25—H25	119.0 (24)	C55—C49—H49	120.9 (25)
C52—C25—H25	119.1 (24)	C48—C50—H50	113.6 (25)
C12—C27—H27	107.7 (21)	C59—C50—H50	126.7 (25)
C47—C27—H27	123.0 (21)	C53—C51—H51	116.8 (27)
C62—C29—H29	120.4 (24)	C54—C51—H51	122.5 (27)
C65—C29—H29	118.6 (25)	C25—C52—H52	115.2 (28)

C44—C53—H53	118.6 (29)	C29—C62—H62	122.0 (34)
C51—C53—H53	120.7 (29)	C45—C63—H63	120.6 (33)
C41—C54—H54	119.0 (25)	C58—C63—H63	119.3 (33)
C51—C54—H54	120.1 (25)	C55—C64—H64	118.1 (35)
C49—C55—H55	118.8 (27)	C56—C64—H64	119.5 (36)
C64—C55—H55	121.5 (27)	C29—C65—H65	121.7 (29)
C35—C56—H56	120.9 (26)	C67—C65—H65	118.4 (29)
C64—C56—H56	117.6 (26)	C47—C66—H66A	120.2 (40)
C39—C57—H57	119.1 (24)	C47—C66—H66B	109.0 (40)
C61—C57—H57	122.2 (24)	C47—C66—H66C	110.8 (64)
C52—C58—H58	118.0 (31)	H66A—C66—H66B	89.8 (57)
C63—C58—H58	122.1 (31)	H66A—C66—H66C	116.4 (73)
C46—C59—H59	117.2 (31)	H66B—C66—H66C	107.3 (76)
C50—C59—H59	122.2 (31)	C43—C67—H67	120.9 (44)
O7—C60—H60A	106.2 (25)	C65—C67—H67	119.1 (44)
O7—C60—H60B	111.0 (30)	C47—C68—H68A	106.7 (50)
O7—C60—H60C	104.7 (58)	C47—C68—H68B	123.5 (35)
H60A—C60—H60B	119.7 (38)	C47—C68—H68C	106.1 (29)
H60A—C60—H60C	106.4 (63)	H68A—C68—H68B	112.8 (59)
H60B—C60—H60C	107.8 (65)	H68A—C68—H68C	97.8 (59)
C24—C61—H61	114.4 (45)	H68B—C68—H68C	106.5 (45)
C57—C61—H61	123.1 (45)		
O2—Al1—O3—C12	78.6 (4)	Al1—O4—C17—C23	−101.5 (8)
O3—Al1—O2—C21	69.4 (3)	Al1—O4—C17—C24	77.6 (7)
O2—Al1—O4—C17	177.1 (8)	Al1—O5—C11—C18	143.7 (9)
O4—Al1—O2—C21	−44.2 (3)	Al1—O5—C11—C22	−35.5 (7)
O2—Al1—O5—C11	−120.3 (8)	C60—O7—C12—O3	2.0 (5)
O5—Al1—O2—C21	−174.9 (4)	C60—O7—C12—C27	−179.0 (6)
O4—Al1—O3—C12	−164.4 (4)	C10—C8—C16—C37	−0.2 (4)
O3—Al1—O4—C17	65.1 (7)	C16—C8—C10—C38	1.6 (4)
O3—Al1—O5—C11	−7.9 (7)	C10—C8—C18—C11	−53.5 (4)
O5—Al1—O3—C12	−37.0 (4)	C10—C8—C18—C34	126.8 (5)
O4—Al1—O5—C11	112.7 (8)	C18—C8—C10—C38	−175.1 (5)
O5—Al1—O4—C17	−56.9 (7)	C16—C8—C18—C11	129.9 (5)
Al1—O2—C21—C9	−92.5 (4)	C16—C8—C18—C34	−49.8 (4)
Al1—O2—C21—C26	89.1 (4)	C18—C8—C16—C37	176.5 (6)
Al1—O3—C12—O7	−177.0 (6)	C20—C9—C21—O2	−9.4 (3)
Al1—O3—C12—C27	4.2 (3)	C20—C9—C21—C26	169.1 (5)

C21—C9—C20—C62	137.6 (6)	C11—C18—C34—C42	2.6 (4)
C20—C9—C30—C19	−172.3 (6)	C13—C19—C30—C9	1.8 (4)
C30—C9—C20—C43	125.1 (5)	C9—C20—C43—C67	−170.4 (6)
C30—C9—C20—C62	−48.9 (5)	C9—C20—C62—C29	172.6 (7)
C30—C9—C21—O2	177.0 (5)	C43—C20—C62—C29	−1.5 (5)
C21—C9—C30—C19	1.5 (4)	C62—C20—C43—C67	3.8 (5)
C30—C9—C21—C26	−4.5 (4)	O2—C21—C26—C13	−177.5 (5)
C8—C10—C38—C40	−2.2 (4)	O2—C21—C26—C36	6.6 (3)
O5—C11—C18—C8	0.1 (3)	C9—C21—C26—C13	4.1 (4)
O5—C11—C18—C34	179.8 (5)	C9—C21—C26—C36	−171.8 (5)
O5—C11—C22—C15	0.9 (4)	C11—C22—C32—C42	1.3 (4)
O5—C11—C22—C32	178.2 (6)	C15—C22—C32—C42	178.7 (6)
C22—C11—C18—C8	179.3 (5)	C17—C23—C28—C25	−48.5 (4)
C18—C11—C22—C15	−178.3 (5)	C17—C23—C28—C45	134.8 (6)
C18—C11—C22—C32	−0.9 (4)	C17—C23—C39—C57	1.2 (5)
C22—C11—C18—C34	−1.0 (4)	C39—C23—C28—C25	133.1 (6)
O3—C12—C27—C47	170.6 (7)	C39—C23—C28—C45	−43.7 (5)
O7—C12—C27—C47	−8.3 (4)	C28—C23—C39—C57	179.7 (7)
C19—C13—C26—C21	−0.7 (4)	C17—C24—C35—C31	43.2 (5)
C26—C13—C19—C30	−2.2 (4)	C17—C24—C35—C56	−137.3 (6)
C19—C13—C26—C36	175.4 (6)	C17—C24—C61—C57	0.6 (5)
C33—C15—C22—C11	−53.1 (4)	C61—C24—C35—C31	−139.8 (6)
C33—C15—C22—C32	129.6 (5)	C61—C24—C35—C56	39.7 (5)
C22—C15—C33—C48	178.3 (6)	C35—C24—C61—C57	−176.5 (7)
C46—C15—C22—C11	125.9 (5)	C52—C25—C28—C23	−175.5 (7)
C46—C15—C22—C32	−51.4 (4)	C52—C25—C28—C45	1.4 (5)
C22—C15—C46—C59	−176.7 (6)	C28—C25—C52—C58	−0.4 (5)
C46—C15—C33—C48	−0.8 (4)	C13—C26—C36—C41	−125.2 (5)
C33—C15—C46—C59	2.3 (4)	C13—C26—C36—C44	47.8 (4)
C8—C16—C37—C40	−0.6 (5)	C21—C26—C36—C41	50.7 (4)
O4—C17—C23—C28	−1.0 (4)	C21—C26—C36—C44	−136.3 (5)
O4—C17—C23—C39	177.4 (6)	C12—C27—C47—C66	−177.7 (7)
O4—C17—C24—C35	−1.2 (4)	C12—C27—C47—C68	−1.0 (6)
O4—C17—C24—C61	−178.3 (6)	C23—C28—C45—C63	175.9 (7)
C24—C17—C23—C28	180.0 (6)	C25—C28—C45—C63	−1.1 (5)
C23—C17—C24—C35	177.8 (6)	C65—C29—C62—C20	−1.6 (6)
C24—C17—C23—C39	−1.6 (4)	C62—C29—C65—C67	2.4 (6)
C23—C17—C24—C61	0.8 (4)	C49—C31—C35—C24	−178.1 (7)

C49—C31—C35—C56	2.4 (5)	H10—C10—C38—C40	−176.7 (23)
C22—C32—C42—C34	0.2 (4)	H10—C10—C38—H38	0.9 (33)
C15—C33—C48—C50	−1.9 (5)	O3—C12—C27—H27	−5.8 (23)
C18—C34—C42—C32	−2.2 (4)	O7—C12—C27—H27	175.3 (23)
C24—C35—C56—C64	179.8 (8)	C26—C13—C19—H19	−179.8 (25)
C31—C35—C56—C64	−0.6 (6)	H13—C13—C19—C30	175.6 (23)
C26—C36—C41—C54	171.1 (6)	H13—C13—C19—H19	−1.9 (33)
C26—C36—C44—C53	−172.1 (7)	H13—C13—C26—C21	−178.7 (21)
C41—C36—C44—C53	1.0 (5)	H13—C13—C26—C36	−2.6 (21)
C44—C36—C41—C54	−2.0 (4)	C22—C15—C33—H33	−6.8 (33)
C16—C37—C40—C38	0.0 (5)	C22—C15—C46—H46	−3.2 (24)
C10—C38—C40—C37	1.4 (4)	C46—C15—C33—H33	174.2 (33)
C23—C39—C57—C61	0.1 (5)	C33—C15—C46—H46	175.8 (24)
C36—C41—C54—C51	0.9 (5)	C8—C16—C37—H37	170.9 (27)
C20—C43—C67—C65	−3.0 (5)	H16—C16—C37—C40	178.4 (26)
C36—C44—C53—C51	1.1 (5)	H16—C16—C37—H37	−10.2 (36)
C28—C45—C63—C58	−0.2 (5)	C8—C18—C34—H34	7.9 (24)
C15—C46—C59—C50	−1.2 (5)	C11—C18—C34—H34	−171.8 (25)
C33—C48—C50—C59	3.0 (5)	C13—C19—C30—H30	−173.3 (24)
C31—C49—C55—C64	−1.1 (6)	H19—C19—C30—C9	179.4 (24)
C48—C50—C59—C46	−1.5 (5)	H19—C19—C30—H30	4.3 (33)
C53—C51—C54—C41	1.2 (5)	C9—C20—C43—H43	7.2 (36)
C54—C51—C53—C44	−2.2 (6)	C9—C20—C62—H62	−12.9 (38)
C25—C52—C58—C63	−0.9 (5)	C62—C20—C43—H43	−178.6 (36)
C49—C55—C64—C56	2.9 (7)	C43—C20—C62—H62	172.9 (38)
C35—C56—C64—C55	−2.0 (6)	C11—C22—C32—H32	178.5 (27)
C39—C57—C61—C24	−1.0 (5)	C15—C22—C32—H32	−4.1 (26)
C52—C58—C63—C45	1.2 (6)	C17—C23—C39—H39	179.3 (30)
C29—C65—C67—C43	−0.2 (6)	C28—C23—C39—H39	−2.2 (29)
C12—O7—C60—H60A	175.9 (26)	C17—C24—C61—H61	179.6 (49)
C12—O7—C60—H60B	44.2 (32)	C35—C24—C61—H61	2.5 (49)
C12—O7—C60—H60C	−71.7 (60)	C28—C25—C52—H52	168.4 (31)
C16—C8—C10—H10	175.9 (24)	H25—C25—C28—C23	1.1 (27)
C10—C8—C16—H16	−179.2 (25)	H25—C25—C28—C45	178.0 (28)
C18—C8—C10—H10	−0.8 (23)	H25—C25—C52—C58	−177.1 (28)
C18—C8—C16—H16	−2.4 (25)	H25—C25—C52—H52	−8.2 (41)
C20—C9—C30—H30	3.2 (21)	H27—C27—C47—C66	−1.8 (26)
C21—C9—C30—H30	177.0 (22)	H27—C27—C47—C68	174.8 (26)

C25—C28—C45—H45	175.7 (33)	C20—C43—C67—H67	−179.1 (50)
C65—C29—C62—H62	−175.7 (40)	H43—C43—C67—C65	179.6 (39)
C62—C29—C65—H65	−176.5 (34)	H43—C43—C67—H67	3.4 (62)
H29—C29—C62—C20	168.7 (29)	C36—C44—C53—H53	179.8 (36)
H29—C29—C62—H62	−5.5 (48)	H44—C44—C53—C51	−170.3 (32)
H29—C29—C65—C67	−168.0 (29)	H44—C44—C53—H53	8.4 (47)
H29—C29—C65—H65	13.1 (43)	C28—C45—C63—H63	177.4 (40)
C35—C31—C49—H49	179.8 (29)	H45—C45—C63—C58	−176.9 (34)
H31—C31—C35—C24	−3.8 (24)	H45—C45—C63—H63	0.7 (51)
H31—C31—C35—C56	176.7 (25)	C15—C46—C59—H59	178.6 (35)
H31—C31—C49—C55	−176.1 (24)	H46—C46—C59—C50	−174.6 (25)
H31—C31—C49—H49	5.3 (36)	H46—C46—C59—H59	5.2 (41)
C22—C32—C42—H42	174.9 (26)	C27—C47—C66—H66A	−3.4 (46)
H32—C32—C42—C34	−176.9 (28)	C27—C47—C66—H66B	−104.8 (44)
H32—C32—C42—H42	−2.3 (37)	C27—C47—C66—H66C	137.2 (68)
C15—C33—C48—H48	−177.8 (28)	C27—C47—C68—H68A	89.1 (52)
H33—C33—C48—C50	−177.0 (32)	C27—C47—C68—H68B	−44.2 (41)
H33—C33—C48—H48	7.1 (42)	C27—C47—C68—H68C	−167.3 (31)
C18—C34—C42—H42	−177.0 (26)	C68—C47—C66—H66A	179.6 (46)
H34—C34—C42—C32	171.7 (27)	C68—C47—C66—H66B	78.2 (44)
H34—C34—C42—H42	−3.1 (36)	C68—C47—C66—H66C	−39.8 (68)
C24—C35—C56—H56	−16.2 (31)	C66—C47—C68—H68A	−94.2 (52)
C31—C35—C56—H56	163.3 (32)	C66—C47—C68—H68B	132.5 (41)
C26—C36—C41—H41	−9.9 (30)	C66—C47—C68—H68C	9.4 (30)
C26—C36—C44—H44	0.0 (29)	C33—C48—C50—H50	−176.1 (27)
C44—C36—C41—H41	177.0 (31)	H48—C48—C50—C59	178.7 (30)
C41—C36—C44—H44	173.1 (29)	H48—C48—C50—H50	−0.3 (39)
C16—C37—C40—H40	178.9 (30)	C31—C49—C55—H55	177.6 (31)
H37—C37—C40—C38	−171.0 (29)	H49—C49—C55—C64	177.5 (30)
H37—C37—C40—H40	8.0 (40)	H49—C49—C55—H55	−3.9 (41)
C10—C38—C40—H40	−177.6 (28)	C48—C50—C59—H59	178.7 (36)
H38—C38—C40—C37	−176.0 (27)	H50—C50—C59—C46	177.5 (31)
H38—C38—C40—H40	5.0 (38)	H50—C50—C59—H59	−2.4 (46)
C23—C39—C57—H57	−179.3 (29)	C54—C51—C53—H53	179.2 (37)
H39—C39—C57—C61	−177.9 (32)	C53—C51—C54—H54	174.9 (29)
H39—C39—C57—H57	2.7 (42)	H51—C51—C53—C44	−169.8 (31)
C36—C41—C54—H54	−172.8 (29)	H51—C51—C53—H53	11.5 (46)
H41—C41—C54—C51	−178.1 (31)	H51—C51—C54—C41	168.1 (32)