Appendix

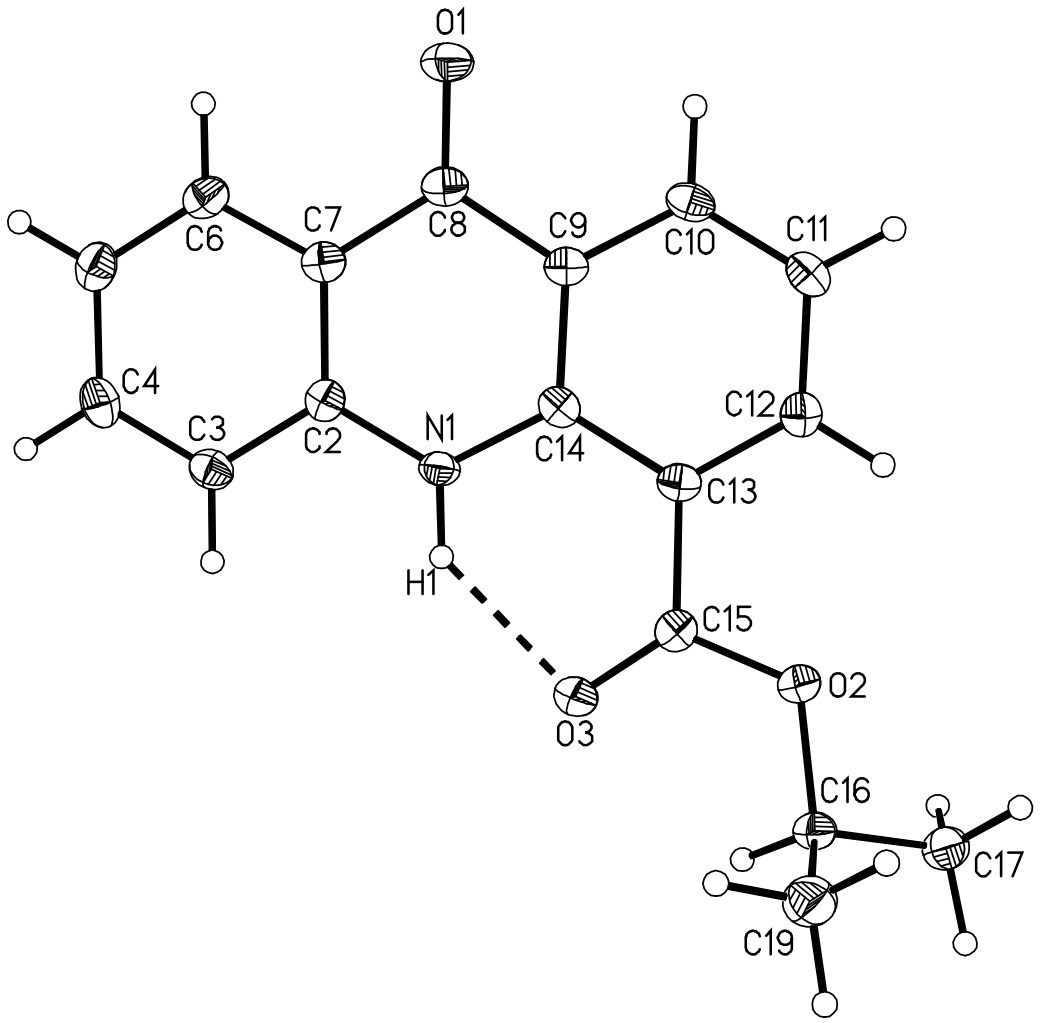

Table 1. Crystal data and structure refinement for *iso*-propyl-9-aminoacridan-4-carboxylate (**22**).

Identification code	twin5
Empirical formula	C17 H15 N O3
Formula weight	281.30
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1

Unit cell dimensions	a = 7.9450(10) Å	α= 77.264(2)°.
	b = 8.4506(11) Å	β= 88.763(4)°.
	c = 11.1255(12) Å	γ = 67.982(4)°.
Volume	673.91(14) $Å^3$	
Z	2	
Density (calculated)	1.386 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	296	
Crystal size	0.38 x 0.24 x 0.06 mm^3	
Theta range for data collection	2.67 to 30.57°.	
Index ranges	-11<=h<=11, -11<=k<=12, 0<=l<=15	
Reflections collected	25508	
Independent reflections	3964 [R(int) = 0.0346]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9943 and 0.8977	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3964 / 1 / 200	
Goodness-of-fit on F^2	0.944	
Final R indices [I>2sigma(I)]	R1 = 0.0440, wR2 = 0.1055	
R indices (all data)	R1 = 0.0774, wR2 = 0.1175	
Largest diff. peak and hole	0.440 and -0.227 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for *iso*-propyl-9-aminoacridan-4-carboxylate (**22**).

N(1)-C(14)	1.3696(15)
N(1)-C(2)	1.3772(15)
N(1)-H(1)	0.890(11)
O(1)-C(8)	1.2368(14)
C(2)-C(7)	1.4025(16)
C(2)-C(3)	1.4046(16)
O(2)-C(15)	1.3338(14)
O(2)-C(16)	1.4697(14)
C(3)-C(4)	1.3757(17)
C(3)-H(3)	0.9500
O(3)-C(15)	1.2200(14)
C(4)-C(5)	1.3997(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3719(17)
C(5)-H(5)	0.9500
C(6)-C(7)	1.4054(16)
C(6)-H(6)	0.9500
C(7)-C(8)	1.4625(16)
C(8)-C(9)	1.4745(16)
C(9)-C(10)	1.3961(16)
C(9)-C(14)	1.4082(16)
C(10)-C(11)	1.3769(17)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3922(16)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3865(16)
C(12)-H(12)	0.9500
C(13)-C(14)	1.4261(16)
C(13)-C(15)	1.4827(16)
C(16)-C(17)	1.5063(18)
C(16)-C(19)	1.5102(17)
C(16)-H(16)	0.973(12)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

C(17)-H(17C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(14)-N(1)-C(2)	122.80(10)
C(14)-N(1)-H(1)	115.6(8)
C(2)-N(1)-H(1)	121.6(8)
N(1)-C(2)-C(7)	120.36(11)
N(1)-C(2)-C(3)	119.78(11)
C(7)-C(2)-C(3)	119.86(11)
C(15)-O(2)-C(16)	118.89(9)
C(4)-C(3)-C(2)	119.86(11)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	120.77(12)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(6)-C(5)-C(4)	119.55(12)
C(6)-C(5)-H(5)	120.2
C(4)-C(5)-H(5)	120.2
C(5)-C(6)-C(7)	121.09(11)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(2)-C(7)-C(6)	118.85(11)
C(2)-C(7)-C(8)	120.46(11)
C(6)-C(7)-C(8)	120.69(11)
O(1)-C(8)-C(7)	122.39(11)
O(1)-C(8)-C(9)	121.83(11)
C(7)-C(8)-C(9)	115.77(10)
C(10)-C(9)-C(14)	119.73(11)
C(10)-C(9)-C(8)	119.69(10)
C(14)-C(9)-C(8)	120.58(11)
C(11)-C(10)-C(9)	121.30(11)
C(11)-C(10)-H(10)	119.4
C(9)-C(10)-H(10)	119.4

C(10)-C(11)-C(12)	119.13(11)
C(10)-C(11)-H(11)	120.4
C(12)-C(11)-H(11)	120.4
C(13)-C(12)-C(11)	121.89(11)
C(13)-C(12)-H(12)	119.1
C(11)-C(12)-H(12)	119.1
C(12)-C(13)-C(14)	118.82(11)
C(12)-C(13)-C(15)	120.30(11)
C(14)-C(13)-C(15)	120.88(10)
N(1)-C(14)-C(9)	119.84(11)
N(1)-C(14)-C(13)	121.04(10)
C(9)-C(14)-C(13)	119.13(11)
O(3)-C(15)-O(2)	123.66(11)
O(3)-C(15)-C(13)	124.73(11)
O(2)-C(15)-C(13)	111.61(10)
O(2)-C(16)-C(17)	104.84(9)
O(2)-C(16)-C(19)	108.33(10)
C(17)-C(16)-C(19)	113.64(10)
O(2)-C(16)-H(16)	107.2(7)
C(17)-C(16)-H(16)	110.6(8)
C(19)-C(16)-H(16)	111.8(7)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for *iso*-propyl-9-aminoacridan-4-carboxylate (**22**).

C(14)-N(1)-C(2)-C(7)	-4.44(18)
C(14)-N(1)-C(2)-C(3)	175.45(10)
N(1)-C(2)-C(3)-C(4)	179.42(11)
C(7)-C(2)-C(3)-C(4)	-0.70(17)
C(2)-C(3)-C(4)-C(5)	-0.44(19)
C(3)-C(4)-C(5)-C(6)	0.78(19)
C(4)-C(5)-C(6)-C(7)	0.01(18)
N(1)-C(2)-C(7)-C(6)	-178.66(11)
C(3)-C(2)-C(7)-C(6)	1.45(17)
N(1)-C(2)-C(7)-C(8)	1.55(17)
C(3)-C(2)-C(7)-C(8)	-178.34(10)
C(5)-C(6)-C(7)-C(2)	-1.12(18)
C(5)-C(6)-C(7)-C(8)	178.68(11)
C(2)-C(7)-C(8)-O(1)	-178.27(11)
C(6)-C(7)-C(8)-O(1)	1.94(18)
C(2)-C(7)-C(8)-C(9)	2.38(16)
C(6)-C(7)-C(8)-C(9)	-177.41(11)
O(1)-C(8)-C(9)-C(10)	-3.06(18)
C(7)-C(8)-C(9)-C(10)	176.30(10)
O(1)-C(8)-C(9)-C(14)	176.87(11)
C(7)-C(8)-C(9)-C(14)	-3.77(17)
C(14)-C(9)-C(10)-C(11)	-0.94(18)
C(8)-C(9)-C(10)-C(11)	178.99(11)
C(9)-C(10)-C(11)-C(12)	0.63(18)
C(10)-C(11)-C(12)-C(13)	-0.38(18)
C(11)-C(12)-C(13)-C(14)	0.43(17)
C(11)-C(12)-C(13)-C(15)	-179.90(11)
C(2)-N(1)-C(14)-C(9)	2.99(17)
C(2)-N(1)-C(14)-C(13)	-176.80(11)
C(10)-C(9)-C(14)-N(1)	-178.81(10)
C(8)-C(9)-C(14)-N(1)	1.26(17)
C(10)-C(9)-C(14)-C(13)	0.98(17)
C(8)-C(9)-C(14)-C(13)	-178.95(10)
C(12)-C(13)-C(14)-N(1)	179.07(10)

C(15)-C(13)-C(14)-N(1)	-0.60(17)
C(12)-C(13)-C(14)-C(9)	-0.72(17)
C(15)-C(13)-C(14)-C(9)	179.61(10)
C(16)-O(2)-C(15)-O(3)	0.30(17)
C(16)-O(2)-C(15)-C(13)	-179.55(9)
C(12)-C(13)-C(15)-O(3)	-176.87(11)
C(14)-C(13)-C(15)-O(3)	2.79(19)
C(12)-C(13)-C(15)-O(2)	2.97(16)
C(14)-C(13)-C(15)-O(2)	-177.36(10)
C(15)-O(2)-C(16)-C(17)	148.05(10)
C(15)-O(2)-C(16)-C(19)	-90.30(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bonds for *iso*-propyl-9-aminoacridan-4-carboxylate (**22**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)	0.890(11)	1.957(12)	2.6791(13)	137.2(11)

Symmetry transformations used to generate equivalent atoms:

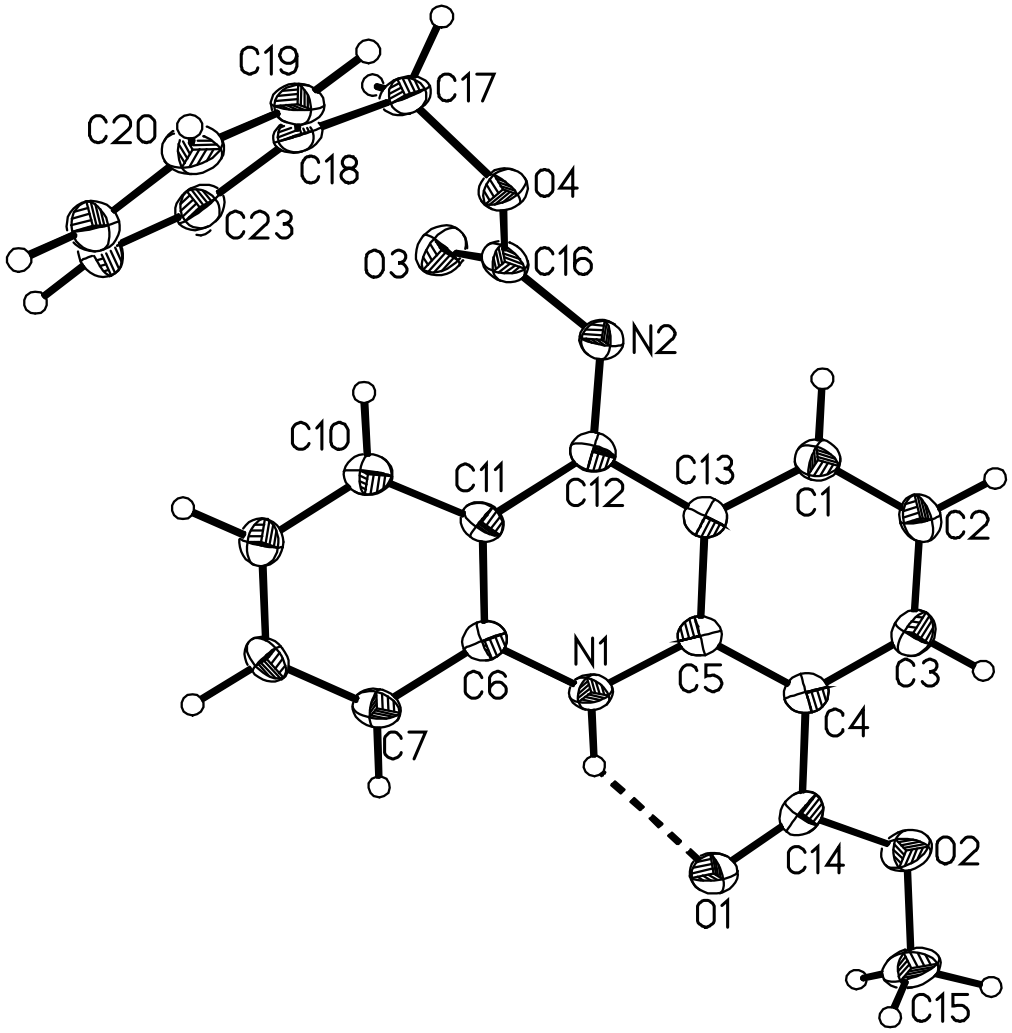

Table 1. Crystal data and structure refinement for methyl-9-benzyloxycarbonylaminoacridine-4-carboxylate (**45**).

Identification code	x81821_0m
Empirical formula	C23 H18 N2 O4
Formula weight	386.39
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P2(1)/n	
Unit cell dimensions	a = 9.528(2) Å	α= 90°.
	b = 8.325(2) Å	β= 100.896(8)°.
	c = 23.478(6) Å	γ = 90°.
Volume	1828.7(8) $Å^3$	
Z	4	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	808	
Crystal size	0.62 x 0.18 x 0.04 mm^3	
Theta range for data collection	2.50 to 30.10°.	
Index ranges	-13<=h<=13, -10<=k<=11, -33<=l<=33	
Reflections collected	36840	
Independent reflections	5356 [R(int) = 0.1126]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9961 and 0.7106	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5356 / 0 / 267	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0643, wR2 = 0.1249	
R indices (all data)	R1 = 0.1640, wR2 = 0.1563	
Largest diff. peak and hole	0.251 and -0.345 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for methyl-9-benzyloxycarbonylaminoacridine-4-carboxylate (**45**).

N(1)-C(5)	1.368(3)
N(1)-C(6)	1.376(3)
N(1)-H(1N)	0.90(2)
N(2)-C(12)	1.292(3)
N(2)-C(16)	1.381(3)
O(1)-C(14)	1.215(3)
O(2)-C(14)	1.343(3)
O(2)-C(15)	1.450(3)
O(3)-C(16)	1.212(3)
O(4)-C(16)	1.351(3)
O(4)-C(17)	1.462(3)
C(1)-C(2)	1.376(3)
C(1)-C(13)	1.397(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.382(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.387(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.424(3)
C(4)-C(14)	1.471(3)
C(5)-C(13)	1.411(3)
C(6)-C(11)	1.405(3)
C(6)-C(7)	1.407(3)
C(7)-C(8)	1.367(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.391(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.371(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.409(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.462(3)
C(12)-C(13)	1.468(3)
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(17)-C(18)	1.501(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.390(3)
C(18)-C(23)	1.393(3)
C(19)-C(20)	1.394(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.372(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.386(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.384(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500

C(5)-N(1)-C(6)	122.81(18)
C(5)-N(1)-H(1N)	114.6(15)
C(6)-N(1)-H(1N)	122.6(15)
C(12)-N(2)-C(16)	126.38(19)
C(14)-O(2)-C(15)	115.87(18)
C(16)-O(4)-C(17)	117.78(18)
C(2)-C(1)-C(13)	121.0(2)
C(2)-C(1)-H(1)	119.5
C(13)-C(1)-H(1)	119.5
C(1)-C(2)-C(3)	120.0(2)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	121.5(2)
C(2)-C(3)-H(3)	119.3
C(4)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	118.85(19)
C(3)-C(4)-C(14)	120.8(2)
C(5)-C(4)-C(14)	120.39(19)
N(1)-C(5)-C(13)	119.33(19)

N(1)-C(5)-C(4)	121.28(18)
C(13)-C(5)-C(4)	119.38(19)
N(1)-C(6)-C(11)	120.85(19)
N(1)-C(6)-C(7)	118.83(18)
C(11)-C(6)-C(7)	120.32(19)
C(8)-C(7)-C(6)	119.91(19)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.7(2)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(10)-C(9)-C(8)	119.7(2)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	121.6(2)
C(9)-C(10)-H(10)	119.2
C(11)-C(10)-H(10)	119.2
C(6)-C(11)-C(10)	117.61(19)
C(6)-C(11)-C(12)	119.00(19)
C(10)-C(11)-C(12)	123.35(18)
N(2)-C(12)-C(11)	127.5(2)
N(2)-C(12)-C(13)	116.36(19)
C(11)-C(12)-C(13)	116.12(18)
C(1)-C(13)-C(5)	119.30(19)
C(1)-C(13)-C(12)	120.33(18)
C(5)-C(13)-C(12)	120.27(19)
O(1)-C(14)-O(2)	122.1(2)
O(1)-C(14)-C(4)	125.4(2)
O(2)-C(14)-C(4)	112.47(19)
O(2)-C(15)-H(15A)	109.5
O(2)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
O(2)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(3)-C(16)-O(4)	125.0(2)

O(3)-C(16)-N(2)	125.5(2)
O(4)-C(16)-N(2)	109.13(19)
O(4)-C(17)-C(18)	108.35(17)
O(4)-C(17)-H(17A)	110.0
C(18)-C(17)-H(17A)	110.0
O(4)-C(17)-H(17B)	110.0
C(18)-C(17)-H(17B)	110.0
H(17A)-C(17)-H(17B)	108.4
C(19)-C(18)-C(23)	119.2(2)
C(19)-C(18)-C(17)	120.5(2)
C(23)-C(18)-C(17)	120.2(2)
C(18)-C(19)-C(20)	120.3(2)
C(18)-C(19)-H(19)	119.8
C(20)-C(19)-H(19)	119.8
C(21)-C(20)-C(19)	120.2(2)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	119.8(2)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	120.7(2)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(18)	119.9(2)
C(22)-C(23)-H(23)	120.0
C(18)-C(23)-H(23)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for methyl-9-benzyloxycarbonylaminoacridine-4-carboxylate (**45**).

C(13)-C(1)-C(2)-C(3)	0.5(3)
C(1)-C(2)-C(3)-C(4)	-0.4(3)
C(2)-C(3)-C(4)-C(5)	-0.5(3)
C(2)-C(3)-C(4)-C(14)	-179.9(2)
C(6)-N(1)-C(5)-C(13)	-4.5(3)
C(6)-N(1)-C(5)-C(4)	176.21(19)
C(3)-C(4)-C(5)-N(1)	-179.39(19)
C(14)-C(4)-C(5)-N(1)	0.1(3)
C(3)-C(4)-C(5)-C(13)	1.3(3)
C(14)-C(4)-C(5)-C(13)	-179.23(19)
C(5)-N(1)-C(6)-C(11)	3.6(3)
C(5)-N(1)-C(6)-C(7)	-176.28(19)
N(1)-C(6)-C(7)-C(8)	178.75(19)
C(11)-C(6)-C(7)-C(8)	-1.1(3)
C(6)-C(7)-C(8)-C(9)	-2.4(3)
C(7)-C(8)-C(9)-C(10)	3.4(3)
C(8)-C(9)-C(10)-C(11)	-0.8(3)
N(1)-C(6)-C(11)-C(10)	-176.27(19)
C(7)-C(6)-C(11)-C(10)	3.6(3)
N(1)-C(6)-C(11)-C(12)	6.1(3)
C(7)-C(6)-C(11)-C(12)	-174.00(19)
C(9)-C(10)-C(11)-C(6)	-2.7(3)
C(9)-C(10)-C(11)-C(12)	174.8(2)
C(16)-N(2)-C(12)-C(11)	-11.6(4)
C(16)-N(2)-C(12)-C(13)	167.3(2)
C(6)-C(11)-C(12)-N(2)	164.9(2)
C(10)-C(11)-C(12)-N(2)	-12.6(3)
C(6)-C(11)-C(12)-C(13)	-14.0(3)
C(10)-C(11)-C(12)-C(13)	168.52(19)
C(2)-C(1)-C(13)-C(5)	0.3(3)
C(2)-C(1)-C(13)-C(12)	-175.9(2)
N(1)-C(5)-C(13)-C(1)	179.44(19)
C(4)-C(5)-C(13)-C(1)	-1.3(3)
N(1)-C(5)-C(13)-C(12)	-4.4(3)

C(4)-C(5)-C(13)-C(12)	174.95(19)
N(2)-C(12)-C(13)-C(1)	10.4(3)
C(11)-C(12)-C(13)-C(1)	-170.55(19)
N(2)-C(12)-C(13)-C(5)	-165.76(19)
C(11)-C(12)-C(13)-C(5)	13.3(3)
C(15)-O(2)-C(14)-O(1)	-5.1(3)
C(15)-O(2)-C(14)-C(4)	174.94(18)
C(3)-C(4)-C(14)-O(1)	177.8(2)
C(5)-C(4)-C(14)-O(1)	-1.7(3)
C(3)-C(4)-C(14)-O(2)	-2.2(3)
C(5)-C(4)-C(14)-O(2)	178.31(18)
C(17)-O(4)-C(16)-O(3)	5.5(3)
C(17)-O(4)-C(16)-N(2)	179.05(16)
C(12)-N(2)-C(16)-O(3)	-71.5(3)
C(12)-N(2)-C(16)-O(4)	115.0(2)
C(16)-O(4)-C(17)-C(18)	102.3(2)
O(4)-C(17)-C(18)-C(19)	88.7(2)
O(4)-C(17)-C(18)-C(23)	-87.6(2)
C(23)-C(18)-C(19)-C(20)	-0.1(3)
C(17)-C(18)-C(19)-C(20)	-176.4(2)
C(18)-C(19)-C(20)-C(21)	0.8(3)
C(19)-C(20)-C(21)-C(22)	-0.7(3)
C(20)-C(21)-C(22)-C(23)	-0.1(3)
C(21)-C(22)-C(23)-C(18)	0.8(3)
C(19)-C(18)-C(23)-C(22)	-0.7(3)
C(17)-C(18)-C(23)-C(22)	175.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bonds for methyl-9-benzyloxycarbonylaminoacridine-4-carboxylate (**45**). [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(1)	0.90(2)	1.93(2)	2.670(2)	138(2)

Symmetry transformations used to generate equivalent atoms: