UNIVERSITAT DE BARCELONA

Síntesis enantioselectiva de alcaloides oxindólicos a partir de lactamas bicíclicas quirales

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Table 1. Crystal data and structure refinement for compound 32.

Identification code	Jb42	
Empirical formula	C23 H26 N2 O4 S	
Formula weight	426.52	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.055(2) Å	α= 90°.
	b = 10.084(2) Å	β= 90°.
	c = 20.606(2) Å	γ = 90°.
Volume	2089.3(6) $Å^3$	
Z	4	
Density (calculated)	1.356 Mg/m^3	
Absorption coefficient	0.188 mm^{-1}	
F(000)	904	
Crystal size	0.32 x 0.28 x 0.10 mm^3	
Theta range for data collection	1.98 to 24.97°.	
Index ranges	-11<=h<=11, 0<=k<=11, 0<=l<=24	
Reflections collected	3970	
Independent reflections	3655 [R(int) = 0.0236]	
Completeness to theta = 24.97°	100.0 %	
Max. and min. transmission	0.9814 and 0.9423	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3655 / 0 / 273	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0898	
R indices (all data)	R1 = 0.0584, wR2 = 0.0991	
Absolute structure parameter	-0.14(9)	
Largest diff. peak and hole	0.155 and -0.177 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 32. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-4012(3)	4965(3)	2053(1)	49(1)
C(3)	-3144(3)	6977(2)	1514(1)	49(1)
C(4)	-1903(3)	7138(3)	1090(1)	56(1)
C(4A)	-1174(2)	5784(3)	1107(1)	45(1)
C(5)	-230(2)	5636(3)	1675(1)	45(1)
C(6)	1026(3)	5291(2)	1463(1)	47(1)
C(8)	-284(3)	5514(3)	512(1)	57(1)
C(8A)	-2377(2)	4831(2)	1138(1)	42(1)
C(9)	-2134(3)	3408(2)	1330(1)	51(1)
C(10)	-3461(3)	2780(3)	1498(1)	55(1)
C(11)	-4034(3)	3480(3)	2087(1)	58(1)
C(31)	-4374(3)	7613(3)	1234(2)	61(1)
C(51)	-446(3)	5783(3)	2332(1)	64(1)
C(52)	590(3)	5568(4)	2762(1)	70(1)
C(53)	1825(3)	5218(3)	2543(2)	69(1)
C(54)	2074(3)	5097(3)	1888(2)	62(1)
C(71)	2041(2)	2758(2)	575(1)	46(1)
C(72)	1013(3)	1985(3)	342(1)	49(1)
C(73)	948(3)	662(3)	506(1)	52(1)
C(74)	1903(3)	76(3)	896(1)	51(1)
C(75)	2917(3)	864(3)	1130(1)	62(1)
C(76)	2987(3)	2189(3)	980(2)	61(1)
C(77)	1833(4)	-1380(3)	1057(2)	81(1)
N(2)	-3279(2)	5526(2)	1578(1)	43(1)
N(7)	1050(2)	5235(2)	775(1)	54(1)
O(1)	-4638(2)	5656(2)	2445(1)	68(1)
O(31)	-4691(2)	7088(2)	608(1)	67(1)
O(71)	3446(2)	4875(2)	566(1)	80(1)
O(72)	1778(2)	4577(2)	-310(1)	78(1)
S(7)	2159(1)	4437(1)	356(1)	59(1)

Table 3. Bond lengths [Å] and angles [°] for compound 32.

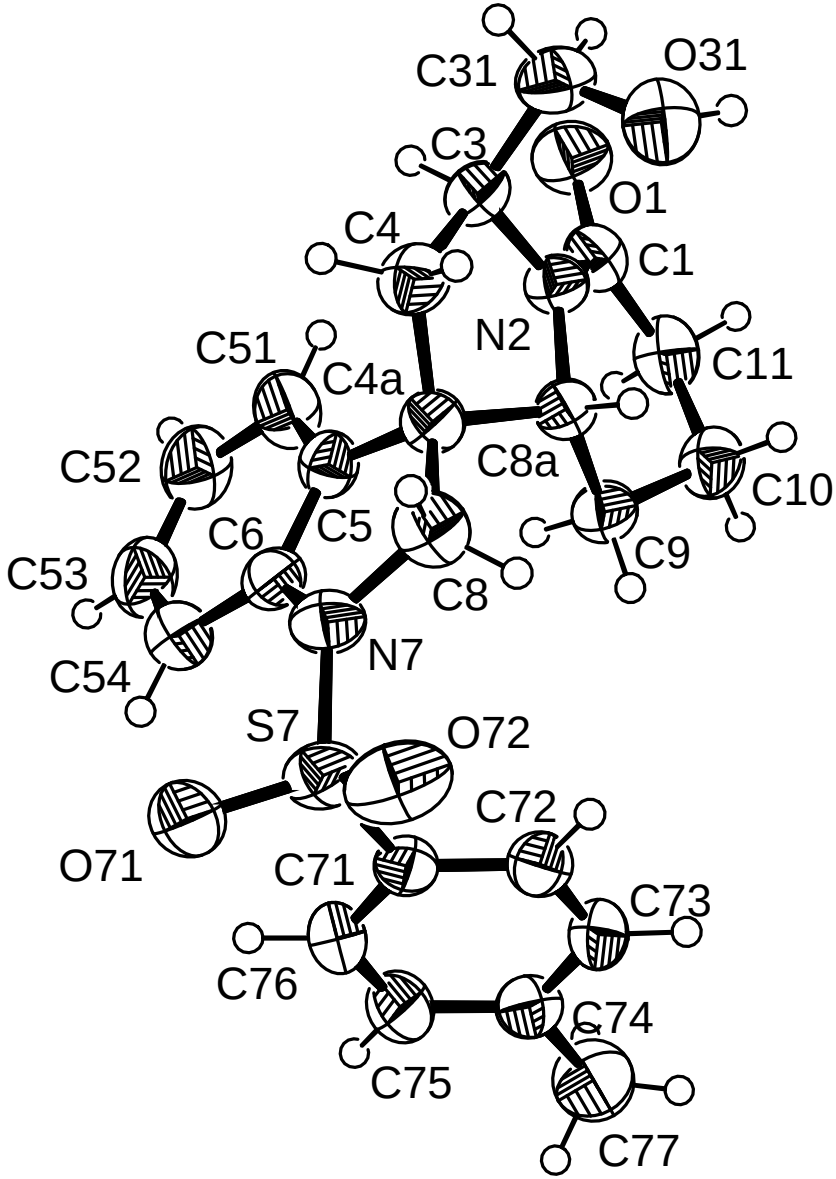
C(1)-O(1)	1.238(3)
C(1)-N(2)	1.349(3)
C(1)-C(11)	1.498(4)
C(3)-N(2)	1.475(3)
C(3)-C(31)	1.508(4)
C(3)-C(4)	1.532(4)
C(4)-C(4A)	1.551(4)
C(4A)-C(5)	1.514(3)
C(4A)-C(8)	1.541(3)
C(4A)-C(8A)	1.546(3)
C(5)-C(6)	1.381(4)
C(5)-C(51)	1.380(3)
C(6)-C(54)	1.385(4)
C(6)-N(7)	1.418(3)
C(8)-N(7)	1.474(3)
C(8A)-N(2)	1.462(3)
C(8A)-C(9)	1.508(3)
C(9)-C(10)	1.518(4)
C(10)-C(11)	1.517(4)
C(31)-O(31)	1.430(3)
C(51)-C(52)	1.385(4)
C(52)-C(53)	1.368(4)
C(53)-C(54)	1.378(4)
C(71)-C(72)	1.381(3)
C(71)-C(76)	1.389(4)
C(71)-S(7)	1.756(3)
C(72)-C(73)	1.377(4)
C(73)-C(74)	1.385(4)
C(74)-C(75)	1.380(4)
C(74)-C(77)	1.506(4)
C(75)-C(76)	1.373(4)
N(7)-S(7)	1.624(2)
O(71)-S(7)	1.435(2)
O(72)-S(7)	1.431(2)

O(1)-C(1)-N(2)	120.9(3)
O(1)-C(1)-C(11)	121.7(3)
N(2)-C(1)-C(11)	117.4(2)
N(2)-C(3)-C(31)	112.4(2)
N(2)-C(3)-C(4)	103.4(2)
C(31)-C(3)-C(4)	113.9(2)
C(3)-C(4)-C(4A)	106.2(2)
C(5)-C(4A)-C(8)	103.5(2)
C(5)-C(4A)-C(8A)	113.4(2)
C(8)-C(4A)-C(8A)	112.2(2)
C(5)-C(4A)-C(4)	113.6(2)
C(8)-C(4A)-C(4)	114.3(2)
C(8A)-C(4A)-C(4)	100.28(19)
C(6)-C(5)-C(51)	118.8(2)
C(6)-C(5)-C(4A)	110.7(2)
C(51)-C(5)-C(4A)	130.5(2)
C(5)-C(6)-C(54)	122.1(2)
C(5)-C(6)-N(7)	110.0(2)
C(54)-C(6)-N(7)	127.9(2)
N(7)-C(8)-C(4A)	105.6(2)
N(2)-C(8A)-C(9)	113.2(2)
N(2)-C(8A)-C(4A)	102.31(19)
C(9)-C(8A)-C(4A)	118.4(2)
C(8A)-C(9)-C(10)	108.3(2)
C(9)-C(10)-C(11)	108.9(2)
C(1)-C(11)-C(10)	115.0(2)
O(31)-C(31)-C(3)	111.7(2)
C(5)-C(51)-C(52)	119.5(3)
C(53)-C(52)-C(51)	120.8(3)
C(52)-C(53)-C(54)	120.7(3)
C(53)-C(54)-C(6)	118.0(3)
C(72)-C(71)-C(76)	119.2(2)
C(72)-C(71)-S(7)	120.3(2)
C(76)-C(71)-S(7)	120.5(2)
C(73)-C(72)-C(71)	119.8(2)

C(72)-C(73)-C(74)	121.5(2)
C(75)-C(74)-C(73)	118.0(3)
C(75)-C(74)-C(77)	121.3(3)
C(73)-C(74)-C(77)	120.7(3)
C(76)-C(75)-C(74)	121.3(3)
C(75)-C(76)-C(71)	120.2(3)
C(1)-N(2)-C(8A)	126.0(2)
C(1)-N(2)-C(3)	122.1(2)
C(8A)-N(2)-C(3)	111.24(19)
C(6)-N(7)-C(8)	110.1(2)
C(6)-N(7)-S(7)	124.29(19)
C(8)-N(7)-S(7)	121.59(18)
O(72)-S(7)-O(71)	120.06(14)
O(72)-S(7)-N(7)	106.13(13)
O(71)-S(7)-N(7)	107.80(13)
O(72)-S(7)-C(71)	108.91(13)
O(71)-S(7)-C(71)	106.24(14)
N(7)-S(7)-C(71)	107.10(12)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 32. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(1)	62(2)	37(1)	2(1)	-1(1)	0(1)
C(3)	56(2)	39(1)	53(2)	-3(1)	1(1)	-1(1)
C(4)	60(2)	41(1)	67(2)	7(1)	7(1)	-5(1)
C(4A)	45(1)	46(2)	45(1)	0(1)	5(1)	-2(1)
C(5)	47(1)	46(1)	42(1)	-1(1)	2(1)	-7(1)
C(6)	50(1)	42(2)	49(2)	-4(1)	4(1)	-1(1)
C(8)	56(2)	70(2)	45(1)	4(1)	9(1)	-2(2)
C(8A)	45(1)	42(1)	39(1)	0(1)	1(1)	0(1)
C(9)	54(2)	42(1)	59(2)	-1(1)	-5(1)	4(1)
C(10)	62(2)	44(2)	59(2)	7(1)	-6(1)	-6(1)
C(11)	61(2)	61(2)	52(2)	13(1)	-2(1)	-13(1)
C(31)	68(2)	51(2)	63(2)	0(2)	0(2)	11(1)
C(51)	55(2)	89(2)	47(2)	-12(2)	5(1)	-8(2)
C(52)	78(2)	88(2)	44(2)	-10(2)	-5(1)	-9(2)
C(53)	72(2)	68(2)	65(2)	-7(2)	-24(2)	-4(2)
C(54)	53(2)	63(2)	71(2)	-10(2)	-7(2)	4(2)
C(71)	42(1)	49(1)	47(1)	-7(1)	8(1)	-1(1)
C(72)	49(1)	55(2)	42(1)	-5(1)	-3(1)	4(1)
C(73)	51(1)	57(2)	50(2)	-6(1)	-8(1)	-4(1)
C(74)	53(2)	51(2)	51(2)	-2(1)	2(1)	3(1)
C(75)	53(2)	66(2)	65(2)	-1(2)	-16(2)	6(2)
C(76)	43(1)	63(2)	76(2)	-13(2)	-8(1)	-6(1)
C(77)	83(2)	56(2)	103(3)	12(2)	-6(2)	1(2)
N(2)	44(1)	42(1)	44(1)	2(1)	6(1)	1(1)
N(7)	55(1)	57(2)	50(1)	-5(1)	10(1)	6(1)
O(1)	67(1)	85(2)	54(1)	-7(1)	17(1)	4(1)
O(31)	71(1)	66(1)	64(1)	12(1)	-7(1)	-6(1)
O(71)	53(1)	67(1)	120(2)	-13(1)	32(1)	-17(1)
O(72)	110(2)	72(1)	52(1)	9(1)	31(1)	9(1)
S(7)	60(1)	51(1)	64(1)	-2(1)	26(1)	-3(1)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C10
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C5
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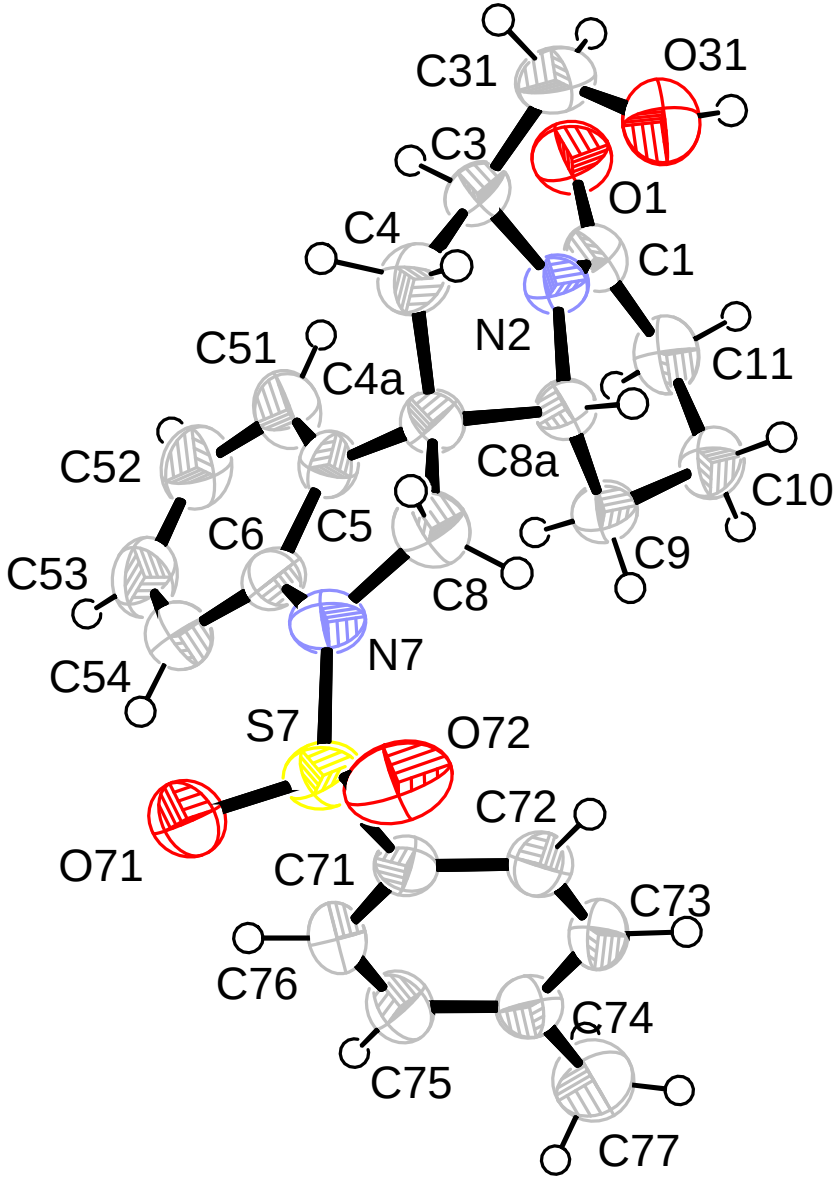
C53
C8
N7
C54
S7
O72
C72
O71
C71
C73
C76
C74
C75
C77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C5
C9
C53
C8
N7
C54
S7
O72
C72
O71
C71
C73
C76
C74
C75
C77

Table 1. Crystal data and structure refinement for compound 42a.

Identification code	Jb99	
Empirical formula	C32 H34 Br2 N4 O4	
Formula weight	698.45	
Temperature	200(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 11.2150(1) Å	α= 90°.
	b = 9.7912(1) Å	β= 92.710(1)°.
	c = 13.7473(1) Å	γ = 90°.
Volume	1507.88(2) $Å^3$	
Z	2	
Density (calculated)	1.538 Mg/m^3	
Absorption coefficient	3.768 mm^{-1}	
F(000)	712	
Crystal size	0.33 x 0.12 x 0.08 mm^3	
Theta range for data collection	3.22 to 64.94°.	
Index ranges	-13<=h<=12, -11<=k<=11, -16<=l<=16	
Reflections collected	24316	
Independent reflections	5063 [R(int) = 0.0265]	
Completeness to theta = 64.94°	99.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5063 / 1 / 379	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0234, wR2 = 0.0585	
R indices (all data)	R1 = 0.0245, wR2 = 0.0595	
Absolute structure parameter	-0.03(1)	
Largest diff. peak and hole	0.475 and -0.464 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For compound 42a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-5781(1)	-9492(1)	-8885(1)	45(1)
Br(2)	-8692(1)	-8714(1)	-4367(1)	57(1)
N(1)	-4513(2)	-5636(2)	-8058(1)	26(1)
N(9)	-6613(2)	-4778(2)	-5330(1)	29(1)
N(19)	-9646(2)	-5002(2)	-3116(1)	25(1)
N(27)	-11396(2)	-6243(2)	-317(2)	30(1)
O(2)	-2805(2)	-6331(2)	-8680(1)	39(1)
O(8)	-7762(1)	-4611(2)	-6754(1)	34(1)
O(20)	-8001(2)	-4142(2)	-3758(1)	45(1)
O(26)	-12510(1)	-6895(2)	-1683(1)	33(1)
C(2)	-3428(2)	-5383(3)	-8392(2)	29(1)
C(3)	-3010(2)	-3918(3)	-8395(2)	40(1)
C(4)	-3953(3)	-2879(3)	-8171(2)	40(1)
C(5)	-4619(2)	-3354(3)	-7290(2)	34(1)
C(6)	-5268(2)	-4659(2)	-7556(2)	26(1)
C(7)	-5728(2)	-5559(2)	-6729(2)	24(1)
C(8)	-6842(2)	-4925(2)	-6301(2)	26(1)
C(10)	-5468(2)	-5220(3)	-5040(2)	28(1)
C(11)	-4942(2)	-5229(3)	-4111(2)	35(1)
C(12)	-3796(2)	-5763(3)	-3992(2)	39(1)
C(13)	-3215(2)	-6278(3)	-4776(2)	37(1)
C(14)	-3747(2)	-6255(3)	-5711(2)	32(1)
C(15)	-4888(2)	-5716(2)	-5844(2)	25(1)
C(16)	-5990(2)	-6895(2)	-7286(2)	27(1)
C(17)	-4951(2)	-7044(2)	-7974(2)	27(1)
C(18)	-5293(2)	-7594(3)	-8983(2)	34(1)
C(20)	-8970(2)	-3946(3)	-3387(2)	30(1)
C(21)	-9417(2)	-2525(3)	-3198(2)	33(1)
C(22)	-10708(2)	-2467(3)	-2921(2)	32(1)
C(23)	-10878(2)	-3497(3)	-2117(2)	30(1)
C(24)	-10699(2)	-4914(2)	-2517(2)	24(1)

C(25)	-10446(2)	-6098(2)	-1790(2)	24(1)
C(26)	-11593(2)	-6484(2)	-1282(2)	26(1)
C(28)	-10226(2)	-5772(2)	-100(2)	26(1)
C(29)	-9724(2)	-5400(3)	794(2)	32(1)
C(30)	-8548(2)	-4937(3)	831(2)	36(1)
C(31)	-7909(2)	-4861(3)	2(2)	36(1)
C(32)	-8436(2)	-5234(3)	-903(2)	31(1)
C(33)	-9606(2)	-5694(2)	-947(2)	25(1)
C(34)	-9992(2)	-7201(3)	-2466(2)	29(1)
C(35)	-9229(2)	-6422(3)	-3183(2)	26(1)
C(36)	-9398(2)	-6907(3)	-4233(2)	36(1)

Table 3. Bond lengths [Å] and angles [°] for compound 42a.

Br(1)-C(18)	1.943(3)
Br(2)-C(36)	1.950(3)
N(1)-C(2)	1.343(3)
N(1)-C(17)	1.470(3)
N(1)-C(6)	1.471(3)
N(9)-C(8)	1.355(3)
N(9)-C(10)	1.396(3)
N(19)-C(20)	1.346(3)
N(19)-C(35)	1.471(3)
N(19)-C(24)	1.474(3)
N(27)-C(26)	1.355(3)
N(27)-C(28)	1.409(3)
O(2)-C(2)	1.238(3)
O(8)-C(8)	1.219(3)
O(20)-C(20)	1.237(3)
O(26)-C(26)	1.213(3)
C(2)-C(3)	1.509(4)
C(3)-C(4)	1.510(4)
C(4)-C(5)	1.526(4)
C(5)-C(6)	1.507(3)
C(6)-C(7)	1.546(3)
C(7)-C(15)	1.510(3)
C(7)-C(16)	1.537(3)
C(7)-C(8)	1.537(3)
C(10)-C(11)	1.381(3)
C(10)-C(15)	1.396(3)
C(11)-C(12)	1.391(4)
C(12)-C(13)	1.381(4)
C(13)-C(14)	1.391(4)
C(14)-C(15)	1.389(3)
C(16)-C(17)	1.543(3)
C(17)-C(18)	1.520(3)
C(20)-C(21)	1.505(4)
C(21)-C(22)	1.516(4)

C(22)-C(23)	1.515(4)
C(23)-C(24)	1.509(3)
C(24)-C(25)	1.547(3)
C(25)-C(33)	1.511(3)
C(25)-C(34)	1.527(3)
C(25)-C(26)	1.540(3)
C(28)-C(29)	1.376(3)
C(28)-C(33)	1.386(3)
C(29)-C(30)	1.393(4)
C(30)-C(31)	1.376(4)
C(31)-C(32)	1.401(3)
C(32)-C(33)	1.386(3)
C(34)-C(35)	1.538(3)
C(35)-C(36)	1.522(3)

C(2)-N(1)-C(17)	120.7(2)
C(2)-N(1)-C(6)	126.3(2)
C(17)-N(1)-C(6)	111.77(18)
C(8)-N(9)-C(10)	112.17(19)
C(20)-N(19)-C(35)	121.58(19)
C(20)-N(19)-C(24)	125.9(2)
C(35)-N(19)-C(24)	110.87(19)
C(26)-N(27)-C(28)	111.8(2)
O(2)-C(2)-N(1)	120.3(2)
O(2)-C(2)-C(3)	122.1(2)
N(1)-C(2)-C(3)	117.6(2)
C(2)-C(3)-C(4)	114.7(2)
C(3)-C(4)-C(5)	109.3(2)
C(6)-C(5)-C(4)	108.3(2)
N(1)-C(6)-C(5)	112.52(18)
N(1)-C(6)-C(7)	101.18(19)
C(5)-C(6)-C(7)	118.62(19)
C(15)-C(7)-C(16)	114.33(19)
C(15)-C(7)-C(8)	102.69(18)
C(16)-C(7)-C(8)	113.20(18)
C(15)-C(7)-C(6)	115.67(18)

C(16)-C(7)-C(6)	100.49(18)
C(8)-C(7)-C(6)	110.91(19)
O(8)-C(8)-N(9)	126.4(2)
O(8)-C(8)-C(7)	126.1(2)
N(9)-C(8)-C(7)	107.48(18)
C(11)-C(10)-C(15)	122.4(2)
C(11)-C(10)-N(9)	127.8(2)
C(15)-C(10)-N(9)	109.8(2)
C(10)-C(11)-C(12)	117.6(3)
C(13)-C(12)-C(11)	120.9(2)
C(12)-C(13)-C(14)	121.2(2)
C(15)-C(14)-C(13)	118.7(2)
C(14)-C(15)-C(10)	119.3(2)
C(14)-C(15)-C(7)	132.9(2)
C(10)-C(15)-C(7)	107.86(19)
C(7)-C(16)-C(17)	104.67(18)
N(1)-C(17)-C(18)	109.4(2)
N(1)-C(17)-C(16)	102.98(18)
C(18)-C(17)-C(16)	115.3(2)
C(17)-C(18)-Br(1)	109.60(18)
O(20)-C(20)-N(19)	120.8(2)
O(20)-C(20)-C(21)	121.4(2)
N(19)-C(20)-C(21)	117.8(2)
C(20)-C(21)-C(22)	114.1(2)
C(23)-C(22)-C(21)	108.3(2)
C(24)-C(23)-C(22)	108.85(19)
N(19)-C(24)-C(23)	112.4(2)
N(19)-C(24)-C(25)	100.91(17)
C(23)-C(24)-C(25)	118.50(19)
C(33)-C(25)-C(34)	115.97(18)
C(33)-C(25)-C(26)	102.66(18)
C(34)-C(25)-C(26)	114.4(2)
C(33)-C(25)-C(24)	112.83(19)
C(34)-C(25)-C(24)	101.17(18)
C(26)-C(25)-C(24)	110.17(18)
O(26)-C(26)-N(27)	126.8(2)

O(26)-C(26)-C(25)	125.7(2)
N(27)-C(26)-C(25)	107.49(19)
C(29)-C(28)-C(33)	122.4(2)
C(29)-C(28)-N(27)	127.8(2)
C(33)-C(28)-N(27)	109.8(2)
C(28)-C(29)-C(30)	117.7(2)
C(31)-C(30)-C(29)	121.1(2)
C(30)-C(31)-C(32)	120.5(2)
C(33)-C(32)-C(31)	118.8(2)
C(32)-C(33)-C(28)	119.5(2)
C(32)-C(33)-C(25)	132.3(2)
C(28)-C(33)-C(25)	108.16(19)
C(25)-C(34)-C(35)	104.5(2)
N(19)-C(35)-C(36)	109.17(19)
N(19)-C(35)-C(34)	103.84(19)
C(36)-C(35)-C(34)	113.9(2)
C(35)-C(36)-Br(2)	109.83(17)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 42a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	53(1)	33(1)	50(1)	-14(1)	4(1)	-9(1)
Br(2)	85(1)	47(1)	39(1)	-16(1)	-4(1)	28(1)
N(1)	24(1)	28(1)	26(1)	-5(1)	10(1)	-6(1)
N(9)	24(1)	37(1)	27(1)	-5(1)	10(1)	4(1)
N(19)	25(1)	32(1)	20(1)	-3(1)	7(1)	7(1)
N(27)	29(1)	35(1)	27(1)	0(1)	12(1)	-2(1)
O(2)	34(1)	51(1)	33(1)	0(1)	18(1)	1(1)
O(8)	24(1)	41(1)	38(1)	-2(1)	1(1)	4(1)
O(20)	39(1)	55(1)	42(1)	-6(1)	25(1)	0(1)
O(26)	25(1)	34(1)	40(1)	-2(1)	3(1)	1(1)
C(2)	25(1)	42(2)	22(1)	1(1)	6(1)	-4(1)
C(3)	37(2)	49(2)	36(1)	2(1)	12(1)	-16(1)
C(4)	44(2)	34(2)	42(2)	4(1)	6(1)	-13(1)
C(5)	33(1)	29(1)	39(1)	-4(1)	8(1)	-6(1)
C(6)	22(1)	28(1)	27(1)	-3(1)	4(1)	-2(1)
C(7)	21(1)	27(1)	23(1)	-4(1)	6(1)	-2(1)
C(8)	22(1)	26(1)	30(1)	-2(1)	5(1)	-3(1)
C(10)	29(1)	29(1)	25(1)	2(1)	5(1)	-4(1)
C(11)	38(1)	41(2)	26(1)	-1(1)	5(1)	-8(1)
C(12)	36(1)	44(2)	35(1)	9(1)	-7(1)	-14(1)
C(13)	24(1)	38(1)	49(2)	7(1)	-4(1)	-5(1)
C(14)	24(1)	32(1)	41(1)	0(1)	4(1)	1(1)
C(15)	22(1)	25(1)	27(1)	0(1)	3(1)	-3(1)
C(16)	26(1)	26(1)	28(1)	-6(1)	7(1)	-5(1)
C(17)	27(1)	28(1)	27(1)	-5(1)	7(1)	-4(1)
C(18)	39(1)	34(1)	31(1)	-9(1)	9(1)	-6(1)
C(20)	33(1)	38(1)	19(1)	0(1)	7(1)	0(1)
C(21)	37(2)	34(1)	28(1)	2(1)	6(1)	-4(1)
C(22)	39(1)	29(1)	29(1)	-1(1)	1(1)	6(1)
C(23)	31(1)	33(1)	27(1)	0(1)	7(1)	8(1)
C(24)	22(1)	31(1)	21(1)	0(1)	3(1)	6(1)

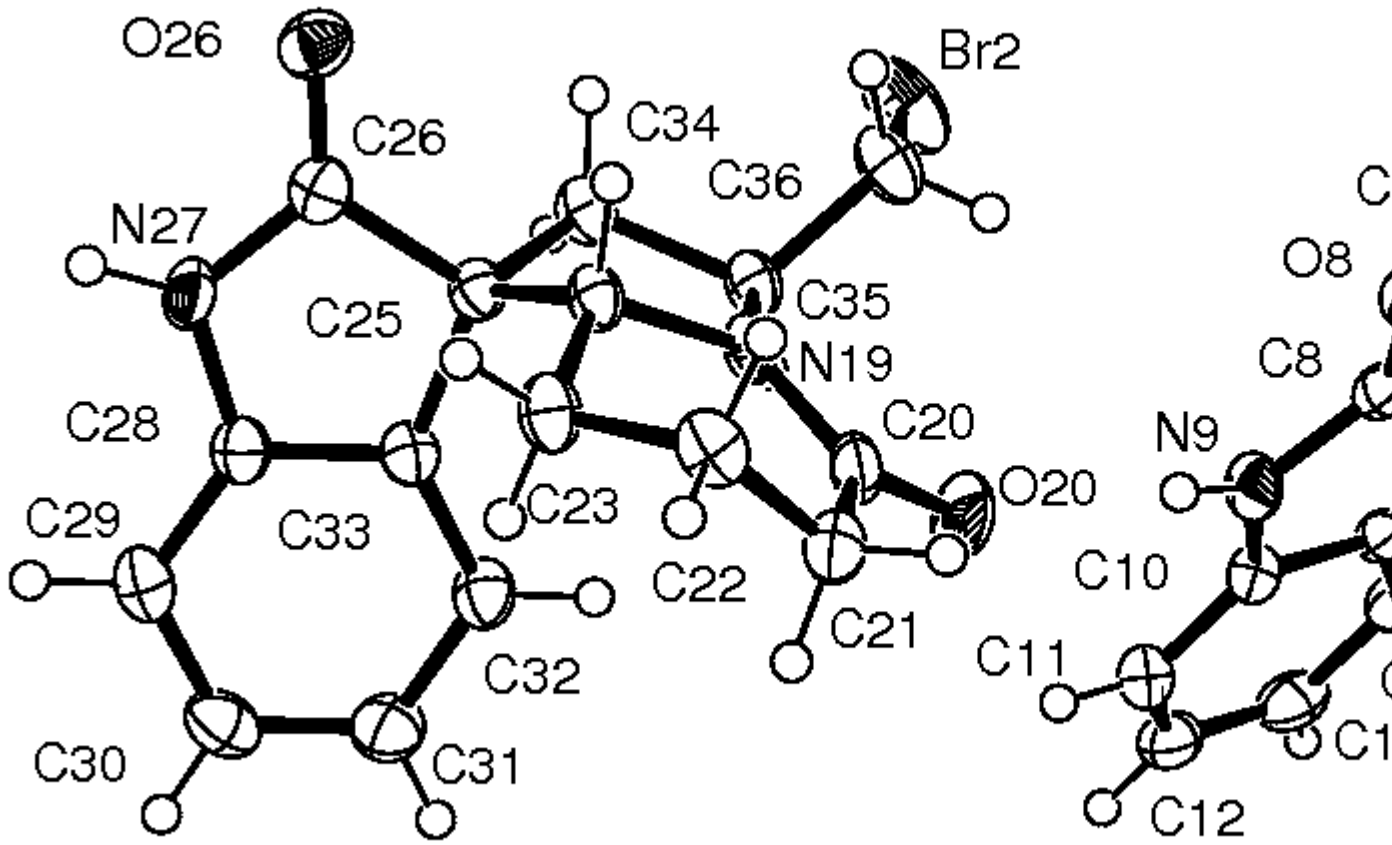
C(25)	22(1)	27(1)	23(1)	0(1)	2(1)	3(1)
C(26)	26(1)	24(1)	30(1)	0(1)	4(1)	4(1)
C(28)	29(1)	26(1)	25(1)	3(1)	4(1)	3(1)
C(29)	40(1)	33(1)	24(1)	2(1)	4(1)	5(1)
C(30)	44(2)	35(1)	29(1)	-1(1)	-8(1)	1(1)
C(31)	30(1)	42(2)	36(1)	3(1)	-4(1)	-1(1)
C(32)	24(1)	39(1)	29(1)	2(1)	3(1)	5(1)
C(33)	24(1)	27(1)	23(1)	2(1)	1(1)	4(1)
C(34)	29(1)	30(1)	28(1)	-3(1)	4(1)	6(1)
C(35)	27(1)	30(1)	22(1)	-2(1)	4(1)	6(1)
C(36)	41(2)	40(2)	26(1)	-7(1)	2(1)	13(1)

Table 5. Hydrogen bonds for compound 42a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9)-H(9)...O(20)	0.88	1.95	2.792(3)	161.0
N(27)-H(27)...O(2)#1	0.88	1.96	2.812(3)	163.7

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z+1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C26
C34
Br2
C36
N27
C25
C35
N19
C28
C20
C23
O20
C29
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C30
C31
O8
C8
N9
C10
C11
C12

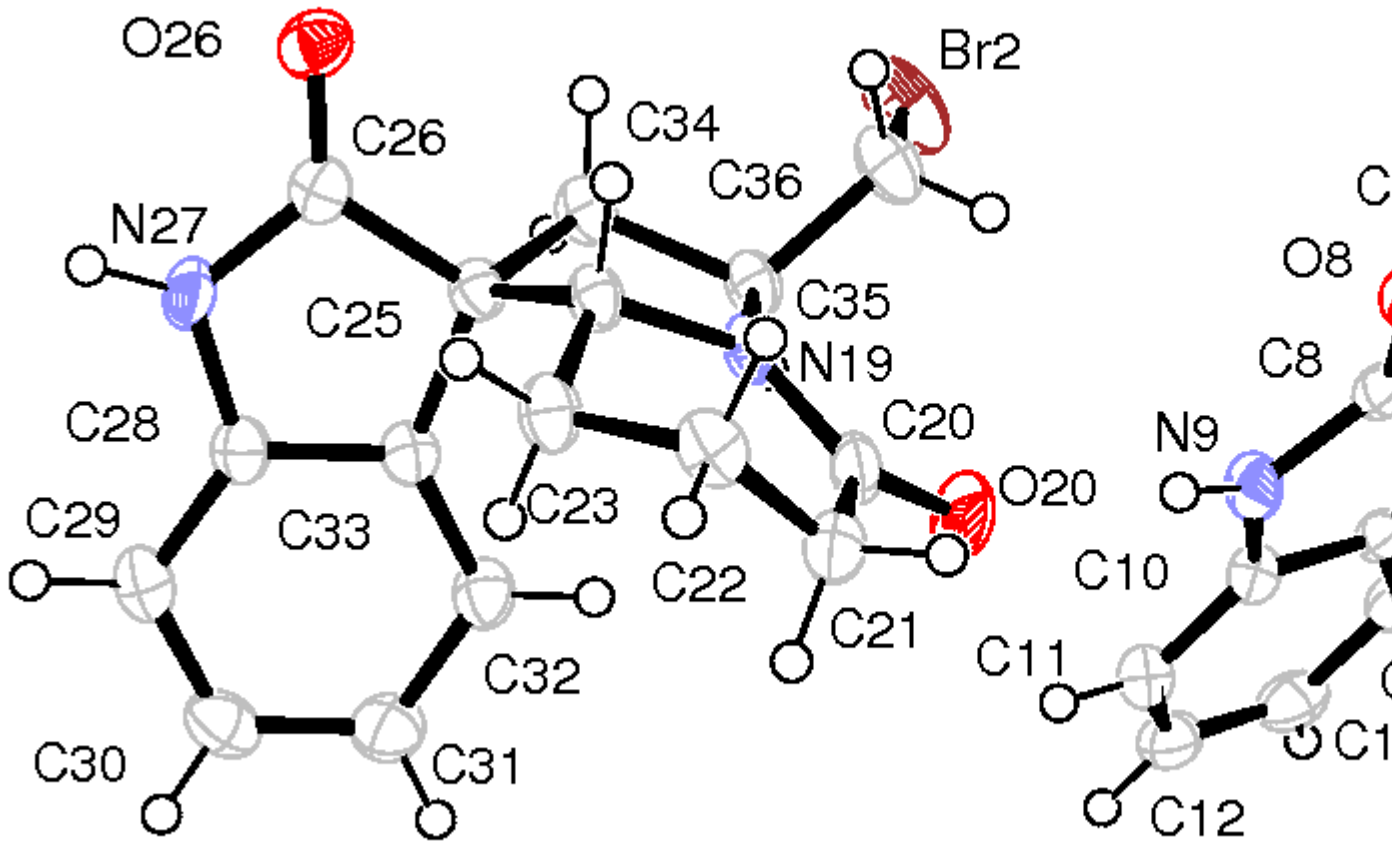

O26
C26
C34
Br2
C36
N27
C25
C35
N19
C28
C20
O20
C29
C33
C23
C22
C21
C32
C30
C31
O8
C8
N9
C10
C11
C12

Table 1. Crystal data and structure refinement for compound 53a.

Identification code	Jb114	
Empirical formula	C17 H20 N2 O3	
Formula weight	300.35	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.5333(13) Å	α= 90°.
	b = 13.2057(17) Å	β= 90°.
	c = 13.303(3) Å	γ = 90°.
Volume	1499.1(5) $Å^3$	
Z	4	
Density (calculated)	1.331 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	640	
Crystal size	0.45 x 0.21 x 0.18 mm^3	
Theta range for data collection	2.173 to 24.964°.	
Index ranges	0<=h<=10, -15<=k<=15, 0<=l<=15	
Reflections collected	3060	
Independent reflections	2637 [R(int) = 0.0421]	
Completeness to theta = 25.242°	97.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2637 / 0 / 201	
Goodness-of-fit on F^2	0.974	
Final R indices [I>2sigma(I)]	R1 = 0.0565, wR2 = 0.1294	
R indices (all data)	R1 = 0.0914, wR2 = 0.1417	
Largest diff. peak and hole	0.320 and -0.145 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For compound 53a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(8)	1462(4)	3211(3)	-702(3)	59(1)
O(14)	6145(4)	4130(3)	3025(2)	51(1)
O(19)	3895(5)	1677(3)	1966(3)	61(1)
N(7)	639(5)	4845(3)	-460(3)	48(1)
N(15)	4620(4)	3837(3)	1685(3)	36(1)
C(1)	1981(5)	5301(4)	950(3)	38(1)
C(2)	2427(7)	5950(4)	1714(4)	51(1)
C(3)	1786(7)	6920(4)	1742(4)	61(2)
C(4)	723(8)	7221(4)	1015(5)	70(2)
C(5)	255(7)	6572(4)	255(4)	59(2)
C(6)	911(6)	5631(4)	228(3)	42(1)
C(8)	1460(6)	4013(4)	-229(4)	42(1)
C(9)	2392(5)	4214(4)	730(3)	36(1)
C(10)	4158(5)	3980(4)	616(3)	38(1)
C(11)	5189(6)	4738(4)	76(3)	45(1)
C(12)	6870(6)	4500(5)	313(4)	56(1)
C(13)	7196(6)	4582(5)	1429(4)	56(1)
C(14)	5957(6)	4166(4)	2107(4)	41(1)
C(16)	3316(5)	3449(4)	2295(3)	40(1)
C(17)	1930(5)	3474(4)	1570(4)	44(1)
C(18)	4875(7)	4744(5)	-1055(4)	67(2)
C(19)	3639(7)	2405(4)	2718(4)	50(1)

Table 3. Bond lengths [Å] and angles [°] for compound 53a.

O(8)-C(8)	1.231(6)
O(14)-C(14)	1.232(5)
O(19)-C(19)	1.404(5)
N(7)-C(8)	1.340(6)
N(7)-C(6)	1.403(6)
N(15)-C(14)	1.344(6)
N(15)-C(16)	1.470(6)
N(15)-C(10)	1.488(5)
C(1)-C(2)	1.382(7)
C(1)-C(6)	1.395(6)
C(1)-C(9)	1.506(7)
C(2)-C(3)	1.393(8)
C(3)-C(4)	1.385(8)
C(4)-C(5)	1.384(8)
C(5)-C(6)	1.364(7)
C(8)-C(9)	1.527(6)
C(9)-C(17)	1.536(6)
C(9)-C(10)	1.545(7)
C(10)-C(11)	1.514(7)
C(11)-C(12)	1.502(7)
C(11)-C(18)	1.528(7)
C(12)-C(13)	1.515(7)
C(13)-C(14)	1.494(7)
C(16)-C(19)	1.514(7)
C(16)-C(17)	1.527(6)
C(8)-N(7)-C(6)	111.7(4)
C(14)-N(15)-C(16)	121.7(4)
C(14)-N(15)-C(10)	125.7(4)
C(16)-N(15)-C(10)	111.8(3)
C(2)-C(1)-C(6)	119.5(5)
C(2)-C(1)-C(9)	132.0(5)
C(6)-C(1)-C(9)	108.4(4)
C(1)-C(2)-C(3)	118.8(5)

C(4)-C(3)-C(2)	120.2(5)
C(5)-C(4)-C(3)	121.4(5)
C(6)-C(5)-C(4)	117.8(6)
C(5)-C(6)-C(1)	122.3(5)
C(5)-C(6)-N(7)	128.6(5)
C(1)-C(6)-N(7)	109.1(4)
O(8)-C(8)-N(7)	126.1(5)
O(8)-C(8)-C(9)	125.2(4)
N(7)-C(8)-C(9)	108.7(4)
C(1)-C(9)-C(8)	102.0(4)
C(1)-C(9)-C(17)	113.9(4)
C(8)-C(9)-C(17)	111.3(4)
C(1)-C(9)-C(10)	115.9(4)
C(8)-C(9)-C(10)	113.0(4)
C(17)-C(9)-C(10)	101.2(4)
N(15)-C(10)-C(11)	112.5(4)
N(15)-C(10)-C(9)	100.9(3)
C(11)-C(10)-C(9)	118.7(4)
C(12)-C(11)-C(10)	108.5(4)
C(12)-C(11)-C(18)	112.0(5)
C(10)-C(11)-C(18)	111.6(4)
C(11)-C(12)-C(13)	111.5(4)
C(14)-C(13)-C(12)	115.8(4)
O(14)-C(14)-N(15)	120.8(5)
O(14)-C(14)-C(13)	121.3(5)
N(15)-C(14)-C(13)	117.9(4)
N(15)-C(16)-C(19)	112.6(4)
N(15)-C(16)-C(17)	103.3(3)
C(19)-C(16)-C(17)	113.3(4)
C(16)-C(17)-C(9)	106.0(4)
O(19)-C(19)-C(16)	112.8(4)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 53a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

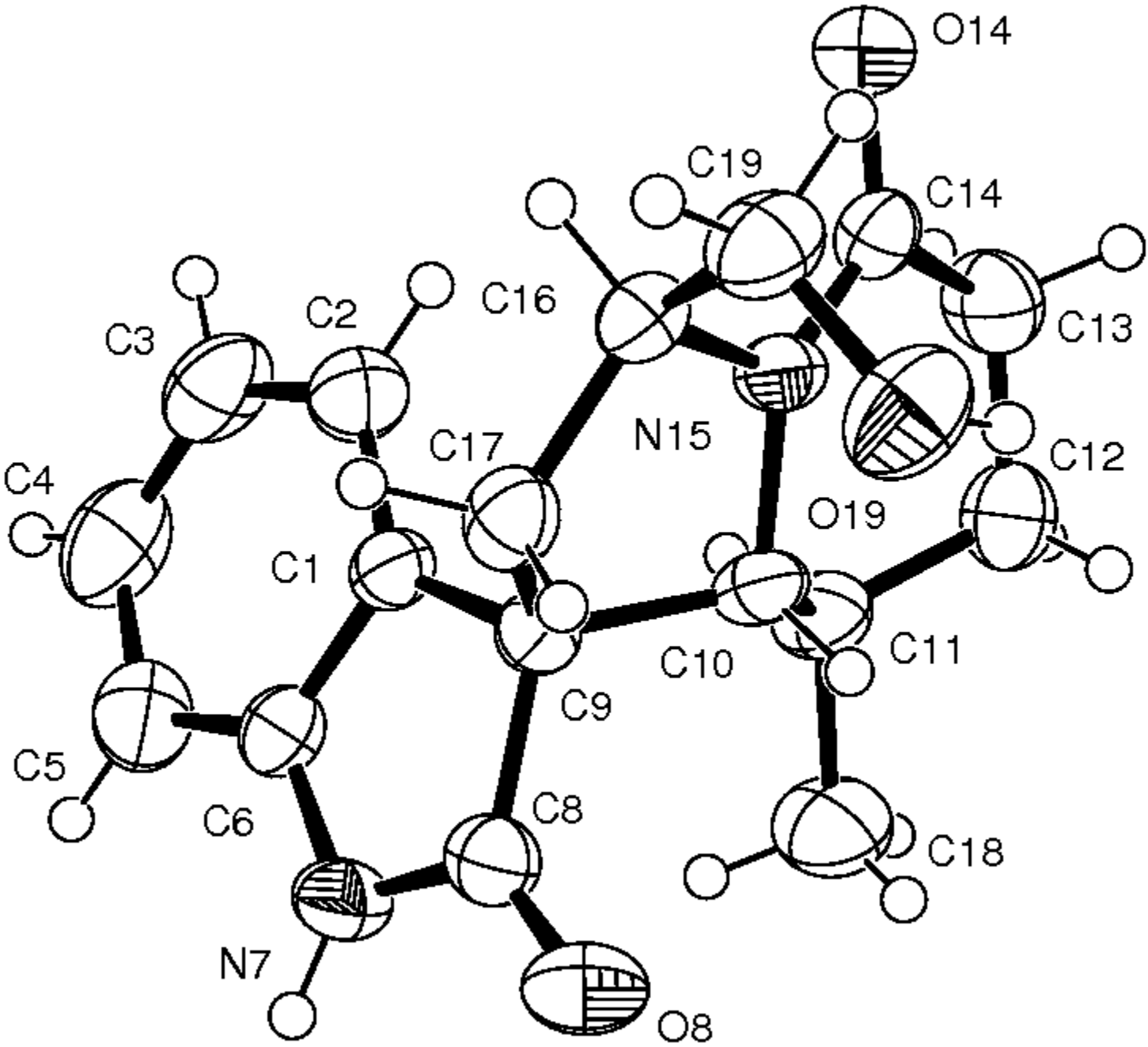
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(8)	59(2)	62(2)	56(2)	-17(2)	-10(2)	-6(2)
O(14)	51(2)	65(2)	37(2)	-6(2)	-8(2)	9(2)
O(19)	73(3)	48(2)	63(2)	-11(2)	12(2)	2(2)
N(7)	42(2)	67(3)	33(2)	-3(2)	-5(2)	1(2)
N(15)	33(2)	46(2)	29(2)	-3(2)	-1(2)	-2(2)
C(1)	35(3)	45(3)	35(2)	-2(2)	4(2)	-3(2)
C(2)	49(3)	54(3)	49(3)	-10(3)	-3(3)	-4(3)
C(3)	71(4)	49(4)	64(4)	-20(3)	11(4)	-6(3)
C(4)	87(5)	47(3)	78(4)	2(3)	18(4)	17(3)
C(5)	62(4)	61(4)	52(3)	13(3)	8(3)	12(3)
C(6)	39(3)	52(3)	36(3)	2(2)	9(2)	0(2)
C(8)	37(3)	47(3)	42(3)	-2(3)	0(2)	-2(3)
C(9)	29(3)	43(3)	36(3)	-5(2)	0(2)	-1(2)
C(10)	42(3)	42(3)	30(2)	-9(2)	-2(2)	-2(2)
C(11)	43(3)	57(3)	37(3)	2(3)	7(2)	-5(3)
C(12)	41(3)	72(4)	54(3)	-2(3)	10(3)	-5(3)
C(13)	35(3)	71(4)	61(3)	-1(3)	-2(3)	-6(3)
C(14)	41(3)	38(3)	42(3)	-9(2)	-2(2)	6(2)
C(16)	39(3)	49(3)	31(2)	-4(2)	2(2)	3(2)
C(17)	36(3)	48(3)	47(3)	-1(3)	3(2)	-4(2)
C(18)	63(4)	95(5)	44(3)	9(3)	5(3)	-7(3)
C(19)	60(4)	48(3)	42(3)	6(3)	9(3)	3(3)

Table 5. Hydrogen bonds for compound 53a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(19)-H(19)...O(8)#1	0.82	1.98	2.766(5)	161.4
N(7)-H(7)...O(14)#2	0.86	2.11	2.865(5)	146.4
N(7)-H(7)...O(19)#3	0.86	2.64	3.205(5)	124.1
C(19)-H(19A)...O(14)	0.97	2.62	3.151(6)	114.7

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,-z #2 -x+1/2,-y+1,z-1/2 #3 x-1/2,-y+1/2,-z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C16
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C3
C13
C17
N15
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C10
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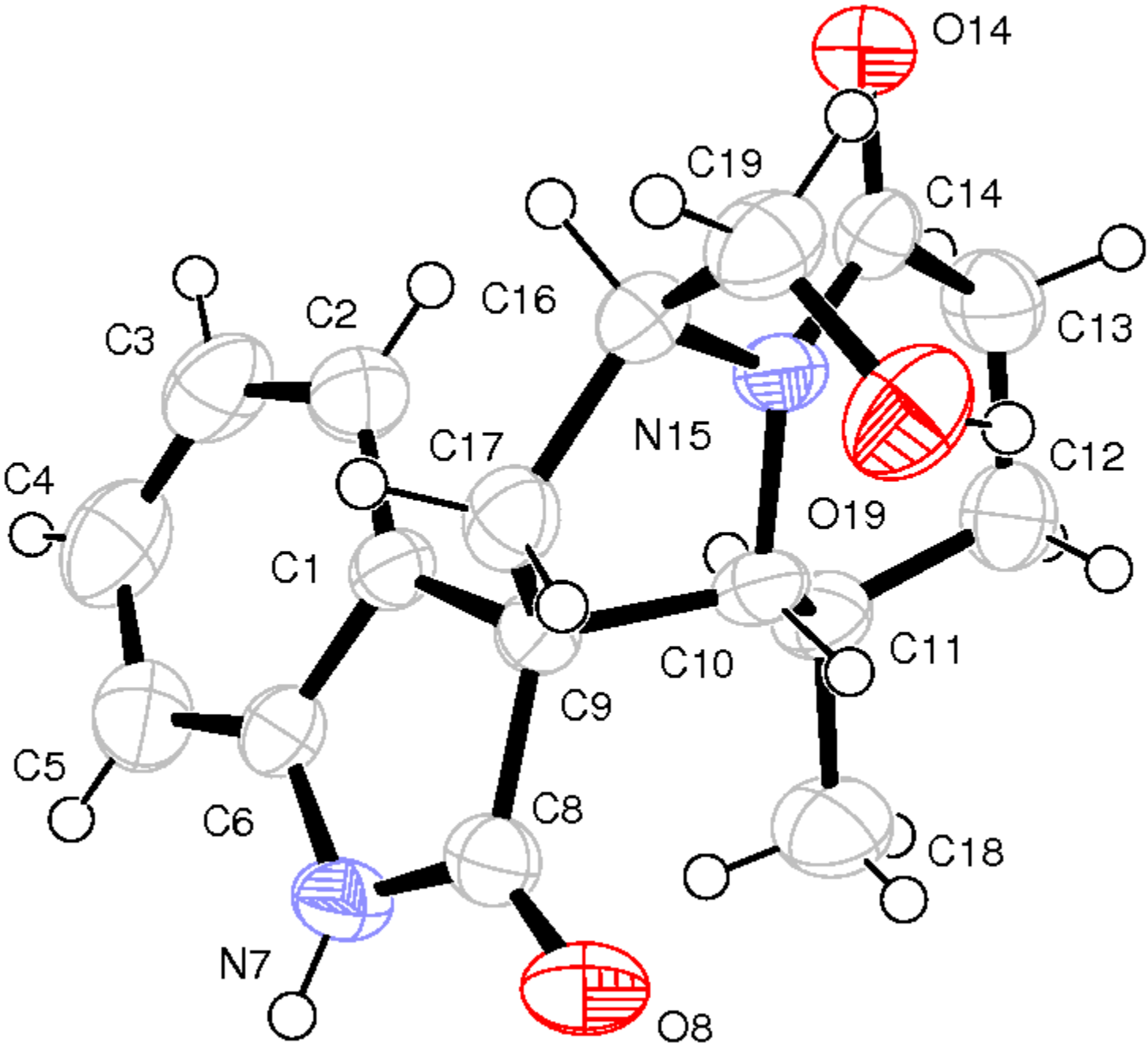
C5
C6
C8
C18
N7
O8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C10
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C9
C5
C6
C8
C18
N7
O8

Table 1. Crystal data and structure refinement for compound 60.

Identification code	Jb100	
Empirical formula	C17 H20 N2 O3	
Formula weight	300.35	
Temperature	200(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.06750(10) Å	α= 90°.
	b = 10.0328(2) Å	β= 90°.
	c = 18.4788(2) Å	γ = 90°.
Volume	1495.67(4) $Å^3$	
Z	4	
Density (calculated)	1.334 Mg/m^3	
Absorption coefficient	0.749 mm^{-1}	
F(000)	640	
Crystal size	0.35 x 0.22 x 0.16 mm^3	
Theta range for data collection	4.786 to 64.931°.	
Index ranges	-8<=h<=9, -11<=k<=11, -20<=l<=21	
Reflections collected	12166	
Independent reflections	2521 [R(int) = 0.0232]	
Completeness to theta = 67.684°	93.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2521 / 2 / 212	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.1025	
R indices (all data)	R1 = 0.0386, wR2 = 0.1047	
Absolute structure parameter	0.00(8)	
Extinction coefficient	0.0059(10)	
Largest diff. peak and hole	0.349 and -0.276 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 60. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-2610(3)	-11027(2)	-3107(1)	29(1)
N(9)	-2133(3)	-9447(2)	-5453(1)	36(1)
O(2)	-3192(3)	-10969(2)	-1924(1)	57(1)
O(8)	-2216(3)	-11724(2)	-5400(1)	44(1)
O(18)	-6726(3)	-12700(3)	-3149(1)	55(1)
C(2)	-2161(4)	-10844(3)	-2420(1)	40(1)
C(3)	-427(5)	-10434(4)	-2278(2)	61(1)
C(4)*	234(7)	-9539(7)	-2899(3)	44(2)
C(4A)*	767(8)	-10414(11)	-2849(3)	44(3)
C(5)	54(4)	-10139(3)	-3604(2)	45(1)
C(6)	-1506(3)	-10978(3)	-3751(1)	31(1)
C(7)	-2741(3)	-10351(2)	-4316(1)	29(1)
C(8)	-2307(3)	-10618(3)	-5116(1)	31(1)
C(10)	-2426(3)	-8367(3)	-4985(1)	33(1)
C(11)	-2378(4)	-7030(3)	-5147(2)	46(1)
C(12)	-2732(4)	-6142(3)	-4594(2)	49(1)
C(13)	-3137(4)	-6591(3)	-3909(2)	47(1)
C(14)	-3163(4)	-7952(3)	-3754(1)	38(1)
C(15)	-2805(3)	-8847(3)	-4299(1)	30(1)
C(16)	-4398(3)	-11029(3)	-4121(1)	33(1)
C(17)	-4356(3)	-11247(3)	-3300(1)	32(1)
C(18)	-4980(4)	-12613(3)	-3072(1)	44(1)
C(61)	-1003(4)	-12403(3)	-3944(2)	46(1)

* disordered position: partial occupation factor for C(4) is 0.69(1), and for C(4A) is 0.39(1).

Table 3. Bond lengths [Å] and angles [°] for compound 60.

N(1)-C(2)	1.332(3)
N(1)-C(17)	1.470(3)
N(1)-C(6)	1.488(3)
N(9)-C(8)	1.338(3)
N(9)-C(10)	1.407(3)
O(2)-C(2)	1.244(4)
O(8)-C(8)	1.229(3)
O(18)-C(18)	1.419(4)
C(2)-C(3)	1.481(4)
C(3)-C(4A)	1.429(5)
C(3)-C(4)	1.551(6)
C(4)-C(5)	1.442(6)
C(4A)-C(5)	1.533(5)
C(5)-C(6)	1.539(4)
C(6)-C(61)	1.528(4)
C(6)-C(7)	1.574(3)
C(7)-C(15)	1.511(4)
C(7)-C(8)	1.542(3)
C(7)-C(16)	1.543(4)
C(10)-C(11)	1.375(4)
C(10)-C(15)	1.389(3)
C(11)-C(12)	1.385(4)
C(12)-C(13)	1.384(4)
C(13)-C(14)	1.395(4)
C(14)-C(15)	1.379(4)
C(16)-C(17)	1.533(3)
C(17)-C(18)	1.519(4)
C(2)-N(1)-C(17)	120.8(2)
C(2)-N(1)-C(6)	126.5(2)
C(17)-N(1)-C(6)	112.60(19)
C(8)-N(9)-C(10)	111.85(19)
O(2)-C(2)-N(1)	120.4(3)
O(2)-C(2)-C(3)	121.9(2)

N(1)-C(2)-C(3)	117.6(3)
C(4A)-C(3)-C(2)	120.6(3)
C(2)-C(3)-C(4)	110.8(3)
C(5)-C(4)-C(3)	113.1(4)
C(3)-C(4A)-C(5)	114.9(4)
C(4)-C(5)-C(6)	118.1(3)
C(4A)-C(5)-C(6)	111.7(4)
N(1)-C(6)-C(61)	108.3(2)
N(1)-C(6)-C(5)	111.4(2)
C(61)-C(6)-C(5)	109.6(2)
N(1)-C(6)-C(7)	99.51(19)
C(61)-C(6)-C(7)	112.8(2)
C(5)-C(6)-C(7)	114.6(2)
C(15)-C(7)-C(8)	101.59(18)
C(15)-C(7)-C(16)	113.9(2)
C(8)-C(7)-C(16)	110.13(19)
C(15)-C(7)-C(6)	114.1(2)
C(8)-C(7)-C(6)	115.0(2)
C(16)-C(7)-C(6)	102.56(19)
O(8)-C(8)-N(9)	126.0(2)
O(8)-C(8)-C(7)	125.4(2)
N(9)-C(8)-C(7)	108.5(2)
C(11)-C(10)-C(15)	122.9(2)
C(11)-C(10)-N(9)	127.8(2)
C(15)-C(10)-N(9)	109.3(2)
C(10)-C(11)-C(12)	117.4(3)
C(13)-C(12)-C(11)	121.0(3)
C(12)-C(13)-C(14)	120.6(3)
C(15)-C(14)-C(13)	119.0(3)
C(14)-C(15)-C(10)	119.1(2)
C(14)-C(15)-C(7)	132.2(2)
C(10)-C(15)-C(7)	108.7(2)
C(17)-C(16)-C(7)	106.0(2)
N(1)-C(17)-C(18)	112.7(2)
N(1)-C(17)-C(16)	103.9(2)
C(18)-C(17)-C(16)	113.3(2)

O(18)-C(18)-C(17)	110.9(3)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 60. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

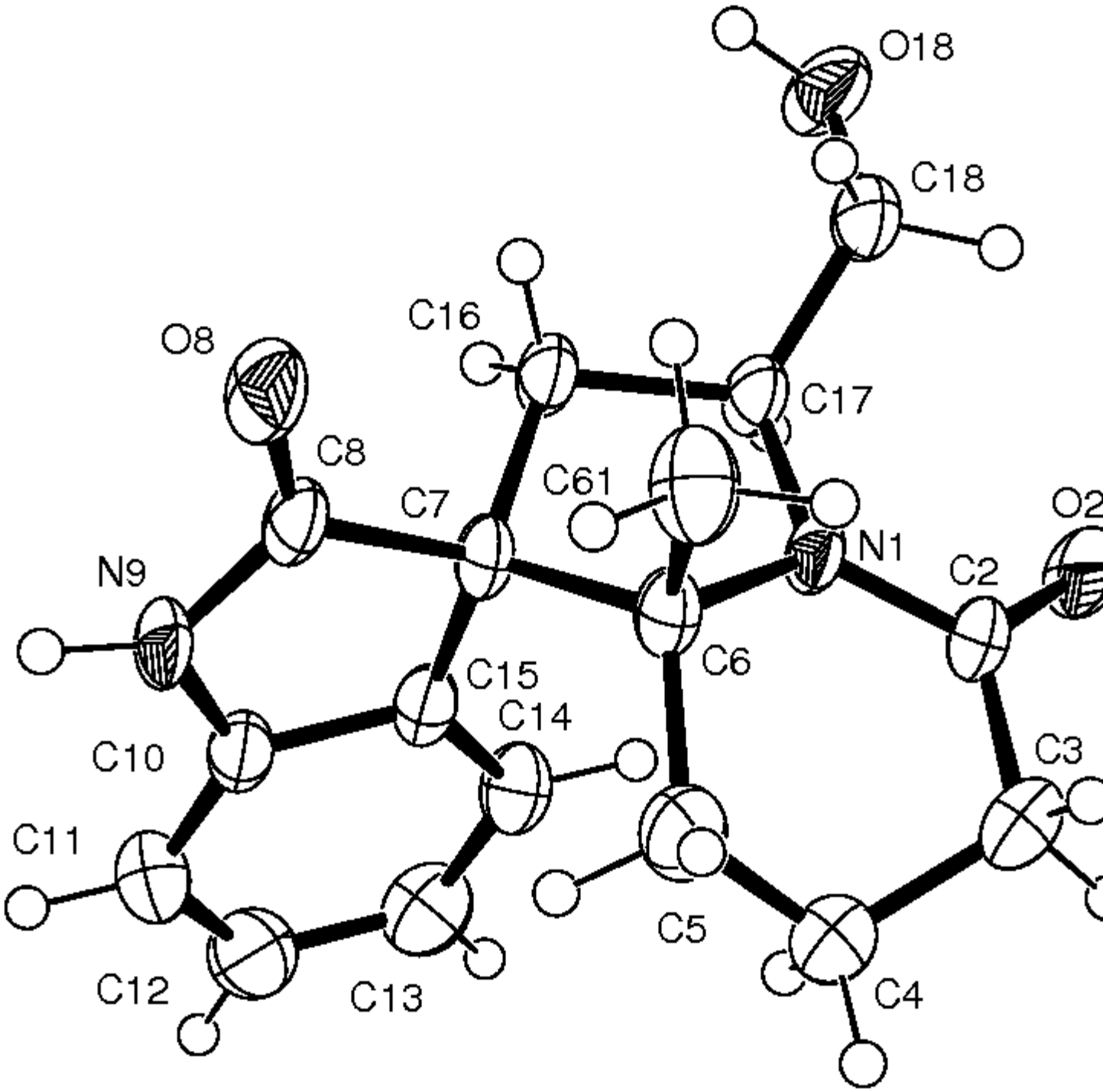
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	33(1)	39(1)	15(1)	-1(1)	-1(1)	-2(1)
N(9)	43(1)	51(1)	15(1)	2(1)	5(1)	-4(1)
O(2)	75(2)	81(2)	15(1)	-5(1)	2(1)	-30(1)
O(8)	60(1)	48(1)	24(1)	-8(1)	7(1)	2(1)
O(18)	49(1)	90(2)	26(1)	-8(1)	3(1)	-31(1)
C(2)	54(2)	46(2)	19(1)	2(1)	-7(1)	-10(1)
C(3)	62(2)	78(2)	43(2)	13(2)	-27(2)	-24(2)
C(4)	40(3)	49(4)	42(3)	1(2)	-7(2)	-4(3)
C(4A)	30(4)	61(6)	40(4)	-8(4)	-5(3)	-2(4)
C(5)	33(1)	56(2)	44(2)	11(1)	-6(1)	-1(1)
C(6)	32(1)	41(1)	21(1)	2(1)	3(1)	3(1)
C(7)	34(1)	38(1)	16(1)	0(1)	2(1)	2(1)
C(8)	33(1)	45(1)	16(1)	-3(1)	2(1)	-1(1)
C(10)	32(1)	44(1)	23(1)	3(1)	-1(1)	-2(1)
C(11)	52(2)	49(2)	36(2)	12(1)	-2(1)	-4(1)
C(12)	56(2)	39(1)	52(2)	5(1)	-5(2)	2(1)
C(13)	49(2)	45(2)	46(2)	-10(1)	-1(1)	7(1)
C(14)	41(2)	45(2)	28(1)	-2(1)	2(1)	7(1)
C(15)	27(1)	41(1)	22(1)	2(1)	-1(1)	2(1)
C(16)	33(1)	48(1)	17(1)	2(1)	-1(1)	-5(1)
C(17)	31(1)	46(1)	19(1)	-2(1)	2(1)	-3(1)
C(18)	49(2)	60(2)	22(1)	5(1)	-1(1)	-19(2)
C(61)	54(2)	48(2)	35(2)	0(1)	6(1)	14(1)

Table 5. Hydrogen bonds for compound 60 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9)-H(9)...O(2)#1	0.88	1.90	2.762(3)	166.6
O(18)-H(18)...O(8)#2	0.84	1.94	2.771(3)	168.1
C(16)-H(16B)...O(8)#2	0.99	2.62	3.322(3)	127.8
C(18)-H(18B)...O(2)	0.99	2.47	3.050(3)	116.8
C(61)-H(61B)...O(8)#3	0.98	2.63	3.402(4)	135.9

Symmetry transformations used to generate equivalent atoms:

#1 -x-1/2,-y-2,z-1/2 #2 x-1/2,-y-5/2,-z-1 #3 x+1/2,-y-5/2,-z-1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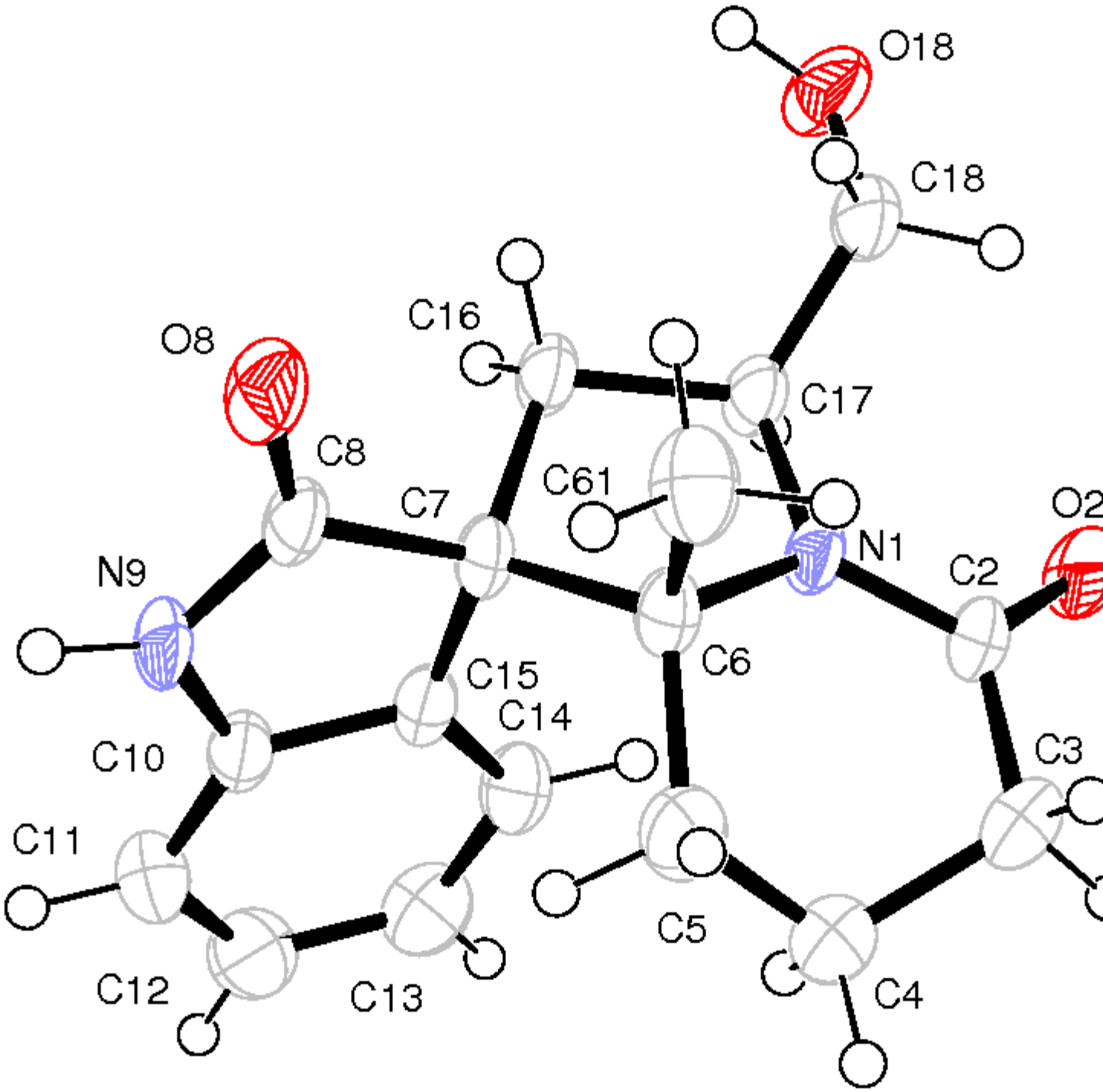
C16
O8
C17
C8
C61
C7
O2
N1
N9
C2
C6
C15
C14
C10
C3
C11
C5
C12
C13
C4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C18
C16
O8
C17
C8
C61
C7
O2
N1
N9
C2
C6
C15
C14
C10
C3
C11
C5
C12
C13
C4