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Crystal Engineering Studies on Ionic Crystals of Pyridine and Carboxylic Acid Derivatives Containing Amide Functional Groups.

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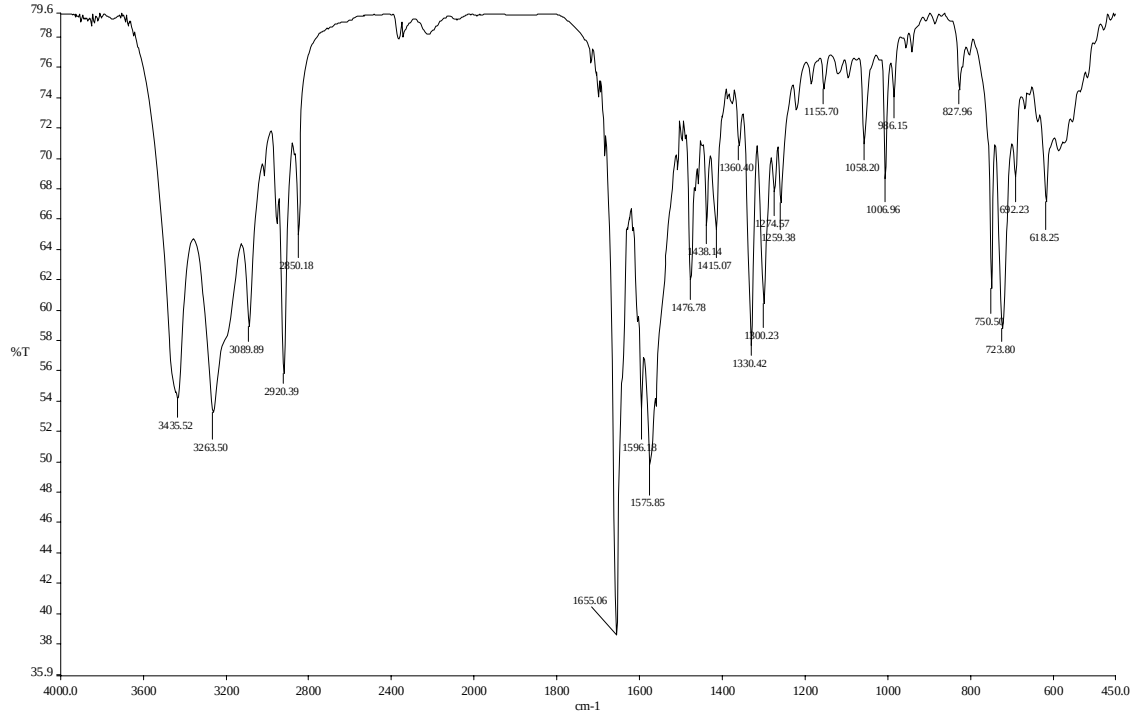
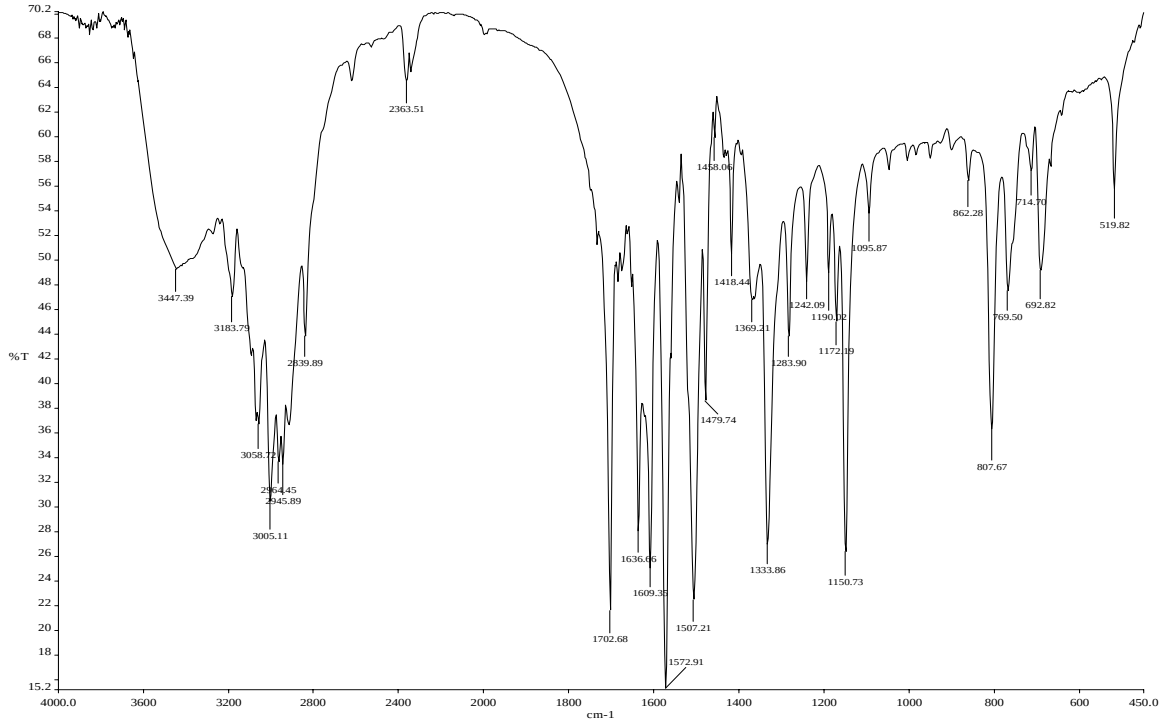
Supporting Information (29 pages)
IR and ^{1}HNMR spectra
Crystallographic information

IR:

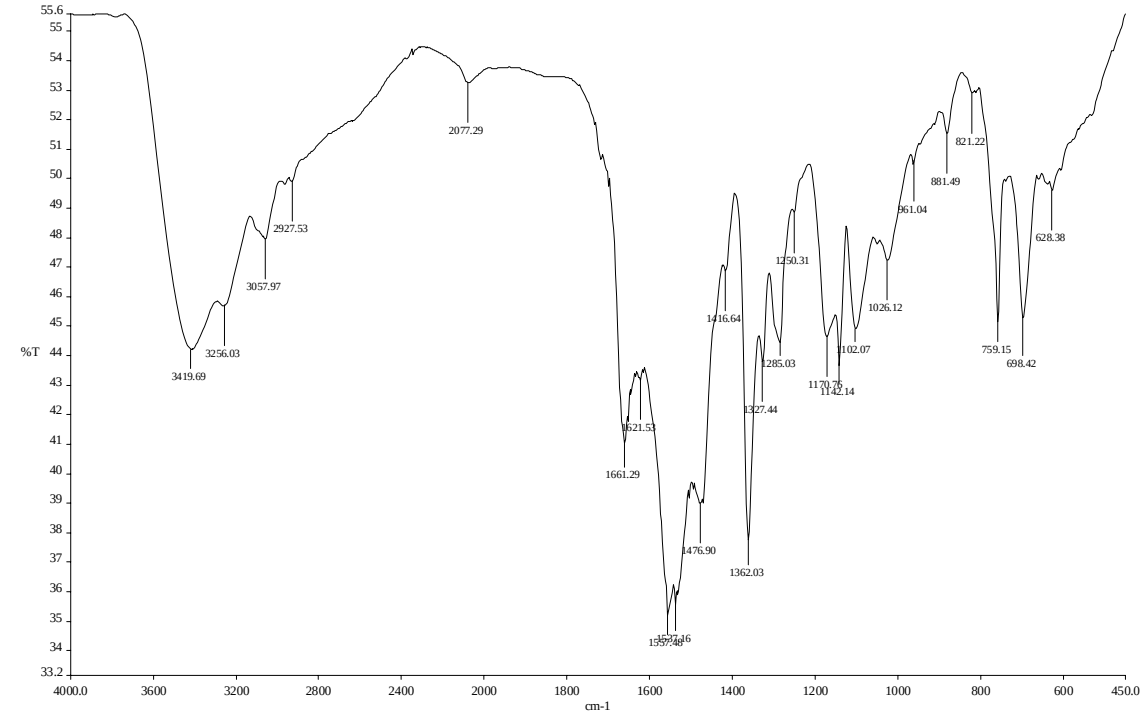
Compound (4):



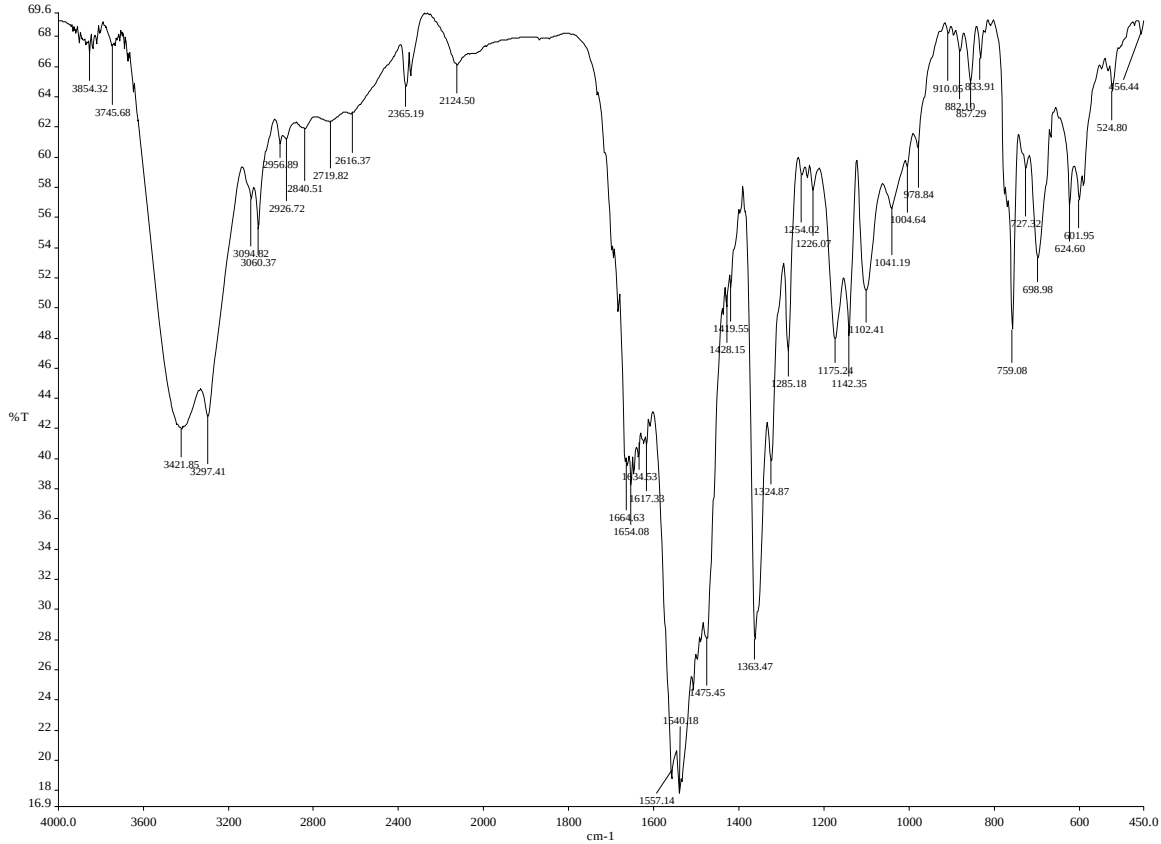
Compound (6):



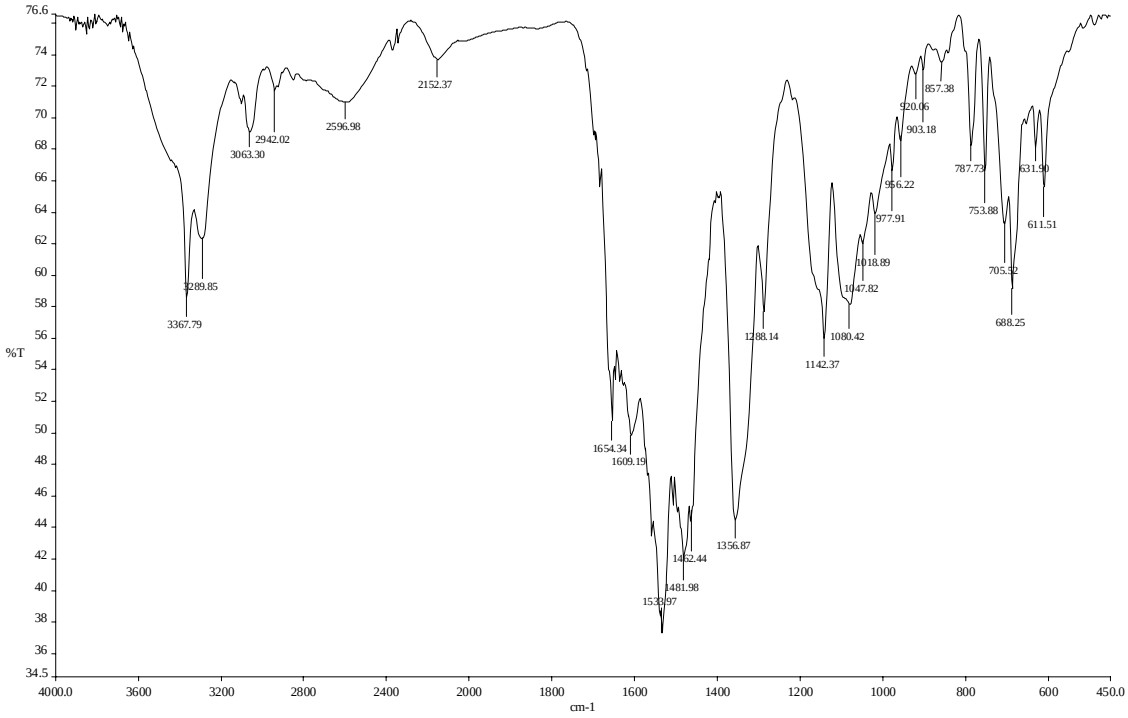
Compound (9):



Compound (10):



Compound (11):


%T
cm-1
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2942.02
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1654.34
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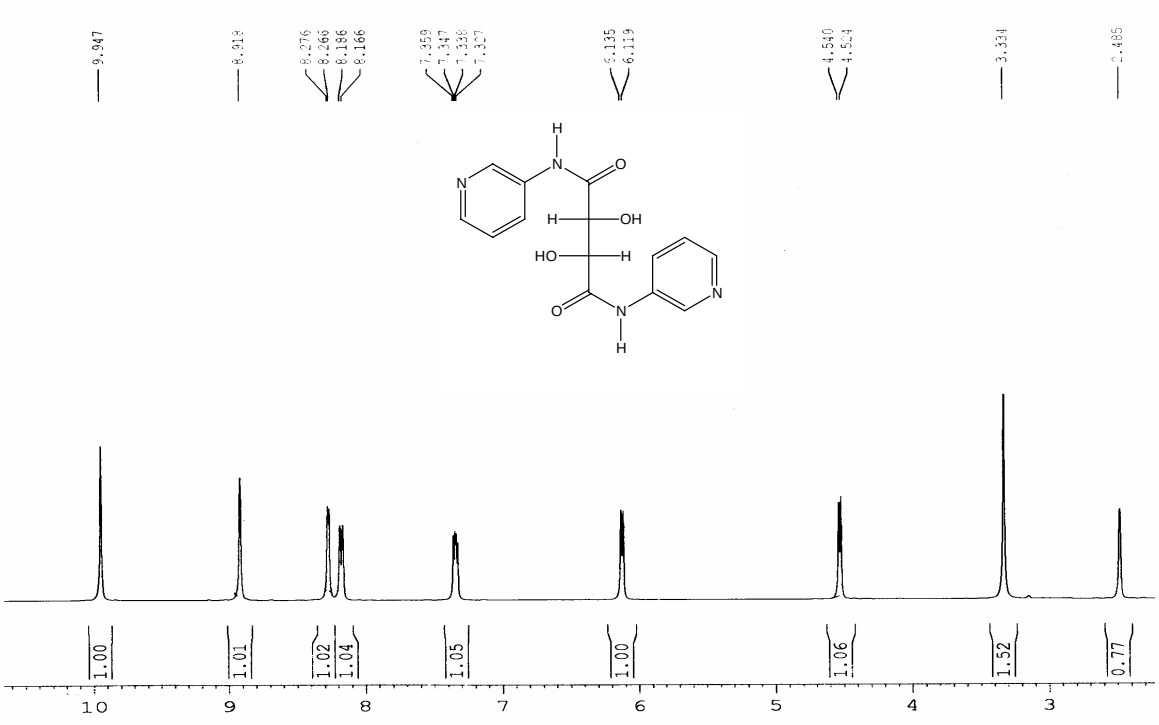
1481.98
1462.44
1356.87
1288.14
1142.37
1080.42
1047.82
1018.89
977.91
956.22
920.06
903.18
857.38
787.73
753.88
705.52
688.25
631.90
611.51

^{1}H NMR:

N,N'-bis(3-pyridyl)tartaramide, [(R,R)-2]:



N,N'-bis[(2-pyridyl) methyl]isophthalamide (4):

Table 1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C20 H22 N4 O4	
Formula weight	382.42	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.0386(11) Å	α= 82.513(5)°.
	b = 11.2021(18) Å	β= 75.156(4)°.
	c = 13.298(2) Å	γ = 72.127(4)°.
Volume	963.1(3) $Å^3$	
Z	2	
Density (calculated)	1.319 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	404	
Crystal size	0.23 x 0.18 x 0.12 mm^3	
Theta range for data collection	1.59 to 26.00°.	
Index ranges	-8<=h<=8, -13<=k<=13, -16<=l<=16	
Reflections collected	12267	
Independent reflections	3740 [R(int) = 0.0339]	
Completeness to theta = 26.00°	98.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.989 and 0.980	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3740 / 0 / 265	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0544, wR2 = 0.1531	
R indices (all data)	R1 = 0.0751, wR2 = 0.1630	
Largest diff. peak and hole	0.195 and -0.215 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(11)	6563(3)	1618(2)	9693(1)	56(1)
O(12)	8874(3)	1344(2)	5885(1)	59(1)
N(11)	3284(3)	1765(2)	10512(1)	47(1)
N(12)	6509(3)	1574(2)	4950(1)	45(1)
C(11)	4412(3)	1332(2)	8682(2)	37(1)
C(12)	5874(3)	1375(2)	7766(2)	37(1)
C(13)	5566(3)	1196(2)	6811(2)	38(1)
C(14)	3769(4)	927(2)	6793(2)	43(1)
C(15)	2319(4)	858(2)	7702(2)	46(1)
C(16)	2623(4)	1069(2)	8642(2)	44(1)
C(17)	4837(3)	1578(2)	9677(2)	41(1)
C(18)	7134(4)	1366(2)	5841(2)	41(1)
N(21)	2790(3)	3531(2)	12748(2)	49(1)
C(21)	3075(3)	3332(2)	11745(2)	41(1)
C(22)	2456(5)	4695(3)	13000(2)	68(1)
C(23)	2374(5)	5703(3)	12299(3)	82(1)
C(24)	2672(5)	5497(3)	11275(3)	81(1)
C(25)	3027(4)	4291(3)	10989(2)	62(1)
C(26)	3478(4)	1980(2)	11529(2)	44(1)
N(31)	7881(3)	3369(2)	2564(1)	49(1)
C(31)	7676(3)	3099(2)	3588(2)	40(1)

C(32)	7791(4)	4557(3)	2214(2)	61(1)
C(33)	7497(4)	5504(3)	2833(2)	67(1)
C(34)	7286(4)	5228(3)	3881(2)	66(1)
C(35)	7372(4)	4016(2)	4264(2)	53(1)
C(36)	7827(4)	1751(2)	3937(2)	47(1)
O(1W)	9125(3)	1832(3)	874(2)	94(1)
O(2W)	2490(4)	1983(3)	4615(2)	102(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

O(11)-C(17)	1.235(3)	O(1W)-H(1W2)	0.86(4)
O(12)-C(18)	1.233(3)	O(1W)-H(2W2)	0.85(5)
N(11)-C(17)	1.331(3)	O(2W)-H(1W1)	0.82(4)
N(11)-C(26)	1.450(3)	O(2W)-H(2W1)	0.83(4)
N(11)-H(11)	0.8600		
N(12)-C(18)	1.336(3)	C(17)-N(11)-C(26)	123.4(2)
N(12)-C(36)	1.455(3)	C(17)-N(11)-H(11)	118.3
N(12)-H(12)	0.8600	C(26)-N(11)-H(11)	118.3
C(11)-C(12)	1.385(3)	C(18)-N(12)-C(36)	123.5(2)
C(11)-C(16)	1.394(3)	C(18)-N(12)-H(12)	118.2
C(11)-C(17)	1.504(3)	C(36)-N(12)-H(12)	118.2
C(12)-C(13)	1.391(3)	C(12)-C(11)-C(16)	118.82(19)
C(12)-H(12A)	0.9300	C(12)-C(11)-C(17)	118.03(19)
C(13)-C(14)	1.393(3)	C(16)-C(11)-C(17)	123.15(19)
C(13)-C(18)	1.501(3)	C(11)-C(12)-C(13)	121.4(2)
C(14)-C(15)	1.378(3)	C(11)-C(12)-H(12A)	119.3
C(14)-H(14)	0.9300	C(13)-C(12)-H(12A)	119.3
C(15)-C(16)	1.381(3)	C(14)-C(13)-C(12)	118.5(2)
C(15)-H(15)	0.9300	C(14)-C(13)-C(18)	122.99(19)
C(16)-H(16)	0.9300	C(12)-C(13)-C(18)	118.4(2)
N(21)-C(22)	1.324(3)	C(15)-C(14)-C(13)	120.6(2)
N(21)-C(21)	1.335(3)	C(15)-C(14)-H(14)	119.7
C(21)-C(25)	1.371(3)	C(13)-C(14)-H(14)	119.7
C(21)-C(26)	1.505(3)	C(16)-C(15)-C(14)	120.2(2)
C(22)-C(23)	1.364(5)	C(16)-C(15)-H(15)	119.9
C(22)-H(22)	0.9300	C(14)-C(15)-H(15)	119.9
C(23)-C(24)	1.363(5)	C(15)-C(16)-C(11)	120.4(2)
C(23)-H(23)	0.9300	C(15)-C(16)-H(16)	119.8
C(24)-C(25)	1.383(4)	C(11)-C(16)-H(16)	119.8
C(24)-H(24)	0.9300	O(11)-C(17)-N(11)	122.6(2)
C(25)-H(25)	0.9300	O(11)-C(17)-C(11)	120.13(19)
C(26)-H(26A)	0.9700	N(11)-C(17)-C(11)	117.3(2)
C(26)-H(26B)	0.9700	O(12)-C(18)-N(12)	122.9(2)
N(31)-C(31)	1.337(3)	O(12)-C(18)-C(13)	121.0(2)
N(31)-C(32)	1.340(3)	N(12)-C(18)-C(13)	116.1(2)
C(31)-C(35)	1.384(3)	C(22)-N(21)-C(21)	118.0(2)
C(31)-C(36)	1.500(3)	N(21)-C(21)-C(25)	121.8(2)
C(32)-C(33)	1.361(4)	N(21)-C(21)-C(26)	114.29(19)
C(32)-H(32)	0.9300	C(25)-C(21)-C(26)	123.9(2)
C(33)-C(34)	1.367(4)	N(21)-C(22)-C(23)	124.0(3)
C(33)-H(33)	0.9300	N(21)-C(22)-H(22)	118.0
C(34)-C(35)	1.376(4)	C(23)-C(22)-H(22)	118.0
C(34)-H(34)	0.9300	C(24)-C(23)-C(22)	117.9(3)
C(35)-H(35)	0.9300	C(24)-C(23)-H(23)	121.0
C(36)-H(36A)	0.9700	C(22)-C(23)-H(23)	121.0
C(36)-H(36B)	0.9700	C(23)-C(24)-C(25)	119.3(3)

C(23)-C(24)-H(24)	120.4	C(32)-C(33)-C(34)	118.1(3)
C(25)-C(24)-H(24)	120.4	C(32)-C(33)-H(33)	120.9
C(21)-C(25)-C(24)	119.0(3)	C(34)-C(33)-H(33)	120.9
C(21)-C(25)-H(25)	120.5	C(33)-C(34)-C(35)	119.0(3)
C(24)-C(25)-H(25)	120.5	C(33)-C(34)-H(34)	120.5
N(11)-C(26)-C(21)	115.64(19)	C(35)-C(34)-H(34)	120.5
N(11)-C(26)-H(26A)	108.4	C(34)-C(35)-C(31)	119.8(2)
C(21)-C(26)-H(26A)	108.4	C(34)-C(35)-H(35)	120.1
N(11)-C(26)-H(26B)	108.4	C(31)-C(35)-H(35)	120.1
C(21)-C(26)-H(26B)	108.4	N(12)-C(36)-C(31)	114.29(19)
H(26A)-C(26)-H(26B)	107.4	N(12)-C(36)-H(36A)	108.7
C(31)-N(31)-C(32)	117.6(2)	C(31)-C(36)-H(36A)	108.7
N(31)-C(31)-C(35)	121.2(2)	N(12)-C(36)-H(36B)	108.7
N(31)-C(31)-C(36)	115.50(19)	C(31)-C(36)-H(36B)	108.7
C(35)-C(31)-C(36)	123.3(2)	H(36A)-C(36)-H(36B)	107.6
N(31)-C(32)-C(33)	124.2(3)	H(1W2)-O(1W)-H(2W2)	103(4)
N(31)-C(32)-H(32)	117.9	H(1W1)-O(2W)-H(2W1)	111(4)
C(33)-C(32)-H(32)	117.9		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. 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(11)	53(1)	85(1)	40(1)	-7(1)	-13(1)	-29(1)
O(12)	48(1)	90(1)	42(1)	5(1)	-10(1)	-28(1)
N(11)	48(1)	65(1)	32(1)	-7(1)	-10(1)	-19(1)
N(12)	51(1)	58(1)	29(1)	3(1)	-7(1)	-24(1)
C(11)	44(1)	38(1)	32(1)	-1(1)	-11(1)	-14(1)
C(12)	42(1)	38(1)	32(1)	1(1)	-10(1)	-15(1)
C(13)	47(1)	37(1)	33(1)	3(1)	-10(1)	-14(1)
C(14)	54(1)	51(1)	31(1)	1(1)	-14(1)	-22(1)
C(15)	47(1)	56(2)	41(1)	-1(1)	-12(1)	-24(1)
C(16)	48(1)	52(1)	34(1)	-1(1)	-6(1)	-19(1)
C(17)	48(1)	42(1)	34(1)	0(1)	-11(1)	-16(1)
C(18)	48(1)	43(1)	34(1)	-1(1)	-7(1)	-16(1)
N(21)	53(1)	58(1)	41(1)	-8(1)	-13(1)	-19(1)
C(21)	37(1)	55(1)	33(1)	1(1)	-5(1)	-18(1)
C(22)	72(2)	70(2)	72(2)	-23(2)	-18(2)	-27(2)
C(23)	76(2)	59(2)	116(3)	-20(2)	-7(2)	-33(2)
C(24)	77(2)	56(2)	98(3)	20(2)	-4(2)	-27(2)
C(25)	71(2)	61(2)	47(2)	10(1)	-1(1)	-23(1)
C(26)	55(1)	51(1)	27(1)	-1(1)	-8(1)	-16(1)
N(31)	49(1)	64(1)	32(1)	3(1)	-8(1)	-18(1)
C(31)	36(1)	50(1)	32(1)	-3(1)	-4(1)	-14(1)
C(32)	58(2)	72(2)	47(2)	20(1)	-13(1)	-19(1)
C(33)	59(2)	50(2)	81(2)	11(2)	-11(2)	-10(1)
C(34)	70(2)	48(2)	72(2)	-13(1)	-1(1)	-16(1)
C(35)	64(2)	54(2)	41(1)	-7(1)	-4(1)	-20(1)
C(36)	61(2)	52(1)	28(1)	-5(1)	-4(1)	-20(1)
O(1W)	56(1)	172(3)	67(1)	-57(2)	-1(1)	-43(1)
O(2W)	70(2)	173(3)	73(2)	59(2)	-38(1)	-56(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4.

	x	y	z	U(eq)
H(11)	2103	1759	10445	57
H(12)	5262	1605	4977	54
H(12A)	7088	1528	7790	44
H(14)	3545	793	6163	52
H(15)	1131	669	7683	55
H(16)	1629	1035	9251	53
H(22)	2266	4834	13698	81
H(23)	2123	6506	12513	98
H(24)	2636	6161	10774	97
H(25)	3231	4132	10294	75
H(26A)	4855	1525	11601	53
H(26B)	2534	1626	12056	53
H(32)	7940	4748	1501	74
H(33)	7441	6315	2552	80
H(34)	7088	5850	4328	79
H(35)	7227	3813	4975	64
H(36A)	7478	1367	3422	56
H(36B)	9237	1314	3962	56
H(1W1)	2440(60)	2420(40)	4070(30)	112
H(2W1)	1370(70)	1850(40)	4880(30)	112
H(1W2)	8440(70)	2260(40)	1410(30)	123
H(2W2)	8210(70)	1630(40)	690(30)	123

Table 1. Crystal data and structure refinement for **6**.

Identification code	**6**	
Empirical formula	C23 H24 N4 O10	
Formula weight	516.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.905(3) Å	α= 90.683(11)°.
	b = 11.360(4) Å	β= 109.965(9)°.
	c = 13.005(4) Å	γ = 110.006(10)°.
Volume	1149.6(6) $Å^3$	
Z	2	
Density (calculated)	1.492 Mg/m^3	
Absorption coefficient	0.119 mm^{-1}	
F(000)	540	
Crystal size	0.18 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.93 to 26.19°.	
Index ranges	-11<=h<=11, -13<=k<=14, -16<=l<=14	
Reflections collected	14716	
Independent reflections	4515 [R(int) = 0.0593]	
Completeness to theta = 26.19°	97.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.988 and 0.979	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4515 / 0 / 355	
Goodness-of-fit on F^2	1.013	

Final R indices [I>2sigma(I)]	R1 = 0.0720, wR2 = 0.2186
R indices (all data)	R1 = 0.1196, wR2 = 0.2357
Largest diff. peak and hole	0.311 and -0.309 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(11)	10583(4)	2838(3)	1352(3)	49(1)
O(12)	11545(4)	2371(4)	3048(3)	55(1)
O(13)	7976(4)	1718(3)	5306(3)	52(1)
O(14)	5340(4)	1736(4)	4604(3)	54(1)
O(15)	3501(4)	3206(3)	1013(3)	49(1)
O(16)	4869(4)	3281(3)	-127(2)	44(1)
C(11)	8781(5)	2530(4)	2381(3)	32(1)
C(12)	8536(5)	2271(4)	3363(3)	34(1)
C(13)	7034(5)	2215(4)	3498(3)	32(1)
C(14)	5801(5)	2468(4)	2644(3)	31(1)
C(15)	6030(5)	2743(4)	1655(3)	30(1)
C(16)	7510(5)	2742(4)	1518(3)	32(1)
C(17)	10438(5)	2567(4)	2316(4)	36(1)
C(18)	6770(6)	1867(4)	4555(3)	38(1)
C(19)	4700(5)	3089(4)	777(3)	34(1)
O(6A)	2705(4)	211(4)	9716(3)	54(1)
N(1A)	4258(5)	1306(4)	6244(3)	48(1)
N(2A)	1140(5)	620(4)	8059(3)	41(1)
C(1A)	2672(6)	1314(5)	5810(4)	50(1)
C(2A)	1638(6)	1102(5)	6415(4)	45(1)
C(3A)	2253(6)	856(4)	7495(4)	36(1)
C(4A)	3929(6)	863(4)	7945(4)	41(1)
C(5A)	4872(6)	1088(5)	7281(4)	47(1)
C(6A)	1412(6)	334(4)	9113(4)	38(1)
C(7A)	-107(6)	197(5)	9446(4)	43(1)
O(6B)	-2148(4)	4963(4)	-4883(3)	51(1)
N(1B)	2220(5)	3843(4)	-1597(4)	46(1)
N(2B)	-2285(4)	4360(4)	-3238(3)	41(1)
C(1B)	1923(6)	4117(4)	-2625(4)	44(1)
C(2B)	463(5)	4301(4)	-3221(4)	39(1)
C(3B)	-747(5)	4201(4)	-2737(3)	34(1)
C(4B)	-400(6)	3918(5)	-1661(4)	48(1)
C(5B)	1089(6)	3753(5)	-1114(4)	53(1)
C(6B)	-2906(6)	4718(5)	-4258(4)	40(1)
C(7B)	-4655(6)	4778(6)	-4480(4)	58(2)
O(1W)	7721(5)	313(4)	6861(3)	53(1)
O(2W)	5978(5)	4297(4)	-1746(3)	59(1)

Table 3. Bond lengths [Å] and angles [°] for **6**.

O(11)-C(17)	1.331(5)	C(11)-C(12)	1.386(6)
O(12)-C(17)	1.201(5)	C(11)-C(17)	1.493(5)
O(13)-C(18)	1.244(5)	C(12)-C(13)	1.387(5)
O(14)-C(18)	1.255(5)	C(13)-C(14)	1.383(6)
O(15)-C(19)	1.255(5)	C(13)-C(18)	1.507(5)
O(16)-C(19)	1.247(5)	C(14)-C(15)	1.392(5)
C(11)-C(16)	1.387(6)	C(15)-C(16)	1.389(5)

C(15)-C(19)	1.506(5)	O(12)-C(17)-O(11)	122.3(4)
O(6A)-C(6A)	1.207(5)	O(12)-C(17)-C(11)	124.3(4)
N(1A)-C(1A)	1.334(6)	O(11)-C(17)-C(11)	113.3(4)
N(1A)-C(5A)	1.332(6)	O(13)-C(18)-O(14)	125.0(4)
N(2A)-C(6A)	1.371(6)	O(13)-C(18)-C(13)	117.6(4)
N(2A)-C(3A)	1.383(5)	O(14)-C(18)-C(13)	117.3(4)
C(1A)-C(2A)	1.369(6)	O(16)-C(19)-O(15)	123.5(4)
C(2A)-C(3A)	1.392(6)	O(16)-C(19)-C(15)	119.0(3)
C(3A)-C(4A)	1.402(6)	O(15)-C(19)-C(15)	117.5(4)
C(4A)-C(5A)	1.367(6)	C(1A)-N(1A)-C(5A)	120.6(4)
C(6A)-C(7A)	1.516(6)	C(6A)-N(2A)-C(3A)	128.3(4)
C(7A)-C(7A)#1	1.483(9)	N(1A)-C(1A)-C(2A)	121.0(5)
O(6B)-C(6B)	1.202(5)	C(1A)-C(2A)-C(3A)	119.1(4)
N(1B)-C(1B)	1.334(6)	N(2A)-C(3A)-C(2A)	116.6(4)
N(1B)-C(5B)	1.335(6)	N(2A)-C(3A)-C(4A)	124.1(4)
N(2B)-C(3B)	1.377(5)	C(2A)-C(3A)-C(4A)	119.3(4)
N(2B)-C(6B)	1.378(5)	C(5A)-C(4A)-C(3A)	117.6(4)
C(1B)-C(2B)	1.355(6)	N(1A)-C(5A)-C(4A)	122.4(5)
C(2B)-C(3B)	1.397(6)	O(6A)-C(6A)-N(2A)	124.7(4)
C(3B)-C(4B)	1.393(6)	O(6A)-C(6A)-C(7A)	123.3(4)
C(4B)-C(5B)	1.352(6)	N(2A)-C(6A)-C(7A)	112.0(4)
C(6B)-C(7B)	1.510(6)	C(7A)#1-C(7A)-C(6A)	113.1(5)
C(7B)-C(7B)#2	1.457(9)	C(1B)-N(1B)-C(5B)	120.9(4)
		C(3B)-N(2B)-C(6B)	128.5(4)
C(16)-C(11)-C(12)	119.6(4)	N(1B)-C(1B)-C(2B)	121.5(4)
C(16)-C(11)-C(17)	123.3(4)	C(1B)-C(2B)-C(3B)	118.6(4)
C(12)-C(11)-C(17)	117.1(4)	N(2B)-C(3B)-C(4B)	116.1(4)
C(13)-C(12)-C(11)	121.1(4)	N(2B)-C(3B)-C(2B)	125.3(4)
C(12)-C(13)-C(14)	118.6(4)	C(4B)-C(3B)-C(2B)	118.6(4)
C(12)-C(13)-C(18)	119.8(4)	C(5B)-C(4B)-C(3B)	119.5(4)
C(14)-C(13)-C(18)	121.6(4)	N(1B)-C(5B)-C(4B)	120.9(4)
C(15)-C(14)-C(13)	121.1(3)	O(6B)-C(6B)-N(2B)	124.5(4)
C(14)-C(15)-C(16)	119.4(4)	O(6B)-C(6B)-C(7B)	124.6(4)
C(14)-C(15)-C(19)	119.1(3)	N(2B)-C(6B)-C(7B)	110.9(4)
C(16)-C(15)-C(19)	121.5(3)	C(7B)#2-C(7B)-C(6B)	113.8(5)
C(11)-C(16)-C(15)	120.0(4)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+2 #2 -x-1,-y+1,-z-1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. 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(11)	35(2)	86(3)	46(2)	22(2)	29(2)	33(2)
O(12)	38(2)	93(3)	54(2)	30(2)	23(2)	42(2)
O(13)	44(2)	83(3)	34(2)	29(2)	15(2)	28(2)
O(14)	41(2)	97(3)	37(2)	26(2)	25(2)	29(2)
O(15)	40(2)	86(2)	50(2)	34(2)	30(2)	43(2)
O(16)	38(2)	81(2)	32(2)	27(2)	19(1)	36(2)
C(11)	29(2)	37(2)	36(2)	10(2)	16(2)	16(2)
C(12)	27(2)	45(2)	32(2)	16(2)	12(2)	17(2)
C(13)	33(2)	40(2)	29(2)	13(2)	16(2)	15(2)
C(14)	24(2)	44(2)	31(2)	10(2)	15(2)	16(2)
C(15)	26(2)	38(2)	30(2)	10(2)	14(2)	14(2)
C(16)	33(2)	42(2)	31(2)	12(2)	19(2)	18(2)
C(17)	32(2)	43(2)	41(3)	12(2)	20(2)	18(2)

C(18)	40(3)	50(3)	28(2)	14(2)	17(2)	16(2)
C(19)	29(2)	47(3)	33(2)	17(2)	16(2)	19(2)
O(6A)	42(2)	92(3)	40(2)	24(2)	24(2)	31(2)
N(1A)	46(2)	68(3)	41(2)	10(2)	31(2)	18(2)
N(2A)	39(2)	65(3)	32(2)	17(2)	24(2)	23(2)
C(1A)	48(3)	76(4)	37(3)	17(2)	26(2)	25(3)
C(2A)	41(3)	63(3)	40(3)	15(2)	25(2)	22(2)
C(3A)	37(2)	46(3)	34(2)	9(2)	23(2)	17(2)
C(4A)	40(3)	57(3)	36(2)	10(2)	22(2)	21(2)
C(5A)	38(3)	60(3)	51(3)	8(2)	25(2)	17(2)
C(6A)	38(3)	47(3)	36(2)	9(2)	22(2)	14(2)
C(7A)	47(3)	61(3)	37(3)	18(2)	27(2)	27(2)
O(6B)	42(2)	91(3)	36(2)	28(2)	21(2)	37(2)
N(1B)	33(2)	60(3)	50(3)	16(2)	8(2)	29(2)
N(2B)	30(2)	73(3)	33(2)	23(2)	15(2)	31(2)
C(1B)	32(2)	49(3)	54(3)	7(2)	15(2)	19(2)
C(2B)	35(2)	52(3)	34(2)	10(2)	14(2)	20(2)
C(3B)	31(2)	44(2)	32(2)	11(2)	10(2)	19(2)
C(4B)	42(3)	79(4)	34(3)	23(2)	17(2)	30(3)
C(5B)	46(3)	77(4)	41(3)	27(3)	14(2)	31(3)
C(6B)	32(2)	62(3)	33(2)	20(2)	14(2)	26(2)
C(7B)	36(3)	110(4)	47(3)	42(3)	20(2)	45(3)
O(1W)	45(2)	84(3)	41(2)	28(2)	20(2)	31(2)
O(2W)	68(3)	75(3)	58(2)	25(2)	46(2)	33(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(11O)	11590(70)	2870(40)	1290(40)	50
H(12)	9392	2133	3941	40
H(14)	4802	2455	2732	37
H(16)	7648	2883	847	38
H(1AN)	4870(60)	1440(40)	5740(40)	50
H(2A)	150	657	7704	49
H(1A)	2263	1467	5084	60
H(2A1)	539	1121	6109	53
H(4A)	4383	720	8669	49
H(5A)	5983	1088	7563	57
H(7A1)	-266	1000	9444	52
H(7A2)	-1136	-423	8902	52
H(1BN)	3070(70)	3650(40)	-1190(40)	50
H(2B)	-2945	4217	-2864	49
H(1B)	2737	4184	-2940	53
H(2B1)	270	4489	-3938	46
H(4B)	-1186	3843	-1321	58
H(5B)	1328	3575	-393	63
H(7B1)	-5449	3941	-4485	69
H(7B2)	-4577	5339	-3879	69
H(1W1)	7640(60)	810(50)	6360(40)	50
H(2W1)	6880(70)	-490(50)	6550(40)	50
H(1W2)	5990(60)	3860(50)	-1210(40)	50
H(2W2)	6370(70)	5090(50)	-1460(40)	50

Table 1. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	C24 H20 N4 O12	
Formula weight	556.44	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21	
Unit cell dimensions	a = 5.4156(4) Å	α= 90°.
	b = 13.4490(11) Å	β= 97.840(2)°.
	c = 16.3970(13) Å	γ = 90°.
Volume	1183.10(16) $Å^3$	
Z	2	
Density (calculated)	1.562 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	576	
Crystal size	0.19 x 0.14 x 0.10 mm^3	
Theta range for data collection	1.25 to 26.50°.	
Index ranges	-6<=h<=6, -16<=k<=15, -20<=l<=19	
Reflections collected	15369	
Independent reflections	4375 [R(int) = 0.0208]	
Completeness to theta = 26.50°	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.987 and 0.979	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4375 / 1 / 379	
Goodness-of-fit on F^2	1.115	
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0982	
R indices (all data)	R1 = 0.0408, wR2 = 0.1175	
Absolute structure parameter	-0.8(8)	
Largest diff. peak and hole	0.285 and -0.407 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(21)	-17463(3)	8344(2)	5137(1)	37(1)
N(22)	-21969(3)	9337(1)	3466(1)	33(1)
N(31)	-31884(3)	12860(2)	-13(1)	39(1)
N(32)	-26797(3)	12305(1)	1615(1)	30(1)
O(12)	-25134(3)	6719(2)	1072(1)	58(1)
O(13)	-23925(3)	3863(1)	2467(1)	59(1)
O(14)	-20323(3)	3295(1)	3070(1)	48(1)
O(15)	-15126(4)	5417(2)	4273(2)	77(1)
O(16)	-16918(3)	3989(1)	3980(1)	47(1)
O(17)	-16072(4)	8224(2)	2826(1)	64(1)
O(18)	-19109(3)	8693(1)	1900(1)	48(1)
O(41)	-26988(3)	10765(1)	1046(1)	48(1)
O(42)	-25333(2)	11545(1)	3126(1)	30(1)
O(43)	-21232(3)	11476(1)	2178(1)	36(1)
O(44)	-19527(2)	10702(1)	3641(1)	35(1)
O(11)	-22844(3)	8059(1)	1152(1)	53(1)
C(10)	-21431(3)	6653(1)	2017(1)	29(1)
C(11)	-22098(3)	5683(2)	2188(1)	32(1)
C(12)	-20698(3)	5050(1)	2745(1)	29(1)
C(13)	-18493(3)	5435(2)	3186(1)	31(1)

C(14)	-17836(3)	6403(2)	3023(1)	33(1)
C(15)	-19190(3)	7025(1)	2449(1)	29(1)
C(16)	-23265(4)	7176(2)	1371(1)	37(1)
C(17)	-21762(4)	4009(2)	2765(1)	36(1)
C(18)	-16702(4)	4927(2)	3864(1)	40(1)
C(19)	-18037(4)	8050(2)	2389(1)	35(1)
C(21)	-20748(3)	8735(2)	4096(1)	29(1)
C(22)	-18550(4)	8999(2)	4583(1)	34(1)
C(23)	-18372(4)	7445(2)	5266(1)	41(1)
C(24)	-20568(5)	7158(2)	4803(2)	44(1)
C(25)	-21746(4)	7805(2)	4225(1)	38(1)
C(31)	-28436(3)	12818(2)	1033(1)	29(1)
C(32)	-30250(4)	12330(2)	499(1)	35(1)
C(33)	-31889(5)	13850(2)	-48(1)	46(1)
C(34)	-30126(5)	14364(2)	467(2)	50(1)
C(35)	-28392(4)	13852(2)	1007(1)	42(1)
C(41)	-26429(3)	11312(2)	1629(1)	29(1)
C(42)	-25245(3)	10877(1)	2458(1)	27(1)
C(43)	-22514(3)	10637(2)	2410(1)	29(1)
C(44)	-21199(3)	10237(1)	3237(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for **7**.

N(21)-C(23)	1.333(3)	C(24)-C(25)	1.377(3)
N(21)-C(22)	1.343(3)	C(31)-C(32)	1.388(2)
N(22)-C(44)	1.350(2)	C(31)-C(35)	1.392(3)
N(22)-C(21)	1.404(2)	C(33)-C(34)	1.372(3)
N(31)-C(33)	1.333(3)	C(34)-C(35)	1.383(3)
N(31)-C(32)	1.339(3)	C(41)-C(42)	1.538(2)
N(32)-C(41)	1.350(3)	C(42)-C(43)	1.526(3)
N(32)-C(31)	1.395(2)	C(43)-C(44)	1.540(2)
O(12)-C(16)	1.228(3)		
O(13)-C(17)	1.222(2)	C(23)-N(21)-C(22)	124.41(17)
O(14)-C(17)	1.293(3)	C(44)-N(22)-C(21)	126.12(14)
O(15)-C(18)	1.207(3)	C(33)-N(31)-C(32)	123.80(18)
O(16)-C(18)	1.284(3)	C(41)-N(32)-C(31)	125.42(15)
O(17)-C(19)	1.221(3)	C(11)-C(10)-C(15)	117.43(16)
O(18)-C(19)	1.266(3)	C(11)-C(10)-C(16)	114.21(16)
O(41)-C(41)	1.212(2)	C(15)-C(10)-C(16)	128.35(17)
O(42)-C(42)	1.423(2)	C(10)-C(11)-C(12)	124.76(16)
O(43)-C(43)	1.405(2)	C(11)-C(12)-C(13)	117.39(17)
O(44)-C(44)	1.219(2)	C(11)-C(12)-C(17)	113.79(15)
O(11)-C(16)	1.270(3)	C(13)-C(12)-C(17)	128.78(16)
C(10)-C(11)	1.392(3)	C(14)-C(13)-C(12)	117.92(17)
C(10)-C(15)	1.411(2)	C(14)-C(13)-C(18)	113.89(16)
C(10)-C(16)	1.522(2)	C(12)-C(13)-C(18)	128.16(18)
C(11)-C(12)	1.395(3)	C(13)-C(14)-C(15)	124.77(16)
C(12)-C(13)	1.407(2)	C(14)-C(15)-C(10)	117.67(17)
C(12)-C(17)	1.517(3)	C(14)-C(15)-C(19)	113.91(16)
C(13)-C(14)	1.385(3)	C(10)-C(15)-C(19)	128.40(17)
C(13)-C(18)	1.532(2)	O(12)-C(16)-O(11)	121.68(18)
C(14)-C(15)	1.391(3)	O(12)-C(16)-C(10)	118.08(19)
C(15)-C(19)	1.523(3)	O(11)-C(16)-C(10)	120.24(18)
C(21)-C(22)	1.387(2)	O(13)-C(17)-O(14)	122.0(2)
C(21)-C(25)	1.390(3)	O(13)-C(17)-C(12)	119.06(19)
C(23)-C(24)	1.376(3)	O(14)-C(17)-C(12)	118.90(16)

O(15)-C(18)-O(16)	121.73(19)	N(31)-C(32)-C(31)	119.61(19)
O(15)-C(18)-C(13)	119.3(2)	N(31)-C(33)-C(34)	118.63(19)
O(16)-C(18)-C(13)	118.96(18)	C(33)-C(34)-C(35)	119.9(2)
O(17)-C(19)-O(18)	121.9(2)	C(34)-C(35)-C(31)	120.3(2)
O(17)-C(19)-C(15)	117.87(19)	O(41)-C(41)-N(32)	124.58(16)
O(18)-C(19)-C(15)	120.19(17)	O(41)-C(41)-C(42)	119.73(18)
C(22)-C(21)-C(25)	117.67(17)	N(32)-C(41)-C(42)	115.69(16)
C(22)-C(21)-N(22)	123.82(18)	O(42)-C(42)-C(43)	107.94(14)
C(25)-C(21)-N(22)	118.48(16)	O(42)-C(42)-C(41)	112.79(15)
N(21)-C(22)-C(21)	118.97(19)	C(43)-C(42)-C(41)	108.96(15)
N(21)-C(23)-C(24)	118.48(19)	O(43)-C(43)-C(42)	111.23(15)
C(25)-C(24)-C(23)	119.1(2)	O(43)-C(43)-C(44)	109.47(15)
C(24)-C(25)-C(21)	121.32(17)	C(42)-C(43)-C(44)	111.30(15)
C(32)-C(31)-N(32)	121.84(17)	O(44)-C(44)-N(22)	122.92(16)
C(32)-C(31)-C(35)	117.82(17)	O(44)-C(44)-C(43)	121.26(17)
N(32)-C(31)-C(35)	120.22(16)	N(22)-C(44)-C(43)	115.79(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. 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(21)	37(1)	36(1)	34(1)	1(1)	-14(1)	-2(1)
N(22)	30(1)	29(1)	34(1)	6(1)	-13(1)	-8(1)
N(31)	39(1)	39(1)	33(1)	2(1)	-14(1)	0(1)
N(32)	30(1)	23(1)	31(1)	3(1)	-11(1)	-4(1)
O(12)	49(1)	49(1)	63(1)	14(1)	-33(1)	-8(1)
O(13)	49(1)	36(1)	82(1)	6(1)	-28(1)	-19(1)
O(14)	54(1)	23(1)	59(1)	6(1)	-18(1)	-8(1)
O(15)	78(1)	45(1)	88(1)	14(1)	-60(1)	-13(1)
O(16)	45(1)	34(1)	55(1)	13(1)	-20(1)	-2(1)
O(17)	63(1)	42(1)	74(1)	20(1)	-36(1)	-31(1)
O(18)	51(1)	28(1)	60(1)	13(1)	-11(1)	-6(1)
O(41)	70(1)	31(1)	36(1)	-7(1)	-18(1)	7(1)
O(42)	27(1)	33(1)	29(1)	-2(1)	-2(1)	-3(1)
O(43)	34(1)	32(1)	43(1)	10(1)	5(1)	-4(1)
O(44)	34(1)	28(1)	38(1)	1(1)	-6(1)	-8(1)
O(11)	48(1)	42(1)	62(1)	22(1)	-18(1)	-3(1)
C(10)	28(1)	27(1)	30(1)	2(1)	-5(1)	1(1)
C(11)	27(1)	29(1)	36(1)	-1(1)	-8(1)	-6(1)
C(12)	29(1)	26(1)	31(1)	2(1)	-6(1)	-4(1)
C(13)	28(1)	28(1)	33(1)	2(1)	-7(1)	-3(1)
C(14)	28(1)	30(1)	37(1)	3(1)	-13(1)	-6(1)
C(15)	31(1)	22(1)	31(1)	1(1)	-4(1)	-3(1)
C(16)	31(1)	38(1)	38(1)	7(1)	-8(1)	2(1)
C(17)	39(1)	29(1)	37(1)	1(1)	-9(1)	-8(1)
C(18)	36(1)	35(1)	43(1)	7(1)	-16(1)	-1(1)
C(19)	40(1)	27(1)	36(1)	2(1)	-3(1)	-8(1)
C(21)	31(1)	28(1)	25(1)	3(1)	-4(1)	-3(1)
C(22)	36(1)	29(1)	34(1)	2(1)	-11(1)	-4(1)
C(23)	50(1)	34(1)	36(1)	9(1)	-11(1)	4(1)
C(24)	55(1)	31(1)	41(1)	10(1)	-9(1)	-9(1)
C(25)	38(1)	34(1)	37(1)	6(1)	-11(1)	-7(1)
C(31)	28(1)	28(1)	27(1)	3(1)	-4(1)	-3(1)
C(32)	38(1)	29(1)	33(1)	3(1)	-11(1)	-1(1)

C(33)	53(1)	42(1)	39(1)	9(1)	-13(1)	10(1)
C(34)	69(2)	26(1)	50(1)	6(1)	-16(1)	1(1)
C(35)	50(1)	30(1)	41(1)	3(1)	-12(1)	-5(1)
C(41)	29(1)	27(1)	30(1)	2(1)	-5(1)	-2(1)
C(42)	28(1)	23(1)	28(1)	3(1)	-5(1)	-3(1)
C(43)	31(1)	24(1)	30(1)	4(1)	-1(1)	0(1)
C(44)	24(1)	25(1)	30(1)	2(1)	-1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(21N)	-15970(60)	8560(20)	5430(20)	58
H(22)	-23335	9111	3202	39
H(31N)	-33140(50)	12420(30)	-383(19)	50
H(32)	-25949	12650	1997	35
H(14O)	-18520(70)	3610(30)	3510(30)	84
H(42O)	-26730(60)	11480(20)	3314(18)	50
H(43O)	-21210(60)	11920(30)	2460(20)	55
H(11O)	-21190(60)	8390(30)	1530(20)	70
H(11)	-23586	5439	1909	38
H(14)	-16383	6655	3318	40
H(22A)	-17839	9621	4527	41
H(23)	-17541	7021	5660	49
H(24)	-21248	6535	4879	53
H(25)	-23238	7616	3914	46
H(32A)	-30330	11640	497	41
H(33)	-33063	14186	-414	56
H(34)	-30097	15055	453	60
H(35)	-27193	14200	1354	50
H(42)	-26119	10263	2566	33
H(43)	-22450	10121	1991	34

Table 1. Crystal data and structure refinement for **9**.

Identification code	**9**	
Empirical formula	C84 H86 N12 O40	
Formula weight	1903.65	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.0159(7) Å	α= 82.806(3)°.
	b = 12.6743(13) Å	β= 87.915(3)°.
	c = 25.156(3) Å	γ = 80.682(3)°.
Volume	2189.7(4) $Å^3$	
Z	1	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	994	
Crystal size	0.24 x 0.19 x 0.12 mm^3	
Theta range for data collection	0.82 to 26.57°.	
Index ranges	-7<=h<=8, -15<=k<=15, -31<=l<=31	
Reflections collected	28849	
Independent reflections	8917 [R(int) = 0.0690]	

Completeness to theta = 26.57°	97.5 %
Absorption correction	Empirical
Max. and min. transmission	0.986 and 0.974
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8917 / 0 / 658
Goodness-of-fit on F^2	0.987
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1453
R indices (all data)	R1 = 0.1271, wR2 = 0.1801
Largest diff. peak and hole	0.452 and -0.355 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(11A)	13213(5)	-1032(2)	-2054(1)	63(1)
O(12A)	12251(4)	-1188(2)	-1202(1)	47(1)
O(13A)	9998(3)	488(2)	-460(1)	45(1)
O(14A)	13202(3)	230(2)	-399(1)	46(1)
O(15A)	10409(4)	4364(2)	-1350(1)	63(1)
O(16A)	10611(4)	4652(2)	-2225(1)	64(1)
O(17A)	11647(4)	3720(2)	-2979(1)	62(1)
O(18A)	13306(4)	2156(2)	-3112(1)	57(1)
C(1A)	12233(4)	557(2)	-1667(1)	30(1)
C(2A)	11766(4)	1104(2)	-1217(1)	29(1)
C(3A)	11362(4)	2221(2)	-1293(1)	34(1)
C(4A)	11418(4)	2825(2)	-1792(1)	32(1)
C(5A)	11989(4)	2276(2)	-2240(1)	32(1)
C(6A)	12352(4)	1156(2)	-2162(1)	34(1)
C(7A)	12563(5)	-643(2)	-1611(1)	35(1)
C(8A)	11710(5)	543(2)	-651(1)	33(1)
C(9A)	10792(5)	4028(3)	-1784(2)	43(1)
C(10A)	12345(5)	2739(3)	-2816(1)	42(1)
O(1B)	13543(3)	-11192(2)	4037(1)	51(1)
O(2B)	15132(3)	-10522(2)	4616(1)	45(1)
O(3B)	12945(4)	-8456(2)	4051(1)	52(1)
O(4B)	11837(4)	-7479(2)	4704(1)	47(1)
C(1B)	10648(4)	-11067(2)	4953(1)	31(1)
C(2B)	11694(4)	-10295(2)	4704(1)	28(1)
C(3B)	11022(4)	-9211(2)	4749(1)	28(1)
C(4B)	13567(4)	-10690(2)	4420(1)	32(1)
C(5B)	12042(4)	-8341(2)	4466(1)	33(1)
C(1)	3664(4)	6281(2)	2342(1)	32(1)
C(2)	3921(4)	6152(2)	1802(1)	33(1)
C(3)	3679(4)	7032(2)	1409(1)	32(1)
C(4)	3267(4)	8061(2)	1565(1)	32(1)
C(5)	3059(4)	8209(2)	2101(1)	30(1)
C(6)	3222(4)	7318(2)	2486(1)	32(1)
O(11)	4732(4)	4420(2)	2630(1)	59(1)
N(11)	3076(4)	5391(2)	3224(1)	41(1)
N(12)	4468(4)	3708(2)	4483(1)	38(1)
C(11)	4650(5)	4397(2)	4042(1)	36(1)
C(12)	5776(6)	3572(3)	4871(1)	48(1)
C(13)	7323(6)	4112(3)	4835(2)	55(1)
C(14)	7514(6)	4817(3)	4383(2)	59(1)
C(15)	6181(5)	4967(3)	3984(2)	50(1)
C(16)	3095(5)	4491(3)	3638(1)	42(1)

C(17)	3872(5)	5291(2)	2746(1)	36(1)
O(21)	4547(4)	5947(2)	705(1)	54(1)
N(21)	3167(4)	7640(2)	465(1)	38(1)
N(22)	5808(5)	8359(2)	-489(1)	45(1)
C(21)	5114(5)	7438(2)	-360(1)	36(1)
C(22)	7497(6)	8420(3)	-746(2)	56(1)
C(23)	8599(6)	7524(3)	-884(2)	67(1)
C(24)	7991(7)	6548(3)	-745(2)	79(1)
C(25)	6230(6)	6517(3)	-487(2)	60(1)
C(26)	3159(5)	7471(3)	-95(1)	39(1)
C(27)	3852(5)	6825(2)	836(1)	34(1)
O(31)	1850(4)	10081(2)	1919(1)	53(1)
N(31)	3069(4)	9494(2)	2737(1)	37(1)
N(32)	-132(4)	11915(2)	2962(1)	48(1)
C(31)	671(5)	10884(2)	3086(1)	35(1)
C(32)	-1886(6)	12318(3)	3148(2)	65(1)
C(33)	-2930(7)	11690(4)	3471(2)	74(1)
C(34)	-2181(6)	10617(4)	3597(2)	66(1)
C(35)	-393(5)	10217(3)	3402(1)	51(1)
C(36)	2703(5)	10567(2)	2899(1)	39(1)
C(37)	2601(4)	9342(2)	2241(1)	33(1)
O(1W)	5792(8)	3106(3)	1885(2)	130(2)
O(2W)	11386(5)	3280(3)	2237(2)	103(2)
O(3W)	12040(6)	-7474(3)	5844(1)	90(1)
O(4W)	7347(5)	4231(2)	1051(1)	75(1)
O(5W)	8300(5)	22873(3)	-3808(1)	74(1)

Table 3. Bond lengths [Å] and angles [°] for **9**.

O(11A)-C(7A)	1.312(4)	C(3B)-C(5B)	1.502(4)
O(12A)-C(7A)	1.198(4)	C(1)-C(2)	1.389(4)
O(13A)-C(8A)	1.287(4)	C(1)-C(6)	1.391(4)
O(14A)-C(8A)	1.226(4)	C(1)-C(17)	1.504(4)
O(15A)-C(9A)	1.226(4)	C(2)-C(3)	1.387(4)
O(16A)-C(9A)	1.278(4)	C(3)-C(4)	1.392(4)
O(17A)-C(10A)	1.283(4)	C(3)-C(27)	1.494(4)
O(18A)-C(10A)	1.222(4)	C(4)-C(5)	1.382(4)
C(1A)-C(6A)	1.381(4)	C(5)-C(6)	1.386(4)
C(1A)-C(2A)	1.401(4)	C(5)-C(37)	1.503(4)
C(1A)-C(7A)	1.490(4)	O(11)-C(17)	1.233(4)
C(2A)-C(3A)	1.388(4)	N(11)-C(17)	1.318(4)
C(2A)-C(8A)	1.513(4)	N(11)-C(16)	1.445(4)
C(3A)-C(4A)	1.387(4)	N(12)-C(11)	1.340(4)
C(4A)-C(5A)	1.412(4)	N(12)-C(12)	1.341(4)
C(4A)-C(9A)	1.519(4)	C(11)-C(15)	1.382(4)
C(5A)-C(6A)	1.391(4)	C(11)-C(16)	1.497(5)
C(5A)-C(10A)	1.521(4)	C(12)-C(13)	1.368(5)
O(1B)-C(4B)	1.220(4)	C(13)-C(14)	1.373(5)
O(2B)-C(4B)	1.279(4)	C(14)-C(15)	1.370(5)
O(3B)-C(5B)	1.214(4)	O(21)-C(27)	1.221(3)
O(4B)-C(5B)	1.296(4)	N(21)-C(27)	1.342(4)
C(1B)-C(3B)#1	1.388(4)	N(21)-C(26)	1.452(4)
C(1B)-C(2B)	1.391(4)	N(22)-C(21)	1.335(4)
C(2B)-C(3B)	1.396(4)	N(22)-C(22)	1.338(5)
C(2B)-C(4B)	1.516(4)	C(21)-C(25)	1.363(5)
C(3B)-C(1B)#1	1.388(4)	C(21)-C(26)	1.499(5)

C(22)-C(23)	1.342(5)	C(2)-C(1)-C(6)	118.8(3)
C(23)-C(24)	1.374(6)	C(2)-C(1)-C(17)	118.5(3)
C(24)-C(25)	1.378(5)	C(6)-C(1)-C(17)	122.6(3)
O(31)-C(37)	1.220(3)	C(3)-C(2)-C(1)	121.2(3)
N(31)-C(37)	1.348(4)	C(2)-C(3)-C(4)	118.7(3)
N(31)-C(36)	1.449(4)	C(2)-C(3)-C(27)	118.1(3)
N(32)-C(32)	1.344(5)	C(4)-C(3)-C(27)	123.1(3)
N(32)-C(31)	1.339(4)	C(5)-C(4)-C(3)	120.9(3)
C(31)-C(35)	1.378(5)	C(6)-C(5)-C(4)	119.5(3)
C(31)-C(36)	1.493(5)	C(6)-C(5)-C(37)	122.4(3)
C(32)-C(33)	1.346(6)	C(4)-C(5)-C(37)	118.1(3)
C(33)-C(34)	1.378(6)	C(5)-C(6)-C(1)	120.7(3)
C(34)-C(35)	1.372(5)	C(17)-N(11)-C(16)	122.7(3)
C(6A)-C(1A)-C(2A)	118.4(3)	C(11)-N(12)-C(12)	119.8(3)
C(6A)-C(1A)-C(7A)	121.1(3)	N(12)-C(11)-C(15)	120.3(3)
C(2A)-C(1A)-C(7A)	120.4(3)	N(12)-C(11)-C(16)	115.1(3)
C(3A)-C(2A)-C(1A)	118.4(3)	C(15)-C(11)-C(16)	124.6(3)
C(3A)-C(2A)-C(8A)	118.1(3)	N(12)-C(12)-C(13)	122.4(3)
C(1A)-C(2A)-C(8A)	123.5(2)	C(12)-C(13)-C(14)	118.0(4)
C(2A)-C(3A)-C(4A)	123.4(3)	C(15)-C(14)-C(13)	120.2(4)
C(3A)-C(4A)-C(5A)	118.2(3)	C(14)-C(15)-C(11)	119.3(3)
C(3A)-C(4A)-C(9A)	114.2(3)	N(11)-C(16)-C(11)	114.2(3)
C(5A)-C(4A)-C(9A)	127.6(3)	O(11)-C(17)-N(11)	121.6(3)
C(6A)-C(5A)-C(4A)	117.9(3)	O(11)-C(17)-C(1)	121.0(3)
C(6A)-C(5A)-C(10A)	113.1(3)	N(11)-C(17)-C(1)	117.4(3)
C(4A)-C(5A)-C(10A)	129.0(3)	C(27)-N(21)-C(26)	120.3(3)
C(1A)-C(6A)-C(5A)	123.6(3)	C(21)-N(22)-C(22)	123.4(3)
O(12A)-C(7A)-O(11A)	124.0(3)	N(22)-C(21)-C(25)	117.3(3)
O(12A)-C(7A)-C(1A)	123.0(3)	N(22)-C(21)-C(26)	118.9(3)
O(11A)-C(7A)-C(1A)	112.9(3)	C(25)-C(21)-C(26)	123.8(3)
O(14A)-C(8A)-O(13A)	124.7(3)	N(22)-C(22)-C(23)	120.1(4)
O(14A)-C(8A)-C(2A)	120.8(3)	C(22)-C(23)-C(24)	119.0(4)
O(13A)-C(8A)-C(2A)	114.4(3)	C(23)-C(24)-C(25)	119.3(4)
O(15A)-C(9A)-O(16A)	122.0(3)	C(21)-C(25)-C(24)	120.7(4)
O(15A)-C(9A)-C(4A)	118.3(3)	N(21)-C(26)-C(21)	112.9(3)
O(16A)-C(9A)-C(4A)	119.6(3)	O(21)-C(27)-N(21)	120.4(3)
O(18A)-C(10A)-O(17A)	121.8(3)	O(21)-C(27)-C(3)	122.1(3)
O(18A)-C(10A)-C(5A)	118.4(3)	N(21)-C(27)-C(3)	117.4(3)
O(17A)-C(10A)-C(5A)	119.8(3)	C(37)-N(31)-C(36)	119.7(3)
C(3B)#1-C(1B)-C(2B)	121.8(3)	C(32)-N(32)-C(31)	122.6(3)
C(1B)-C(2B)-C(3B)	118.8(3)	N(32)-C(31)-C(35)	117.7(3)
C(1B)-C(2B)-C(4B)	117.5(3)	N(32)-C(31)-C(36)	117.2(3)
C(3B)-C(2B)-C(4B)	123.7(3)	C(35)-C(31)-C(36)	125.0(3)
C(1B)#1-C(3B)-C(2B)	119.4(3)	N(32)-C(32)-C(33)	120.9(4)
C(1B)#1-C(3B)-C(5B)	119.7(3)	C(32)-C(33)-C(34)	118.5(4)
C(2B)-C(3B)-C(5B)	120.9(3)	C(35)-C(34)-C(33)	119.9(4)
O(1B)-C(4B)-O(2B)	122.9(3)	C(34)-C(35)-C(31)	120.4(4)
O(1B)-C(4B)-C(2B)	119.9(3)	N(31)-C(36)-C(31)	113.1(3)
O(2B)-C(4B)-C(2B)	117.1(3)	O(31)-C(37)-N(31)	122.1(3)
O(3B)-C(5B)-O(4B)	124.7(3)	O(31)-C(37)-C(5)	121.5(3)
O(3B)-C(5B)-C(3B)	121.7(3)	N(31)-C(37)-C(5)	116.4(3)
O(4B)-C(5B)-C(3B)	113.6(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y-2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9**. 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(11A)	105(2)	34(1)	45(2)	-9(1)	19(2)	2(2)
O(12A)	71(2)	32(1)	37(1)	2(1)	1(1)	-9(1)
O(13A)	40(2)	50(1)	34(1)	9(1)	10(1)	5(1)
O(14A)	48(2)	45(1)	42(1)	-7(1)	-9(1)	5(1)
O(15A)	89(2)	34(1)	65(2)	-13(1)	3(2)	-2(1)
O(16A)	90(2)	30(1)	65(2)	11(1)	11(2)	-1(1)
O(17A)	83(2)	44(2)	49(2)	15(1)	14(2)	4(1)
O(18A)	66(2)	61(2)	34(1)	5(1)	9(1)	6(1)
C(1A)	31(2)	27(2)	30(2)	-2(1)	4(1)	-3(1)
C(2A)	24(2)	30(2)	31(2)	0(1)	3(1)	-3(1)
C(3A)	34(2)	31(2)	35(2)	-5(1)	4(1)	-3(1)
C(4A)	29(2)	26(2)	39(2)	2(1)	3(1)	-7(1)
C(5A)	25(2)	33(2)	35(2)	1(1)	3(1)	-5(1)
C(6A)	35(2)	33(2)	31(2)	-2(1)	5(1)	-4(1)
C(7A)	39(2)	31(2)	33(2)	-4(1)	-1(2)	-2(1)
C(8A)	41(2)	25(2)	30(2)	-9(1)	6(2)	5(1)
C(9A)	42(2)	30(2)	56(2)	-3(2)	5(2)	-6(2)
C(10A)	39(2)	42(2)	40(2)	8(2)	2(2)	-7(2)
O(1B)	43(2)	63(2)	53(2)	-33(1)	13(1)	-10(1)
O(2B)	24(1)	68(2)	47(1)	-21(1)	6(1)	-9(1)
O(3B)	68(2)	52(2)	42(1)	-13(1)	24(1)	-27(1)
O(4B)	62(2)	31(1)	52(2)	-11(1)	22(1)	-20(1)
C(1B)	31(2)	23(2)	38(2)	-6(1)	2(1)	-2(1)
C(2B)	27(2)	30(2)	27(2)	-3(1)	3(1)	-7(1)
C(3B)	27(2)	31(2)	26(2)	-4(1)	2(1)	-10(1)
C(4B)	30(2)	32(2)	33(2)	-5(1)	7(1)	-4(1)
C(5B)	31(2)	34(2)	34(2)	-5(1)	3(2)	-10(1)
C(1)	34(2)	28(2)	30(2)	-1(1)	0(1)	-2(1)
C(2)	40(2)	21(2)	37(2)	-4(1)	-1(2)	-1(1)
C(3)	35(2)	27(2)	32(2)	-4(1)	2(1)	-3(1)
C(4)	35(2)	28(2)	31(2)	3(1)	0(1)	-3(1)
C(5)	31(2)	23(2)	34(2)	-5(1)	1(1)	-2(1)
C(6)	36(2)	30(2)	30(2)	-6(1)	0(1)	-3(1)
O(11)	99(2)	28(1)	44(1)	-1(1)	16(1)	8(1)
N(11)	57(2)	30(1)	33(2)	1(1)	5(1)	-3(1)
N(12)	49(2)	24(1)	40(2)	3(1)	5(1)	-6(1)
C(11)	47(2)	25(2)	34(2)	-1(1)	7(2)	-7(1)
C(12)	64(3)	35(2)	40(2)	5(2)	-4(2)	-1(2)
C(13)	55(3)	46(2)	63(3)	-4(2)	-14(2)	-2(2)
C(14)	45(2)	56(2)	80(3)	-6(2)	1(2)	-19(2)
C(15)	55(2)	45(2)	50(2)	4(2)	10(2)	-20(2)
C(16)	58(2)	36(2)	34(2)	1(1)	4(2)	-13(2)
C(17)	46(2)	27(2)	34(2)	-3(1)	-2(2)	-3(1)
O(21)	86(2)	33(1)	36(1)	-5(1)	0(1)	12(1)
N(21)	50(2)	30(1)	31(1)	-3(1)	2(1)	5(1)
N(22)	48(2)	29(2)	56(2)	-8(1)	4(2)	-1(1)
C(21)	44(2)	31(2)	32(2)	-1(1)	0(2)	-2(2)
C(22)	51(3)	47(2)	72(3)	-3(2)	7(2)	-17(2)
C(23)	49(3)	71(3)	84(3)	-21(2)	30(2)	-17(2)
C(24)	69(3)	54(3)	113(4)	-31(3)	42(3)	-4(2)
C(25)	64(3)	36(2)	81(3)	-18(2)	22(2)	-9(2)

C(26)	45(2)	41(2)	29(2)	-3(1)	1(2)	-2(2)
C(27)	39(2)	26(2)	34(2)	-2(1)	1(2)	-2(1)
O(31)	73(2)	28(1)	53(2)	0(1)	-19(1)	1(1)
N(31)	46(2)	27(1)	36(2)	-5(1)	-1(1)	-2(1)
N(32)	46(2)	36(2)	61(2)	-9(1)	7(2)	-2(1)
C(31)	41(2)	34(2)	33(2)	-10(1)	0(2)	-5(2)
C(32)	49(3)	52(2)	90(3)	-16(2)	5(2)	8(2)
C(33)	50(3)	88(4)	82(3)	-26(3)	21(2)	-2(2)
C(34)	50(3)	92(3)	56(3)	-2(2)	12(2)	-25(2)
C(35)	52(3)	51(2)	48(2)	4(2)	4(2)	-9(2)
C(36)	43(2)	30(2)	44(2)	-9(1)	3(2)	-7(2)
C(37)	32(2)	27(2)	39(2)	0(1)	1(1)	-6(1)
O(1W)	260(6)	41(2)	78(2)	-19(2)	25(3)	15(3)
O(2W)	88(3)	41(2)	163(4)	23(2)	35(3)	2(2)
O(3W)	86(3)	130(3)	56(2)	-24(2)	-4(2)	-9(2)
O(4W)	71(2)	51(2)	99(2)	-21(2)	-13(2)	8(2)
O(5W)	75(2)	73(2)	83(2)	-42(2)	13(2)	-19(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9**.

	x	y	z	U(eq)
H(11O)	13490(60)	-1690(30)	-1984(17)	76
H(13A)	10000	0	0	53
H(17O)	11220(60)	4140(30)	-2692(18)	75
H(3A)	11036	2582	-995	40
H(6A)	12694	791	-2458	40
H(2BO)	15000	-10000	5000	54
H(4BO)	12810(50)	-6930(30)	4575(14)	56
H(1B)	11079	-11789	4919	37
H(2)	4261	5463	1702	40
H(4)	3129	8658	1306	38
H(6)	3034	7415	2846	38
H(11)	2522	6018	3291	49
H(12)	5627	3094	5176	57
H(13)	8217	4004	5108	66
H(14)	8552	5195	4346	71
H(15)	6306	5447	3678	60
H(16A)	3256	3832	3472	51
H(16B)	1853	4559	3824	51
H(21)	2732	8265	559	46
H(22N)	5050(50)	8960(30)	-429(14)	50
H(22)	7908	9083	-830	68
H(23)	9758	7564	-1071	80
H(24)	8759	5915	-824	94
H(25)	5798	5859	-399	72
H(26A)	2265	8047	-286	47
H(26B)	2699	6798	-122	47
H(31)	3583	8957	2957	44
H(32N)	640(50)	12330(30)	2707(14)	50
H(32)	-2384	13040	3052	78
H(33)	-4130	11974	3605	88
H(34)	-2886	10165	3813	79
H(35)	105	9491	3485	61

H(36A)	2986	11080	2599	46
H(36B)	3571	10602	3186	46
H(1W1)	5570(90)	3560(50)	2140(30)	156
H(2W1)	7420(100)	3240(50)	1910(30)	156
H(1W2)	10770(80)	3930(50)	2270(20)	123
H(2W2)	12380(90)	3230(50)	2190(30)	123
H(1W3)	11830(80)	-8180(40)	6000(20)	108
H(2W3)	12710(80)	-7650(50)	6130(20)	108
H(1W4)	6330(70)	4800(40)	929(18)	89
H(2W4)	8430(60)	4740(40)	1179(17)	89
H(1W5)	7620(70)	22450(40)	-3918(19)	89
H(2W5)	9500(70)	22830(40)	-3925(19)	89

Table 1. Crystal data and structure refinement for **10**.

Identification code	**10**	
Empirical formula	C30 H24 N4 O10	
Formula weight	600.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.862(4) Å	α= 90°.
	b = 16.423(3) Å	β= 103.089(6)°.
	c = 7.4789(13) Å	γ = 90°.
Volume	2615.4(8) $Å^3$	
Z	4	
Density (calculated)	1.525 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	1248	
Crystal size	0.18 x 0.13 x 0.10 mm^3	
Theta range for data collection	1.57 to 25.49°.	
Index ranges	-26<=h<=26, -19<=k<=19, -9<=l<=8	
Reflections collected	15940	
Independent reflections	2433 [R(int) = 0.1259]	
Completeness to theta = 25.49°	100.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.988 and 0.982	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2433 / 0 / 206	
Goodness-of-fit on F^2	0.848	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1328	
R indices (all data)	R1 = 0.1319, wR2 = 0.1632	
Largest diff. peak and hole	0.241 and -0.238 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	4848(1)	7710(1)	-281(3)	58(1)
O(2)	4133(1)	8254(1)	1025(4)	61(1)
O(3)	3466(1)	10881(2)	-165(4)	71(1)
O(4)	4090(1)	11930(1)	471(4)	62(1)
C(1)	4848(1)	9168(2)	167(4)	32(1)
C(2)	4425(1)	9790(2)	220(4)	35(1)
C(3)	4548(1)	10612(2)	57(4)	32(1)
C(4)	3991(2)	11156(2)	108(4)	44(1)
C(5)	4597(2)	8314(2)	325(4)	42(1)
N(11)	6696(1)	2936(2)	-1207(4)	41(1)
N(12)	6151(1)	3424(2)	2087(4)	44(1)
C(11)	6976(1)	3258(2)	424(5)	39(1)
C(12)	6850(2)	3155(2)	-2782(5)	47(1)
C(13)	7307(2)	3728(2)	-2758(5)	50(1)
C(14)	7610(2)	4062(2)	-1100(5)	50(1)
C(15)	7444(2)	3821(2)	486(5)	45(1)
C(16)	6728(2)	2997(2)	2046(5)	49(1)
O(21)	6670(1)	4558(2)	3186(4)	67(1)
C(21)	5000	4197(3)	2500	43(1)
C(22)	5555(2)	4617(2)	2564(4)	40(1)
C(23)	5549(2)	5460(2)	2571(5)	54(1)
C(24)	5000	5880(3)	2500	63(2)
C(25)	6167(2)	4201(2)	2639(5)	44(1)

Table 3. Bond lengths [Å] and angles [°] for **10**.

O(1)-C(5)	1.266(4)	C(24)-C(23)#2	1.375(4)
O(2)-C(5)	1.246(4)	C(2)-C(1)-C(3)#1	117.6(2)
O(3)-C(4)	1.206(4)	C(2)-C(1)-C(5)	115.0(3)
O(4)-C(4)	1.307(4)	C(3)#1-C(1)-C(5)	127.4(3)
C(1)-C(2)	1.385(4)	C(3)-C(2)-C(1)	124.8(3)
C(1)-C(3)#1	1.416(4)	C(2)-C(3)-C(1)#1	117.6(3)
C(1)-C(5)	1.521(4)	C(2)-C(3)-C(4)	113.5(3)
C(2)-C(3)	1.387(4)	C(1)#1-C(3)-C(4)	128.9(3)
C(3)-C(1)#1	1.416(4)	O(3)-C(4)-O(4)	120.4(3)
C(3)-C(4)	1.518(4)	O(3)-C(4)-C(3)	120.8(3)
N(11)-C(11)	1.343(4)	O(4)-C(4)-C(3)	118.7(3)
N(11)-C(12)	1.345(4)	O(2)-C(5)-O(1)	123.3(3)
N(12)-C(25)	1.340(4)	O(2)-C(5)-C(1)	116.6(3)
N(12)-C(16)	1.451(4)	O(1)-C(5)-C(1)	120.0(3)
C(11)-C(15)	1.372(4)	C(11)-N(11)-C(12)	122.5(3)
C(11)-C(16)	1.499(5)	C(25)-N(12)-C(16)	120.3(3)
C(12)-C(13)	1.370(5)	N(11)-C(11)-C(15)	118.6(3)
C(13)-C(14)	1.380(5)	N(11)-C(11)-C(16)	116.6(3)
C(14)-C(15)	1.374(4)	C(15)-C(11)-C(16)	124.7(3)
O(21)-C(25)	1.229(4)	N(11)-C(12)-C(13)	119.9(3)
C(21)-C(22)#2	1.387(4)	C(14)-C(13)-C(12)	119.0(3)
C(21)-C(22)	1.387(4)	C(13)-C(14)-C(15)	119.6(3)
C(22)-C(23)	1.385(4)	C(11)-C(15)-C(14)	120.3(3)
C(22)-C(25)	1.492(5)	N(12)-C(16)-C(11)	110.8(3)
C(23)-C(24)	1.375(4)	C(22)#2-C(21)-C(22)	120.4(4)

C(23)-C(22)-C(21)	119.2(3)	C(23)#2-C(24)-C(23)	119.7(5)
C(23)-C(22)-C(25)	117.8(3)	O(21)-C(25)-N(12)	121.1(3)
C(21)-C(22)-C(25)	123.0(3)	O(21)-C(25)-C(22)	121.4(3)
C(22)-C(23)-C(24)	120.7(4)	N(12)-C(25)-C(22)	117.5(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. 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(1)	59(2)	30(1)	81(2)	-6(1)	9(1)	-4(1)
O(2)	67(2)	44(2)	79(2)	2(1)	27(2)	-19(1)
O(3)	33(2)	62(2)	120(2)	-7(2)	17(2)	4(1)
O(4)	48(2)	43(2)	93(2)	-16(1)	11(2)	9(1)
C(1)	32(2)	26(2)	34(2)	2(1)	-1(1)	-1(1)
C(2)	27(2)	36(2)	39(2)	1(1)	6(1)	-3(1)
C(3)	31(2)	28(2)	33(2)	-1(1)	0(1)	3(1)
C(4)	42(2)	39(2)	49(2)	-5(2)	8(2)	7(2)
C(5)	46(2)	32(2)	45(2)	3(2)	4(2)	-6(2)
N(11)	33(2)	34(2)	56(2)	4(1)	9(1)	1(1)
N(12)	36(2)	37(2)	62(2)	-4(1)	15(1)	-4(1)
C(11)	30(2)	35(2)	51(2)	2(2)	6(2)	6(2)
C(12)	46(2)	42(2)	51(2)	-2(2)	5(2)	-1(2)
C(13)	47(2)	47(2)	58(2)	9(2)	14(2)	-1(2)
C(14)	33(2)	41(2)	74(3)	10(2)	12(2)	-5(2)
C(15)	35(2)	42(2)	54(2)	-6(2)	4(2)	-1(2)
C(16)	45(2)	47(2)	56(2)	2(2)	12(2)	7(2)
O(21)	48(2)	58(2)	91(2)	-15(1)	9(2)	-15(1)
C(21)	53(3)	26(2)	52(3)	0	16(2)	0
C(22)	48(2)	35(2)	39(2)	-2(1)	11(2)	-6(2)
C(23)	70(3)	34(2)	62(2)	-3(2)	22(2)	-11(2)
C(24)	83(4)	31(3)	83(4)	0	35(3)	0
C(25)	44(2)	41(2)	47(2)	-1(2)	11(2)	-9(2)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **10**.

	x	y	z	U(eq)
H(3O)	4556(17)	12102(18)	410(40)	50
H(2)	4029	9646	376	41
H(11N)	6353(15)	2523(19)	-1210(40)	50
H(12)	5796	3177	1755	53
H(12A)	6646	2917	-3885	56
H(13)	7412	3889	-3842	60
H(14)	7924	4448	-1056	59
H(15)	7650	4042	1607	53
H(16A)	6650	2415	1982	59
H(16B)	7039	3108	3167	59
H(21)	5000	3631	2500	51
H(23)	5920	5745	2625	65
H(24)	5000	6447	2500	76

Table 1. Crystal data and structure refinement for **11**.

Identification code	**11**	
Empirical formula	C30 H24 N4 O10	
Formula weight	600.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 8.7408(13) Å	α= 90°.
	b = 13.509(2) Å	β= 91.307(5)°.
	c = 22.629(4) Å	γ = 90°.
Volume	2671.4(7) $Å^3$	
Z	4	
Density (calculated)	1.493 Mg/m^3	
Absorption coefficient	0.114 mm^{-1}	
F(000)	1248	
Crystal size	0.14 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.76 to 25.00°.	
Index ranges	-10<=h<=10, -16<=k<=16, -26<=l<=26	
Reflections collected	30994	
Independent reflections	4702 [R(int) = 0.1526]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.991 and 0.984	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4702 / 0 / 409	
Goodness-of-fit on F^2	0.814	
Final R indices [I>2sigma(I)]	R1 = 0.0632, wR2 = 0.1362	
R indices (all data)	R1 = 0.1679, wR2 = 0.1727	
Largest diff. peak and hole	0.170 and -0.212 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(11)	6265(4)	17332(2)	1182(1)	82(1)
O(12)	5182(4)	16617(3)	1920(2)	98(1)
O(13)	4048(3)	15037(2)	2166(1)	68(1)
O(14)	3342(3)	13669(2)	1707(1)	67(1)
O(15)	5522(3)	12288(2)	138(1)	65(1)
O(16)	7377(4)	12852(2)	-371(2)	98(1)
O(17)	8541(4)	14392(3)	-615(1)	91(1)
O(18)	8519(4)	15915(3)	-342(1)	93(1)
C(10)	5842(4)	15599(3)	1086(2)	41(1)
C(11)	5081(4)	14703(3)	1208(1)	37(1)
C(12)	5320(4)	13917(3)	822(2)	39(1)
C(13)	6282(4)	13937(3)	348(1)	36(1)
C(14)	7045(4)	14830(3)	231(2)	40(1)
C(15)	6780(4)	15624(3)	605(2)	42(1)
C(16)	5754(5)	16595(3)	1411(2)	58(1)
C(17)	4070(4)	14456(3)	1724(2)	50(1)
C(18)	6387(5)	12963(3)	18(2)	52(1)
C(19)	8113(5)	15078(4)	-271(2)	54(1)
N(11A)	10782(4)	12135(2)	597(1)	60(1)
N(12A)	13899(4)	9245(3)	564(2)	67(1)

C(11A)	12658(4)	10787(3)	548(2)	50(1)
C(12A)	13013(5)	9907(3)	281(2)	59(1)
C(13A)	14439(5)	9372(3)	1110(2)	70(1)
C(14A)	14114(5)	10233(3)	1397(2)	67(1)
C(15A)	13240(5)	10944(3)	1111(2)	60(1)
C(16A)	11698(5)	11522(3)	210(2)	65(1)
C(21A)	9917(4)	17229(3)	1896(2)	47(1)
C(22A)	8864(4)	17486(3)	2317(2)	49(1)
C(23A)	8434(5)	19024(3)	1888(2)	61(1)
C(24A)	9445(6)	18811(3)	1457(2)	69(1)
C(25A)	10195(5)	17916(3)	1462(2)	64(1)
C(26A)	10783(5)	16271(3)	1958(2)	60(1)
O(31A)	9172(3)	10896(2)	786(1)	72(1)
O(32A)	8650(4)	15215(2)	2568(1)	82(1)
N(21A)	9987(4)	15399(2)	1746(1)	51(1)
N(22A)	8172(4)	18356(3)	2304(2)	52(1)
C(31A)	8754(4)	12406(3)	1288(2)	45(1)
C(32A)	9249(4)	13358(3)	1446(2)	44(1)
C(33A)	8502(4)	13894(3)	1875(2)	44(1)
C(34A)	7275(5)	13468(3)	2155(2)	60(1)
C(35A)	6755(5)	12545(4)	1990(2)	67(1)
C(36A)	7482(5)	12022(3)	1556(2)	63(1)
C(37A)	9571(5)	11763(3)	866(2)	51(1)
C(38A)	9037(5)	14894(3)	2091(2)	51(1)

Table 3. Bond lengths [Å] and angles [°] for **11**.

O(11)-C(16)	1.213(5)	C(21A)-C(26A)	1.504(5)
O(12)-C(16)	1.266(5)	C(22A)-N(22A)	1.322(5)
O(13)-C(17)	1.273(5)	C(23A)-N(22A)	1.328(5)
O(14)-C(17)	1.239(5)	C(23A)-C(24A)	1.361(6)
O(15)-C(18)	1.220(5)	C(24A)-C(25A)	1.375(6)
O(16)-C(18)	1.257(5)	C(26A)-N(21A)	1.445(5)
O(17)-C(19)	1.272(5)	O(31A)-C(37A)	1.233(4)
O(18)-C(19)	1.198(5)	O(32A)-C(38A)	1.218(4)
C(10)-C(15)	1.378(5)	N(21A)-C(38A)	1.341(5)
C(10)-C(11)	1.411(5)	C(31A)-C(36A)	1.380(5)
C(10)-C(16)	1.537(5)	C(31A)-C(32A)	1.400(5)
C(11)-C(12)	1.393(5)	C(31A)-C(37A)	1.488(5)
C(11)-C(17)	1.519(5)	C(32A)-C(33A)	1.388(5)
C(12)-C(13)	1.379(5)	C(33A)-C(34A)	1.383(5)
C(13)-C(14)	1.406(5)	C(33A)-C(38A)	1.506(5)
C(13)-C(18)	1.516(5)	C(34A)-C(35A)	1.376(6)
C(14)-C(15)	1.390(5)	C(35A)-C(36A)	1.377(6)
C(14)-C(19)	1.524(5)		
N(11A)-C(37A)	1.332(5)	C(15)-C(10)-C(11)	117.8(3)
N(11A)-C(16A)	1.458(5)	C(15)-C(10)-C(16)	113.2(4)
N(12A)-C(12A)	1.336(5)	C(11)-C(10)-C(16)	129.0(4)
N(12A)-C(13A)	1.324(6)	C(12)-C(11)-C(10)	117.0(3)
C(11A)-C(12A)	1.372(5)	C(12)-C(11)-C(17)	114.4(3)
C(11A)-C(15A)	1.379(5)	C(10)-C(11)-C(17)	128.6(3)
C(11A)-C(16A)	1.498(5)	C(13)-C(12)-C(11)	125.1(3)
C(13A)-C(14A)	1.367(6)	C(12)-C(13)-C(14)	117.6(3)
C(14A)-C(15A)	1.379(5)	C(12)-C(13)-C(18)	114.2(3)
C(21A)-C(25A)	1.377(5)	C(14)-C(13)-C(18)	128.1(3)
C(21A)-C(22A)	1.383(5)	C(15)-C(14)-C(13)	117.5(3)

C(15)-C(14)-C(19)	113.4(3)
C(13)-C(14)-C(19)	129.0(3)
C(10)-C(15)-C(14)	124.9(3)
O(11)-C(16)-O(12)	121.8(4)
O(11)-C(16)-C(10)	119.4(4)
O(12)-C(16)-C(10)	118.8(4)
O(14)-C(17)-O(13)	122.5(4)
O(14)-C(17)-C(11)	118.2(4)
O(13)-C(17)-C(11)	119.2(4)
O(15)-C(18)-O(16)	120.4(4)
O(15)-C(18)-C(13)	119.7(3)
O(16)-C(18)-C(13)	119.9(4)
O(18)-C(19)-O(17)	120.9(4)
O(18)-C(19)-C(14)	119.8(4)
O(17)-C(19)-C(14)	119.3(4)
C(37A)-N(11A)-C(16A)	120.9(3)
C(12A)-N(12A)-C(13A)	123.4(4)
C(12A)-C(11A)-C(15A)	117.2(4)
C(12A)-C(11A)-C(16A)	118.7(4)
C(15A)-C(11A)-C(16A)	124.1(3)
N(12A)-C(12A)-C(11A)	120.3(4)
N(12A)-C(13A)-C(14A)	118.8(4)
C(15A)-C(14A)-C(13A)	119.2(4)
C(14A)-C(15A)-C(11A)	121.1(4)
N(11A)-C(16A)-C(11A)	112.3(3)
C(25A)-C(21A)-C(22A)	116.9(4)
C(25A)-C(21A)-C(26A)	123.4(4)
C(22A)-C(21A)-C(26A)	119.5(4)
N(22A)-C(22A)-C(21A)	121.3(4)
N(22A)-C(23A)-C(24A)	119.3(4)
C(23A)-C(24A)-C(25A)	119.8(4)
C(24A)-C(25A)-C(21A)	120.4(4)
N(21A)-C(26A)-C(21A)	115.6(3)
C(38A)-N(21A)-C(26A)	121.4(3)
C(22A)-N(22A)-C(23A)	122.3(4)
C(36A)-C(31A)-C(32A)	118.8(4)
C(36A)-C(31A)-C(37A)	117.8(4)
C(32A)-C(31A)-C(37A)	123.4(3)
C(33A)-C(32A)-C(31A)	120.6(4)
C(34A)-C(33A)-C(32A)	119.1(4)
C(34A)-C(33A)-C(38A)	117.6(4)
C(32A)-C(33A)-C(38A)	123.2(4)
C(35A)-C(34A)-C(33A)	120.5(4)
C(34A)-C(35A)-C(36A)	120.2(4)
C(35A)-C(36A)-C(31A)	120.6(4)
O(31A)-C(37A)-N(11A)	121.1(4)
O(31A)-C(37A)-C(31A)	120.6(4)
N(11A)-C(37A)-C(31A)	118.2(3)
O(32A)-C(38A)-N(21A)	121.5(4)
O(32A)-C(38A)-C(33A)	121.1(4)
N(21A)-C(38A)-C(33A)	117.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. 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(11)	106(3)	44(2)	95(3)	-15(2)	-4(2)	-8(2)
O(12)	131(3)	80(2)	86(3)	-42(2)	46(2)	-16(2)
O(13)	76(2)	83(2)	45(2)	-9(2)	19(2)	10(2)
O(14)	69(2)	71(2)	63(2)	5(2)	26(2)	-11(2)
O(15)	81(2)	41(2)	74(2)	-13(2)	22(2)	-9(2)
O(16)	118(3)	66(2)	113(3)	-34(2)	70(2)	-16(2)
O(17)	101(3)	95(3)	79(2)	-12(2)	59(2)	-10(2)
O(18)	112(3)	70(2)	98(3)	26(2)	45(2)	-20(2)
C(10)	42(2)	41(2)	39(2)	0(2)	-2(2)	8(2)
C(11)	37(2)	47(2)	28(2)	-1(2)	5(2)	7(2)
C(12)	42(2)	39(2)	35(2)	8(2)	3(2)	0(2)
C(13)	36(2)	41(2)	31(2)	1(2)	2(2)	4(2)
C(14)	39(2)	45(2)	36(2)	5(2)	2(2)	3(2)
C(15)	43(2)	33(2)	49(2)	7(2)	-3(2)	-5(2)
C(16)	55(3)	59(3)	61(3)	-16(2)	-1(2)	7(2)
C(17)	44(3)	61(3)	44(3)	4(2)	3(2)	9(2)
C(18)	54(3)	60(3)	42(3)	-3(2)	11(2)	12(2)
C(19)	46(3)	71(3)	47(3)	7(2)	9(2)	0(2)
N(11A)	73(3)	32(2)	77(3)	-8(2)	13(2)	1(2)
N(12A)	72(3)	45(2)	85(3)	-23(2)	14(2)	-1(2)
C(11A)	54(3)	39(2)	56(3)	-11(2)	16(2)	-9(2)
C(12A)	62(3)	50(3)	64(3)	-10(2)	2(2)	3(2)
C(13A)	69(3)	51(3)	89(4)	1(3)	4(3)	3(2)
C(14A)	74(3)	68(3)	58(3)	-5(2)	-5(2)	2(3)
C(15A)	82(3)	41(2)	58(3)	-19(2)	7(2)	-1(2)
C(16A)	87(3)	45(2)	62(3)	-6(2)	6(2)	6(2)
C(21A)	43(2)	50(2)	47(2)	-14(2)	2(2)	-2(2)
C(22A)	49(2)	50(2)	48(2)	-9(2)	2(2)	0(2)
C(23A)	72(3)	47(3)	64(3)	-10(2)	-5(3)	10(2)
C(24A)	98(4)	55(3)	55(3)	-1(2)	10(3)	-6(3)
C(25A)	82(3)	58(3)	53(3)	-14(2)	24(2)	-9(3)
C(26A)	49(3)	57(3)	73(3)	-21(2)	-1(2)	3(2)
O(31A)	84(2)	39(2)	93(2)	-3(2)	-10(2)	-10(2)
O(32A)	119(3)	77(2)	50(2)	-4(2)	30(2)	15(2)
N(21A)	60(2)	47(2)	46(2)	-10(2)	4(2)	2(2)
N(22A)	48(2)	53(2)	55(2)	-20(2)	8(2)	4(2)
C(31A)	41(2)	40(2)	53(2)	15(2)	-4(2)	1(2)
C(32A)	40(2)	46(2)	44(2)	12(2)	5(2)	1(2)
C(33A)	41(2)	54(2)	38(2)	13(2)	8(2)	7(2)
C(34A)	61(3)	65(3)	55(3)	27(2)	17(2)	17(2)
C(35A)	51(3)	70(3)	81(3)	40(3)	11(3)	7(3)
C(36A)	55(3)	50(3)	82(3)	29(2)	-3(3)	-2(2)
C(37A)	52(3)	36(2)	65(3)	11(2)	-7(2)	-4(2)
C(38A)	59(3)	55(3)	39(3)	1(2)	7(2)	17(2)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **11**.

	x	y	z	U(eq)
H(12O)	4860(40)	15970(30)	2111(15)	50
H(16O)	7960(40)	13350(30)	-476(16)	50
H(12)	4789	13333	890	47
H(15)	7273	16218	525	50
H(11A)	11027	12745	652	72
H(12N)	14110(40)	8720(30)	309(15)	50
H(12A)	12635	9770	-98	71
H(13A)	15028	8883	1294	84
H(14A)	14479	10340	1781	80
H(15A)	13039	11538	1302	72
H(16A)	12360	11944	-18	78
H(16B)	11025	11172	-65	78
H(22A)	8638	17038	2614	58
H(23A)	7933	19631	1891	74
H(24A)	9628	19269	1160	83
H(25A)	10894	17774	1170	77
H(26A)	11731	16332	1747	72
H(26B)	11048	16174	2373	72
H(21A)	10127	15200	1390	61
H(22N)	7530(40)	18560(20)	2652(15)	50
H(32A)	10087	13634	1260	52
H(34A)	6797	13809	2457	72
H(35A)	5909	12273	2172	81
H(36A)	7112	11403	1442	75