Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Information

Propensity of formation of zipper architecture vs. Lincoln log arrangement in solvated molecular complexes of melamine with hydroxybenzoic acids

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Index

Crystallographic Information for **2**

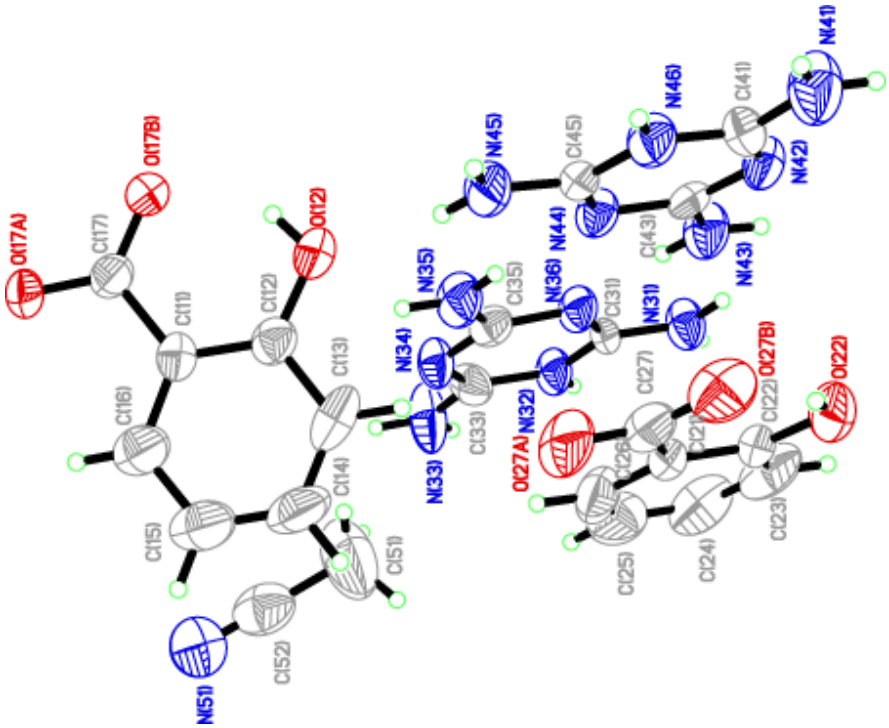


Figure 1. ORTEP drawing of the asymmetric unit of the complex **2**.

Table 1. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	$C_{22}\ H_{27}\ N_{13}\ O_6$	
Formula weight	569.57	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 16.691(8) Å	α= 90°.
	b = 8.577(4) Å	β= 117.83(3)°.
	c = 20.692(8) Å	γ = 90°.
Volume	2620(2) Å^3	
Z	4	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	1192	
Crystal size	0.14 x 0.11 x 0.09 mm^3	

Theta range for data collection	2.00 to 25.00°.
Index ranges	-15<=h<=18, -10<=k<=10, -24<=l<=3
Reflections collected	5980
Independent reflections	4203 [R(int) = 0.0539]
Completeness to theta = 25.00°	91.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9902 and 0.9848
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4203 / 0 / 371
Goodness-of-fit on F^2	0.689
Final *R* indices [I>2sigma(I)]	*R*1 = 0.0712, *wR*2 = 0.1620
R indices (all data)	*R*1 = 0.1660, *wR*2 = 0.1805
Largest diff. peak and hole	0.358 and -0.341 e.Å^{-3}

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

	x	y	z	U(eq)
N(31)	3562(2)	2574(5)	6962(2)	54(1)
N(32)	2205(3)	1953(5)	6005(2)	47(1)
N(33)	845(3)	1271(6)	5076(2)	79(2)
N(34)	1766(3)	2885(5)	4829(2)	49(1)
N(35)	2790(3)	4466(5)	4700(2)	59(1)
N(36)	3222(3)	3545(5)	5836(2)	45(1)
N(41)	7030(3)	8609(6)	6397(2)	78(2)
N(42)	6003(3)	6920(5)	6474(2)	47(1)
N(43)	4925(3)	5300(5)	6450(2)	57(1)
N(44)	4623(3)	6380(5)	5367(2)	43(1)
N(45)	4432(3)	7637(5)	4311(2)	56(1)
N(46)	5732(3)	8092(5)	5378(2)	52(1)
C(31)	2993(3)	2707(6)	6264(2)	35(1)
C(33)	1599(4)	2047(7)	5286(3)	48(2)
C(35)	2570(4)	3590(6)	5131(3)	42(1)
C(41)	6256(4)	7862(7)	6093(3)	51(2)
C(43)	5209(4)	6238(7)	6089(3)	41(2)
C(45)	4931(4)	7352(6)	5023(3)	40(1)
O(12)	2705(2)	6033(4)	3294(2)	60(1)
O(17A)	662(2)	5303(4)	1197(2)	58(1)
O(17B)	2057(2)	4761(4)	2048(2)	53(1)
C(11)	1205(4)	6567(6)	2339(2)	40(1)
C(12)	1906(4)	6809(6)	3035(3)	44(2)
C(13)	1797(5)	7863(7)	3504(3)	64(2)
C(14)	1010(5)	8658(8)	3277(3)	75(2)
C(15)	314(4)	8416(7)	2600(4)	71(2)
C(16)	401(4)	7381(7)	2126(3)	60(2)
C(17)	1318(4)	5474(6)	1827(3)	42(2)
O(22)	4695(2)	8961(5)	7162(2)	66(1)
O(27A)	3229(3)	9949(5)	5007(2)	76(1)

O(27B)	4493(3)	10182(5)	6030(2)	72(1)
C(21)	3350(4)	8579(6)	6045(2)	38(1)
C(22)	3884(4)	8268(6)	6782(3)	45(2)
C(23)	3563(5)	7283(7)	7146(3)	70(2)
C(24)	2745(5)	6606(7)	6780(4)	76(2)
C(25)	2214(4)	6904(8)	6053(4)	77(2)
C(26)	2527(4)	7885(7)	5687(3)	63(2)
C(27)	3723(4)	9628(7)	5655(3)	51(2)
N(51)	-1457(4)	6287(7)	2940(3)	88(2)
C(51)	117(4)	5915(9)	4073(3)	122(3)
C(52)	-781(5)	6106(8)	3437(4)	73(2)

Table 3. Bond lengths [Å] and angles [°] for **2**.

N(31)-C(31)	1.311(5)	C(31)-N(31)-H(31B)	120.0
N(31)-H(31B)	0.8600	C(31)-N(31)-H(32B)	120.0
N(31)-H(32B)	0.8599	H(31B)-N(31)-H(32B)	120.0
N(32)-C(31)	1.334(5)	C(31)-N(32)-C(33)	120.2(4)
N(32)-C(33)	1.356(5)	C(31)-N(32)-H(32)	119.9
N(32)-H(32)	0.8600	C(33)-N(32)-H(32)	119.9
N(33)-C(33)	1.306(6)	C(33)-N(33)-H(33B)	120.0
N(33)-H(33B)	0.8599	C(33)-N(33)-H(33A)	120.0
N(33)-H(33A)	0.8601	H(33B)-N(33)-H(33A)	120.0
N(34)-C(33)	1.318(6)	C(33)-N(34)-C(35)	114.5(5)
N(34)-C(35)	1.333(6)	C(35)-N(35)-H(35A)	119.9
N(35)-C(35)	1.341(6)	C(35)-N(35)-H(35B)	120.1
N(35)-H(35A)	0.8600	H(35A)-N(35)-H(35B)	120.0
N(35)-H(35B)	0.8600	C(31)-N(36)-C(35)	113.5(5)
N(36)-C(31)	1.327(6)	C(41)-N(41)-H(41B)	119.9
N(36)-C(35)	1.354(6)	C(41)-N(41)-H(41A)	120.1
N(41)-C(41)	1.311(6)	H(41B)-N(41)-H(41A)	120.0
N(41)-H(41B)	0.8600	C(43)-N(42)-C(41)	114.8(5)
N(41)-H(41A)	0.8600	C(43)-N(43)-H(43A)	120.0
N(42)-C(43)	1.321(6)	C(43)-N(43)-H(43B)	120.0
N(42)-C(41)	1.326(6)	H(43A)-N(43)-H(43B)	120.0
N(43)-C(43)	1.327(6)	C(45)-N(44)-C(43)	112.4(5)
N(43)-H(43A)	0.8600	C(45)-N(45)-H(45B)	120.0
N(43)-H(43B)	0.8600	C(45)-N(45)-H(45A)	120.0
N(44)-C(45)	1.344(6)	H(45B)-N(45)-H(45A)	120.0
N(44)-C(43)	1.357(5)	C(41)-N(46)-C(45)	120.3(5)
N(45)-C(45)	1.333(5)	C(41)-N(46)-H(46)	119.9
N(45)-H(45B)	0.8601	C(45)-N(46)-H(46)	119.8
N(45)-H(45A)	0.8600	N(31)-C(31)-N(36)	119.7(5)
N(46)-C(41)	1.336(6)	N(31)-C(31)-N(32)	118.2(5)
N(46)-C(45)	1.346(6)	N(36)-C(31)-N(32)	122.1(4)
N(46)-H(46)	0.8600	N(33)-C(33)-N(34)	122.1(5)
O(12)-C(12)	1.358(5)	N(33)-C(33)-N(32)	116.4(5)
O(12)-H(12)	0.8201	N(34)-C(33)-N(32)	121.4(5)
O(17A)-C(17)	1.258(5)	N(34)-C(35)-N(35)	118.1(5)
O(17B)-C(17)	1.257(5)	N(34)-C(35)-N(36)	128.2(5)
C(11)-C(12)	1.382(6)	N(35)-C(35)-N(36)	113.7(5)
C(11)-C(16)	1.389(6)	N(41)-C(41)-N(42)	121.9(6)
C(11)-C(17)	1.492(7)	N(41)-C(41)-N(46)	116.6(6)
C(12)-C(13)	1.399(7)	N(42)-C(41)-N(46)	121.5(5)
C(13)-C(14)	1.355(7)	N(42)-C(43)-N(43)	116.9(5)

C(13)-H(13)	0.9300	N(42)-C(43)-N(44)	128.9(5)
C(14)-C(15)	1.355(7)	N(43)-C(43)-N(44)	114.3(5)
C(14)-H(14)	0.9300	N(45)-C(45)-N(44)	120.2(5)
C(15)-C(16)	1.380(7)	N(45)-C(45)-N(46)	117.8(5)
C(15)-H(4A)	0.9300	N(44)-C(45)-N(46)	122.1(5)
C(16)-H(15)	0.9300	C(12)-O(12)-H(12)	109.4
O(22)-C(22)	1.345(6)	C(12)-C(11)-C(16)	118.5(5)
O(22)-H(22)	0.8201	C(12)-C(11)-C(17)	120.6(5)
O(27A)-C(27)	1.233(6)	C(16)-C(11)-C(17)	120.9(5)
O(27B)-C(27)	1.245(6)	O(12)-C(12)-C(11)	122.4(5)
C(21)-C(26)	1.356(6)	O(12)-C(12)-C(13)	117.7(5)
C(21)-C(22)	1.385(6)	C(11)-C(12)-C(13)	119.9(6)
C(21)-C(27)	1.523(7)	C(14)-C(13)-C(12)	120.3(6)
C(22)-C(23)	1.395(7)	C(14)-C(13)-H(13)	119.9
C(23)-C(24)	1.345(7)	C(12)-C(13)-H(13)	119.9
C(23)-H(23)	0.9300	C(15)-C(14)-C(13)	120.4(6)
C(24)-C(25)	1.368(7)	C(15)-C(14)-H(14)	119.8
C(24)-H(24)	0.9300	C(13)-C(14)-H(14)	119.8
C(25)-C(26)	1.387(8)	C(14)-C(15)-C(16)	120.6(6)
C(25)-H(25)	0.9300	C(14)-C(15)-H(4A)	119.7
C(26)-H(26)	0.9300	C(16)-C(15)-H(4A)	119.7
N(51)-C(52)	1.128(7)	C(15)-C(16)-C(11)	120.3(6)
C(51)-C(52)	1.470(8)	C(15)-C(16)-H(15)	119.9
C(51)-H(51B)	0.9600	C(11)-C(16)-H(15)	119.9
C(51)-H(1B)	0.9600	O(17B)-C(17)-O(17A)	123.5(5)
C(51)-H(51A)	0.9600	O(17B)-C(17)-C(11)	118.3(5)
		O(17A)-C(17)-C(11)	118.2(5)
		C(22)-O(22)-H(22)	109.4
		C(26)-C(21)-C(22)	119.0(5)
		C(26)-C(21)-C(27)	122.0(5)
		C(22)-C(21)-C(27)	119.0(5)
		O(22)-C(22)-C(21)	120.9(5)
		O(22)-C(22)-C(23)	119.1(5)
		C(21)-C(22)-C(23)	119.9(6)
		C(24)-C(23)-C(22)	120.2(6)
		C(24)-C(23)-H(23)	119.9
		C(22)-C(23)-H(23)	119.9
		C(23)-C(24)-C(25)	120.3(7)
		C(23)-C(24)-H(24)	119.9
		C(25)-C(24)-H(24)	119.9
		C(24)-C(25)-C(26)	119.8(6)
		C(24)-C(25)-H(25)	120.1
		C(26)-C(25)-H(25)	120.1
		C(21)-C(26)-C(25)	120.8(6)
		C(21)-C(26)-H(26)	119.6
		C(25)-C(26)-H(26)	119.6
		O(27A)-C(27)-O(27B)	124.4(6)
		O(27A)-C(27)-C(21)	118.5(6)
		O(27B)-C(27)-C(21)	117.0(5)
		C(52)-C(51)-H(51B)	109.5
		C(52)-C(51)-H(1B)	109.5
		H(51B)-C(51)-H(1B)	109.5
		C(52)-C(51)-H(51A)	109.5
		H(51B)-C(51)-H(51A)	109.5
		H(1B)-C(51)-H(51A)	109.5
		N(51)-C(52)-C(51)	177.7(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. 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(31)	47(3)	79(4)	34(2)	7(2)	17(2)	-10(3)
N(32)	50(3)	60(3)	27(2)	9(2)	16(2)	0(3)
N(33)	69(4)	114(5)	36(3)	10(3)	10(3)	-37(4)
N(34)	50(3)	61(3)	29(2)	6(2)	12(2)	-2(3)
N(35)	65(3)	76(4)	38(2)	12(2)	26(2)	0(3)
N(36)	54(3)	50(3)	29(2)	8(2)	17(2)	6(3)
N(41)	76(4)	106(5)	49(3)	-4(3)	28(3)	-24(4)
N(42)	54(3)	54(3)	34(2)	-6(2)	22(3)	-10(3)
N(43)	66(3)	70(3)	36(2)	6(2)	25(2)	-7(3)
N(44)	48(3)	51(3)	34(2)	-1(2)	23(2)	-7(3)
N(45)	55(3)	82(4)	33(2)	9(2)	23(2)	4(3)
N(46)	51(3)	70(4)	40(3)	0(2)	25(2)	-6(3)
C(31)	24(3)	46(4)	28(3)	-7(3)	7(3)	-2(3)
C(33)	45(4)	56(4)	44(4)	16(3)	21(3)	10(4)
C(35)	51(4)	39(4)	41(3)	2(3)	27(3)	2(3)
C(41)	34(4)	66(5)	46(4)	-14(3)	12(3)	-6(4)
C(43)	45(4)	44(4)	36(3)	-9(3)	22(3)	8(3)
C(45)	32(4)	50(4)	35(3)	-12(3)	13(3)	2(3)
O(12)	62(3)	80(3)	33(2)	-6(2)	19(2)	11(3)
O(17A)	37(2)	94(3)	32(2)	-14(2)	8(2)	2(2)
O(17B)	49(3)	70(3)	38(2)	-2(2)	19(2)	16(2)
C(11)	42(4)	44(4)	32(3)	0(3)	16(3)	-5(3)
C(12)	53(4)	47(4)	38(3)	4(3)	25(3)	2(3)
C(13)	98(6)	62(5)	43(3)	-14(3)	41(4)	-16(4)
C(14)	101(6)	79(5)	69(5)	5(4)	61(5)	29(5)
C(15)	85(5)	68(5)	80(5)	6(4)	55(5)	17(4)
C(16)	77(5)	55(4)	60(4)	8(3)	42(4)	14(4)
C(17)	46(4)	45(4)	38(3)	-3(3)	22(3)	0(3)
O(22)	68(3)	89(3)	35(2)	1(2)	20(2)	4(3)
O(27A)	102(3)	94(3)	36(2)	16(2)	37(2)	15(3)
O(27B)	87(3)	77(3)	77(3)	0(2)	59(3)	-12(3)
C(21)	38(4)	44(4)	32(3)	-4(3)	17(3)	1(3)
C(22)	38(4)	53(4)	36(3)	-15(3)	12(3)	1(3)
C(23)	125(7)	57(5)	56(4)	16(4)	65(5)	18(5)
C(24)	117(6)	55(5)	85(5)	-7(4)	70(5)	-13(5)
C(25)	63(5)	88(6)	98(5)	-24(4)	53(5)	-20(4)
C(26)	62(5)	77(5)	51(4)	-25(3)	26(4)	-18(4)
C(27)	68(5)	44(4)	48(4)	-2(3)	33(4)	7(4)
N(51)	89(5)	96(5)	74(4)	4(4)	33(3)	12(4)
C(51)	96(6)	164(8)	74(5)	29(5)	13(5)	6(6)
C(52)	93(6)	71(5)	79(5)	11(5)	61(5)	8(6)

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

	x	y	z	U(eq)
H(31B)	3423	2012	7239	65
H(32B)	4075	3049	7142	65
H(32)	2081	1406	6295	56
H(33B)	437	1298	4625	94
H(33A)	755	734	5387	94
H(35A)	2415	4559	4243	70
H(35B)	3304	4935	4880	70
H(41B)	7391	8495	6856	93
H(41A)	7178	9212	6138	93
H(43A)	5253	5160	6912	68
H(43B)	4412	4831	6222	68
H(45B)	4625	8276	4094	67
H(45A)	3918	7182	4069	67
H(46)	5906	8716	5143	62
H(12)	2698	5459	2975	89
H(13)	2267	8019	3973	77
H(14)	947	9374	3588	89
H(4A)	-228	8953	2454	86
H(15)	-81	7228	1662	72
H(22)	4790	9543	6891	98
H(23)	3916	7094	7643	84
H(24)	2540	5932	7023	91
H(25)	1644	6450	5804	93
H(26)	2169	8069	5190	76
H(51B)	183	6647	4446	183
H(1B)	578	6098	3929	183
H(51A)	175	4873	4260	183

Crystallographic Information for **3**

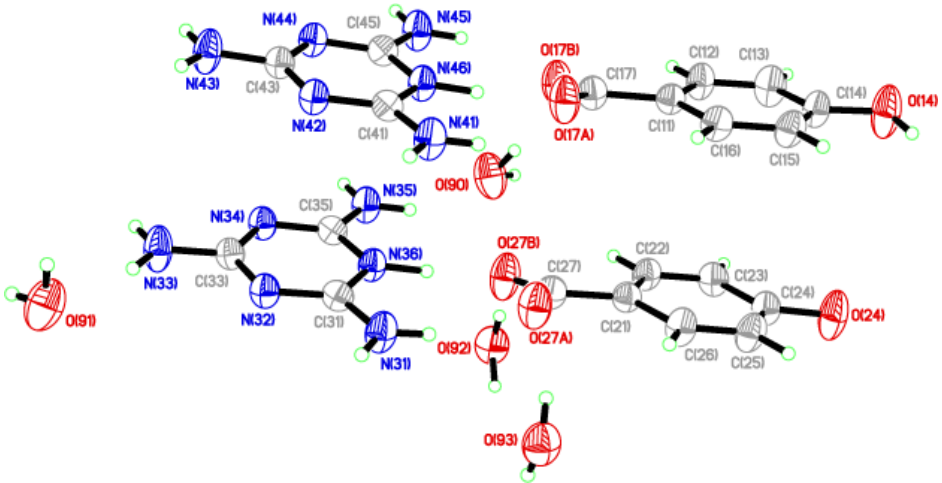


Figure 2. ORTEP drawing of the asymmetric unit of the complex **3**.

Table 1. Crystal data and structure refinement for **3**.

Identification code	**3**	
Empirical formula	$C_{10}\ H_{16}\ N_6\ O_5$	
Formula weight	300.29	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 7.571 Å	α= 87.120(5)°.
	b = 10.8570(10) Å	β= 85.510(5)°.
	c = 16.4770(10) Å	γ = 82.630(5)°.
Volume	1337.96(15) $Å^3$	
Z	4	
Density (calculated)	1.491 Mg/m^3	
Absorption coefficient	0.121 mm^{-1}	
F(000)	632	
Crystal size	0.16 x 0.11 x 0.10 mm^3	
Theta range for data collection	2.22 to 25.23°.	
Index ranges	-9<=h<=9, -13<=k<=13, -19<=l<=19	
Reflections collected	25272	
Independent reflections	4818 [R(int) = 0.0560]	
Completeness to theta = 25.23°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9880 and 0.9809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4818 / 2 / 379	
Goodness-of-fit on F^2	0.944	
Final R indices [I>2sigma(I)]	$R1$ = 0.0459, $wR2$ = 0.1032	
R indices (all data)	$R1$ = 0.0837, $wR2$ = 0.1119	
Largest diff. peak and hole	0.195 and -0.258 $e.Å^{-3}$	

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

	x	y	z	U(eq)
N(31)	3446(2)	4124(2)	954(1)	43(1)
N(32)	4256(2)	3259(2)	-289(1)	33(1)
N(33)	5145(3)	2287(2)	-1465(1)	47(1)
N(34)	6137(2)	1290(2)	-308(1)	33(1)
N(35)	6985(2)	394(2)	918(1)	39(1)
N(36)	5224(2)	2265(2)	923(1)	33(1)
C(31)	4298(3)	3225(2)	510(1)	31(1)
C(33)	5181(3)	2277(2)	-671(1)	30(1)
C(35)	6116(3)	1309(2)	496(1)	29(1)
N(41)	7951(2)	4579(2)	1065(1)	41(1)
N(42)	8847(2)	3685(2)	-157(1)	32(1)
N(43)	9901(2)	2690(2)	-1318(1)	44(1)
N(44)	10708(2)	1707(2)	-131(1)	33(1)
N(45)	11458(2)	834(2)	1117(1)	44(1)
N(46)	9675(2)	2697(2)	1082(1)	34(1)
C(41)	8825(3)	3663(2)	647(1)	30(1)
C(43)	9813(3)	2694(2)	-520(1)	31(1)
C(45)	10619(3)	1731(2)	674(1)	31(1)
O(14)	10186(2)	2647(2)	6471(1)	62(1)
O(17A)	9534(2)	3112(1)	2645(1)	49(1)
O(17B)	10456(2)	1100(1)	2819(1)	48(1)
C(11)	10019(3)	2324(2)	3985(1)	32(1)
C(12)	10792(3)	1365(2)	4479(1)	39(1)
C(13)	10829(3)	1483(2)	5302(1)	46(1)
C(14)	10081(3)	2576(2)	5656(1)	37(1)
C(15)	9287(3)	3537(2)	5175(1)	39(1)
C(16)	9262(3)	3413(2)	4354(1)	36(1)
C(17)	10006(3)	2171(2)	3093(1)	36(1)
O(24)	4989(2)	2394(2)	6330(1)	58(1)
O(27A)	4404(2)	3865(1)	2599(1)	49(1)
O(27B)	5284(2)	1847(1)	2505(1)	51(1)
C(21)	4943(3)	2667(2)	3816(1)	32(1)
C(22)	5698(3)	1579(2)	4202(1)	34(1)
C(23)	5741(3)	1471(2)	5030(1)	37(1)
C(24)	5004(3)	2445(2)	5505(1)	36(1)
C(25)	4251(3)	3538(2)	5132(1)	42(1)
C(26)	4226(3)	3647(2)	4305(1)	39(1)
C(27)	4879(3)	2794(2)	2921(1)	37(1)
O(91)	3412(2)	4246(2)	-2591(1)	60(1)
O(93)	1108(2)	5343(1)	2697(1)	50(1)
O(90)	8250(2)	-715(2)	2474(1)	59(1)
O(92)	3718(2)	-382(1)	2810(1)	50(1)

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

N(31)-C(31)	1.320(3)	C(31)-N(31)-H(31B)	120.1
N(31)-H(31B)	0.8600	C(31)-N(31)-H(31A)	119.9
N(31)-H(31A)	0.8599	H(31B)-N(31)-H(31A)	120.0
N(32)-C(31)	1.317(3)	C(31)-N(32)-C(33)	115.76(18)
N(32)-C(33)	1.353(3)	C(33)-N(33)-H(34B)	120.0
N(33)-C(33)	1.311(3)	C(33)-N(33)-H(33B)	120.0
N(33)-H(34B)	0.8600	H(34B)-N(33)-H(33B)	120.0
N(33)-H(33B)	0.8601	C(35)-N(34)-C(33)	115.31(18)
N(34)-C(35)	1.325(3)	C(35)-N(35)-H(45A)	120.0
N(34)-C(33)	1.355(3)	C(35)-N(35)-H(45B)	120.0
N(35)-C(35)	1.317(2)	H(45A)-N(35)-H(45B)	120.0
N(35)-H(45A)	0.8601	C(35)-N(36)-C(31)	118.82(18)
N(35)-H(45B)	0.8600	C(35)-N(36)-H(36)	116.8
N(36)-C(35)	1.359(3)	C(31)-N(36)-H(36)	124.2
N(36)-C(31)	1.363(3)	N(32)-C(31)-N(31)	121.7(2)
N(36)-H(36)	1.0469	N(32)-C(31)-N(36)	122.01(19)
N(41)-C(41)	1.316(3)	N(31)-C(31)-N(36)	116.3(2)
N(41)-H(41B)	0.8601	N(33)-C(33)-N(32)	116.77(19)
N(41)-H(41A)	0.8599	N(33)-C(33)-N(34)	117.29(19)
N(42)-C(41)	1.321(3)	N(32)-C(33)-N(34)	125.95(19)
N(42)-C(43)	1.358(3)	N(35)-C(35)-N(34)	120.90(19)
N(43)-C(43)	1.313(3)	N(35)-C(35)-N(36)	117.0(2)
N(43)-H(43B)	0.8601	N(34)-C(35)-N(36)	122.15(19)
N(43)-H(43A)	0.8601	C(41)-N(41)-H(41B)	120.0
N(44)-C(45)	1.324(3)	C(41)-N(41)-H(41A)	120.0
N(44)-C(43)	1.353(3)	H(41B)-N(41)-H(41A)	120.0
N(45)-C(45)	1.314(3)	C(41)-N(42)-C(43)	115.49(18)
N(45)-H(26A)	0.8601	C(43)-N(43)-H(43B)	120.1
N(45)-H(26B)	0.8600	C(43)-N(43)-H(43A)	120.0
N(46)-C(41)	1.360(3)	H(43B)-N(43)-H(43A)	120.0
N(46)-C(45)	1.366(3)	C(45)-N(44)-C(43)	115.91(18)
N(46)-H(46)	1.0203	C(45)-N(45)-H(26A)	119.9
O(14)-C(14)	1.358(2)	C(45)-N(45)-H(26B)	120.1
O(14)-H(14)	0.8973	H(26A)-N(45)-H(26B)	120.0
O(17A)-C(17)	1.261(3)	C(41)-N(46)-C(45)	118.97(18)
O(17B)-C(17)	1.265(2)	C(41)-N(46)-H(46)	116.9
C(11)-C(12)	1.387(3)	C(45)-N(46)-H(46)	124.1
C(11)-C(16)	1.392(3)	N(41)-C(41)-N(42)	121.0(2)
C(11)-C(17)	1.488(3)	N(41)-C(41)-N(46)	116.8(2)
C(12)-C(13)	1.372(3)	N(42)-C(41)-N(46)	122.21(19)
C(12)-H(12)	0.9300	N(43)-C(43)-N(44)	116.70(19)
C(13)-C(14)	1.383(3)	N(43)-C(43)-N(42)	117.51(19)
C(13)-H(13)	0.9300	N(44)-C(43)-N(42)	125.78(19)
C(14)-C(15)	1.382(3)	N(45)-C(45)-N(44)	121.4(2)
C(15)-C(16)	1.368(3)	N(45)-C(45)-N(46)	116.9(2)
C(15)-H(15)	0.9300	N(44)-C(45)-N(46)	121.63(19)
C(16)-H(16)	0.9300	C(14)-O(14)-H(14)	108.9
O(24)-C(24)	1.357(2)	C(12)-C(11)-C(16)	117.8(2)
O(24)-H(24)	0.8743	C(12)-C(11)-C(17)	120.20(19)
O(27A)-C(27)	1.273(2)	C(16)-C(11)-C(17)	122.05(19)
O(27B)-C(27)	1.256(3)	C(13)-C(12)-C(11)	121.4(2)
C(21)-C(22)	1.391(3)	C(13)-C(12)-H(12)	119.3
C(21)-C(26)	1.395(3)	C(11)-C(12)-H(12)	119.3
C(21)-C(27)	1.479(3)	C(12)-C(13)-C(14)	120.0(2)
C(22)-C(23)	1.366(3)	C(12)-C(13)-H(13)	120.0
C(22)-H(22)	0.9300	C(14)-C(13)-H(13)	120.0

C(23)-C(24)	1.381(3)	O(14)-C(14)-C(15)	123.2(2)
C(23)-H(23)	0.9300	O(14)-C(14)-C(13)	117.3(2)
C(24)-C(25)	1.385(3)	C(15)-C(14)-C(13)	119.5(2)
C(25)-C(26)	1.363(3)	C(16)-C(15)-C(14)	120.2(2)
C(25)-H(25)	0.9300	C(16)-C(15)-H(15)	119.9
C(26)-H(26)	0.9300	C(14)-C(15)-H(15)	119.9
O(91)-H(91A)	0.9548	C(15)-C(16)-C(11)	121.2(2)
O(91)-H(91B)	0.7620	C(15)-C(16)-H(16)	119.4
O(93)-H(93B)	0.8408	C(11)-C(16)-H(16)	119.4
O(93)-H(93A)	0.8678	O(17A)-C(17)-O(17B)	122.8(2)
O(90)-H(92A)	0.8459	O(17A)-C(17)-C(11)	118.66(19)
O(90)-H(90A)	0.8811	O(17B)-C(17)-C(11)	118.5(2)
O(92)-H(92B)	0.8980	C(24)-O(24)-H(24)	114.5
O(92)-H(0AA)	0.8507	C(22)-C(21)-C(26)	117.6(2)
		C(22)-C(21)-C(27)	121.94(19)
		C(26)-C(21)-C(27)	120.4(2)
		C(23)-C(22)-C(21)	121.3(2)
		C(23)-C(22)-H(22)	119.3
		C(21)-C(22)-H(22)	119.3
		C(22)-C(23)-C(24)	120.2(2)
		C(22)-C(23)-H(23)	119.9
		C(24)-C(23)-H(23)	119.9
		O(24)-C(24)-C(23)	123.2(2)
		O(24)-C(24)-C(25)	117.53(19)
		C(23)-C(24)-C(25)	119.3(2)
		C(26)-C(25)-C(24)	120.3(2)
		C(26)-C(25)-H(25)	119.8
		C(24)-C(25)-H(25)	119.8
		C(25)-C(26)-C(21)	121.2(2)
		C(25)-C(26)-H(26)	119.4
		C(21)-C(26)-H(26)	119.4
		O(27B)-C(27)-O(27A)	122.3(2)
		O(27B)-C(27)-C(21)	119.1(2)
		O(27A)-C(27)-C(21)	118.60(19)
		H(91A)-O(91)-H(91B)	107.7
		H(93B)-O(93)-H(93A)	109.7
		H(92A)-O(90)-H(90A)	99.8
		H(92B)-O(92)-H(0AA)	107.1

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. 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(31)	55(1)	36(1)	33(1)	-5(1)	-4(1)	15(1)
N(32)	40(1)	27(1)	30(1)	0(1)	-5(1)	2(1)
N(33)	71(2)	37(1)	28(1)	-3(1)	-9(1)	18(1)
N(34)	40(1)	28(1)	29(1)	0(1)	-6(1)	2(1)
N(35)	49(1)	32(1)	32(1)	-2(1)	-7(1)	8(1)
N(36)	39(1)	29(1)	28(1)	-2(1)	-3(1)	4(1)
C(31)	32(1)	27(1)	34(1)	2(1)	-5(1)	-2(1)
C(33)	35(1)	26(1)	30(1)	2(1)	-5(1)	-2(1)
C(35)	31(1)	24(1)	34(1)	0(1)	-5(1)	-3(1)

N(41)	54(1)	34(1)	33(1)	-2(1)	-6(1)	11(1)
N(42)	39(1)	28(1)	29(1)	-1(1)	-4(1)	4(1)
N(43)	63(1)	37(1)	27(1)	-2(1)	-3(1)	17(1)
N(44)	40(1)	28(1)	29(1)	-2(1)	-2(1)	2(1)
N(45)	55(1)	38(1)	33(1)	-2(1)	-10(1)	16(1)
N(46)	42(1)	32(1)	27(1)	-3(1)	-5(1)	6(1)
C(41)	31(1)	24(1)	34(1)	-2(1)	-5(1)	-2(1)
C(43)	34(1)	28(1)	30(1)	0(1)	-4(1)	-1(1)
C(45)	33(1)	25(1)	35(1)	-3(1)	-4(1)	0(1)
O(14)	98(2)	49(1)	32(1)	-5(1)	-15(1)	25(1)
O(17A)	75(1)	37(1)	33(1)	-1(1)	-13(1)	10(1)
O(17B)	68(1)	36(1)	38(1)	-10(1)	-10(1)	10(1)
C(11)	33(1)	30(1)	32(1)	-2(1)	-3(1)	2(1)
C(12)	49(2)	30(1)	34(1)	-5(1)	-6(1)	10(1)
C(13)	61(2)	34(1)	38(2)	2(1)	-11(1)	15(1)
C(14)	48(2)	33(1)	28(1)	-3(1)	-4(1)	5(1)
C(15)	47(2)	29(1)	36(2)	-5(1)	0(1)	8(1)
C(16)	41(1)	28(1)	36(1)	2(1)	-5(1)	7(1)
C(17)	40(2)	32(1)	35(1)	-4(1)	-6(1)	4(1)
O(24)	92(1)	46(1)	29(1)	-2(1)	-8(1)	20(1)
O(27A)	72(1)	37(1)	34(1)	4(1)	-9(1)	9(1)
O(27B)	82(1)	34(1)	33(1)	-4(1)	-6(1)	9(1)
C(21)	33(1)	30(1)	31(1)	-2(1)	-3(1)	-1(1)
C(22)	39(1)	27(1)	35(1)	-6(1)	-2(1)	4(1)
C(23)	44(2)	28(1)	36(2)	1(1)	-9(1)	6(1)
C(24)	43(2)	31(1)	32(1)	-1(1)	-7(1)	3(1)
C(25)	55(2)	31(1)	37(2)	-7(1)	0(1)	10(1)
C(26)	52(2)	28(1)	32(1)	1(1)	-5(1)	9(1)
C(27)	40(2)	35(1)	35(1)	-1(1)	-3(1)	0(1)
O(91)	85(1)	46(1)	47(1)	-10(1)	8(1)	-2(1)
O(93)	60(1)	40(1)	48(1)	-7(1)	-5(1)	4(1)
O(90)	87(1)	45(1)	46(1)	5(1)	-22(1)	-3(1)
O(92)	59(1)	39(1)	48(1)	1(1)	-7(1)	5(1)

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

	x	y	z	U(eq)
H(31B)	2842	4752	723	52
H(31A)	3495	4082	1474	52
H(34B)	4552	2898	-1718	57
H(33B)	5714	1682	-1734	57
H(45A)	7574	-226	672	46
H(45B)	6961	418	1440	46
H(36)	5202	2168	1559	39
H(41B)	7386	5207	816	49
H(41A)	7948	4553	1587	49
H(43B)	10507	2080	-1569	53
H(43A)	9353	3298	-1591	53
H(26A)	12082	215	883	53
H(26B)	11383	866	1639	53
H(46)	9585	2758	1700	41
H(14)	9535	3351	6638	93
H(12)	11297	626	4247	46

H(13)	11356	829	5623	55
H(15)	8769	4271	5410	46
H(16)	8729	4068	4036	43
H(24)	5499	1694	6539	87
H(22)	6184	911	3890	41
H(23)	6269	739	5275	44
H(25)	3760	4201	5448	51
H(26)	3721	4387	4063	46
H(91A)	4253	4834	-2641	91
H(91B)	3628	3811	-2944	91
H(93B)	375	4824	2692	75
H(93A)	2180	4956	2722	75
H(92A)	8443	-1270	2847	89
H(90A)	8865	-149	2636	89
H(92B)	2616	35	2872	74
H(0AA)	4448	157	2764	74

Crystallographic Information of **4**

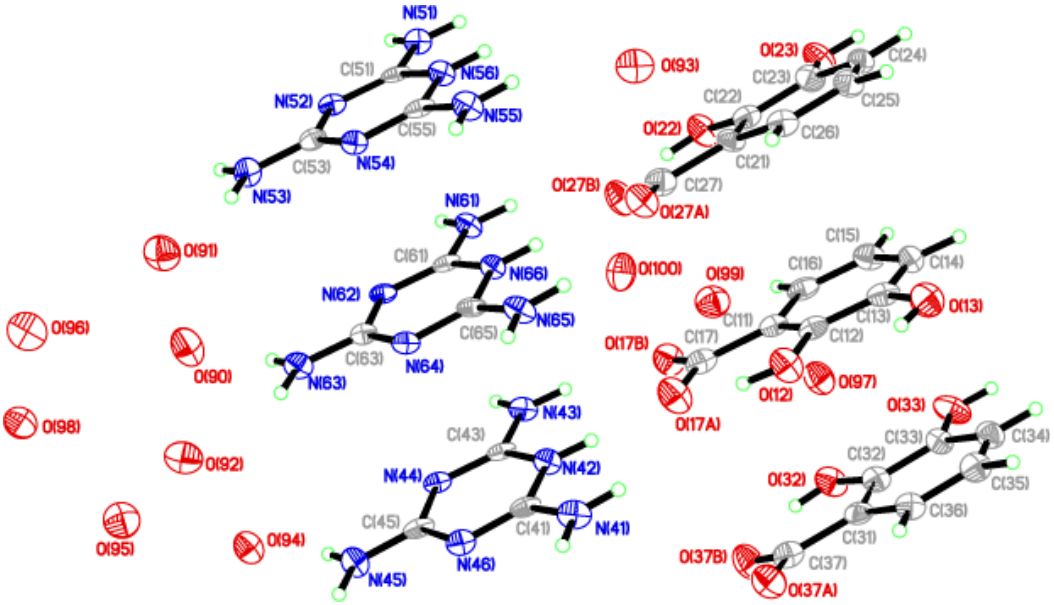


Figure 3. ORTEP drawing of the asymmetric unit of the complex **4**.

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

Identification code	**4**
Empirical formula	$C_{30}\ H_{36}\ N_{18}\ O_{23}$
Formula weight	1016.77
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$

Unit cell dimensions	a = 10.8110(10) Å	α= 82.230(4)°.
	b = 12.2980(10) Å	β= 79.120(5)°.
	c = 19.5800(10) Å	γ = 64.530(5)°.
Volume	2303.7(3) Å^3	
Z	2	
Density (calculated)	1.466 Mg/m^3	
Absorption coefficient	0.127 mm^{-1}	
F(000)	1052	
Crystal size	0.18 x 0.15 x 0.11 mm^3	
Theta range for data collection	2.15 to 25.24°.	
Index ranges	-12<=h<=12, -14<=k<=14, -23<=l<=23	
Reflections collected	43060	
Independent reflections	8323 [R(int) = 0.0794]	
Completeness to theta = 25.24°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9861 and 0.9774	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8323 / 569 / 640	
Goodness-of-fit on F^2	1.112	
Final R indices [I>2sigma(I)]	R1 = 0.0797, wR2 = 0.2058	
R indices (all data)	R1 = 0.1432, wR2 = 0.2257	
Largest diff. peak and hole	0.536 and -0.364 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(22)	6799(3)	3890(3)	1680(2)	32(1)
O(23)	7804(3)	3948(3)	353(2)	34(1)
O(27A)	6296(3)	2669(3)	2779(2)	33(1)
O(27B)	7054(3)	681(3)	2785(2)	30(1)
C(21)	7438(4)	1742(4)	1710(2)	21(1)
C(22)	7371(4)	2820(4)	1364(2)	23(1)
C(23)	7902(5)	2851(4)	658(2)	26(1)
C(24)	8496(4)	1805(4)	306(2)	25(1)
C(25)	8564(4)	710(4)	651(2)	27(1)
C(26)	8054(4)	678(4)	1344(2)	24(1)
C(27)	6897(5)	1691(4)	2463(2)	28(1)
O(32)	176(3)	4147(3)	1495(2)	32(1)
O(33)	1234(3)	4063(3)	138(2)	36(1)

O(37A)	-393(3)	3012(3)	2635(2)	36(1)
O(37B)	409(3)	1019(3)	2703(2)	34(1)
C(31)	784(4)	2000(4)	1600(2)	23(1)
C(32)	725(4)	3067(4)	1204(2)	23(1)
C(33)	1274(4)	3014(4)	510(2)	22(1)
C(34)	1868(5)	1929(4)	197(2)	27(1)
C(35)	1940(5)	876(4)	587(2)	28(1)
C(36)	1412(4)	908(4)	1267(2)	24(1)
C(37)	229(5)	2007(4)	2353(2)	26(1)
N(51)	8736(3)	4508(3)	4052(2)	21(1)
N(52)	8118(3)	3604(3)	5087(2)	19(1)
N(53)	7499(4)	2627(3)	6077(2)	23(1)
N(54)	8184(3)	1622(3)	5072(2)	19(1)
N(55)	8921(4)	712(3)	4028(2)	24(1)
N(56)	8811(3)	2609(3)	4044(2)	20(1)
C(51)	8533(4)	3586(4)	4409(2)	18(1)
C(53)	7930(4)	2626(4)	5398(2)	19(1)
C(55)	8622(4)	1642(3)	4399(2)	17(1)
N(61)	5385(3)	4409(3)	4133(2)	21(1)
N(62)	4742(3)	3553(3)	5174(2)	18(1)
N(63)	4121(4)	2610(3)	6175(2)	23(1)
N(64)	4778(3)	1576(3)	5182(2)	18(1)
N(65)	5544(3)	630(3)	4147(2)	23(1)
N(66)	5440(3)	2528(3)	4144(2)	18(1)
C(61)	5168(4)	3503(4)	4500(2)	17(1)
C(63)	4544(4)	2571(3)	5498(2)	17(1)
C(65)	5242(4)	1568(4)	4502(2)	18(1)
N(41)	2169(4)	542(3)	4245(2)	25(1)
N(42)	2058(4)	2452(3)	4214(2)	21(1)
N(43)	2043(3)	4327(3)	4176(2)	22(1)
N(44)	1365(3)	3513(3)	5228(2)	18(1)
N(45)	667(4)	2615(3)	6229(2)	24(1)
N(46)	1388(4)	1533(3)	5258(2)	20(1)
C(41)	1858(4)	1509(4)	4593(2)	20(1)
C(43)	1805(4)	3445(3)	4554(2)	18(1)
C(45)	1148(4)	2548(3)	5562(2)	18(1)
O(12)	4145(3)	579(3)	1998(2)	33(1)
O(13)	5178(3)	68(3)	671(2)	34(1)
O(17A)	3106(3)	2079(3)	2909(2)	38(1)
O(17B)	2764(3)	4012(3)	2678(2)	33(1)
C(11)	3801(4)	2657(4)	1751(2)	23(1)
C(12)	4251(4)	1491(4)	1545(2)	22(1)
C(13)	4793(4)	1230(4)	861(2)	25(1)
C(14)	4916(5)	2105(4)	379(2)	28(1)
C(15)	4494(5)	3285(4)	579(2)	29(1)
C(16)	3956(4)	3534(4)	1257(2)	25(1)
C(17)	3195(5)	2942(4)	2488(2)	28(1)
O(94)	108(3)	4474(3)	7163(2)	32(1)
O(95)	1624(3)	3065(3)	8211(2)	42(1)
O(97)	1007(4)	6169(3)	1039(2)	39(1)
O(96)	5603(4)	1829(3)	8462(2)	42(1)
O(99)	2035(4)	7511(3)	1713(2)	46(1)
O(92)	3540(3)	1162(3)	7433(2)	34(1)
O(91)	7081(3)	789(3)	7053(2)	38(1)
O(90)	3804(4)	4448(3)	7138(2)	45(1)
O(100)	3585(4)	5831(3)	2700(2)	45(1)
O(93)	9868(3)	-945(3)	2648(2)	33(1)
O(98)	3116(3)	3845(3)	8884(2)	35(1)

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

O(22)-C(22)	1.369(5)	C(22)-C(21)-C(26)	119.4(4)
O(23)-C(23)	1.368(5)	C(22)-C(21)-C(27)	120.7(4)
O(27A)-C(27)	1.277(5)	C(26)-C(21)-C(27)	119.9(4)
O(27B)-C(27)	1.271(5)	O(22)-C(22)-C(21)	123.2(4)
C(21)-C(22)	1.384(6)	O(22)-C(22)-C(23)	116.7(4)
C(21)-C(26)	1.413(6)	C(21)-C(22)-C(23)	120.1(4)
C(21)-C(27)	1.483(6)	O(23)-C(23)-C(24)	123.5(4)
C(22)-C(23)	1.395(6)	O(23)-C(23)-C(22)	116.6(4)
C(23)-C(24)	1.381(6)	C(24)-C(23)-C(22)	119.9(4)
C(24)-C(25)	1.401(6)	C(23)-C(24)-C(25)	120.5(4)
C(25)-C(26)	1.366(6)	C(26)-C(25)-C(24)	119.6(4)
O(32)-C(32)	1.356(5)	C(25)-C(26)-C(21)	120.5(4)
O(33)-C(33)	1.381(5)	O(27B)-C(27)-O(27A)	121.1(4)
O(37A)-C(37)	1.271(5)	O(27B)-C(27)-C(21)	119.9(4)
O(37B)-C(37)	1.267(5)	O(27A)-C(27)-C(21)	118.9(4)
C(31)-C(36)	1.406(6)	C(36)-C(31)-C(32)	118.4(4)
C(31)-C(32)	1.413(6)	C(36)-C(31)-C(37)	119.9(4)
C(31)-C(37)	1.483(6)	C(32)-C(31)-C(37)	121.7(4)
C(32)-C(33)	1.375(6)	O(32)-C(32)-C(33)	118.5(4)
C(33)-C(34)	1.381(6)	O(32)-C(32)-C(31)	121.8(4)
C(34)-C(35)	1.391(6)	C(33)-C(32)-C(31)	119.7(4)
C(35)-C(36)	1.344(6)	C(32)-C(33)-C(34)	120.4(4)
N(51)-C(51)	1.329(5)	C(32)-C(33)-O(33)	118.7(4)
N(52)-C(51)	1.318(5)	C(34)-C(33)-O(33)	120.9(4)
N(52)-C(53)	1.350(5)	C(33)-C(34)-C(35)	120.0(4)
N(53)-C(53)	1.324(5)	C(36)-C(35)-C(34)	120.5(4)
N(54)-C(55)	1.315(5)	C(35)-C(36)-C(31)	120.9(4)
N(54)-C(53)	1.365(5)	O(37B)-C(37)-O(37A)	121.5(4)
N(55)-C(55)	1.325(5)	O(37B)-C(37)-C(31)	119.8(4)
N(56)-C(55)	1.368(5)	O(37A)-C(37)-C(31)	118.7(4)
N(56)-C(51)	1.373(5)	C(51)-N(52)-C(53)	116.2(4)
N(61)-C(61)	1.326(5)	C(55)-N(54)-C(53)	115.9(3)
N(62)-C(61)	1.313(5)	C(55)-N(56)-C(51)	118.3(4)
N(62)-C(63)	1.368(5)	N(52)-C(51)-N(51)	121.0(4)
N(63)-C(63)	1.318(5)	N(52)-C(51)-N(56)	122.0(4)
N(64)-C(65)	1.330(5)	N(51)-C(51)-N(56)	117.0(4)
N(64)-C(63)	1.352(5)	N(53)-C(53)-N(52)	117.4(4)
N(65)-C(65)	1.315(5)	N(53)-C(53)-N(54)	117.2(4)
N(66)-C(61)	1.362(5)	N(52)-C(53)-N(54)	125.3(4)
N(66)-C(65)	1.366(5)	N(54)-C(55)-N(55)	121.4(4)
N(41)-C(41)	1.335(5)	N(54)-C(55)-N(56)	122.2(4)
N(42)-C(41)	1.366(5)	N(55)-C(55)-N(56)	116.4(4)
N(42)-C(43)	1.368(5)	C(61)-N(62)-C(63)	115.7(4)
N(43)-C(43)	1.319(5)	C(65)-N(64)-C(63)	116.3(3)
N(44)-C(43)	1.317(5)	C(61)-N(66)-C(65)	118.6(4)
N(44)-C(45)	1.364(5)	N(62)-C(61)-N(61)	120.7(4)
N(45)-C(45)	1.312(5)	N(62)-C(61)-N(66)	122.8(4)
N(46)-C(41)	1.303(5)	N(61)-C(61)-N(66)	116.4(4)
N(46)-C(45)	1.358(5)	N(63)-C(63)-N(64)	118.7(4)
O(12)-C(12)	1.364(5)	N(63)-C(63)-N(62)	116.2(4)
O(13)-C(13)	1.388(5)	N(64)-C(63)-N(62)	125.1(4)
O(17A)-C(17)	1.279(5)	N(65)-C(65)-N(64)	121.3(4)
O(17B)-C(17)	1.275(5)	N(65)-C(65)-N(66)	117.1(4)
C(11)-C(16)	1.393(6)	N(64)-C(65)-N(66)	121.5(4)
C(11)-C(12)	1.393(6)	C(41)-N(42)-C(43)	118.3(4)
C(11)-C(17)	1.489(6)	C(43)-N(44)-C(45)	116.0(4)
C(12)-C(13)	1.377(6)	C(41)-N(46)-C(45)	115.7(4)

C(13)-C(14)	1.367(6)	N(46)-C(41)-N(41)	120.9(4)
C(14)-C(15)	1.408(6)	N(46)-C(41)-N(42)	122.9(4)
C(15)-C(16)	1.364(6)	N(41)-C(41)-N(42)	116.2(4)
		N(44)-C(43)-N(43)	121.4(4)
		N(44)-C(43)-N(42)	121.8(4)
		N(43)-C(43)-N(42)	116.9(4)
		N(45)-C(45)-N(46)	117.9(4)
		N(45)-C(45)-N(44)	116.9(4)
		N(46)-C(45)-N(44)	125.2(4)
		C(16)-C(11)-C(12)	118.5(4)
		C(16)-C(11)-C(17)	121.3(4)
		C(12)-C(11)-C(17)	120.2(4)
		O(12)-C(12)-C(13)	117.6(4)
		O(12)-C(12)-C(11)	122.1(4)
		C(13)-C(12)-C(11)	120.3(4)
		C(14)-C(13)-C(12)	120.6(4)
		C(14)-C(13)-O(13)	121.0(4)
		C(12)-C(13)-O(13)	118.4(4)
		C(13)-C(14)-C(15)	120.1(4)
		C(16)-C(15)-C(14)	118.9(4)
		C(15)-C(16)-C(11)	121.7(4)
		O(17B)-C(17)-O(17A)	122.3(4)
		O(17B)-C(17)-C(11)	120.5(4)
		O(17A)-C(17)-C(11)	117.2(4)

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(22)	38(2)	21(2)	31(2)	-5(1)	5(2)	-10(2)
O(23)	40(2)	26(2)	31(2)	-2(2)	7(2)	-13(2)
O(27A)	41(2)	24(2)	27(2)	-9(1)	5(2)	-11(2)
O(27B)	36(2)	23(2)	31(2)	-3(1)	2(2)	-13(2)
C(21)	15(2)	19(2)	26(2)	-6(2)	3(2)	-5(2)
C(22)	18(3)	19(2)	33(3)	-4(2)	-5(2)	-7(2)
C(23)	22(3)	21(2)	29(3)	-1(2)	-2(2)	-5(2)
C(24)	17(3)	31(3)	23(2)	-4(2)	-1(2)	-6(2)
C(25)	17(3)	25(3)	30(3)	-6(2)	-1(2)	-1(2)
C(26)	20(3)	16(2)	32(3)	1(2)	-5(2)	-5(2)
C(27)	26(3)	25(3)	33(3)	-2(2)	-3(2)	-12(2)
O(32)	31(2)	20(2)	38(2)	-9(2)	6(2)	-7(2)
O(33)	30(2)	28(2)	40(2)	6(2)	6(2)	-9(2)
O(37A)	45(2)	30(2)	31(2)	-7(2)	4(2)	-14(2)
O(37B)	37(2)	28(2)	34(2)	2(2)	-2(2)	-13(2)
C(31)	12(2)	25(2)	28(2)	-1(2)	-6(2)	-5(2)
C(32)	14(2)	15(2)	33(3)	-7(2)	-1(2)	2(2)
C(33)	20(3)	18(2)	23(2)	2(2)	-3(2)	-4(2)
C(34)	22(3)	31(3)	26(3)	-2(2)	-2(2)	-8(2)
C(35)	22(3)	21(2)	35(3)	-6(2)	-3(2)	-4(2)
C(36)	21(3)	19(2)	30(3)	-1(2)	-3(2)	-6(2)
C(37)	22(3)	17(2)	38(3)	-7(2)	-3(2)	-7(2)
N(51)	23(2)	12(2)	28(2)	-3(2)	-3(2)	-6(2)
N(52)	14(2)	12(2)	28(2)	-3(2)	-3(2)	-4(2)
N(53)	32(2)	15(2)	26(2)	-1(2)	-4(2)	-14(2)

N(54)	19(2)	14(2)	23(2)	-3(2)	-1(2)	-8(2)
N(55)	29(2)	16(2)	29(2)	-6(2)	2(2)	-11(2)
N(56)	23(2)	13(2)	25(2)	-7(2)	2(2)	-9(2)
C(51)	7(2)	11(2)	34(3)	-4(2)	-4(2)	-2(2)
C(53)	14(2)	13(2)	27(2)	0(2)	-6(2)	-3(2)
C(55)	11(2)	7(2)	34(3)	-2(2)	-5(2)	-4(2)
N(61)	22(2)	13(2)	24(2)	-4(2)	3(2)	-6(2)
N(62)	12(2)	14(2)	26(2)	-2(2)	-2(2)	-4(2)
N(63)	29(2)	16(2)	28(2)	-4(2)	0(2)	-14(2)
N(64)	16(2)	13(2)	26(2)	-4(2)	0(2)	-6(2)
N(65)	25(2)	12(2)	28(2)	-2(2)	4(2)	-8(2)
N(66)	21(2)	13(2)	21(2)	-2(2)	0(2)	-9(2)
C(61)	10(2)	12(2)	29(3)	-1(2)	-6(2)	-4(2)
C(63)	13(2)	10(2)	25(2)	2(2)	-5(2)	-2(2)
C(65)	11(2)	12(2)	29(3)	-1(2)	-1(2)	-4(2)
N(41)	24(2)	13(2)	36(2)	-5(2)	1(2)	-6(2)
N(42)	23(2)	13(2)	26(2)	-4(2)	0(2)	-8(2)
N(43)	21(2)	13(2)	31(2)	-8(2)	3(2)	-7(2)
N(44)	14(2)	12(2)	29(2)	-5(2)	-2(2)	-4(2)
N(45)	39(2)	15(2)	24(2)	-5(2)	1(2)	-17(2)
N(46)	20(2)	12(2)	29(2)	-4(2)	-3(2)	-5(2)
C(41)	10(2)	13(2)	35(3)	-5(2)	-4(2)	-2(2)
C(43)	10(2)	10(2)	33(3)	-4(2)	-4(2)	-4(2)
C(45)	9(2)	6(2)	37(3)	-3(2)	-6(2)	1(2)
O(12)	38(2)	26(2)	31(2)	-3(2)	0(2)	-12(2)
O(13)	32(2)	29(2)	36(2)	-5(2)	-2(2)	-8(2)
O(17A)	47(2)	29(2)	34(2)	-5(2)	4(2)	-16(2)
O(17B)	36(2)	24(2)	36(2)	-9(2)	1(2)	-11(2)
C(11)	18(3)	25(2)	30(2)	-2(2)	-5(2)	-11(2)
C(12)	20(3)	20(2)	30(2)	3(2)	-8(2)	-10(2)
C(13)	18(3)	18(2)	39(3)	-2(2)	-4(2)	-8(2)
C(14)	25(3)	39(3)	21(2)	-3(2)	-2(2)	-13(2)
C(15)	26(3)	23(3)	36(3)	-3(2)	0(2)	-12(2)
C(16)	19(3)	16(2)	41(3)	1(2)	-8(2)	-8(2)
C(17)	21(3)	25(3)	40(3)	-5(2)	-6(2)	-10(2)
O(94)	41(2)	24(2)	30(2)	-7(1)	2(2)	-14(2)
O(95)	34(2)	35(2)	45(2)	-6(2)	-3(2)	-5(2)
O(97)	48(2)	33(2)	35(2)	-3(2)	2(2)	-18(2)
O(96)	46(2)	27(2)	49(2)	-5(2)	-2(2)	-13(2)
O(99)	37(2)	41(2)	53(2)	-6(2)	-5(2)	-10(2)
O(92)	33(2)	24(2)	44(2)	1(2)	-2(2)	-12(2)
O(91)	44(2)	33(2)	39(2)	4(2)	-5(2)	-21(2)
O(90)	69(3)	42(2)	34(2)	-6(2)	2(2)	-34(2)
O(100)	56(3)	42(2)	40(2)	-9(2)	-11(2)	-20(2)
O(93)	32(2)	25(2)	41(2)	-2(2)	-4(2)	-11(2)
O(98)	34(2)	30(2)	36(2)	-6(2)	1(2)	-11(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(22)	6501	3778	2100	47
H(23)	8155	3873	-68	52
H(24A)	8861	1827	-174	30

H(25A)	8962	-6	405	32
H(26A)	8114	-66	1581	29
H(32)	-124	4062	1918	48
H(33)	1611	3910	-275	54
H(34A)	2227	1901	-285	33
H(35A)	2365	129	371	33
H(36A)	1465	182	1526	29
H(51A)	8593	5144	4268	25
H(51B)	9013	4484	3600	25
H(53A)	7346	3250	6308	27
H(53B)	7365	2005	6298	27
H(55A)	8828	63	4233	29
H(55B)	9213	743	3578	29
H(56)	9103	2606	3592	24
H(61A)	5244	5052	4340	25
H(61B)	5670	4366	3681	25
H(63A)	3996	1995	6412	27
H(63B)	3963	3251	6390	27
H(65A)	5440	-10	4359	27
H(65B)	5850	642	3698	27
H(66)	5736	2517	3694	22
H(41A)	2056	-91	4464	30
H(41B)	2485	537	3797	30
H(42)	2342	2422	3762	25
H(43A)	1909	4977	4374	26
H(43B)	2337	4264	3726	26
H(45A)	510	2014	6465	29
H(45B)	501	3262	6441	29
H(12)	3802	838	2397	49
H(13)	5036	-359	1024	51
H(14A)	5286	1917	-92	34
H(15A)	4583	3896	247	34
H(16A)	3679	4326	1395	30

Crystallographic Information of **5**

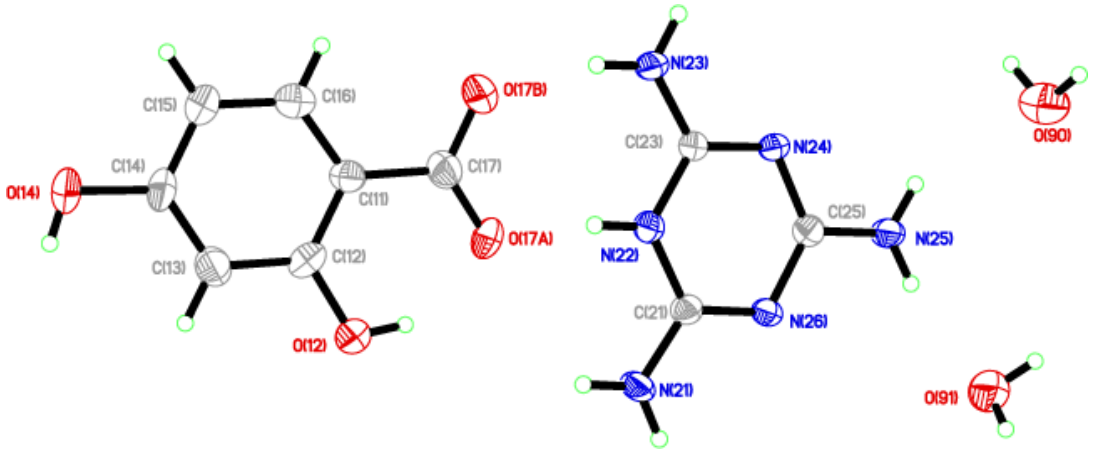


Figure 4. ORTEP drawing of the asymmetric unit of the complex **5**.

Table 1. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	$C_{10}\ H_{16}\ N_6\ O_6$	
Formula weight	316.29	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.7880(10) Å	α= 90°.
	b = 12.1600(10) Å	β= 96.560(5)°.
	c = 7.161 Å	γ = 90°.
Volume	1365.78(14) Å^3	
Z	4	
Density (calculated)	1.538 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	664	
Crystal size	0.14 x 0.13 x 0.08 mm^3	
Theta range for data collection	2.12 to 25.10°.	
Index ranges	-18<=h<=18, -14<=k<=13, -8<=l<=8	
Reflections collected	13382	
Independent reflections	2437 [R(int) = 0.0556]	
Completeness to theta = 25.10°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9898 and 0.9823	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2437 / 2 / 223	
Goodness-of-fit on F^2	0.900	
Final R indices [I>2sigma(I)]	R1 = 0.0659, wR2 = 0.1608	
R indices (all data)	R1 = 0.1108, wR2 = 0.1773	
Largest diff. peak and hole	0.818 and -0.224 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(21)	920(2)	4346(2)	4135(4)	33(1)
N(22)	861(2)	2468(2)	4268(4)	24(1)
N(23)	874(2)	589(2)	4183(4)	29(1)
N(24)	-298(2)	1492(2)	2744(4)	23(1)
N(25)	-1441(2)	2501(2)	1476(4)	31(1)
N(26)	-279(2)	3475(2)	2716(4)	23(1)
C(21)	486(2)	3437(2)	3685(5)	22(1)
C(23)	468(2)	1510(2)	3711(4)	20(1)
C(25)	-657(2)	2487(2)	2338(4)	22(1)
O(12)	3649(2)	3962(2)	2417(4)	45(1)
O(14)	6292(2)	2241(2)	4488(5)	52(1)
O(17A)	2401(2)	2722(2)	1179(4)	41(1)
O(17B)	2503(2)	914(2)	1447(4)	46(1)
C(11)	3739(2)	1984(3)	2406(5)	29(1)
C(12)	4097(2)	3025(3)	2742(5)	31(1)
C(13)	4957(2)	3123(3)	3469(5)	36(1)
C(14)	5442(2)	2203(3)	3804(5)	34(1)
C(15)	5097(2)	1161(3)	3449(5)	39(1)
C(16)	4251(2)	1076(3)	2761(5)	39(1)
C(17)	2827(2)	1872(3)	1633(5)	35(1)
O(90)	-2931(2)	860(3)	653(5)	59(1)
O(91)	-2510(2)	4443(3)	501(5)	55(1)

Table 3. Bond lengths [Å] and angles [°] for **5**.

N(21)-C(21)	1.320(4)	C(21)-N(21)-H(21A)	120.0
N(21)-H(21A)	0.8600	C(21)-N(21)-H(21B)	120.0
N(21)-H(21B)	0.8600	H(21A)-N(21)-H(21B)	120.0
N(22)-C(23)	1.359(4)	C(23)-N(22)-C(21)	118.9(3)
N(22)-C(21)	1.362(4)	C(23)-N(22)-H(22)	120(3)
N(22)-H(22)	0.85(5)	C(21)-N(22)-H(22)	121(3)
N(23)-C(23)	1.315(4)	C(23)-N(23)-H(23B)	120.0
N(23)-H(23B)	0.8600	C(23)-N(23)-H(23A)	120.0
N(23)-H(23A)	0.8600	H(23B)-N(23)-H(23A)	120.0
N(24)-C(23)	1.323(4)	C(23)-N(24)-C(25)	115.7(3)
N(24)-C(25)	1.354(4)	C(25)-N(25)-H(25A)	120.0
N(25)-C(25)	1.318(4)	C(25)-N(25)-H(25B)	120.0
N(25)-H(25A)	0.8600	H(25A)-N(25)-H(25B)	120.0
N(25)-H(25B)	0.8600	C(21)-N(26)-C(25)	115.4(3)
N(26)-C(21)	1.324(4)	N(21)-C(21)-N(26)	121.0(3)
N(26)-C(25)	1.356(4)	N(21)-C(21)-N(22)	117.0(3)
O(12)-C(12)	1.347(4)	N(26)-C(21)-N(22)	122.0(3)
O(12)-H(12)	0.8200	N(23)-C(23)-N(24)	120.7(3)
O(14)-C(14)	1.376(4)	N(23)-C(23)-N(22)	117.5(3)
O(14)-H(14)	0.81(3)	N(24)-C(23)-N(22)	121.8(3)
O(17A)-C(17)	1.256(4)	N(25)-C(25)-N(24)	117.4(3)
O(17B)-C(17)	1.273(4)	N(25)-C(25)-N(26)	116.8(3)
C(11)-C(16)	1.375(5)	N(24)-C(25)-N(26)	125.8(3)
C(11)-C(12)	1.396(5)	C(12)-O(12)-H(12)	109.5

C(11)-C(17)	1.489(5)	C(14)-O(14)-H(14)	108(2)
C(12)-C(13)	1.403(5)	C(16)-C(11)-C(12)	118.6(3)
C(13)-C(14)	1.361(5)	C(16)-C(11)-C(17)	121.2(3)
C(13)-H(13)	0.9300	C(12)-C(11)-C(17)	120.2(3)
C(14)-C(15)	1.392(5)	O(12)-C(12)-C(11)	122.9(3)
C(15)-C(16)	1.373(5)	O(12)-C(12)-C(13)	117.3(3)
C(15)-H(15)	0.9300	C(11)-C(12)-C(13)	119.8(3)
C(16)-H(16)	0.9300	C(14)-C(13)-C(12)	119.8(3)
O(90)-H(90A)	0.800(18)	C(14)-C(13)-H(13)	120.1
O(90)-H(90B)	0.814(19)	C(12)-C(13)-H(13)	120.1
O(91)-H(91B)	0.83(3)	C(13)-C(14)-O(14)	122.8(3)
O(91)-H(914)	0.89(5)	C(13)-C(14)-C(15)	121.1(3)
		O(14)-C(14)-C(15)	116.2(3)
		C(16)-C(15)-C(14)	118.5(3)
		C(16)-C(15)-H(15)	120.7
		C(14)-C(15)-H(15)	120.7
		C(15)-C(16)-C(11)	122.3(3)
		C(15)-C(16)-H(16)	118.9
		C(11)-C(16)-H(16)	118.9
		O(17A)-C(17)-O(17B)	122.0(3)
		O(17A)-C(17)-C(11)	119.1(3)
		O(17B)-C(17)-C(11)	118.9(3)
		H(90A)-O(90)-H(90B)	97(4)
		H(91B)-O(91)-H(914)	97(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. 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)	25(2)	18(1)	51(2)	1(1)	-14(1)	-4(1)
N(22)	20(2)	21(1)	30(2)	3(1)	-4(1)	0(1)
N(23)	23(2)	17(1)	46(2)	1(1)	-7(1)	1(1)
N(24)	21(2)	16(1)	31(2)	0(1)	-1(1)	2(1)
N(25)	23(2)	19(1)	47(2)	0(1)	-12(1)	1(1)
N(26)	21(2)	17(1)	31(2)	1(1)	-3(1)	-1(1)
C(21)	23(2)	19(2)	24(2)	2(1)	-1(2)	1(1)
C(23)	19(2)	18(2)	24(2)	1(1)	2(1)	0(1)
C(25)	23(2)	23(2)	20(2)	-2(2)	1(1)	0(1)
O(12)	32(2)	29(1)	71(2)	-1(1)	-8(1)	3(1)
O(14)	22(2)	47(2)	84(2)	6(2)	-12(1)	1(1)
O(17A)	26(1)	41(2)	52(2)	5(1)	-10(1)	8(1)
O(17B)	32(2)	36(2)	67(2)	2(1)	-8(1)	-7(1)
C(11)	32(2)	24(2)	30(2)	1(2)	3(2)	-1(2)
C(12)	33(2)	30(2)	31(2)	2(2)	4(2)	10(2)
C(13)	32(2)	35(2)	38(2)	3(2)	-1(2)	-5(2)
C(14)	21(2)	43(2)	36(2)	4(2)	-3(2)	4(2)
C(15)	29(2)	37(2)	48(3)	3(2)	-2(2)	5(2)
C(16)	41(2)	28(2)	46(3)	1(2)	2(2)	-1(2)
C(17)	31(2)	35(2)	37(2)	-5(2)	0(2)	-4(2)
O(90)	63(2)	39(2)	77(3)	6(2)	15(2)	-1(2)
O(91)	37(2)	43(2)	83(3)	-10(2)	-1(2)	2(2)

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

	x	y	z	U(eq)
H(21A)	707	4975	3797	39
H(21B)	1417	4308	4765	39
H(23B)	642	-33	3864	35
H(23A)	1371	610	4812	35
H(25A)	-1703	1893	1193	37
H(25B)	-1689	3118	1195	37
H(22)	1350(30)	2450(30)	4910(60)	64(14)
H(12)	3162	3814	1963	67
H(13)	5195	3814	3722	43
H(15)	5432	535	3673	46
H(16)	4017	381	2528	46
H(14)	6410(20)	2870(20)	4770(40)	10(9)
H(90A)	-2630(20)	370(20)	360(50)	36(12)
H(90B)	-3170(30)	520(40)	1420(60)	90(20)
H(91B)	-2940(20)	4050(20)	490(40)	7(8)
H(914)	-2600(30)	4840(40)	1500(70)	90(20)

Crystallographic Information of **6**

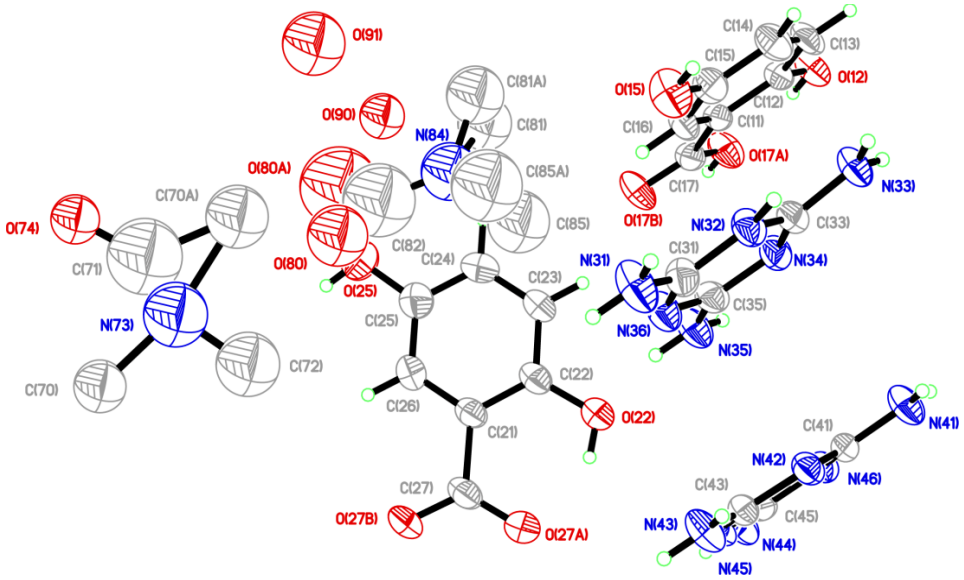


Figure 5. ORTEP drawing of the asymmetric unit of the complex **6**.

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

Identification code	**6**	
Empirical formula	$C_{26}\ H_{24}\ N_{14}\ O_{12}$	
Formula weight	724.59	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C* 2/*c*	
Unit cell dimensions	*a* = 38.011(5) Å	α= 90°.
	b = 9.212(5) Å	β= 99.440(5)°.
	c = 20.430(5) Å	γ = 90°.
Volume	7057(4) Å^3	
Z	8	
Density (calculated)	1.364 Mg/m^3	
Absorption coefficient	0.111 mm^{-1}	
F(000)	2992	
Crystal size	0.17 x 0.14 x 0.09 mm^3	
Theta range for data collection	2.13 to 25.24°.	
Index ranges	-45<=h<=45, -11<=k<=11, -24<=l<=24	
Reflections collected	34754	
Independent reflections	6376 [R(int) = 0.0515]	
Completeness to theta = 25.24°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9901 and 0.9814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6376 / 0 / 429	
Goodness-of-fit on F^2	1.049	
Final *R* indices [I>2sigma(I)]	*R*1 = 0.0929, *wR*2 = 0.2892	
R indices (all data)	*R*1 = 0.1533, *wR*2 = 0.3227	
Largest diff. peak and hole	1.163 and -0.592 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(80)	5002(3)	7059(14)	4042(6)	116(4)
O(80A)	5011(7)	5880(30)	3837(11)	204(10)
N(84)	5438(2)	6583(8)	3433(3)	106(2)
C(81)	5625(5)	5278(19)	3213(10)	99(6)
C(81A)	5510(5)	5480(20)	2913(10)	110(6)
C(82)	5188(5)	6297(19)	3839(8)	173(6)
C(85)	5748(5)	7690(20)	3598(10)	123(6)
C(85A)	5499(6)	8080(30)	3201(12)	155(8)
O(12)	7388(1)	3030(3)	2747(2)	46(1)
O(15)	6276(1)	6948(4)	2402(2)	61(1)
O(17A)	7208(1)	2338(4)	3826(2)	52(1)
O(17B)	6730(1)	3264(4)	4159(2)	56(1)
C(11)	6880(1)	4098(5)	3143(2)	34(1)
C(12)	7110(1)	3986(5)	2677(2)	35(1)
C(13)	7059(1)	4879(5)	2118(2)	45(1)
C(14)	6782(1)	5864(5)	2018(2)	44(1)
C(15)	6556(1)	5977(5)	2477(2)	44(1)
C(16)	6608(1)	5095(5)	3040(2)	40(1)
C(17)	6933(1)	3197(5)	3756(2)	37(1)
O(91)	4853(2)	2882(7)	3101(3)	141(2)
O(74)	3755(1)	8606(4)	3742(2)	66(1)
N(73)	4233(2)	9910(8)	4199(4)	113(2)
C(70)	4004(3)	10278(14)	4810(6)	75(4)
C(70A)	4382(4)	9282(18)	3426(8)	108(5)
C(71)	4061(3)	9228(14)	3868(6)	157(4)
C(72)	4564(2)	10602(9)	4418(4)	112(3)
O(22)	6623(1)	6873(4)	5692(2)	51(1)
O(25)	5444(1)	3322(5)	5170(2)	87(1)
O(27A)	6387(1)	7832(4)	6703(2)	51(1)
O(27B)	5869(1)	7085(4)	6955(2)	58(1)
C(21)	6070(1)	6054(5)	6007(2)	38(1)
C(22)	6325(1)	6023(5)	5589(2)	40(1)
C(23)	6281(1)	5113(6)	5047(2)	48(1)
C(24)	5987(2)	4223(6)	4915(3)	60(2)
C(25)	5732(2)	4236(6)	5324(3)	58(2)
C(26)	5771(1)	5152(6)	5866(2)	50(1)
C(27)	6110(1)	7053(5)	6603(2)	44(1)
N(31)	6005(1)	11416(5)	3215(2)	56(1)
N(32)	6487(1)	10536(4)	2801(2)	38(1)
N(33)	6956(1)	9641(4)	2352(2)	44(1)
N(34)	6881(1)	8873(4)	3393(2)	37(1)
N(35)	6759(1)	8105(4)	4387(2)	47(1)
N(36)	6373(1)	9758(4)	3834(2)	41(1)
C(31)	6289(1)	10561(5)	3303(2)	40(1)
C(33)	6776(1)	9672(5)	2861(2)	35(1)
C(35)	6668(1)	8948(5)	3857(2)	36(1)
O(90)	5410(1)	1593(4)	4011(2)	80(1)
N(41)	7725(1)	9955(5)	4512(2)	48(1)
N(42)	7619(1)	8970(4)	5501(2)	35(1)
N(43)	7485(1)	8120(4)	6471(2)	43(1)
N(44)	7120(1)	9908(4)	5963(2)	38(1)
N(45)	6788(1)	11741(4)	5402(2)	51(1)

N(46)	7261(1)	10853(4)	4976(2)	36(1)
C(41)	7536(1)	9903(5)	5009(2)	34(1)
C(43)	7403(1)	9028(5)	5968(2)	34(1)
C(45)	7055(1)	10805(5)	5458(2)	34(1)

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

O(80)-C(82)	1.123(18)	C(82)-O(80)-O(80A)	39.4(14)
O(80)-O(80A)	1.17(2)	C(82)-O(80A)-O(80)	67(2)
O(80A)-C(82)	0.77(3)	C(82)-N(84)-C(85A)	121.7(13)
N(84)-C(82)	1.385(17)	C(82)-N(84)-C(81)	115.5(11)
N(84)-C(85A)	1.49(2)	C(85A)-N(84)-C(81)	122.7(13)
N(84)-C(81)	1.502(19)	C(82)-N(84)-C(81A)	120.5(12)
N(84)-C(81A)	1.53(2)	C(85A)-N(84)-C(81A)	110.0(13)
N(84)-C(85)	1.551(19)	C(81)-N(84)-C(81A)	27.3(9)
C(81)-C(81A)	0.71(2)	C(82)-N(84)-C(85)	124.5(12)
C(85)-C(85A)	1.20(3)	C(85A)-N(84)-C(85)	46.3(10)
O(12)-C(12)	1.363(5)	C(81)-N(84)-C(85)	102.2(10)
O(12)-H(12)	0.8200	C(81A)-N(84)-C(85)	111.9(11)
O(15)-C(15)	1.379(6)	C(81A)-C(81)-N(84)	78(3)
O(15)-H(15)	0.8200	C(81)-C(81A)-N(84)	74(2)
O(17A)-C(17)	1.299(5)	O(80A)-C(82)-O(80)	73(3)
O(17A)-H(17A)	0.8200	O(80A)-C(82)-N(84)	141(3)
O(17B)-C(17)	1.220(5)	O(80)-C(82)-N(84)	129.6(18)
C(11)-C(16)	1.373(6)	C(85A)-C(85)-N(84)	64.2(15)
C(11)-C(12)	1.398(6)	C(85)-C(85A)-N(84)	69.6(15)
C(11)-C(17)	1.489(6)	C(12)-O(12)-H(12)	109.5
C(12)-C(13)	1.394(6)	C(15)-O(15)-H(15)	109.5
C(13)-C(14)	1.380(7)	C(17)-O(17A)-H(17A)	109.5
C(13)-H(13)	0.9300	C(16)-C(11)-C(12)	118.9(4)
C(14)-C(15)	1.374(6)	C(16)-C(11)-C(17)	119.8(4)
C(14)-H(14)	0.9300	C(12)-C(11)-C(17)	121.3(4)
C(15)-C(16)	1.396(6)	O(12)-C(12)-C(13)	118.0(4)
C(16)-H(16)	0.9300	O(12)-C(12)-C(11)	122.4(4)
O(74)-C(71)	1.285(13)	C(13)-C(12)-C(11)	119.6(4)
N(73)-C(71)	1.066(12)	C(14)-C(13)-C(12)	120.8(4)
N(73)-C(72)	1.414(10)	C(14)-C(13)-H(13)	119.6
N(73)-C(70)	1.672(14)	C(12)-C(13)-H(13)	119.6
N(73)-C(70A)	1.854(18)	C(15)-C(14)-C(13)	119.6(4)
C(70A)-C(71)	1.635(18)	C(15)-C(14)-H(14)	120.2
O(22)-C(22)	1.366(6)	C(13)-C(14)-H(14)	120.2
O(22)-H(22)	0.8200	C(14)-C(15)-O(15)	122.0(4)
O(25)-C(25)	1.377(6)	C(14)-C(15)-C(16)	119.8(5)
O(25)-H(25)	0.8200	O(15)-C(15)-C(16)	118.1(4)
O(27A)-C(27)	1.263(6)	C(11)-C(16)-C(15)	121.2(4)
O(27B)-C(27)	1.254(5)	C(11)-C(16)-H(16)	119.4
C(21)-C(22)	1.390(6)	C(15)-C(16)-H(16)	119.4
C(21)-C(26)	1.400(7)	O(17B)-C(17)-O(17A)	123.0(4)
C(21)-C(27)	1.514(6)	O(17B)-C(17)-C(11)	121.7(4)
C(22)-C(23)	1.378(6)	O(17A)-C(17)-C(11)	115.3(4)
C(23)-C(24)	1.375(7)	C(71)-N(73)-C(72)	152.7(11)
C(23)-H(23)	0.9300	C(71)-N(73)-C(70)	104.5(10)
C(24)-C(25)	1.380(7)	C(72)-N(73)-C(70)	102.6(8)
C(24)-H(24)	0.9300	C(71)-N(73)-C(70A)	61.2(9)
C(25)-C(26)	1.382(7)	C(72)-N(73)-C(70A)	91.8(7)
C(26)-H(26)	0.9300	C(70)-N(73)-C(70A)	165.6(9)

N(31)-C(31)	1.323(6)	C(71)-C(70A)-N(73)	34.9(6)
N(31)-H(31A)	0.8600	N(73)-C(71)-O(74)	146.5(13)
N(31)-H(31B)	0.8600	N(73)-C(71)-C(70A)	83.9(11)
N(32)-C(33)	1.346(6)	O(74)-C(71)-C(70A)	129.6(12)
N(32)-C(31)	1.369(6)	C(22)-O(22)-H(22)	109.5
N(32)-H(32)	1.01(6)	C(25)-O(25)-H(25)	109.5
N(33)-C(33)	1.337(5)	C(22)-C(21)-C(26)	119.0(4)
N(33)-H(33B)	0.8600	C(22)-C(21)-C(27)	121.2(4)
N(33)-H(33A)	0.8600	C(26)-C(21)-C(27)	119.7(4)
N(34)-C(33)	1.318(5)	O(22)-C(22)-C(23)	117.4(4)
N(34)-C(35)	1.346(5)	O(22)-C(22)-C(21)	122.5(4)
N(35)-C(35)	1.331(5)	C(23)-C(22)-C(21)	120.1(5)
N(35)-H(35B)	0.8600	C(24)-C(23)-C(22)	120.5(5)
N(35)-H(5B)	0.8600	C(24)-C(23)-H(23)	119.8
N(36)-C(31)	1.308(6)	C(22)-C(23)-H(23)	119.8
N(36)-C(35)	1.341(6)	C(23)-C(24)-C(25)	120.2(5)
N(41)-C(41)	1.337(5)	C(23)-C(24)-H(24)	119.9
N(41)-H(41B)	0.8600	C(25)-C(24)-H(24)	119.9
N(41)-H(41A)	0.8600	O(25)-C(25)-C(24)	118.0(5)
N(42)-C(41)	1.321(5)	O(25)-C(25)-C(26)	122.1(5)
N(42)-C(43)	1.357(5)	C(24)-C(25)-C(26)	119.9(5)
N(43)-C(43)	1.322(5)	C(25)-C(26)-C(21)	120.2(5)
N(43)-H(43B)	0.8600	C(25)-C(26)-H(26)	119.9
N(43)-H(43A)	0.8600	C(21)-C(26)-H(26)	119.9
N(44)-C(45)	1.314(5)	O(27B)-C(27)-O(27A)	124.2(4)
N(44)-C(43)	1.345(6)	O(27B)-C(27)-C(21)	119.3(5)
N(45)-C(45)	1.322(6)	O(27A)-C(27)-C(21)	116.4(4)
N(45)-H(45A)	0.8600	C(31)-N(31)-H(31A)	120.0
N(45)-H(45B)	0.8600	C(31)-N(31)-H(31B)	120.0
N(46)-C(41)	1.354(6)	H(31A)-N(31)-H(31B)	120.0
N(46)-C(45)	1.357(5)	C(33)-N(32)-C(31)	118.8(4)
		C(33)-N(32)-H(32)	113(4)
		C(31)-N(32)-H(32)	128(4)
		C(33)-N(33)-H(33B)	120.0
		C(33)-N(33)-H(33A)	120.0
		H(33B)-N(33)-H(33A)	120.0
		C(33)-N(34)-C(35)	114.7(4)
		C(35)-N(35)-H(35B)	120.0
		C(35)-N(35)-H(5B)	120.0
		H(35B)-N(35)-H(5B)	120.0
		C(31)-N(36)-C(35)	115.7(4)
		N(36)-C(31)-N(31)	122.2(4)
		N(36)-C(31)-N(32)	121.5(4)
		N(31)-C(31)-N(32)	116.4(4)
		N(34)-C(33)-N(33)	120.4(4)
		N(34)-C(33)-N(32)	122.5(4)
		N(33)-C(33)-N(32)	117.1(4)
		N(35)-C(35)-N(36)	117.4(4)
		N(35)-C(35)-N(34)	115.9(4)
		N(36)-C(35)-N(34)	126.7(4)
		C(41)-N(41)-H(41B)	120.0
		C(41)-N(41)-H(41A)	120.0
		H(41B)-N(41)-H(41A)	120.0
		C(41)-N(42)-C(43)	114.4(4)
		C(43)-N(43)-H(43B)	120.0
		C(43)-N(43)-H(43A)	120.0
		H(43B)-N(43)-H(43A)	120.0
		C(45)-N(44)-C(43)	115.6(4)
		C(45)-N(45)-H(45A)	120.0
		C(45)-N(45)-H(45B)	120.0

	H(45A)-N(45)-H(45B)	120.0
	C(41)-N(46)-C(45)	118.4(4)
	N(42)-C(41)-N(41)	120.7(4)
	N(42)-C(41)-N(46)	122.9(4)
	N(41)-C(41)-N(46)	116.4(4)
	N(43)-C(43)-N(44)	118.2(4)
	N(43)-C(43)-N(42)	115.5(4)
	N(44)-C(43)-N(42)	126.3(4)
	N(44)-C(45)-N(45)	121.4(4)
	N(44)-C(45)-N(46)	122.2(4)
	N(45)-C(45)-N(46)	116.3(4)

Symmetry transformations used to generate equivalent atoms:

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(12)	53(2)	54(2)	34(2)	5(2)	17(2)	14(2)
O(15)	58(2)	65(2)	62(2)	15(2)	16(2)	15(2)
O(17A)	64(2)	62(2)	31(2)	17(2)	15(2)	7(2)
O(17B)	69(2)	68(2)	38(2)	11(2)	30(2)	6(2)
C(11)	40(3)	36(3)	28(2)	-5(2)	10(2)	-9(2)
C(12)	41(3)	38(3)	30(2)	-5(2)	11(2)	-5(2)
C(13)	59(3)	52(3)	27(2)	2(2)	21(2)	-6(3)
C(14)	56(3)	44(3)	35(3)	10(2)	13(2)	6(3)
C(15)	46(3)	47(3)	40(3)	2(2)	8(2)	-2(2)
C(16)	40(3)	50(3)	33(3)	3(2)	15(2)	3(2)
C(17)	42(3)	37(3)	32(2)	-3(2)	8(2)	-5(2)
O(22)	51(2)	63(2)	42(2)	-13(2)	19(2)	-11(2)
O(25)	74(3)	97(3)	95(3)	-41(3)	32(2)	-43(3)
O(27A)	52(2)	60(2)	42(2)	-12(2)	12(2)	-6(2)
O(27B)	52(2)	82(3)	44(2)	-20(2)	22(2)	-2(2)
C(21)	39(3)	46(3)	29(2)	-2(2)	9(2)	6(2)
C(22)	44(3)	46(3)	32(3)	0(2)	12(2)	3(2)
C(23)	49(3)	60(3)	38(3)	-9(2)	19(2)	-3(3)
C(24)	64(4)	71(4)	46(3)	-22(3)	16(3)	-10(3)
C(25)	56(3)	64(4)	58(3)	-13(3)	20(3)	-15(3)
C(26)	41(3)	65(3)	47(3)	-7(3)	17(2)	-5(3)
C(27)	48(3)	54(3)	34(3)	-5(2)	14(2)	6(3)
N(31)	53(3)	71(3)	48(3)	19(2)	22(2)	19(2)
N(32)	38(2)	47(2)	30(2)	8(2)	9(2)	1(2)
N(33)	47(2)	55(3)	33(2)	7(2)	19(2)	3(2)
N(34)	39(2)	43(2)	30(2)	5(2)	10(2)	-3(2)
N(35)	54(3)	57(3)	35(2)	12(2)	18(2)	8(2)
N(36)	40(2)	51(2)	35(2)	9(2)	12(2)	8(2)
C(31)	39(3)	41(3)	42(3)	0(2)	13(2)	-4(2)
C(33)	35(3)	42(3)	27(2)	0(2)	9(2)	-2(2)
C(35)	44(3)	39(3)	26(2)	2(2)	8(2)	-4(2)
N(41)	53(3)	62(3)	31(2)	10(2)	17(2)	8(2)
N(42)	41(2)	39(2)	26(2)	4(2)	8(2)	-1(2)
N(43)	53(2)	46(2)	32(2)	10(2)	19(2)	2(2)
N(44)	43(2)	47(2)	26(2)	-2(2)	16(2)	1(2)
N(45)	60(3)	58(3)	40(2)	7(2)	25(2)	11(2)
N(46)	41(2)	39(2)	30(2)	0(2)	12(2)	-1(2)
C(41)	33(2)	42(3)	26(2)	-4(2)	8(2)	-9(2)

C(43)	41(3)	35(3)	27(2)	-6(2)	6(2)	-12(2)
C(45)	37(3)	38(3)	27(2)	-1(2)	9(2)	-5(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(12)	7397	2589	3098	69
H(15)	6275	7417	2061	91
H(17A)	7219	1881	4173	77
H(13)	7213	4809	1810	53
H(14)	6748	6448	1641	53
H(16)	6456	5184	3350	48
H(22)	6622	7370	6025	76
H(25)	5321	3366	5464	130
H(23)	6452	5100	4769	58
H(24)	5961	3611	4548	72
H(26)	5598	5170	6139	60
H(31A)	5869	11456	3512	67
H(31B)	5957	11931	2861	67
H(33B)	7141	9098	2369	52
H(33A)	6886	10165	2006	52
H(35B)	6631	8094	4696	57
H(5B)	6947	7570	4420	57
H(32)	6459	11170	2390	90
H(41B)	7902	9376	4510	57
H(41A)	7669	10566	4194	57
H(43B)	7358	8103	6783	51
H(43A)	7664	7546	6486	51
H(45A)	6653	11773	5701	61
H(45B)	6750	12319	5068	61

Crystallographic Information of **7**

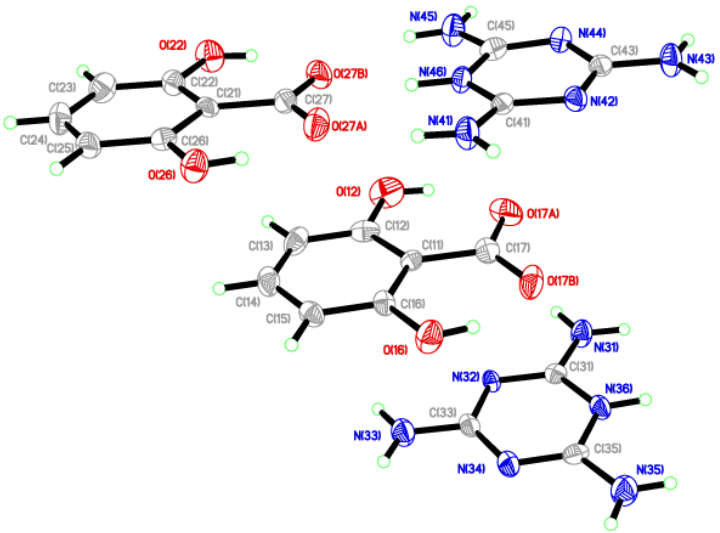


Figure 6. ORTEP drawing of the asymmetric unit of the complex **7**.

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

Identification code	**7**	
Empirical formula	$C_{10}H_{12}N_6O_4$	
Formula weight	280.26	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.3720(10) Å	α= 90.000(7)°.
	b = 8.5490(10) Å	β= 114.23°.
	c = 20.671(2) Å	γ = 90°.
Volume	2316.0(4) Å^3	
Z	8	
Density (calculated)	1.607 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	1168	
Crystal size	0.16 x 0.12 x 0.11 mm^3	
Theta range for data collection	2.16 to 25.24°.	
Index ranges	-17<=h<=17, -10<=k<=10, -24<=l<=24	
Reflections collected	21344	
Independent reflections	4184 [R(int) = 0.0849]	
Completeness to theta = 25.24°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9861 and 0.9798	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4184 / 0 / 361	
Goodness-of-fit on F^2	0.771	
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.0838	
R indices (all data)	R1 = 0.1371, wR2 = 0.0984	
Largest diff. peak and hole	0.261 and -0.237 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)
O(12)	6621(2)	7318(3)	7670(1)	42(1)
O(16)	9928(2)	6160(2)	7739(1)	32(1)

O(17A)	7822(2)	5448(3)	8598(1)	40(1)
O(17B)	9387(2)	5009(2)	8661(1)	34(1)
C(11)	8289(2)	6693(4)	7747(2)	18(1)
C(12)	7364(3)	7496(4)	7426(2)	24(1)
C(13)	7168(3)	8469(4)	6856(2)	29(1)
C(14)	7895(3)	8654(4)	6587(2)	29(1)
C(15)	8822(3)	7877(4)	6887(2)	23(1)
C(16)	9013(2)	6913(4)	7460(2)	19(1)
C(17)	8510(3)	5666(4)	8376(2)	26(1)
O(22)	4295(2)	7340(2)	5395(1)	34(1)
O(26)	7322(2)	6172(2)	5051(1)	29(1)
O(27A)	7010(2)	4877(2)	6023(1)	32(1)
O(27B)	5615(2)	5412(2)	6206(1)	31(1)
C(21)	5826(3)	6691(4)	5257(2)	19(1)
C(22)	4899(3)	7505(4)	5037(2)	23(1)
C(23)	4588(3)	8502(4)	4464(2)	32(1)
C(24)	5203(3)	8729(4)	4104(2)	30(1)
C(25)	6116(3)	7960(4)	4303(2)	27(1)
C(26)	6426(2)	6938(4)	4871(2)	22(1)
C(27)	6168(3)	5597(4)	5863(1)	25(1)
N(31)	9181(2)	7137(3)	10230(1)	27(1)
N(32)	9552(2)	8517(3)	9406(1)	20(1)
N(33)	10008(2)	9745(3)	8607(1)	29(1)
N(34)	11203(2)	8111(3)	9383(1)	24(1)
N(35)	12316(2)	6417(3)	10202(1)	33(1)
N(36)	10735(2)	6781(3)	10195(1)	22(1)
C(31)	9812(2)	7516(4)	9930(2)	18(1)
C(33)	10269(3)	8764(3)	9147(2)	22(1)
C(35)	11417(2)	7137(4)	9916(2)	23(1)
N(41)	8139(2)	2704(3)	7075(1)	28(1)
N(42)	7931(2)	1459(3)	7999(1)	21(1)
N(43)	7584(2)	264(3)	8862(1)	29(1)
N(44)	6356(2)	1931(3)	8136(1)	25(1)
N(45)	5242(2)	3762(3)	7410(1)	33(1)
N(46)	6709(2)	3228(3)	7263(1)	23(1)
C(41)	7608(3)	2446(4)	7453(2)	21(1)
C(43)	7281(3)	1242(4)	8320(2)	22(1)
C(45)	6104(3)	2948(4)	7615(2)	24(1)

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

O(12)-C(12)	1.365(4)	C(12)-C(11)-C(16)	117.2(3)
O(16)-C(16)	1.361(4)	C(12)-C(11)-C(17)	121.7(3)
O(17A)-C(17)	1.265(3)	C(16)-C(11)-C(17)	121.1(3)
O(17B)-C(17)	1.281(3)	O(12)-C(12)-C(13)	118.0(3)
C(11)-C(12)	1.398(4)	O(12)-C(12)-C(11)	120.3(3)
C(11)-C(16)	1.408(4)	C(13)-C(12)-C(11)	121.7(3)
C(11)-C(17)	1.490(4)	C(12)-C(13)-C(14)	119.5(3)
C(12)-C(13)	1.373(4)	C(13)-C(14)-C(15)	120.9(3)
C(13)-C(14)	1.378(4)	C(16)-C(15)-C(14)	119.1(3)
C(14)-C(15)	1.387(4)	O(16)-C(16)-C(15)	117.8(3)
C(15)-C(16)	1.376(4)	O(16)-C(16)-C(11)	120.7(3)
O(22)-C(22)	1.360(4)	C(15)-C(16)-C(11)	121.5(3)
O(26)-C(26)	1.353(4)	O(17A)-C(17)-O(17B)	122.4(3)
O(27A)-C(27)	1.275(3)	O(17A)-C(17)-C(11)	119.0(3)
O(27B)-C(27)	1.275(3)	O(17B)-C(17)-C(11)	118.5(3)
C(21)-C(22)	1.403(4)	C(22)-C(21)-C(26)	117.5(3)
C(21)-C(26)	1.411(4)	C(22)-C(21)-C(27)	122.1(3)
C(21)-C(27)	1.476(4)	C(26)-C(21)-C(27)	120.4(3)

C(22)-C(23)	1.377(4)	O(22)-C(22)-C(23)	118.6(3)
C(23)-C(24)	1.382(4)	O(22)-C(22)-C(21)	120.3(3)
C(24)-C(25)	1.371(4)	C(23)-C(22)-C(21)	121.1(3)
C(25)-C(26)	1.383(4)	C(22)-C(23)-C(24)	119.7(3)
N(31)-C(31)	1.331(4)	C(25)-C(24)-C(23)	121.1(3)
N(32)-C(31)	1.308(3)	C(24)-C(25)-C(26)	119.5(3)
N(32)-C(33)	1.358(4)	O(26)-C(26)-C(25)	118.6(3)
N(33)-C(33)	1.323(3)	O(26)-C(26)-C(21)	120.3(3)
N(34)-C(35)	1.314(4)	C(25)-C(26)-C(21)	121.1(3)
N(34)-C(33)	1.348(4)	O(27A)-C(27)-O(27B)	122.5(3)
N(35)-C(35)	1.331(4)	O(27A)-C(27)-C(21)	118.5(3)
N(36)-C(35)	1.359(4)	O(27B)-C(27)-C(21)	119.0(3)
N(36)-C(31)	1.363(4)	C(31)-N(32)-C(33)	115.0(3)
N(41)-C(41)	1.316(4)	C(35)-N(34)-C(33)	114.8(3)
N(42)-C(41)	1.330(3)	C(35)-N(36)-C(31)	118.6(3)
N(42)-C(43)	1.362(4)	N(32)-C(31)-N(31)	121.8(3)
N(43)-C(43)	1.320(3)	N(32)-C(31)-N(36)	122.3(3)
N(44)-C(45)	1.314(4)	N(31)-C(31)-N(36)	116.0(3)
N(44)-C(43)	1.357(4)	N(33)-C(33)-N(34)	117.5(3)
N(45)-C(45)	1.330(4)	N(33)-C(33)-N(32)	115.7(3)
N(46)-C(41)	1.362(4)	N(34)-C(33)-N(32)	126.8(3)
N(46)-C(45)	1.364(4)	N(34)-C(35)-N(35)	121.0(3)
		N(34)-C(35)-N(36)	122.5(3)
		N(35)-C(35)-N(36)	116.5(3)
		C(41)-N(42)-C(43)	115.4(3)
		C(45)-N(44)-C(43)	115.2(3)
		C(41)-N(46)-C(45)	119.7(3)
		N(41)-C(41)-N(42)	121.7(3)
		N(41)-C(41)-N(46)	117.2(3)
		N(42)-C(41)-N(46)	121.1(3)
		N(43)-C(43)-N(44)	117.2(3)
		N(43)-C(43)-N(42)	116.5(3)
		N(44)-C(43)-N(42)	126.3(3)
		N(44)-C(45)-N(45)	121.0(3)
		N(44)-C(45)-N(46)	122.1(3)
		N(45)-C(45)-N(46)	116.9(3)

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}
O(12)	36(2)	57(2)	39(1)	-8(1)	22(1)	-4(1)
O(16)	28(2)	40(2)	29(1)	7(1)	12(1)	8(1)
O(17A)	56(2)	49(2)	24(1)	-8(1)	25(1)	-25(1)
O(17B)	48(2)	27(1)	19(1)	1(1)	6(1)	6(1)
C(11)	22(2)	17(2)	13(2)	-5(2)	6(2)	-3(2)
C(12)	25(2)	28(2)	23(2)	-14(2)	14(2)	-6(2)
C(13)	27(2)	25(2)	26(2)	1(2)	2(2)	9(2)
C(14)	44(3)	24(2)	17(2)	0(2)	11(2)	-1(2)
C(15)	30(2)	22(2)	23(2)	-2(2)	15(2)	-3(2)
C(16)	26(2)	13(2)	18(2)	-1(2)	10(2)	3(2)
C(17)	40(2)	18(2)	16(2)	-6(2)	9(2)	-5(2)
O(22)	33(2)	42(2)	37(1)	4(1)	23(1)	3(1)
O(26)	28(2)	36(2)	25(1)	3(1)	13(1)	5(1)

O(27A)	36(2)	30(1)	26(1)	5(1)	8(1)	6(1)
O(27B)	43(2)	33(2)	23(1)	1(1)	18(1)	-8(1)
C(21)	25(2)	13(2)	19(2)	-3(2)	10(2)	-5(2)
C(22)	28(2)	25(2)	20(2)	-1(2)	14(2)	-1(2)
C(23)	30(2)	31(2)	30(2)	2(2)	9(2)	7(2)
C(24)	38(2)	27(2)	24(2)	7(2)	11(2)	7(2)
C(25)	34(2)	29(2)	21(2)	-3(2)	15(2)	-8(2)
C(26)	21(2)	22(2)	21(2)	-3(2)	7(2)	-2(2)
C(27)	36(2)	21(2)	14(2)	-4(2)	8(2)	-6(2)
N(31)	25(2)	35(2)	25(2)	9(1)	13(1)	6(1)
N(32)	23(2)	22(2)	15(1)	5(1)	9(1)	-3(1)
N(33)	30(2)	31(2)	27(1)	7(1)	14(1)	2(1)
N(34)	27(2)	25(2)	22(2)	5(1)	11(1)	0(1)
N(35)	28(2)	37(2)	34(2)	8(1)	14(2)	6(2)
N(36)	27(2)	22(2)	20(1)	4(1)	12(1)	-1(1)
C(31)	21(2)	19(2)	14(2)	-5(2)	8(2)	-3(2)
C(33)	33(2)	15(2)	15(2)	-3(2)	7(2)	-7(2)
C(35)	17(2)	24(2)	24(2)	-4(2)	5(2)	-3(2)
N(41)	30(2)	33(2)	24(2)	9(1)	12(1)	4(1)
N(42)	26(2)	21(2)	18(1)	1(1)	9(1)	-1(1)
N(43)	32(2)	34(2)	25(1)	13(1)	15(1)	6(1)
N(44)	26(2)	26(2)	21(2)	4(1)	6(1)	0(1)
N(45)	29(2)	40(2)	31(2)	13(1)	13(2)	9(2)
N(46)	25(2)	23(2)	17(1)	5(1)	5(1)	3(1)
C(41)	25(2)	21(2)	14(2)	-2(2)	4(2)	-7(2)
C(43)	30(2)	18(2)	14(2)	-4(2)	5(2)	-5(2)
C(45)	21(2)	27(2)	23(2)	-5(2)	8(2)	-
2(2)						

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

	x	y	z	U(eq)
H(12)	6824	6698	8016	63
H(16)	9967	5630	8092	48
H(13)	6536	9010	6648	34
H(14)	7758	9323	6192	34
H(15)	9319	8009	6698	28
H(22)	4566	6703	5730	52
H(26)	7423	5590	5401	44
H(23)	3952	9032	4316	38
H(24)	4990	9430	3714	36
H(25)	6532	8128	4052	32
H(31A)	9375	6460	10581	33
H(31B)	8571	7563	10076	33
H(33A)	9404	10194	8439	34
H(33B)	10439	9949	8414	34
H(35A)	12779	6591	10034	39
H(35B)	12448	5768	10559	39
H(36)	10859	6119	10570	26
H(41A)	7910	3363	6716	34
H(41B)	8723	2219	7181	34
H(43A)	8179	-206	8997	35
H(43B)	7191	82	9086	35
H(45A)	4831	3623	7624	40
H(45B)	5082	4439	7060	40
H(46)	6504	3943	6879	27

Thermo gravimetric Analysis

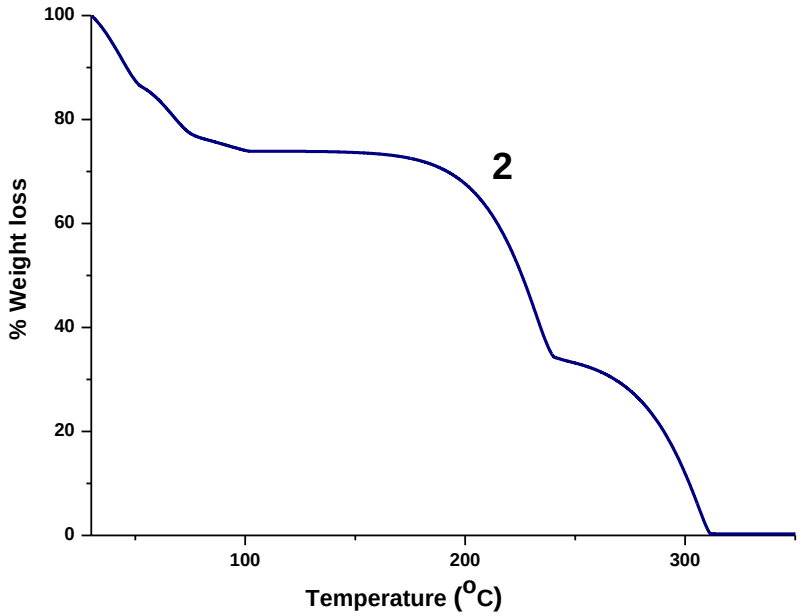


Figure 7. TG plot for the complex **2**.

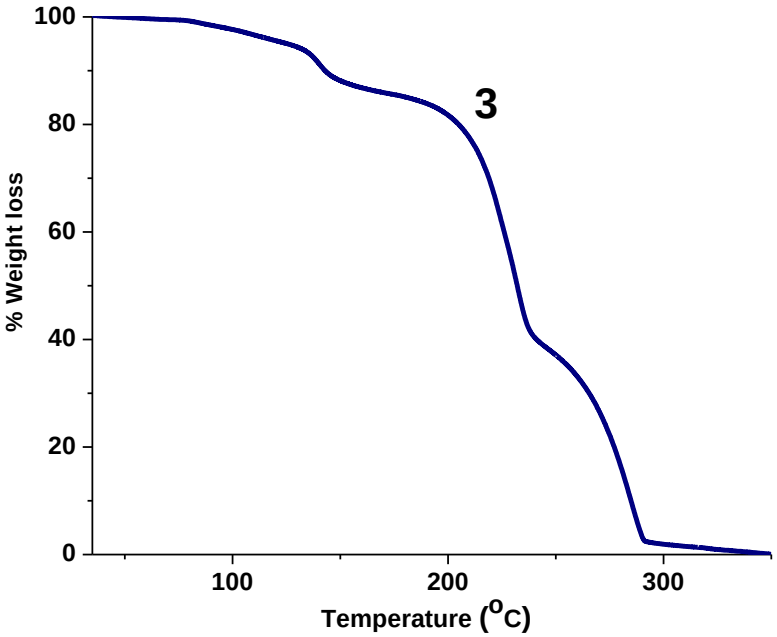


Figure 8. TG plot for the complex **3**.

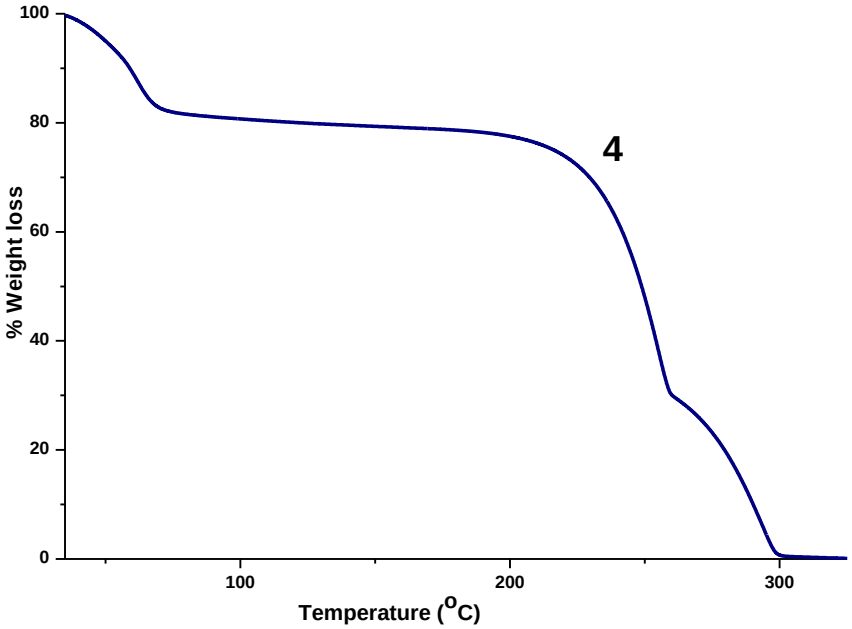


Figure 9. TG plot for the complex **4**.

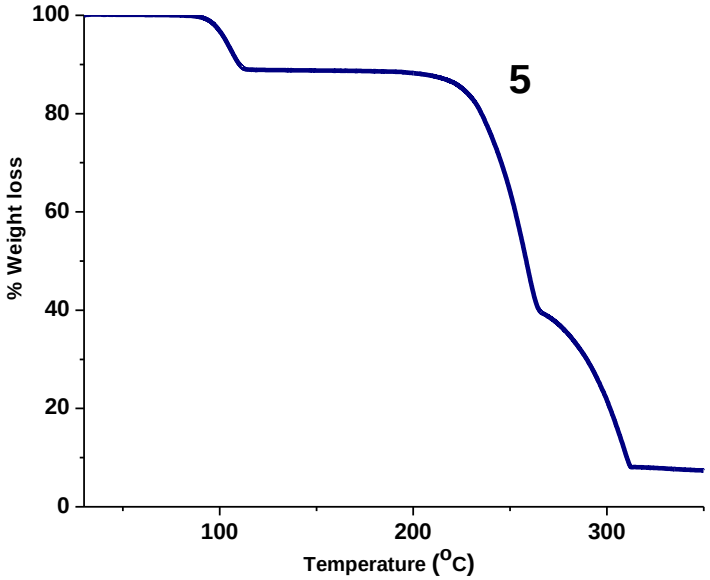


Figure 10. TG plot for the complex **5**.

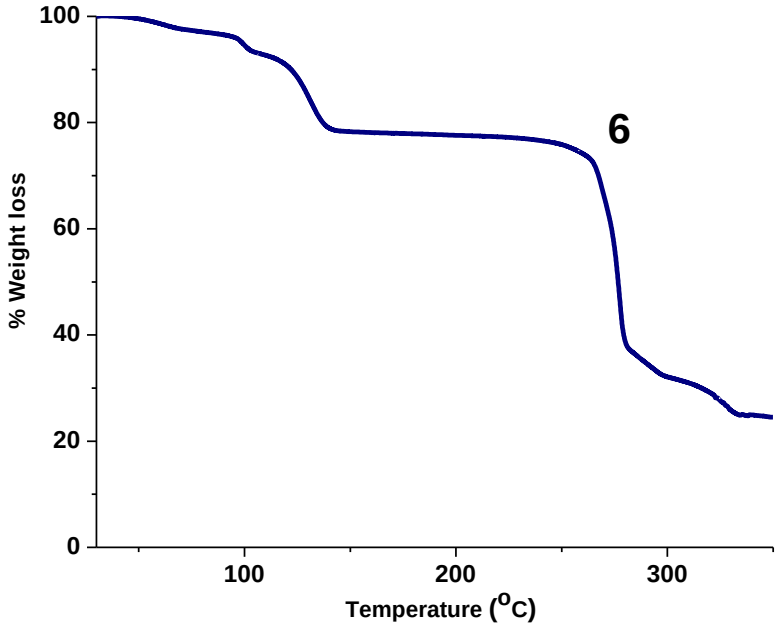


Figure 11. TG plot for the complex **6**.

PXRD Analysis

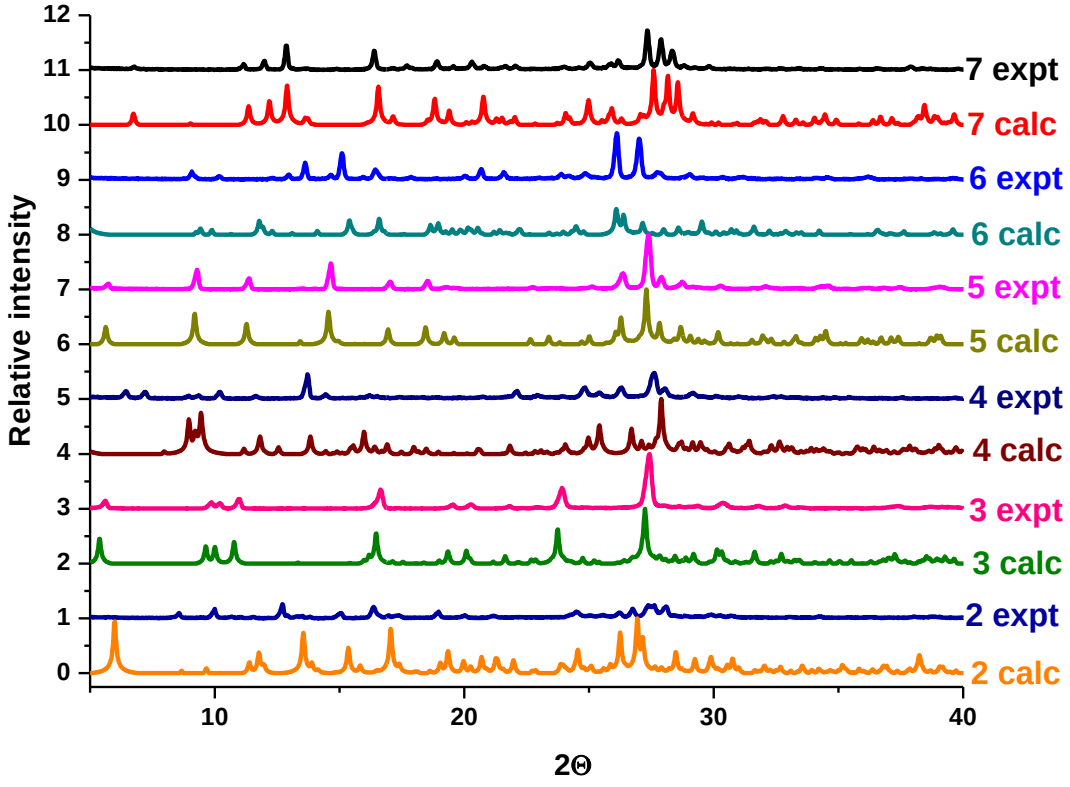
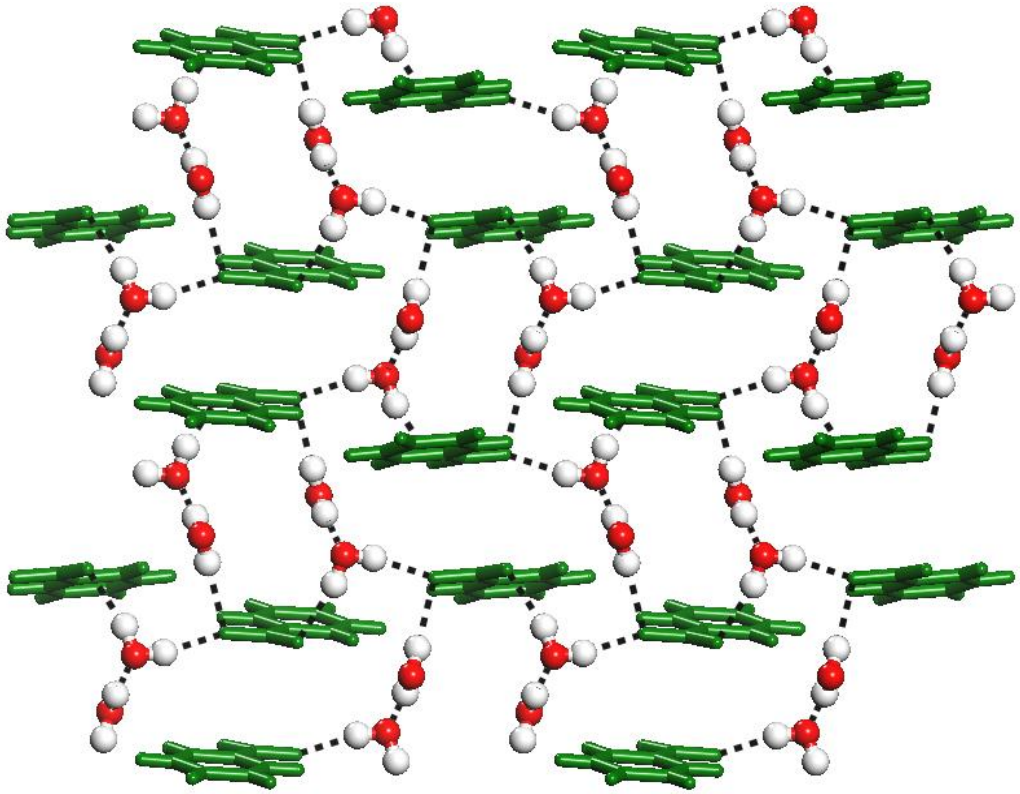
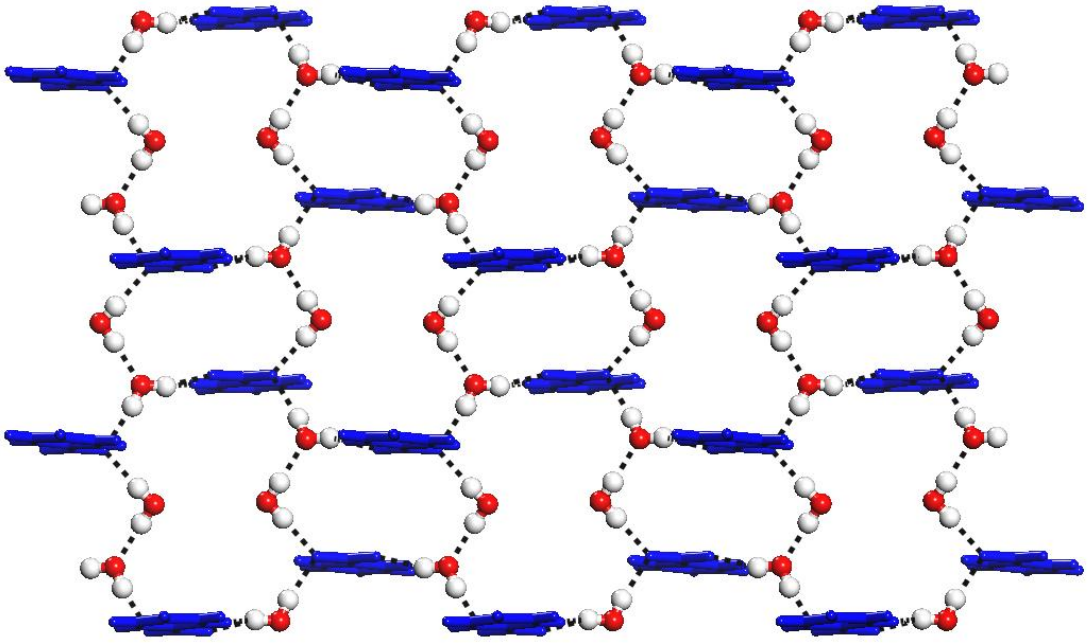


Figure 12. Combined PXRD plot for the complexes. The deviation of the experimental and the calculated pattern for the complexes **2** and **4** is due to the loss of solvent molecules from the crystal lattice, as evident from the TG plots.



(a)



(b)

Figure 13. The arrangement of water molecules in the crystal lattice of the two polymorphic structures of the **BA-ML** complex. (a) Monoclinic form, (b) orthorhombic form.

Table S1. Conformational analysis of dihydroxybenzoic acids.*

DHBA	Refcode	*Syn-syn*	*Anti-anti*	*Syn-anti*
23DHB	MOZDEL	✓		
24DHB	ACHRES	✓		
	TEVWOH	✓		
	DEYREF	✓		
	GIDLUB	✓		
	HUHDUK	✓		
	HUHFAS	✓		
	IDUBUF	✓		
	MOZCIO	✓		
	HEFTUI			✓
	TEZXIG			✓
25DHB	DUCROJ	✓		
	XAQQOW	✓		
	ZEZHIV	✓		
	CUSZIA	✓		
	EWINAZ	✓		
	RACBED	✓		
	AJAGUN			✓
	DAVPAS			✓
	MOZDIP			✓
	NEKDEN			✓
	NURFOW			✓
	GULLUF			✓
26DHB	DEXTOQ	✓		
	KEZHED	✓		
	KEZHAZ	✓		
	QIRGUT	✓		
	LEWRUA	✓		
	LEWPOS	✓		
	LEZJIH	✓		
	LOLDAS	✓		
	LOLDEW	✓		
	REZHAG	✓		
	RIBLUJ	✓		
	HUZDOV	✓		✓

*When the –OH group is pointing towards the carboxyl group it is considered as *syn* conformation and when pointing away it is considered as *anti*.