

Supplementary Information

Crystallographic data

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

Empirical formula	$C_{12}H_{16}N_2O_3$	
Formula weight	236.27	
Temperature	93(2)°K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P 2_12_12_1$	
Unit cell dimensions	$a = 5.6585(6)$ Å	$\alpha = 90^\circ$
	$b = 7.9422(8)$ Å	$\beta = 90^\circ$
	$c = 26.129(3)$ Å	$\gamma = 90^\circ$
Volume	$1174.3(2)$ Å ³	
Z	4	
Density (calculated)	1.336 Mg/m ³	
Absorption coefficient	0.097 mm ⁻¹	
F(000)	504	
Crystal size	0.63 x 0.17 x 0.12 mm ³	
Theta range for data collection	1.56 to 28.22°.	
Index ranges	$-6 \leq h \leq 7, -10 \leq k \leq 10, -34 \leq l \leq 30$	
Reflections collected	9555	
Independent reflections	2838 [R(int) = 0.0288]	
Completeness to $\theta = 28.22^\circ$	99.5 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.988 and 0.942	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2838 / 0 / 157	
Goodness-of-fit on F ²	1.029	
Final R indices [I > 2σ(I)]	R1 = 0.0364, wR2 = 0.0848	
R indices (all data)	R1 = 0.0442, wR2 = 0.0874	
Absolute structure parameter	0.6(10)	
Largest diff. peak and hole	0.250 and -0.204 eÅ ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) For compound **6**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6484(2)	4584(1)	11218(1)	17(1)
C(2)	4856(3)	5842(2)	11118(1)	19(1)
O(2)	3435(2)	6367(1)	11429(1)	30(1)
N(3)	4953(2)	6461(2)	10623(1)	19(1)
C(4)	6471(2)	5979(2)	10239(1)	16(1)
O(4)	6235(2)	6627(1)	9806(1)	19(1)
C(5)	8204(2)	4729(2)	10374(1)	17(1)
C(5A)	9986(3)	4162(2)	9987(1)	21(1)
C(6)	8085(2)	4077(2)	10852(1)	17(1)
C(1')	6339(2)	1860(2)	11662(1)	17(1)
C(2')	6423(2)	3754(2)	11729(1)	16(1)
C(3')	8659(3)	4091(2)	12048(1)	20(1)
C(4')	10333(3)	2597(2)	11949(1)	20(1)
C(5')	8762(2)	1133(2)	11791(1)	18(1)
C(6')	6680(3)	793(2)	12136(1)	22(1)
C(7')	9797(3)	-255(2)	11474(1)	24(1)
O(7')	10858(2)	486(1)	11031(1)	29(1)

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

N(1)-C(6)	1.3771(17)	C(7')-C(5')-C(4')	118.97(12)
N(1)-C(2)	1.3835(17)	C(7')-C(5')-C(6')	120.25(13)
N(1)-C(2')	1.4888(16)	O(7')-C(7')-C(5')	107.94(12)
C(2)-O(2)	1.2171(17)		
C(2)-N(3)	1.3863(17)		
N(3)-C(4)	1.3743(17)		
C(4)-O(4)	1.2502(16)		
C(4)-C(5)	1.4398(19)		
C(5)-C(6)	1.3536(19)		
C(5)-C(5A)	1.4972(19)		
C(1')-C(6')	1.5142(19)		
C(2')-C(1')	1.5149(19)		
C(3')-C(2')	1.5386(19)		
C(4')-C(3')	1.540(2)		
C(5')-C(1')	1.5254(19)		
C(5')-C(4')	1.520(2)		
C(5')-C(6')	1.5086(19)		
C(5')-C(7')	1.497(2)		
C(7')-O(7')	1.4310(18)		
C(6)-N(1)-C(2)	121.21(11)		
C(6)-N(1)-C(2')	120.54(11)		
C(2)-N(1)-C(2')	118.23(11)		
O(2)-C(2)-N(1)	124.17(12)		
O(2)-C(2)-N(3)	121.88(13)		
N(1)-C(2)-N(3)	113.94(12)		
C(4)-N(3)-C(2)	127.39(12)		
O(4)-C(4)-N(3)	118.61(13)		
O(4)-C(4)-C(5)	125.36(13)		
N(3)-C(4)-C(5)	116.03(11)		
C(6)-C(5)-C(4)	117.14(12)		
C(6)-C(5)-C(5A)	122.79(13)		
C(4)-C(5)-C(5A)	120.04(12)		
C(5)-C(6)-N(1)	124.16(13)		
N(1)-C(2')-C(1')	109.66(11)		
N(1)-C(2')-C(3')	112.92(11)		
C(1')-C(2')-C(3')	105.12(11)		
C(2')-C(3')-C(4')	106.30(11)		
C(2')-C(1')-C(5')	108.80(12)		
C(4')-C(5')-C(1')	107.21(11)		
C(5')-C(4')-C(3')	105.98(11)		
C(5')-C(6')-C(1')	60.61(9)		
C(6')-C(1')-C(2')	117.20(12)		
C(6')-C(1')-C(5')	59.51(9)		
C(6')-C(5')-C(1')	59.88(9)		
C(6')-C(5')-C(4')	115.56(12)		
C(7')-C(5')-C(1')	120.53(12)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	17(1)	19(1)	13(1)	2(1)	1(1)	2(1)
C(2)	21(1)	20(1)	17(1)	1(1)	1(1)	2(1)
O(2)	33(1)	34(1)	23(1)	6(1)	10(1)	18(1)
N(3)	20(1)	19(1)	19(1)	4(1)	1(1)	7(1)
C(4)	16(1)	16(1)	17(1)	-2(1)	1(1)	-4(1)
O(4)	21(1)	21(1)	16(1)	3(1)	-1(1)	0(1)
C(5)	17(1)	17(1)	16(1)	-1(1)	0(1)	-2(1)
C(5A)	22(1)	23(1)	19(1)	1(1)	4(1)	2(1)
C(6)	16(1)	17(1)	18(1)	-2(1)	0(1)	3(1)
C(1')	15(1)	21(1)	17(1)	1(1)	0(1)	0(1)
C(2')	17(1)	21(1)	11(1)	2(1)	2(1)	3(1)
C(3')	22(1)	21(1)	16(1)	-2(1)	-1(1)	-1(1)
C(4')	15(1)	26(1)	18(1)	2(1)	-2(1)	0(1)
C(5')	17(1)	21(1)	15(1)	2(1)	0(1)	3(1)
C(6')	23(1)	23(1)	19(1)	5(1)	4(1)	1(1)
C(7')	30(1)	20(1)	21(1)	3(1)	2(1)	5(1)
O(7')	43(1)	25(1)	20(1)	-2(1)	11(1)	6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **6**.

	x	y	z	U(eq)
H(3A)	3949	7234	10547	23
H(5AA)	11001	3329	10138	32
H(5AB)	10914	5108	9878	32
H(5AC)	9186	3685	9698	32
H(6A)	9152	3234	10939	20
H(1'A)	5459	1390	11372	21
H(2'A)	5025	4131	11918	20
H(3'A)	8269	4164	12409	24
H(3'B)	9395	5139	11943	24
H(4'A)	11445	2867	11678	24
H(4'B)	11212	2319	12256	24
H(6'A)	6642	1356	12465	26
H(6'B)	6018	-334	12135	26
H(7'A)	10975	-864	11670	28
H(7'B)	8569	-1040	11373	28
H(7'C)	11000(40)	-290(20)	10792(7)	35

Table 6. Torsion angles [°] for compound **6**.

N(1)-C(2)-N(3)-C(4)	-0.9(2)
N(1)-C(2')-C(1')-C(5')	105.38(13)
N(1)-C(2')-C(1')-C(6')	170.06(11)
C(2)-N(1)-C(6)-C(5)	-0.6(2)
C(2)-N(1)-C(2')-C(1')	128.38(13)
C(2)-N(1)-C(2')-C(3')	-114.76(13)
C(2)-N(3)-C(4)-O(4)	176.90(13)
C(2)-N(3)-C(4)-C(5)	-2.2(2)
O(2)-C(2)-N(3)-C(4)	179.78(13)
N(3)-C(4)-C(5)-C(5A)	-178.08(13)
N(3)-C(4)-C(5)-C(6)	3.90(18)
O(4)-C(4)-C(5)-C(6)	-175.16(13)
O(4)-C(4)-C(5)-C(5A)	2.9(2)
C(4)-C(5)-C(6)-N(1)	-2.7(2)
C(5A)-C(5)-C(6)-N(1)	179.31(13)
C(6)-N(1)-C(2)-O(2)	-178.36(14)
C(6)-N(1)-C(2)-N(3)	2.35(19)
C(6)-N(1)-C(2')-C(1')	-50.03(17)
C(6)-N(1)-C(2')-C(3')	66.83(16)
C(1')-C(5')-C(7')-O(7')	82.02(16)
C(1')-C(5')-C(4')-C(3')	14.62(15)
C(2')-N(1)-C(2)-O(2)	3.2(2)
C(2')-N(1)-C(2)-N(3)	-176.05(12)
C(2')-N(1)-C(6)-C(5)	177.81(13)
C(2')-C(1')-C(6')-C(5')	-96.77(14)
C(3')-C(2')-C(1')-C(5')	-16.28(14)
C(3')-C(2')-C(1')-C(6')	48.40(16)
C(4')-C(3')-C(2')-N(1)	-94.32(13)
C(4')-C(3')-C(2')-C(1')	25.19(14)
C(4')-C(5')-C(1')-C(6')	-110.02(13)
C(4')-C(5')-C(1')-C(2')	1.08(15)
C(4')-C(5')-C(6')-C(1')	95.84(12)
C(4')-C(5')-C(7')-O(7')	-53.96(17)
C(5')-C(4')-C(3')-C(2')	-24.76(15)
C(6')-C(5')-C(1')-C(2')	111.10(13)
C(6')-C(5')-C(4')-C(3')	-49.64(15)
C(6')-C(5')-C(7')-O(7')	152.71(12)
C(7')-C(5')-C(1')-C(2')	-139.40(13)
C(7')-C(5')-C(1')-C(6')	109.51(15)
C(7')-C(5')-C(4')-C(3')	155.82(12)
C(7')-C(5')-C(6')-C(1')	-109.97(14)

Table 7. Hydrogen bonds for **6** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(3)-H(3A)...O(4)#1	0.86	2.01	2.8264(15)	159.0
O(7')-H(7'C)...O(4)#2	0.883(18)	1.892(18)	2.7650(15)	169.5(17)

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, -y+3/2, -z+2$ #2 $x+1/2, -y+1/2, -z+2$