7. X-Ray Single Crystal Diffraction Structure and Data of **3a**

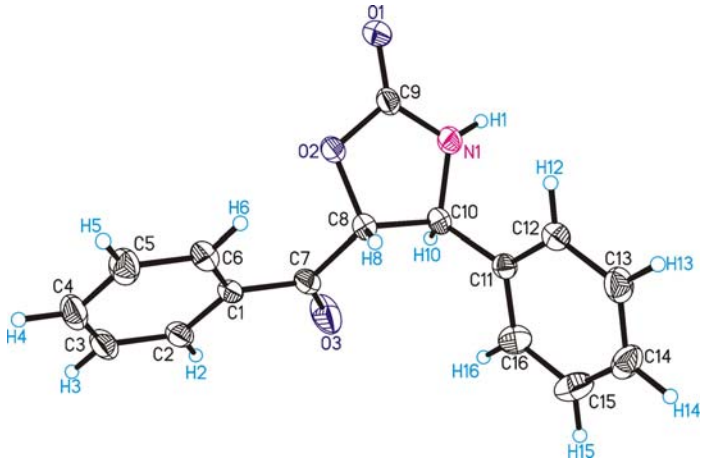
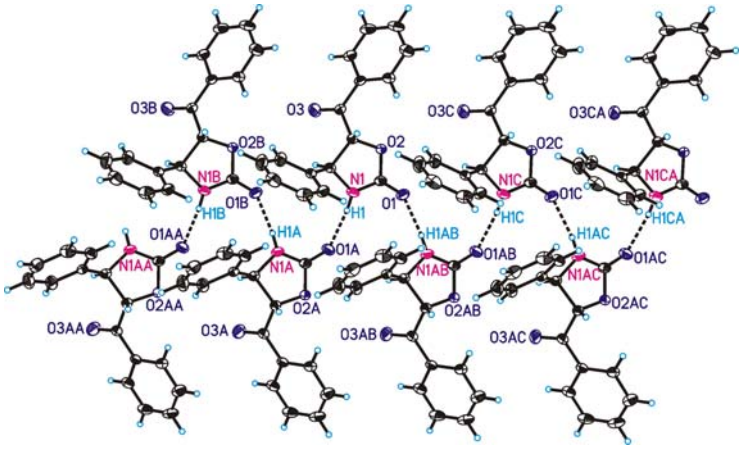
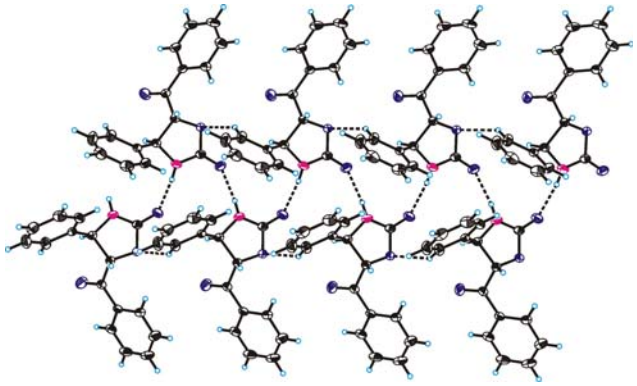


Fig1. ORTEP drawing.

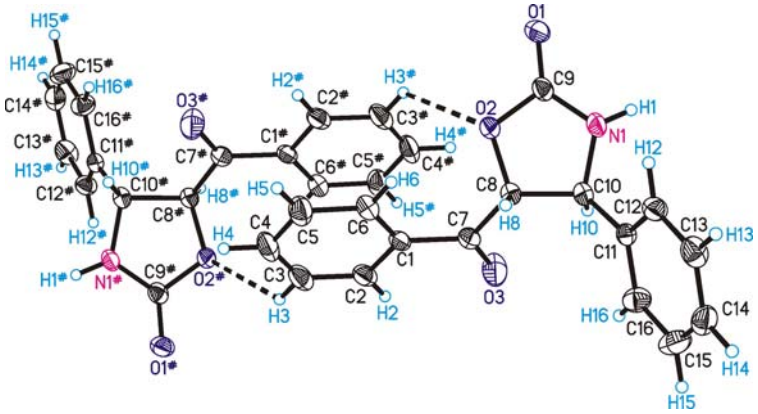


N1-H1…O1[1#] (symmetry code 1#: x, 1.5-y, 0.5+z) hydrogen bond (H1…O1[1#]: 2.051 Å; N1…O1[1#]: 2.905 Å, 172°). 1D N-H…O hydrogen bond chain along c axis.

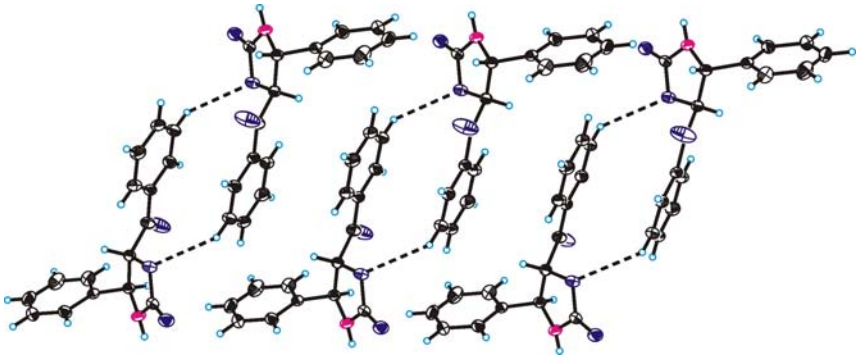


C16-H16…O2[3#] (symmetry code 3#: x, y, 1+z) hydrogen bond (H16…O2[3#]: 2.526 Å; C16…O2[3#]: 3.331 Å, 145.0°). Two parallel 1D C-H…O hydrogen bond chains along c axis. 1D

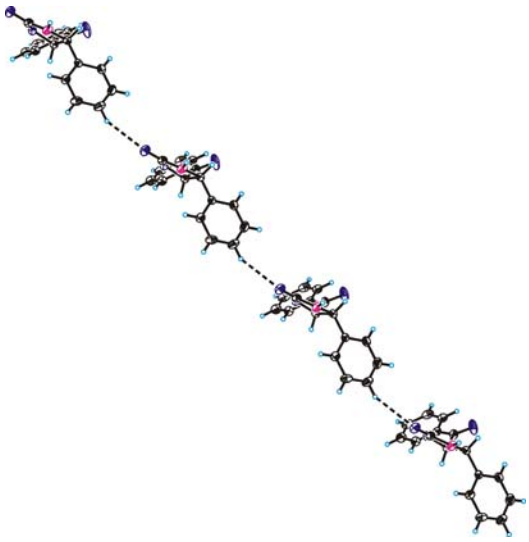
N-H…O hydrogen bond chain is also shown.



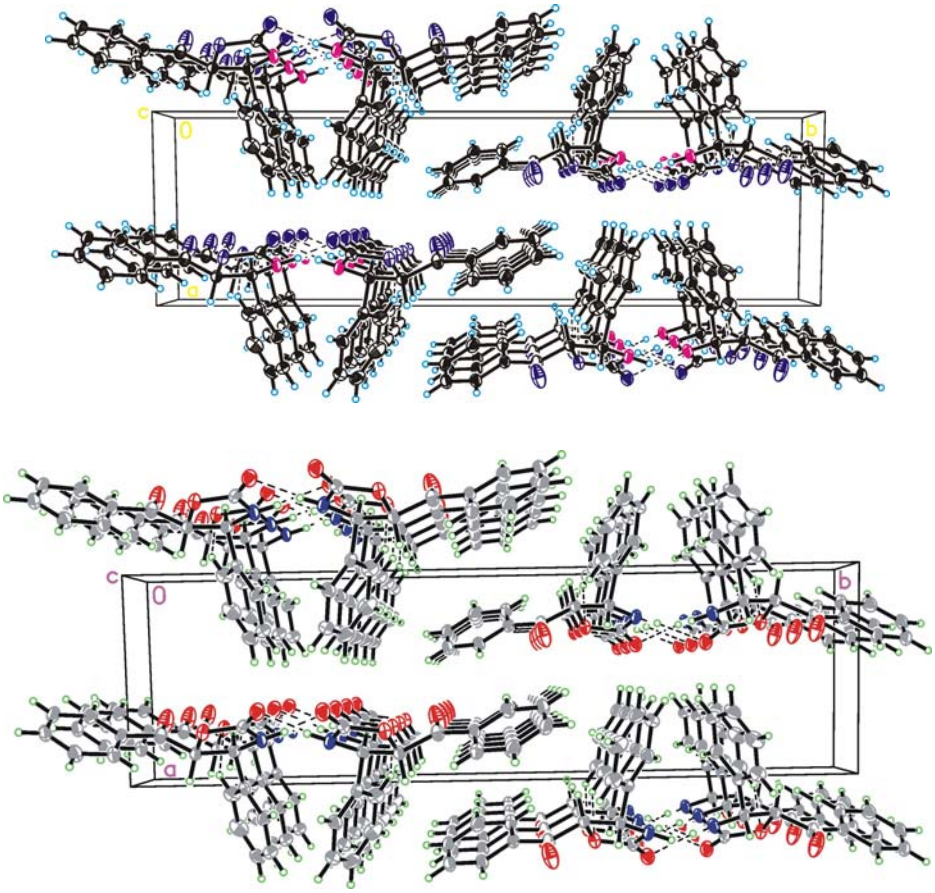
C3-H3…O2$^{4\#}$ (symmetry code 4#: 1-x, 1-y, 1-z) hydrogen bond (H3…O2$^{4\#}$: 2.784 Å; C3…O2$^{4\#}$: 3.457 Å, 130.1°) C-H…O hydrogen bond dimer with C1-C2-C3-C4-C5-C6, C1#-C2#-C3#-C4#-C5#-C6#, (symmetry code #: 1-x, 1-y, 1-z), π-π stacking in a distance of 3.4423 Å.



π-π stacking of the dimmer along a axis also forms 1D chain. C1-C2-C3-C4-C5-C6, C1##-C2##-C3##-C4##-C5##-C6##, (symmetry code #: -x, 1-y, 1-z), π-π stacking with distance of 3.5478Å.



C14-H14…O1$^{2\#}$ (symmetry code 2#: 1-x, y, 1+z) hydrogen bond (H14…O1$^{2\#}$: 2.820 Å; C14…O1$^{2\#}$: 3.678 Å, 153.9°). 1D C-H…O hydrogen bond chain along the line of x=z.



Cell packing

Table 1. Crystal data and structure refinement for T.

Identification code	t	
Empirical formula	C16 H13 N O3	
Formula weight	267.27	
Temperature	292(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 7.8191(5) Å	α= 90°.
	b = 26.657(2) Å	β= 98.6590(10)°.
	c = 6.3613(7) Å	γ = 90°.
Volume	1310.8(2) $Å^3$	
Z	4	
Density (calculated)	1.354 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	560	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.53 to 27.00°.	
Index ranges	-9<=h<=9, -28<=k<=34, -7<=l<=8	
Reflections collected	9625	
Independent reflections	2837 [R(int) = 0.0457]	
Completeness to theta = 27.00°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2837 / 1 / 184	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1299	
R indices (all data)	R1 = 0.0959, wR2 = 0.1459	
Largest diff. peak and hole	0.158 and -0.165 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	2604(3)	5236(1)	5940(3)	43(1)
C(2)	3490(3)	4818(1)	6877(4)	53(1)
C(3)	3607(3)	4386(1)	5714(5)	65(1)
C(4)	2828(3)	4362(1)	3634(5)	68(1)
C(5)	1938(3)	4769(1)	2687(4)	65(1)
C(6)	1835(3)	5206(1)	3829(4)	52(1)
C(7)	2566(3)	5695(1)	7238(4)	49(1)
C(8)	1752(3)	6171(1)	6180(3)	40(1)
C(9)	2941(3)	6830(1)	4583(3)	45(1)
C(10)	1786(3)	6632(1)	7647(3)	41(1)
C(11)	63(2)	6727(1)	8381(3)	38(1)
C(12)	-1246(3)	6999(1)	7186(4)	51(1)
C(13)	-2838(3)	7049(1)	7868(4)	63(1)
C(14)	-3134(3)	6836(1)	9729(5)	66(1)
C(15)	-1847(4)	6573(1)	10929(4)	72(1)
C(16)	-258(3)	6516(1)	10261(4)	57(1)
N(1)	2311(2)	7016(1)	6253(3)	51(1)
O(3)	3124(3)	5705(1)	9115(3)	93(1)
O(2)	2721(2)	6322(1)	4508(2)	46(1)
O(1)	3597(2)	7048(1)	3231(3)	58(1)

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

C(1)-C(6)	1.389(3)
C(1)-C(2)	1.398(3)
C(1)-C(7)	1.479(3)
C(2)-C(3)	1.379(3)
C(3)-C(4)	1.372(4)
C(4)-C(5)	1.378(4)
C(5)-C(6)	1.382(3)
C(7)-O(3)	1.208(2)
C(7)-C(8)	1.529(3)
C(8)-O(2)	1.453(2)
C(8)-C(10)	1.541(3)
C(9)-O(1)	1.214(2)
C(9)-N(1)	1.332(3)
C(9)-O(2)	1.365(2)
C(10)-N(1)	1.454(3)
C(10)-C(11)	1.512(3)
C(11)-C(16)	1.379(3)
C(11)-C(12)	1.384(3)
C(12)-C(13)	1.385(3)
C(13)-C(14)	1.364(3)
C(14)-C(15)	1.362(4)
C(15)-C(16)	1.381(4)

C(6)-C(1)-C(2)	118.8(2)
C(6)-C(1)-C(7)	123.04(19)
C(2)-C(1)-C(7)	118.2(2)
C(3)-C(2)-C(1)	120.4(2)
C(4)-C(3)-C(2)	120.1(2)
C(3)-C(4)-C(5)	120.4(2)
C(4)-C(5)-C(6)	120.0(3)
C(5)-C(6)-C(1)	120.4(2)
O(3)-C(7)-C(1)	122.3(2)
O(3)-C(7)-C(8)	118.9(2)
C(1)-C(7)-C(8)	118.87(18)

O(2)-C(8)-C(7)	108.87(15)
O(2)-C(8)-C(10)	105.01(15)
C(7)-C(8)-C(10)	115.29(17)
O(1)-C(9)-N(1)	129.3(2)
O(1)-C(9)-O(2)	120.92(19)
N(1)-C(9)-O(2)	109.74(18)
N(1)-C(10)-C(11)	114.66(17)
N(1)-C(10)-C(8)	99.97(16)
C(11)-C(10)-C(8)	112.67(16)
C(16)-C(11)-C(12)	118.3(2)
C(16)-C(11)-C(10)	119.09(19)
C(12)-C(11)-C(10)	122.54(18)
C(11)-C(12)-C(13)	120.3(2)
C(14)-C(13)-C(12)	120.6(2)
C(15)-C(14)-C(13)	119.6(2)
C(14)-C(15)-C(16)	120.5(2)
C(11)-C(16)-C(15)	120.8(2)
C(9)-N(1)-C(10)	113.37(17)
C(9)-O(2)-C(8)	109.03(15)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	46(1)	32(1)	52(1)	6(1)	15(1)	-1(1)
C(2)	53(1)	41(1)	68(2)	12(1)	18(1)	4(1)
C(3)	60(2)	36(1)	104(2)	7(1)	28(2)	6(1)
C(4)	60(2)	38(1)	110(2)	-18(1)	30(2)	-8(1)
C(5)	65(2)	54(2)	78(2)	-18(1)	14(1)	-10(1)
C(6)	60(1)	37(1)	59(2)	-2(1)	9(1)	-2(1)
C(7)	63(1)	38(1)	46(1)	7(1)	10(1)	5(1)
C(8)	42(1)	34(1)	42(1)	-1(1)	5(1)	1(1)
C(9)	43(1)	35(1)	56(1)	3(1)	9(1)	7(1)
C(10)	43(1)	34(1)	44(1)	-3(1)	2(1)	0(1)
C(11)	43(1)	33(1)	39(1)	-5(1)	5(1)	-4(1)
C(12)	52(1)	44(1)	57(1)	8(1)	14(1)	5(1)
C(13)	44(1)	53(2)	91(2)	0(1)	12(1)	6(1)
C(14)	53(2)	64(2)	87(2)	-23(2)	31(1)	-16(1)
C(15)	77(2)	89(2)	53(2)	-2(1)	23(1)	-23(2)
C(16)	59(2)	67(2)	44(1)	4(1)	3(1)	-5(1)
N(1)	58(1)	32(1)	67(1)	-10(1)	23(1)	-8(1)
O(3)	165(2)	63(1)	44(1)	4(1)	-6(1)	37(1)
O(2)	62(1)	34(1)	42(1)	2(1)	10(1)	6(1)
O(1)	67(1)	45(1)	68(1)	12(1)	24(1)	3(1)

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

	x	y	z	U(eq)
H(2)	4004	4831	8293	64
H(3)	4215	4111	6339	78
H(4)	2900	4069	2859	81
H(5)	1407	4750	1279	78
H(6)	1247	5482	3180	62
H(8)	553	6100	5555	47
H(10)	2686	6589	8884	49
H(12)	-1057	7148	5919	61
H(13)	-3713	7231	7051	75
H(14)	-4207	6870	10176	79
H(15)	-2040	6430	12206	86
H(16)	606	6333	11089	69
H(1)	2640(30)	7308(5)	6730(30)	61