

X-ray Data Collection, Structure Solution and Refinement for **9**.

A colorless crystal of approximate dimensions 0.13 x 0.17 x 0.30 mm was mounted on a glass fiber and transferred to a Bruker CCD platform diffractometer. The SMART<sup>1</sup> program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a hemisphere of diffraction data). The raw frame data was processed using SAINT<sup>2</sup> and SADABS<sup>3</sup> to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL<sup>4</sup> program. The diffraction symmetry was  $2/m$  and the systematic absences were consistent with the monoclinic space groups  $Cc$  or  $C2/c$ . It was later determined that the centrosymmetric space group  $C2/c$  was correct.

The structure was solved by direct methods and refined on  $F^2$  by full-matrix least-squares techniques. The analytical scattering factors<sup>5</sup> for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined ( $x, y, z$  and  $U_{iso}$ ).

At convergence,  $wR2 = 0.0884$  and  $GOF = 1.055$  for 145 variables refined against 1797 unique data (As a comparison for refinement on  $F$ ,  $R1 = 0.0368$  for those 1541 data with  $I > 2.0\sigma(I)$ ).

## References.

1. SMART Software Users Guide, Version 4.21, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
2. SAINT Software Users Guide, Version 4.05, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
3. Sheldrick, G. M. SADABS, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
4. Sheldrick, G. M. SHELXTL Version 5.10, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
5. International Tables for X-Ray Crystallography 1992, Vol. C., Dordrecht: Kluwer Academic Publishers.

## Definitions:

$$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$$

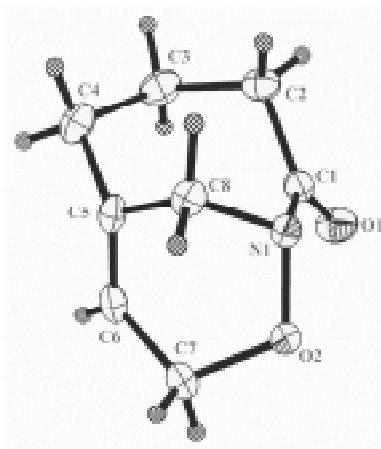
$$R1 = \sum||F_o| - |F_c|| / \sum|F_o|$$

$Goof = S = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$  where  $n$  is the number of reflections and  $p$  is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

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

Identification code	<b>9</b>	
Empirical formula	C <sub>8</sub> H <sub>11</sub> N O <sub>2</sub>	
Formula weight	153.18	
Temperature	158 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 25.133(2) Å	α = 90°.
	b = 5.5289(4) Å	β = 109.0120(10)°.
	c = 11.6527(9) Å	γ = 90°.
Volume	1530.9(2) Å <sup>3</sup>	
Z	8	
Density (calculated)	1.329 Mg/m <sup>3</sup>	
Absorption coefficient	0.096 mm <sup>-1</sup>	
F(000)	656	
Crystal size	0.30 x 0.17 x 0.13 mm <sup>3</sup>	
Theta range for data collection	1.71 to 28.32°.	
Index ranges	-33 ≤ h ≤ 32, -7 ≤ k ≤ 7, -15 ≤ l ≤ 13	
Reflections collected	4616	
Independent reflections	1797 [R(int) = 0.0254]	
Completeness to theta = 28.32°	94.2 %	
Absorption correction	None	
Max. and min. transmission	0.9876 and 0.9718	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	1797 / 0 / 145	
Goodness-of-fit on F <sup>2</sup>	1.055	
Final R indices [I > 2σ(I)]	R1 = 0.0368, wR2 = 0.0838	
R indices (all data)	R1 = 0.0449, wR2 = 0.0884	
Extinction coefficient	0.0024(8)	
Largest diff. peak and hole	0.237 and -0.196 e.Å <sup>-3</sup>	



**Please Note: The atom numbering has changed from that used in the paper.**

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

	x	y	z	$U(\text{eq})$
C(1)	4017(1)	-704(2)	3913(1)	21(1)
C(2)	4434(1)	-2645(2)	4563(1)	24(1)
C(3)	4439(1)	-2952(3)	5883(1)	30(1)
C(4)	3899(1)	-4054(3)	6033(1)	30(1)
C(5)	3399(1)	-2891(2)	5115(1)	22(1)
C(6)	3162(1)	-799(2)	5245(1)	25(1)
C(7)	2807(1)	416(3)	4111(1)	26(1)
C(8)	3287(1)	-3629(2)	3812(1)	21(1)
N(1)	3469(1)	-1491(2)	3268(1)	19(1)
O(1)	4149(1)	1418(2)	3940(1)	31(1)
O(2)	3069(1)	401(2)	3131(1)	23(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **9**.

C(1)-O(1)	1.2168(14)
C(1)-N(1)	1.4065(15)
C(1)-C(2)	1.5184(17)
C(2)-C(3)	1.5441(18)
C(2)-H(2A)	0.974(15)
C(2)-H(2B)	0.949(16)
C(3)-C(4)	1.547(2)
C(3)-H(3A)	0.991(17)
C(3)-H(3B)	0.969(17)
C(4)-C(5)	1.5038(17)
C(4)-H(4A)	0.986(16)
C(4)-H(4B)	1.018(17)
C(5)-C(6)	1.3331(18)
C(5)-C(8)	1.5064(16)
C(6)-C(7)	1.4923(18)

C(6)-H(6A)	0.946(17)
C(7)-O(2)	1.4920(14)
C(7)-H(7A)	0.986(16)
C(7)-H(7B)	0.983(17)
C(8)-N(1)	1.4827(15)
C(8)-H(8A)	0.967(14)
C(8)-H(8B)	0.970(15)
N(1)-O(2)	1.4239(12)

O(1)-C(1)-N(1)	121.55(11)
O(1)-C(1)-C(2)	122.08(11)
N(1)-C(1)-C(2)	116.37(10)
C(1)-C(2)-C(3)	110.80(10)
C(1)-C(2)-H(2A)	106.7(9)
C(3)-C(2)-H(2A)	108.8(8)
C(1)-C(2)-H(2B)	112.3(9)
C(3)-C(2)-H(2B)	110.1(9)
H(2A)-C(2)-H(2B)	108.0(12)
C(2)-C(3)-C(4)	115.67(11)
C(2)-C(3)-H(3A)	107.5(9)
C(4)-C(3)-H(3A)	109.4(9)
C(2)-C(3)-H(3B)	106.8(9)
C(4)-C(3)-H(3B)	111.3(10)
H(3A)-C(3)-H(3B)	105.5(13)
C(5)-C(4)-C(3)	108.12(10)
C(5)-C(4)-H(4A)	109.2(9)
C(3)-C(4)-H(4A)	110.5(9)
C(5)-C(4)-H(4B)	111.3(9)
C(3)-C(4)-H(4B)	108.6(9)
H(4A)-C(4)-H(4B)	109.1(13)
C(6)-C(5)-C(4)	126.20(12)
C(6)-C(5)-C(8)	113.95(11)
C(4)-C(5)-C(8)	116.16(11)
C(5)-C(6)-C(7)	116.75(11)
C(5)-C(6)-H(6A)	122.4(10)
C(7)-C(6)-H(6A)	120.2(10)

O(2)-C(7)-C(6)	112.92(10)
O(2)-C(7)-H(7A)	105.9(9)
C(6)-C(7)-H(7A)	112.0(9)
O(2)-C(7)-H(7B)	102.6(9)
C(6)-C(7)-H(7B)	113.6(9)
H(7A)-C(7)-H(7B)	109.1(13)
N(1)-C(8)-C(5)	103.43(9)
N(1)-C(8)-H(8A)	106.5(8)
C(5)-C(8)-H(8A)	112.9(8)
N(1)-C(8)-H(8B)	110.6(8)
C(5)-C(8)-H(8B)	113.3(8)
H(8A)-C(8)-H(8B)	109.7(12)
C(1)-N(1)-O(2)	111.47(9)
C(1)-N(1)-C(8)	113.79(9)
O(2)-N(1)-C(8)	109.15(8)
N(1)-O(2)-C(7)	112.98(8)

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **9**. 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 <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	22(1)	19(1)	23(1)	1(1)	11(1)	1(1)
C(2)	20(1)	19(1)	32(1)	-1(1)	7(1)	0(1)
C(3)	26(1)	31(1)	26(1)	2(1)	-2(1)	3(1)
C(4)	35(1)	31(1)	22(1)	7(1)	5(1)	1(1)
C(5)	23(1)	24(1)	19(1)	4(1)	7(1)	-6(1)
C(6)	27(1)	31(1)	20(1)	0(1)	13(1)	-4(1)
C(7)	25(1)	30(1)	29(1)	5(1)	16(1)	3(1)
C(8)	22(1)	20(1)	20(1)	-1(1)	4(1)	-5(1)
N(1)	21(1)	19(1)	19(1)	1(1)	7(1)	2(1)
O(1)	26(1)	19(1)	48(1)	3(1)	12(1)	-2(1)
O(2)	22(1)	26(1)	22(1)	7(1)	10(1)	7(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **9**.

	x	y	z	U(eq)
H(2A)	4804(6)	-2100(30)	4575(12)	27(4)
H(2B)	4361(6)	-4150(30)	4151(13)	30(4)
H(3A)	4508(6)	-1340(30)	6274(14)	35(4)
H(3B)	4767(7)	-3910(30)	6301(15)	37(4)
H(4A)	3885(6)	-3730(30)	6855(15)	36(4)
H(4B)	3904(7)	-5870(30)	5904(14)	39(4)
H(6A)	3253(7)	10(30)	5999(15)	37(4)
H(7A)	2437(7)	-380(30)	3763(14)	32(4)
H(7B)	2749(6)	2150(30)	4213(14)	33(4)
H(8A)	2891(6)	-3850(30)	3374(13)	24(3)
H(8B)	3494(6)	-5060(30)	3724(12)	23(3)

Table 6. Torsion angles [ $^\circ$ ] for **9**.

O(1)-C(1)-C(2)-C(3)	88.37(14)
N(1)-C(1)-C(2)-C(3)	-91.99(12)
C(1)-C(2)-C(3)-C(4)	68.66(15)
C(2)-C(3)-C(4)-C(5)	-43.17(16)
C(3)-C(4)-C(5)-C(6)	-84.70(15)
C(3)-C(4)-C(5)-C(8)	72.22(14)
C(4)-C(5)-C(6)-C(7)	160.02(12)
C(8)-C(5)-C(6)-C(7)	2.66(15)
C(5)-C(6)-C(7)-O(2)	-43.84(16)
C(6)-C(5)-C(8)-N(1)	53.80(13)
C(4)-C(5)-C(8)-N(1)	-105.96(12)
O(1)-C(1)-N(1)-O(2)	-24.67(14)
C(2)-C(1)-N(1)-O(2)	155.69(9)
O(1)-C(1)-N(1)-C(8)	-148.62(11)
C(2)-C(1)-N(1)-C(8)	31.74(14)

C(5)-C(8)-N(1)-C(1)	52.19(12)
C(5)-C(8)-N(1)-O(2)	-73.01(11)
C(1)-N(1)-O(2)-C(7)	-93.10(11)
C(8)-N(1)-O(2)-C(7)	33.44(12)
C(6)-C(7)-O(2)-N(1)	23.32(14)

---

### X-ray Data Collection, Structure Solution and Refinement for **10**.

A colorless crystal of approximate dimensions 0.24 x 0.27 x 0.40 mm was mounted on a glass fiber and transferred to a Bruker CCD platform diffractometer. The SMART<sup>1</sup> program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a hemisphere of diffraction data). The raw frame data was processed using SAINT<sup>2</sup> and SADABS<sup>3</sup> to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL<sup>4</sup> program. The diffraction symmetry was  $2/m$  and the systematic absences were consistent with the monoclinic space groups  $Cc$  or  $C2/c$ . It was later determined that the centrosymmetric space group  $C2/c$  was correct.

The structure was solved by direct methods and refined on  $F^2$  by full-matrix least-squares techniques. The analytical scattering factors<sup>5</sup> for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined ( $x, y, z$  and  $U_{iso}$ ).

At convergence,  $wR2 = 0.0849$  and  $GOF = 1.020$  for 162 variables refined against 2001 unique data (As a comparison for refinement on  $F$ ,  $R1 = 0.0337$  for those 1854 data with  $I > 2.0\sigma(I)$ ).

### References.

6. SMART Software Users Guide, Version 4.21, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
  7. SAINT Software Users Guide, Version 4.05, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
  8. Sheldrick, G. M. SADABS, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
  9. Sheldrick, G. M. SHELXTL Version 5.10, Bruker Analytical X-Ray Systems, Inc.; Madison, WI 1997.
  10. International Tables for X-Ray Crystallography 1992, Vol. C., Dordrecht: Kluwer Academic Publishers.
-



Definitions:

$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$$

$$R1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$$

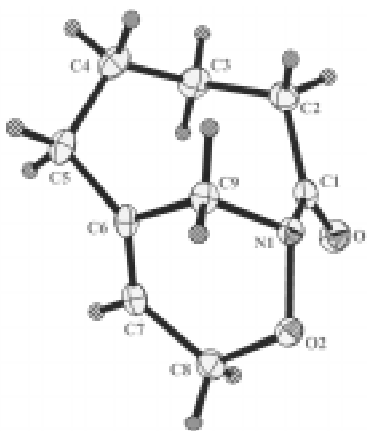
Goof = S =  $[\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$  where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

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

Identification code	<b>10</b>	
Empirical formula	C <sub>9</sub> H <sub>13</sub> N O <sub>2</sub>	
Formula weight	167.20	
Temperature	158 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 24.2267(16) Å	α = 90°.
	b = 6.0297(4) Å	β = 99.5230(10)°.
	c = 11.6827(8) Å	γ = 90°.
Volume	1683.1(2) Å <sup>3</sup>	
Z	8	
Density (calculated)	1.320 Mg/m <sup>3</sup>	
Absorption coefficient	0.093 mm <sup>-1</sup>	
F(000)	720	
Crystal size	0.40 x 0.27 x 0.24 mm <sup>3</sup>	
Theta range for data collection	1.70 to 28.32°.	
Index ranges	-31 ≤ h ≤ 29, -7 ≤ k ≤ 8, -15 ≤ l ≤ 14	
Reflections collected	5201	
Independent reflections	2001 [R(int) = 0.0153]	
Completeness to theta = 28.32°	95.6 %	
Absorption correction	None	
Max. and min. transmission	0.9780 and 0.9636	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	

Data / restraints / parameters	2001 / 0 / 162
Goodness-of-fit on $F^2$	1.020
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0337, wR2 = 0.0824
R indices (all data)	R1 = 0.0368, wR2 = 0.0849
Extinction coefficient	0.0040(9)
Largest diff. peak and hole	0.330 and -0.189 e. $\text{\AA}^{-3}$



**Please Note: The atom numbering has changed from that used in the paper.**

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

	x	y	z	U(eq)
C(1)	4007(1)	641(2)	5171(1)	18(1)
C(2)	4467(1)	2266(2)	5010(1)	21(1)
C(3)	4532(1)	2637(2)	3720(1)	24(1)
C(4)	4209(1)	4604(2)	3093(1)	24(1)
C(5)	3597(1)	4133(2)	2525(1)	21(1)
C(6)	3295(1)	2778(2)	3307(1)	17(1)
C(7)	3100(1)	742(2)	3049(1)	19(1)
C(8)	2908(1)	-763(2)	3925(1)	21(1)
C(9)	3317(1)	3523(2)	4551(1)	17(1)
N(1)	3491(1)	1575(1)	5282(1)	17(1)
O(1)	4087(1)	-1356(1)	5226(1)	25(1)
O(2)	3044(1)	22(1)	5121(1)	19(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **10**.

C(1)-O(1)	1.2194(13)
C(1)-N(1)	1.3977(12)
C(1)-C(2)	1.5183(14)
C(2)-C(3)	1.5570(14)
C(2)-H(2A)	0.976(13)
C(2)-H(2B)	0.979(13)
C(3)-C(4)	1.5385(15)
C(3)-H(3A)	1.006(14)
C(3)-H(3B)	0.977(14)
C(4)-C(5)	1.5461(15)
C(4)-H(4A)	0.991(13)
C(4)-H(4B)	0.994(15)
C(5)-C(6)	1.5034(13)

C(5)-H(5A)	0.968(13)
C(5)-H(5B)	0.989(13)
C(6)-C(7)	1.3323(14)
C(6)-C(9)	1.5137(13)
C(7)-C(8)	1.4971(14)
C(7)-H(7A)	0.951(14)
C(8)-O(2)	1.4608(12)
C(8)-H(8A)	0.990(14)
C(8)-H(8B)	0.994(14)
C(9)-N(1)	1.4721(12)
C(9)-H(9A)	0.968(12)
C(9)-H(9B)	0.976(13)
N(1)-O(2)	1.4209(10)

O(1)-C(1)-N(1)	121.93(9)
O(1)-C(1)-C(2)	122.09(9)
N(1)-C(1)-C(2)	115.97(8)
C(1)-C(2)-C(3)	113.96(8)
C(1)-C(2)-H(2A)	111.3(8)
C(3)-C(2)-H(2A)	109.8(8)
C(1)-C(2)-H(2B)	104.9(8)
C(3)-C(2)-H(2B)	109.1(8)
H(2A)-C(2)-H(2B)	107.5(11)
C(4)-C(3)-C(2)	116.56(9)
C(4)-C(3)-H(3A)	110.6(8)
C(2)-C(3)-H(3A)	108.3(8)
C(4)-C(3)-H(3B)	108.0(8)
C(2)-C(3)-H(3B)	105.5(8)
H(3A)-C(3)-H(3B)	107.4(11)
C(3)-C(4)-C(5)	116.03(9)
C(3)-C(4)-H(4A)	108.5(8)
C(5)-C(4)-H(4A)	111.4(7)
C(3)-C(4)-H(4B)	108.2(8)
C(5)-C(4)-H(4B)	107.0(8)
H(4A)-C(4)-H(4B)	105.1(11)
C(6)-C(5)-C(4)	111.52(8)

C(6)-C(5)-H(5A)	108.3(8)
C(4)-C(5)-H(5A)	109.6(7)
C(6)-C(5)-H(5B)	111.7(8)
C(4)-C(5)-H(5B)	108.6(8)
H(5A)-C(5)-H(5B)	107.0(10)
C(7)-C(6)-C(5)	123.62(9)
C(7)-C(6)-C(9)	116.46(8)
C(5)-C(6)-C(9)	118.64(9)
C(6)-C(7)-C(8)	122.86(9)
C(6)-C(7)-H(7A)	121.2(8)
C(8)-C(7)-H(7A)	115.7(8)
O(2)-C(8)-C(7)	114.31(8)
O(2)-C(8)-H(8A)	107.9(8)
C(7)-C(8)-H(8A)	107.9(8)
O(2)-C(8)-H(8B)	103.0(8)
C(7)-C(8)-H(8B)	113.0(8)
H(8A)-C(8)-H(8B)	110.5(11)
N(1)-C(9)-C(6)	106.35(7)
N(1)-C(9)-H(9A)	109.8(7)
C(6)-C(9)-H(9A)	113.0(7)
N(1)-C(9)-H(9B)	106.0(8)
C(6)-C(9)-H(9B)	112.4(8)
H(9A)-C(9)-H(9B)	109.1(10)
C(1)-N(1)-O(2)	113.35(8)
C(1)-N(1)-C(9)	116.23(7)
O(2)-N(1)-C(9)	108.10(7)
N(1)-O(2)-C(8)	112.69(7)

---

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **10**. 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 <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	18(1)	22(1)	12(1)	1(1)	1(1)	2(1)
C(2)	17(1)	25(1)	22(1)	0(1)	2(1)	-1(1)
C(3)	19(1)	28(1)	25(1)	2(1)	9(1)	1(1)
C(4)	27(1)	24(1)	24(1)	4(1)	11(1)	-2(1)
C(5)	28(1)	21(1)	16(1)	3(1)	7(1)	3(1)
C(6)	18(1)	19(1)	14(1)	2(1)	3(1)	6(1)
C(7)	21(1)	22(1)	13(1)	-1(1)	1(1)	4(1)
C(8)	23(1)	20(1)	18(1)	-2(1)	2(1)	-2(1)
C(9)	19(1)	17(1)	15(1)	0(1)	5(1)	3(1)
N(1)	17(1)	19(1)	14(1)	1(1)	3(1)	-1(1)
O(1)	23(1)	22(1)	29(1)	5(1)	3(1)	4(1)
O(2)	18(1)	24(1)	16(1)	1(1)	5(1)	-3(1)

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

	x	y	z	U(eq)
H(2A)	4416(5)	3690(20)	5376(11)	22(3)
H(2B)	4811(5)	1600(20)	5427(12)	27(3)
H(3A)	4431(6)	1220(20)	3282(12)	27(3)
H(3B)	4931(6)	2890(20)	3731(12)	30(3)
H(4A)	4231(5)	5870(20)	3640(11)	23(3)
H(4B)	4410(6)	5110(20)	2465(12)	34(4)
H(5A)	3593(5)	3320(20)	1809(11)	21(3)
H(5B)	3407(6)	5560(20)	2316(11)	24(3)
H(7A)	3107(5)	110(20)	2306(12)	25(3)
H(8A)	3092(5)	-2220(20)	3878(11)	27(3)

H(9A)	3577(5)	4730(20)	4766(10)	16(3)
H(9B)	2950(5)	3950(20)	4718(11)	21(3)
H(8B)	2495(6)	-940(20)	3810(12)	28(3)

---

Table 6. Torsion angles [°] for **10**.

O(1)-C(1)-C(2)-C(3)	85.35(12)
N(1)-C(1)-C(2)-C(3)	-96.25(10)
C(1)-C(2)-C(3)-C(4)	93.42(11)
C(2)-C(3)-C(4)-C(5)	-86.43(12)
C(3)-C(4)-C(5)-C(6)	43.21(12)
C(4)-C(5)-C(6)-C(7)	-116.27(11)
C(4)-C(5)-C(6)-C(9)	50.31(12)
C(5)-C(6)-C(7)-C(8)	166.91(9)
C(9)-C(6)-C(7)-C(8)	0.07(14)
C(6)-C(7)-C(8)-O(2)	-10.19(14)
C(7)-C(6)-C(9)-N(1)	38.49(11)
C(5)-C(6)-C(9)-N(1)	-129.04(9)
O(1)-C(1)-N(1)-O(2)	-17.37(12)
C(2)-C(1)-N(1)-O(2)	164.23(7)
O(1)-C(1)-N(1)-C(9)	-143.53(9)
C(2)-C(1)-N(1)-C(9)	38.07(11)
C(6)-C(9)-N(1)-C(1)	58.97(10)
C(6)-C(9)-N(1)-O(2)	-69.78(9)
C(1)-N(1)-O(2)-C(8)	-68.54(9)
C(9)-N(1)-O(2)-C(8)	61.82(9)
C(7)-C(8)-O(2)-N(1)	-21.31(11)

---