

# The Effect of Varying Substituents on the Equilibrium Distribution and Conformation of Macrocyclic Steroidal N–Acyl Hydrazones

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## Supplementary Data 2. Crystallographic data and structure refinement for 10.

These crystals were only weakly diffracting and, the molecule suffered from severe disorder around the *iso*-nicotinate groups. By comparison with conventional small molecule crystallography, the R-factors rather large; while this limits the precision with which one can determine bond lengths and angles, it does not detract from our ability to draw conclusions concerning the geometry of the N–acyl hydrazone.

## Supplementary Data 2. Crystallographic data and structure refinement for 10.

Identification code	js9937 (10)	
Empirical formula	C <sub>78</sub> H <sub>98</sub> Cl <sub>4</sub> N <sub>6</sub> O <sub>10</sub>	
Formula weight	1421.42	
Temperature	180(2) K	
Wavelength	0.71069 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2	
Unit cell dimensions	a = 21.2775(15) Å	α = 90°.
	b = 20.0853(15) Å	β = 90°.
	c = 20.3763(9) Å	γ = 90°.
Volume	8708.1(10) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.084 Mg/m <sup>3</sup>	
Absorption coefficient	0.189 mm <sup>-1</sup>	
F(000)	3024	
Crystal size	0.23 x 0.23 x 0.20 mm <sup>3</sup>	
Theta range for data collection	3.52 to 22.52°.	
Index ranges	-22 ≤ h ≤ 22, -21 ≤ k ≤ 21, -21 ≤ l ≤ 21	
Reflections collected	22500	
Independent reflections	11348 [R(int) = 0.1034]	
Completeness to theta = 22.50°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	11348 / 35 / 771	

Goodness-of-fit on $F^2$	1.448
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.1432$ , $wR_2 = 0.3681$
R indices (all data)	$R_1 = 0.1859$ , $wR_2 = 0.4052$
Absolute structure parameter	-0.1(3)
Largest diff. peak and hole	1.566 and -1.243 e.Å <sup>-3</sup>

**Table 1.1** 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	$U(\text{eq})$
O(1)	4464(4)	703(4)	6971(3)	70(2)
O(2)	9036(4)	1262(5)	4657(4)	101(3)
O(3)	8280(3)	1598(3)	3979(3)	65(2)
O(4)	5849(3)	620(4)	-1989(3)	67(2)
O(5)	1340(4)	1432(5)	288(4)	90(2)
O(6)	2078(3)	1793(3)	966(3)	60(2)
N(1)	5459(4)	741(4)	6638(4)	62(2)
N(2)	5902(4)	929(4)	6186(3)	52(2)
N(3)	4857(4)	781(4)	-1700(4)	54(2)
N(4)	4434(4)	949(3)	-1218(3)	51(2)
C(1)	1509(5)	2696(5)	2449(5)	60(3)
C(2)	1922(5)	2529(5)	1863(5)	65(3)
C(3)	1633(5)	1966(5)	1475(4)	57(2)
C(4)	1512(5)	1358(5)	1892(4)	58(2)
C(5)	1139(5)	1515(4)	2510(5)	55(2)
C(6)	1018(5)	889(5)	2927(5)	60(2)
C(7)	1614(5)	674(5)	3304(5)	62(3)
C(8)	1920(5)	1237(4)	3683(4)	54(2)
C(9)	2011(4)	1846(4)	3235(4)	48(2)
C(10)	1404(4)	2077(5)	2900(4)	55(2)
C(11)	2396(5)	2402(4)	3569(4)	49(2)
C(12)	3007(5)	2183(4)	3895(4)	53(2)
C(13)	2898(5)	1575(5)	4346(4)	57(2)
C(14)	2527(5)	1015(4)	3964(4)	56(3)
C(15)	2558(6)	453(4)	4428(5)	71(3)
C(16)	3165(6)	538(5)	4835(5)	70(3)
C(17)	3451(5)	1196(5)	4606(5)	62(3)
C(18)	2509(6)	1836(5)	4928(4)	68(3)
C(19)	911(5)	2339(5)	3444(4)	63(3)
C(20)	3888(5)	1531(4)	5106(4)	54(2)
C(21)	4344(7)	2048(6)	4777(6)	93(4)
C(22)	4272(5)	1040(5)	5515(4)	64(3)
C(23)	4661(5)	1397(5)	6022(5)	62(3)
C(24)	4852(6)	911(5)	6585(4)	64(3)
C(25)	6467(5)	739(5)	6298(4)	58(3)
C(26)	6970(5)	892(4)	5862(4)	51(2)
C(27)	7595(6)	764(5)	6024(5)	67(3)
C(28)	8083(6)	922(5)	5602(5)	73(3)
C(29)	7948(5)	1199(4)	4984(4)	55(2)
C(30)	7331(5)	1339(4)	4832(4)	53(2)
C(31)	6847(5)	1189(5)	5242(4)	55(2)
C(32)	8491(7)	1344(6)	4552(5)	70(3)
C(33)	8858(5)	2579(4)	2549(4)	54(2)

C(34)	8452(5)	2375(5)	3106(5)	62(3)
C(35)	8757(5)	1800(5)	3474(4)	58(3)
C(36)	8902(5)	1221(5)	3059(5)	60(3)
C(37)	9299(4)	1416(4)	2453(4)	52(2)
C(38)	9448(5)	833(5)	1985(5)	66(3)
C(39)	8851(5)	592(5)	1625(5)	64(3)
C(40)	8546(5)	1154(4)	1244(5)	55(2)
C(41)	8410(4)	1716(4)	1727(4)	48(2)
C(42)	9008(4)	1997(4)	2056(4)	49(2)
C(43)	8012(4)	2302(4)	1393(4)	48(2)
C(44)	7400(4)	2025(4)	1105(4)	51(2)
C(45)	7541(4)	1462(4)	602(4)	46(2)
C(46)	7933(5)	918(4)	939(4)	55(2)
C(47)	7940(6)	359(4)	445(5)	72(3)
C(48)	7311(6)	435(5)	74(5)	75(3)
C(49)	6979(4)	1049(4)	344(4)	49(2)
C(50)	7899(5)	1773(5)	20(4)	57(2)
C(51)	9475(5)	2263(5)	1539(5)	61(3)
C(52)	6501(5)	1419(5)	-121(4)	55(2)
C(53)	6046(6)	1837(6)	278(6)	83(3)
C(54)	6156(5)	894(5)	-563(4)	58(2)
C(55)	5672(5)	1268(5)	-1004(4)	58(2)
C(56)	5475(5)	864(4)	-1581(4)	51(2)
C(57)	3851(5)	823(4)	-1369(4)	49(2)
C(58)	3350(4)	1006(4)	-912(4)	48(2)
C(59)	2720(5)	956(4)	-1094(5)	57(3)
C(60)	2244(5)	1119(5)	-660(4)	58(3)
C(61)	2382(4)	1354(4)	-46(4)	46(2)
C(62)	3009(5)	1426(5)	127(5)	60(3)
C(63)	3490(5)	1262(5)	-278(4)	57(2)
C(64)	1876(5)	1525(5)	404(5)	58(3)
O(8)	3418(3)	1922(3)	3377(3)	65(2)
C(65)	3677(11)	2303(7)	2933(8)	80(3)
O(7)	3667(10)	2899(7)	3019(9)	100(2)
C(66)	3976(11)	1934(11)	2378(9)	105(4)
C(67)	3925(12)	1247(11)	2314(11)	176(3)
C(68)	4195(14)	928(9)	1778(13)	176(3)
N(5)	4516(12)	1296(14)	1307(10)	176(3)
C(69)	4566(12)	1982(14)	1371(10)	176(3)
C(70)	4296(13)	2302(9)	1907(12)	176(3)
C(65')	3761(12)	2389(8)	3094(11)	80(3)
O(7')	3768(13)	2984(8)	3188(11)	100(2)
C(66')	4206(12)	2088(12)	2606(12)	105(4)
C(67')	4490(15)	2422(11)	2087(14)	176(3)
C(68')	4925(14)	2094(17)	1693(13)	176(3)
N(5')	5075(13)	1433(17)	1818(15)	176(3)
C(69')	4791(16)	1099(12)	2336(16)	176(3)
C(70')	4357(14)	1426(13)	2730(12)	176(3)
O(10)	7019(3)	1748(3)	1608(3)	58(2)

C(71)	6706(6)	2131(6)	2006(6)	80(3)
O(9)	6637(5)	2709(5)	1874(4)	100(2)
C(72)	6434(6)	1790(6)	2578(5)	105(4)
C(73)	6068(7)	2137(5)	3027(7)	176(3)
C(74)	5817(7)	1809(8)	3568(6)	176(3)
N(6)	5932(7)	1134(8)	3658(6)	176(3)
C(75)	6298(8)	787(5)	3209(8)	176(3)
C(76)	6549(6)	1115(6)	2668(6)	176(3)
CI(1)	10370(7)	-1562(8)	9566(6)	142(1)
CI(2)	9696(7)	-1132(8)	8467(6)	142(1)
C(77)	9790(20)	-1080(30)	9283(9)	153(7)
CI(3)	8638(4)	520(4)	8530(4)	142(1)
CI(4)	7441(3)	740(4)	7972(4)	142(1)
C(78)	8208(6)	893(13)	7955(11)	153(7)
CI(5)	5741(8)	3199(6)	4642(7)	142(1)
CI(6)	5735(8)	4532(6)	5014(7)	142(1)
C(79)	5328(14)	3907(11)	4660(30)	153(7)
CI(7)	1614(4)	822(4)	-3519(4)	142(1)
CI(8)	2848(4)	916(4)	-3075(4)	142(1)
C(80)	2112(6)	1204(12)	-3018(12)	153(7)

**Table 1.2.** Bond lengths [Å] and angles [°] for **10**

O(1)-C(24)	1.215(12)	O(2)-C(32)	1.191(14)
O(3)-C(32)	1.350(12)	O(3)-C(35)	1.500(11)
O(4)-C(56)	1.253(11)	O(5)-C(64)	1.180(12)
O(6)-C(64)	1.337(11)	O(6)-C(3)	1.447(11)
N(1)-C(24)	1.341(13)	N(1)-N(2)	1.371(11)
N(1)-H(1)	0.8800	N(2)-C(25)	1.281(12)
N(3)-C(56)	1.347(12)	N(3)-N(4)	1.374(10)
N(3)-H(3)	0.8800	N(4)-C(57)	1.302(12)
C(1)-C(2)	1.519(13)	C(1)-C(10)	1.563(13)
C(1)-H(1A)	0.9900	C(1)-H(1B)	0.9900
C(2)-C(3)	1.510(13)	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	C(3)-C(4)	1.509(13)
C(3)-H(3A)	1.0000	C(4)-C(5)	1.523(13)
C(4)-H(4A)	0.9900	C(4)-H(4B)	0.9900
C(5)-C(10)	1.490(13)	C(5)-C(6)	1.539(13)
C(5)-H(5)	1.0000	C(6)-C(7)	1.546(15)
C(6)-H(6A)	0.9900	C(6)-H(6B)	0.9900
C(7)-C(8)	1.517(13)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-C(14)	1.480(14)
C(8)-C(9)	1.539(12)	C(8)-H(8)	1.0000
C(9)-C(10)	1.533(13)	C(9)-C(11)	1.544(12)
C(9)-H(9)	1.0000	C(10)-C(19)	1.615(13)
C(11)-C(12)	1.525(13)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	C(12)-O(8)	1.467(11)
C(12)-C(13)	1.547(12)	C(12)-H(12)	1.0000
C(13)-C(17)	1.496(14)	C(13)-C(18)	1.538(14)
C(13)-C(14)	1.580(13)	C(14)-C(15)	1.474(12)
C(14)-H(14)	1.0000	C(15)-C(16)	1.546(15)
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-C(17)	1.529(13)	C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900	C(17)-C(20)	1.534(13)
C(17)-H(17)	1.0000	C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800	C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800	C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800	C(20)-C(22)	1.529(13)
C(20)-C(21)	1.571(15)	C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800	C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800	C(22)-C(23)	1.505(13)
C(22)-H(22A)	0.9900	C(22)-H(22B)	0.9900
C(23)-C(24)	1.560(14)	C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900	C(25)-C(26)	1.424(14)
C(25)-H(25)	0.9500	C(26)-C(27)	1.395(15)
C(26)-C(31)	1.423(13)	C(27)-C(28)	1.385(15)
C(27)-H(27)	0.9500	C(28)-C(29)	1.407(14)
C(28)-H(28)	0.9500	C(29)-C(30)	1.378(14)
C(29)-C(32)	1.481(16)	C(30)-C(31)	1.359(13)
C(30)-H(30)	0.9500	C(31)-H(31)	0.9500

C(33)-C(34)	1.485(13)	C(33)-C(42)	1.574(12)
C(33)-H(33A)	0.9900	C(33)-H(33B)	0.9900
C(34)-C(35)	1.521(14)	C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900	C(35)-C(36)	1.471(14)
C(35)-H(35)	1.0000	C(36)-C(37)	1.547(13)
C(36)-H(36A)	0.9900	C(36)-H(36B)	0.9900
C(37)-C(38)	1.542(13)	C(37)-C(42)	1.549(12)
C(37)-H(37)	1.0000	C(38)-C(39)	1.545(15)
C(38)-H(38A)	0.9900	C(38)-H(38B)	0.9900
C(39)-C(40)	1.516(13)	C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900	C(40)-C(46)	1.521(13)
C(40)-C(41)	1.526(12)	C(40)-H(40)	1.0000
C(41)-C(42)	1.545(13)	C(41)-C(43)	1.602(11)
C(41)-H(41)	1.0000	C(42)-C(51)	1.545(13)
C(43)-C(44)	1.534(13)	C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900	C(44)-O(10)	1.419(11)
C(44)-C(45)	1.555(12)	C(44)-H(44)	1.0000
C(45)-C(46)	1.538(12)	C(45)-C(50)	1.542(13)
C(45)-C(49)	1.547(13)	C(46)-C(47)	1.507(12)
C(46)-H(46)	1.0000	C(47)-C(48)	1.543(16)
C(47)-H(47A)	0.9900	C(47)-H(47B)	0.9900
C(48)-C(49)	1.523(13)	C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900	C(49)-C(52)	1.577(12)
C(49)-H(49)	1.0000	C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800	C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800	C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800	C(52)-C(53)	1.519(15)
C(52)-C(54)	1.570(13)	C(52)-H(52)	1.0000
C(53)-H(53A)	0.9800	C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800	C(54)-C(55)	1.560(13)
C(54)-H(54A)	0.9900	C(54)-H(54B)	0.9900
C(55)-C(56)	1.488(13)	C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900	C(57)-C(58)	1.463(13)
C(57)-H(57)	0.9500	C(58)-C(59)	1.394(14)
C(58)-C(63)	1.422(13)	C(59)-C(60)	1.384(14)
C(59)-H(59)	0.9500	C(60)-C(61)	1.369(12)
C(60)-H(60)	0.9500	C(61)-C(62)	1.386(14)
C(61)-C(64)	1.456(14)	C(62)-C(63)	1.356(13)
C(62)-H(62)	0.9500	C(63)-H(63)	0.9500
O(8)-C(65)	1.306(9)	O(8)-C(65')	1.322(9)
C(65)-O(7)	1.210(8)	C(65)-C(66)	1.495(9)
C(66)-C(67)	1.3900	C(66)-C(70)	1.3900
C(67)-C(68)	1.3900	C(67)-H(67)	0.9500
C(68)-N(5)	1.3900	C(68)-H(68)	0.9500
N(5)-C(69)	1.3900	C(69)-C(70)	1.3900
C(69)-H(69)	0.9500	C(70)-H(70)	0.9500
C(65')-O(7')	1.210(9)	C(65')-C(66')	1.501(9)
C(66')-C(67')	1.3900	C(66')-C(70')	1.3900
C(67')-C(68')	1.3900	C(67')-H(67')	0.9500

C(68')-N(5')	1.3900	C(68')-H(68')	0.9500
N(5')-C(69')	1.3900	C(69')-C(70')	1.3900
C(69')-H(69')	0.9500	C(70')-H(70')	0.9500
O(10)-C(71)	1.303(13)	C(71)-O(9)	1.199(13)
C(71)-C(72)	1.469(14)	C(72)-C(73)	1.3900
C(72)-C(76)	1.3900	C(73)-C(74)	1.3900
C(73)-H(73)	0.9500	C(74)-N(6)	1.3900
C(74)-H(74)	0.9500	N(6)-C(75)	1.3900
C(75)-C(76)	1.3900	C(75)-H(75)	0.9500
C(76)-H(76)	0.9500	Cl(1)-C(77)	1.675(11)
Cl(2)-C(77)	1.677(11)	C(77)-H(77A)	0.9900
C(77)-H(77B)	0.9900	Cl(3)-C(78)	1.665(11)
Cl(4)-C(78)	1.661(11)	C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900	Cl(5)-C(79)	1.673(11)
Cl(6)-C(79)	1.683(11)	C(79)-H(79A)	0.9900
C(79)-H(79B)	0.9900	Cl(7)-C(80)	1.660(11)
Cl(8)-C(80)	1.673(11)	C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900	C(32)-O(3)-C(35)	118.1(8)
C(64)-O(6)-C(3)	120.1(8)	C(24)-N(1)-N(2)	122.6(8)
C(24)-N(1)-H(1)	118.7	N(2)-N(1)-H(1)	118.7
C(25)-N(2)-N(1)	116.3(7)	C(56)-N(3)-N(4)	118.7(8)
C(56)-N(3)-H(3)	120.7	N(4)-N(3)-H(3)	120.7
C(57)-N(4)-N(3)	113.9(7)	C(2)-C(1)-C(10)	111.6(7)
C(2)-C(1)-H(1A)	109.3	C(10)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1B)	109.3	C(10)-C(1)-H(1B)	109.3
H(1A)-C(1)-H(1B)	108.0	C(3)-C(2)-C(1)	110.0(8)
C(3)-C(2)-H(2A)	109.7	C(1)-C(2)-H(2A)	109.7
C(3)-C(2)-H(2B)	109.7	C(1)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2	O(6)-C(3)-C(4)	108.7(7)
O(6)-C(3)-C(2)	106.8(8)	C(4)-C(3)-C(2)	112.4(8)
O(6)-C(3)-H(3A)	109.6	C(4)-C(3)-H(3A)	109.6
C(2)-C(3)-H(3A)	109.6	C(3)-C(4)-C(5)	112.7(8)
C(3)-C(4)-H(4A)	109.0	C(5)-C(4)-H(4A)	109.1
C(3)-C(4)-H(4B)	109.1	C(5)-C(4)-H(4B)	109.0
H(4A)-C(4)-H(4B)	107.8	C(10)-C(5)-C(4)	113.6(8)
C(10)-C(5)-C(6)	112.9(8)	C(4)-C(5)-C(6)	111.9(8)
C(10)-C(5)-H(5)	105.9	C(4)-C(5)-H(5)	105.9
C(6)-C(5)-H(5)	105.9	C(5)-C(6)-C(7)	111.5(8)
C(5)-C(6)-H(6A)	109.3	C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3	C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0	C(8)-C(7)-C(6)	113.4(8)
C(8)-C(7)-H(7A)	108.9	C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7B)	108.9	C(6)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7	C(14)-C(8)-C(7)	110.2(8)
C(14)-C(8)-C(9)	111.1(8)	C(7)-C(8)-C(9)	110.1(7)
C(14)-C(8)-H(8)	108.5	C(7)-C(8)-H(8)	108.4
C(9)-C(8)-H(8)	108.5	C(10)-C(9)-C(8)	113.5(7)
C(10)-C(9)-C(11)	115.1(7)	C(8)-C(9)-C(11)	112.3(7)
C(10)-C(9)-H(9)	104.9	C(8)-C(9)-H(9)	104.9



C(11)-C(9)-H(9)	104.9	C(5)-C(10)-C(9)	109.1(7)
C(5)-C(10)-C(1)	110.1(7)	C(9)-C(10)-C(1)	112.5(8)
C(5)-C(10)-C(19)	111.5(8)	C(9)-C(10)-C(19)	109.9(7)
C(1)-C(10)-C(19)	103.7(7)	C(12)-C(11)-C(9)	115.8(7)
C(12)-C(11)-H(11A)	108.3	C(9)-C(11)-H(11A)	108.3
C(12)-C(11)-H(11B)	108.3	C(9)-C(11)-H(11B)	108.3
H(11A)-C(11)-H(11B)	107.4	O(8)-C(12)-C(11)	107.4(7)
O(8)-C(12)-C(13)	103.6(7)	C(11)-C(12)-C(13)	111.0(8)
O(8)-C(12)-H(12)	111.5	C(11)-C(12)-H(12)	111.5
C(13)-C(12)-H(12)	111.5	C(17)-C(13)-C(18)	108.9(8)
C(17)-C(13)-C(12)	119.6(8)	C(18)-C(13)-C(12)	105.7(8)
C(17)-C(13)-C(14)	101.9(7)	C(18)-C(13)-C(14)	110.6(8)
C(12)-C(13)-C(14)	110.1(7)	C(15)-C(14)-C(8)	121.1(9)
C(15)-C(14)-C(13)	101.9(7)	C(8)-C(14)-C(13)	114.3(7)
C(15)-C(14)-H(14)	106.1	C(8)-C(14)-H(14)	106.1
C(13)-C(14)-H(14)	106.1	C(14)-C(15)-C(16)	107.3(8)
C(14)-C(15)-H(15A)	110.3	C(16)-C(15)-H(15A)	110.3
C(14)-C(15)-H(15B)	110.3	C(16)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.5	C(17)-C(16)-C(15)	105.3(7)
C(17)-C(16)-H(16A)	110.7	C(15)-C(16)-H(16A)	110.7
C(17)-C(16)-H(16B)	110.7	C(15)-C(16)-H(16B)	110.7
H(16A)-C(16)-H(16B)	108.8	C(13)-C(17)-C(16)	103.6(8)
C(13)-C(17)-C(20)	119.2(8)	C(16)-C(17)-C(20)	114.7(8)
C(13)-C(17)-H(17)	106.1	C(16)-C(17)-H(17)	106.1
C(20)-C(17)-H(17)	106.1	C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5	H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(22)-C(20)-C(17)	113.8(7)
C(22)-C(20)-C(21)	109.1(9)	C(17)-C(20)-C(21)	112.4(8)
C(22)-C(20)-H(20)	107.0	C(17)-C(20)-H(20)	107.0
C(21)-C(20)-H(20)	107.1	C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5	C(23)-C(22)-C(20)	111.2(8)
C(23)-C(22)-H(22A)	109.4	C(20)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22B)	109.4	C(20)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0	C(22)-C(23)-C(24)	110.5(8)
C(22)-C(23)-H(23A)	109.5	C(24)-C(23)-H(23A)	109.6
C(22)-C(23)-H(23B)	109.5	C(24)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	108.1	O(1)-C(24)-N(1)	121.0(9)
O(1)-C(24)-C(23)	121.0(10)	N(1)-C(24)-C(23)	118.0(9)
N(2)-C(25)-C(26)	121.9(9)	N(2)-C(25)-H(25)	119.0
C(26)-C(25)-H(25)	119.0	C(27)-C(26)-C(31)	117.5(9)
C(27)-C(26)-C(25)	122.0(9)	C(31)-C(26)-C(25)	120.5(9)
C(28)-C(27)-C(26)	121.8(9)	C(28)-C(27)-H(27)	119.1
C(26)-C(27)-H(27)	119.1	C(27)-C(28)-C(29)	119.5(11)

C(27)-C(28)-H(28)	120.2	C(29)-C(28)-H(28)	120.2
C(30)-C(29)-C(28)	118.5(10)	C(30)-C(29)-C(32)	124.6(9)
C(28)-C(29)-C(32)	116.8(10)	C(31)-C(30)-C(29)	122.5(8)
C(31)-C(30)-H(30)	118.7	C(29)-C(30)-H(30)	118.7
C(30)-C(31)-C(26)	120.0(9)	C(30)-C(31)-H(31)	120.0
C(26)-C(31)-H(31)	120.0	O(2)-C(32)-O(3)	122.1(10)
O(2)-C(32)-C(29)	128.6(9)	O(3)-C(32)-C(29)	109.3(10)
C(34)-C(33)-C(42)	113.6(7)	C(34)-C(33)-H(33A)	108.8
C(42)-C(33)-H(33A)	108.8	C(34)-C(33)-H(33B)	108.8
C(42)-C(33)-H(33B)	108.8	H(33A)-C(33)-H(33B)	107.7
C(33)-C(34)-C(35)	109.7(8)	C(33)-C(34)-H(34A)	109.7
C(35)-C(34)-H(34A)	109.7	C(33)-C(34)-H(34B)	109.7
C(35)-C(34)-H(34B)	109.7	H(34A)-C(34)-H(34B)	108.2
C(36)-C(35)-O(3)	108.8(8)	C(36)-C(35)-C(34)	114.0(7)
O(3)-C(35)-C(34)	104.8(8)	C(36)-C(35)-H(35)	109.7
O(3)-C(35)-H(35)	109.7	C(34)-C(35)-H(35)	109.7
C(35)-C(36)-C(37)	111.9(7)	C(35)-C(36)-H(36A)	109.2
C(37)-C(36)-H(36A)	109.2	C(35)-C(36)-H(36B)	109.2
C(37)-C(36)-H(36B)	109.2	H(36A)-C(36)-H(36B)	107.9
C(38)-C(37)-C(36)	114.4(8)	C(38)-C(37)-C(42)	109.4(7)
C(36)-C(37)-C(42)	112.9(7)	C(38)-C(37)-H(37)	106.5
C(36)-C(37)-H(37)	106.5	C(42)-C(37)-H(37)	106.5
C(37)-C(38)-C(39)	111.2(8)	C(37)-C(38)-H(38A)	109.4
C(39)-C(38)-H(38A)	109.4	C(37)-C(38)-H(38B)	109.4
C(39)-C(38)-H(38B)	109.4	H(38A)-C(38)-H(38B)	108.0
C(40)-C(39)-C(38)	111.2(8)	C(40)-C(39)-H(39A)	109.4
C(38)-C(39)-H(39A)	109.4	C(40)-C(39)-H(39B)	109.4
C(38)-C(39)-H(39B)	109.4	H(39A)-C(39)-H(39B)	108.0
C(39)-C(40)-C(46)	110.1(7)	C(39)-C(40)-C(41)	107.5(7)
C(46)-C(40)-C(41)	109.3(8)	C(39)-C(40)-H(40)	109.9
C(46)-C(40)-H(40)	109.9	C(41)-C(40)-H(40)	109.9
C(40)-C(41)-C(42)	113.1(7)	C(40)-C(41)-C(43)	111.7(7)
C(42)-C(41)-C(43)	110.6(7)	C(40)-C(41)-H(41)	107.0
C(42)-C(41)-H(41)	107.0	C(43)-C(41)-H(41)	107.0
C(51)-C(42)-C(41)	111.2(7)	C(51)-C(42)-C(37)	111.1(8)
C(41)-C(42)-C(37)	106.3(7)	C(51)-C(42)-C(33)	107.9(7)
C(41)-C(42)-C(33)	112.4(7)	C(37)-C(42)-C(33)	107.9(7)
C(44)-C(43)-C(41)	110.1(7)	C(44)-C(43)-H(43A)	109.6
C(41)-C(43)-H(43A)	109.6	C(44)-C(43)-H(43B)	109.6
C(41)-C(43)-H(43B)	109.6	H(43A)-C(43)-H(43B)	108.1
O(10)-C(44)-C(43)	110.6(7)	O(10)-C(44)-C(45)	107.5(6)
C(43)-C(44)-C(45)	110.6(7)	O(10)-C(44)-H(44)	109.4
C(43)-C(44)-H(44)	109.4	C(45)-C(44)-H(44)	109.4
C(46)-C(45)-C(50)	111.2(7)	C(46)-C(45)-C(49)	100.9(6)
C(50)-C(45)-C(49)	109.8(7)	C(46)-C(45)-C(44)	109.1(7)
C(50)-C(45)-C(44)	107.9(7)	C(49)-C(45)-C(44)	117.7(7)
C(47)-C(46)-C(40)	119.8(9)	C(47)-C(46)-C(45)	103.6(7)
C(40)-C(46)-C(45)	115.2(7)	C(47)-C(46)-H(46)	105.7
C(40)-C(46)-H(46)	105.7	C(45)-C(46)-H(46)	105.7

C(46)-C(47)-C(48)	104.2(8)	C(46)-C(47)-H(47A)	110.9
C(48)-C(47)-H(47A)	110.9	C(46)-C(47)-H(47B)	110.9
C(48)-C(47)-H(47B)	110.9	H(47A)-C(47)-H(47B)	108.9
C(49)-C(48)-C(47)	107.8(7)	C(49)-C(48)-H(48A)	110.1
C(47)-C(48)-H(48A)	110.2	C(49)-C(48)-H(48B)	110.1
C(47)-C(48)-H(48B)	110.1	H(48A)-C(48)-H(48B)	108.5
C(48)-C(49)-C(45)	101.4(7)	C(48)-C(49)-C(52)	117.6(7)
C(45)-C(49)-C(52)	116.6(7)	C(48)-C(49)-H(49)	106.8
C(45)-C(49)-H(49)	106.8	C(52)-C(49)-H(49)	106.8
C(45)-C(50)-H(50A)	109.5	C(45)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5	C(45)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5	H(50B)-C(50)-H(50C)	109.5
C(42)-C(51)-H(51A)	109.5	C(42)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5	C(42)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5	H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(54)	112.3(8)	C(53)-C(52)-C(49)	110.4(7)
C(54)-C(52)-C(49)	109.2(7)	C(53)-C(52)-H(52)	108.3
C(54)-C(52)-H(52)	108.2	C(49)-C(52)-H(52)	108.3
C(52)-C(53)-H(53A)	109.5	C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5	C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5	H(53B)-C(53)-H(53C)	109.5
C(55)-C(54)-C(52)	108.4(7)	C(55)-C(54)-H(54A)	110.0
C(52)-C(54)-H(54A)	110.0	C(55)-C(54)-H(54B)	110.0
C(52)-C(54)-H(54B)	110.0	H(54A)-C(54)-H(54B)	108.4
C(56)-C(55)-C(54)	112.2(8)	C(56)-C(55)-H(55A)	109.2
C(54)-C(55)-H(55A)	109.2	C(56)-C(55)-H(55B)	109.2
C(54)-C(55)-H(55B)	109.2	H(55A)-C(55)-H(55B)	107.9
O(4)-C(56)-N(3)	116.9(8)	O(4)-C(56)-C(55)	124.0(9)
N(3)-C(56)-C(55)	119.0(9)	N(4)-C(57)-C(58)	119.6(8)
N(4)-C(57)-H(57)	120.2	C(58)-C(57)-H(57)	120.2
C(59)-C(58)-C(63)	117.9(9)	C(59)-C(58)-C(57)	120.9(8)
C(63)-C(58)-C(57)	121.1(9)	C(60)-C(59)-C(58)	121.1(9)
C(60)-C(59)-H(59)	119.4	C(58)-C(59)-H(59)	119.4
C(61)-C(60)-C(59)	120.5(10)	C(61)-C(60)-H(60)	119.7
C(59)-C(60)-H(60)	119.7	C(60)-C(61)-C(62)	118.3(9)
C(60)-C(61)-C(64)	119.8(9)	C(62)-C(61)-C(64)	121.9(8)
C(63)-C(62)-C(61)	123.2(9)	C(63)-C(62)-H(62)	118.4
C(61)-C(62)-H(62)	118.4	C(62)-C(63)-C(58)	118.8(9)
C(62)-C(63)-H(63)	120.6	C(58)-C(63)-H(63)	120.6
O(5)-C(64)-O(6)	123.1(10)	O(5)-C(64)-C(61)	123.6(9)
O(6)-C(64)-C(61)	113.3(9)	C(65)-O(8)-C(65')	18.0(18)
C(65)-O(8)-C(12)	122.7(9)	C(65')-O(8)-C(12)	112.9(10)
O(7)-C(65)-O(8)	118.2(15)	O(7)-C(65)-C(66)	127.4(14)
O(8)-C(65)-C(66)	114.4(13)	C(67)-C(66)-C(70)	120.0
C(67)-C(66)-C(65)	122.1(16)	C(70)-C(66)-C(65)	117.9(16)
C(68)-C(67)-C(66)	120.0	C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0	C(67)-C(68)-N(5)	120.0
C(67)-C(68)-H(68)	120.0	N(5)-C(68)-H(68)	120.0
C(69)-N(5)-C(68)	120.0	C(70)-C(69)-N(5)	120.0

C(70)-C(69)-H(69)	120.0	N(5)-C(69)-H(69)	120.0
C(69)-C(70)-C(66)	120.0	C(69)-C(70)-H(70)	120.0
C(66)-C(70)-H(70)	120.0	O(7')-C(65')-O(8)	129.7(19)
O(7')-C(65')-C(66')	119.7(16)	O(8)-C(65')-C(66')	110.5(15)
C(67')-C(66')-C(70')	120.0	C(67')-C(66')-C(65')	125.7(18)
C(70')-C(66')-C(65')	114.2(18)	C(66')-C(67')-C(68')	120.0
C(66')-C(67')-H(67')	120.0	C(68')-C(67')-H(67')	120.0
N(5')-C(68')-C(67')	120.0	N(5')-C(68')-H(68')	120.0
C(67')-C(68')-H(68')	120.0	C(69')-N(5')-C(68')	120.0
C(70')-C(69')-N(5')	120.0	C(70')-C(69')-H(69')	120.0
N(5')-C(69')-H(69')	120.0	C(69')-C(70')-C(66')	120.0
C(69')-C(70')-H(70')	120.0	C(66')-C(70')-H(70')	120.0
C(71)-O(10)-C(44)	120.7(8)	O(9)-C(71)-O(10)	119.6(11)
O(9)-C(71)-C(72)	125.5(12)	O(10)-C(71)-C(72)	114.8(10)
C(73)-C(72)-C(76)	120.0	C(73)-C(72)-C(71)	120.6(10)
C(76)-C(72)-C(71)	119.4(10)	C(72)-C(73)-C(74)	120.0
C(72)-C(73)-H(73)	120.0	C(74)-C(73)-H(73)	120.0
N(6)-C(74)-C(73)	120.0	N(6)-C(74)-H(74)	120.0
C(73)-C(74)-H(74)	120.0	C(75)-N(6)-C(74)	120.0
N(6)-C(75)-C(76)	120.0	N(6)-C(75)-H(75)	120.0
C(76)-C(75)-H(75)	120.0	C(75)-C(76)-C(72)	120.0
C(75)-C(76)-H(76)	120.0	C(72)-C(76)-H(76)	120.0
Cl(1)-C(77)-Cl(2)	113.0(9)	Cl(1)-C(77)-H(77A)	109.0
Cl(2)-C(77)-H(77A)	109.0	Cl(1)-C(77)-H(77B)	109.0
Cl(2)-C(77)-H(77B)	109.0	H(77A)-C(77)-H(77B)	107.8
Cl(4)-C(78)-Cl(3)	116.3(9)	Cl(4)-C(78)-H(78A)	108.2
Cl(3)-C(78)-H(78A)	108.2	Cl(4)-C(78)-H(78B)	108.2
Cl(3)-C(78)-H(78B)	108.2	H(78A)-C(78)-H(78B)	107.4
Cl(5)-C(79)-Cl(6)	112.0(9)	Cl(5)-C(79)-H(79A)	109.2
Cl(6)-C(79)-H(79A)	109.2	Cl(5)-C(79)-H(79B)	109.2
Cl(6)-C(79)-H(79B)	109.2	H(79A)-C(79)-H(79B)	107.9
Cl(7)-C(80)-Cl(8)	113.3(8)	Cl(7)-C(80)-H(80A)	108.9
Cl(8)-C(80)-H(80A)	108.9	Cl(7)-C(80)-H(80B)	108.9
Cl(8)-C(80)-H(80B)	108.9	H(80A)-C(80)-H(80B)	107.7

Symmetry transformations used to generate equivalent atoms:

**Table 1.3.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **10**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^*2U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
O(1)	69(5)	89(5)	51(4)	-8(4)	-3(4)	2(4)
O(2)	51(5)	166(9)	85(5)	58(6)	-10(4)	-10(5)
O(3)	65(4)	85(4)	44(3)	14(3)	-4(3)	-10(4)
O(4)	53(4)	90(5)	57(4)	4(4)	-6(4)	0(4)
O(5)	60(5)	141(7)	70(4)	-39(5)	6(4)	11(5)
O(6)	48(4)	86(4)	47(3)	-3(3)	8(3)	-4(3)
N(1)	49(5)	88(6)	48(4)	32(4)	6(4)	21(4)
N(2)	54(6)	60(5)	42(4)	-1(3)	-2(4)	8(4)
N(3)	39(5)	65(5)	57(4)	-8(4)	-1(4)	1(4)
N(4)	50(5)	49(4)	55(4)	8(3)	3(4)	6(4)
C(1)	52(6)	53(5)	75(6)	-5(5)	-3(5)	11(5)
C(2)	58(6)	62(6)	74(6)	-1(5)	15(5)	4(5)
C(3)	44(6)	76(6)	49(5)	-16(5)	1(4)	11(5)
C(4)	44(6)	68(6)	61(5)	3(5)	-6(5)	0(5)
C(5)	46(6)	48(5)	70(6)	4(5)	8(5)	-13(4)
C(6)	48(6)	64(6)	67(6)	-4(5)	-2(5)	-6(5)
C(7)	64(7)	67(6)	56(5)	3(5)	6(5)	-15(5)
C(8)	54(6)	49(5)	59(5)	-5(4)	-9(5)	-4(5)
C(9)	43(5)	50(5)	52(5)	-3(4)	15(4)	8(4)
C(10)	47(6)	69(6)	47(5)	1(5)	7(4)	9(5)
C(11)	61(6)	42(5)	45(5)	2(4)	-5(4)	-2(4)
C(12)	51(6)	51(5)	56(5)	6(4)	-3(5)	3(4)
C(13)	61(6)	56(6)	53(5)	12(5)	-5(5)	-7(5)
C(14)	83(8)	41(5)	43(5)	3(4)	8(5)	-4(5)
C(15)	102(9)	31(5)	81(7)	4(5)	-25(7)	-12(5)
C(16)	91(8)	49(5)	69(6)	25(5)	-20(6)	0(5)
C(17)	60(7)	58(6)	68(6)	4(5)	-16(5)	-10(5)
C(18)	79(7)	82(7)	41(5)	-5(5)	9(5)	-16(6)
C(19)	62(7)	79(6)	49(5)	-7(5)	4(5)	12(5)
C(20)	70(7)	43(5)	49(5)	-5(4)	-16(5)	-4(5)
C(21)	107(10)	90(8)	82(7)	30(7)	-44(7)	-29(8)
C(22)	77(7)	70(6)	46(5)	-7(5)	-13(5)	10(6)
C(23)	67(7)	57(6)	62(6)	-2(5)	-17(5)	13(5)
C(24)	71(8)	85(7)	34(5)	-11(5)	6(5)	8(6)
C(25)	69(8)	70(6)	36(5)	2(4)	-2(5)	6(6)
C(26)	56(7)	40(5)	59(5)	5(4)	7(5)	-5(4)
C(27)	80(9)	56(6)	66(6)	4(5)	-5(6)	10(6)
C(28)	71(8)	82(7)	66(6)	1(6)	0(6)	7(6)
C(29)	67(7)	44(5)	54(5)	4(4)	1(5)	-8(5)
C(30)	59(7)	58(5)	42(5)	1(4)	-10(5)	-4(5)
C(31)	57(6)	63(6)	46(5)	-6(4)	-2(5)	1(5)
C(32)	79(9)	84(7)	47(6)	7(5)	-8(6)	-12(6)
C(33)	54(6)	51(5)	57(5)	7(5)	-9(5)	-10(4)
C(34)	53(6)	72(6)	61(6)	-18(5)	8(5)	-9(5)
C(35)	47(6)	81(7)	47(5)	11(5)	4(5)	-12(5)

C(36)	48(6)	66(6)	67(6)	22(5)	-6(5)	0(5)
C(37)	39(5)	52(5)	66(5)	11(5)	6(5)	7(4)
C(38)	68(7)	48(5)	81(7)	-1(5)	-8(6)	7(5)
C(39)	58(6)	54(6)	80(7)	1(5)	-6(5)	5(5)
C(40)	56(6)	42(5)	67(6)	4(4)	-4(5)	-5(4)
C(41)	45(5)	43(5)	55(5)	11(4)	-4(4)	1(4)
C(42)	55(6)	46(5)	45(5)	0(4)	-1(4)	-11(4)
C(43)	57(6)	37(4)	51(5)	6(4)	-16(5)	2(4)
C(44)	54(6)	49(5)	51(5)	-13(4)	-5(5)	-2(4)
C(45)	40(5)	37(4)	62(5)	-6(4)	-5(4)	6(4)
C(46)	70(7)	40(5)	54(5)	-9(4)	-20(5)	-3(5)
C(47)	106(9)	47(5)	64(6)	-18(5)	-29(6)	26(6)
C(48)	103(9)	57(6)	65(6)	-8(5)	-36(6)	6(6)
C(49)	54(6)	56(5)	39(4)	-9(4)	-10(4)	14(4)
C(50)	64(7)	62(6)	44(5)	-6(4)	-5(5)	2(5)
C(51)	49(6)	60(6)	72(6)	14(5)	-1(5)	-2(5)
C(52)	54(6)	59(5)	51(5)	-3(5)	-6(4)	0(5)
C(53)	78(8)	80(7)	92(8)	-16(6)	-26(7)	26(6)
C(54)	61(6)	64(6)	50(5)	5(5)	-13(5)	-3(5)
C(55)	52(6)	64(6)	58(5)	8(5)	-17(5)	-5(5)
C(56)	59(7)	51(5)	44(5)	14(5)	-5(5)	-7(5)
C(57)	49(6)	50(5)	49(5)	-7(4)	2(5)	1(4)
C(58)	53(6)	41(5)	50(5)	-2(4)	0(5)	-8(4)
C(59)	79(8)	40(5)	52(5)	7(4)	-13(5)	-1(5)
C(60)	64(7)	60(6)	51(5)	1(5)	-2(5)	9(5)
C(61)	40(6)	45(5)	53(5)	-1(4)	-7(4)	7(4)
C(62)	67(7)	57(6)	55(5)	0(5)	4(6)	11(5)
C(63)	56(6)	62(6)	53(5)	-1(5)	-4(5)	7(5)
C(64)	53(7)	55(5)	65(6)	-5(5)	-31(5)	0(5)
O(8)	65(4)	73(4)	58(4)	14(3)	-7(3)	-6(4)
O(10)	54(4)	71(4)	49(3)	-3(3)	0(3)	-4(3)

**Table 1.4.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for **10**.

	x	y	z	U(eq)
H(1)	5578	500	6976	74
H(3)	4726	622	-2078	64
H(1A)	1097	2861	2291	72
H(1B)	1709	3056	2707	72
H(2A)	1967	2926	1579	78
H(2B)	2345	2398	2017	78
H(3A)	1231	2119	1272	68
H(4A)	1919	1156	2018	69
H(4B)	1278	1026	1628	69
H(5)	716	1668	2357	66
H(6A)	881	521	2637	72
H(6B)	676	980	3243	72
H(7A)	1502	314	3615	75
H(7B)	1923	491	2989	75
H(8)	1636	1367	4052	65
H(9)	2284	1684	2869	58
H(11A)	2497	2745	3236	59
H(11B)	2128	2615	3907	59
H(12)	3211	2558	4137	63
H(14)	2797	888	3582	67
H(15A)	2567	25	4186	86
H(15B)	2185	454	4719	86
H(16A)	3067	555	5310	84
H(16B)	3458	165	4754	84
H(17)	3718	1087	4217	75
H(18A)	2454	1479	5251	101
H(18B)	2096	1982	4770	101
H(18C)	2727	2212	5132	101
H(19A)	1086	2729	3668	95
H(19B)	832	1986	3765	95
H(19C)	515	2462	3230	95
H(20)	3615	1785	5417	65
H(21A)	4663	2187	5096	139
H(21B)	4104	2437	4632	139
H(21C)	4550	1842	4398	139
H(22A)	3985	723	5735	77
H(22B)	4553	782	5222	77
H(23A)	4416	1772	6207	75
H(23B)	5043	1581	5814	75
H(25)	6552	489	6684	70
H(27)	7689	563	6435	81
H(28)	8507	843	5729	88
H(30)	7240	1549	4425	64
H(31)	6427	1282	5113	66
H(33A)	9259	2755	2725	65

H(33B)	8649	2944	2307	65
H(34A)	8035	2236	2940	75
H(34B)	8391	2756	3408	75
H(35)	9148	1958	3697	70
H(36A)	8504	1013	2911	72
H(36B)	9134	887	3322	72
H(37)	9712	1579	2624	63
H(38A)	9629	459	2240	79
H(38B)	9764	978	1659	79
H(39A)	8963	227	1320	77
H(39B)	8548	414	1949	77
H(40)	8838	1315	893	66
H(41)	8143	1524	2084	57
H(43A)	7914	2648	1724	58
H(43B)	8264	2512	1040	58
H(44)	7164	2392	882	61
H(46)	7671	755	1313	66
H(47A)	7964	-78	667	87
H(47B)	8300	404	141	87
H(48A)	7390	489	-402	90
H(48B)	7048	35	140	90
H(49)	6735	900	738	59
H(50A)	7972	1433	-316	85
H(50B)	8304	1947	174	85
H(50C)	7650	2137	-167	85
H(51A)	9886	2337	1746	91
H(51B)	9318	2684	1360	91
H(51C)	9519	1937	1184	91
H(52)	6745	1724	-414	66
H(53A)	5803	2124	-16	125
H(53B)	6281	2112	590	125
H(53C)	5759	1543	519	125
H(54A)	6464	655	-841	70
H(54B)	5936	563	-284	70
H(55A)	5297	1381	-739	69
H(55B)	5861	1690	-1160	69
H(57)	3753	613	-1774	59
H(59)	2616	807	-1523	68
H(60)	1818	1069	-789	70
H(62)	3105	1597	549	71
H(63)	3914	1318	-141	68
H(67)	3706	996	2636	211
H(68)	4161	458	1734	211
H(69)	4785	2234	1049	211
H(70)	4331	2771	1951	211
H(67')	4387	2874	2002	211
H(68')	5119	2323	1339	211
H(69')	4894	647	2422	211
H(70')	4162	1198	3085	211



H(73)	5990	2598	2966	211
H(74)	5567	2046	3875	211
H(75)	6376	326	3270	211
H(76)	6799	878	2361	211
H(77A)	9873	-612	9403	183
H(77B)	9389	-1213	9498	183
H(78A)	8270	1379	7995	183
H(78B)	8372	757	7521	183
H(79A)	4935	3832	4913	183
H(79B)	5212	4036	4210	183
H(80A)	1964	1150	-2561	183
H(80B)	2112	1686	-3120	183

**Table 1.5.** Torsion angles [°] for **10**.

C(24)-N(1)-N(2)-C(25)	179.3(9)	C(56)-N(3)-N(4)-C(57)	-177.1(8)
C(10)-C(1)-C(2)-C(3)	57.3(10)	C(64)-O(6)-C(3)-C(4)	85.7(10)
C(64)-O(6)-C(3)-C(2)	-152.7(8)	C(1)-C(2)-C(3)-O(6)	-174.8(7)
C(1)-C(2)-C(3)-C(4)	-55.6(11)	O(6)-C(3)-C(4)-C(5)	170.1(7)
C(2)-C(3)-C(4)-C(5)	52.1(11)	C(3)-C(4)-C(5)-C(10)	-50.9(11)
C(3)-C(4)-C(5)-C(6)	179.8(8)	C(10)-C(5)-C(6)-C(7)	-53.8(11)
C(4)-C(5)-C(6)-C(7)	75.9(10)	C(5)-C(6)-C(7)-C(8)	50.2(11)
C(6)-C(7)-C(8)-C(14)	-173.1(8)	C(6)-C(7)-C(8)-C(9)	-50.2(11)
C(14)-C(8)-C(9)-C(10)	176.9(7)	C(7)-C(8)-C(9)-C(10)	54.5(10)
C(14)-C(8)-C(9)-C(11)	-50.4(10)	C(7)-C(8)-C(9)-C(11)	-172.7(8)
C(4)-C(5)-C(10)-C(9)	-72.2(10)	C(6)-C(5)-C(10)-C(9)	56.6(10)
C(4)-C(5)-C(10)-C(1)	51.7(10)	C(6)-C(5)-C(10)-C(1)	-179.5(8)
C(4)-C(5)-C(10)-C(19)	166.2(8)	C(6)-C(5)-C(10)-C(19)	-65.0(10)
C(8)-C(9)-C(10)-C(5)	-57.7(9)	C(11)-C(9)-C(10)-C(5)	171.0(7)
C(8)-C(9)-C(10)-C(1)	179.8(7)	C(11)-C(9)-C(10)-C(1)	48.5(10)
C(8)-C(9)-C(10)-C(19)	64.9(10)	C(11)-C(9)-C(10)-C(19)	-66.5(10)
C(2)-C(1)-C(10)-C(5)	-55.6(10)	C(2)-C(1)-C(10)-C(9)	66.3(10)
C(2)-C(1)-C(10)-C(19)	-175.0(8)	C(10)-C(9)-C(11)-C(12)	-179.0(7)
C(8)-C(9)-C(11)-C(12)	49.1(10)	C(9)-C(11)-C(12)-O(8)	63.0(9)
C(9)-C(11)-C(12)-C(13)	-49.6(10)	O(8)-C(12)-C(13)-C(17)	52.8(10)
C(11)-C(12)-C(13)-C(17)	167.8(8)	O(8)-C(12)-C(13)-C(18)	176.0(8)
C(11)-C(12)-C(13)-C(18)	-69.1(9)	O(8)-C(12)-C(13)-C(14)	-64.6(9)
C(11)-C(12)-C(13)-C(14)	50.4(10)	C(7)-C(8)-C(14)-C(15)	-59.7(11)
C(9)-C(8)-C(14)-C(15)	177.9(8)	C(7)-C(8)-C(14)-C(13)	177.7(7)
C(9)-C(8)-C(14)-C(13)	55.4(10)	C(17)-C(13)-C(14)-C(15)	43.6(10)
C(18)-C(13)-C(14)-C(15)	-72.1(10)	C(12)-C(13)-C(14)-C(15)	171.5(8)
C(17)-C(13)-C(14)-C(8)	176.1(8)	C(18)-C(13)-C(14)-C(8)	60.4(10)
C(12)-C(13)-C(14)-C(8)	-56.0(10)	C(8)-C(14)-C(15)-C(16)	-156.5(9)
C(13)-C(14)-C(15)-C(16)	-28.2(11)	C(14)-C(15)-C(16)-C(17)	3.3(12)
C(18)-C(13)-C(17)-C(16)	75.4(10)	C(12)-C(13)-C(17)-C(16)	-163.0(8)
C(14)-C(13)-C(17)-C(16)	-41.5(9)	C(18)-C(13)-C(17)-C(20)	-53.4(11)
C(12)-C(13)-C(17)-C(20)	68.1(12)	C(14)-C(13)-C(17)-C(20)	-170.4(8)
C(15)-C(16)-C(17)-C(13)	24.6(11)	C(15)-C(16)-C(17)-C(20)	156.2(9)

C(13)-C(17)-C(20)-C(22)	158.7(9)	C(16)-C(17)-C(20)-C(22)	35.1(13)
C(13)-C(17)-C(20)-C(21)	-76.6(12)	C(16)-C(17)-C(20)-C(21)	159.8(10)
C(17)-C(20)-C(22)-C(23)	-176.5(9)	C(21)-C(20)-C(22)-C(23)	57.1(11)
C(20)-C(22)-C(23)-C(24)	159.4(9)	N(2)-N(1)-C(24)-O(1)	175.3(9)
N(2)-N(1)-C(24)-C(23)	-6.0(14)	C(22)-C(23)-C(24)-O(1)	-70.2(11)
C(22)-C(23)-C(24)-N(1)	111.1(11)	N(1)-N(2)-C(25)-C(26)	179.1(8)
N(2)-C(25)-C(26)-C(27)	171.3(9)	N(2)-C(25)-C(26)-C(31)	-8.2(14)
C(31)-C(26)-C(27)-C(28)	0.4(14)	C(25)-C(26)-C(27)-C(28)	-179.1(9)
C(26)-C(27)-C(28)-C(29)	-2.0(15)	C(27)-C(28)-C(29)-C(30)	3.4(14)
C(27)-C(28)-C(29)-C(32)	-178.8(9)	C(28)-C(29)-C(30)-C(31)	-3.4(14)
C(32)-C(29)-C(30)-C(31)	179.1(9)	C(29)-C(30)-C(31)-C(26)	1.8(14)
C(27)-C(26)-C(31)-C(30)	-0.2(13)	C(25)-C(26)-C(31)-C(30)	179.3(8)
C(35)-O(3)-C(32)-O(2)	-2.0(16)	C(35)-O(3)-C(32)-C(29)	178.2(8)
C(30)-C(29)-C(32)-O(2)	176.9(12)	C(28)-C(29)-C(32)-O(2)	-0.7(17)
C(30)-C(29)-C(32)-O(3)	-3.3(14)	C(28)-C(29)-C(32)-O(3)	179.2(8)
C(42)-C(33)-C(34)-C(35)	56.9(10)	C(32)-O(3)-C(35)-C(36)	88.4(10)
C(32)-O(3)-C(35)-C(34)	-149.3(8)	C(33)-C(34)-C(35)-C(36)	-56.0(11)
C(33)-C(34)-C(35)-O(3)	-174.8(7)	O(3)-C(35)-C(36)-C(37)	170.0(7)
C(34)-C(35)-C(36)-C(37)	53.5(11)	C(35)-C(36)-C(37)-C(38)	-178.0(8)
C(35)-C(36)-C(37)-C(42)	-52.1(10)	C(36)-C(37)-C(38)-C(39)	69.4(10)
C(42)-C(37)-C(38)-C(39)	-58.4(10)	C(37)-C(38)-C(39)-C(40)	57.5(11)
C(38)-C(39)-C(40)-C(46)	-175.5(8)	C(38)-C(39)-C(40)-C(41)	-56.5(11)
C(39)-C(40)-C(41)-C(42)	61.2(9)	C(46)-C(40)-C(41)-C(42)	-179.2(7)
C(39)-C(40)-C(41)-C(43)	-173.2(8)	C(46)-C(40)-C(41)-C(43)	-53.7(9)
C(40)-C(41)-C(42)-C(51)	58.5(9)	C(43)-C(41)-C(42)-C(51)	-67.7(9)
C(40)-C(41)-C(42)-C(37)	-62.5(9)	C(43)-C(41)-C(42)-C(37)	171.3(7)
C(40)-C(41)-C(42)-C(33)	179.6(6)	C(43)-C(41)-C(42)-C(33)	53.4(9)
C(38)-C(37)-C(42)-C(51)	-62.3(10)	C(36)-C(37)-C(42)-C(51)	169.1(8)
C(38)-C(37)-C(42)-C(41)	58.8(9)	C(36)-C(37)-C(42)-C(41)	-69.8(9)
C(38)-C(37)-C(42)-C(33)	179.6(8)	C(36)-C(37)-C(42)-C(33)	51.0(10)
C(34)-C(33)-C(42)-C(51)	-175.3(8)	C(34)-C(33)-C(42)-C(41)	61.7(10)
C(34)-C(33)-C(42)-C(37)	-55.2(10)	C(40)-C(41)-C(43)-C(44)	56.5(10)
C(42)-C(41)-C(43)-C(44)	-176.5(7)	C(41)-C(43)-C(44)-O(10)	61.8(9)
C(41)-C(43)-C(44)-C(45)	-57.1(9)	O(10)-C(44)-C(45)-C(46)	-64.4(9)
C(43)-C(44)-C(45)-C(46)	56.4(9)	O(10)-C(44)-C(45)-C(50)	174.6(7)
C(43)-C(44)-C(45)-C(50)	-64.6(9)	O(10)-C(44)-C(45)-C(49)	49.7(9)
C(43)-C(44)-C(45)-C(49)	170.5(7)	C(39)-C(40)-C(46)-C(47)	-61.7(11)
C(41)-C(40)-C(46)-C(47)	-179.6(8)	C(39)-C(40)-C(46)-C(45)	173.5(8)
C(41)-C(40)-C(46)-C(45)	55.6(10)	C(50)-C(45)-C(46)-C(47)	-70.5(10)
C(49)-C(45)-C(46)-C(47)	45.9(10)	C(44)-C(45)-C(46)-C(47)	170.5(8)
C(50)-C(45)-C(46)-C(40)	62.3(10)	C(49)-C(45)-C(46)-C(40)	178.8(8)
C(44)-C(45)-C(46)-C(40)	-56.6(10)	C(40)-C(46)-C(47)-C(48)	-159.9(9)
C(45)-C(46)-C(47)-C(48)	-29.8(11)	C(46)-C(47)-C(48)-C(49)	2.4(12)
C(47)-C(48)-C(49)-C(45)	25.5(10)	C(47)-C(48)-C(49)-C(52)	153.9(9)
C(46)-C(45)-C(49)-C(48)	-43.1(8)	C(50)-C(45)-C(49)-C(48)	74.4(8)
C(44)-C(45)-C(49)-C(48)	-161.6(7)	C(46)-C(45)-C(49)-C(52)	-172.1(7)
C(50)-C(45)-C(49)-C(52)	-54.6(9)	C(44)-C(45)-C(49)-C(52)	69.4(10)
C(48)-C(49)-C(52)-C(53)	158.9(10)	C(45)-C(49)-C(52)-C(53)	-80.3(11)
C(48)-C(49)-C(52)-C(54)	34.9(12)	C(45)-C(49)-C(52)-C(54)	155.8(8)

C(53)-C(52)-C(54)-C(55)	55.4(10)	C(49)-C(52)-C(54)-C(55)	178.3(8)
C(52)-C(54)-C(55)-C(56)	161.3(8)	N(4)-N(3)-C(56)-O(4)	170.2(7)
N(4)-N(3)-C(56)-C(55)	-13.5(12)	C(54)-C(55)-C(56)-O(4)	-55.3(12)
C(54)-C(55)-C(56)-N(3)	128.6(9)	N(3)-N(4)-C(57)-C(58)	-177.2(7)
N(4)-C(57)-C(58)-C(59)	171.8(8)	N(4)-C(57)-C(58)-C(63)	-6.0(12)
C(63)-C(58)-C(59)-C(60)	-3.1(12)	C(57)-C(58)-C(59)-C(60)	179.0(8)
C(58)-C(59)-C(60)-C(61)	1.9(13)	C(59)-C(60)-C(61)-C(62)	0.3(13)
C(59)-C(60)-C(61)-C(64)	179.9(8)	C(60)-C(61)-C(62)-C(63)	-1.4(14)
C(64)-C(61)-C(62)-C(63)	179.1(9)	C(61)-C(62)-C(63)-C(58)	0.2(14)
C(59)-C(58)-C(63)-C(62)	2.0(12)	C(57)-C(58)-C(63)-C(62)	179.9(8)
C(3)-O(6)-C(64)-O(5)	1.9(14)	C(3)-O(6)-C(64)-C(61)	-177.5(7)
C(60)-C(61)-C(64)-O(5)	5.3(15)	C(62)-C(61)-C(64)-O(5)	-175.2(10)
C(60)-C(61)-C(64)-O(6)	-175.3(8)	C(62)-C(61)-C(64)-O(6)	4.3(12)
C(11)-C(12)-O(8)-C(65)	70.3(16)	C(13)-C(12)-O(8)-C(65)	-172.2(14)
C(11)-C(12)-O(8)-C(65')	87.4(17)	C(13)-C(12)-O(8)-C(65')	-155.0(16)
C(65')-O(8)-C(65)-O(7)	-48(4)	C(12)-O(8)-C(65)-O(7)	13(3)
C(65')-O(8)-C(65)-C(66)	129(6)	C(12)-O(8)-C(65)-C(66)	-169.0(14)
O(7)-C(65)-C(66)-C(67)	-176(2)	O(8)-C(65)-C(66)-C(67)	6(3)
O(7)-C(65)-C(66)-C(70)	2(4)	O(8)-C(65)-C(66)-C(70)	-176.0(16)
C(70)-C(66)-C(67)-C(68)	0.0	C(65)-C(66)-C(67)-C(68)	178(2)
C(66)-C(67)-C(68)-N(5)	0.0	C(67)-C(68)-N(5)-C(69)	0.0
C(68)-N(5)-C(69)-C(70)	0.0	N(5)-C(69)-C(70)-C(66)	0.0
C(67)-C(66)-C(70)-C(69)	0.0	C(65)-C(66)-C(70)-C(69)	-178(2)
C(65)-O(8)-C(65')-O(7')	124(8)	C(12)-O(8)-C(65')-O(7')	-2(4)
C(65)-O(8)-C(65')-C(66')	-58(4)	C(12)-O(8)-C(65')-C(66')	175.7(17)
O(7')-C(65')-C(66')-C(67')	-23(4)	O(8)-C(65')-C(66')-C(67')	159.0(18)
O(7')-C(65')-C(66')-C(70')	154(3)	O(8)-C(65')-C(66')-C(70')	-25(3)
C(70')-C(66')-C(67')-C(68')	0.0	C(65')-C(66')-C(67')-C(68')	176(3)
C(66')-C(67')-C(68')-N(5')	0.0	C(67')-C(68')-N(5')-C(69')	0.0
C(68')-N(5')-C(69')-C(70')	0.0	N(5')-C(69')-C(70')-C(66')	0.0
C(67')-C(66')-C(70')-C(69')	0.0	C(65')-C(66')-C(70')-C(69')	-176(2)
C(43)-C(44)-O(10)-C(71)	75.8(11)	C(45)-C(44)-O(10)-C(71)	-163.3(8)
C(44)-O(10)-C(71)-O(9)	14.6(16)	C(44)-O(10)-C(71)-C(72)	-168.5(9)
O(9)-C(71)-C(72)-C(73)	-0.8(18)	O(10)-C(71)-C(72)-C(73)	-177.5(8)
O(9)-C(71)-C(72)-C(76)	179.6(12)	O(10)-C(71)-C(72)-C(76)	2.8(14)
C(76)-C(72)-C(73)-C(74)	0.0	C(71)-C(72)-C(73)-C(74)	-179.6(11)
C(72)-C(73)-C(74)-N(6)	0.0	C(73)-C(74)-N(6)-C(75)	0.0
C(74)-N(6)-C(75)-C(76)	0.0	N(6)-C(75)-C(76)-C(72)	0.0
C(73)-C(72)-C(76)-C(75)	0.0	C(71)-C(72)-C(76)-C(75)	179.7(11)

Symmetry transformations used to generate equivalent atoms: