Supporting Information

Table 1. Crystallographic Data for crystal 3a and 3b.

Compound	**3a**	**3b**
Molecular formula	$C_{20}H_{14}N_2O$	$C_{20}H_{14}N_2O$
Molecular weight	298.33	298.33
Temperature(K)	298(2)	298(2)
Wavelength (nm)	0.071073	0.071073
Crystal system	Tetragonal	Monoclinic
Space group	I4(1)/a	P2(1)/n
a (Å)	21.5111(7)	10.7240(6)
b (Å)	21.5111(7)	8.9019(5)
c (Å)	13.2377(9)	6.1894(8)
α (°)	90.00	90.00
β (°)	90.00	102.039(4)
γ (°)	90.00	90.00
V (Å^3)	6125.4(5)	1511.51(14)
Z	16	4
ρ (cald.) (Mg m^{-3})	1.1294	1.311
μ (mm^{-1})	0.081	0.082
F(000)	2496	624
Crystal size (mm)	0.16 × 0.13 × 0.10	0.32 x 0.29 x 0.28
θ range for data collection (°)	1.81 to 27.64	2.09 to 27.56
h/k/l (max, min)	-28 , 24/ -25 , 28/ -17 , 15	-10,13/-11,10/ -21,20
Reflections collected	25513	13247
Independent reflections	3576 [*R* (int) = 0.0566]	3460 [R(int) = 0.0332]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	3576/0/209	3460 / 0 / 209
Goodness-of-fit on F^2	1.002	1.050
Final $R1$[a],$wR2$ [b] indices [$I > 2\sigma(I)$]	0.0534, 0.1359	0.0430, 0.1012

*R*1,*wR*2 indices (all data)	0.1103, 0.1682	0.0688, 0.1163
Largest diff. Peak and hole ($e.nm^{-3}$)	482 and -186	118 and -188

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for c. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	3a					3b			
	x	y	z	U(eq)		x	y	z	U(eq)
O(1)	9877(1)	4366(1)	2208(1)	80(1)	O(1)	2826(1)	4971(1)	1664(1)	58(1)
N(1)	9092(1)	4860(1)	838(1)	56(1)	N(1)	5071(1)	5534(1)	1158(1)	43(1)
N(2)	7419(1)	6531(1)	1206(1)	56(1)	N(2)	7400(1)	12207(1)	-823(1)	50(1)
C(1)	9477(1)	4397(1)	531(2)	52(1)	C(1)	4980(1)	4257(2)	1604(1)	42(1)
C(2)	9888(1)	4143(1)	1255(2)	57(1)	C(2)	3816(1)	4001(2)	1868(1)	46(1)
C(3)	10281(1)	3674(1)	1005(2)	69(1)	C(3)	3695(2)	2762(2)	2350(1)	56(1)
C(4)	10275(1)	3431(1)	22(2)	75(1)	C(4)	4699(2)	1741(2)	2572(1)	61(1)
C(5)	9887(1)	3657(1)	694(2)	69(1)	C(5)	5822(2)	1938(2)	2314(1)	57(1)
C(6)	9478(1)	4152(1)	463(2)	58(1)	C(6)	5990(1)	3209(2)	1824(1)	46(1)
C(7)	9069(1)	4431(1)	1154(2)	71(1)	C(7)	7109(2)	3520(2)	1532(1)	54(1)
C(8)	8694(1)	4902(1)	-853(2)	74(1)	C(8)	7198(1)	4798(2)	1088(1)	51(1)
C(9)	8708(1)	5111(1)	162(2)	58(1)	C(9)	6164(1)	5810(2)	922(1)	43(1)
C(10)	8276(1)	5591(1)	506(2)	67(1)	C(10)	6235(1)	7246(2)	491(1)	47(1)
C(11)	8207(1)	5751(1)	1470(2)	66(1)	C(11)	7288(1)	8015(2)	484(1)	46(1)
C(12)	7740(1)	6188(1)	1857(2)	58(1)	C(12)	7337(1)	9464(2)	57(1)	42(1)
C(13)	7638(1)	6214(1)	2908(2)	68(1)	C(13)	6417(2)	9850(2)	-629(1)	51(1)
C(14)	7198(1)	6596(1)	3290(2)	69(1)	C(14)	6483(2)	11219(2)	-1040(1)	54(1)
C(15)	6843(1)	6969(1)	2629(2)	55(1)	C(15)	8350(1)	11860(2)	-147(1)	43(1)
C(16)	6379(1)	7383(1)	2953(2)	69(1)	C(16)	9358(2)	12894(2)	90(1)	52(1)
C(17)	6064(1)	7735(1)	2277(2)	72(1)	C(17)	10310(2)	12630(2)	769(1)	59(1)
C(18)	6195(1)	7692(1)	1241(2)	68(1)	C(18)	10308(2)	11317(2)	1244(1)	60(1)
C(19)	6639(1)	7292(1)	900(2)	59(1)	C(19)	9362(1)	10284(2)	1028(1)	51(1)
C(20)	6975(1)	6921(1)	1583(1)	50(1)	C(20)	8356(1)	10507(1)	323(1)	41(1)

Table 3 Bond lengths [A] and angles [deg] for crystal 3a and 3b.

3a		3b	
O(1)-C(2)	1.350(2)	O(1)-C(2)	1.3543(18)
O(1)-H(1)	0.8200	O(1)-H(1)	0.8200
N(1)-C(9)	1.332(3)	N(1)-C(9)	1.3286(18)
N(1)-C(1)	1.358(2)	N(1)-C(1)	1.3621(17)
N(2)-C(12)	1.328(3)	N(2)-C(14)	1.3117(19)
N(2)-C(20)	1.366(2)	N(2)-C(15)	1.3667(18)
C(1)-C(2)	1.413(3)	C(1)-C(6)	1.418(2)

C(1)-C(6)	1.418(3)	C(1)-C(2)	1.419(2)
C(2)-C(3)	1.359(3)	C(2)-C(3)	1.374(2)
C(3)-C(4)	1.402(3)	C(3)-C(4)	1.397(2)
C(3)-H(3)	0.9300	C(3)-H(3)	0.9300
C(4)-C(5)	1.354(3)	C(4)-C(5)	1.366(2)
C(4)-H(4)	0.9300	C(4)-H(4)	0.9300
C(5)-C(6)	1.413(3)	C(5)-C(6)	1.415(2)
C(5)-H(5)	0.9300	C(5)-H(5)	0.9300
C(6)-C(7)	1.404(3)	C(6)-C(7)	1.406(2)
C(7)-C(8)	1.355(3)	C(7)-C(8)	1.360(2)
C(7)-H(7)	0.9300	C(7)-H(7)	0.9300
C(8)-C(9)	1.416(3)	C(8)-C(9)	1.410(2)
C(8)-H(8)	0.9300	C(8)-H(8)	0.9300
C(9)-C(10)	1.463(3)	C(9)-C(10)	1.4660(19)
C(10)-C(11)	1.330(3)	C(10)-C(11)	1.323(2)
C(10)-H(10)	0.9300	C(10)-H(10)	0.9300
C(11)-C(12)	1.468(3)	C(11)-C(12)	1.4699(19)
C(11)-H(11)	0.9300	C(11)-H(11)	0.9300
C(12)-C(13)	1.410(3)	C(12)-C(13)	1.367(2)
C(13)-C(14)	1.353(3)	C(12)-C(20)	1.4299(19)
C(13)-H(13)	0.9300	C(13)-C(14)	1.397(2)
C(14)-C(15)	1.411(3)	C(13)-H(13)	0.9300
C(14)-H(14)	0.9300	C(14)-H(14)	0.9300
C(15)-C(16)	1.405(3)	C(15)-C(16)	1.410(2)
C(15)-C(20)	1.417(3)	C(15)-C(20)	1.4236(19)
C(16)-C(17)	1.353(3)	C(16)-C(17)	1.356(2)
C(16)-H(16)	0.9300	C(16)-H(16)	0.9300
C(17)-C(18)	1.403(3)	C(17)-C(18)	1.399(2)
C(17)-H(17)	0.9300	C(17)-H(17)	0.9300
C(18)-C(19)	1.363(3)	C(18)-C(19)	1.360(2)
C(18)-H(18)	0.9300	C(18)-H(18)	0.9300
C(19)-C(20)	1.405(3)	C(19)-C(20)	1.411(2)
C(19)-H(19)	0.9300	C(19)-H(19)	0.9300
C(2)-O(1)-H(1)	109.5	C(2)-O(1)-H(1)	109.5
C(9)-N(1)-C(1)	118.29(17)	C(9)-N(1)-C(1)	118.14(12)
C(12)-N(2)-C(20)	117.96(17)	C(14)-N(2)-C(15)	117.06(12)
N(1)-C(1)-C(2)	117.52(18)	N(1)-C(1)-C(6)	123.14(13)
N(1)-C(1)-C(6)	123.48(19)	N(1)-C(1)-C(2)	117.29(13)
C(2)-C(1)-C(6)	119.00(19)	C(6)-C(1)-C(2)	119.55(13)
O(1)-C(2)-C(3)	120.2(2)	O(1)-C(2)-C(3)	119.20(14)
O(1)-C(2)-C(1)	119.06(19)	O(1)-C(2)-C(1)	121.23(12)
C(3)-C(2)-C(1)	120.8(2)	C(3)-C(2)-C(1)	119.56(14)
C(2)-C(3)-C(4)	119.9(2)	C(2)-C(3)-C(4)	120.59(15)
C(2)-C(3)-H(3)	120.1	C(2)-C(3)-H(3)	119.7

C(4)-C(3)-H(3)	120.1	C(4)-C(3)-H(3)	119.7
C(5)-C(4)-C(3)	121.3(2)	C(5)-C(4)-C(3)	121.31(15)
C(5)-C(4)-H(4)	119.3	C(5)-C(4)-H(4)	119.3
C(3)-C(4)-H(4)	119.3	C(3)-C(4)-H(4)	119.3
C(4)-C(5)-C(6)	120.3(2)	C(4)-C(5)-C(6)	119.84(15)
C(4)-C(5)-H(5)	119.9	C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	119.9	C(6)-C(5)-H(5)	120.1
C(7)-C(6)-C(5)	124.9(2)	C(7)-C(6)-C(5)	124.30(15)
C(7)-C(6)-C(1)	116.4(2)	C(7)-C(6)-C(1)	116.59(13)
C(5)-C(6)-C(1)	118.8(2)	C(5)-C(6)-C(1)	119.12(14)
C(8)-C(7)-C(6)	120.1(2)	C(8)-C(7)-C(6)	120.08(14)
C(8)-C(7)-H(7)	119.9	C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	119.9	C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.2(2)	C(7)-C(8)-C(9)	119.73(14)
C(7)-C(8)-H(8)	119.9	C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	119.9	C(9)-C(8)-H(8)	120.1
N(1)-C(9)-C(8)	121.5(2)	N(1)-C(9)-C(8)	122.23(13)
N(1)-C(9)-C(10)	118.07(19)	N(1)-C(9)-C(10)	115.73(12)
C(8)-C(9)-C(10)	120.4(2)	C(8)-C(9)-C(10)	122.03(13)
C(11)-C(10)-C(9)	123.5(2)	C(11)-C(10)-C(9)	125.77(14)
C(11)-C(10)-H(10)	118.2	C(11)-C(10)-H(10)	117.1
C(9)-C(10)-H(10)	118.2	C(9)-C(10)-H(10)	117.1
C(10)-C(11)-C(12)	125.2(2)	C(10)-C(11)-C(12)	124.92(14)
C(10)-C(11)-H(11)	117.4	C(10)-C(11)-H(11)	117.5
C(12)-C(11)-H(11)	117.4	C(12)-C(11)-H(11)	117.5
N(2)-C(12)-C(13)	122.4(2)	C(13)-C(12)-C(20)	117.28(12)
N(2)-C(12)-C(11)	119.03(19)	C(13)-C(12)-C(11)	120.83(13)
C(13)-C(12)-C(11)	118.5(2)	C(20)-C(12)-C(11)	121.87(12)
C(14)-C(13)-C(12)	120.2(2)	C(12)-C(13)-C(14)	120.47(14)
C(14)-C(13)-H(13)	119.9	C(12)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.9	C(14)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	119.4(2)	N(2)-C(14)-C(13)	124.50(14)
C(13)-C(14)-H(14)	120.3	N(2)-C(14)-H(14)	117.7
C(15)-C(14)-H(14)	120.3	C(13)-C(14)-H(14)	117.7
C(16)-C(15)-C(14)	123.7(2)	N(2)-C(15)-C(16)	118.06(13)
C(16)-C(15)-C(20)	119.1(2)	N(2)-C(15)-C(20)	122.63(12)
C(14)-C(15)-C(20)	117.19(19)	C(16)-C(15)-C(20)	119.30(13)
C(17)-C(16)-C(15)	120.6(2)	C(17)-C(16)-C(15)	120.78(14)
C(17)-C(16)-H(16)	119.7	C(17)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.7	C(15)-C(16)-H(16)	119.6
C(16)-C(17)-C(18)	120.5(2)	C(16)-C(17)-C(18)	120.21(14)
C(16)-C(17)-H(17)	119.7	C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.7	C(18)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	120.4(2)	C(19)-C(18)-C(17)	120.68(15)

C(19)-C(18)-H(18)	119.8	C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.8	C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	120.4(2)	C(18)-C(19)-C(20)	121.05(14)
C(18)-C(19)-H(19)	119.8	C(18)-C(19)-H(19)	119.5
C(20)-C(19)-H(19)	119.8	C(20)-C(19)-H(19)	119.5
N(2)-C(20)-C(19)	118.30(17)	C(19)-C(20)-C(15)	117.94(12)
N(2)-C(20)-C(15)	122.76(18)	C(19)-C(20)-C(12)	124.01(12)
C(19)-C(20)-C(15)	118.94(19)	C(15)-C(20)-C(12)	118.04(12)

Table 4 Anisotropic displacement parameters (A^2 x 10^3) for crystal 3a and 3b. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	3a							3b					
	U11	U22	U33	U23	U13	U12		U11	U22	U33	U23	U13	U12
O(1)	86(1)	92(1)	61(1)	-11(1)	-13(1)	23(1)	O(1)	49(1)	56(1)	71(1)	11(1)	20(1)	-6(1)
N(1)	57(1)	57(1)	54(1)	-1(1)	2(1)	2(1)	N(1)	42(1)	41(1)	45(1)	1(1)	7(1)	-6(1)
N(2)	58(1)	59(1)	51(1)	-4(1)	-2(1)	3(1)	N(2)	53(1)	47(1)	51(1)	7(1)	13(1)	-1(1)
C(1)	51(1)	51(1)	54(1)	2(1)	6(1)	0(1)	C(1)	48(1)	38(1)	38(1)	-3(1)	5(1)	-8(1)
C(2)	58(1)	62(1)	52(1)	-3(1)	2(1)	0(1)	C(2)	51(1)	45(1)	43(1)	-3(1)	8(1)	-11(1)
C(3)	65(1)	73(2)	69(2)	-1(1)	-1(1)	15(1)	C(3)	66(1)	55(1)	48(1)	1(1)	14(1)	-17(1)
C(4)	78(2)	71(2)	77(2)	-4(1)	15(1)	17(1)	C(4)	85(1)	46(1)	48(1)	7(1)	7(1)	-16(1)
C(5)	75(2)	73(2)	59(1)	-8(1)	12(1)	9(1)	C(5)	71(1)	43(1)	50(1)	4(1)	-2(1)	-2(1)
C(6)	60(1)	62(1)	50(1)	0(1)	7(1)	-2(1)	C(6)	54(1)	39(1)	43(1)	-3(1)	3(1)	-4(1)
C(7)	79(2)	86(2)	49(1)	-7(1)	1(1)	9(1)	C(7)	53(1)	42(1)	65(1)	-4(1)	7(1)	5(1)
C(8)	77(2)	90(2)	54(1)	2(1)	-5(1)	18(1)	C(8)	46(1)	45(1)	65(1)	-6(1)	17(1)	-2(1)
C(9)	59(1)	63(1)	53(1)	2(1)	2(1)	5(1)	C(9)	45(1)	39(1)	45(1)	-3(1)	9(1)	-6(1)
C(10)	67(2)	71(2)	61(1)	4(1)	-2(1)	16(1)	C(10)	46(1)	43(1)	51(1)	2(1)	12(1)	-1(1)
C(11)	68(2)	67(1)	63(1)	-1(1)	-7(1)	13(1)	C(11)	46(1)	42(1)	51(1)	2(1)	10(1)	-4(1)
C(12)	61(1)	56(1)	57(1)	-3(1)	-4(1)	1(1)	C(12)	43(1)	40(1)	45(1)	-2(1)	14(1)	-2(1)
C(13)	77(2)	73(2)	54(1)	4(1)	-6(1)	11(1)	C(13)	50(1)	51(1)	50(1)	2(1)	7(1)	-10(1)
C(14)	81(2)	79(2)	46(1)	-2(1)	0(1)	3(1)	C(14)	54(1)	56(1)	49(1)	6(1)	4(1)	-2(1)
C(15)	58(1)	57(1)	51(1)	-6(1)	-1(1)	-3(1)	C(15)	43(1)	40(1)	50(1)	0(1)	16(1)	2(1)
C(16)	73(2)	77(2)	57(1)	-15(1)	5(1)	7(1)	C(16)	53(1)	40(1)	66(1)	3(1)	20(1)	-5(1)
C(17)	71(2)	72(2)	74(2)	-10(1)	5(1)	16(1)	C(17)	49(1)	48(1)	79(1)	-3(1)	12(1)	-12(1)
C(18)	67(2)	71(2)	67(1)	0(1)	-3(1)	11(1)	C(18)	49(1)	57(1)	67(1)	1(1)	0(1)	-6(1)
C(19)	58(1)	64(1)	55(1)	-1(1)	-3(1)	4(1)	C(19)	48(1)	47(1)	58(1)	5(1)	8(1)	-2(1)
C(20)	51(1)	51(1)	50(1)	-6(1)	-1(1)	-4(1)	C(20)	40(1)	37(1)	46(1)	-2(1)	13(1)	0(1)

Table 5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for crystal 3a and 3b.

3a	3b

	x	y	z	U(eq)		x	y	z	U(eq)
H(1)	9615	4642	2251	120	H(1)	3032	5676	1396	87
H(3)	10553	3514	1485	83	H(3)	2938	2600	2531	67
H(4)	10544	3107	-141	90	H(4)	4600	912	2901	73
H(5)	9889	3487	-1339	83	H(5)	6474	1238	2459	68
H(7)	9055	4293	-1819	86	H(7)	7789	2850	1642	65
H(8)	8427	5089	-1313	88	H(8)	7937	5004	894	62
H(10)	8035	5795	25	80	H(10)	5472	7652	196	56
H(11)	8477	5573	1936	79	H(11)	8056	7607	771	56
H(13)	7873	5967	3339	82	H(13)	5743	9198	-823	61
H(14)	7129	6614	3983	82	H(14)	5832	11445	-1500	65
H(16)	6288	7416	3637	83	H(16)	9369	13767	-224	62
H(17)	5757	8007	2502	87	H(17)	10966	13323	919	71
H(18)	5979	7939	785	82	H(18)	10961	11149	1712	72
H(19)	6719	7263	212	71	H(19)	9378	9416	1350	61

Table 6 Torsion angles [deg] for 3a and 3b.

3a		**3b**	
C(9)-N(1)-C(1)-C(2)	179.02(19)	C(9)-N(1)-C(1)-C(6)	-0.34(19)
C(9)-N(1)-C(1)-C(6)	-2.1(3)	C(9)-N(1)-C(1)-C(2)	178.49(12)
N(1)-C(1)-C(2)-O(1)	0.5(3)	N(1)-C(1)-C(2)-O(1)	1.63(19)
C(6)-C(1)-C(2)-O(1)	-178.5(2)	C(6)-C(1)-C(2)-O(1)	-179.49(12)
N(1)-C(1)-C(2)-C(3)	179.3(2)	N(1)-C(1)-C(2)-C(3)	-177.22(12)
C(6)-C(1)-C(2)-C(3)	0.3(3)	C(6)-C(1)-C(2)-C(3)	1.7(2)
O(1)-C(2)-C(3)-C(4)	177.9(2)	O(1)-C(2)-C(3)-C(4)	-179.91(13)
C(1)-C(2)-C(3)-C(4)	-0.9(3)	C(1)-C(2)-C(3)-C(4)	-1.0(2)
C(2)-C(3)-C(4)-C(5)	0.5(4)	C(2)-C(3)-C(4)-C(5)	-0.3(2)
C(3)-C(4)-C(5)-C(6)	0.5(4)	C(3)-C(4)-C(5)-C(6)	1.1(2)
C(4)-C(5)-C(6)-C(7)	178.3(2)	C(4)-C(5)-C(6)-C(7)	179.56(14)
C(4)-C(5)-C(6)-C(1)	-1.0(3)	C(4)-C(5)-C(6)-C(1)	-0.4(2)
N(1)-C(1)-C(6)-C(7)	2.4(3)	N(1)-C(1)-C(6)-C(7)	-2.10(19)
C(2)-C(1)-C(6)-C(7)	-178.7(2)	C(2)-C(1)-C(6)-C(7)	179.09(13)
N(1)-C(1)-C(6)-C(5)	-178.3(2)	N(1)-C(1)-C(6)-C(5)	177.87(12)
C(2)-C(1)-C(6)-C(5)	0.6(3)	C(2)-C(1)-C(6)-C(5)	-0.93(19)
C(5)-C(6)-C(7)-C(8)	179.7(2)	C(5)-C(6)-C(7)-C(8)	-177.81(14)
C(1)-C(6)-C(7)-C(8)	-0.9(3)	C(1)-C(6)-C(7)-C(8)	2.2(2)
C(6)-C(7)-C(8)-C(9)	-0.7(4)	C(6)-C(7)-C(8)-C(9)	0.0(2)
C(1)-N(1)-C(9)-C(8)	0.3(3)	C(1)-N(1)-C(9)-C(8)	2.76(19)
C(1)-N(1)-C(9)-C(10)	177.34(19)	C(1)-N(1)-C(9)-C(10)	-176.27(12)
C(7)-C(8)-C(9)-N(1)	1.0(4)	C(7)-C(8)-C(9)-N(1)	-2.7(2)
C(7)-C(8)-C(9)-C(10)	-175.9(2)	C(7)-C(8)-C(9)-C(10)	176.30(14)
N(1)-C(9)-C(10)-C(11)	-6.1(4)	N(1)-C(9)-C(10)-C(11)	152.78(15)

C(8)-C(9)-C(10)-C(11)	171.0(2)	C(8)-C(9)-C(10)-C(11)	-26.2(2)
C(9)-C(10)-C(11)-C(12)	-174.1(2)	C(9)-C(10)-C(11)-C(12)	-179.12(13)
C(20)-N(2)-C(12)-C(13)	0.0(3)	C(10)-C(11)-C(12)-C(13)	-26.6(2)
C(20)-N(2)-C(12)-C(11)	178.19(18)	C(10)-C(11)-C(12)-C(20)	155.01(14)
C(10)-C(11)-C(12)-N(2)	-11.4(4)	C(20)-C(12)-C(13)-C(14)	-0.4(2)
C(10)-C(11)-C(12)-C(13)	166.9(2)	C(11)-C(12)-C(13)-C(14)	-178.87(13)
N(2)-C(12)-C(13)-C(14)	0.2(4)	C(15)-N(2)-C(14)-C(13)	0.0(2)
C(11)-C(12)-C(13)-C(14)	-177.9(2)	C(12)-C(13)-C(14)-N(2)	0.9(2)
C(12)-C(13)-C(14)-C(15)	-0.1(4)	C(14)-N(2)-C(15)-C(16)	178.94(14)
C(13)-C(14)-C(15)-C(16)	-179.5(2)	C(14)-N(2)-C(15)-C(20)	-1.2(2)
C(13)-C(14)-C(15)-C(20)	-0.3(3)	N(2)-C(15)-C(16)-C(17)	178.27(14)
C(14)-C(15)-C(16)-C(17)	178.9(2)	C(20)-C(15)-C(16)-C(17)	-1.6(2)
C(20)-C(15)-C(16)-C(17)	-0.3(3)	C(15)-C(16)-C(17)-C(18)	0.3(2)
C(15)-C(16)-C(17)-C(18)	-0.1(4)	C(16)-C(17)-C(18)-C(19)	0.6(3)
C(16)-C(17)-C(18)-C(19)	0.6(4)	C(17)-C(18)-C(19)-C(20)	-0.2(3)
C(17)-C(18)-C(19)-C(20)	-0.8(3)	C(18)-C(19)-C(20)-C(15)	-1.1(2)
C(12)-N(2)-C(20)-C(19)	179.18(19)	C(18)-C(19)-C(20)-C(12)	179.48(14)
C(12)-N(2)-C(20)-C(15)	-0.5(3)	N(2)-C(15)-C(20)-C(19)	-177.91(13)
C(18)-C(19)-C(20)-N(2)	-179.32(19)	C(16)-C(15)-C(20)-C(19)	1.95(19)
C(18)-C(19)-C(20)-C(15)	0.3(3)	N(2)-C(15)-C(20)-C(12)	1.56(19)
C(16)-C(15)-C(20)-N(2)	179.8(2)	C(16)-C(15)-C(20)-C(12)	-178.57(13)
C(14)-C(15)-C(20)-N(2)	0.6(3)	C(13)-C(12)-C(20)-C(19)	178.75(13)
C(16)-C(15)-C(20)-C(19)	0.2(3)	C(11)-C(12)-C(20)-C(19)	-2.8(2)
C(14)-C(15)-C(20)-C(19)	-179.0(2)	C(13)-C(12)-C(20)-C(15)	-0.69(19)
		C(11)-C(12)-C(20)-C(15)	177.74(12)

Table 7 Hydrogen bonds for 3a and 3b [A and deg.].

3a					3b				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)#1	0.82	2.23	2.696(2)	116.1	O(1)-H(1)...N(2)#1	0.82	2.11	2.8438(15)	149.2
O(1)-H(1)...N(2)#2	0.82	2.49	3.099(2)	132.5	O(1)-H(1)...N(1)#2	0.82	2.301	2.7463(16)	114.63
Symmetry Code: #1 x,y,z #2 y+1/4,-x+5/4,z+1/4					Symmetry Code: #1 -x+1,-y+2,-z #2 x,y,z				