A Novel Synthesis of 5-Functionalized Oxazolidin-2-ones from Enantiomerically Pure 2-Substituted *N*-[(*R*)-(+)- α -Methylbenzyl]aziridines

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Supporting Information

X-Ray crystallographic data for **6a** and **6b**.

6a

6b

Crystallographic studies of **6a** and **6b**.

Preliminary examination and data collection for compounds **6a** and **6b** were performed with MoK α radiation ($\lambda = 0.7107 \text{ \AA}$) on an MXC3 diffractometer (MAC Science) at 130(1) K. Cell constants and an orientation matrix for data collection were determined from the least-squares analysis, using setting angles of 26 reflections in the range of $20^\circ \leq 2\theta \leq 28^\circ$ for **6a** and 22 reflections in the range of $20^\circ \leq 2\theta \leq 28^\circ$ for **6b**. For both compounds, intensity data were collected with the ω -scan with $3^\circ \leq 2\theta \leq 50^\circ$ and two standard reflections monitored every 100 reflections throughout the data collection process showed no significant trends.

The **6a** crystallizes in the space group $D_2^4-P2_12_12_1$ of the orthorhombic system with four formula units in a cell dimensions: $a=15.237(4) \text{ \AA}$, $b=22.307(5) \text{ \AA}$, $c=6.417(2) \text{ \AA}$, and $V=2186.2(11) \text{ \AA}^3$. Equivalent reflection has been checked for Laue symmetry. The transparent needle shaped crystal of dimension $0.64 \times 0.18 \times 0.15 \text{ mm}^3$ was used to collect 1800 unique (F_o^2 0) and 1041 (F_o^2 2 (F_o^2)) reflections. The **6b** crystallizes in the space group $C_2^2-P2_1$ of the monoclinic system with two formula units in a cell dimensions: $a=14.167(5) \text{ \AA}$, $b=6.346(2) \text{ \AA}$, $c=12.483(4) \text{ \AA}$, $\beta=108.64(2)^\circ$, and $V=1063.4(6) \text{ \AA}^3$. The transparent polyhedron crystal of dimension $0.84 \times 0.28 \times 0.26 \text{ mm}^3$ was used to collect 1667

unique ($F_o^2 > 0$) and 1308 ($F_o^2 \geq 2(F_o^2)$) reflections.

The initial positions for all non-hydrogen atoms were obtained by using direct methods of the SHELXS-86 program (1). The structure was refined with the use of the SHELXL-97 program (2). Positional and thermal parameters for non-hydrogen atoms were refined using a full-matrix least-squares refinement procedure. Atomic positions of hydrogen atoms were generated with riding model technique of SHELXL-97 (2). The final cycle of refinement performed with $wR2 = 0.1301$ on $F_o^2 (F_o^2 > 0)$ for **6a** and $wR2 = 0.0838$ on $F_o^2 (F_o^2 > 0)$ for **6b** and the conventional R index based on the reflections having $F_o^2 \geq 2(F_o^2)$ is 0.0584 for **6a** and 0.0393 for **6b**. Crystal data and crystallographic details are described in Table 1. None of the structures shows additional potential symmetry, as tested by the MISSYM algorithm in the PLATON suite of program (3,4). Final values of atomic parameters and equivalent isotropic displacement parameters are given in Table 2 for **6a** and Table 3 for **6b**. Final anisotropic displacement parameters appear Table 4 for non-hydrogen atoms. Bond distances and angles are given in Table 5 and 6, respectively.

(1) Sheldrick, G. M. *Acta Crystallogr.* **1990**, A46, 467 - 473.

(2) Sheldrick, G. M. SHELXL97. Program for the Refinement of Crystal Structure.

University of Göttingen, Germany, **1997**.

(3) Le Page, Y. J. *Appl. Crystallogr.*, **1987**, 20, 264-269.

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Table 1. Crystal Data and Structure Refinement for **6a** and **6b**.

	6a	6b
Formula	C ₂₂ H ₃₁ NO ₄	C ₂₂ H ₃₁ NO ₄
Formula Weight, amu	373.48	373.48
Space Group	D ₂ ⁴ -P2 ₁ 2 ₁ 2 ₁	C ₂ ² -P2 ₁
a, Å	15.273(4)	14.167(5)
b, Å	22.307(5)	6.346(2)
c, Å	6.417(2)	12.483(4)
β , deg.		108.64(2)
V, Å ³	2186.2(11)	1063.4(6)
Radiation	Graphite monochromated MoK α (λ = 0.7107 Å)	
Z, Temperature, K	4, 130 (1)	2, 130 (1)
Scan Type	-2	-2
Scan Rate	4.0 /min (in θ)	5.0 /min (in θ)
Scan Width, deg.	1.0 + 0.35 tan θ	0.9 + 0.35 tan θ
$2\theta_{max}$, deg.	50.0	50.0
No. of Reflections Measured	Total	1806
	Unique	1742
No. Observations ($F_o^2 > 0$)	1800	1667 ($R_{int} = 0.0145$)
No. Unique data with $F_o^2 > 2\sigma(F_o^2)$	1041	1308
No. Variables	249	249
Reflection / Parameter Ratio	13.83	14.94
wR2 ($F_o^2 > 0$)	0.1301	0.0838
R (on F_o^2 for $F_o^2 > 2\sigma(F_o^2)$)	0.0584	0.0393
Goodness of Fit Indicator	1.029	1.026
Max Shift / Error in Final Cycle	< 0.0005	< 0.0005
Maximum peak in Final Diff. Map	0.217 e ⁻ /Å ³	0.112 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.188 e ⁻ /Å ³	0.097 e ⁻ /Å ³

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **6a**.

Atom	x	y	z	U_{eq}^a
C(1)	1703(4)	4029(2)	12171(8)	47(2)
C(2)	1928(4)	4625(3)	11146(9)	58(2)
C(3)	1348(4)	4019(3)	8679(10)	63(2)
C(4)	777(4)	3172(3)	10693(9)	57(2)
C(5)	1470(4)	2692(3)	10808(11)	63(2)
C(6)	1621(5)	2349(3)	12557(13)	87(2)
C(7)	2266(7)	1906(4)	12559(18)	114(3)
C(8)	2762(6)	1810(4)	10830(2)	105(3)
C(9)	2625(6)	2139(4)	9106(17)	104(3)
C(10)	1988(5)	2575(3)	9079(12)	82(2)
C(11)	108(4)	3156(3)	12439(13)	81(2)
C(12)	1324(5)	5139(3)	11582(10)	68(2)
C(13)	390(4)	5600(3)	14166(10)	58(2)
C(14)	-322(4)	5275(3)	15347(10)	61(2)
C(15)	-971(4)	5739(3)	16163(11)	81(2)
C(16)	-534(5)	6211(3)	17482(12)	86(2)
C(17)	207(5)	6537(3)	16357(12)	80(2)
C(18)	844(4)	6078(3)	15466(9)	64(2)
C(19)	-727(5)	4769(3)	14100(13)	86(2)
C(20)	-1258(5)	4356(3)	15500(14)	139(4)
C(21)	-1286(6)	4967(4)	12237(16)	152(4)
C(22)	661(5)	6983(3)	17724(14)	112(3)
N	1165(3)	3767(2)	10541(7)	52(1)
O(1)	1866(3)	4502(2)	8941(6)	69(1)
O(2)	1101(4)	3850(2)	6984(6)	98(2)
O(3)	1132(5)	5498(3)	10341(8)	165(3)
O(4)	1052(2)	5158(2)	13538(6)	56(1)
H(1A)	2222	3791	12444	57
H(1B)	1377	4084	13455	57
H(2)	2530	4738	11499	69
H(4)	454	3105	9393	68
H(6)	1289	2413	13752	104

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **6a**. (continued)

Atom	x	y	z	U_{eq}^a
H(7)	2357	1675	13747	136
H(8)	3196	1518	10846	126
H(9)	2963	2072	7924	125
H(10)	1902	2798	7870	98
H(11A)	-335	3453	12186	122
H(11B)	393	3239	13741	122
H(11C)	-157	2766	12496	122
H(13)	138	5785	12919	69
H(14)	-44	5092	16568	74
H(15A)	-1259	5930	14993	98
H(15B)	-1416	5537	16985	98
H(16A)	-302	6023	18729	103
H(16B)	-970	6501	17914	103
H(17)	-50	6757	15184	96
H(18A)	1272	6284	14606	76
H(18B)	1155	5887	16604	76
H(19)	-243	4531	13538	104
H(20A)	-1766	4565	16000	209
H(20B)	-905	4233	16662	209
H(20C)	-1437	4009	14723	209
H(21A)	-1788	5184	12728	229
H(21B)	-1475	4620	11475	229
H(21C)	-945	5220	11341	229
H(22A)	1126	7172	16957	169
H(22B)	900	6782	18919	169
H(22C)	250	7282	18172	169

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **6b**.

Atom	x	y	z	U_{eq}^a
C(1)	11400(2)	3542(6)	9426(3)	51(1)
C(2)	11279(2)	5182(6)	10278(3)	45(1)
C(3)	9937(3)	5454(6)	8658(3)	47(1)
C(4)	10313(3)	2882(6)	7375(3)	52(1)
C(5)	10904(2)	3629(6)	6622(3)	47(1)
C(6)	10892(3)	2453(7)	5681(3)	62(1)
C(7)	11371(3)	3140(9)	4939(3)	75(1)
C(8)	11875(3)	5011(10)	5135(4)	81(2)
C(9)	11902(3)	6201(9)	6065(4)	79(1)
C(10)	11421(3)	5489(7)	6799(3)	61(1)
C(11)	10412(3)	526(7)	7616(3)	73(1)
C(12)	12088(3)	6814(6)	10516(3)	46(1)
C(13)	13801(2)	7333(6)	11620(3)	50(1)
C(14)	14182(2)	7751(6)	12883(3)	46(1)
C(15)	15239(3)	8617(7)	13194(3)	63(1)
C(16)	15930(3)	7219(8)	12803(3)	68(1)
C(17)	15552(3)	6888(8)	11538(3)	70(1)
C(18)	14497(2)	5981(8)	11210(3)	67(1)
C(19)	13468(3)	9100(6)	13289(3)	59(1)
C(20)	13740(3)	9071(9)	14571(3)	91(2)
C(21)	13360(3)	11370(8)	12861(4)	90(2)
C(22)	16233(3)	5498(12)	11133(4)	121(2)
N	10565(2)	4046(4)	8439(2)	45(1)
O(1)	10331(2)	6161(4)	9746(2)	53(1)
O(2)	9151(2)	6080(5)	8038(2)	66(1)
O(3)	12065(2)	8360(5)	9968(2)	82(1)
O(4)	12863(2)	6179(4)	11367(2)	55(1)
H(1A)	12028	3712	9282	61
H(1B)	11352	2117	9685	61
H(2)	11283	4489	10982	54
H(4)	9609	3160	6968	62
H(6)	10554	1174	5547	75

Table 3. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **6b**. (continued)

Atom	x	y	z	U_{eq}^a
H(7)	11351	2334	4309	90
H(8)	12200	5480	4640	97
H(9)	12243	7477	6198	94
H(10)	11448	6295	7430	73
H(11A)	10043	156	8114	109
H(11B)	11101	176	7966	109
H(11C)	10153	-238	6919	109
H(13)	13685	8676	11211	60
H(14)	14228	6380	13258	55
H(15A)	15219	10003	12859	76
H(15B)	15505	8778	14008	76
H(16A)	16586	7856	13013	82
H(16B)	15991	5865	13179	82
H(17)	15516	8266	11173	84
H(18A)	14233	5856	10394	80
H(18B)	14525	4579	11528	80
H(19)	12808	8449	12988	71
H(20A)	14370	9761	14900	137
H(20B)	13787	7638	14830	137
H(20C)	13236	9794	14791	137
H(21A)	13194	11374	12053	135
H(21B)	13977	12106	13191	135
H(21C)	12842	12058	13071	135
H(22A)	16202	4081	11389	181
H(22B)	16904	6009	11430	181
H(22C)	16026	5519	10322	181

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6a** and **6b**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
6a						
C(1)	55(4)	49(4)	37(3)	0(3)	1(3)	7(3)
C(2)	53(4)	73(4)	47(4)	2(4)	4(3)	4(4)
C(3)	75(5)	75(5)	37(4)	-4(4)	0(4)	-13(4)
C(4)	55(4)	69(4)	47(4)	0(4)	5(4)	-15(4)
C(5)	67(4)	61(4)	60(5)	-8(4)	-3(5)	-14(4)
C(6)	94(6)	84(6)	82(6)	6(5)	-8(5)	-2(5)
C(7)	119(8)	90(7)	131(9)	31(7)	-33(8)	-3(7)
C(8)	88(6)	87(7)	139(9)	-22(8)	-12(8)	6(5)
C(9)	92(7)	116(8)	103(7)	-28(7)	-4(6)	14(6)
C(10)	79(5)	94(6)	72(5)	-17(5)	1(5)	-4(5)
C(11)	69(4)	75(5)	99(5)	10(5)	15(4)	-18(4)
C(12)	73(5)	85(5)	47(4)	17(4)	-7(4)	14(4)
C(13)	49(4)	69(4)	55(4)	9(4)	-1(4)	18(4)
C(14)	49(4)	64(4)	71(4)	11(4)	15(4)	8(4)
C(15)	54(4)	99(5)	91(5)	-2(5)	22(4)	18(4)
C(16)	82(5)	93(5)	83(5)	-2(5)	16(5)	41(5)
C(17)	88(5)	73(5)	78(5)	7(5)	15(5)	25(5)
C(18)	67(4)	65(4)	59(4)	8(4)	11(4)	2(4)
C(19)	61(4)	86(5)	112(6)	-11(6)	19(5)	-12(4)
C(20)	111(7)	122(7)	186(10)	-20(7)	59(8)	-45(6)
C(21)	115(7)	187(9)	156(9)	-31(8)	-50(8)	-28(8)
C(22)	142(7)	74(5)	121(7)	-22(6)	36(7)	1(6)
N	62(3)	62(3)	34(3)	3(3)	-6(3)	-13(3)
O(1)	86(3)	78(3)	43(3)	-1(3)	24(3)	-23(3)
O(2)	160(5)	102(4)	32(2)	-8(3)	-11(3)	-28(4)
O(3)	252(8)	177(6)	65(4)	48(4)	48(5)	142(6)
O(4)	58(3)	65(3)	44(2)	11(2)	7(2)	11(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for OX (I) and **6b**.
(continued)

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
6b						
C(1)	45(2)	47(2)	53(2)	-5(2)	4(2)	4(2)
C(2)	36(2)	50(2)	48(2)	0(2)	12(2)	-4(2)
C(3)	42(2)	44(2)	54(2)	-2(2)	13(2)	-4(2)
C(4)	51(2)	47(2)	49(2)	-7(2)	5(2)	1(2)
C(5)	49(2)	42(2)	44(2)	4(2)	8(2)	8(2)
C(6)	59(2)	69(3)	53(2)	-8(2)	12(2)	6(2)
C(7)	71(3)	101(4)	52(3)	-3(3)	20(2)	13(3)
C(8)	67(3)	111(5)	66(3)	18(3)	26(2)	14(3)
C(9)	78(3)	77(3)	85(3)	10(3)	32(3)	-10(3)
C(10)	70(3)	52(3)	64(2)	-2(2)	25(2)	1(2)
C(11)	103(3)	51(3)	60(2)	-9(2)	22(2)	-16(3)
C(12)	48(2)	50(3)	37(2)	0(2)	11(2)	0(2)
C(13)	42(2)	55(3)	48(2)	7(2)	7(2)	-13(2)
C(14)	47(2)	50(2)	38(2)	3(2)	9(2)	-8(2)
C(15)	53(2)	79(3)	51(2)	-14(2)	7(2)	-14(3)
C(16)	47(2)	94(4)	59(2)	-10(2)	11(2)	-6(2)
C(17)	54(2)	100(4)	57(2)	-5(2)	22(2)	-7(3)
C(18)	59(2)	88(3)	53(2)	-12(2)	16(2)	-13(3)
C(19)	57(2)	58(3)	61(2)	-7(2)	17(2)	-3(2)
C(20)	98(3)	110(5)	74(3)	-19(3)	38(3)	0(3)
C(21)	87(3)	65(3)	120(4)	5(3)	36(3)	7(3)
C(22)	77(3)	178(6)	126(4)	-59(5)	58(3)	-24(4)
N	42(2)	46(2)	43(2)	-3(2)	8(1)	9(2)
O(1)	40(1)	63(2)	56(2)	-14(1)	14(1)	1(1)
O(2)	43(2)	68(2)	75(2)	-5(2)	0(1)	14(2)
O(3)	63(2)	70(2)	92(2)	36(2)	-4(2)	-12(2)
O(4)	46(1)	60(2)	48(1)	12(1)	2(1)	-14(1)

The anisotropic displacement factor exponent takes the form:

$$-2 \quad {}^2[h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^{*}b^{*}U_{12} + 2klb^{*}c^{*}U_{23} + 2hla^{*}c^{*}U_{13}]$$

Table 5. Selected Bond Lengths(Å) for **6a** and **6b**.

atom	atom	distance	atom	atom	distance
6a					
C(1)	N	1.453(6)	C(1)	C(2)	1.523(7)
C(2)	O(1)	1.444(7)	C(2)	C(12)	1.498(8)
C(3)	O(2)	1.211(6)	C(3)	O(1)	1.349(7)
C(3)	N	1.350(7)	C(4)	N	1.458(6)
C(4)	C(5)	1.507(8)	C(4)	C(11)	1.517(8)
C(5)	C(6)	1.378(9)	C(5)	C(10)	1.387(8)
C(6)	C(7)	1.395(10)	C(7)	C(8)	1.358(11)
C(8)	C(9)	1.345(11)	C(9)	C(10)	1.376(9)
C(12)	O(3)	1.166(7)	C(12)	O(4)	1.322(7)
C(13)	O(4)	1.469(6)	C(13)	C(14)	1.510(7)
C(13)	C(18)	1.522(7)	C(14)	C(19)	1.515(8)
C(14)	C(15)	1.526(7)	C(15)	C(16)	1.507(8)
C(16)	C(17)	1.528(9)	C(17)	C(22)	1.497(9)
C(17)	C(18)	1.523(8)	C(19)	C(20)	1.522(9)
C(19)	C(21)	1.533(10)			
6b					
C(1)	N	1.445(4)	C(1)	C(2)	1.536(5)
C(2)	O(1)	1.435(4)	C(2)	C(12)	1.503(5)
C(3)	O(2)	1.202(4)	C(3)	N	1.349(4)
C(3)	O(1)	1.369(4)	C(4)	N	1.461(4)
C(4)	C(5)	1.521(5)	C(4)	C(11)	1.522(6)
C(5)	C(10)	1.369(5)	C(5)	C(6)	1.387(5)
C(6)	C(7)	1.384(5)	C(7)	C(8)	1.367(7)
C(8)	C(9)	1.375(6)	C(9)	C(10)	1.382(5)
C(12)	O(3)	1.191(4)	C(12)	O(4)	1.323(4)
C(13)	O(4)	1.461(4)	C(13)	C(18)	1.514(5)
C(13)	C(14)	1.517(4)	C(14)	C(15)	1.525(5)
C(14)	C(19)	1.530(5)	C(15)	C(16)	1.513(6)
C(16)	C(17)	1.511(5)	C(17)	C(22)	1.509(6)
C(17)	C(18)	1.530(5)	C(19)	C(20)	1.522(5)
C(19)	C(21)	1.527(6)			

Table 6. Selected Bond Angles(°) for **6a** and **6b**.

atom	atom	atom	angle	atom	atom	atom	angle
6a							
N	C(1)	C(2)	99.7(4)	O(1)	C(2)	C(12)	106.7(5)
O(1)	C(2)	C(1)	104.0(5)	C(12)	C(2)	C(1)	116.7(5)
O(2)	C(3)	O(1)	122.9(6)	O(2)	C(3)	N	127.0(6)
O(1)	C(3)	N	110.1(5)	N	C(4)	C(5)	111.4(5)
N	C(4)	C(11)	110.1(5)	C(5)	C(4)	C(11)	114.9(6)
C(6)	C(5)	C(10)	116.9(7)	C(6)	C(5)	C(4)	123.5(7)
C(10)	C(5)	C(4)	119.6(7)	C(5)	C(6)	C(7)	120.8(9)
C(8)	C(7)	C(6)	120.3(9)	C(9)	C(8)	C(7)	120.0(9)
C(8)	C(9)	C(10)	120.4(9)	C(9)	C(10)	C(5)	121.7(8)
O(3)	C(12)	O(4)	123.2(6)	O(3)	C(12)	C(2)	123.6(6)
O(4)	C(12)	C(2)	113.2(6)	O(4)	C(13)	C(14)	108.2(4)
O(4)	C(13)	C(18)	107.9(4)	C(14)	C(13)	C(18)	112.9(5)
C(13)	C(14)	C(19)	112.7(5)	C(13)	C(14)	C(15)	108.4(5)
C(19)	C(14)	C(15)	114.9(5)	C(16)	C(15)	C(14)	112.3(5)
C(15)	C(16)	C(17)	113.3(6)	C(22)	C(17)	C(18)	111.7(6)
C(22)	C(17)	C(16)	112.6(7)	C(18)	C(17)	C(16)	109.2(5)
C(13)	C(18)	C(17)	112.7(5)	C(14)	C(19)	C(20)	110.9(6)
C(14)	C(19)	C(21)	115.2(7)	C(20)	C(19)	C(21)	109.7(6)
C(3)	N	C(1)	110.7(5)	C(3)	N	C(4)	121.5(5)
C(1)	N	C(4)	123.3(5)	C(3)	O(1)	C(2)	108.2(5)
C(12)	O(4)	C(13)	119.9(5)				
6b							
N	C(1)	C(2)	101.5(3)	O(1)	C(2)	C(12)	109.5(3)
O(1)	C(2)	C(1)	105.5(2)	C(12)	C(2)	C(1)	110.9(3)
O(2)	C(3)	N	128.6(3)	O(2)	C(3)	O(1)	122.0(4)
N	C(3)	O(1)	109.4(3)	N	C(4)	C(5)	112.4(3)
N	C(4)	C(11)	109.7(3)	C(5)	C(4)	C(11)	113.2(4)
C(10)	C(5)	C(6)	117.5(4)	C(10)	C(5)	C(4)	122.7(3)
C(6)	C(5)	C(4)	119.7(4)	C(7)	C(6)	C(5)	121.5(4)
C(8)	C(7)	C(6)	119.6(5)	C(7)	C(8)	C(9)	120.1(4)
C(8)	C(9)	C(10)	119.6(5)	C(5)	C(10)	C(9)	121.8(4)

Table 6. Selected Bond Angles(°) for **6a** and **6b**. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	C(12)	O(4)	125.2(4)	O(3)	C(12)	C(2)	125.1(3)
O(4)	C(12)	C(2)	109.5(3)	O(4)	C(13)	C(18)	106.8(3)
O(4)	C(13)	C(14)	108.0(3)	C(18)	C(13)	C(14)	113.3(3)
C(13)	C(14)	C(15)	108.8(3)	C(13)	C(14)	C(19)	112.9(3)
C(15)	C(14)	C(19)	114.4(3)	C(16)	C(15)	C(14)	113.0(4)
C(17)	C(16)	C(15)	111.7(3)	C(22)	C(17)	C(16)	112.4(4)
C(22)	C(17)	C(18)	111.4(4)	C(16)	C(17)	C(18)	108.7(3)
C(13)	C(18)	C(17)	112.5(4)	C(20)	C(19)	C(21)	110.0(4)
C(20)	C(19)	C(14)	111.7(3)	C(21)	C(19)	C(14)	114.5(4)
C(3)	N	C(1)	112.8(3)	C(3)	N	C(4)	122.2(3)
C(1)	N	C(4)	124.0(3)	C(3)	O(1)	C(2)	110.0(3)
C(12)	O(4)	C(13)	119.0(3)				