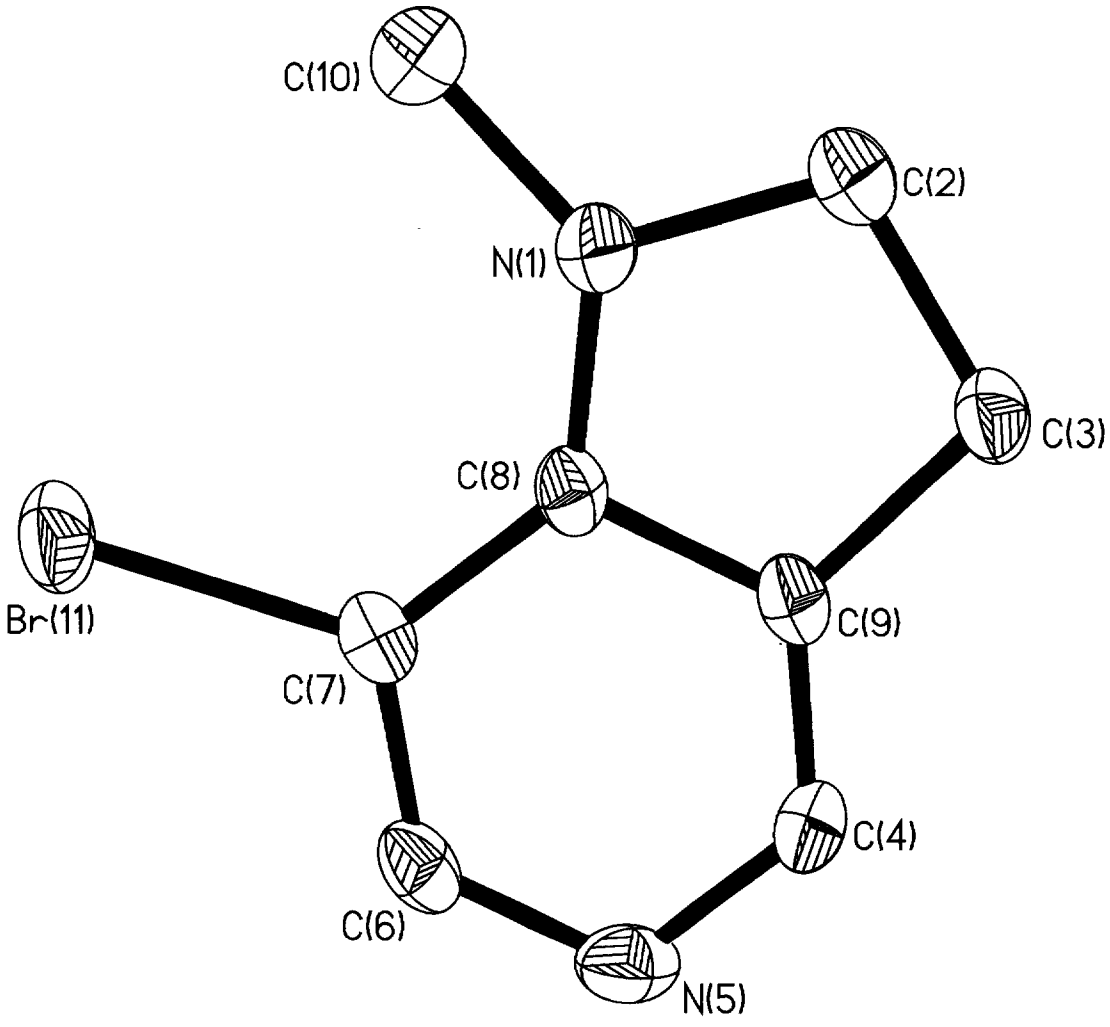


An ORTEP plot for aryl bromide (18).

Table 1. Crystal data and structure refinement for aryl bromide **18**.

Empirical formula	C8 H9 Br N2	
Formula weight	213.08	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.7576(15) Å	α= 90°.
	b = 13.231(3) Å	β= 110.010(4)°.
	c = 8.2134(16) Å	γ = 90°.
Volume	792.1(3) $Å^3$	
Z	4	
Density (calculated)	1.787 Mg/m^3	
Absorption coefficient	5.119 mm^{-1}	
F(000)	424	
Crystal size	0.50 x 0.48 x 0.45 mm^3	
Theta range for data collection	2.79 to 28.26°.	
Index ranges	-6<=h<=10, -16<=k<=17, -10<=l<=10	
Reflections collected	4053	
Independent reflections	1747 [R(int) = 0.1367]	
Completeness to theta = 28.26°	88.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2066 and 0.1840	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1747 / 0 / 100	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1217	
R indices (all data)	R1 = 0.0612, wR2 = 0.1270	
Largest diff. peak and hole	0.916 and -1.272 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for aryl bromide **18**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(11)	7978(1)	2401(1)	3891(1)	34(1)
N(1)	12112(4)	1553(2)	6801(4)	28(1)
N(5)	7482(5)	-111(3)	6655(5)	31(1)
C(2)	13614(5)	962(3)	7993(5)	28(1)
C(3)	12689(5)	134(3)	8718(5)	26(1)
C(4)	9221(5)	-300(3)	7668(5)	28(1)
C(6)	7249(5)	684(3)	5591(5)	27(1)
C(7)	8653(5)	1301(2)	5472(5)	24(1)
C(8)	10458(4)	1095(2)	6547(4)	20(1)
C(9)	10677(5)	256(2)	7645(5)	23(1)
C(10)	12596(6)	2298(3)	5738(6)	33(1)

Table 3. Bond lengths [Å] and angles [°] for aryl bromide **18**.

Br(11)-C(7)	1.901(3)
N(1)-C(8)	1.369(4)
N(1)-C(10)	1.448(5)
N(1)-C(2)	1.465(4)
N(5)-C(6)	1.340(5)
N(5)-C(4)	1.344(5)
C(2)-C(3)	1.536(5)
C(3)-C(9)	1.516(5)
C(4)-C(9)	1.354(6)
C(6)-C(7)	1.391(5)
C(7)-C(8)	1.403(5)
C(8)-C(9)	1.404(4)
C(8)-N(1)-C(10)	129.2(3)
C(8)-N(1)-C(2)	110.8(3)
C(10)-N(1)-C(2)	117.1(3)
C(6)-N(5)-C(4)	115.7(3)
N(1)-C(2)-C(3)	105.6(3)
C(9)-C(3)-C(2)	102.9(3)
N(5)-C(4)-C(9)	123.7(3)
N(5)-C(6)-C(7)	124.9(3)
C(6)-C(7)-C(8)	118.6(3)
C(6)-C(7)-Br(11)	117.3(2)
C(8)-C(7)-Br(11)	124.1(2)
N(1)-C(8)-C(7)	133.8(3)
N(1)-C(8)-C(9)	110.6(3)
C(7)-C(8)-C(9)	115.7(3)
C(4)-C(9)-C(8)	121.4(3)
C(4)-C(9)-C(3)	129.2(3)
C(8)-C(9)-C(3)	109.4(3)

Symmetry transformations used to generate equivalent atoms:

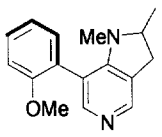
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for aryl bromide **18**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(11)	32(1)	34(1)	27(1)	8(1)	0(1)	7(1)
N(1)	24(2)	31(2)	24(2)	7(1)	4(1)	-2(1)
N(5)	24(2)	42(2)	29(2)	-3(1)	10(1)	-9(1)
C(2)	24(2)	32(2)	24(2)	-1(1)	4(2)	2(1)
C(3)	23(2)	32(2)	19(2)	4(1)	3(1)	3(1)
C(4)	31(2)	30(2)	22(2)	9(1)	8(2)	3(1)
C(6)	20(2)	37(2)	18(2)	-3(1)	0(1)	4(1)
C(7)	22(2)	24(2)	22(2)	-2(1)	4(2)	4(1)
C(8)	22(2)	25(2)	12(2)	-1(1)	4(1)	4(1)
C(9)	21(2)	26(2)	18(2)	1(1)	3(1)	5(1)
C(10)	33(2)	30(2)	34(2)	5(2)	10(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for aryl bromide **18**.

	x	y	z	U(eq)
H(2A)	14385	1386	8921	33
H(2B)	14364	665	7386	33
H(3A)	13134	-531	8562	31
H(3B)	12900	241	9940	31
H(4A)	9437	-844	8429	33
H(6A)	6059	834	4879	32
H(10A)	11506	2635	5016	49
H(10B)	13181	1969	5025	49
H(10C)	13420	2784	6470	49

Single-crystal X-ray data for biaryl (22)



22

Crystal data for $C_{16}H_{18}N_2O$; M =254.32. Crystallizes from ethyl acetate as colorless blocks; crystal dimensions 0.40 x 0.21 x 0.21 mm. Orthorhombic, a = 7.461(6), b = 8.350(8), c = 21.315(18) Å, U = 1328 (2) $Å^3$, Z = 4, D_c = 1.272 Mg/m^3, space group $P2_12_12_1$ (D_2^4 , No.19), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.080 mm^{-1}, F(000) =544.

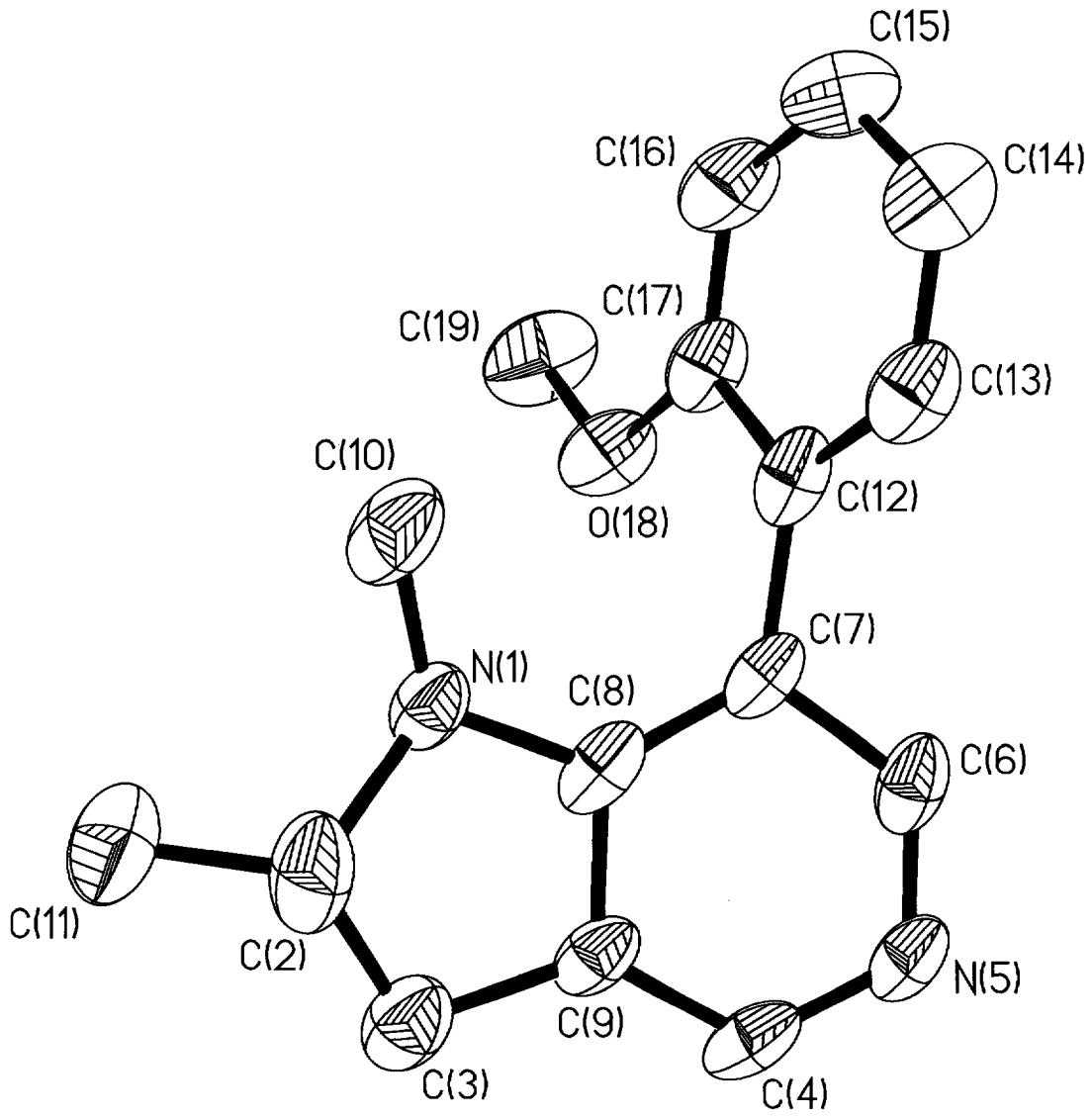
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 45 reflections (θ range 1.91< 28.72°).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 8858 reflections measured, all of which were corrected for Lorentz and polarization effects and for absorption by semi-empirical methods (maximum and minimum transmission coefficients of 0.9833 and 0.9685) 1505 independent reflections exceeded the significance level $|F|/\sigma(|F|) > 4.0$. The structure was solved by direct methods and refined by full matrix least squares methods on F^2. Hydrogen atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Refinement converged at a final R= 0.1018(wR2=0.2882 for all 3208 unique data, 172 parameters, mean and maximum δ/σ 0.000, 0.000), with allowance for the thermal anisotropy of all non-hydrogen atoms. Minimum and maximum final electron density -0.389 and 0.447e A^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.1159 * P)^2 + 0.000 * P]$ where $P=(Fo^2 + 2 * Fc^2)/3$ was used in the latter stages of refinement. Complex scattering factors were taken from the program package **SHELXTL**[Y] as implemented on the Viglen Pentium computer.

Reference Y SHELXTL version, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD

Supplementary material

anisotropic thermal vibrational parameters with e.s.d.s
hydrogen atom position parameters
observed structure amplitudes and calculated structure factors.



An ORTEP plot for biaryl (22).

Table 1. Crystal data and structure refinement for biaryl **22**.

Empirical formula	C16 H18 N2 O	
Formula weight	254.32	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.461(6) Å	α= 90°.
	b = 8.350(8) Å	β= 90°.
	c = 21.315(18) Å	γ = 90°.
Volume	1328(2) $Å^3$	
Z	4	
Density (calculated)	1.272 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	544	
Crystal size	0.40 x 0.21 x 0.21 mm^3	
Theta range for data collection	1.91 to 28.72°.	
Index ranges	-5<=h<=9, -10<=k<=10, -28<=l<=27	
Reflections collected	8858	
Independent reflections	3208 [R(int) = 0.2981]	
Completeness to theta = 28.72°	94.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9833 and 0.9685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3208 / 0 / 172	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.1018, wR2 = 0.2239	
R indices (all data)	R1 = 0.1799, wR2 = 0.2882	
Absolute structure parameter	-3(5)	
Largest diff. peak and hole	0.447 and -0.389 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for biaryl **22**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(18)	-213(4)	3783(4)	8633(2)	49(1)
N(1)	3355(5)	5169(5)	9317(2)	38(1)
N(5)	4356(5)	314(5)	9201(2)	40(1)
C(2)	4366(8)	5553(7)	9893(3)	57(2)
C(3)	4451(7)	3995(6)	10246(3)	50(2)
C(4)	4600(6)	1198(6)	9711(3)	42(1)
C(6)	3672(6)	1040(6)	8710(3)	42(1)
C(7)	3214(5)	2669(5)	8672(3)	32(1)
C(8)	3548(6)	3558(5)	9205(3)	37(1)
C(9)	4230(6)	2796(5)	9740(3)	37(1)
C(10)	3276(8)	6336(6)	8821(3)	55(2)
C(11)	3657(10)	6936(7)	10246(4)	73(2)
C(12)	2422(6)	3268(5)	8079(3)	38(1)
C(13)	3350(6)	3263(6)	7525(3)	44(1)
C(14)	2622(7)	3825(7)	6983(3)	54(2)
C(15)	877(7)	4420(8)	6980(3)	55(2)
C(16)	-91(7)	4412(7)	7525(3)	53(2)
C(17)	651(6)	3840(6)	8067(3)	40(1)
C(19)	-2052(7)	4230(8)	8643(4)	65(2)

Table 3. Bond lengths [Å] and angles [°] for biaryl **22**.

O(18)-C(17)	1.369(7)
O(18)-C(19)	1.422(6)
N(1)-C(8)	1.373(6)
N(1)-C(10)	1.439(7)
N(1)-C(2)	1.476(8)
N(5)-C(6)	1.314(7)
N(5)-C(4)	1.325(7)
C(2)-C(11)	1.476(9)
C(2)-C(3)	1.505(9)
C(3)-C(9)	1.480(8)
C(4)-C(9)	1.364(7)
C(6)-C(7)	1.405(6)
C(7)-C(8)	1.379(7)
C(7)-C(12)	1.483(8)
C(8)-C(9)	1.403(7)
C(12)-C(13)	1.369(8)
C(12)-C(17)	1.405(7)
C(13)-C(14)	1.360(9)
C(14)-C(15)	1.394(8)
C(15)-C(16)	1.368(9)
C(16)-C(17)	1.368(8)

C(17)-O(18)-C(19)	117.2(5)
C(8)-N(1)-C(10)	122.7(5)
C(8)-N(1)-C(2)	107.7(4)
C(10)-N(1)-C(2)	119.0(4)
C(6)-N(5)-C(4)	116.8(4)
N(1)-C(2)-C(11)	114.3(5)
N(1)-C(2)-C(3)	104.5(4)
C(11)-C(2)-C(3)	115.8(6)
C(9)-C(3)-C(2)	102.5(5)
N(5)-C(4)-C(9)	123.7(5)
N(5)-C(6)-C(7)	125.9(5)
C(8)-C(7)-C(6)	115.5(5)
C(8)-C(7)-C(12)	126.3(4)
C(6)-C(7)-C(12)	118.2(5)
N(1)-C(8)-C(7)	130.6(5)
N(1)-C(8)-C(9)	110.0(5)

C(7)-C(8)-C(9)	119.4(4)
C(4)-C(9)-C(8)	118.7(5)
C(4)-C(9)-C(3)	132.3(6)
C(8)-C(9)-C(3)	109.0(4)
C(13)-C(12)-C(17)	117.5(5)
C(13)-C(12)-C(7)	122.2(4)
C(17)-C(12)-C(7)	120.3(5)
C(14)-C(13)-C(12)	122.0(5)
C(13)-C(14)-C(15)	120.1(6)
C(16)-C(15)-C(14)	119.1(6)
C(15)-C(16)-C(17)	120.4(5)
C(16)-C(17)-O(18)	124.5(4)
C(16)-C(17)-C(12)	121.0(6)
O(18)-C(17)-C(12)	114.5(5)

Symmetry transformations used to generate equivalent atoms:

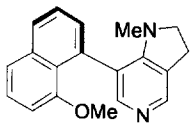
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for biaryl **22**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(18)	18(2)	57(2)	71(3)	6(2)	-2(2)	7(2)
N(1)	29(2)	29(2)	57(3)	-2(2)	-5(2)	1(2)
N(5)	35(2)	24(2)	62(3)	1(2)	-1(2)	4(2)
C(2)	54(3)	38(3)	79(5)	-14(3)	3(3)	-9(3)
C(3)	38(3)	40(3)	72(4)	-3(3)	-5(3)	2(2)
C(4)	30(2)	29(2)	67(4)	16(3)	-4(3)	1(2)
C(6)	24(2)	34(3)	68(4)	-13(3)	1(2)	2(2)
C(7)	17(2)	24(2)	55(3)	7(2)	9(2)	0(2)
C(8)	19(2)	24(2)	67(4)	6(2)	5(2)	-2(2)
C(9)	21(2)	30(2)	60(4)	4(2)	-4(2)	2(2)
C(10)	60(4)	27(3)	78(5)	5(3)	-5(3)	-3(2)
C(11)	89(5)	40(3)	89(6)	-7(4)	-3(5)	5(3)
C(12)	22(2)	29(2)	64(4)	-7(3)	2(2)	-2(2)
C(13)	24(2)	40(3)	67(4)	-1(3)	1(3)	1(2)
C(14)	39(3)	52(3)	71(5)	8(3)	5(3)	-5(2)
C(15)	43(3)	59(4)	64(4)	19(3)	-7(3)	-1(3)
C(16)	27(2)	55(3)	77(5)	4(3)	-7(3)	12(2)
C(17)	20(2)	39(3)	60(4)	-2(3)	6(2)	4(2)
C(19)	25(2)	85(4)	85(5)	17(4)	13(3)	18(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for biaryl **22**.

	x	y	z	U(eq)
H(2A)	5592	5821	9765	69
H(3A)	5594	3869	10457	60
H(3B)	3493	3918	10552	60
H(4A)	5048	700	10068	50
H(6A)	3474	420	8354	50
H(10A)	2578	5918	8479	83
H(10B)	4467	6568	8677	83
H(10C)	2729	7299	8975	83
H(11A)	3659	7867	9982	109
H(11B)	4398	7128	10607	109
H(11C)	2454	6711	10379	109
H(13A)	4514	2864	7519	53
H(14A)	3289	3811	6615	65
H(15A)	377	4818	6612	66
H(16A)	-1261	4797	7527	64
H(19A)	-2504	4146	9063	98
H(19B)	-2720	3531	8372	98
H(19C)	-2172	5315	8499	98

Single-crystal X-ray data for biaryl (35)



35

Crystal data for $C_{19}H_{19}ClN_2O$; M =326.81, crystallizes from dichloromethane/ethyl acetate as colorless blocks; crystal dimensions 0.32 x 0.16 x 0.15mm. Monoclinic, a = 7.194(3), b = 23.993(7), c = 9.667(3) Å, β =106.41(4)° U =1600.5(9) Å^3, Z = 4, D_c = 1.356 Mg/m^3, space group $P2_1/n$ (a non-standard setting of $P2_1/c$ C_2^5 h No.14), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.245 mm^{-1}, F(000) = 688.

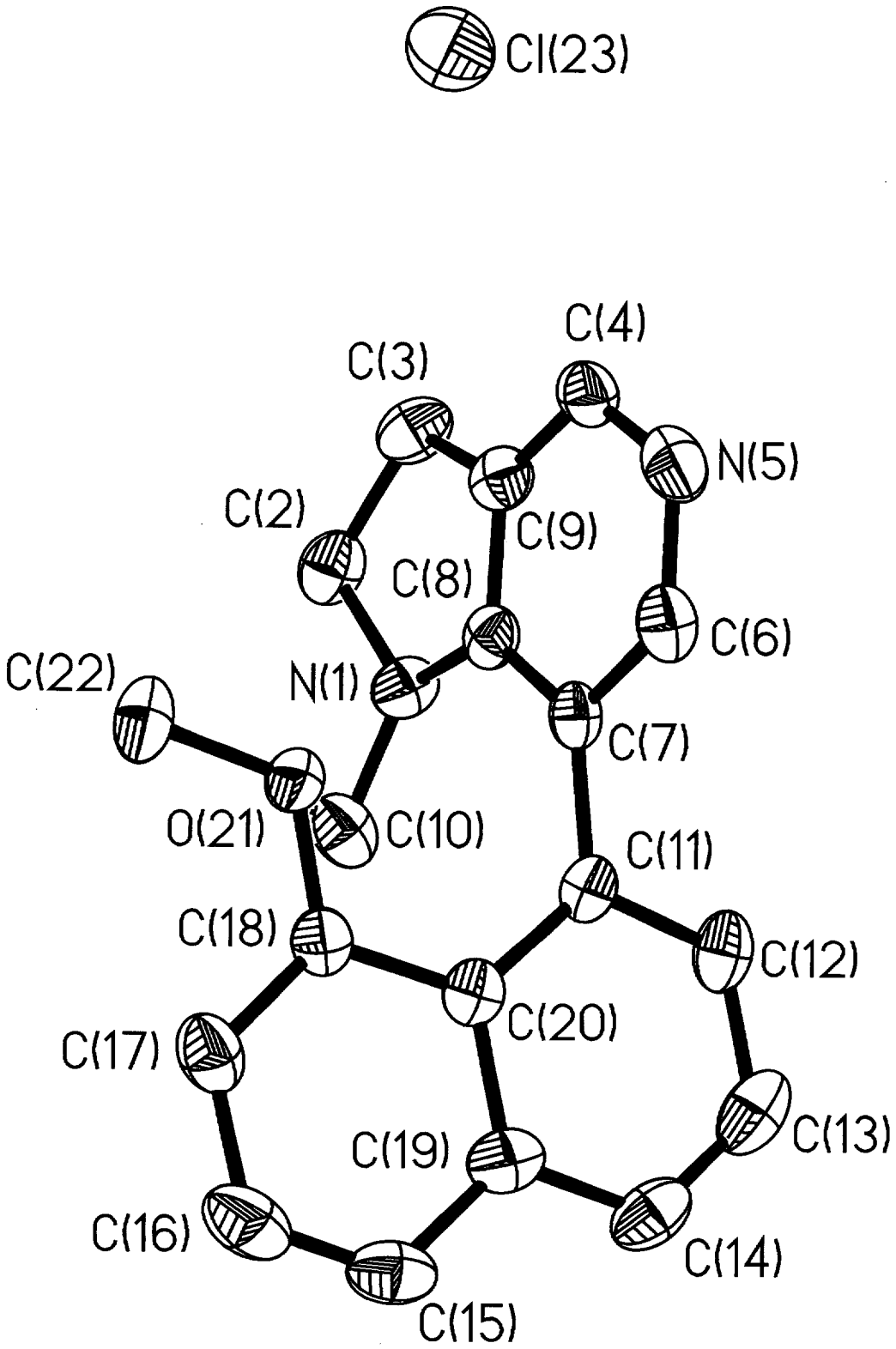
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 48 reflections (θ range 1.70< 23.30).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 10487 reflections measured, all of which were corrected for Lorentz and polarization effects and for absorption by semi empirical methods based on symmetry -equivalent and repeated reflections (minimum and maximum transmission coefficients 0.9257 and 0.9642) 2157 independent reflections exceeded the significance level $|F|/\sigma(|F|) > 4.0$ The structure was solved by direct methods and refined by full matrix least squares methods on F^2. Hydrogen atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2(1.5 for methyl groups) times U_{eq} of the carrier atom. Refinement converged at a final R= 0.0833(wR_2=0.2691, for all 3821 data, 208 parameters, mean and maximum δ/σ 0.000, 0.000) with allowance for the thermal anisotropy of all non-hydrogen atoms. Minimum and maximum final electron density -0.833 and 0.539e Å^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.1715*P)^2 + 0.00*P]$ where $P=(Fo^2 + 2 * Fc^2)/3$ was used in the latter stages of refinement. Complex scattering factors were taken from the program package SHELXTL[Y] as implemented on the Viglen Pentium computer.

Reference Y SHELXL version, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD

Supplementary material

anisotropic thermal vibrational parameters with e.s.d.s
hydrogen atom position parameters
observed structure amplitudes and calculated structure factors.



An ORTEP plot for biaryl (35).

Table 1. Crystal data and structure refinement for biaryl **35**.

Empirical formula	C19 H19 Cl N2 O	
Formula weight	326.81	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.194(3) Å	α= 90°.
	b = 23.993(7) Å	β= 106.41(4)°.
	c = 9.667(3) Å	γ = 90°.
Volume	1600.5(9) $Å^3$	
Z	4	
Density (calculated)	1.356 Mg/m^3	
Absorption coefficient	0.245 mm^{-1}	
F(000)	688	
Crystal size	0.32 x 0.16 x 0.15 mm^3	
Theta range for data collection	1.70 to 28.31°.	
Index ranges	-8<=h<=9, -31<=k<=27, -12<=l<=9	
Reflections collected	10487	
Independent reflections	3821 [R(int) = 0.0750]	
Completeness to theta = 28.31°	96.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9642 and 0.9257	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3821 / 0 / 208	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0832, wR2 = 0.2310	
R indices (all data)	R1 = 0.1333, wR2 = 0.2675	
Largest diff. peak and hole	0.535 and -0.835 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for biaryl **35**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(23)	11236(2)	-500(1)	9385(1)	71(1)
N(1)	10350(4)	1262(1)	5180(3)	34(1)
N(5)	15416(4)	902(1)	8295(3)	40(1)
O(21)	13936(3)	907(1)	3805(2)	32(1)
C(2)	9030(5)	821(2)	5375(4)	41(1)
C(3)	10040(5)	569(1)	6860(4)	41(1)
C(4)	13702(5)	640(1)	8192(3)	35(1)
C(6)	15479(5)	1297(1)	7337(3)	34(1)
C(7)	13909(4)	1465(1)	6210(3)	28(1)
C(8)	12144(5)	1190(1)	6110(3)	29(1)
C(9)	12079(5)	781(1)	7137(4)	33(1)
C(10)	9839(5)	1554(2)	3814(4)	41(1)
C(11)	14232(4)	1939(1)	5283(3)	28(1)
C(12)	14421(5)	2461(1)	5915(4)	37(1)
C(13)	14797(5)	2939(1)	5191(4)	45(1)
C(14)	14994(5)	2896(1)	3851(4)	40(1)
C(15)	15021(5)	2334(2)	1737(4)	42(1)
C(16)	14882(5)	1841(2)	1063(4)	47(1)
C(17)	14530(5)	1350(2)	1733(4)	37(1)
C(18)	14294(4)	1369(1)	3088(3)	29(1)
C(19)	14815(4)	2373(1)	3136(4)	34(1)
C(20)	14441(4)	1884(1)	3860(3)	28(1)
C(22)	13885(5)	381(1)	3110(4)	42(1)

Table 3. Bond lengths [Å] and angles [°] for biaryl **35**.

N(1)-C(8)	1.359(4)
N(1)-C(10)	1.447(4)
N(1)-C(2)	1.470(4)
N(5)-C(6)	1.335(4)
N(5)-C(4)	1.363(5)
O(21)-C(18)	1.370(4)
O(21)-C(22)	1.425(4)
C(2)-C(3)	1.537(5)
C(3)-C(9)	1.504(5)
C(4)-C(9)	1.358(5)
C(6)-C(7)	1.389(4)
C(7)-C(8)	1.409(4)
C(7)-C(11)	1.506(4)
C(8)-C(9)	1.406(5)
C(11)-C(12)	1.382(4)
C(11)-C(20)	1.432(4)
C(12)-C(13)	1.409(5)
C(13)-C(14)	1.347(6)
C(14)-C(19)	1.422(5)
C(15)-C(16)	1.342(5)
C(15)-C(19)	1.404(5)
C(16)-C(17)	1.400(5)
C(17)-C(18)	1.368(5)
C(18)-C(20)	1.432(4)
C(19)-C(20)	1.428(4)

C(8)-N(1)-C(10)	127.9(3)
C(8)-N(1)-C(2)	110.5(3)
C(10)-N(1)-C(2)	117.3(3)
C(6)-N(5)-C(4)	119.0(3)
C(18)-O(21)-C(22)	117.6(3)
N(1)-C(2)-C(3)	104.5(3)
C(9)-C(3)-C(2)	102.3(3)
C(9)-C(4)-N(5)	120.5(3)
N(5)-C(6)-C(7)	124.7(3)
C(6)-C(7)-C(8)	115.9(3)
C(6)-C(7)-C(11)	117.2(3)
C(8)-C(7)-C(11)	126.8(3)

N(1)-C(8)-C(9)	109.9(3)
N(1)-C(8)-C(7)	130.9(3)
C(9)-C(8)-C(7)	119.1(3)
C(4)-C(9)-C(8)	120.8(3)
C(4)-C(9)-C(3)	129.6(3)
C(8)-C(9)-C(3)	109.6(3)
C(12)-C(11)-C(20)	118.9(3)
C(12)-C(11)-C(7)	115.7(3)
C(20)-C(11)-C(7)	125.3(3)
C(11)-C(12)-C(13)	121.8(3)
C(14)-C(13)-C(12)	120.2(3)
C(13)-C(14)-C(19)	121.0(3)
C(16)-C(15)-C(19)	120.8(3)
C(15)-C(16)-C(17)	121.0(3)
C(18)-C(17)-C(16)	120.2(3)
C(17)-C(18)-O(21)	123.3(3)
C(17)-C(18)-C(20)	121.1(3)
O(21)-C(18)-C(20)	115.6(3)
C(15)-C(19)-C(14)	120.4(3)
C(15)-C(19)-C(20)	120.2(3)
C(14)-C(19)-C(20)	119.4(3)
C(19)-C(20)-C(11)	118.8(3)
C(19)-C(20)-C(18)	116.7(3)
C(11)-C(20)-C(18)	124.5(3)

Symmetry transformations used to generate equivalent atoms:

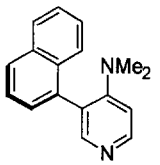
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for biaryl **35**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(23)	70(1)	63(1)	65(1)	8(1)	-4(1)	9(1)
N(1)	24(1)	33(1)	43(2)	4(1)	7(1)	0(1)
N(5)	43(2)	45(2)	30(2)	-4(1)	6(1)	2(1)
O(21)	39(1)	26(1)	31(1)	-4(1)	11(1)	-3(1)
C(2)	31(2)	44(2)	51(2)	-6(2)	15(2)	-9(1)
C(3)	38(2)	35(2)	57(2)	3(2)	20(2)	-1(1)
C(4)	44(2)	34(2)	27(2)	-3(1)	13(1)	2(1)
C(6)	29(2)	41(2)	31(2)	-8(1)	9(1)	-2(1)
C(7)	27(2)	31(2)	26(2)	-8(1)	8(1)	-1(1)
C(8)	32(2)	27(2)	31(2)	-6(1)	13(1)	1(1)
C(9)	37(2)	29(2)	36(2)	-3(1)	18(1)	3(1)
C(10)	29(2)	58(2)	34(2)	-1(2)	7(1)	-1(2)
C(11)	25(2)	27(2)	34(2)	-5(1)	9(1)	-2(1)
C(12)	33(2)	37(2)	43(2)	-13(2)	11(1)	-1(1)
C(13)	35(2)	30(2)	68(3)	-8(2)	10(2)	-1(1)
C(14)	27(2)	31(2)	61(2)	5(2)	11(2)	-2(1)
C(15)	35(2)	48(2)	45(2)	14(2)	17(2)	0(2)
C(16)	41(2)	68(3)	34(2)	7(2)	17(2)	-2(2)
C(17)	35(2)	49(2)	30(2)	-7(2)	13(1)	-3(2)
C(18)	25(2)	33(2)	30(2)	-4(1)	9(1)	-2(1)
C(19)	22(2)	35(2)	43(2)	8(1)	8(1)	1(1)
C(20)	20(1)	31(2)	32(2)	-2(1)	8(1)	0(1)
C(22)	45(2)	35(2)	43(2)	-14(2)	7(2)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for biaryl **35**.

	x	y	z	U(eq)
H(5A)	16441	814	8966	48
H(2A)	8851	541	4623	49
H(2B)	7776	974	5359	49
H(3A)	9454	700	7589	50
H(3B)	9999	165	6831	50
H(4A)	13642	362	8849	42
H(6A)	16661	1473	7431	41
H(10A)	10808	1830	3817	61
H(10B)	8605	1733	3671	61
H(10C)	9765	1293	3047	61
H(12A)	14297	2497	6842	45
H(13A)	14909	3285	5641	54
H(14A)	15251	3214	3385	48
H(15A)	15257	2655	1273	50
H(16A)	15022	1824	136	56
H(17A)	14457	1011	1256	45
H(22A)	13623	92	3718	63
H(22B)	15114	312	2935	63
H(22C)	12885	384	2210	63

Single-crystal X-ray data for biaryl (38)



38

Crystal data for $C_{17}H_{16}N_2$; M = 248.32. Crystallizes from dichloromethane/petrol as colorless blocks; crystal dimensions 0.40 x 0.32 x 0.32 mm. Monoclinic, a = 7.1351(12), b = 7.1394(12), c = 13.279(2) Å, β =104.452°(3), U = 655.03(19) Å^3, Z = 2, D_c = 1.259 Mg/m^3, space group $P2_1$ (C_2^2, No.4), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.075 mm^{-1}, F(000) = 264.

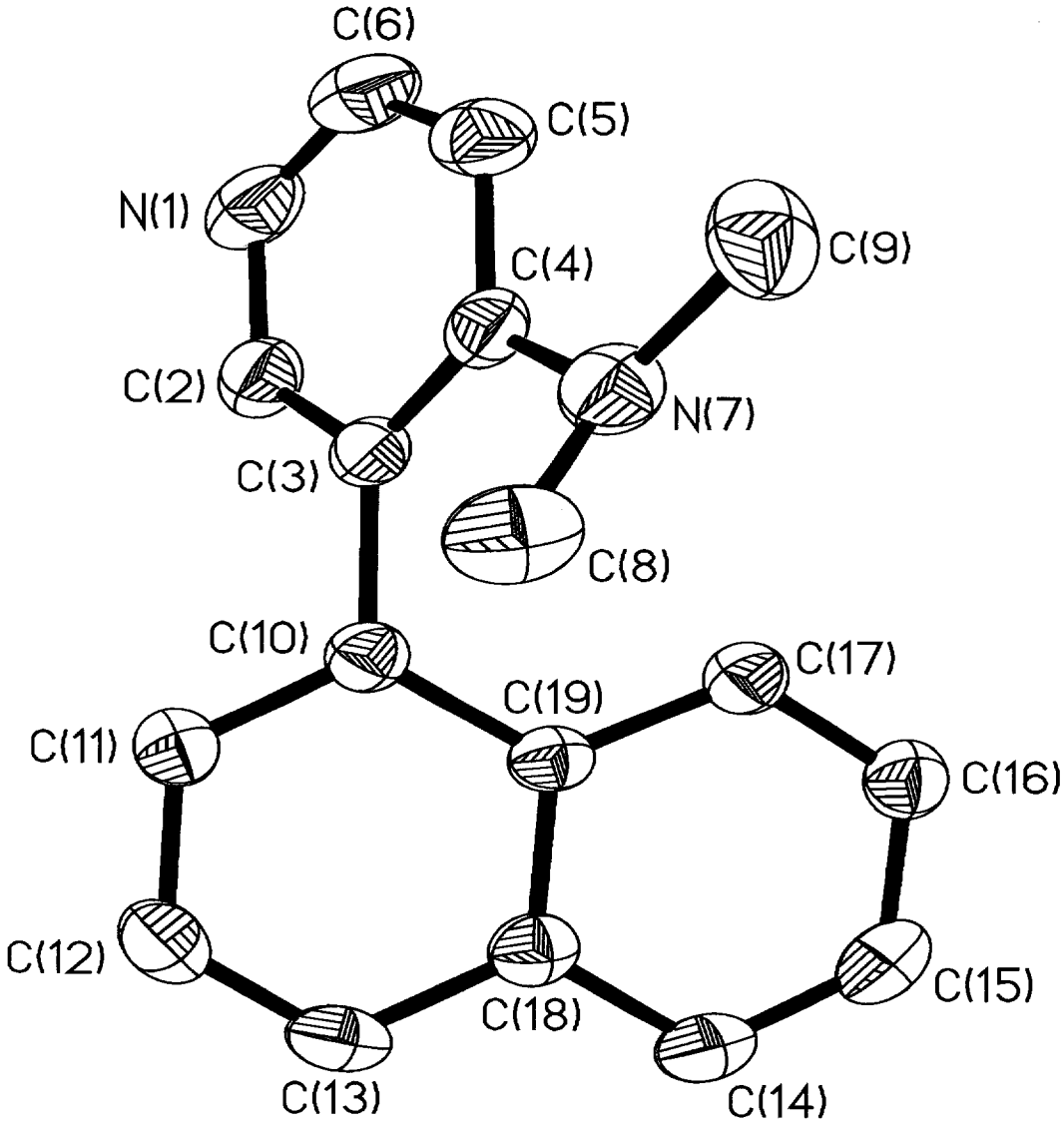
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 48 reflections (θ range 1.58< 28.30°).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 4356 reflections measured, all of which were corrected for Lorentz and polarization effects and for absorption by semi empirical methods based on symmetry-equivalent and repeated reflections (minimum and maximum transmission coefficients 0.9707 and 0.9765) 2403 independent reflections exceeded the significance level $|F|/\sigma(|F|) > 4.0$. The structure was solved by direct methods and refined by full matrix least squares methods on F^2. Hydrogen atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Refinement converged at a final R= 0.0651 (wR_2 = 0.2159, for all 2957 data, 172 parameters, mean and maximum δ/σ 0.000, 0.000) with allowance for the thermal anisotropy of all non-hydrogen atoms. Minimum and maximum final electron density -0.219 and 0.502 e.Å^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.1563*P)^2 + 0.00*P]$ where $P=(Fo^2 + 2 * Fc^2)/3$ was used in the latter stages of refinement. Complex scattering factors were taken from the program package SHELXTL[Y] as implemented on the Viglen Pentium computer.

Reference Y SHELXTL version, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD

Supplementary material

anisotropic thermal vibrational parameters with e.s.d.s
hydrogen atom position parameters
observed structure amplitudes and calculated structure factors.



An ORTEP plot for biaryl (38).

Table 1. Crystal data and structure refinement for biaryl **38**.

Empirical formula	C17 H16 N2	
Formula weight	248.32	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 7.1351(12) Å	α= 90°.
	b = 7.1394(12) Å	β= 104.452(3)°.
	c = 13.279(2) Å	γ = 90°.
Volume	655.03(19) $Å^3$	
Z	2	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	264	
Crystal size	0.40 x 0.32 x 0.32 mm^3	
Theta range for data collection	1.58 to 28.30°.	
Index ranges	-8<=h<=9, -8<=k<=9, -17<=l<=10	
Reflections collected	4356	
Independent reflections	2957 [R(int) = 0.0700]	
Completeness to theta = 28.30°	96.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9765 and 0.9707	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2957 / 1 / 172	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0651, wR2 = 0.1768	
R indices (all data)	R1 = 0.0813, wR2 = 0.2159	
Absolute structure parameter	-2(5)	
Largest diff. peak and hole	0.502 and -0.219 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for biaryl **38**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2332(4)	3314(4)	4964(2)	45(1)
N(7)	2700(4)	7204(4)	2609(2)	41(1)
C(2)	3469(4)	3024(4)	4310(2)	37(1)
C(3)	3637(3)	4207(4)	3498(2)	30(1)
C(4)	2575(4)	5903(4)	3363(2)	33(1)
C(5)	1332(4)	6170(5)	4031(2)	41(1)
C(6)	1283(5)	4883(5)	4787(2)	45(1)
C(8)	4590(5)	7731(5)	2460(3)	48(1)
C(9)	1391(5)	8805(5)	2467(3)	53(1)
C(10)	4879(3)	3513(4)	2823(2)	30(1)
C(11)	6821(3)	3215(4)	3254(2)	35(1)
C(12)	8025(4)	2452(5)	2659(2)	39(1)
C(13)	7274(4)	1911(4)	1667(2)	36(1)
C(14)	4468(4)	1527(4)	155(2)	38(1)
C(15)	2536(4)	1754(5)	-292(2)	42(1)
C(16)	1332(4)	2638(5)	250(2)	38(1)
C(17)	2065(4)	3251(4)	1257(2)	32(1)
C(18)	5275(4)	2142(4)	1188(2)	32(1)
C(19)	4058(3)	2997(4)	1761(2)	29(1)

Table 3. Bond lengths [Å] and angles [°] for biaryl **38**.

N(1)-C(6)	1.335(5)
N(1)-C(2)	1.344(3)
N(7)-C(4)	1.384(4)
N(7)-C(9)	1.458(4)
N(7)-C(8)	1.461(4)
C(2)-C(3)	1.398(4)
C(3)-C(4)	1.416(4)
C(3)-C(10)	1.494(3)
C(4)-C(5)	1.415(4)
C(5)-C(6)	1.368(5)
C(10)-C(11)	1.377(3)
C(10)-C(19)	1.434(3)
C(11)-C(12)	1.414(4)
C(12)-C(13)	1.348(4)
C(13)-C(18)	1.419(4)
C(14)-C(15)	1.368(4)
C(14)-C(18)	1.419(4)
C(15)-C(16)	1.401(4)
C(16)-C(17)	1.380(4)
C(17)-C(19)	1.424(3)
C(18)-C(19)	1.426(3)
C(6)-N(1)-C(2)	114.6(3)
C(4)-N(7)-C(9)	117.7(3)
C(4)-N(7)-C(8)	119.9(2)
C(9)-N(7)-C(8)	111.3(3)
N(1)-C(2)-C(3)	126.0(3)
C(2)-C(3)-C(4)	117.9(2)
C(2)-C(3)-C(10)	116.1(2)
C(4)-C(3)-C(10)	125.9(2)
N(7)-C(4)-C(3)	122.5(2)
N(7)-C(4)-C(5)	121.7(3)
C(3)-C(4)-C(5)	115.8(2)
C(6)-C(5)-C(4)	120.3(3)
N(1)-C(6)-C(5)	125.3(3)
C(11)-C(10)-C(19)	119.4(2)
C(11)-C(10)-C(3)	119.2(2)
C(19)-C(10)-C(3)	121.2(2)

C(10)-C(11)-C(12)	121.1(2)
C(13)-C(12)-C(11)	120.5(2)
C(12)-C(13)-C(18)	121.0(2)
C(15)-C(14)-C(18)	120.3(3)
C(14)-C(15)-C(16)	120.8(3)
C(17)-C(16)-C(15)	120.5(2)
C(16)-C(17)-C(19)	120.5(2)
C(14)-C(18)-C(13)	121.2(2)
C(14)-C(18)-C(19)	119.6(2)
C(13)-C(18)-C(19)	119.2(2)
C(17)-C(19)-C(18)	118.2(2)
C(17)-C(19)-C(10)	123.0(2)
C(18)-C(19)-C(10)	118.8(2)

Symmetry transformations used to generate equivalent atoms:

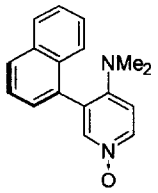
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for biaryl **38**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	50(1)	58(2)	30(1)	-4(1)	15(1)	-14(1)
N(7)	50(1)	35(1)	37(1)	0(1)	11(1)	3(1)
C(2)	38(1)	42(2)	30(1)	2(1)	7(1)	-2(1)
C(3)	28(1)	36(1)	25(1)	-2(1)	7(1)	-3(1)
C(4)	34(1)	38(1)	25(1)	-3(1)	5(1)	-3(1)
C(5)	40(1)	43(2)	43(2)	-13(1)	13(1)	-4(1)
C(6)	48(2)	55(2)	39(2)	-12(1)	21(1)	-13(2)
C(8)	66(2)	35(2)	51(2)	7(1)	29(2)	-2(1)
C(9)	57(2)	38(2)	57(2)	-1(2)	-1(2)	8(1)
C(10)	31(1)	31(1)	28(1)	3(1)	10(1)	1(1)
C(11)	30(1)	42(2)	32(1)	1(1)	7(1)	1(1)
C(12)	28(1)	43(2)	45(2)	4(1)	8(1)	4(1)
C(13)	38(1)	34(1)	44(2)	5(1)	22(1)	7(1)
C(14)	48(2)	36(2)	35(1)	-1(1)	20(1)	3(1)
C(15)	55(2)	44(2)	28(1)	-4(1)	10(1)	-4(1)
C(16)	34(1)	46(2)	34(1)	1(1)	7(1)	-2(1)
C(17)	34(1)	34(1)	30(1)	2(1)	10(1)	1(1)
C(18)	38(1)	28(1)	32(1)	4(1)	13(1)	2(1)
C(19)	32(1)	29(1)	28(1)	1(1)	12(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for biaryl **38**.

	x	y	z	U(eq)
H(2A)	4212	1938	4407	44
H(5A)	544	7225	3956	50
H(6A)	453	5120	5212	54
H(8A)	5419	6652	2558	72
H(8B)	5156	8679	2956	72
H(8C)	4438	8209	1769	72
H(9A)	163	8418	2569	80
H(9B)	1216	9290	1775	80
H(9C)	1933	9761	2962	80
H(11A)	7349	3522	3948	42
H(12A)	9345	2321	2953	47
H(13A)	8078	1379	1292	44
H(14A)	5256	966	-221	46
H(15A)	2015	1317	-963	51
H(16A)	29	2814	-72	46
H(17A)	1251	3833	1610	39

Single-crystal X-ray data for N-oxide of biaryl (38)



N-oxide of (38)

Crystal data for $C_{17}H_{18}N_2O_2$; M = 282.33, crystallizes from dichloromethane/ethyl acetate as colorless blocks; crystal dimensions 0.37 x 0.22 x 0.22 mm. Monoclinic, a = 6.8156(9), b = 7.6023(10), c = 27.838(4) Å, β =96.509(2)° U = 1433.1(3) Å^3, Z = 4, D_c = 1.309 Mg/m^3, space group $P2_1/c$ (C_2^5 *h* No.14), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.087 mm^{-1}, F(000) = 600.

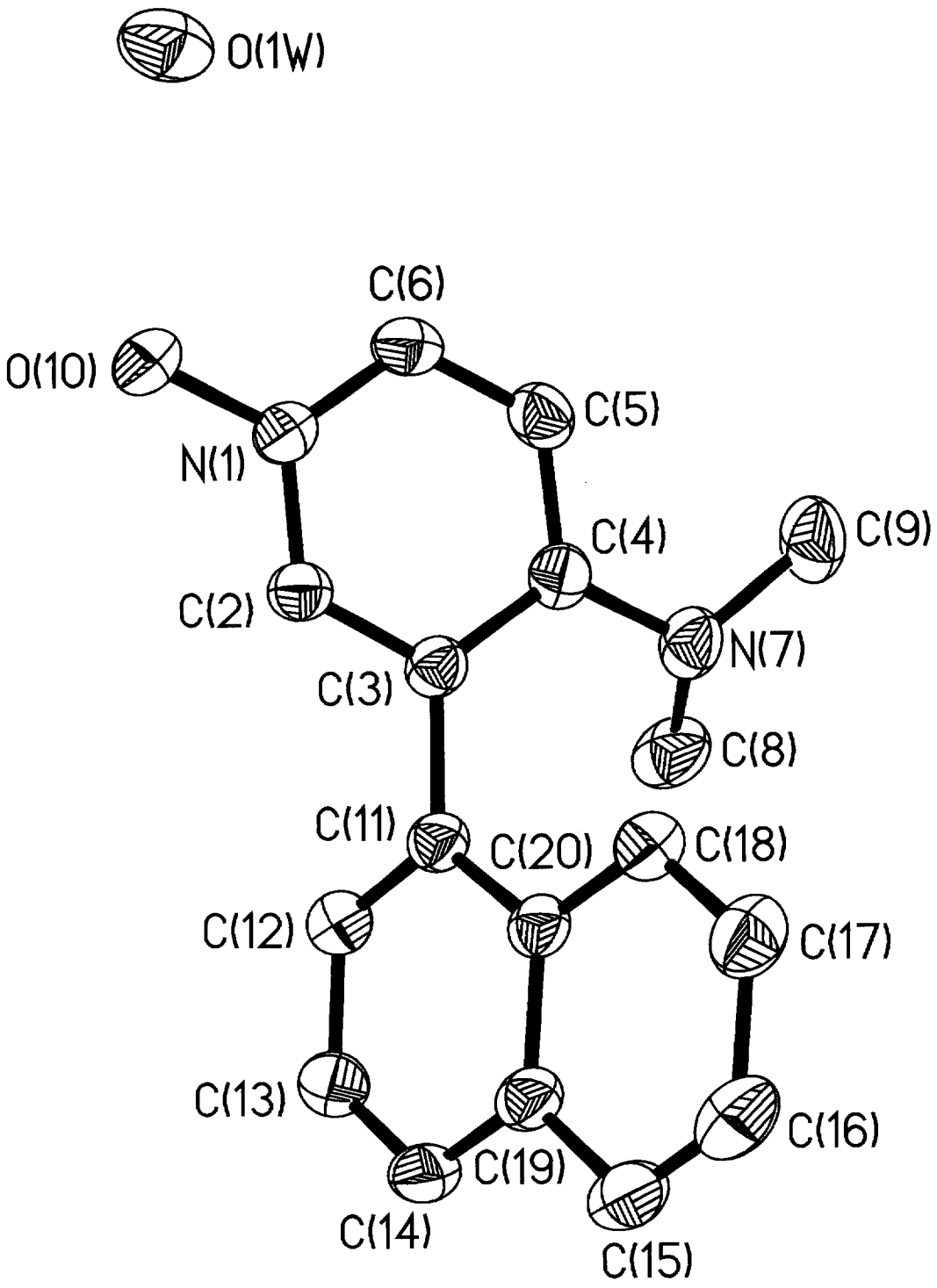
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 66 reflections (θ range 2.78< 28.34°).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 9146 reflections measured, all of which were corrected for Lorentz and polarization effects and for absorption by semi empirical methods based on symmetry-equivalent and repeated reflections (minimum and maximum transmission coefficients 0.9686 and 0.9812), 2491 independent reflections exceeded the significance level $|F|/\sigma(|F|) > 4.0$. The structure was solved by direct methods and refined by full matrix least squares methods on F^2. Hydrogen atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Refinement converged at a final R= 0.0542 (wR_2=0.1716, for all 3410 data, 190 parameters, mean and maximum δ/σ 0.000, 0.001) with allowance for the thermal anisotropy of all non-hydrogen atoms. Minimum and maximum final electron density -0.311 and 0.299 e.Å^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.1026*P)^2 + 0.1535*P]$ where $P=(Fo^2 + 2 * Fc^2)/3$ was used in the latter stages of refinement. Complex scattering factors were taken from the program package SHELXTL^Y as implemented on the Viglen Pentium computer.

Reference Y SHELXTL version, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD

Supplementary material

anisotropic thermal vibrational parameters with e.s.d.s
hydrogen atom position parameters
observed structure amplitudes and calculated structure factors.



An ORTEP plot for *N*-oxide of biaryl (38).

Table 1. Crystal data and structure refinement for *N*-oxide of biaryl **38**.

Empirical formula	C17 H18 N2 O2	
Formula weight	282.33	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.8156(9) Å	α= 90°.
	b = 7.6023(10) Å	β= 96.509(2)°.
	c = 27.838(4) Å	γ = 90°.
Volume	1433.1(3) $Å^3$	
Z	4	
Density (calculated)	1.309 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	600	
Crystal size	0.37 x 0.22 x 0.22 mm^3	
Theta range for data collection	2.78 to 28.34°.	
Index ranges	-7<=h<=9, -8<=k<=9, -35<=l<=36	
Reflections collected	9146	
Independent reflections	3410 [R(int) = 0.0664]	
Completeness to theta = 28.34°	95.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9812 and 0.9686	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3410 / 0 / 190	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1472	
R indices (all data)	R1 = 0.0756, wR2 = 0.1716	
Largest diff. peak and hole	0.299 and -0.311 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *N*-oxide of biaryl **38**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(10)	2805(2)	6446(2)	4901(1)	41(1)
N(1)	3702(2)	7519(2)	5239(1)	32(1)
N(7)	6569(2)	10893(2)	6285(1)	39(1)
C(2)	5309(2)	6954(2)	5528(1)	30(1)
C(3)	6291(2)	8004(2)	5884(1)	30(1)
C(4)	5620(2)	9755(2)	5939(1)	32(1)
C(5)	3936(2)	10264(2)	5639(1)	36(1)
C(6)	3015(2)	9152(2)	5298(1)	35(1)
C(8)	8685(3)	11162(3)	6284(1)	51(1)
C(9)	5559(3)	12553(2)	6358(1)	50(1)
C(11)	7959(2)	7153(2)	6195(1)	30(1)
C(12)	9619(2)	6646(2)	5993(1)	35(1)
C(13)	11196(2)	5788(2)	6270(1)	40(1)
C(14)	11080(2)	5401(2)	6745(1)	38(1)
C(15)	9173(3)	5339(2)	7448(1)	41(1)
C(16)	7495(3)	5722(3)	7650(1)	45(1)
C(17)	5942(3)	6639(2)	7387(1)	42(1)
C(18)	6088(2)	7153(2)	6917(1)	35(1)
C(19)	9376(2)	5838(2)	6964(1)	33(1)
C(20)	7794(2)	6753(2)	6692(1)	30(1)
O(1W)	-1286(2)	6723(2)	4732(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for *N*-oxide of biaryl **38**.

O(10)-N(1)	1.3391(16)
N(1)-C(6)	1.344(2)
N(1)-C(2)	1.3536(18)
N(7)-C(4)	1.3965(19)
N(7)-C(8)	1.457(3)
N(7)-C(9)	1.463(2)
C(2)-C(3)	1.385(2)
C(3)-C(4)	1.421(2)
C(3)-C(11)	1.495(2)
C(4)-C(5)	1.396(2)
C(5)-C(6)	1.369(2)
C(11)-C(12)	1.374(2)
C(11)-C(20)	1.4326(19)
C(12)-C(13)	1.409(2)
C(13)-C(14)	1.366(2)
C(14)-C(19)	1.411(2)
C(15)-C(16)	1.362(3)
C(15)-C(19)	1.422(2)
C(16)-C(17)	1.402(2)
C(17)-C(18)	1.378(2)
C(18)-C(20)	1.416(2)
C(19)-C(20)	1.426(2)
O(10)-N(1)-C(6)	120.74(12)
O(10)-N(1)-C(2)	119.91(12)
C(6)-N(1)-C(2)	119.34(13)
C(4)-N(7)-C(8)	117.87(14)
C(4)-N(7)-C(9)	116.25(14)
C(8)-N(7)-C(9)	111.13(15)
N(1)-C(2)-C(3)	122.41(14)
C(2)-C(3)-C(4)	118.76(13)
C(2)-C(3)-C(11)	116.03(13)
C(4)-C(3)-C(11)	125.17(13)
C(5)-C(4)-N(7)	121.70(14)
C(5)-C(4)-C(3)	116.64(14)
N(7)-C(4)-C(3)	121.64(14)
C(6)-C(5)-C(4)	121.68(14)
N(1)-C(6)-C(5)	121.11(14)

C(12)-C(11)-C(20)	119.56(13)
C(12)-C(11)-C(3)	119.51(13)
C(20)-C(11)-C(3)	120.79(13)
C(11)-C(12)-C(13)	121.29(14)
C(14)-C(13)-C(12)	120.26(15)
C(13)-C(14)-C(19)	120.56(14)
C(16)-C(15)-C(19)	120.70(15)
C(15)-C(16)-C(17)	120.71(15)
C(18)-C(17)-C(16)	120.29(16)
C(17)-C(18)-C(20)	120.73(15)
C(14)-C(19)-C(15)	121.32(14)
C(14)-C(19)-C(20)	119.70(13)
C(15)-C(19)-C(20)	118.96(15)
C(18)-C(20)-C(19)	118.59(13)
C(18)-C(20)-C(11)	122.77(13)
C(19)-C(20)-C(11)	118.57(13)

Symmetry transformations used to generate equivalent atoms:

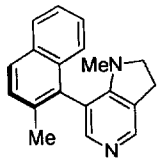
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *N*-oxide of biaryl **38**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(10)	38(1)	43(1)	39(1)	-8(1)	-9(1)	-1(1)
N(1)	32(1)	34(1)	30(1)	-1(1)	-2(1)	0(1)
N(7)	52(1)	29(1)	36(1)	-3(1)	0(1)	-2(1)
C(2)	29(1)	30(1)	30(1)	1(1)	0(1)	2(1)
C(3)	33(1)	29(1)	27(1)	1(1)	1(1)	-1(1)
C(4)	38(1)	28(1)	29(1)	2(1)	3(1)	-1(1)
C(5)	42(1)	30(1)	36(1)	3(1)	5(1)	7(1)
C(6)	32(1)	36(1)	36(1)	4(1)	-1(1)	6(1)
C(8)	54(1)	40(1)	53(1)	-2(1)	-13(1)	-10(1)
C(9)	70(1)	31(1)	49(1)	-8(1)	8(1)	0(1)
C(11)	31(1)	28(1)	30(1)	-1(1)	-1(1)	-1(1)
C(12)	35(1)	37(1)	33(1)	0(1)	2(1)	1(1)
C(13)	33(1)	44(1)	41(1)	-2(1)	1(1)	5(1)
C(14)	34(1)	38(1)	39(1)	-1(1)	-8(1)	4(1)
C(15)	45(1)	40(1)	34(1)	3(1)	-8(1)	-1(1)
C(16)	54(1)	52(1)	29(1)	4(1)	-1(1)	-6(1)
C(17)	41(1)	53(1)	32(1)	-3(1)	5(1)	-4(1)
C(18)	35(1)	37(1)	32(1)	-2(1)	-1(1)	0(1)
C(19)	36(1)	29(1)	32(1)	-1(1)	-5(1)	-2(1)
C(20)	33(1)	25(1)	30(1)	-2(1)	-3(1)	-2(1)
O(1W)	45(1)	51(1)	49(1)	13(1)	1(1)	13(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *N*-oxide of biaryl **38**.

	x	y	z	U(eq)
H(2A)	5769	5819	5487	36
H(5A)	3426	11387	5671	43
H(6A)	1896	9534	5104	42
H(8A)	9312	10055	6236	76
H(8B)	9224	11653	6589	76
H(8C)	8915	11954	6028	76
H(9A)	4170	12341	6357	75
H(9B)	5768	13356	6102	75
H(9C)	6078	13054	6663	75
H(12A)	9702	6872	5668	42
H(13A)	12321	5484	6128	48
H(14A)	12133	4846	6925	46
H(15A)	10197	4745	7628	49
H(16A)	7378	5371	7965	54
H(17A)	4809	6901	7530	50
H(18A)	5055	7770	6747	42
H(1W)	216	6844	4755	58
H(2W)	-1781	5602	4862	58

Single-crystal X-ray data for biaryl (+)-(55)



(+)-55

Crystal data for $C_{19}H_{18}N_2$; M =274.35. Crystallizes from ethyl acetate as colorless blocks; crystal dimensions 0.34 x 0.31 x 0.31 mm. Orthorhombic, a = 7.8911(16), b = 12.503(3), c = 14.477(3) Å, U = 1428.4 (5) Å^3, Z = 4, D_c = 1.276 Mg/m^3, space group $P2_12_12_1$ (D_2^4 , No.19), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.075 mm^{-1}, F(000) =584.

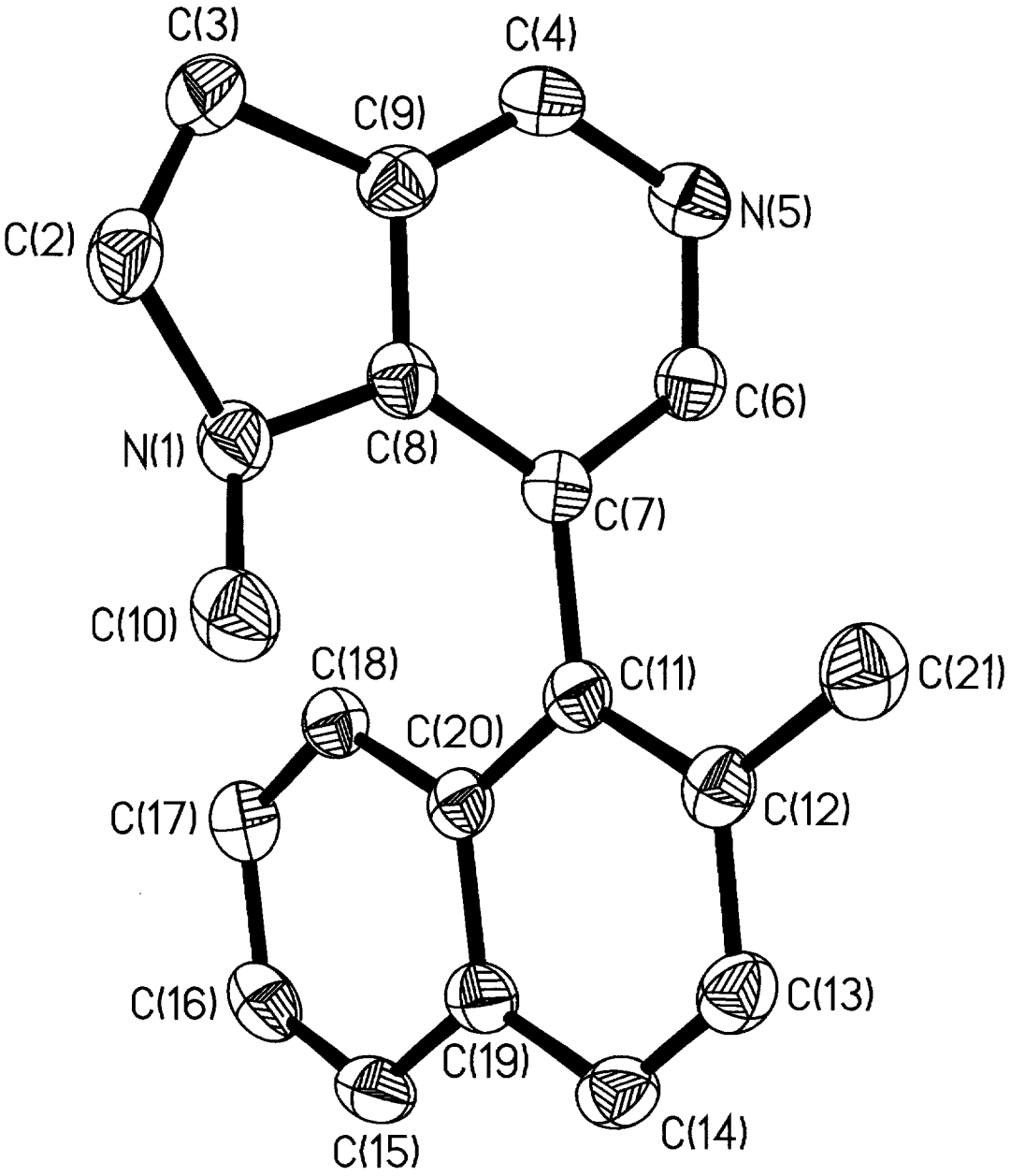
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 45 reflections (θ range 2.15< 28.36°).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 9470 reflections measured, all of which were corrected for Lorentz and polarization effects and for absorption by semi empirical methods based on symmetry-equivalent and repeated reflections (maximum and minimum transmission coefficients of 0.9770 and 0.9748) 1715 independent reflections exceeded the significance level $|F|/\sigma(|F|) > 4.0$. The structure was solved by direct methods and refined by full matrix least squares methods on F^2. Hydrogen atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Refinement converged at a final R= 0.0472(wR2=0.1326 for all 2007 unique data, 190 parameters, mean and maximum δ/σ 0.000, 0.000), with allowance for the thermal anisotropy of all non-hydrogen atoms. Minimum and maximum final electron density -0.231 and 0.307e A^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.0869 * P)^2 + 0.000 * P]$ where $P=(Fo^2 + 2 * Fc^2)/3$ was used in the latter stages of refinement. Complex scattering factors were taken from the program package **SHELXTL**[Y] as implemented on the Viglen Pentium computer.

Reference Y SHELXTL version, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD

Supplementary material

anisotropic thermal vibrational parameters with e.s.d.s
hydrogen atom position parameters
observed structure amplitudes and calculated structure factors.



An ORTEP plot for biaryl (+)-55.