Table 1. Crystal data and structure refinement for biaryl (+)-**55**.

Empirical formula	C19 H18 N2	
Formula weight	274.35	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.8911(16) Å	α= 90°.
	b = 12.503(3) Å	β= 90°.
	c = 14.477(3) Å	γ = 90°.
Volume	1428.4(5) $Å^3$	
Z	4	
Density (calculated)	1.276 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	584	
Crystal size	0.34 x 0.31 x 0.31 mm^3	
Theta range for data collection	2.15 to 28.36°.	
Index ranges	-10<=h<=9, -16<=k<=16, -19<=l<=14	
Reflections collected	9470	
Independent reflections	2007 [R(int) = 0.0534]	
Completeness to theta = 28.36°	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9770 and 0.9748	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2007 / 0 / 190	
Goodness-of-fit on F^2	1.153	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.1267	
R indices (all data)	R1 = 0.0558, wR2 = 0.1326	
Largest diff. peak and hole	0.307 and -0.231 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for biaryl (+)-**55**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	12201(2)	5698(1)	6520(1)	30(1)
N(5)	9448(2)	3016(1)	5663(1)	32(1)
C(2)	13920(3)	5409(2)	6190(2)	35(1)
C(3)	13619(3)	4578(2)	5426(2)	36(1)
C(4)	11048(3)	3257(2)	5380(2)	31(1)
C(6)	8726(3)	3717(2)	6235(2)	28(1)
C(7)	9455(3)	4661(2)	6586(1)	25(1)
C(8)	11125(3)	4858(2)	6293(1)	26(1)
C(9)	11885(3)	4154(2)	5671(2)	29(1)
C(10)	12146(3)	6210(2)	7424(2)	37(1)
C(11)	8440(3)	5368(2)	7200(1)	25(1)
C(12)	8058(3)	5062(2)	8095(1)	29(1)
C(13)	7065(3)	5746(2)	8652(2)	33(1)
C(14)	6471(3)	6702(2)	8334(2)	33(1)
C(15)	6160(3)	8007(2)	7058(2)	34(1)
C(16)	6441(3)	8298(2)	6168(2)	36(1)
C(17)	7430(3)	7636(2)	5587(2)	35(1)
C(18)	8107(3)	6701(2)	5920(2)	29(1)
C(19)	6816(3)	7034(2)	7423(2)	29(1)
C(20)	7817(3)	6365(2)	6845(1)	26(1)
C(21)	8690(3)	4021(2)	8496(2)	38(1)

Table 3. Bond lengths [Å] and angles [°] for biaryl (+)-**55**.

N(1)-C(8)	1.390(3)
N(1)-C(10)	1.457(3)
N(1)-C(2)	1.484(3)
N(5)-C(6)	1.334(3)
N(5)-C(4)	1.361(3)
C(2)-C(3)	1.535(3)
C(3)-C(9)	1.510(3)
C(4)-C(9)	1.367(3)
C(6)-C(7)	1.408(3)
C(7)-C(8)	1.406(3)
C(7)-C(11)	1.487(3)
C(8)-C(9)	1.395(3)
C(11)-C(12)	1.385(3)
C(11)-C(20)	1.436(3)
C(12)-C(13)	1.413(3)
C(12)-C(21)	1.510(3)
C(13)-C(14)	1.364(3)
C(14)-C(19)	1.410(3)
C(15)-C(16)	1.357(3)
C(15)-C(19)	1.424(3)
C(16)-C(17)	1.415(3)
C(17)-C(18)	1.373(3)
C(18)-C(20)	1.422(3)
C(19)-C(20)	1.423(3)
C(8)-N(1)-C(10)	121.76(18)
C(8)-N(1)-C(2)	107.31(17)
C(10)-N(1)-C(2)	115.07(18)
C(6)-N(5)-C(4)	115.92(19)
N(1)-C(2)-C(3)	104.80(17)
C(9)-C(3)-C(2)	102.08(18)
N(5)-C(4)-C(9)	122.5(2)
N(5)-C(6)-C(7)	126.9(2)
C(8)-C(7)-C(6)	114.88(19)
C(8)-C(7)-C(11)	125.54(18)
C(6)-C(7)-C(11)	119.57(18)
N(1)-C(8)-C(9)	111.57(19)
N(1)-C(8)-C(7)	129.27(19)

C(9)-C(8)-C(7)	119.15(19)
C(4)-C(9)-C(8)	120.6(2)
C(4)-C(9)-C(3)	130.8(2)
C(8)-C(9)-C(3)	108.62(19)
C(12)-C(11)-C(20)	120.01(19)
C(12)-C(11)-C(7)	120.86(19)
C(20)-C(11)-C(7)	119.11(18)
C(11)-C(12)-C(13)	119.2(2)
C(11)-C(12)-C(21)	121.7(2)
C(13)-C(12)-C(21)	119.08(19)
C(14)-C(13)-C(12)	121.9(2)
C(13)-C(14)-C(19)	120.5(2)
C(16)-C(15)-C(19)	121.5(2)
C(15)-C(16)-C(17)	119.8(2)
C(18)-C(17)-C(16)	120.3(2)
C(17)-C(18)-C(20)	121.3(2)
C(14)-C(19)-C(20)	119.0(2)
C(14)-C(19)-C(15)	121.9(2)
C(20)-C(19)-C(15)	119.1(2)
C(18)-C(20)-C(19)	118.00(19)
C(18)-C(20)-C(11)	122.59(19)
C(19)-C(20)-C(11)	119.38(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for biaryl (+)-**55**. 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)	23(1)	28(1)	40(1)	0(1)	-1(1)	-2(1)
N(5)	30(1)	31(1)	35(1)	-4(1)	-6(1)	1(1)
C(2)	23(1)	35(1)	46(1)	9(1)	0(1)	-2(1)
C(3)	27(1)	35(1)	47(1)	3(1)	7(1)	2(1)
C(4)	30(1)	31(1)	32(1)	-4(1)	-3(1)	6(1)
C(6)	25(1)	30(1)	31(1)	0(1)	-1(1)	-2(1)
C(7)	24(1)	26(1)	25(1)	1(1)	-2(1)	0(1)
C(8)	24(1)	24(1)	29(1)	4(1)	-3(1)	1(1)
C(9)	25(1)	31(1)	30(1)	2(1)	-1(1)	5(1)
C(10)	31(1)	34(1)	45(1)	-6(1)	-7(1)	-6(1)
C(11)	22(1)	27(1)	27(1)	-2(1)	-1(1)	-4(1)
C(12)	26(1)	33(1)	27(1)	0(1)	-2(1)	-5(1)
C(13)	34(1)	39(1)	25(1)	-3(1)	1(1)	-6(1)
C(14)	30(1)	38(1)	32(1)	-10(1)	2(1)	-4(1)
C(15)	29(1)	30(1)	43(1)	-10(1)	-1(1)	3(1)
C(16)	34(1)	25(1)	50(1)	1(1)	-7(1)	1(1)
C(17)	36(1)	33(1)	34(1)	3(1)	-3(1)	-4(1)
C(18)	28(1)	28(1)	30(1)	-1(1)	1(1)	-3(1)
C(19)	24(1)	30(1)	33(1)	-7(1)	-2(1)	-5(1)
C(20)	22(1)	28(1)	27(1)	-2(1)	-1(1)	-4(1)
C(21)	43(1)	40(1)	30(1)	6(1)	-2(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for biaryl (+)-**55**.

	x	y	z	U(eq)
H(2A)	14591	5106	6687	41
H(2B)	14503	6031	5946	41
H(3A)	13622	4907	4819	44
H(3B)	14466	4016	5444	44
H(4A)	11592	2795	4973	37
H(6A)	7623	3567	6421	34
H(10A)	10992	6369	7582	55
H(10B)	12790	6861	7406	55
H(10C)	12621	5738	7878	55
H(13A)	6809	5539	9253	39
H(14A)	5834	7139	8722	40
H(15A)	5524	8453	7438	41
H(16A)	5984	8931	5940	44
H(17A)	7623	7835	4977	41
H(18A)	8768	6279	5533	35
H(21A)	9341	3645	8039	56
H(21B)	7741	3589	8679	56
H(21C)	9388	4165	9025	56

Single-crystal X-ray data for biaryl (56)

56

Crystal data for $C_{24}H_{22}N_2O$; M = 354.44; crystallizes from ethyl acetate as colorless blocks; crystal dimensions 0.24 x 0.12 x 0.12 mm. Triclinic, a = 9.977(3), b = 9.993(3), c = 10.769(3) Å, α = 107.865(5)° β = 113.068(5)° γ = 93.022(5)°, U = 921.6(4) Å^3, Z = 2, D_c = 1.277 Mg/m^3, space group $P\bar{1}$ (C_i^1, No. 2), Mo-K_α radiation ($\bar{\lambda}$ = 0.71073 Å), μ(Mo-K_α) = 0.078 mm^{-1}, F(000) = 376.

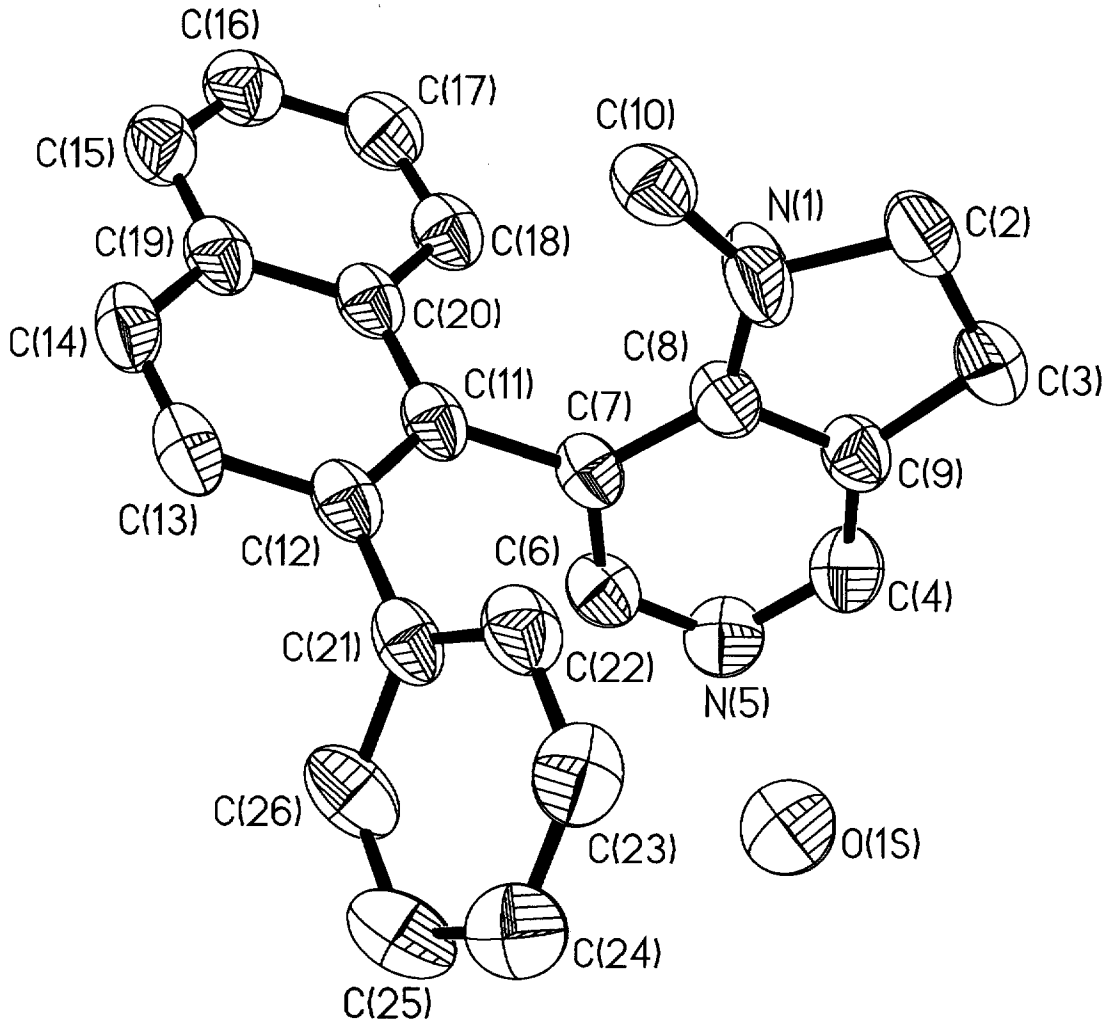
Data collected were measured on a Bruker Smart CCD area detector with Oxford Cryosystems low temperature system. Cell parameters were refined from the setting angles of 26 reflections (θ range 2.18 < 28.30°).

Reflections were measured from a hemisphere of data collected of frames each covering 0.3 degrees in omega. Of the 6108 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 0.9814 and 0.9906), 2424 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 = 0.0564 (wR_2 = 0.1694, for all 4212 data, 252 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 -0.340 and 0.290 e.Å^{-3}. A weighting scheme $w = 1/[\sigma^2(Fo^2) + (0.0942*P)^2 + 0.00*P]$ 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 (56).

Table 1. Crystal data and structure refinement for biaryl **56**.

Empirical formula	C24 H22 N2 O	
Formula weight	354.44	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.977(3) Å	α= 107.865(5)°.
	b = 9.993(3) Å	β= 113.068(5)°.
	c = 10.769(3) Å	γ = 93.022(5)°.
Volume	921.6(4) $Å^3$	
Z	2	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	376	
Crystal size	0.24 x 0.12 x 0.12 mm^3	
Theta range for data collection	2.18 to 28.30°.	
Index ranges	-13<=h<=13, -11<=k<=13, -14<=l<=11	
Reflections collected	6108	
Independent reflections	4212 [R(int) = 0.0479]	
Completeness to theta = 28.30°	91.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9906 and 0.9814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4212 / 0 / 252	
Goodness-of-fit on F^2	0.947	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1475	
R indices (all data)	R1 = 0.0967, wR2 = 0.1694	
Largest diff. peak and hole	0.290 and -0.340 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for biaryl **56**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3491(2)	2780(3)	-2037(2)	89(1)
N(5)	-1018(2)	1117(2)	-3781(2)	54(1)
C(2)	3641(2)	3171(2)	-3182(2)	57(1)
C(3)	2119(2)	2632(2)	-4462(2)	61(1)
C(4)	-329(2)	1588(2)	-4465(2)	52(1)
C(6)	-155(2)	1211(2)	-2433(2)	45(1)
C(7)	1365(2)	1764(2)	-1672(2)	40(1)
C(8)	2037(2)	2229(2)	-2436(2)	46(1)
C(9)	1156(2)	2133(2)	-3850(2)	46(1)
C(10)	4758(2)	2954(2)	-751(2)	50(1)
C(11)	2118(2)	1900(2)	-119(2)	40(1)
C(12)	2488(2)	711(2)	255(2)	41(1)
C(13)	3167(2)	876(2)	1741(2)	48(1)
C(14)	3438(2)	2167(2)	2804(2)	50(1)
C(15)	3207(2)	4725(2)	3539(2)	54(1)
C(16)	2776(2)	5880(2)	3185(2)	55(1)
C(17)	2148(2)	5760(2)	1733(2)	54(1)
C(18)	1944(2)	4494(2)	657(2)	47(1)
C(19)	3019(2)	3389(2)	2465(2)	45(1)
C(20)	2366(2)	3260(2)	984(2)	42(1)
C(21)	2217(2)	-743(2)	-837(2)	43(1)
C(22)	3081(2)	-1086(2)	-1594(2)	50(1)
C(23)	2853(2)	-2465(2)	-2547(2)	57(1)
C(24)	1747(2)	-3527(2)	-2779(2)	58(1)
C(25)	883(2)	-3200(2)	-2036(3)	65(1)
C(26)	1105(2)	-1826(2)	-1084(3)	58(1)
O(1S)	-4053(2)	279(2)	-5640(2)	83(1)

Table 3. Bond lengths [Å] and angles [°] for biaryl **56**.

N(1)-C(8)	1.369(3)
N(1)-C(10)	1.415(3)
N(1)-C(2)	1.460(3)
N(5)-C(6)	1.336(2)
N(5)-C(4)	1.346(3)
C(2)-C(3)	1.521(3)
C(3)-C(9)	1.502(3)
C(4)-C(9)	1.362(3)
C(6)-C(7)	1.392(2)
C(7)-C(8)	1.406(3)
C(7)-C(11)	1.498(3)
C(8)-C(9)	1.398(3)
C(11)-C(12)	1.391(2)
C(11)-C(20)	1.437(3)
C(12)-C(13)	1.423(3)
C(12)-C(21)	1.493(3)
C(13)-C(14)	1.365(3)
C(14)-C(19)	1.417(3)
C(15)-C(16)	1.363(3)
C(15)-C(19)	1.418(3)
C(16)-C(17)	1.401(3)
C(17)-C(18)	1.368(3)
C(18)-C(20)	1.423(3)
C(19)-C(20)	1.427(3)
C(21)-C(22)	1.391(3)
C(21)-C(26)	1.392(3)
C(22)-C(23)	1.386(3)
C(23)-C(24)	1.380(3)
C(24)-C(25)	1.379(3)
C(25)-C(26)	1.383(3)
C(8)-N(1)-C(10)	128.93(18)
C(8)-N(1)-C(2)	110.51(18)
C(10)-N(1)-C(2)	120.53(17)
C(6)-N(5)-C(4)	116.02(16)
N(1)-C(2)-C(3)	105.86(17)
C(9)-C(3)-C(2)	103.23(16)
N(5)-C(4)-C(9)	123.31(19)

N(5)-C(6)-C(7)	126.50(18)
C(6)-C(7)-C(8)	115.39(17)
C(6)-C(7)-C(11)	118.63(16)
C(8)-C(7)-C(11)	125.86(15)
N(1)-C(8)-C(9)	110.39(17)
N(1)-C(8)-C(7)	130.59(18)
C(9)-C(8)-C(7)	119.01(16)
C(4)-C(9)-C(8)	119.76(18)
C(4)-C(9)-C(3)	130.71(19)
C(8)-C(9)-C(3)	109.47(17)
C(12)-C(11)-C(20)	120.06(17)
C(12)-C(11)-C(7)	120.80(17)
C(20)-C(11)-C(7)	119.01(15)
C(11)-C(12)-C(13)	119.17(18)
C(11)-C(12)-C(21)	122.88(17)
C(13)-C(12)-C(21)	117.95(16)
C(14)-C(13)-C(12)	121.47(18)
C(13)-C(14)-C(19)	121.07(18)
C(16)-C(15)-C(19)	121.4(2)
C(15)-C(16)-C(17)	119.7(2)
C(18)-C(17)-C(16)	121.1(2)
C(17)-C(18)-C(20)	120.84(19)
C(14)-C(19)-C(15)	122.49(19)
C(14)-C(19)-C(20)	118.53(18)
C(15)-C(19)-C(20)	118.98(18)
C(18)-C(20)-C(19)	117.99(18)
C(18)-C(20)-C(11)	122.37(17)
C(19)-C(20)-C(11)	119.62(16)
C(22)-C(21)-C(26)	117.77(19)
C(22)-C(21)-C(12)	122.26(17)
C(26)-C(21)-C(12)	119.92(17)
C(23)-C(22)-C(21)	121.01(19)
C(24)-C(23)-C(22)	120.5(2)
C(25)-C(24)-C(23)	119.1(2)
C(24)-C(25)-C(26)	120.7(2)
C(25)-C(26)-C(21)	120.98(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for biaryl **56**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	45(1)	166(2)	59(1)	63(1)	12(1)	-21(1)
N(5)	35(1)	69(1)	55(1)	24(1)	15(1)	13(1)
C(2)	61(1)	63(1)	61(1)	31(1)	35(1)	6(1)
C(3)	74(2)	62(1)	55(1)	32(1)	28(1)	2(1)
C(4)	50(1)	62(1)	49(1)	29(1)	16(1)	21(1)
C(6)	37(1)	51(1)	55(1)	25(1)	22(1)	12(1)
C(7)	36(1)	47(1)	49(1)	28(1)	20(1)	15(1)
C(8)	39(1)	56(1)	49(1)	28(1)	17(1)	7(1)
C(9)	49(1)	49(1)	47(1)	27(1)	20(1)	12(1)
C(10)	40(1)	55(1)	62(1)	27(1)	24(1)	9(1)
C(11)	30(1)	56(1)	48(1)	31(1)	20(1)	12(1)
C(12)	31(1)	55(1)	53(1)	31(1)	24(1)	13(1)
C(13)	44(1)	65(1)	57(1)	40(1)	28(1)	19(1)
C(14)	44(1)	73(1)	47(1)	34(1)	23(1)	13(1)
C(15)	46(1)	71(1)	52(1)	26(1)	26(1)	8(1)
C(16)	50(1)	59(1)	63(1)	20(1)	32(1)	8(1)
C(17)	49(1)	57(1)	68(2)	29(1)	32(1)	16(1)
C(18)	37(1)	58(1)	57(1)	31(1)	23(1)	14(1)
C(19)	36(1)	60(1)	53(1)	30(1)	25(1)	11(1)
C(20)	32(1)	55(1)	52(1)	29(1)	23(1)	13(1)
C(21)	34(1)	58(1)	53(1)	37(1)	21(1)	16(1)
C(22)	40(1)	65(1)	55(1)	28(1)	25(1)	7(1)
C(23)	45(1)	75(2)	54(1)	24(1)	23(1)	15(1)
C(24)	52(1)	56(1)	66(1)	26(1)	19(1)	20(1)
C(25)	52(1)	57(1)	98(2)	40(1)	36(1)	11(1)
C(26)	54(1)	59(1)	89(2)	40(1)	46(1)	19(1)
O(1S)	50(1)	106(1)	81(1)	43(1)	9(1)	19(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for biaryl **56**.

	x	y	z	U(eq)
H(2A)	4382	2722	-3436	68
H(2B)	3934	4203	-2876	68
H(3A)	1772	3396	-4807	73
H(3B)	2140	1849	-5250	73
H(4A)	-896	1538	-5405	63
H(6A)	-616	874	-1956	54
H(10A)	4459	2642	-122	75
H(10B)	5237	3947	-277	75
H(10C)	5436	2391	-981	75
H(13A)	3433	86	1994	58
H(14A)	3904	2246	3767	60
H(15A)	3635	4814	4506	65
H(16A)	2899	6744	3905	67
H(17A)	1865	6553	1496	65
H(18A)	1525	4439	-299	56
H(22A)	3822	-378	-1459	60
H(23A)	3450	-2677	-3035	68
H(24A)	1587	-4449	-3427	70
H(25A)	142	-3912	-2177	78
H(26A)	504	-1623	-601	70
H(1S)	-4600(90)	280(80)	-4870(90)	250(30)
H(2S)	-2760(40)	570(30)	-4790(40)	139(12)