Supporting information for

Determination of Bond Distances and Bond Angles in a Liquid Crystal with Hydrogen Bonding

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Table A1. Crystal data, data collection and refinement characteristics for O-deuterated 5-butoxy-2[(4-butylphenyl)azo]phenol. The data were corrected for Lorentz and polarization effects; absorption correction was not applied since it was judged to be insignificant. The structure was solved by the direct method using the SHELXTL system, and refined by full-matrix least squares on F^2 using all reflections. All the non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were included with idealized parameters except the H atoms on O2, C6, C7 and C10 atoms, which were refined isotropically. The final reliability factors R1=0.054 is based on 2158 "observed reflections" [$I>2\sigma(I)$], and wR^2=0.157 is based on all reflections (3284 unique data).

Crystal data			
Chemical formula	$C_{20}H_{26}N_2O_2$	MW(g/mol)	326.43
Crystal system	Monoclinic	Space group	P2(1)/c
a(Å)	12.2588	α	90°
b(Å)	15.5488	β	99.743°
c(Å)	9.9716	γ	90°
Volume of cell (Å^3)	1873.3	Number of molecules per unit ce (Z)	4
Density (g/cm^3)	1.157	Absorption (mm^{-1})	0.075
Crystal shape	Needle	Crystal color	Transparent red
Data collection conditions			
Radiation	MoKα	Wavelength (Å)	0.71073
Temperature (K)	173	θ range for data collection (°)	2.13-24.98
hmin, hmax	-14, 14	Absorption correction	none
kmin, kmax	-18, 0	Independent reflections	3284
lmin, lmax	0, 11		
Reflections collected	3488		
Refinement			
Refinement mode	Full-matrix least-squares on F^2		
Final R indices	0.0541	wR	0.1352

Goodness of fit	1.003	Number of refined parameters	3284

Table A2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for O-deuterated 5-butoxy-2[(4-butylphenyl)azo]phenol. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x/a**	**y/b**	**z/c**	**U(eq)**
O(1)	2854(1)	6235(1)	-79(2)	54(1)
O(2)	-366(1)	5652(1)	1858(2)	56(1)
N(1)	741(1)	6436(1)	4381(2)	45(1)
N(2)	-231(1)	6112(1)	4328(2)	44(1)
C1′	1188(2)	6357(1)	3199(2)	43(1)
C2′	663(2)	5990(1)	1970(2)	45(1)
C3′	1184(2)	5952(1)	852(3)	48(1)
C4′	2259(2)	6265(1)	942(2)	47(1)
C5′	2799(2)	6625(2)	2164(3)	52(1)
C6′	2275(2)	6678(1)	3256(3)	49(1)
C1	-708(2)	6209(1)	5509(2)	43(1)
C2	-1645(2)	5714(1)	5570(2)	49(1)
C3	-2158(2)	5746(1)	6689(2)	51(1)
C4	-1765(2)	6272(1)	7788(2)	50(1)

Table A3. Bond lengths for O-deuterated 5-butoxy-2[(4-butylphenyl)azo]phenol (Å)

O(2)-C2′	1.354(2)
O(2)-D	0.930(17)
N(1)-N(2)	1.285(2)
N(1)-C1′	1.387(3)
N(2)-C1	1.409(3)
C1′-C2′	1.406(3)
C2′-C3′	1.376(3)
C3′-C4′	1.394(3)
C4′-C5′	1.402(3)
C5′-C6′	1.357(3)
C6′-C1′	1.415(3)
C1-C2	1.393(3)
C2-C3	1.374(3)
C3-C4	1.387(3)

Table A4. Bond angles [°] in the asymmetric ring and the diazo link.

C2′-O(2)-D	103.1(19)
N(2)-N(1)-C1′	115.28(18)
N(1)-N(2)-C1	115.89(18)
O(1)-C4′-C3′	124.5(2)
O(1)-C4′-C5′	115.7(2)
C3′-C4′-C5′	119.8(2)
C4′-C5′-C6′	120.2(2)
C6′-C5′-H5′	124.4(15)
C4′-C5′-H6′	115.3(15)
C5′-C6′-C1′	121.1(2)
C5′-C6′-H6′	123.1(14)
C1′-C6′-H6′	115.8(14)
N(1)-C1′-C2′	126.1(2)
N(1)-C1′-C6′	116.1(2)
C2′-C1′-C6′	117.8(2)
O(2)-C2′-C3′	118.0(2)
O(2)-C2′-C1′	120.8(2)
C1′-C2′-C3′	121.2(2)
C2′-C3′-C4′	119.8(2)
C2′-C3′-H3′	120.8(14)
C4′-C3′-H3′	119.4(14)