Study of the mesomorphic behavior through the structure modification of azo and acetylene pyridinium and imidazolium-based ionic liquid crystals

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Crystallographic data for the NN-11 compound

ORTEP a 50%.

Table 1. Crystal data and structure refinement for NN-II.

Empirical formula	C ₄₈ H ₇₂ I ₂ N ₂ O ₆	
Formula weight	1026.88	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4783(2) Å	$\alpha = 88.5240(10)^\circ$.
	b = 9.6426(2) Å	$\beta = 80.9730(10)^\circ$.
	c = 16.8704(4) Å	$\gamma = 65.4770(10)^\circ$.
Volume	1238.06(5) Å ³	
Z	1	

Density (calculated)	1.377 Mg/m ³
Absorption coefficient	1.316 mm ⁻¹
F(000)	528
Crystal size	0.22 x 0.16 x 0.06 mm ³
Theta range for data collection	1.22 to 33.22°.
Index ranges	-12<=h<=13, -14<=k<=14, -25<=l<=26
Reflections collected	34258
Independent reflections	9436 [R(int) = 0.0131]
Completeness to theta = 33.22°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9252 and 0.7606
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9436 / 0 / 264
Goodness-of-fit on F ²	1.127
Final R indices [I>2sigma(I)]	R1 = 0.0212, wR2 = 0.0549
R indices (all data)	R1 = 0.0239, wR2 = 0.0562
Largest diff. peak and hole	1.106 and -0.380 e.Å ⁻³

Table 2. Bond lengths [Å] and angles [°] for NN-II.

C(2)-N(1)	1.3509(13)
C(2)-C(3)	1.3719(14)
C(3)-C(4)	1.4048(13)
C(4)-C(5)	1.4014(14)
C(4)-C(7)	1.4192(14)
C(5)-C(6)	1.3716(15)
C(6)-N(1)	1.3492(13)
C(7)-C(8)	1.2044(15)
C(8)-C(9)	1.4248(14)
C(9)-C(10)	1.3978(14)
C(9)-C(14)	1.4085(14)
C(10)-C(11)	1.3878(15)
C(11)-C(12)	1.4000(14)
C(12)-O(1)	1.3518(12)
C(12)-C(13)	1.4024(14)

C(13)-C(14)	1.3776(14)
C(15)-O(1)	1.4394(13)
C(15)-C(16)	1.5097(15)
C(16)-C(17)	1.5275(16)
C(17)-C(18)	1.5228(16)
C(18)-C(19)	1.5243(16)
C(19)-C(20)	1.5221(16)
C(20)-C(21)	1.5255(15)
C(21)-C(22)	1.5208(15)
C(22)-C(23)	1.5209(16)
C(23)-C(24)	1.5207(19)
C(25)-N(1)	1.4734(14)

N(1)-C(2)-C(3)	120.74(9)
C(2)-C(3)-C(4)	119.69(9)
C(5)-C(4)-C(3)	118.09(9)
C(5)-C(4)-C(7)	121.07(9)
C(3)-C(4)-C(7)	120.84(9)
C(6)-C(5)-C(4)	119.81(9)
N(1)-C(6)-C(5)	120.75(9)
C(8)-C(7)-C(4)	178.68(11)
C(7)-C(8)-C(9)	178.61(11)
C(10)-C(9)-C(14)	119.04(9)
C(10)-C(9)-C(8)	121.19(9)
C(14)-C(9)-C(8)	119.77(9)
C(11)-C(10)-C(9)	120.75(9)
C(10)-C(11)-C(12)	119.69(9)
O(1)-C(12)-C(11)	124.69(9)
O(1)-C(12)-C(13)	115.40(9)
C(11)-C(12)-C(13)	119.90(9)
C(14)-C(13)-C(12)	120.11(9)
C(13)-C(14)-C(9)	120.51(9)
O(1)-C(15)-C(16)	107.25(9)
C(15)-C(16)-C(17)	111.99(9)
C(18)-C(17)-C(16)	112.50(9)
C(17)-C(18)-C(19)	113.46(9)

C(20)-C(19)-C(18)	113.31(9)
C(19)-C(20)-C(21)	113.19(9)
C(22)-C(21)-C(20)	113.49(9)
C(23)-C(22)-C(21)	113.14(9)
C(24)-C(23)-C(22)	112.78(11)
C(6)-N(1)-C(2)	120.91(9)
C(6)-N(1)-C(25)	119.00(9)
C(2)-N(1)-C(25)	120.09(9)
C(12)-O(1)-C(15)	118.49(8)

Symmetry transformations used to generate equivalent atoms:

Table 3. Hydrogen bonds for NN-II [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1W)-H(1WA)...I(1)#1	0.86	2.69	3.5425(11)	173
O(1W)-H(1WB)...O(2W)#2	0.80	2.06	2.8166(17)	159
O(2W)-H(2WA)...O(1W)#3	0.75	2.05	2.7757(17)	162
O(2W)-H(2WB)...I(1)#3	0.83	2.83	3.6492(10)	168

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 x-1,y+1,z #3 -x,-y+1,-z+1