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Electronic Supplementary Information

Crown ether-containing *N*-salicylidene aniline derivatives: synthesis, characterization and optical properties

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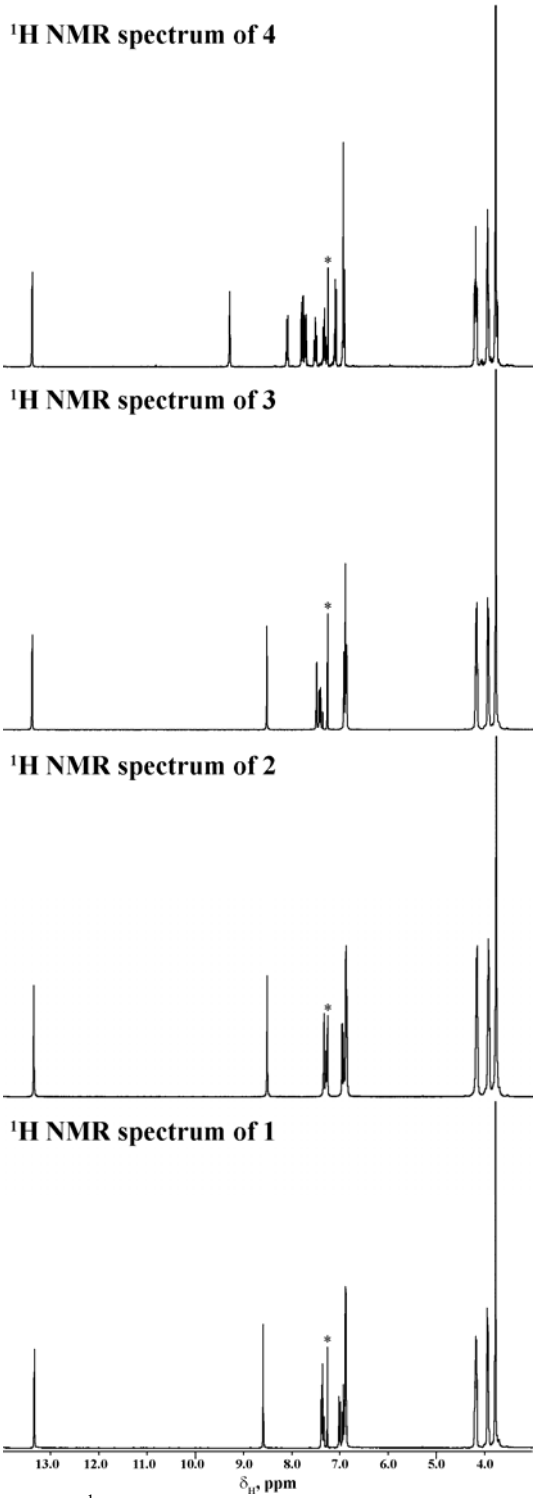

Fig. S1 ^{1}H NMR spectra of **1–4**. The solvent ($CHCl_3$) is marked by an asterisk.

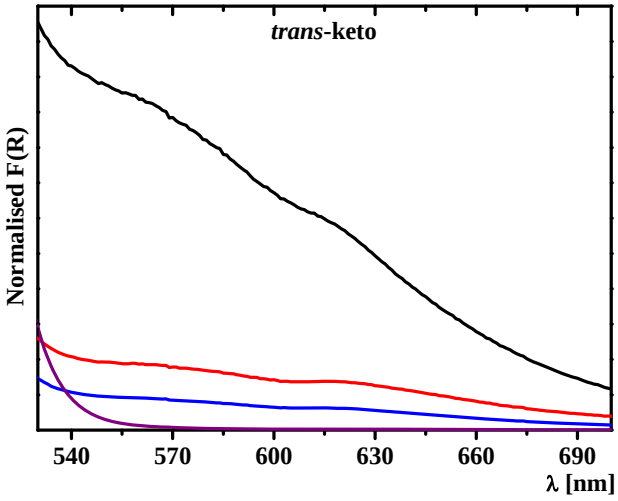

Fig. S2 A zoomed range of the *trans*-keto form of the Kubelka-Munk spectra of **1** (black), **2** (red), **3** (blue) and **4** (purple) at 298 K.

Table S1 Selected bond lengths (Å) and bond angles (°) for **1**

Bond lengths					
O(1)–C(2)	1.348(5)	O(25)–C(24)	1.431(4)	C(10)–C(11)	1.404(4)
O(13)–C(12)	1.362(4)	O(25)–C(26)	1.361(4)	C(10)–C(28)	1.373(5)
O(13)–C(14)	1.420(4)	N(9)–C(8)	1.269(4)	C(11)–C(12)	1.377(5)
O(16)–C(15)	1.413(4)	N(9)–C(10)	1.418(4)	C(12)–C(26)	1.402(4)
O(16)–C(17)	1.415(5)	C(2)–C(3)	1.394(6)	C(14)–C(15)	1.495(5)
O(16)–C(17B)	1.42(4)	C(2)–C(7)	1.395(5)	C(17)–C(18)	1.487(8)
O(19)–C(18)	1.425(6)	C(3)–C(4)	1.367(6)	C(17B)–C(18B)	1.49(4)
O(19)–C(18B)	1.41(2)	C(4)–C(5)	1.374(6)	C(20)–C(21)	1.486(6)
O(19)–C(20)	1.422(5)	C(5)–C(6)	1.383(6)	C(23)–C(24)	1.492(5)
O(22)–C(21)	1.409(5)	C(6)–C(7)	1.382(5)	C(26)–C(27)	1.379(4)
O(22)–C(23)	1.426(4)	C(7)–C(8)	1.450(5)	C(27)–C(28)	1.377(5)
Bond angles					
C(12)–O(13)–C(14)	117.8(3)	C(5)–C(6)–C(7)	121.1(3)	O(16)–C(17)–C(18)	113.0(4)
C(15)–O(16)–C(17)	114.7(4)	C(2)–C(7)–C(6)	118.8(3)	O(19)–C(18)–C(17)	116.4(5)
C(15)–O(16)–C(17B)	102.6(13)	C(2)–C(7)–C(8)	121.9(3)	O(19)–C(20)–C(21)	107.1(3)
C(18)–O(19)–C(20)	113.2(3)	C(6)–C(7)–C(8)	119.3(3)	O(22)–C(21)–C(20)	112.4(3)
C(20)–O(19)–C(18B)	125.1(11)	N(9)–C(8)–C(7)	122.8(3)	O(22)–C(23)–C(24)	111.4(3)
C(21)–O(22)–C(23)	116.6(3)	N(9)–C(10)–C(11)	124.3(3)	O(25)–C(24)–C(23)	107.8(3)
C(24)–O(25)–C(26)	117.4(2)	N(9)–C(10)–C(28)	117.4(3)	O(25)–C(26)–C(12)	115.8(3)
C(8)–N(9)–C(10)	122.2(3)	C(11)–C(10)–C(28)	118.3(3)	O(25)–C(26)–C(27)	125.0(3)
O(1)–C(2)–C(3)	118.7(3)	C(10)–C(11)–C(12)	120.6(3)	C(12)–C(26)–C(27)	119.2(3)
O(1)–C(2)–C(7)	121.5(3)	O(13)–C(12)–C(11)	125.1(3)	C(26)–C(27)–C(28)	120.2(3)
C(3)–C(2)–C(7)	119.8(3)	O(13)–C(12)–C(26)	114.9(3)	C(10)–C(28)–C(27)	121.7(3)
C(2)–C(3)–C(4)	120.0(4)	C(11)–C(12)–C(26)	120.0(3)	O(16)–C(17B)–C(18B)	115(3)
C(3)–C(4)–C(5)	120.8(4)	O(13)–C(14)–C(15)	107.3(3)	O(19)–C(18B)–C(17B)	105(2)
C(4)–C(5)–C(6)	119.5(4)	O(16)–C(15)–C(14)	108.2(2)		
Torsion angles					
C(14)–O(13)–C(12)–C(11)	–13.1(4)	O(1)–C(2)–C(7)–C(8)	0.4(5)	N(9)–C(10)–C(28)–C(27)	178.9(3)
C(14)–O(13)–C(12)–C(26)	166.2(3)	C(3)–C(2)–C(7)–C(6)	1.5(5)	C(11)–C(10)–C(28)–C(27)	–0.1(5)
C(12)–O(13)–C(14)–C(15)	–173.8(3)	C(3)–C(2)–C(7)–C(8)	–178.4(4)	C(10)–C(11)–C(12)–O(13)	178.6(3)
C(17)–O(16)–C(15)–C(14)	–171.8(4)	C(2)–C(3)–C(4)–C(5)	0.8(7)	C(10)–C(11)–C(12)–C(26)	–0.6(5)
C(15)–O(16)–C(17)–C(18)	87.8(6)	C(3)–C(4)–C(5)–C(6)	–0.7(7)	O(13)–C(12)–C(26)–O(25)	–0.1(4)
C(20)–O(19)–C(18)–C(17)	–79.8(5)	C(4)–C(5)–C(6)–C(7)	1.0(6)	O(13)–C(12)–C(26)–C(27)	–179.3(3)
C(18)–O(19)–C(20)–C(21)	–149.6(4)	C(5)–C(6)–C(7)–C(2)	–1.4(6)	C(11)–C(12)–C(26)–O(25)	179.2(3)
C(23)–O(22)–C(21)–C(20)	–84.5(4)	C(5)–C(6)–C(7)–C(8)	178.5(4)	C(11)–C(12)–C(26)–C(27)	0.1(5)
C(21)–O(22)–C(23)–C(24)	124.6(3)	C(2)–C(7)–C(8)–N(9)	0.1(6)	O(13)–C(14)–C(15)–O(16)	68.8(4)
C(26)–O(25)–C(24)–C(23)	178.3(3)	C(6)–C(7)–C(8)–N(9)	–179.8(4)	O(16)–C(17)–C(18)–O(19)	74.0(6)
C(24)–O(25)–C(26)–C(12)	–175.3(3)	C(7)–C(8)–N(9)–C(10)	176.9(3)	O(19)–C(20)–C(21)–O(22)	–169.7(3)
C(24)–O(25)–C(26)–C(27)	3.9(5)	C(11)–C(10)–N(9)–C(8)	–11.0(5)	O(22)–C(23)–C(24)–O(25)	–75.1(3)
O(1)–C(2)–C(3)–C(4)	–180.0(4)	C(28)–C(10)–N(9)–C(8)	170.2(3)	O(25)–C(26)–C(27)–C(28)	–178.6(3)
C(7)–C(2)–C(3)–C(4)	–1.2(6)	N(9)–C(10)–C(11)–C(12)	–178.2(3)	C(12)–C(26)–C(27)–C(28)	0.5(5)
O(1)–C(2)–C(7)–C(6)	–179.8(4)	C(28)–C(10)–C(11)–C(12)	0.6(5)	C(26)–C(27)–C(28)–C(10)	–0.5(6)

Table S2 Selected hydrogen bond lengths (Å) and angles (°) for **1**

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠ (DHA)
O(1)–H(1)···N(9)	0.82	1.90	2.627(4)	147

Table S3 Selected π···π interactions for **1**

Cg(*I*)	Cg(*J*)	Cg–Cg (Å)	Dihedral angle (°)	*β* (°)
Cg(1)	Cg(1)	5.403(2)	85.92	28.23
Cg(1)	Cg(2)	4.665(2)	12.91	37.78
Cg(2)	Cg(1)	4.665(2)	12.91	44.28

Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7); Cg(2): C(10)–C(11)–C(12)–C(26)–C(27)–C(28)

β: angle Cg(*I*) → Cg(*J*) vector and normal to plane I.