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TABLE I

Crystal Data and Experimental Details for the Structure Determination of Na^+-**3**

Chemical Formula	$[Na(C_{23}H_{28.5}N_3O_5)]^{0.5+}(ClO_4^-)_{0.5}$
Formula Weight	499.7
Crystal System	Triclinic
Space Group	$P\bar{1}$
Crystal Color	Colorless
Crystal Dimensions	0.1 x 0.2 x 0.3 mm
Unit Cell Parameters	a= 9.400 (9) Å
	b= 11.467 (10) Å
	c= 12.281 (11) Å
	α= 77.22 (7)°
	β= 87.73 (7)°
	γ= 86.39 (7)°
Volume	1288 $Å^3$
Z	2
Linear Absorption Coefficient	1.59 cm^{-1}
Temperature	20° C
Wavelength of Radiation	0.71073 Å
2θ Range	4.0-45.0°
Total Data Collected	3635
Data Used in Refinement	3388 (R_{int}= 1.61%)
Observed Data	1832 (F>4.0 σ(F))
Goodness of fit	1.89 (unit weights)
Calculated Density	1.288 mg/m^3
Intensity Measurement Method	2θ -θ
R, Unweighted	8.27%

$R= \Sigma \, ||F_o|-|F_c|| / \sum |F_o|$

TABLE II

Atomic Positional Parameters ($x10^4$) and Equivalent Isotropic Displacement Coefficients ($Å^2 \times 10^3$) for the Non-hydrogen Atoms and H29 for Na^+-**3**

atom	x	y	z	U(eq)[a]
Na	4296(4)	9271(3)	2595(3)	44(1)
N1	4123(9)	11571(8)	2205(7)	51(3)
C2	2868(11)	12218(10)	2152(8)	50(4)
C3	1618(11)	11546(10)	2643(8)	56(4)
O4	1861(7)	10300(7)	2687(6)	63(3)
C5	707(11)	9602(11)	3162(11)	75(6)
C6	887(13)	8453(12)	2838(13)	90(7)
O7	2226(8)	7925(7)	3116(8)	81(4)
C8	2493(13)	6774(11)	2812(12)	88(6)
C9	3846(12)	6248(10)	3361(11)	76(5)
N10	5068(9)	6972(7)	2942(7)	50(3)
C11	6156(12)	6748(10)	3775(9)	67(5)
C12	5781(13)	7365(11)	4746(9)	74(5)
O13	5609(8)	8636(7)	4351(6)	63(3)
C14	6861(13)	9225(11)	4468(10)	75(5)
C15	6744(11)	10437(10)	3743(10)	63(5)
O16	6724(7)	10323(6)	2609(6)	56(3)
C17	6660(11)	11428(10)	1809(10)	67(5)
C18	5265(11)	12154(10)	1803(8)	51(4)
C19	5193(13)	13380(10)	1339(9)	66(5)
C20	3909(14)	13999(10)	1270(11)	72(5)
C21	2738(13)	13430(10)	1675(10)	67(5)
C22	5588(11)	6656(9)	1892(9)	60(5)
C23	6755(10)	7369(8)	1258(8)	45(4)
C24	8078(11)	6818(9)	1134(8)	52(4)
C25	9145(10)	7425(10)	491(8)	51(4)
C26	10449(13)	6787(12)	302(10)	73(5)
N26	11493(12)	6286(12)	121(11)	120(6)
C27	8904(11)	8622(9)	-5(8)	49(4)
C28	7592(10)	9203(9)	98(8)	50(4)
C29	6510(10)	8584(9)	718(8)	43(4)
O29	5217(7)	9114(6)	779(6)	55(3)
H29[b]	5242	9559	301	80[c]
Cl30	-663(7)	13852(6)	3951(6)	93(3)
O31	738(13)	13749(21)	4332(16)	34(6)[c]
O32	-1399(29)	14828(24)	4252(30)	305(54)[c]
O33	-1332(20)	12793(20)	4436(27)	177(22)[c]
O34	-637(27)	13993(32)	2790(9)	113(13)[c]
O31'	353(22)	13076(19)	4581(18)	63(8)[c]
O32'	-1406(25)	14512(24)	4659(21)	108(15)[c]
O33'	-1626(23)	13238(22)	3500(24)	104(12)[c]
O34'	27(28)	14655(22)	3097(20)	137(17)[c]

[a] Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij} tensor.

[b] The population parameters for H29 and Cl30 were 0.50 while the population parameter for each of the disordered perchlorate oxygens (O31-O34') was 0.25.

[c] This value is an isotropic displacement coefficient.

TABLE III

Na - Donor Atom Interatomic Distances of Na^+-**3**

	Donor Atom	Interatomic Distance (Å)
Na	N1	2.571 (10)
Na	O4	2.518 (8)
Na	O7	2.533 (9)
Na	N10	2.635 (9)
Na	O13	2.471 (8)
Na	O16	2.651 (8)
Na	O29	2.400 (8)

TABLE IV
Bond Lengths and Angles in **3** of the Na^+-**3** Complex

1	2	3	1-2 Å	1-2-3°
C2	N1	C18	1.349 (13)	117.0 (9)
N1	C2	C3		115.6 (9)
C21	C2	N1	1.383 (15)	123.0(10)
C3	C2	C21	1.480 (14)	121.5(10)
C2	C3	O4		111.3 (8)
C3	O4	C5	1.422 (13)	114.0 (8)
O4	C5	C6	1.418 (13)	108.1(10)
C5	C6	O7	1.457 (20)	110.3(11)
C6	O7	C8	1.384 (14)	113.7(10)
O7	C8	C9	1.454 (17)	105.8(11)
C8	C9	N10	1.493 (17)	112.3 (9)
C9	N10	C11	1.469 (14)	109.6 (8)
C22	N10	C9	1.472 (14)	107.7 (9)
C11	N10	C22	1.447 (14)	112.0 (8)
N10	C11	C12		112.7 (9)
C11	C12	O13	1.534 (18)	110.7 (8)
C12	O13	C14	1.432 (14)	112.4 (8)
O13	C14	C15	1.420 (15)	108.0 (9)
C14	C15	O16	1.476 (16)	108.4(10)
C15	O16	C17	1.428 (14)	114.6 (9)
O16	C17	C18	1.421(12)	114.9 (8)
N1	C18	C17	1.321 (14)	117.3 (9)
N1	C18	C19		122.1(10)
C17	C18	C19	1.508 (15)	120.5(10)
C18	C19	C20	1.394 (15)	119.5(11)
C19	C20	C21	1.357 (17)	119.5(11)
C20	C21	C2	1.337 (17)	119.0(11)
N10	C22	C23		117.1 (9)
C22	C23	C24	1.498 (14)	119.8 (8)
C22	C23	C29		121.5 (8)
C24	C23	C29	1.378 (14)	118.6 (9)
C23	C24	C25		121.3 (9)
C24	C25	C26	1.376 (14)	119.1(10)
C24	C25	C27		119.5 (9)
C26	C25	C27	1.426 (16)	121.3 (9)
N26	C26	C25	1.145 (17)	178.2(13)
C25	C27	C28	1.381 (14)	120.9 (9)
C27	C28	C29	1.379 (14)	119.6 (9)
C23	C29	C28	1.413 (13)	120.1 (9)
O29	C29	C23	1.332 (12)	119.5 (8)
C28	C29	O29	1.382 (13)	120.3 (8)

TABLE V

Bond Lengths and Angles in the Disordered Perchlorate[a] ion of Na^+-**3**

1	2	3	1-2 Å	1-2-3°
O31	Cl30	O32	1.405(15)	109.7(17)
O33	Cl30	O31	1.404(25)	108.4(15)
O34	Cl30	O31	1.398(14)	109.7(14)
O32	Cl30	O33	1.390(31)	110.2(17)
O32	Cl30	O34		110.1(20)
O33	Cl30	O34		108.7(21)
O31'	Cl30	O32'	1.397(21)	108.1(14)
O33'	Cl30	O31'	1.384(28)	111.8(14)
O34'	Cl30	O31'	1.401(24)	109.3(14)
O32'	Cl30	O33'	1.412(28)	109.1(15)
O32'	Cl30	O34'		108.4(16)
O33'	Cl30	O34'		110.0(16)

[a] The two orientations of the disordered perchlorate ion were refined as rigid tetrahedral groups with Cl-O bond lengths of approximately 1.400Å.

TABLE VI

Anisotropic Displacement Coefficients ($Å^2$ x 10^3) for all Atoms Refined Anisotropically of Na^+-**3**

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na	39(2)	46(2)	46(2)	2(2)	5(2)	-8(2)
N1	44(5)	58(6)	50(5)	-3(5)	7(4)	-12(5)
C2	50(7)	58(8)	44(6)	8(6)	0(5)	-19(6)
C3	53(7)	69(8)	44(6)	21(6)	-1(5)	-11(6)
O4	43(4)	61(5)	82(6)	2(4)	12(4)	-10(4)
C5	42(7)	75(9)	99(10)	-6(7)	9(7)	1(8)
C6	51(8)	81(11)	128(13)	-13(7)	5(8)	0(9)
O7	51(5)	68(6)	123(8)	-4(4)	0(5)	-16(5)
C8	76(10)	64(9)	128(13)	-20(8)	28(9)	-29(9)
C9	69(9)	58(8)	91(10)	-7(7)	30(7)	-2(7)
N10	49(5)	47(5)	47(5)	-2(4)	14(4)	1(4)
C11	68(8)	57(8)	61(8)	20(6)	3(6)	8(6)
C12	84(9)	74(9)	56(8)	5(7)	10(7)	-1(7)
O13	61(5)	62(5)	62(5)	5(4)	2(4)	-10(4)
C14	64(8)	90(10)	63(8)	9(8)	-12(6)	-1(7)
C15	49(7)	74(9)	68(8)	1(6)	-6(6)	-19(7)
O16	53(5)	56(5)	58(5)	7(4)	5(4)	-11(4)
C17	61(8)	58(8)	81(9)	-12(6)	20(7)	-14(7)
C18	55(7)	53(8)	46(6)	6(6)	0(5)	-16(5)
C19	74(9)	51(8)	71(8)	0(7)	-6(7)	-11(6)
C20	77(9)	43(7)	91(10)	3(7)	-9(8)	-5(7)
C21	66(8)	50(8)	80(9)	13(7)	0(7)	-7(7)
C22	63(7)	46(7)	67(8)	3(6)	5(6)	-8(6)
C23	48(6)	33(6)	55(7)	-1(5)	5(5)	-10(5)
C24	55(7)	44(7)	53(7)	10(6)	1(6)	-6(5)
C25	36(6)	66(8)	49(7)	8(6)	1(5)	-12(6)
C26	53(8)	83(9)	73(9)	12(7)	6(7)	1(7)
N26	70(8)	124(11)	137(12)	31(8)	33(8)	18(9)
C27	50(7)	53(7)	39(6)	3(6)	2(5)	-4(5)
C28	50(7)	43(6)	51(7)	4(5)	4(5)	-1(5)
C29	46(6)	49(7)	33(6)	10(5)	-1(5)	-14(5)
O29	52(4)	52(5)	53(4)	11(4)	2(3)	-1(4)
Cl30	104(6)	78(5)	90(5)	17(4)	39(4)	-17(4)

The anisotropic displacement exponent takes the form:

$-2\pi^2 (h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

TABLE VII

Hydrogen Atom Coordinates [a](x10^{-4}) and Isotropic Displacement Coefficients (Å^2 x 10^3) for Na^+ -3

	x	y	z	U
H3A	791	11851	2214	80[b]
H3B	1444	11662	3388	80
H5A	-185	10021	2930	80
H5B	733	9446	3962	80
H6A	805	8603	2041	80
H6B	161	7928	3179	80
H8A	2613	6886	2016	80
H8B	1712	6271	3057	80
H9A	4040	5456	3233	80
H9B	3716	6182	4151	80
H11A	6273	5900	4068	80
H11B	7035	7039	3426	80
H12A	6504	7167	5297	80
H12B	4897	7074	5086	80
H14A	7683	8793	4233	80
H14B	6964	9256	5235	80
H15A	7533	10889	3849	80
H15B	5877	10845	3932	80
H17A	6867	11284	1076	80
H17B	7397	11895	1982	80
H19	6047	13776	1062	80
H20	3827	14834	914	80
H21	1825	13856	1666	80
H22A	4790	6762	1409	80
H22B	5896	5823	2044	80
H24	8258	5997	1507	80
H27	9658	9055	-430	80
H28	7430	10036	-244	80
H29	5242	9959	301	80

[a]Positions for all hydrogen atoms except H29, the phenol hydrogen, were calculated.

[b]Values for isotropic displacement coefficients were assigned.

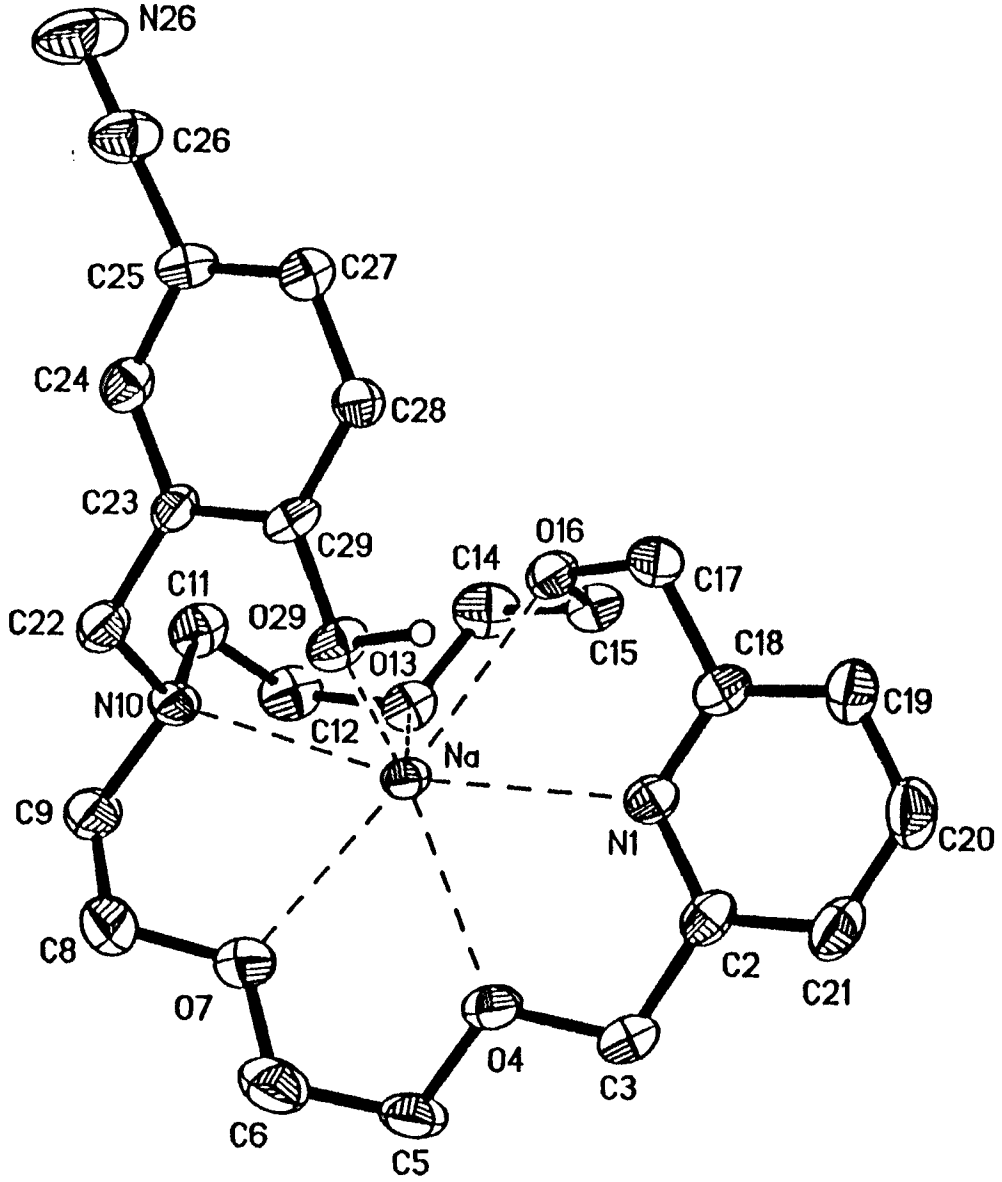

Figure I. A thermal ellipsoid drawing of Na^{+}-**3**. The atoms are drawn at the 40% probability level. The disordered perchlorate ion and hydrogen atoms (except for H29) are omitted for clarity.

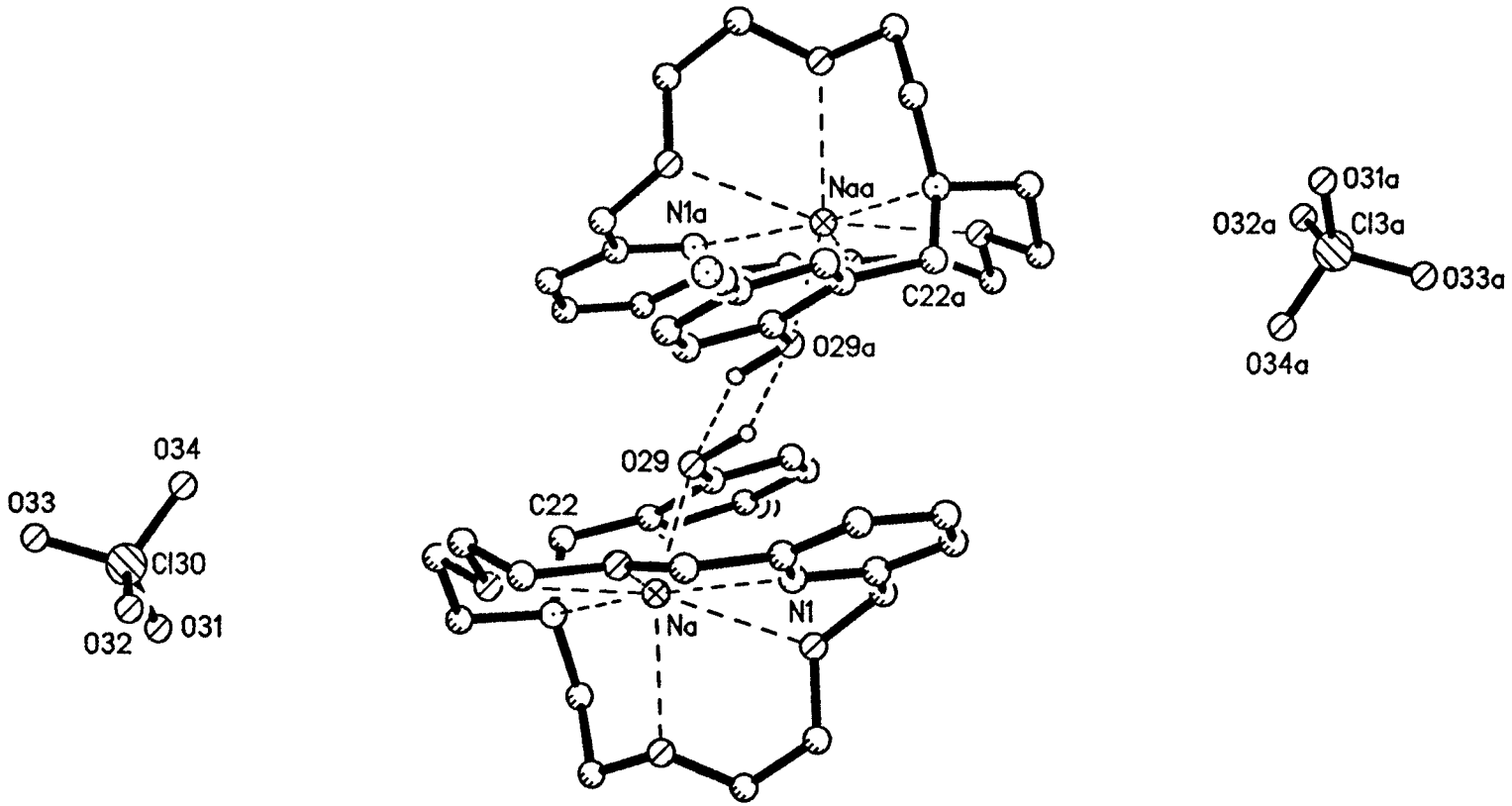

Figure II. A drawing of the dimer formed by the two molecules of Na^{+}-**3** which are related by an inversion center. Only one ClO_4^- and one phenol hydrogen site is occupied for each dimer. H atoms (except for H29 and H29a) and one set of disordered oxygen atoms for each ClO_4^- are omitted for clarity.

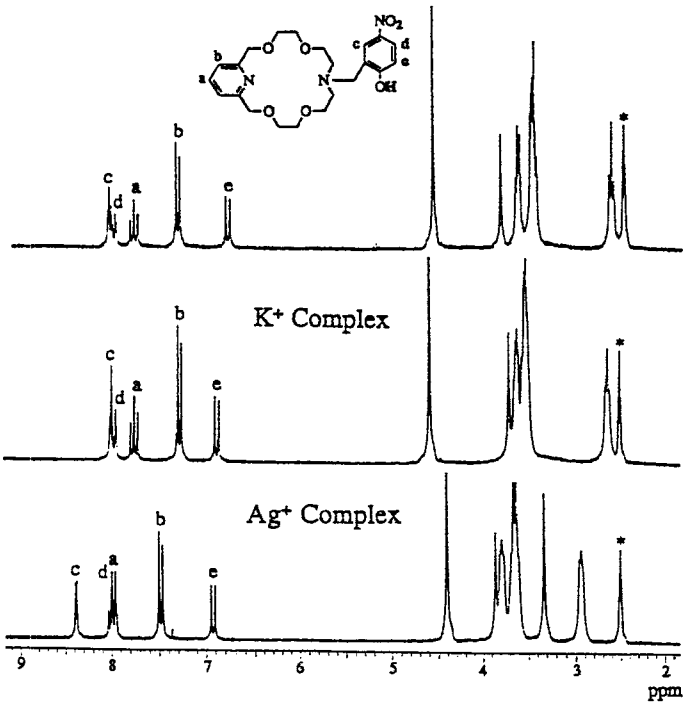

Figure S1. ^{1}H NMR spectra of free **2** and its K^+ and Ag^+ complexes in DMSO-d_6. Peak assignments are shown for aromatic protons. The peaks labeled with an asterisk are attributed to the solvent.

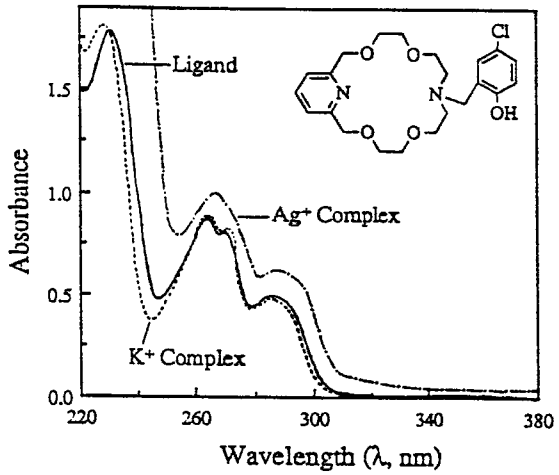

Figure S2. UV-visible spectra of free and complexed **4** in MeOH. [**4**] = 2.00 x 10^{-4} M; [K^+] = 8.82 x 10^{-3} M; [Ag^+] = 9.18 x 10^{-3} M.

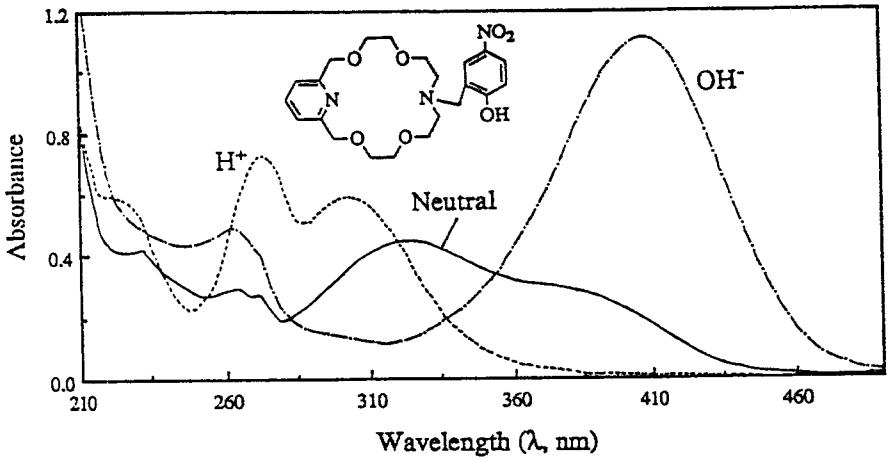

Figure S3. UV-visible spectra of **2** in neutral, acidic, and basic MeOH solutions. [**2**] = 6.63 x 10^{-5} M (neutral solution) and 6.88 x 10^{-5} M (acidic and basic solutions).

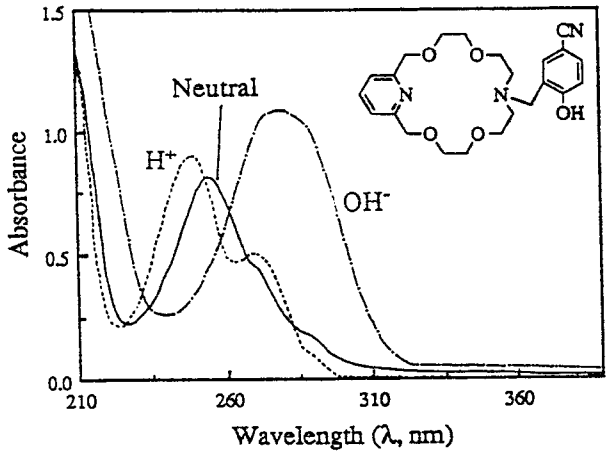

Figure S4. UV-visible spectra of **3** in neutral, acidic, and basic MeOH solutions. [**3**] = 4.37 x 10^{-5} M (neutral solution) and 5.12 x 10^{-5} M (acidic and basic solutions).