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Experimental Section:

Synthesis. Isopropylidene **1** was prepared as described in Davis, J. T.; Tirumala, S.; Jenssen, J. R.; Radler, E.; Fabris, D. *J. Org. Chem.* **1995**, *60*, 4167-4176. Isopropylidene **1** was purified by flash chromatography on silica gel using 10:1 CH_2Cl_2:EtOH as eluant. N^6-Formamidine isoG (**a** in Supplemental Scheme 1) was synthesized according to Seela, F.; Frölich, T. *Helv. Chim. Acta*, **1994**, *77*, 399.

5'-(*tert*-Butyldimethylsilyl)-N^6-formamidine isoG (b). To a solution of N^6-formamidine isoG **a** (0.52 g, 1.53 mmol) in DMF (15 mL) was added NEt_3 (0.61 g, 0.84 mL, 6.03 mmol) and TBDMS-Cl (0.88 g, 5.85 mmol). The reaction mixture was stirred at rt for 48 h, diluted with CH_2Cl_2 (30 mL) and the organic layer was washed with H_2O (15 mL), 0.01 N HCl (15 mL), saturated $NaHCO_3$ (15 mL), and saturated NaCl (15 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo* to give a yellow gum. The crude product was triturated with diethyl ether to give **b** (0.57 g, 83%) as a white solid. R_f 0.75 (CH_2Cl_2/MeOH, 3:2). UV (MeOH), λ_{max} (ε) 227 (24000), 260 (14000), 345 (25000). ^{1}H NMR (400 MHz, DMSO-d_6) δ 0.04 (s, 6 H), 0.86 (s, 9 H), 3.09 (s, 3 H), 3.19 (s, 3 H), 3.71 (dd, J = 4.4, 11.3 Hz, 1 H), 3.81 (dd, J = 3.8, 11.3 Hz, 1 H), 3.89 (ddd, J = 3.8, 4.1, 4.4 Hz, 1 H), 4.07 (ddd, J = 4.1, 5.0, 5.4 Hz, 1 H), 4.38 (ddd, J = 5.0, 5.2, 5.9 Hz, 1 H), 5.18 (d, J = 5.4 Hz, 1 H), 5.51 (d, J = 5.9 Hz, 1 H), 5.69 (d, J = 5.2 Hz, 1 H), 7.97 (s, 1 H), 9.11 (s, 1 H), 11.05 (br s, 1 H). ^{13}C NMR (50 MHz, DMSO-d_6) δ -5.5, 18.0, 25.8, 34.3, 63.0, 69.9, 73.2, 84.3, 86.3, 113.1, 139.3, 154.4, 156.4, 157.7, 161.0. LRMS (FAB), *m/z* (rel int) 73 (100), 207 (88), 453 ([M+1]$^+$, 33). HRMS (FAB), calc. for $C_{19}H_{33}N_6O_5Si$ 453.2282, found 453.2285.

5'-(*tert*-Butyldimethylsilyl)-isoguanosine (c). To a solution of 5'-(*tert*-butyldimethylsilyl)-N^6-formamidine isoG **b** (0.30 g, 0.66 mmol) in CH_3CN (2 mL) was added EtOH (2 mL) and NH_4OH (6 mL). The reaction mixture was stirred at rt

for 16 h after which time TLC indicated the reaction was complete. The solvent was evaporated to give **c** (0.26 g, 100%) as a white solid. This material was used without further purification in the next step. *Rf* 0.58 (CH_2Cl_2/MeOH, 3:2). ^1H NMR (200 MHz, DMSO-d6) δ 0.05 (s, 6 H), 0.87 (s, 9 H), 3.66-3.90 (m, 3H), 4.08 (m, 1 H), 4.31 (dd, *J* = 4.7, 4.7 Hz, 1 H), 5.14 (br s, 1H), 5.22 (br s, 1 H), 5.66 (d, *J* = 4.7 Hz, 1 H), 7.46 (br s, 1 H), 7.90 (s, 1 H). LRMS (FAB), *m/z* (rel int) 73 (100), 75 (27), 152 (69), 398 ($[M+1]^+$, 18). HRMS (FAB), calc. for $C_{16}H_{28}N_5O_5Si$ 398.1860, found 398.1842.

2',3'-Di-*O*-acetyl-5'-(*tert*-Butyldimethylsilyl)-isoguanosine (4). To a suspension of 5'-(*tert*-butyldimethylsilyl)-isoG **c** (0.26 g, 0.66 mmol) in CH_2Cl_2 was added NEt_3 (0.67 g, 0.93 mL, 6.63 mmol) and acetic anhydride (0.68 g, 0.63 mL, 6.63 mmol). The reaction was allowed to stir at rt for 19 h, after which time TLC indicated that the reaction was complete. The reaction was diluted with CH_2Cl_2 (25 mL) and the organic layer was washed with 0.01 N HCl (25 mL), sat $NaHCO_3$ (25 mL), and sat NaCl (25 mL). The organic layer was dried over Na_2SO_4 and concentrated *in vacuo* to give a yellow oil. The ^1H NMR of the crude product showed many acetate signals. Thus, MeOH (10 mL) and CH_2Cl_2 (5 mL) were added and the reaction mixture was refluxed for 72 h. After this time the two spots with R*f* 0.69 and 0.53 (CH_2Cl_2/MeOH, 10:1) were converted to two lower running spots of R*f* 0.41 and 0.27 (major). This mixture was purified by silica gel chromatography to give 2',3'-di-*O*-acetyl-5'-(*tert*-butyldimethylsilyl)-isoG **4** (0.11 g, 34%) as a white solid. R*f* 0.27 (CH_2Cl_2/MeOH, 10:1). UV (MeOH), λ_{max} (ε) 215 (32000), 252 (12000), 295 (12000). ^1H NMR (400 MHz, DMSO-d6) δ 0.07 (s, 6 H), 0.88 (s, 9 H), 2.00 (s, 3H), 2.11 (s, 3H), 3.81 (dd, J = 3.5, 11.3 Hz, 1H), 3.88 (dd, J = 3.5, 11.3 Hz, 1 H), 4.20 (m, 1H), 5.41 (dd, *J* = 2.9, 5.2 Hz, 1 H), 5.70 (dd, J = 5.2, 6.6 Hz, 1H), 5.96 (d, *J* = 6.6 Hz, 1 H), 7.62 (br s, 1 H), 7.91 (s, 1 H), 10.51 (br s, 1H). ^{13}C NMR (50 MHz, CDCl3) δ -5.5, 18.4, 20.4, 20.7, 25.9, 63.1, 71.8, 74.2, 83.7, 83.7, 110.0, 136.5,

151.5, 154.5, 158.0, 169.4, 170.0. LRMS (FAB), *m/z* (rel int) 66 (29), 73 (100), 152 (40), 482 ($[M+1]^+$, 38). HRMS (FAB), calc. for $C_{20}H_{32}N_5O_7Si$ 482.2071, found 482.2056.

Preparation of Potassium and cesium picrate: Potassium picrate was prepared by neutralizing picric acid with an equal molar amount of potassium or cesium hydroxide in EtOH. Solid impurities were removed by filtration. The resulting metal picrate salts, which precipitated from solution, were recrystallized twice from water and dried in a vacuum desiccator for 2 days. The recrystallized metal picrates salts were characterized by ^1H NMR, UV spectroscopy, and elemental analysis. **Warning: Picrate salts are potentially shock sensitive and explosive.**

NMR Experiments: Most NMR experiments were performed on a Bruker AMX-500 NMR spectrometer. The spectrometer ^1H frequency was 500.13 MHz and its ^{133}Cs frequency was 65.6 MHz. The temperature was controlled to ± 0.1° C. The spectral window was 20 ppm for ^1H and 300 ppm for ^{133}Cs. Typical 90° pulse widths were 11 μs for ^1H and 7.4 μs for ^{133}Cs. The ^{133}Cs chemical shifts were referenced relative to 0.5 M CsI in D_2O at 0 °C.

Metal Cation Picrate Extractions. To a glass vial containing 1 mL of a 16 mM solution of isoG **1** or **4** in $CDCl_3$ was added 1 mL of a 4.5 mM solution of metal picrate in distilled water. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer was carefully removed with a syringe and transferred to an NMR tube for measurement. The 500 MHz ^1H NMR spectrum of the sample was recorded at 0 °C. The stoichiometry for $(isoG)_8$-M^+ was determined by comparing the integration of the picrate's ^1H resonance at 8.66 ppm with the integration of the isoG resonances.

Competition Experiment for Potassium Picrate and Cesium Picrate Extraction. To a glass vial containing 1 mL of a 16 mM solution of isoG **4** in $CDCl_3$ was added a 1 mL solution of 4.5 mM potassium picrate and 4.5 mM cesium picrate in H_2O. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer was carefully removed with a syringe and transferred to an NMR tube for measurement. The ^1H NMR (500 MHz) spectrum was recorded at 0 °C. The relative amounts of (isoG)8-K^+ and (isoG)8-Cs^+ were determined by comparing the integration of the H8 resonance of (isoG)8-K^+ at 7.89 ppm, with the integration of the H8 resonance of (isoG)8-Cs^+ at 7.68 ppm.

Metal Picrate Titrations. A series of NMR tubes containing a solution of isoG **4** (2.6 mM) in CD_3CN, and metal cation picrate in CD_3CN in increasing increments (0.02 mM, 0.04 mM, 0.08 mM, 0.16 mM, 0.32 mM) were vortexed for 2 min. The 400 MHz ^1H NMR spectra were recorded at 25 °C. The stoichiometry of the isoG-metal complex was determined by comparing the integration of the picrate's ^1H resonance at 8.66 ppm with the integration of the isoG resonances.

^{133}Cs T1 determination: The inversion-recovery method was used to determine the ^{133}Cs spin lattice relaxation time, T_1, for cesium picrate (10 mM) and (isoG **1**)8-Cs^+ picrate (8 mM) in CD_3CN at 25 °C. The T_1 values were estimated by a null point determination method in a single inversion recovery experiment. Incremental values for τ of 0.05 sec and 0.002 sec were used for cesium picrate and (isoG **1**)8- Cs^+ picrate, respectively, to determine the null point. Selected acquisition parameters of the individual spectra were as follows: spectral window, 200 ppm; relaxation delay 10 s; ^{133}Cs 90 degree pulse 7.3 us; number of scans 300.

Competition of (isoG 4)$_8$-Cs$^+$ with calixarene 5. To a glass vial containing 1 mL of a 16 mM solution of isoG **4** in $CDCl_3$ was added 1 mL of a 4.5 mM solution of cesium picrate in distilled water. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer was carefully removed with a syringe and transferred to an NMR tube for measurement. To this was added 50 mL of a 20 mM solution of calixarene **5**, so that the overall solution was 1.8 mM (isoG **4**)$_8$-Cs$^+$ and 1.8 mM calixarene **5**. The ^{1}H NMR (500 MHz) and ^{133}Cs NMR (65.6 MHz) spectra were recorded at 0°C. The relative amounts of (isoG **4**)$_8$-Cs$^+$ and (isoG **4**)$_4$ were determined by comparing the integration of ^{133}Cs resonance for (isoG)$_8$-Cs$^+$ at -28.4 ppm ppm with the integration of the calixarene-Cs$^+$ resonance at -61.4 ppm. *The uncertainties in calculated K_a values arise from the K_a value for calixarene **5**, reported by Reinhoudt and Ungaro (ref 7a), and from experimental uncertainties in the NMR competition experiments. Our largest experimental uncertainty is due to errors associated with NMR integration. Reinhoudt and Ungaro measured K_a (Cs$^+$) for calixarene **5** in $CHCl_3$ by using Cram's picrate extraction method. They reported a value of log K_a= 8.8, and they noted that this K_a value is only as precise as the picrate extraction method itself. Cram reported that the picrate method is relatively low-precision, with errors between ± 15-50%, depending on the host's R value (JACS, **1979**, 101, 4928). Since calixarene **5** is such a good Cs$^+$ binder, the uncertainty in the reported K_a for calixarene **5** is likely ± 50%. We have made a conservative estimate that the uncertainty in our NMR signal integration is ± 10%.*

Competition of (isoG 1)$_8$-Cs$^+$ with calixarene 5. To a glass vial containing 1 mL of a 16 mM solution of isoG **1** in $CDCl_3$ was added 1 mL of a 4.5 mM solution of cesium picrate in distilled water. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer

was carefully removed with a syringe and transferred to an NMR tube for measurement. To this was added varying amounts of a 20 mM solution of calixarene **5**, so that the overall solution was 1.8 mM (isoG **1**)$_8$-Cs^+ and between 1.8-18 mM in calixarene **5**. The ^{1}H NMR (500 MHz) and ^{133}Cs NMR (65.6 MHz) spectra were recorded at 0°C.

Determination of Cs+/K+ Specificity for Isopropylidene isoG 1. Because of solubility problems for high concentrations of potassium picrate, the more soluble iodide salts were used to determine the Cs+/K+ specificity for isopropylidene **1**. To a glass vial containing 1 mL of a 16 mM solution of isoG **1** in $CDCl_3$ was added 1 mL of a 2.5 M solution of potassium or cesium iodide in distilled water. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer was carefully removed with a syringe and transferred to an NMR tube for measurement. The ^{1}H NMR (500 MHz) spectrum was recorded at 25°C.

Competition Experiment for Cesium Iodide and Potassium Iodide Extraction. To a glass vial containing 1 mL of a 16 mM solution of isoG **1** in $CDCl_3$ was added a 1 mL solution of 2.5 M potassium iodide and 0.005 M cesium iodide in H_2O. This $CDCl_3/H_2O$ mixture was stirred for 1h at rt. The mixture was then transferred to an eppendorf tube and centrifuged for 5 min to force the organic layer to the bottom of the tube. An aliquot (0.5 mL) of the $CDCl_3$ layer was carefully removed with a syringe and transferred to an NMR tube for measurement. The ^{1}H NMR (500 MHz) spectrum was recorded at 25°C. The Cs^+/K^+ specificity was determined by peak integration of the separate K^+ and Cs^+-bound species.

Supplemental Figure Captions

Figure 1. 500 MHz ^{1}H NMR spectrum of diacetate **4** (40 mM) in d$_6$-DMSO at 20 ^{o}C. This spectrum indicates that isoG diacetate is monomeric in d$_6$-DMSO.

Figure 2. A region of the 500 MHz ^{1}H NMR spectrum of isopropylidene **1** (16 mM) in CDCl$_3$ at 0 ^{o}C. A) Before extraction; B) After extraction with water containing 5 mM cesium picrate. Integration of the picrate signal at σ 8.78 ppm and resonances for isopropylidene **1** indicate formation of the octamer, (isoG **1**)$_8$-Cs$^+$ picrate.

Figure 3. A region of the 500 MHz ^{1}H NMR spectrum of diacetate **4** (16 mM) in CDCl$_3$ at 25 ^{o}C. A) After extraction with water containing 4.5 mM cesium picrate; B) After extraction with water containing 4.5 mM potassium picrate. C) After extraction with water containing 4.5 mM potassium picrate and 4.5 mM cesium picrate. Integration of the diacetate's H8 resonance indicates a 57:43 ratio of (isoG **4**)$_8$-K$^+$ to (isoG **4**)$_8$-Cs$^+$.

Figure 4. 400 MHz ^{1}H NMR spectrum of diacetate **4** (2.0 mM) in CD$_3$CN at 25 ^{o}C. A) After titration with 0.50 mM (2 eq. per octamer) potassium picrate; B) After titration with 0.50 mM (2 eq. per octamer) cesium picrate. C) IsoG diacetate **4** (2.5 mM) with 0.31 mM (1 eq per octamer) potassium picrate and 0.31 mM cesium picrate (1 eq per octamer). The two sets of separate resonances for (isoG **4**)$_8$-K$^+$ and (isoG **4**)$_8$-Cs$^+$ show that there is little Cs$^+$/K$^+$ selectivity for diacetate **4**.

Figure 5. Optical spectra of a $CHCl_3$ solution of isoG **1** (0.11 mM) at 20 °C. (A) Before cesium picrate extraction. (B) After extraction of an aqueous cesium picrate (3.0 mM) solution. Integration of the isoG absorption at 295 nm and the picrate absorption at 378 nm indicates formation of (isoG **1**)$_8$-Cs^+.

Figure 6. 65.6 MHz ^{133}Cs NMR spectra in CD_3CN at 25 °C. A) Cesium picrate (10 mM) before titration of isopropylidene **1**. B) After addition of 4 eq of isoG **1**. C) After addition of 8 eq of isoG **1**. D) After addition of 16 eq of isoG **1**. The limiting chemical shift change indicates that isoG 1 binds Cs+ as an octamer in CD_3CN.

Figure 7. Stack plot of spectra from ^{133}Cs inversion-recovery T_1 experiments in CD_3CN at 20 °C A) Cesium picrate (10 mM). Based on the null point determination, the T_1 is 3.25 s. B) For (isoG **1**)$_8$-Cs^+(8 mM). The T_1 is 0.0023 s.

Figure 8. 65.6 MHz ^{133}Cs NMR spectra in $CDCl_3$ at 0 °C. A) For (isoG **4**)$_8$-Cs^+ (2.0 mM); B) For calixarene **5** (2.0 mM); C) For a 1:1 mixture of (isoG **4**)$_8$-Cs^+ and calixarene **5** (both 2.0 mM). Integration of the two signals gives a 1:1 ratio. This experiment shows that (isoG **4**)$_8$ and calixarene **5** have similar Cs^+ association constants.

Figure 9. 500 MHz ^1H NMR spectrum in $CDCl_3$ at 0°C for (isoG **4**)$_8$-Cs^+ (2.0 mM) after addition of 1 eq of calixarene **5**. Integration of isoG tetramer resonances at 7.89 ppm (H8) and 6.15 ppm (H1') to isoG octamer resonances at 7.68 ppm (H8) and 5.86 ppm (H1') gives a 1:1 ratio. This experiment indicates a 50% conversion of (isoG **4**)$_8$-Cs^+ to (isoG **4**)$_4$-Cs^+ upon addition of 1 eq of calixarene **5** which shows that (isoG **4**)$_8$ and calixarene **5** have similar Cs^+ association constants.

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Figure 10. A region of the 500 MHz ^{1}H NMR spectrum for solutions of (isoG **1**)$_8$-Cs^+ and calixarene **5** in $CDCl_3$ at 0 ^{o}C. A) For a solution containing 2 mM (isoG **1**)$_8$-Cs^+. B) For a solution containing 2 mM (isoG **1**)$_8$-Cs^+ and 20 mM calixarene **5**. Even in the presence of 10 equivalents of calixarene **5** (log $K_a(Cs^+)$=8.8) the NH1 peak for (isoG **1**)$_8$-Cs^+ octamer predominates over (isoG **1**)$_4$.

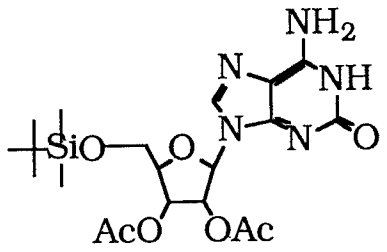
Figure 11. Some 65.6 MHz ^{133}Cs NMR spectra in $CDCl_3$ at 0 ^{o}C. A) For calixarene **5** (2.0 mM); B) For isopropylidene octamer, (isoG **1**)$_8$-Cs^+ (2.0 mM). C) For a solution containing a 1:1 mixture of (isoG **1**)$_8$-Cs^+ (2.0 mM) and calixarene-Cs^+ **5** (2.0 mM). D) For a solution containing a 1:10 mixture of (isoG **1**)$_8$-Cs^+ (2.0 mM) and calixarene **5** (20 mM). The major ^{133}Cs resonances corresponds to that for (isoG **1**)$_8$-Cs^+. There is no evidence for a calixarene-Cs+ peak. There a small amount of an unknown complex at σ= -58.8 ppm.

Table 1. 500 MHz ^{1}H Chemical Shifts (ppm) for isoG diacetate **4**.

Table 2. 65.6 MHz ^{133}Cs Chemical Shifts (ppm) for isoG **1**, isoG **4** and calixarene **5**

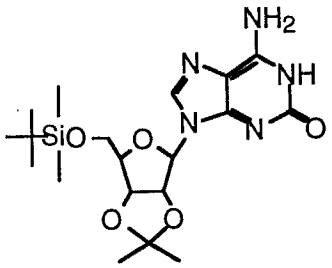
Figure 1

400 MHz ^{1}H NMR
25°C in DMSO-d_6



4

Figure 2 **500 MHz ^{1}H NMR at 25 °C in $CDCl_3$**



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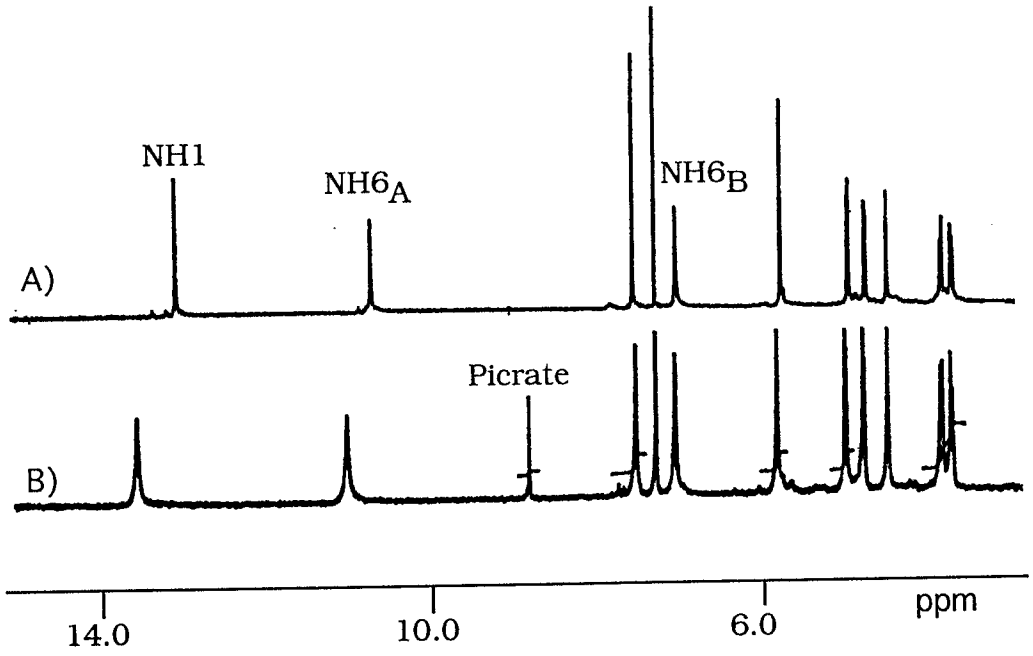
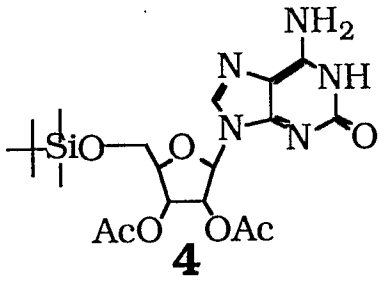


Figure 3



4

500 MHz ^{1}H NMR
0°C in $CDCl_3$

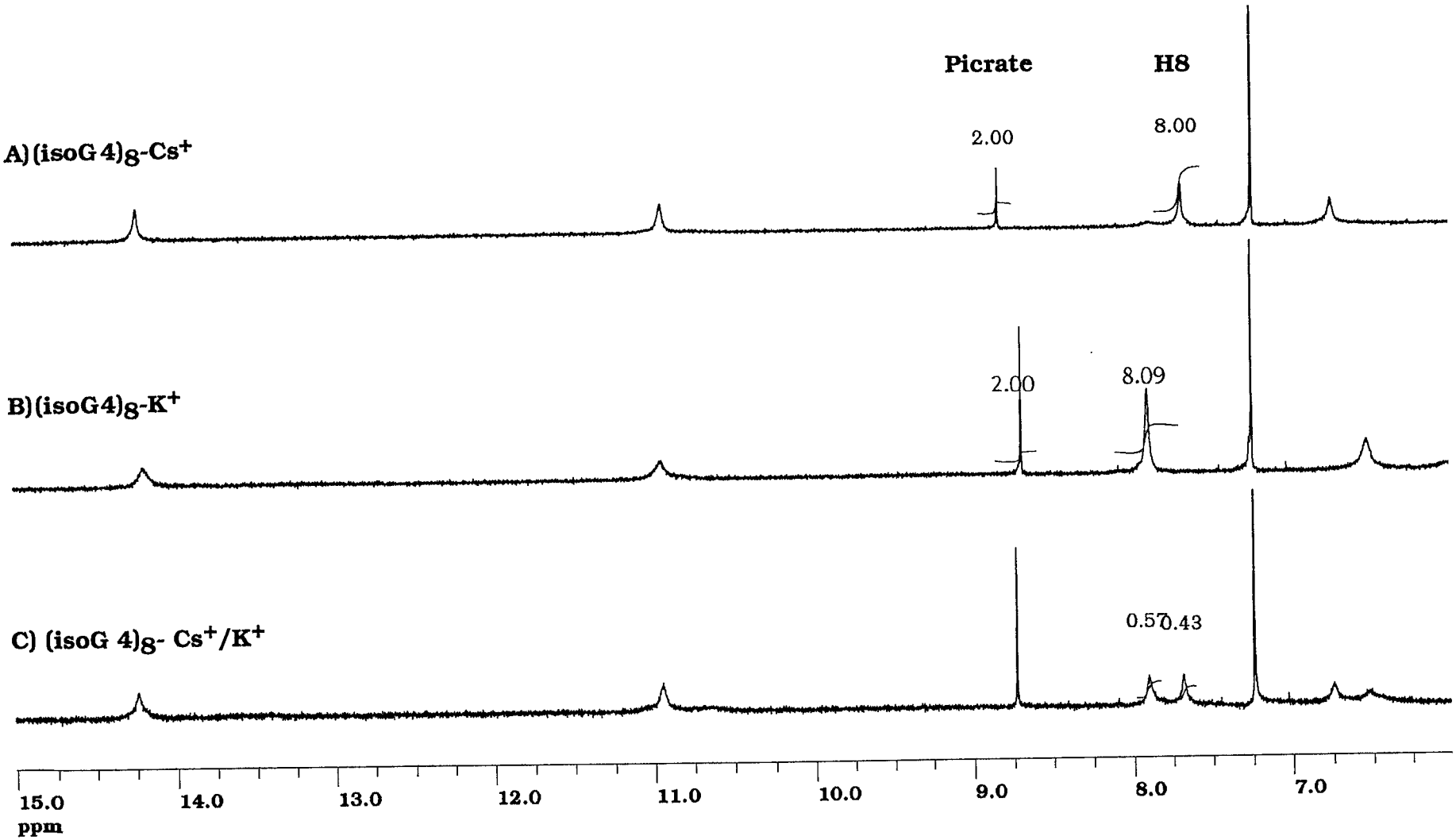
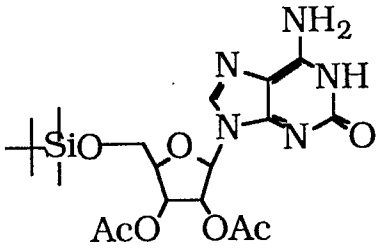


Figure 4

400 MHz ^{1}H NMR
25°C in CD_3CN



4

A) (isoG 4)$_8$-K$^+$

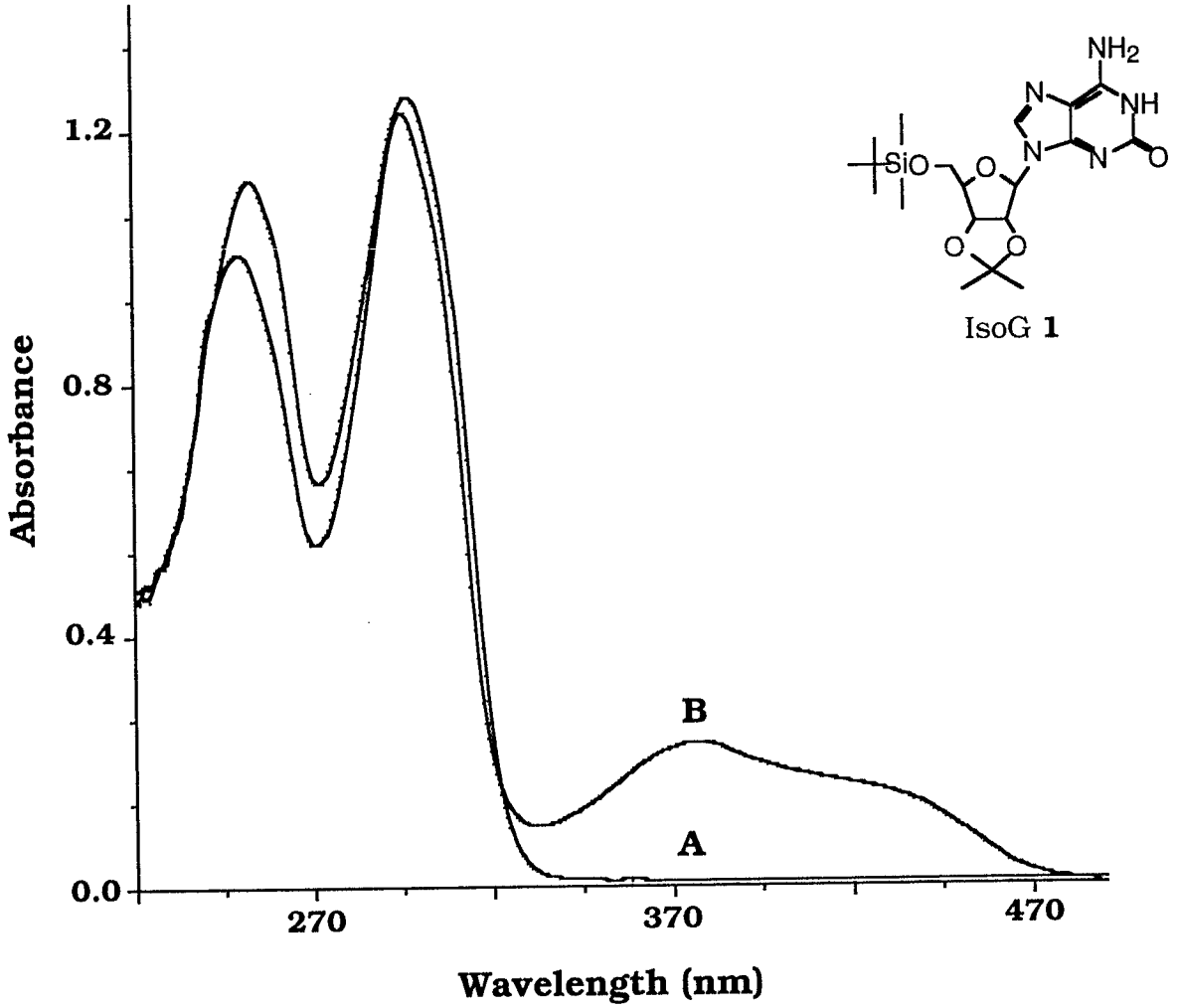
B) (isoG 4)$_8$-Cs$^+$

C) (isoG 4)$_8$-Cs$^+$/K$^+$

15.0 14.0 13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 -0.0

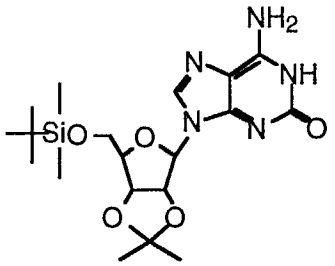
Figure 5

UV Spectra at 25 °C in $CHCl_3$



IsoG **1**

Figure 6 **^{133}Cs NMR (65.6 MHz) at 25 °C in CD_3CN**



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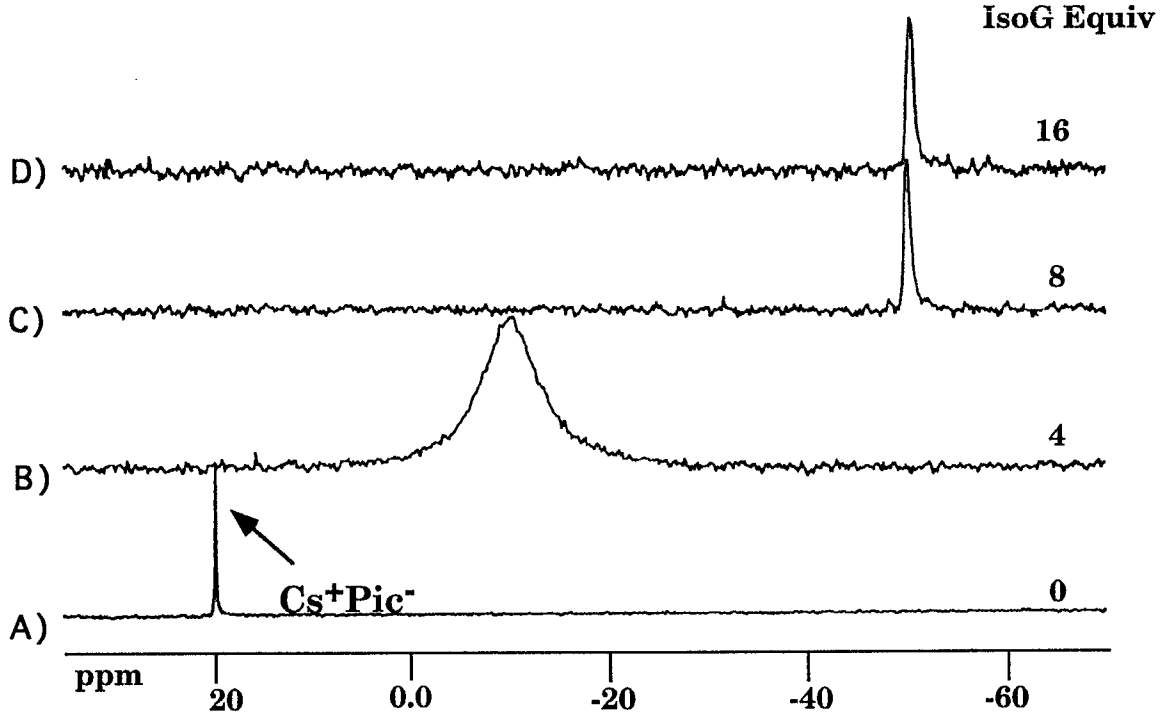


Figure 7

^{133}Cs NMR- T1 Determination

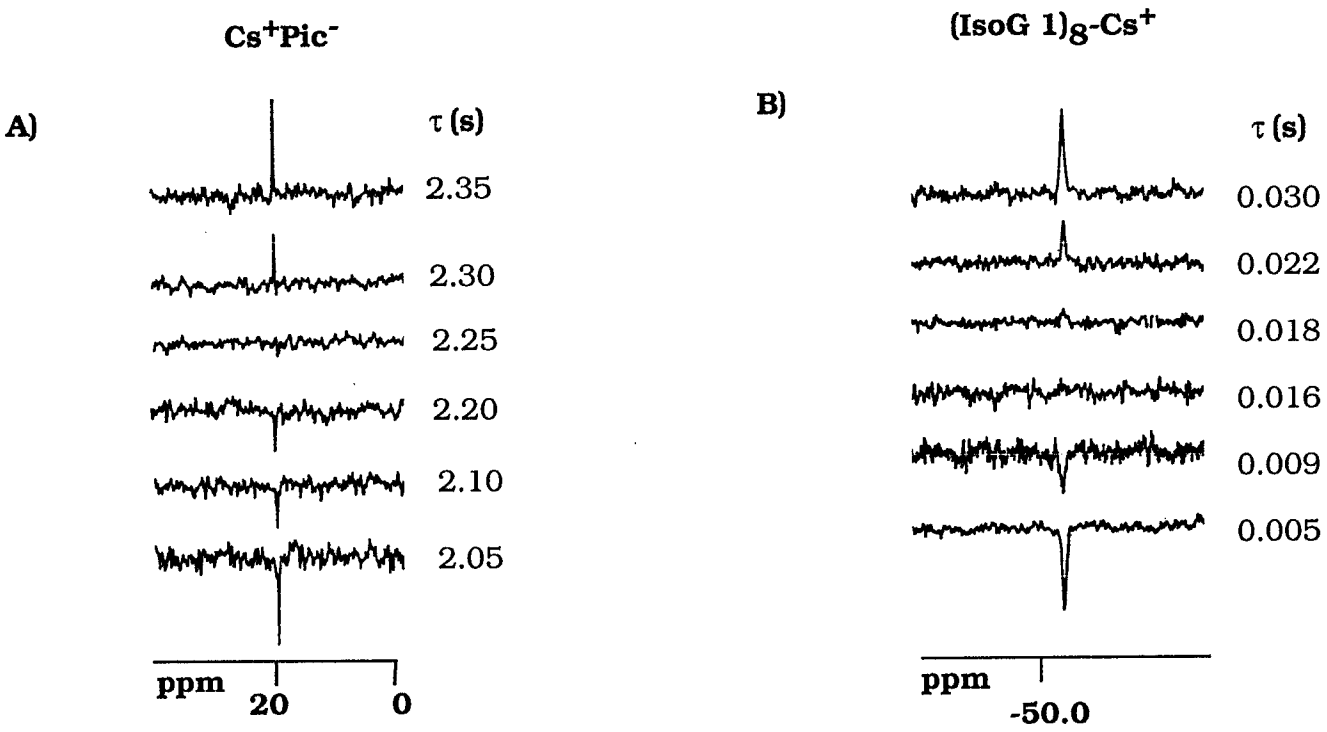
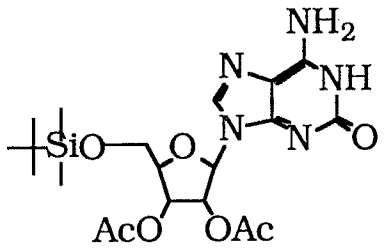


Figure 8

^{133}Cs NMR (65.6 MHz) at 0°C
$CDCl_3$



4

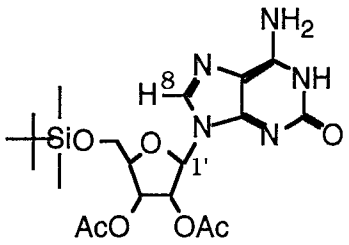
A) (isoG 4)$_8$-Cs$^+$

B) calixarene 5-Cs$^+$

C) (isoG 4)$_8$-Cs$^+$ + 1 eq. calixarene 5

Figure 9

500 MHz ^{1}H NMR
0°C in $CDCl_3$

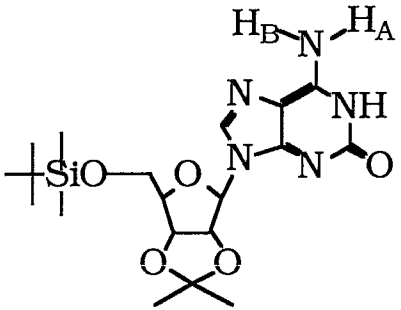


4

(isoG 4)$_8$-Cs$^+$ + 1 eq. calixarene 5

Figure 10

500 MHz ^{1}H NMR
0°C in $CDCl_3$



1

A) (isoG 1)$_8$-Cs$^+$ + 5 eq. calixarene 5

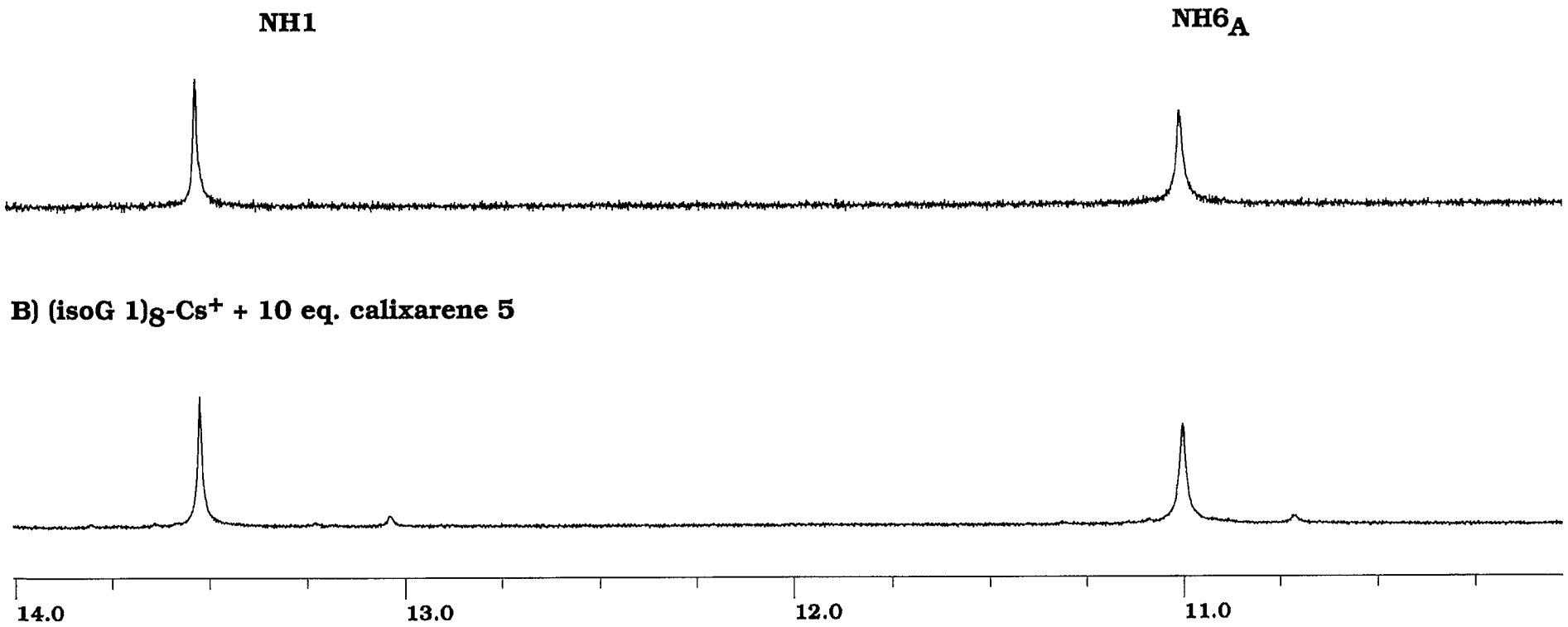
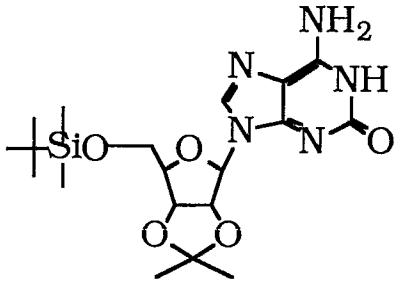


Figure 11

^{133}Cs NMR (65.6 MHz) at 0°C
$CDCl_3$



1

A) calixarene 5-Cs$^+$

B) (isoG 1)$_8$-Cs$^+$

C) (isoG 1)$_8$-Cs$^+$ + calixarene 5-Cs$^+$

D) (isoG 1)$_8$-Cs$^+$+ 10 eq. calixarene 5

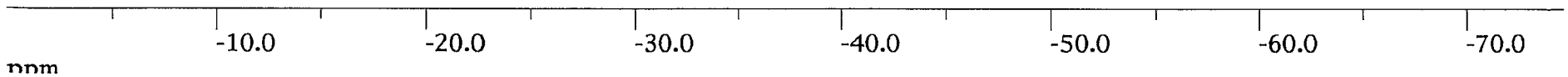


Table 1. ^{1}H NMR chemical shifts (ppm) for isoG diacetate 4.

	Solvent					
Resonance	DMSO-d_6[a]	$CDCl_3$[b]	$CDCl_3$+K$^+$[c]	$CDCl_3$+Cs$^+$[d]	CD_3CN+K$^+$[e]	CD_3CN+Cs$^+$[f]
NH1	10.51		14.21	14.24	14.24	14.02
$NH6_A$	7.62		10.95	10.95	10.84	10.90
$NH6_B$	7.62		6.53	6.74	6.19	6.31
H8	7.91	7.86	7.89	7.68	7.98	7.84
H1'	5.96	6.14	5.74	5.86	5.73	5.63
H2'	5.70	5.55	5.40	5.38	5.38	5.37
H3'	5.41	5.42	5.40	5.38	5.33	5.24
H4'	4.20	4.25	4.33	4.37	4.33	4.33
H5'	3.88	3.90	4.01	4.04	4.09	4.11
H5"	3.81	3.86	3.88	3.93	3.91	3.88
CH_3 A	2.11	2.15	2.15	2.17	2.15	2.11
CH_3 B	2.00	2.02	2.01	2.04	2.08	2.02
tBu	0.88	0.93	0.93	0.94	0.95	0.94
SiMe A	0.07	0.14	0.15	0.16	0.18	0.17
SiMe B	0.07	0.14	0.15	0.16	0.15	0.14

[a] 400 MHz at 25 °C.
[b] 500 MHz at 20 °C.
[c] 500 MHz at 0 °C after extraction of potassium picrate.
[d] 500 MHz at 0 °C after extraction of cesium picrate.
[e] 400 MHz at 25°C with excess potassium picrate.
[f] 400 MHz at 25°C with excess cesium picrate.

Table 2. ^{133}Cs NMR chemical shifts[a]

Species	σ (ppm)
(isoG **1**)8-Cs^+	-28.6
(isoG **4**)8-Cs^+	-55.1
calixarene **5**-Cs^+	-61.4

[a] At 65.6 MHz in $CDCl_3$ at 0 °C. Relative to KI in D_2O at O °C.

Supplemental Scheme