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Supporting Information for:

Supramolecular Hydrogen-bonding Assembly of Silanediols with Bifunctional Heterocycles

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I. General Information

Instruments and Analyses. All nuclear magnetic resonance (NMR) spectra were obtained on Varian VNMRS 600 or Bruker Avance 500 at room temperature. Chemicals shifts were reported in parts per million (δ scale), and referenced according the following standards: ^{1}H signals in chloroform, benzene residual solvent (∂ 7.16) for ^{1}H signals in benzene.

Materials and Purification. Dichloromethane (DCM), diethyl ether (Et_2O), and benzene were obtained from EMD Chemicals. Benzene (C_6D_6) was acquired from Cambridge Isotope Laboratories. 7-azaindole was purchased from Acros Organics. Phenazine, 4,4'-bipyridine, 1,4-dimethoxybenzene, and tetramethylsilane (TMS) were obtained from Sigma Aldrich. 1-tetradecene (TDE) and cyclooctene (COE) were obtained from TCI Chemicals. All chemicals were used as purchased, without further purification.

Dimesitylsilanediol (**1**) was synthesized according to procedures previously reported in the literature and matches spectral data reported.[1,2] Spectral data for **1**: ^{1}H NMR (600 MHz, $CDCl_3$) ∂ 6.72 (s, 4H), 3.41 (s, 2H), 2.30 (s, 12H), 2.20 (s, 6H).

II. Diffusion-ordered NMR Spectroscopy (DOSY) Experiments

^{1}H diffusion-ordered NMR spectroscopy experiments were prepared by adding the appropriate amount of silanediol and binding partner, indicated below, to a vial along with internal standards: tetramethylsilane (TMS), cyclooctene (COE), and 1-tetradecene (TDE). The material was dissolved in 1.0 mL of C_6D_6 and transferred to an NMR tube. The spectra were acquired on a Bruker Avance 500 using a 2D stimulated echo experiment pulse sequence (stegp1s). Experimental parameters transmitter offset (o1p), sweep width (sw), and receiver gain (rg) were obtained from a ^{1}H spectra prior to data acquisition. A linear gradient ramp from 5% to 95% strength with 25 data points (8 scans each) was used. Diffusion constants from the resulting spectra were processed using the T1/T2 relaxation function within the TopSpin 2.1 software after phase correction. Estimated formula weights of NMR-observed species were calculated by graphing log(formula weight) v log(diffusion constant) of the internal standards and fitting a straight line to these data points.[3,4] Using the experimental diffusion constant of $Mes_2Si(OH)_2$, the formula weight of the observed species was calculated using the line of best fit equation.

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[1] Tran, N. T.; Min, T.; Franz, A. K. *Chem. Eur. J.* **2011**, *17*, 9897-9900.

[2] Tran, N. T.; Wilson, S. O.; Franz, A. K. *Org. Lett.* **2012**, *14*, 186.

[3] Li, D.; Sun, C.; Williard, P. G. *J. Am. Chem. Soc.* **2008**, *130*, 11726–11736.

[4] Li, D.; Keresztes, I.; Hopson, R.; Williard, P. G. *Acc. Chem. Res.* **2009**, *42*, 270–280.

$Mes_2Si(OH)_2$ DOSY Self Association Studies

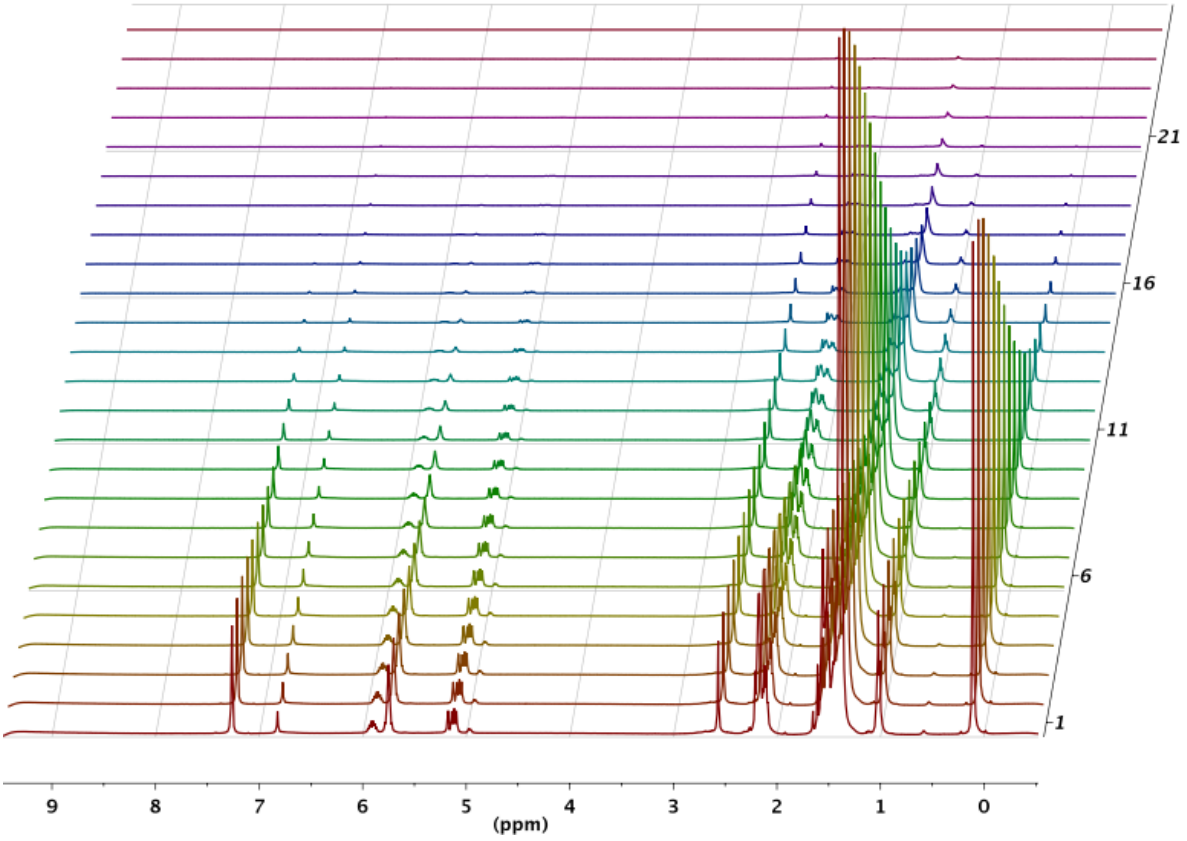


Figure S1. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

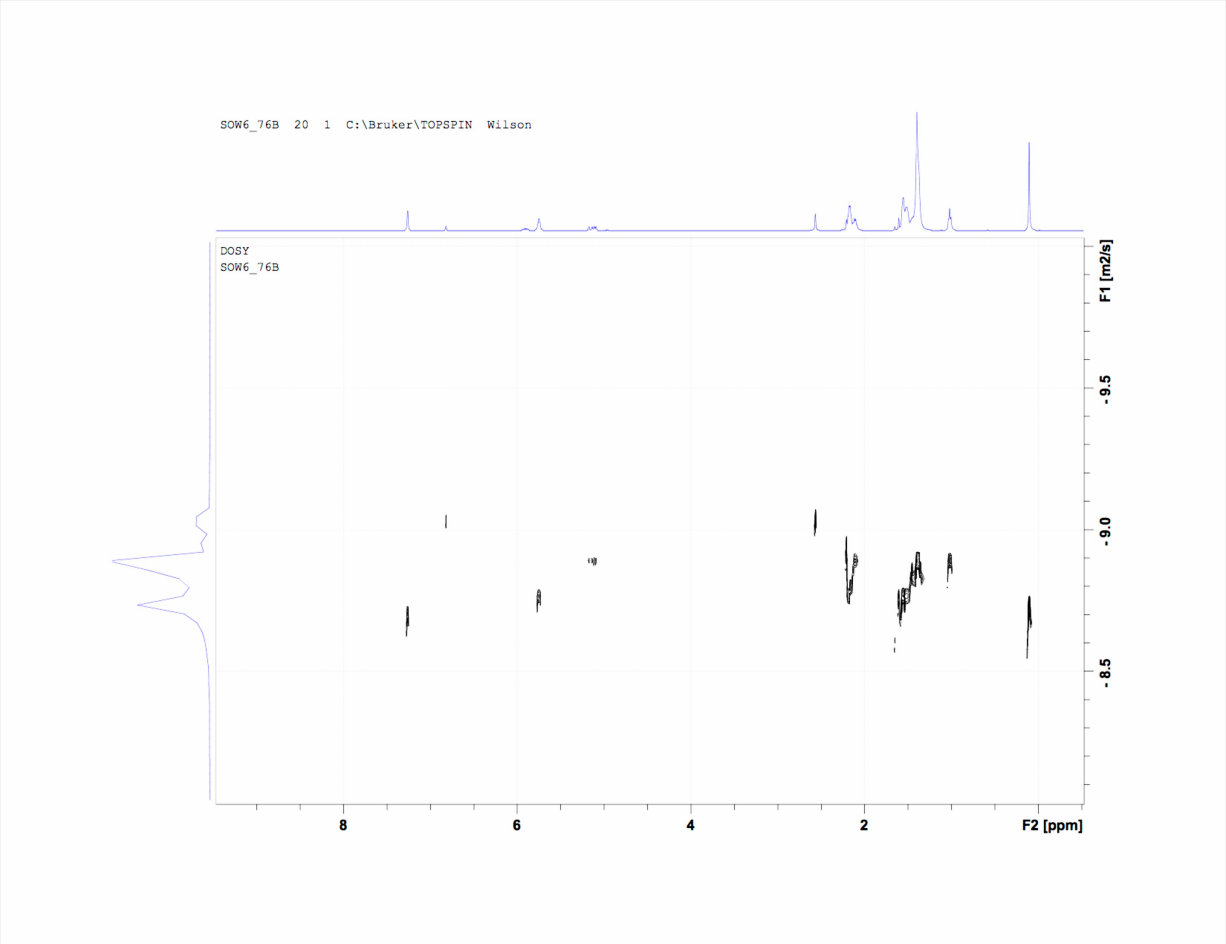


Figure S2. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (10 mM) in C_6D_6 with internal standards.

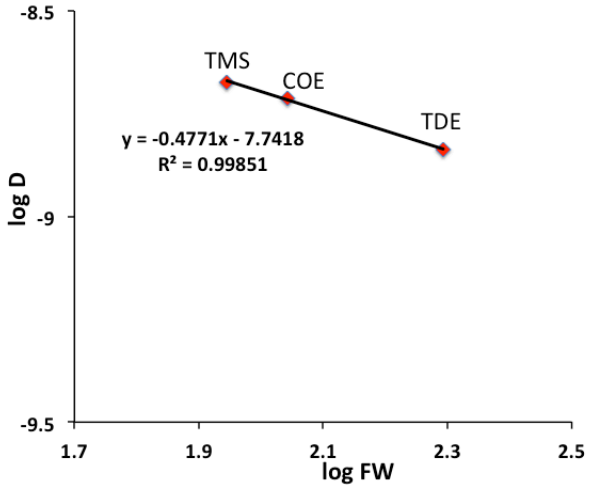


Figure S3. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S1: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 10mM

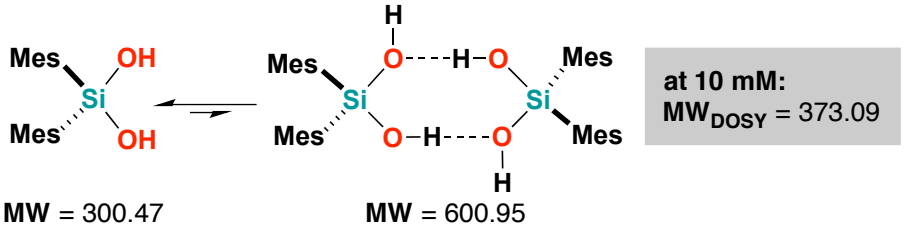


Table S1. Diffusion constants and estimated formula weight of species observed in ^{1}H NMR spectra with 10 mM of $Mes_2Si(OH)_2$ in C_6D_6 suggest self-association but primarily monomeric form.

Molecule	D (m^2/s)	log D	FW (g/mol)	log FW
COE	1.94E-09	-8.712	110.20	2.042
TDE	1.46E-09	-8.837	196.37	2.293
TMS	2.12E-09	-8.673	88.22	1.946
$Mes_2Si(OH)_2$	1.07E-09	-8.969	373.09	2.572

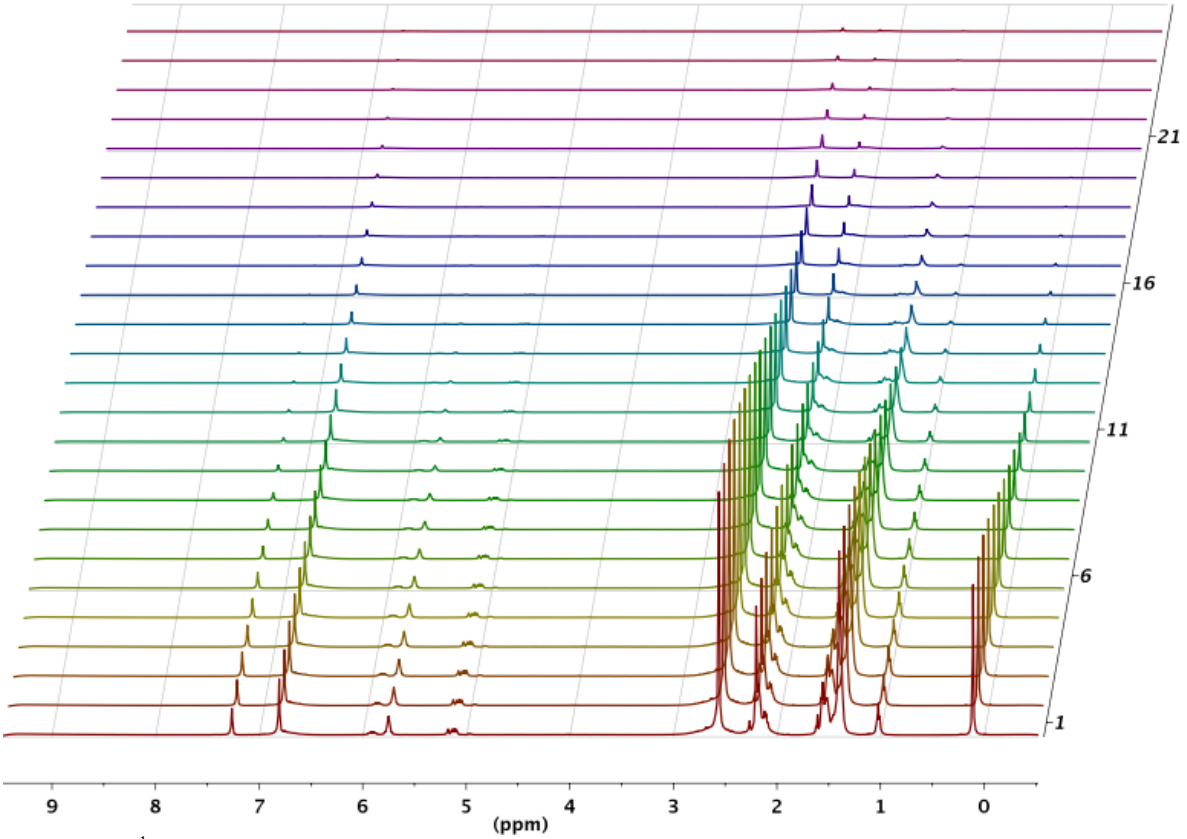


Figure S4. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

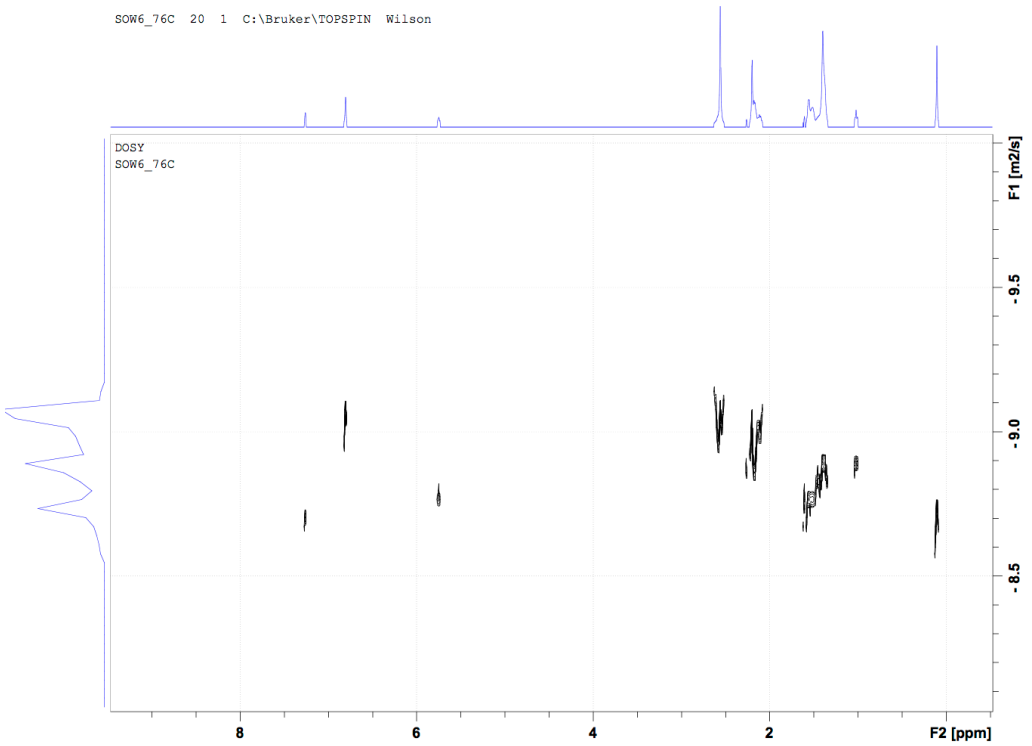


Figure S5. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (100 mM) in C_6D_6 with internal standards.

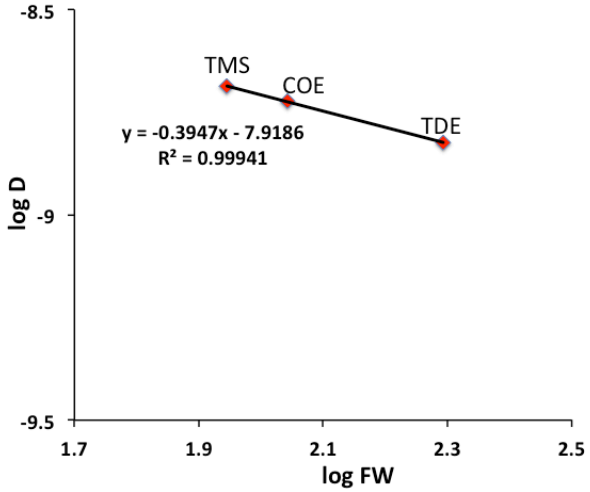
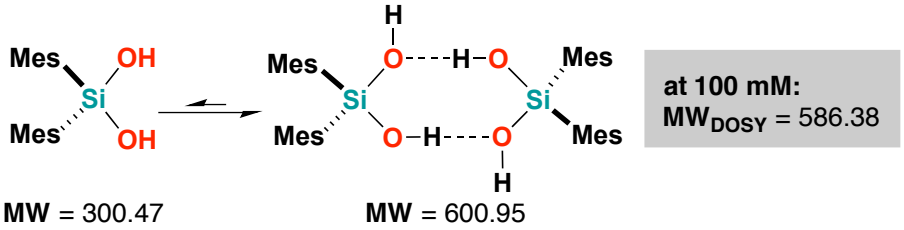


Figure S6. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S2: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 100mM



MW = 300.47 **MW** = 600.95

Table S2. Diffusion constants and estimated formula weight of $Mes_2Si(OH)_2$ species observed in ^1H NMR spectra (100 mM $Mes_2Si(OH)_2$) correlate to a higher order hydrogen-bonded species in equilibrium.

Molecule	**D (m^2/s)**	**log D**	**FW (g/mol)**	**log FW**
COE	1.89E-09	-8.723	110.20	2.042
TDE	1.50E-09	-8.824	196.37	2.293
TMS	2.05E-09	-8.688	88.22	1.946
$Mes_2Si(OH)_2$	9.75E-10	-9.011	586.38	2.768

$Mes_2Si(OH)_2$ DOSY Studies with 7-azaindole

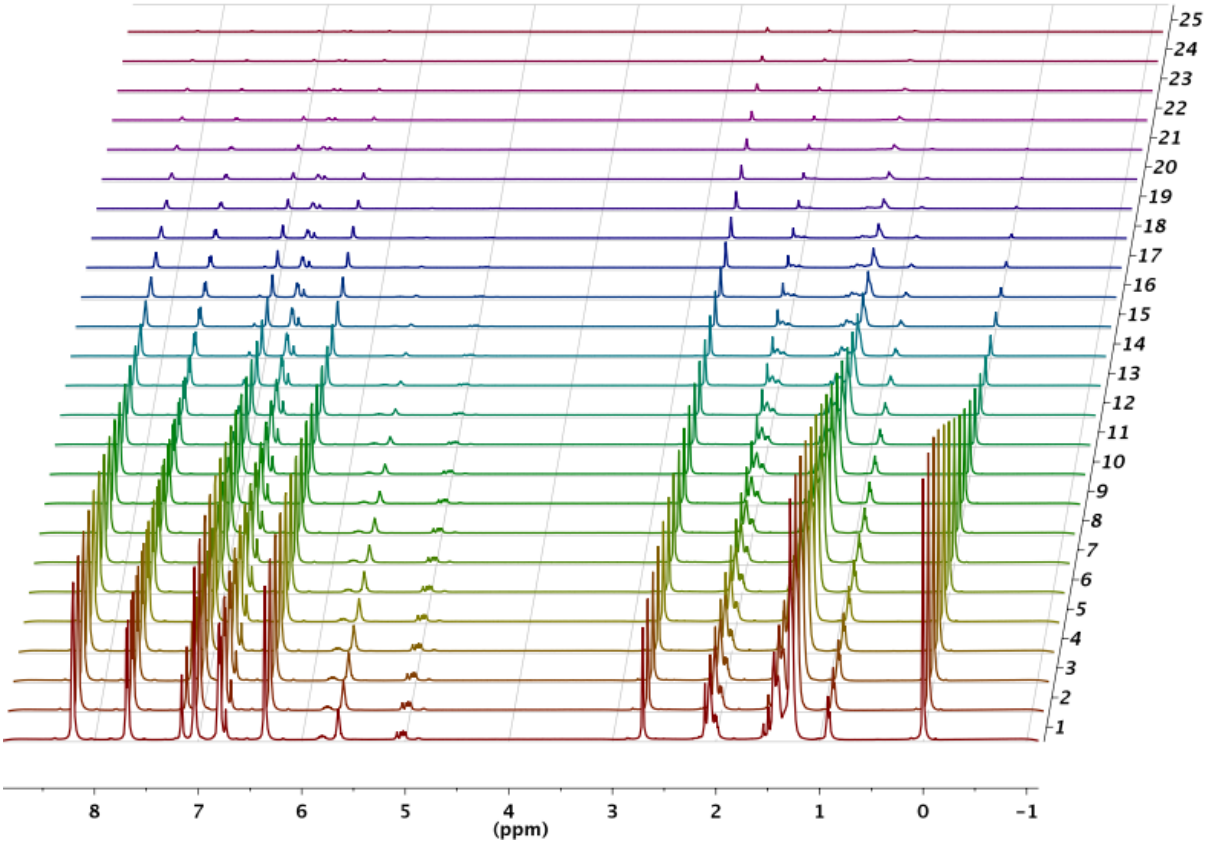


Figure S7. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

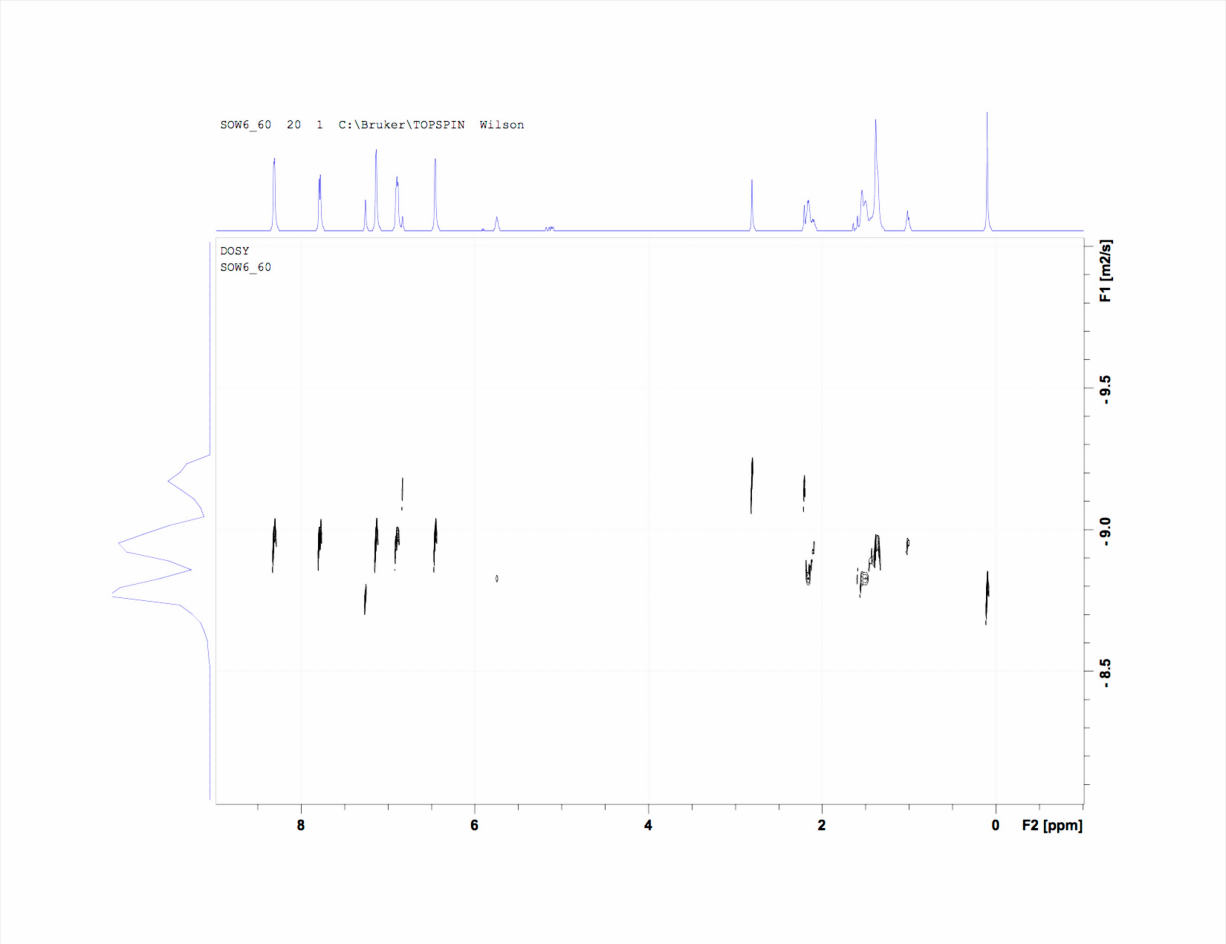


Figure S8. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (10 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards.

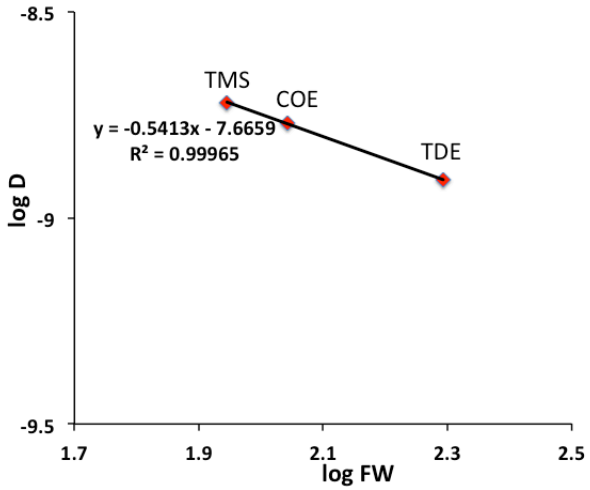


Figure S9. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S3: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 10mM with 7-Azaindole

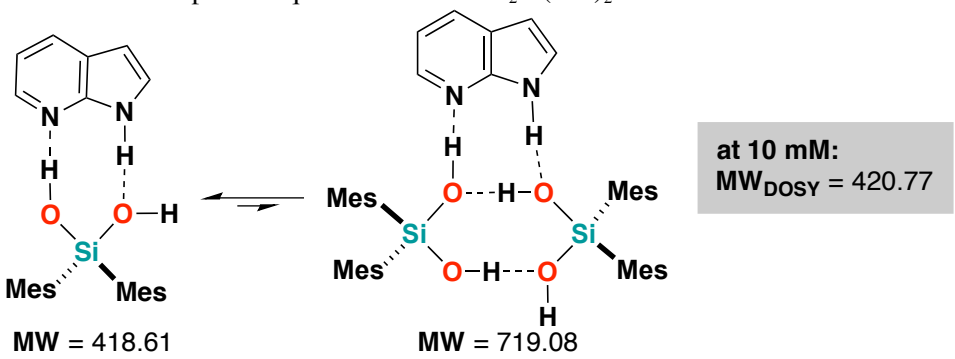


Table S3. Diffusion constants and estimated formula weight of species observed in ^{1}H NMR spectra with 10 mM of $Mes_2Si(OH)_2$ and 50 equivalents of 7-azaindole match corresponding heterodimer.

Molecule	**D (m^2/s)**	**log D**	**FW (g/mol)**	**log FW**
COE	1.70E-09	-8.769	110.20	2.042
TDE	1.24E-09	-8.908	196.37	2.293
TMS	1.90E-09	-8.720	88.22	1.946
$Mes_2Si(OH)_2$	8.20E-10	-9.086	420.77	2.624

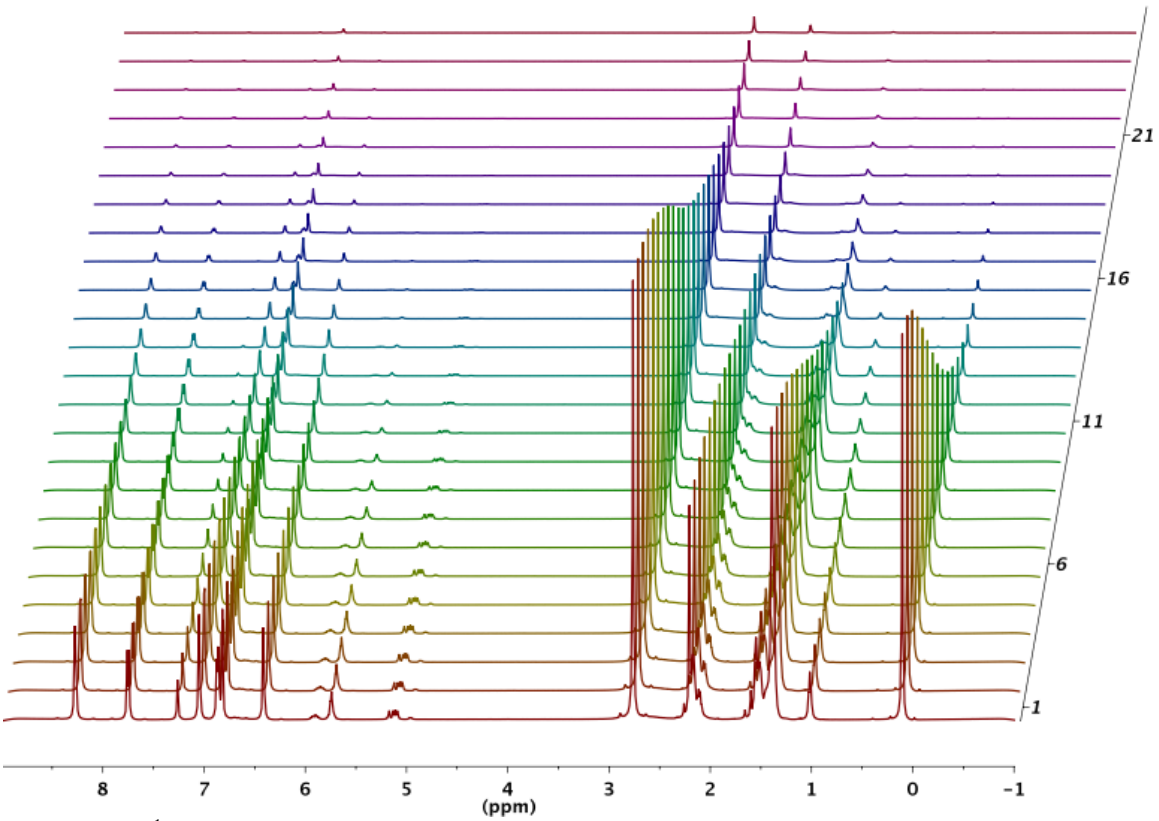


Figure S10. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

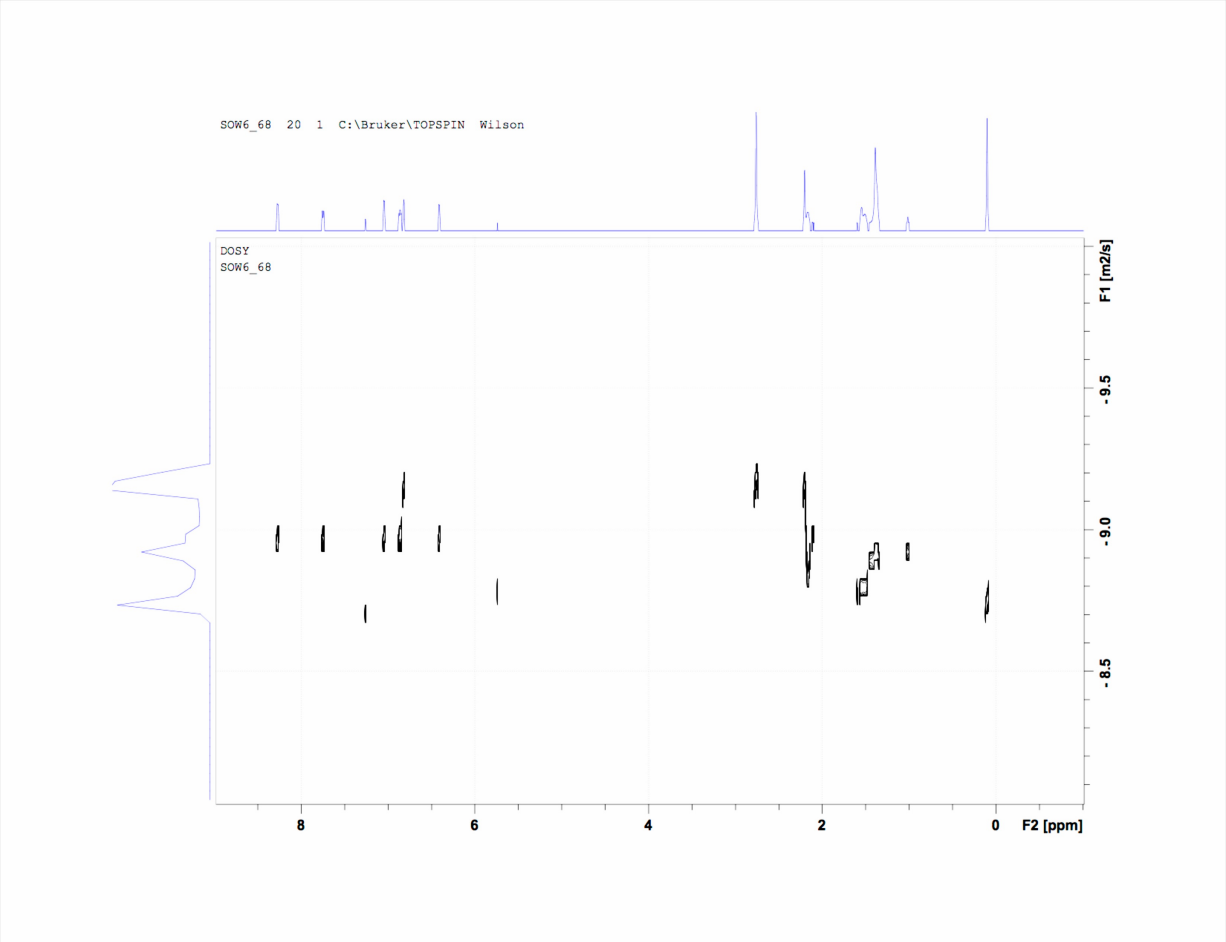


Figure S11. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (100 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards.

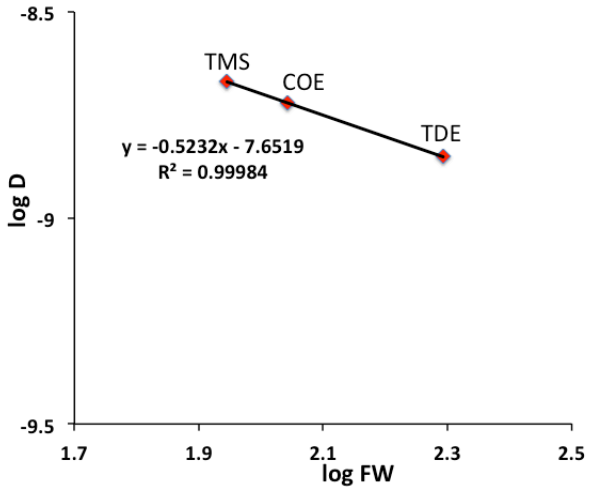


Figure S12. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) and 7-azaindole (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S4: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 100mM with 7-Azaindole

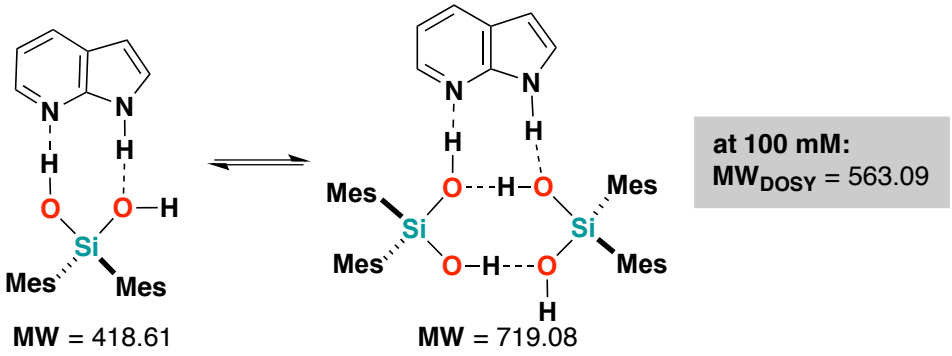


Table S4. Diffusion constants and estimated formula weight of $Mes_2Si(OH)_2$ species observed in ^1H NMR spectra (100 mM $Mes_2Si(OH)_2$ and 500 mM 7-azaindole) correlate to a higher order hydrogen-bonded species in equilibrium.

Molecule	**D (m^2/s)**	**log D**	**FW (g/mol)**	**log FW**
COE	1.90E-09	-8.722	110.20	2.042
TDE	1.41E-09	-8.851	196.37	2.293
TMS	2.14E-09	-8.669	88.22	1.946
$Mes_2Si(OH)_2$	8.11E-10	-9.091	563.09	2.751

$Mes_2Si(OH)_2$ DOSY Studies with 4,4'-bipyridine

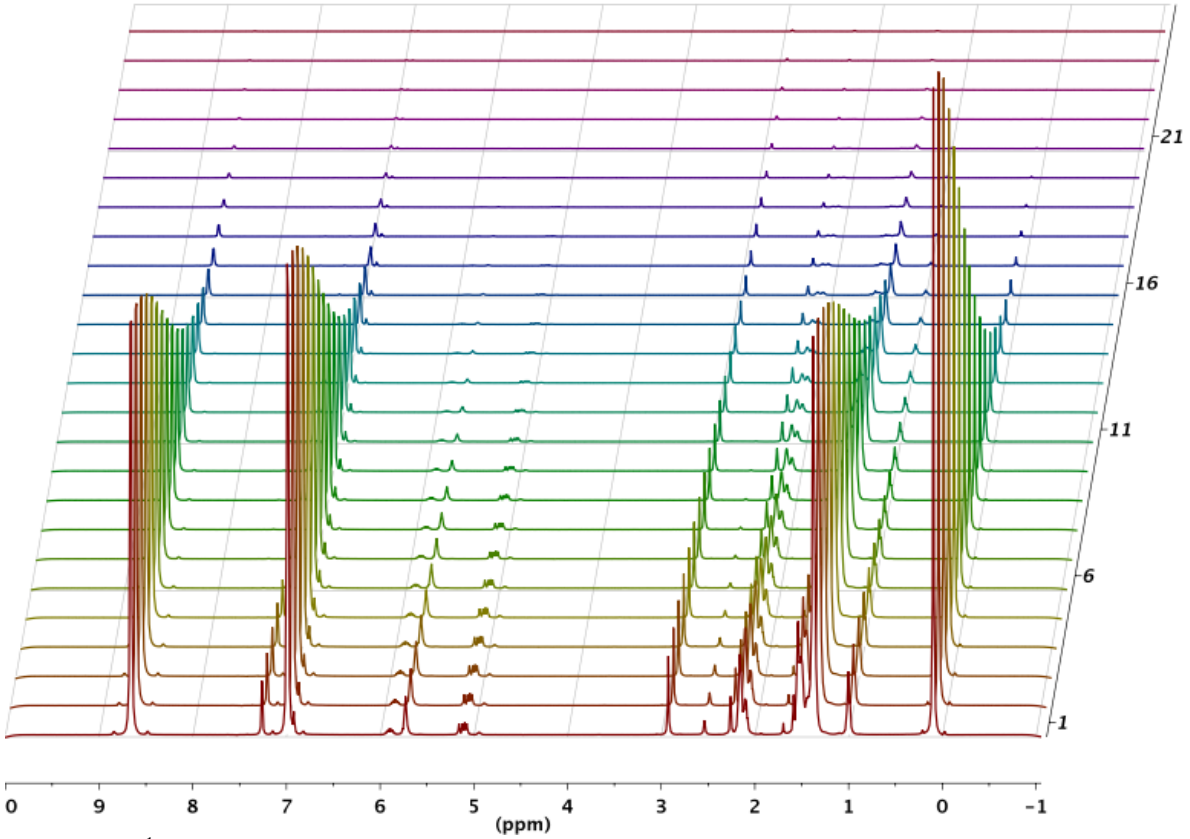


Figure S13. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) and 4,4'-bipyridine (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

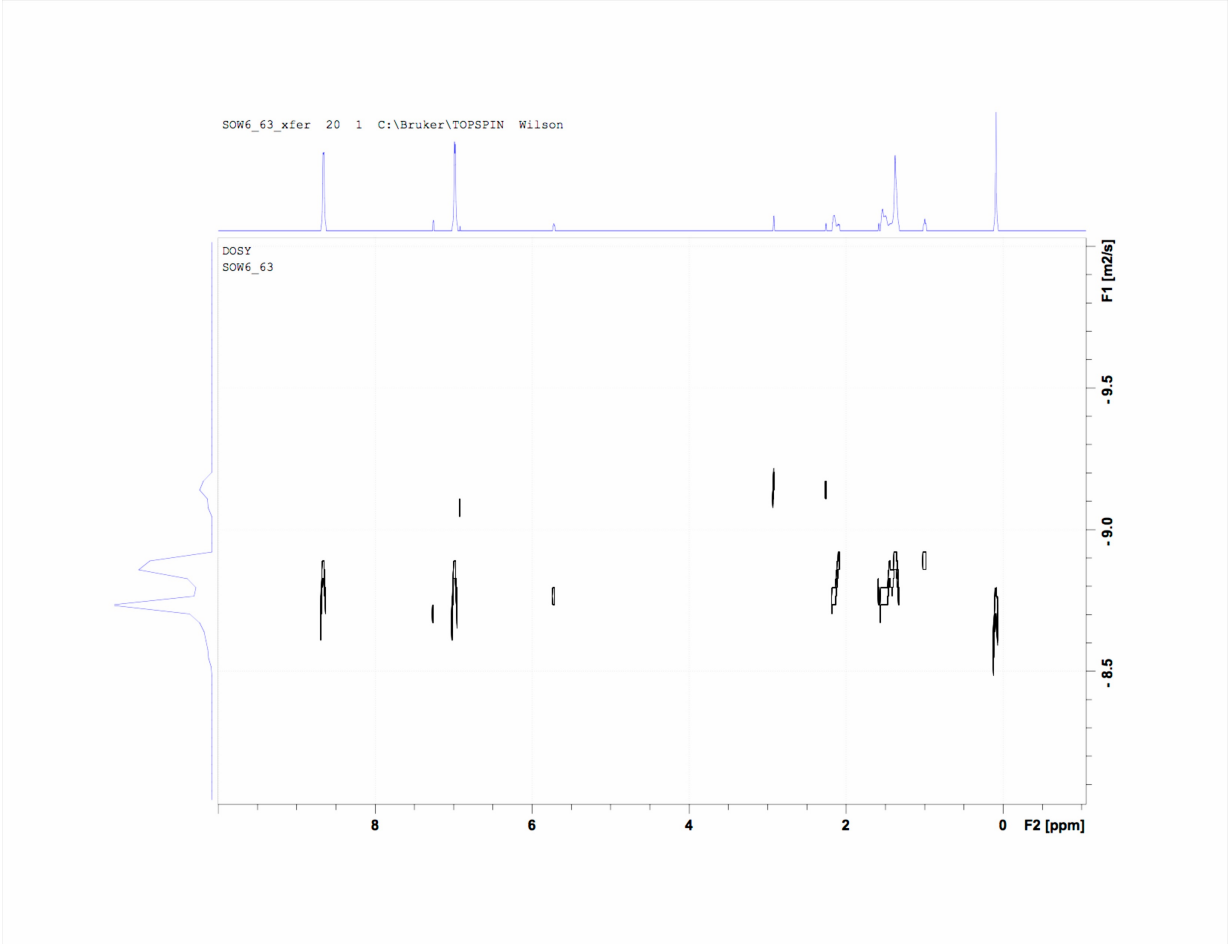


Figure S14. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (10 mM) and 4,4-bipyridine (500 mM) in C_6D_6 with internal standards.

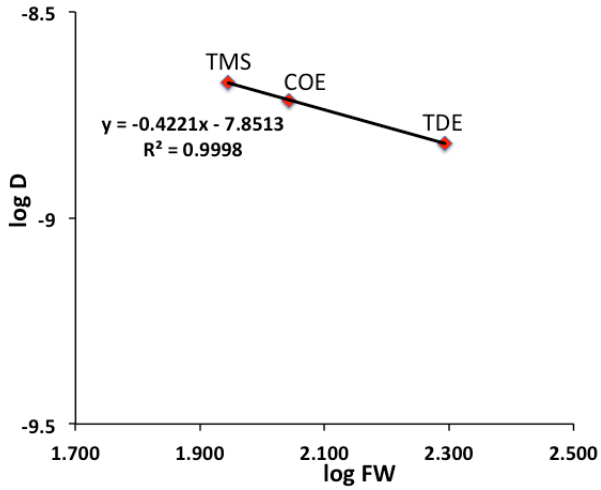


Figure S15. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (10 mM) and 4,4-bipyridine (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S5: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 10mM with 4,4'-Bipyridine

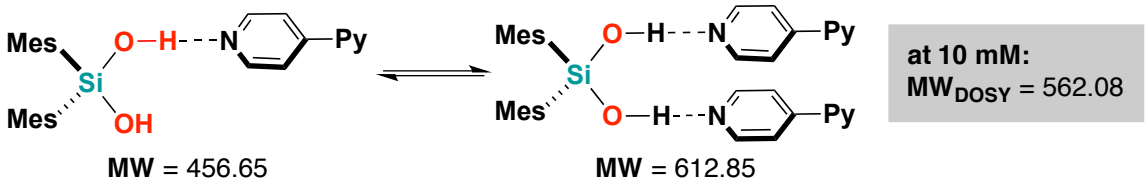


Table S5. Diffusion constants and estimated formula weight of species observed in ^{1}H NMR spectra with 10 mM of $Mes_2Si(OH)_2$ and 50 equivalents of 4,4'-bipyridine correlate to a species in equilibrium between a 1:1 complex and a 1:2 silanediol/bipyridine complex.

Molecule	D (m^2/s)	log D	FW (g/mol)	log FW
COE	1.93E-09	-8.714	110.20	2.042
TDE	1.52E-09	-8.819	196.37	2.293
TMS	2.13E-09	-8.672	88.22	1.946
$Mes_2Si(OH)_2$	9.73E-10	-9.012	562.08	2.750

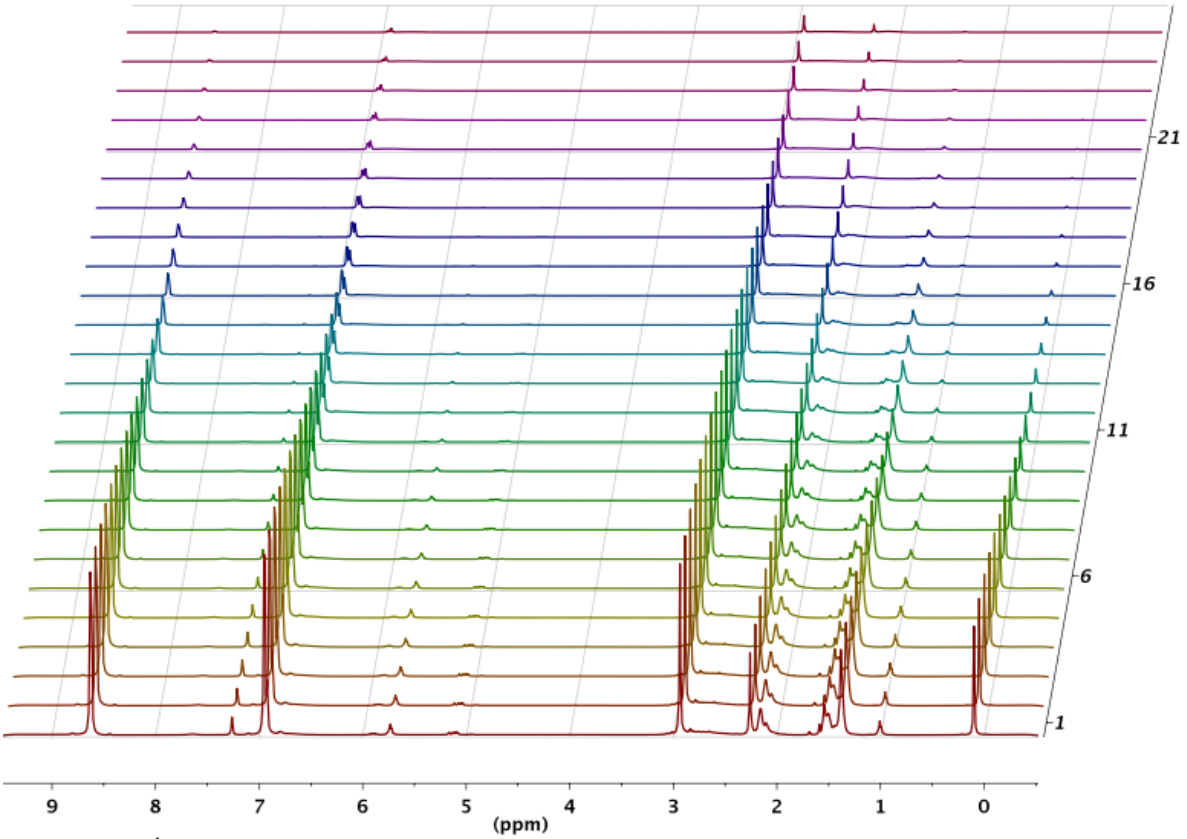


Figure S16. ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) and 4,4'-bipyridine (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

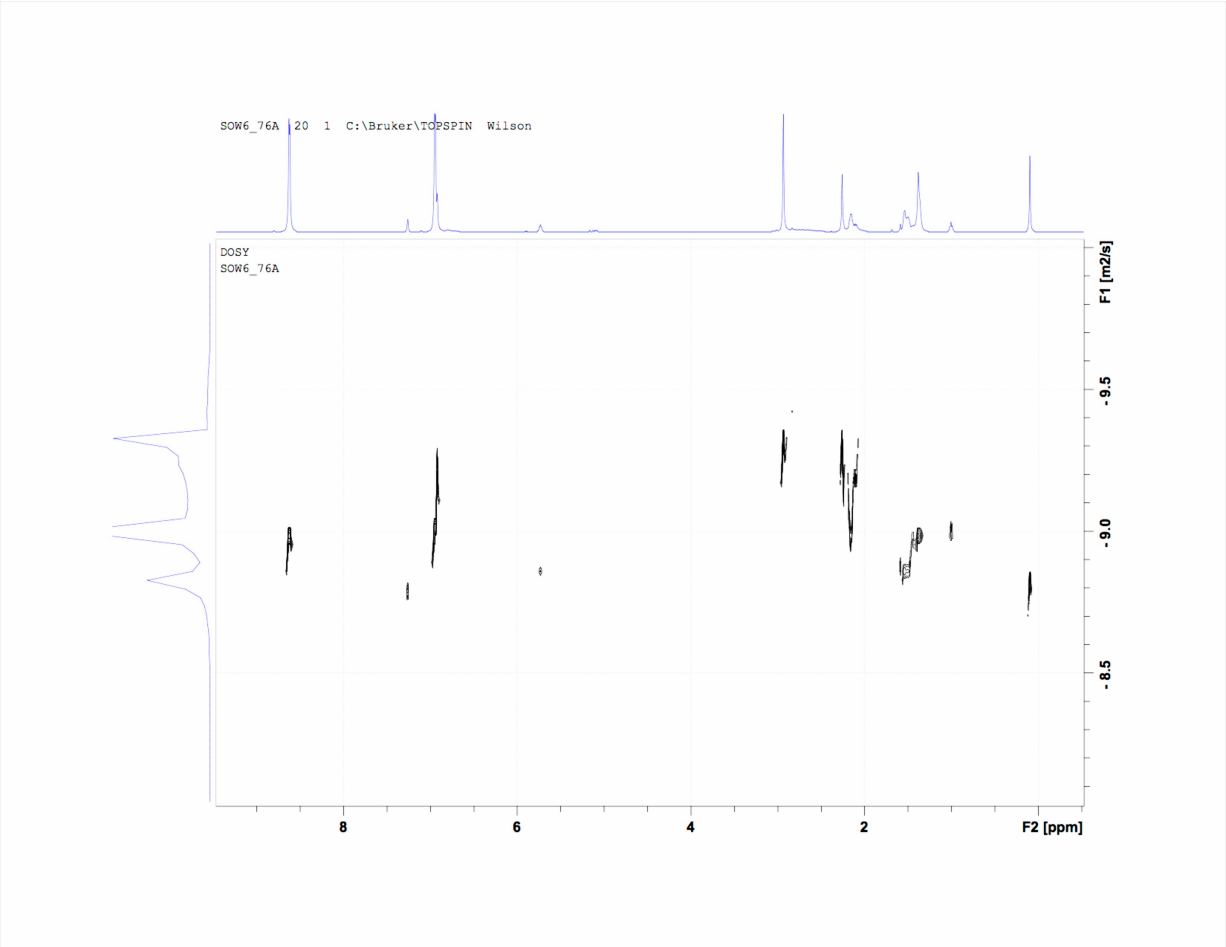


Figure S17. ^{1}H DOSY spectrum of $Mes_2Si(OH)_2$ (100 mM) and 4,4'-bipyridine (500 mM) in C_6D_6 with internal standards.

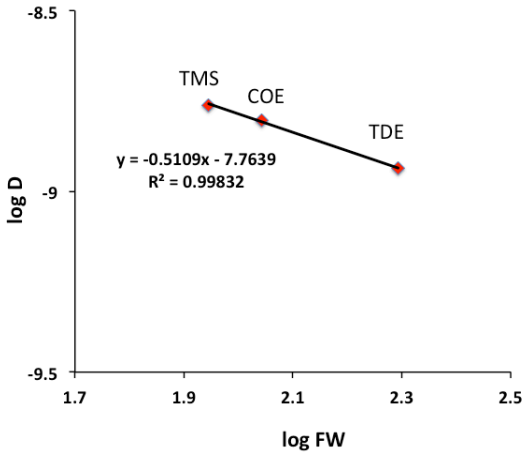


Figure S18. Standard curve for ^{1}H DOSY experiment with $Mes_2Si(OH)_2$ (100 mM) and 4,4'-bipyridine (500 mM) in C_6D_6 with internal standards (TMS, COE, TDE).

Scheme S6: Proposed Equilibrium for $Mes_2Si(OH)_2$ at 100mM with 4,4'-Bipyridine

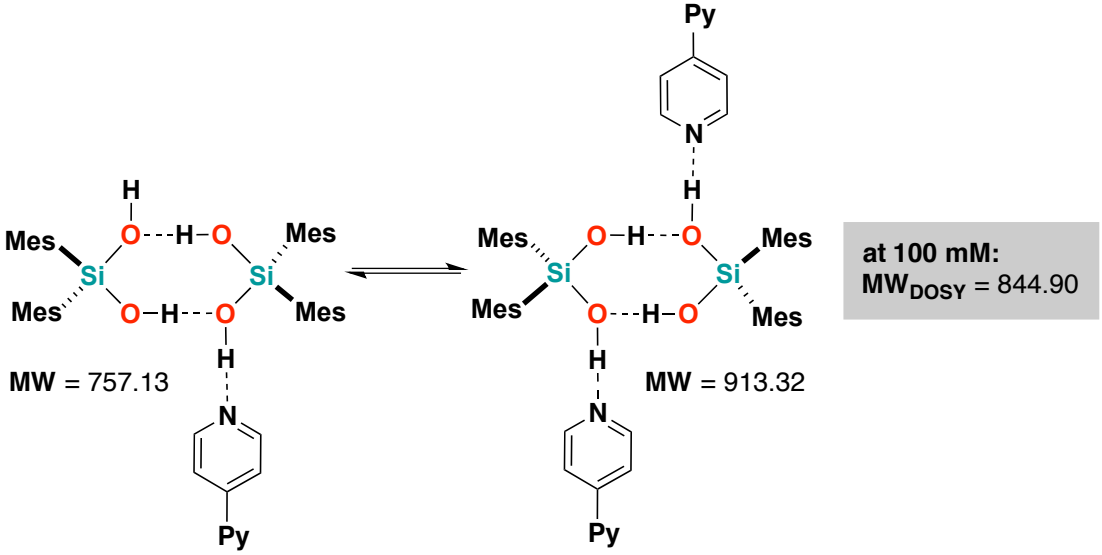


Table S6. Diffusion constants and estimated formula weight of $Mes_2Si(OH)_2$ species observed in ^1H NMR spectra (100 mM $Mes_2Si(OH)_2$ and 500 mM 4,4'-bipyridine) correlate to a higher order hydrogen-bonded species in equilibrium.

Molecule	**D (m^2/s)**	**log D**	**FW (g/mol)**	**log FW**
COE	1.57E-09	-8.803	110.20	2.042
TDE	1.16E-09	-8.937	196.37	2.293
TMS	1.73E-09	-8.761	88.22	1.946
$Mes_2Si(OH)_2$	5.51E-10	-9.259	844.90	2.927

III. NMR Binding Studies

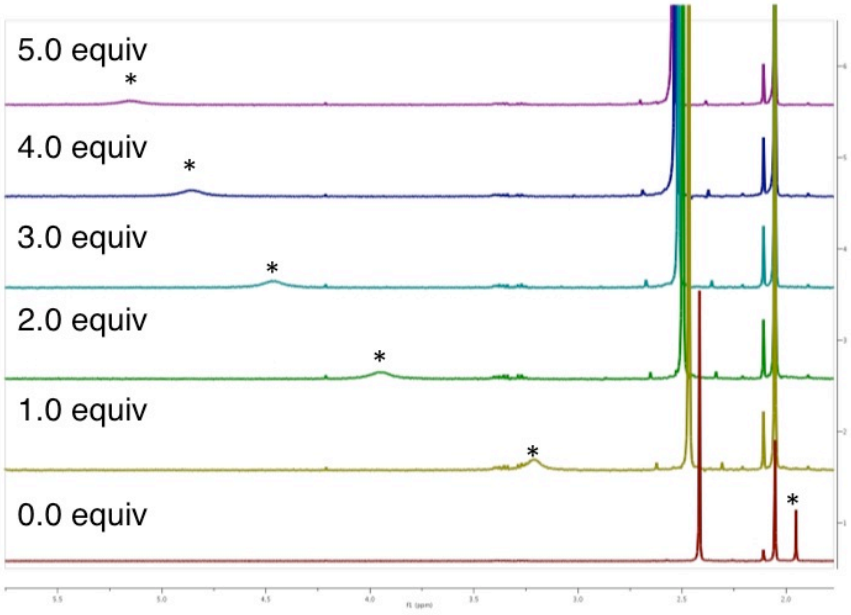


Figure S19. Spectra for $Mes_2Si(OH)_2$ as a 10 mM solution in C_6D_6 with 0-5 equivalents of 7-azaindole. A shift of 3.21 ppm is observed for the SiOH hydroxy protons (indicated with *) when 5.0 equivalents of 7-azaindole are added.

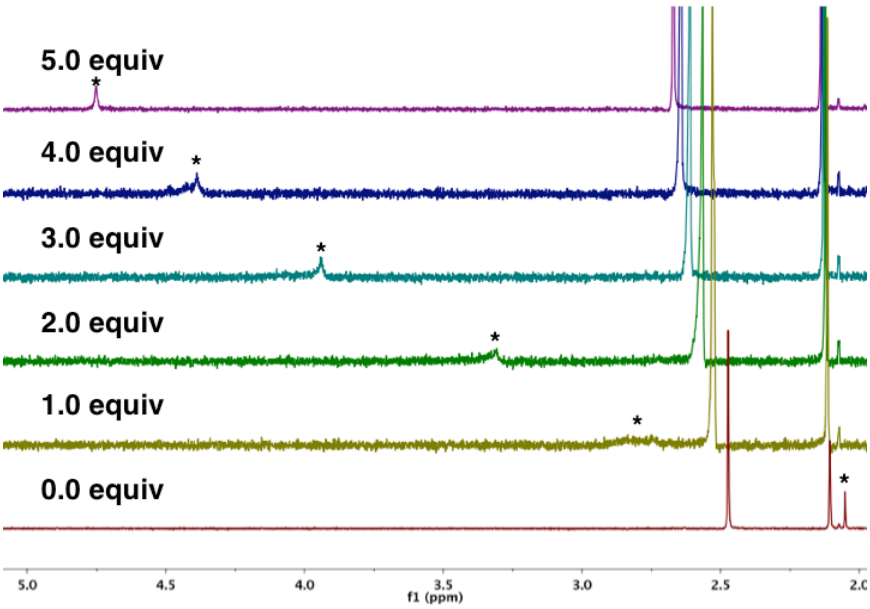


Figure S20. Spectra for $Mes_2Si(OH)_2$ as a 10 mM solution in C_6D_6 with 0-5 equivalents of 4,4'-bipyridine. A shift of 2.70 ppm is observed for the SiOH hydroxy protons (indicated with *) when 5.0 equivalents of 4,4'-bipyridine are added.

III. Crystallography Data

Crystal Growth, Structure Collection and Determination. Crystals were grown from slow evaporation of dimesitylsilanediol with one equivalent of Lewis base in the following solutions: dichloromethane for 4,4'-bipyridine, 1:1 benzene/dichoromethane for phenazine, benzene for 1,4-dimethoxybenzene, and 6:1 benzene/dichoromethane for 7-azaindole. Suitable crystals were mounted on glass fibers with silicone grease and placed in the cold N_2 stream of a Bruker SMART Apex II diffractometer with graphite-monochromated Mo *K*α radiation ($\lambda = 0.71073$ Å) at 90(2) K.[5] Reflections were integrated and corrected for Lorentz and polarization effects, and absorption was corrected by using Blessing's method[6] with the program SADABS.[7] Structures were solved by direct methods and refined using all data (based on F^2) and the software SHELXTL 6.1.[8,9,10] All non-hydrogen atoms were refined anisotropically. In general, as many hydrogen atoms were located on a difference map as possible and then the missing hydrogen atoms were added geometrically. The position and thermal parameters of hydrogen atoms were allowed to refine freely. Full crystallographic data for all crystals can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. For each crystal, a CCDC number and a shortened description of crystal data and structure refinement are provided below.

A. Dimesitylsilanediol with 4,4'-Bipyridine

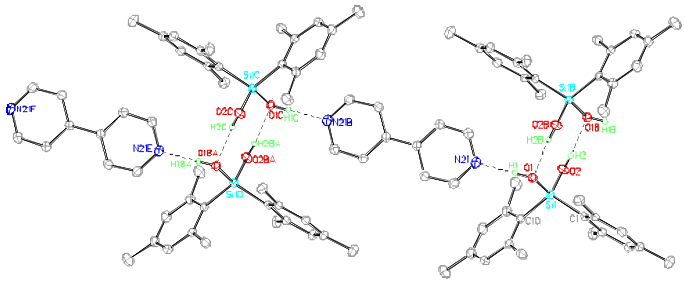


Figure S21. Asymmetric unit repeated multiple times to show linking between two cyclic dimers by 4,4'-bipyridine. Dichloromethane molecules, which are not involved in hydrogen bonding, are omitted for charity. The thermal displacement plot shows 50% probability displacement ellipsoids for non-hydrogens. Selected hydrogens are omitted for clarity. CCDC 958825.

[5] Bruker (2002). SMART (Version 5.054) and SAINT (Version 7.23a). Bruker AXS Inc., Madison, Wisconsin, USA.
[6] Blessing, R. H. *Acta Cryst*. **1995**. *A51*, 33.
[7] Sheldrick, G.M., *SADABS*, Version 2.10; Universitat Gottingen: Gottingen, Germany, 2003.
[8] Sheldrick, G. M. *Acta Cryst*. **2008**. *A64*, 112.
[9] Sheldrick, G. M., **1997**. *SHELXS97* and *SHELXL97*. Universitat Gottingen: Gottingen, Germany.
[10] Sheldrick, G.M., **2002**. *SHELXTL 6.1*. Bruker AXS Inc., Madison, Wisconsin, USA.

Table S7. Crystal data and structure refinement for dimesitylsilanediol with 4,4'-bipyridine solvate.

Identification code	NT110	
Empirical formula	C24 H30 Cl2 N O2 Si	
Formula weight	463.48	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.4628(15) Å	α = 99.002(18)°.
	b = 12.198(3) Å	β = 98.19(2)°.
	c = 12.589(2) Å	γ = 108.44(2)°.
Volume	1191.9(4) $Å^3$	
Z	2	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.343 mm^{-1}	
F(000)	490	
Crystal size	0.59 x 0.44 x 0.37 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Bruker SMART 1000	
Theta range for data collection	3.17 to 27.57°.	
Index ranges	-10<=h<=10, -15<=k<=13, -16<=l<=15	
Reflections collected	8841	
Independent reflections	5204 [R(int) = 0.0141]	
Observed reflections (I > 2sigma(I))	4543	
Completeness to theta = 27.57°	94.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8832 and 0.8237	
Solution method	SHELXS-97 (Sheldrick, 2008)	
Refinement method	SHELXL-97 (Sheldrick, 2008)	
Data / restraints / parameters	5204 / 0 / 391	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0333, wR2 = 0.0895	
R indices (all data)	R1 = 0.0394, wR2 = 0.0937	
Largest diff. peak and hole	0.399 and -0.208 $e.Å^{-3}$	

Table S8. Hydrogen bonds for $Mes_2Si(OH)_2$•4,4'-bipyridine [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#2	0.75(2)	2.00(2)	2.7476(16)	174(2)
O(1)-H(1)...N(21)	0.83(2)	1.88(2)	2.7138(18)	178(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+2 #2 -x+1,-y+1,-z+1

B. Dimesitylsilanediol with Phenazine

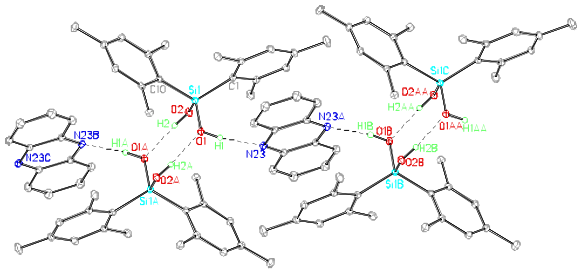


Figure S22. Asymmetric unit repeated multiple times to show linking between two cyclic dimers by phenazine. The thermal displacement plot shows 30% probability displacement ellipsoids for non-hydrogens. Selected hydrogens are omitted for clarity. CCDC 958790.

Table S9. Crystal data and structure refinement for dimesitylsilanediol with phenazine solvate.

Identification code	NT114	
Empirical formula	C24 H28 N O2 Si	
Formula weight	390.56	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.7044(6) Å	α = 90°.
	b = 11.1778(6) Å	β = 107.2130(10)°.
	c = 16.8654(9) Å	γ = 90°.
Volume	2107.66(19) $Å^3$	
Z	4	
Density (calculated)	1.231 Mg/m^3	
Absorption coefficient	0.131 mm^{-1}	
F(000)	836	
Crystal size	0.51 x 0.42 x 0.36 mm^3	
Crystal color and habit	yellow block	
Diffractometer	Bruker SMART APEXII CCD	
Theta range for data collection	2.58 to 27.49°.	
Index ranges	-15<=h<=15, -14<=k<=14, -21<=l<=21	
Reflections collected	23090	
Independent reflections	4821 [R(int) = 0.0156]	
Observed reflections (I > 2sigma(I))	4515	
Completeness to theta = 27.49°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9545 and 0.9364	
Solution method	SHELXS-97 (Sheldrick, 2008)	
Refinement method	SHELXL-97 (Sheldrick, 2008)	
Data / restraints / parameters	4821 / 0 / 365	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0873	
R indices (all data)	R1 = 0.0337, wR2 = 0.0890	
Largest diff. peak and hole	0.404 and -0.289 $e.Å^{-3}$	

Table S10. Hydrogen bonds for $Mes_2Si(OH)_2$• phenazine [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#2	0.828(19)	1.920(19)	2.7446(11)	173.7(18)
O(1)-H(1)...N(23)	0.855(19)	1.946(19)	2.7932(12)	170.8(16)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2 #2 -x+1,-y+1,-z+2

C. Dimesitylsilanediol with 1,4-Dimethoxybenzene

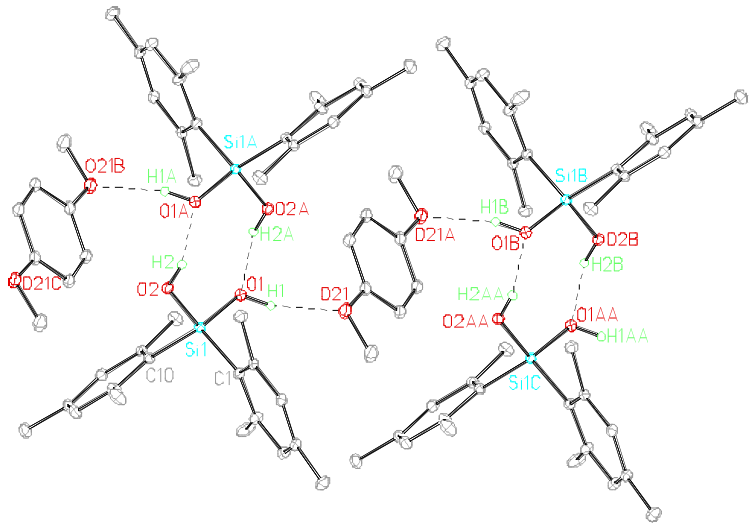


Figure S23. Asymmetric unit repeated multiple times to show linking between two cyclic dimers by 1,4-dimethoxybenzene. The thermal displacement plot shows 30% probability displacement ellipsoids for non-hydrogens. Selected hydrogens are omitted for clarity. CCDC 958824.

Table S11. Crystal data and structure refinement for dimesitylsilanediol with 1,4-dimethoxybenzene.

Identification code	NT116	
Empirical formula	C22 H29 O3 Si	
Formula weight	369.54	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.4092(2) Å	α = 99.15°.
	b = 9.0220(2) Å	β = 97.10°.
	c = 13.4486(3) Å	γ = 93.79°.
Volume	995.76(4) $Å^3$	
Z	2	
Density (calculated)	1.233 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	398	
Crystal size	0.38 x 0.38 x 0.36 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Bruker SMART APEXII CCD	
Theta range for data collection	2.45 to 33.27°.	
Index ranges	-12<=h<=12, -13<=k<=13, -20<=l<=20	
Reflections collected	15470	

Table S11 (continued)

Independent reflections	7069 [R(int) = 0.0157]
Observed reflections (I > 2sigma(I))	6024
Completeness to theta = 33.27°	95.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9530 and 0.9504
Solution method	SHELXS-97 (Sheldrick, 2008)
Refinement method	SHELXL-97 (Sheldrick, 2008)
Data / restraints / parameters	7069 / 0 / 351
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0978
R indices (all data)	R1 = 0.0436, wR2 = 0.1032
Largest diff. peak and hole	0.457 and -0.231 $e.Å^{-3}$

Table S12. Hydrogen bonds for $Mes_2Si(OH)_2$•1,4-dimethoxybenzene [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#2	0.874(18)	1.961(18)	2.8087(9)	163.1(17)
O(1)-H(1)...O(21)	0.857(17)	2.004(17)	2.8399(9)	164.9(15)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x,-y+1,-z

D. Dimesitylsilanediol with 7-Azaindole

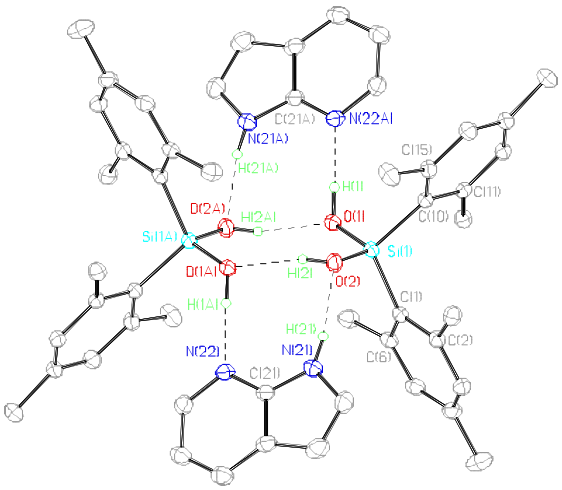


Figure S24. Asymmetric unit repeated once to show cyclic dimer cluster supramolecular motif and intermolecular hydrogen bonding with 7-azaindole. The thermal displacement plot shows 50% probability displacement ellipsoids for non-hydrogens. Selected hydrogens are omitted for clarity. CCDC 958784.

Table S13. Crystal data and structure refinement for dimesitylsilanediol with 7-azaindole.

Identification code	NT67	
Empirical formula	C25 H30 N2 O2 Si	
Formula weight	418.60	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.9457(10) Å	α = 90°.
	b = 11.0271(10) Å	β = 97.9210(10)°.
	c = 17.2592(15) Å	γ = 90°.
Volume	2251.8(3) $Å^3$	
Z	4	
Density (calculated)	1.235 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	896	
Crystal size	0.47 x 0.26 x 0.22 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Bruker SMART 1000	
Theta range for data collection	1.72 to 27.51°.	
Index ranges	-15<=h<=15, -14<=k<=14, -22<=l<=22	
Reflections collected	23897	
Independent reflections	5185 [R(int) = 0.0299]	
Observed reflections (I > 2sigma(I))	4384	
Completeness to theta = 27.51°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9729 and 0.9424	
Solution method	SHELXS-97 (Sheldrick, 2008)	
Refinement method	SHELXL-97 (Sheldrick, 2008)	
Data / restraints / parameters	5185 / 0 / 391	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.1046	
R indices (all data)	R1 = 0.0484, wR2 = 0.1121	
Largest diff. peak and hole	0.601 and -0.300 $e.Å^{-3}$	

Table S14. Hydrogen bonds for $Mes_2Si(OH)_2$•7-azaindole [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(22)#1	0.90(3)	1.79(3)	2.6769(15)	171(3)
O(2)-H(2)...O(1)#1	0.82(2)	1.91(2)	2.7049(14)	166(2)
N(21)-H(21)...O(2)	0.90(2)	2.02(2)	2.9161(16)	172(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z