The Assembly of Amphiphilic Baskets into Stimuli-Responsive Vesicles. Developing a Strategy for the Detection of Organophosphorus Chemical Nerve Agents

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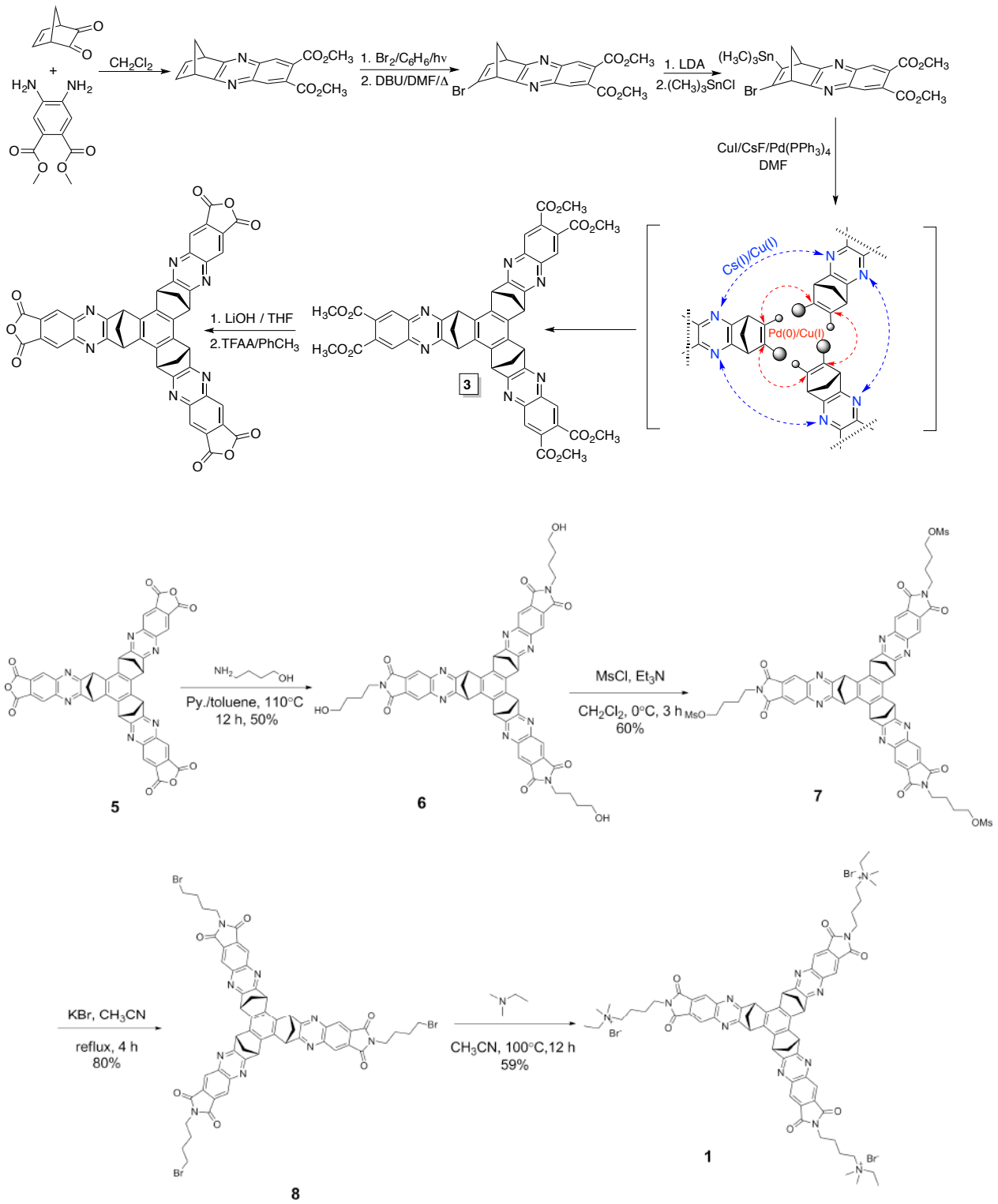
Supporting Information

General methods. All solvents were dried before use following standard procedures. Unless indicated otherwise, all starting materials were obtained from commercial suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on silica-gel plates w/UV254 (200 μm). The ^{1}H NMR spectra were recorded on 500 or 400 MHz spectrophotometers in the indicated solvents. Chemical shifts are expressed in parts per million (δ) using residual solvent protons as internal standard (chloroform: δ 7.26 ppm; MeOD: δ 2.50 ppm; CD_3CN δ 1.94 ppm). Coupling constants values (J) are in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; m, multiplet; and br, broad. The ^{13}C NMR spectra were recorded on a 125 MHz spectrometer in the indicated solvents. Chemical shifts are expressed in parts per million using solvents as internal standards. HRMS (ESI) were measured on a Micromass Q-TOF II spectrometer. Transmission electron microscopy (TEM) images were recorded on FEI Tecnai G2 Spirit TEM microscope working at 80 kV. Dynamic light scattering (DLS) measurements were performed on a Zetasizer NanoZS instrument (ZEN3600).



Scheme S1. Synthesis of basket 1; synthetic details pertaining the preparation of *tris*-anhydride **5** (top scheme) via template-directed protocol are given in Badjic et al. *Org. & Biom. Chem.* **2013** (DOI: 10.1039/C3OB41511B).

Synthesis

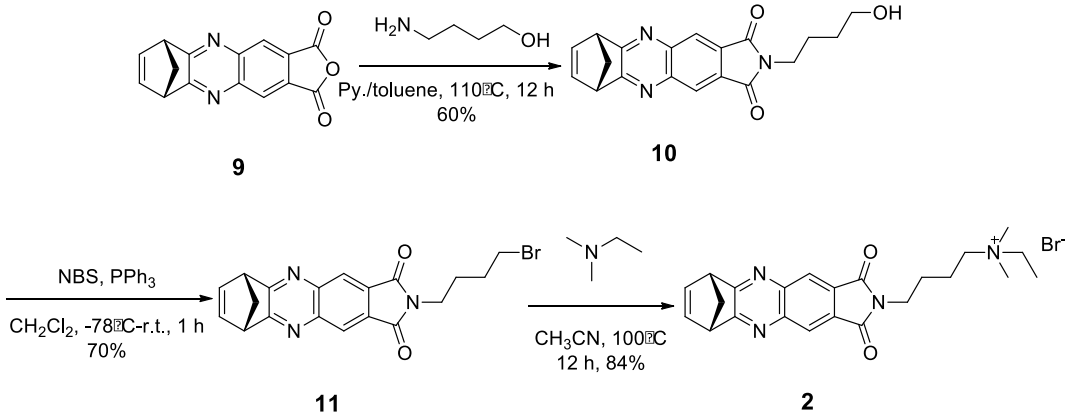
Compound 6: To a suspension of *tris*-anhydride **5** (20 mg, 0.025 mmol) in toluene:pyridine = 4:1 (4.00 mL) was added 4-aminobutan-1-ol (6.8 mg, 0.078 mmol). The mixture was heated to 110 °C for 12 h. Then the mixture was concentrated under reduced pressure and the resulting slurry triturated in dichloromethane (100 mL). The organic phase was washed with aqueous HCl (1.0 M, 30 mL), water (2 × 30 mL) and brine (30 mL), and then dried over sodium sulfate. Upon removal of the solvent, the resulting residue was purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:25) to give compound **6** as a white solid (13 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ (ppm) = 8.25 (s, 6H), 4.78 (s, 6H), 3.74 (t, J = 7.0 Hz, 6H), 3.61 (t, J = 6.4 Hz, 6H), 3.06 (d, J = 9.5 Hz, 3H), 2.96 (d, J = 9.5 Hz, 3H), 1.81 – 1.68 (m, 6H), 1.54 (d, J = 8.5 Hz, 6H). ^{13}C NMR (125 MHz, CD_3OD, 298 K): δ (ppm) = 167.58, 166.33, 143.36, 139.22, 131.10, 125.09, 61.65, 61.48, 49.60, 38.55, 29.94, 25.21. HRMS (ESI): *m/z* Calcd for $C_{57}H_{45}N_9NaO_9$: 1022.3232 $[M+Na]^+$, found: 1022.3185.

Compound 7: To a solution of compound **6** (22 mg, 0.022 mmol) in dry CH_2Cl_2 (2 mL) and at 0 °C was added triethylamine (67 mg, 0.176mmol) followed by CH_3SO_2Cl (15 mg, 0.132 mmol). The mixture was stirred for 2 hours and then water (5 mL) was added to quench the reaction. After the addition of CH_2Cl_2 (50 mL), the organic phase was washed with water (2 × 200 mL) brine (200 mL), and then dried over sodium sulfate. Upon removal of the solvent, the solid residue was purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:100) to give compound **7** as a white solid (16 mg, 60%).^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ (ppm) = 8.22 (s, 6H), 4.76 (s, 6H), 4.18 (t, J = 5.9 Hz, 6H), 3.70 (t, J = 6.6 Hz, 6H), 3.07 (d, J = 9.5 Hz, 3H), 2.97 (s, 9H), 2.94 (d, J = 9.5 Hz, 3H), 1.82–1.69 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm) = 167.10, 165.65, 143.23, 138.86, 130.74, 125.17, 69.18, 49.41, 37.64, 37.43, 29.83, 26.43, 24.60. HRMS (ESI): *m/z* Calcd for $C_{60}H_{51}N_9NaO_{15}S_3$: 1256.2559 $[M+Na]^+$, found: 1256.2545.

Compound 8: To a solution of compound **7** (20 mg, 0.016 mmol) in dry acetonitrile (2 mL) was added KBr (130 mg, 1.1 mmol). The mixture was refluxed for 4 hours, followed by the removal of the solvent under reduced pressure and trituration of the resulting slurry in CH_2Cl_2 (100 mL). The organic phase was washed with water (2 × 30 mL) and brine (30 mL), and dried over sodium sulfate. Upon removal of the solvent, the resulting residue was purified by column chromatography (SiO_2, CH_3OH/CH_2Cl_2 = 1:80) to give compound **8** as a white solid (15 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ (ppm) = 8.23 (s, 6H), 4.76 (s, 6H), 3.70 (t, J = 6.6 Hz, 6H), 3.38 (t, J = 6.2 Hz, 6H), 3.04 (d, J = 9.5 Hz, 3H), 2.93 (d, J = 9.5 Hz, 3H), 1.87–1.73 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm) = 167.03, 165.64, 143.21, 138.85, 130.79, 125.16, 61.26, 49.41, 37.52, 32.83, 29.89, 27.17. HRMS (ESI): *m/z* Calcd for $C_{57}H_{42}Br_3N_9NaO_6$: 1208.0700 $[M+Na]^+$, found: 1256.0702.

Compound 1: To a solution of compound **8** (14 mg, 0.012 mmol) in dry acetonitrile (2 mL) was added *N*,*N*-dimethylethanamine (73 mg, 1.0 mmol). The mixture was refluxed for 12 hours, and then concentrated under a reduced pressure. The solid residue was recrystallized from CH_3OH:$CH_3COOCH_2CH_3$ = 1:10 to give compound **1** (10 mg, 59%). ^{1}H NMR (400 MHz, CD_3CN:$CDCl_3$ = 4:1, 298 K): δ (ppm) = 8.15 (s, 6H), 4.76 (s, 6H), 3.64 (t, J = 6.3 Hz, 6H),

3.31-3.29 (m, 12H), 2.99-2.96 (m, 24H), 1.66 (br, 12H), 1.25 (t, J = 6.0 Hz,, 9H). ^{13}C NMR (125 MHz, CD_3CN:$CDCl_3$ = 4:1, 300 K): δ (ppm) = 167.99, 166.36, 143.85, 139.76, 131.53, 125.31, 62.86, 60.57, 59.74, 50.84, 49.98, 37.19, 24.86, 20.50, 8.51. HRMS (ESI): *m/z* Calcd for $C_{69}H_{75}N_{12}O_6$: 389.1978, $[M-3Br]^{3+}$, found: 389.1981.



Scheme S2 Synthesis of **Model 2**

Compound 10: To a suspension of anhydride **9** (40 mg, 0.15 mmol) in toluene:pyridine = 4:1 (4.0 mL) was added 4-aminobutan-1-ol (14 mg, 0.16 mmol). The mixture was heated to 110 °C for 12 hours followed by the removal of the solvent under reduced pressure and trituration of the slurry in CH_2Cl_2 (100 mL). The organic phase was washed with aqueous HCl (1.0 M, 30 mL), water (2 × 30 mL), brine (30 mL) and then dried over sodium sulfate. Upon removal of the solvent, the resulting solid residue was purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:50) to give compound **10** as a white solid (30 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ (ppm) = 8.33 (s, 2H), 6.92 (t, J = 1.8 Hz, 2H), 4.03 (dd, J = 3.6, 1.7 Hz, 2H), 3.81 (t, J = 7.1 Hz, 2H), 3.71 (t, J = 6.4 Hz, 2H), 2.83 (dt, J = 9.0, 1.7 Hz, 1H), 2.64 (d, J = 9.0 Hz, 1H), 1.88 – 1.77 (m, 2H), 1.69 – 1.60 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm) = 169.02, 167.60, 142.22, 142.02, 130.03, 124.89, 60.68, 59.79, 49.81, 37.18, 30.12, 25.93. HRMS (ESI): *m/z* Calcd for $C_{19}H_{17}N_3NaO_3$: 358.1168, $[M+Na]^+$, found: 358.1197.

Compound 11: To a solution of compound **10** (30 mg, 0.09 mmol) and triphenylphosphine (39 mg, 0.15 mmol) in dry CH_2Cl_2 (2 mL) at −78 ºC was added *N*-bromosuccinimide (25 mg, 0.14 mmol). The mixture was warmed to room temperature and stirred for 1 hour followed by solvent removal under reduced pressure and trituration of the slurry in CH_2Cl_2 (100 mL). The organic phase was washed with aqueous $NaHCO_3$ (30 mL), water (2 × 30 mL), brine (30 mL), and then dried over sodium sulfate. Upon removal of the solvent, the resulting residue was purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:100) to give compound **11** as a white solid (25 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ (ppm) = 8.33 (s, 2H), 6.93 (s, 2H), 4.03 (s, 2H), 3.79-3.77 (m, 2H), 3.46-3.45 (m, 2H), 2.84 (d, J = 8.0 Hz, 1H), 2.64 (d, J = 8.0 Hz, 1H), 1.92 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, 300 K): δ (ppm) = 168.66, 166.95, 142.12, 141.43, 139.77, 125.91, 60.32, 50.55, 49.61, 37.17, 32.13, 29.12. HRMS (ESI): *m/z* Calcd for $C_{19}H_{16}BrN_3NaO_2$: 420.0324, $[M+Na]^+$, found: 420.0298.

Compound 2: To a solution of compound **11** (25 mg, 0.006 mmol) in dry CH_3CN (2 mL) was added *N*,*N*-dimethylethanamine (73 mg, 1.0 mmol). The mixture was refluxed for 12 hours followed by solvent removal under a reduced pressure. The residue was recrystallized in CH_3OH:$CH_3COOCH_2CH_3$ = 1:8 to give compound **1** as a gray solid (24 mg, 84%).^{1}H NMR (400 MHz, $CDCl_3$, 300 K): δ (ppm) = 8.32 (s, 2H), 6.93 (s, 2H), 4.09 – 3.98 (m, 2H), 3.82 (t, J = 6.2 Hz, 2H), 3.77 – 3.64 (m, 4H), 3.37 (s, 6H), 2.84 (d, J = 9.0 Hz, 1H), 2.64 (d, J = 9.0 Hz, 1H), 1.87-1.85 (m, 4H), 1.44 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, 300 K): δ (ppm) = 169.45, 167.62, 142.72, 142.51, 130.46, 125.09, 63.05, 62.93, 60.35, 50.73, 49.61, 37.17, 25.60, 20.09, 8.68. HRMS (ESI): *m*/*z* Calcd for $C_{23}H_{27}N_4O_2$: 391.2129, $[M\text{-}Br]^+$, found: 391.2112.

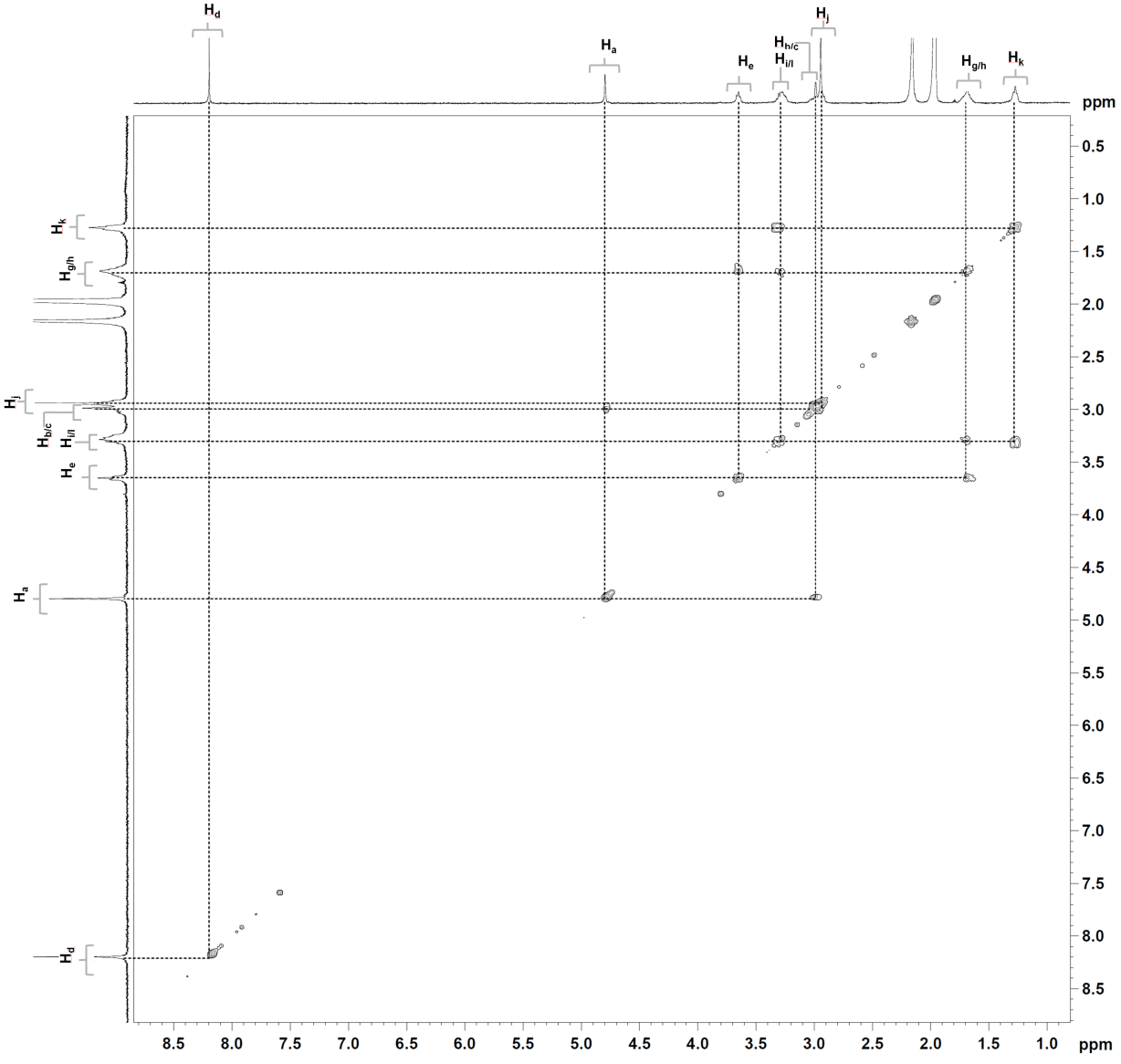


Figure S1. ^{1}H–^{1}H COSY NMR spectrum (500 MHz) of basket **1** (1.0 mM) in CD_3CN at 298.0 K.

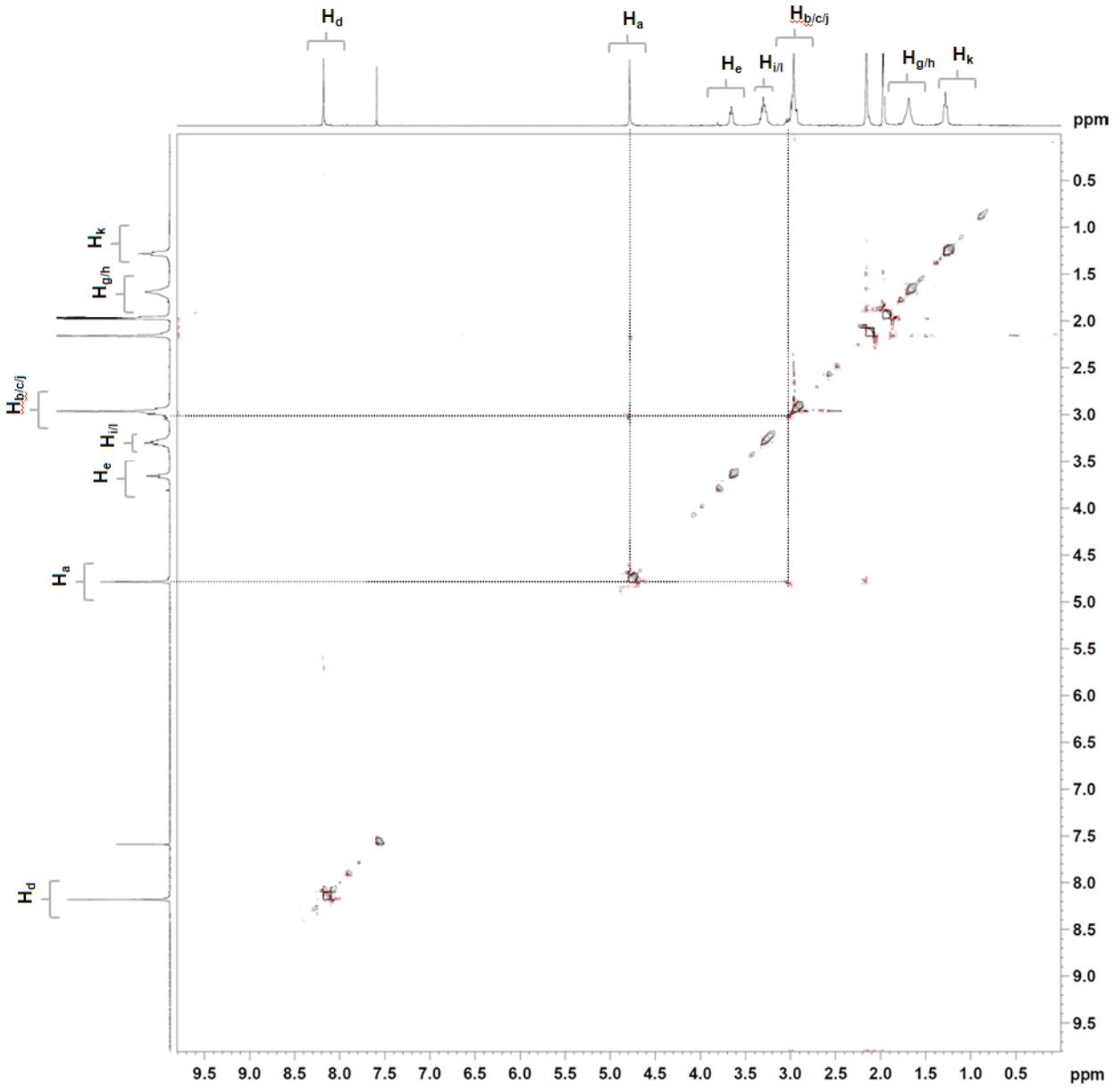


Figure S2. ^{1}H–^{1}H NOESY NMR spectrum (500 MHz) of basket **1** (1.0 mM) in CD_3CN at 298.0 K.

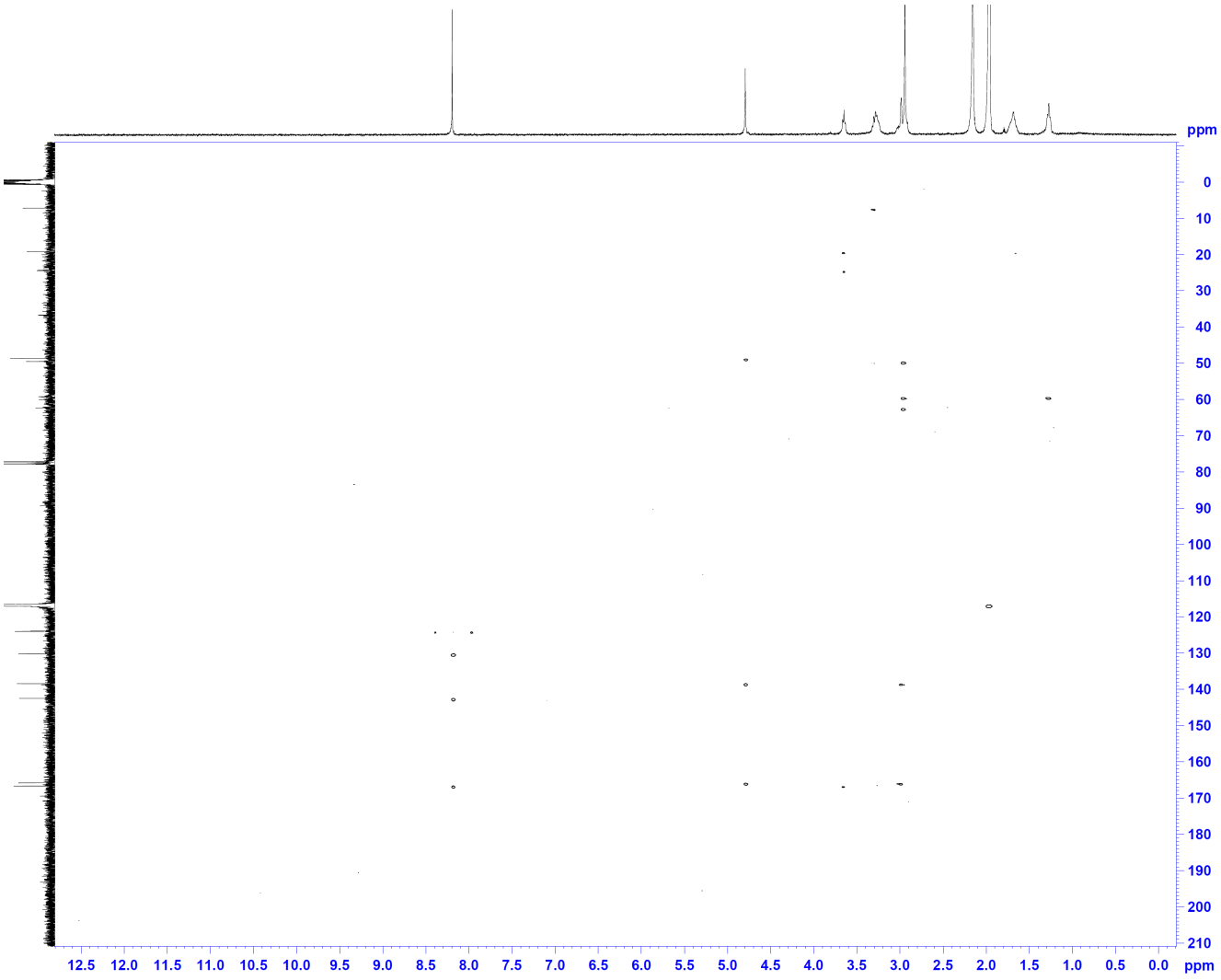


Figure S3. $^{1}H-^{13}C$ HMBC NMR spectrum (500 MHz) of basket **1** (1.0 mM) in CD_3CN at 298.0 K.

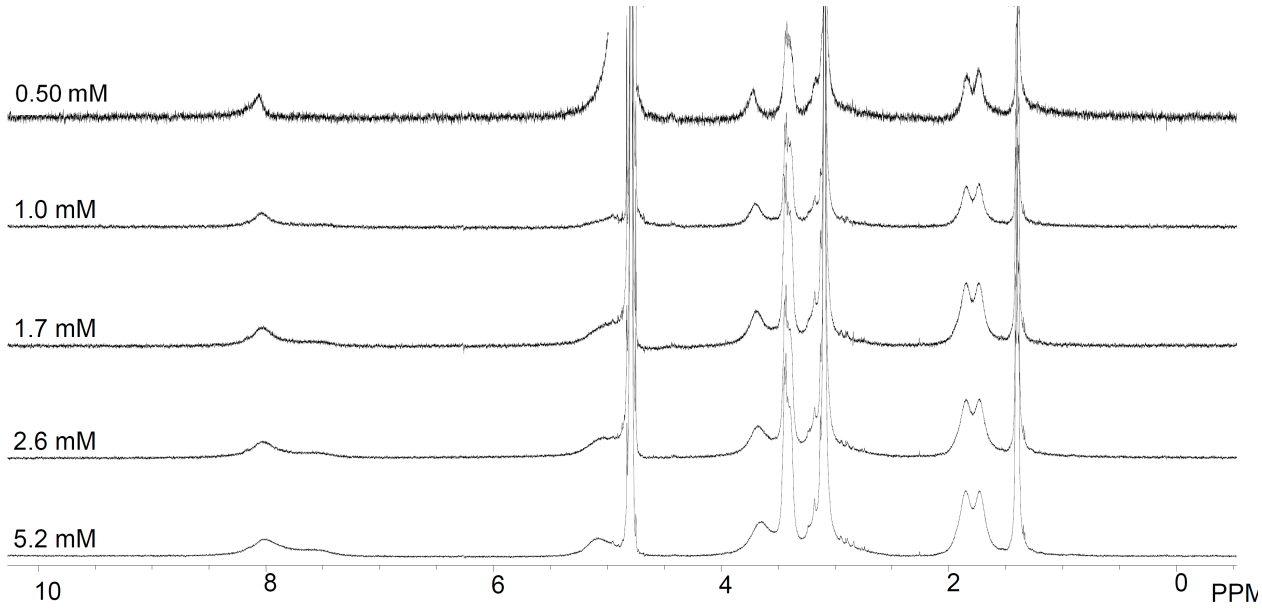


Figure S4. ^{1}H NMR spectra (500 MHz, 298 K) of basket **1** were obtained upon an incremental dilution of its 5.2 mM D_2O solution (from bottom to top).

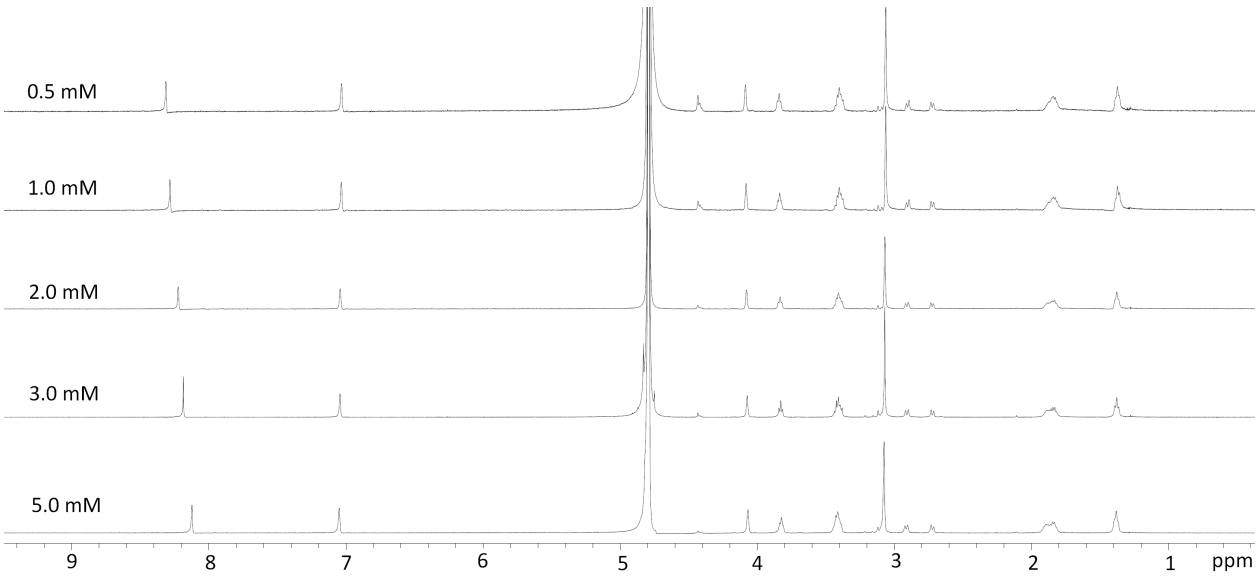


Figure S5. ^{1}H NMR spectra (500 MHz, 298 K) of model compound **2** were obtained upon an incremental dilution of its 5.0 mM D_2O solution (from bottom to top).

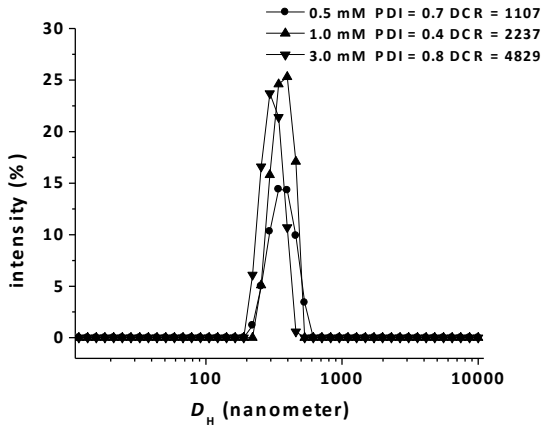
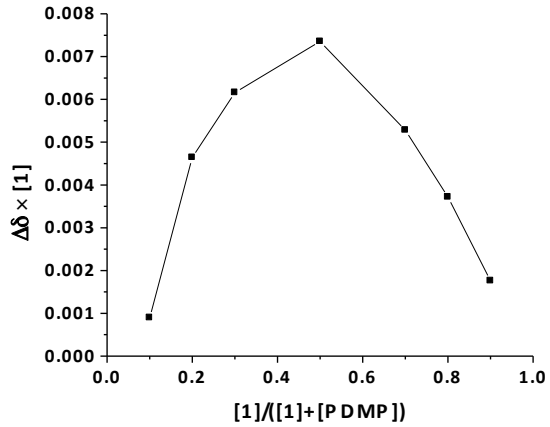


Figure S6. Dynamic light scattering (DLS) measurements of variously concentrated solutions (H_2O, 0.5–3.0 mM) of basket **1** at 298.0 K.



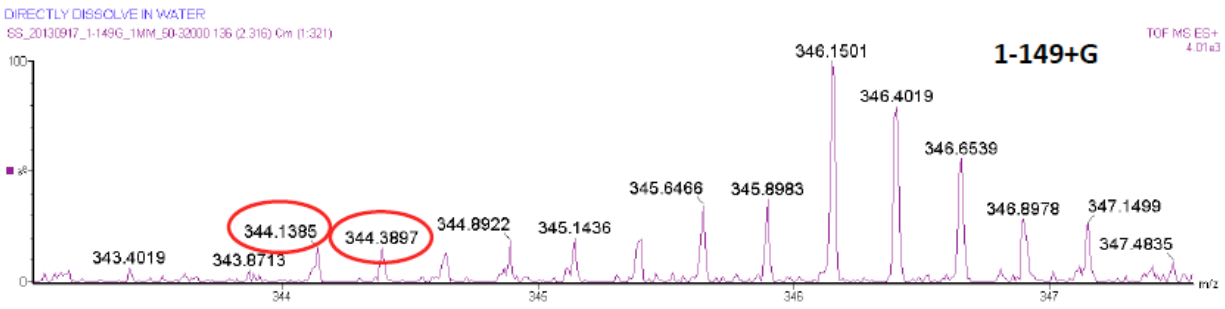


Figure S7. (Top) The Job plot for the interaction of basket **1** and DMPP guest in D_2O was obtained with ^1H NMR spectroscopy at 298 K by measuring the variation in the chemical shift of proton H_j of the host **1**. (Bottom) Low-resolution ESI-MS spectrum of an aqueous solution of **1** and DMPP guest with peaks at m/z = 344 corresponding to [**1**–3Br+Na+DMPP]$^{4+}$ ion.

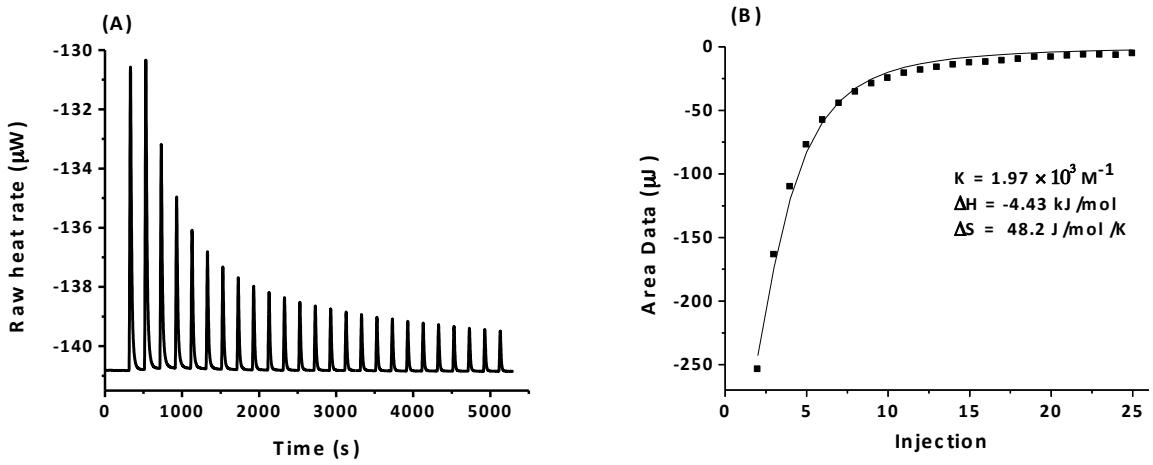


Figure S8. Experimental (A) and integrated (B) ITC data corresponding to the titration of DMPP guest (60.0 mM) to basket **1** (1.0 mM) at 298.0 K. The fitting procedure was completed with the assistance of the single site-binding model.

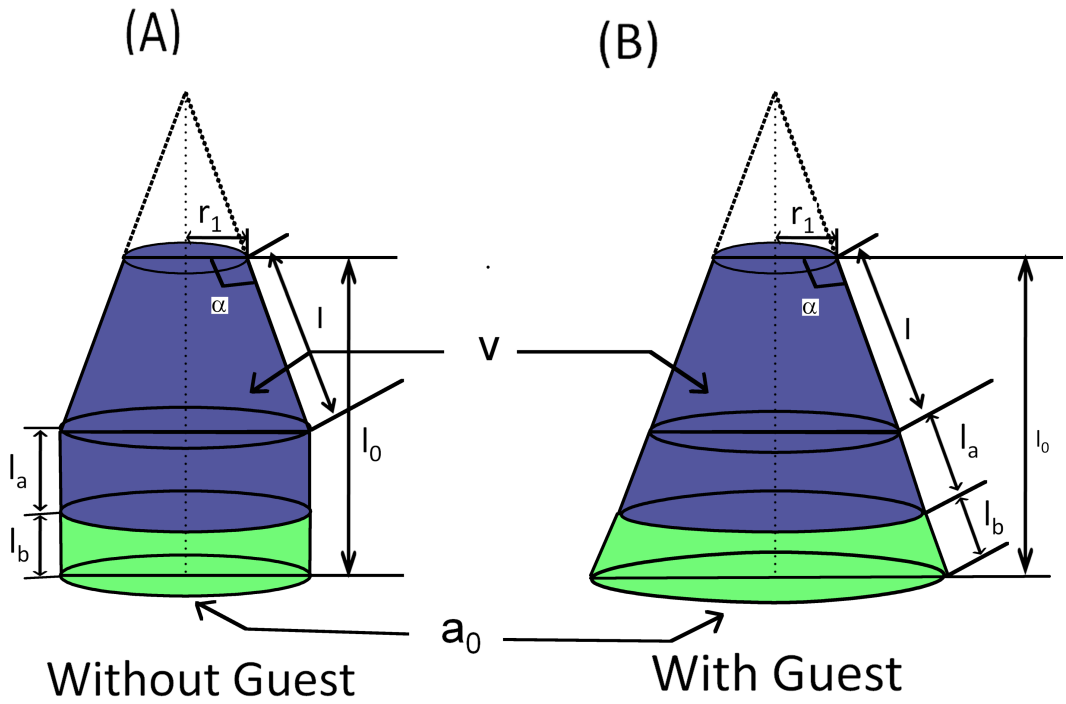


Figure S9. A schematic representation of basket **1** before (A) and after (B) the addition of DMPP guest with the corresponding geometric parameters. On the basis of the crystal structure of hexaester **3**, we estimated the radius of the platform's bottom to r_1 = 3 Å, while the length of the platform's sides to h_2-h_1 = 9 Å

To compute the critical packing parameter *P*, we made the following assumptions:
1. The shape of empty basket (Figure S9) corresponds to a truncated cone.
2. The aliphatic chains are compact without a guest populating the basket's cavity (A, Figure S9). The shape of three aliphatic units is cylindrical, and divided into two parts; hydrophobic (l_a, blue) and hydrophilic (l_b, green).
3. The aliphatic chains are extended along the aromatic arms when DMMP guest populates the inner space of **1** (B, Figure S9). The shape of the aliphatic unit is a truncated cone.
4. The value of used parameters: r_1 = 3 Å, l = 9 Å, l_a = 4 Å, l_b = 3 Å, α = 108° without guest, α = 112° with guest.

$$P = v/(a_0 l_0)$$

while v is the volume of the hydrophobic part (blue), a_0 is the hydrophilic head surface area (green), l_0 is the length of the whole basket.

P ≈ 0.59 for basket **1** without guest (A), while P ≈ 0.32 for basket **1** with guest (B).

Crystallographic Data

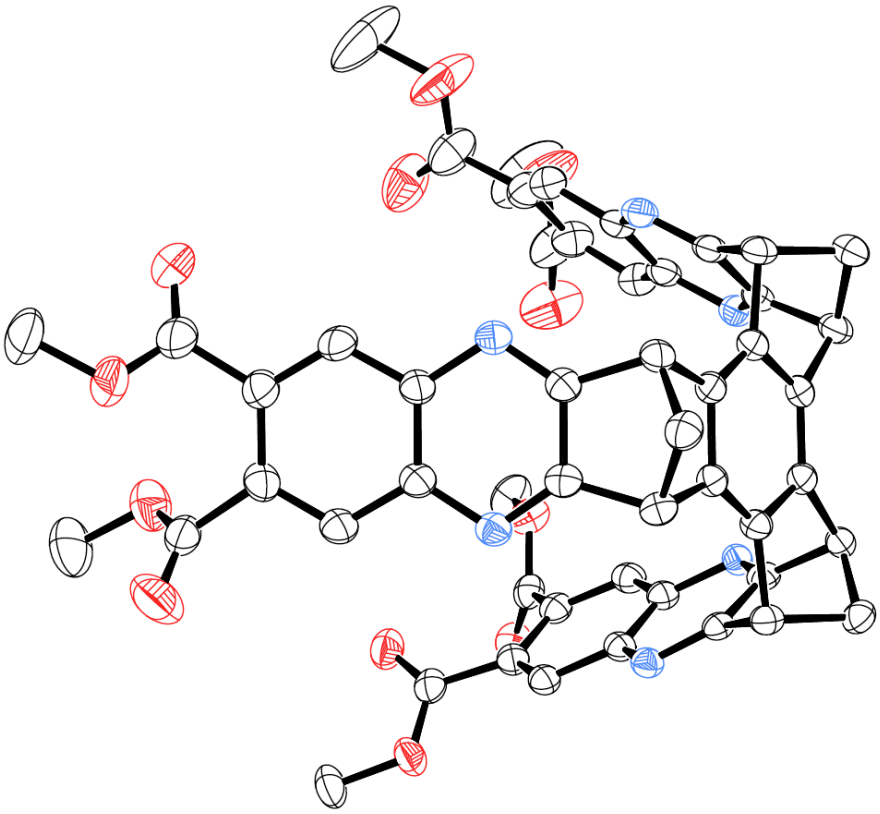


Figure S10. ORTEP plot of compound 3.

The data collection crystal was a colorless chunk, which had been cut from a cluster of crystals. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated a triclinic crystal system. All work was done at 150 K using an Oxford Cryosystems Cryostream Cooler. The data collection strategy was set up to measure a hemisphere of reciprocal space with a redundancy factor of 3.5, which means that 90% of these reflections were measured at least 3.5 times. Phi and omega scans with a frame width of 1.0˚ were used. Data integration was done with Denzo(1), and scaling and merging of the data was done with Scalepack(1). Merging the data and averaging the symmetry equivalent reflections resulted in an Rin value of 0.041.

The structure was solved by the direct methods procedure in SIR2004(2). Full-matrix least-squares refinements based on F2 were performed in SHELXL-2013(3), as incorporated in the WinGX package(4). There are two molecules in the asymmetric unit (labeled as molecules A and B) along with many different solvent molecules. There is one ordered solvent molecule of CH_2Cl_2 [Cl(1C)-C(1C)-Cl(2C)], one ordered ethyl acetate molecule (labeled as D), one CH_2Cl_2 disordered about an inversion center [Cl(1F) and C(1F)], one CH_2Cl_2 and one H_2O molecule disordered about the same site [Cl(1E)-C(1E)-Cl(2E) and O(1H)] and one water molecule

disordered about an inversion center [O(1G)]. One of the methoxy groups of a main molecule [C(19A)] seems to be disordered over two sites, so C(19C) is added as a second site and distance restraints were applied during refinement. Distance restraints were also used for some of the CH_2Cl_2 molecules. For each methyl group, the hydrogen atoms were added at calculated positions using a riding model with U(H) = 1.5 * Ueq(bonded carbon atom). The rest of the hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2 * Ueq(bonded atom). Because the hydrogen atoms of the two water molecules could not be located, they were not included in the model.

The final refinement cycle was based on 17741 intensities, 7 restraints, and 1397 variables and resulted in agreement factors of R1(F) = 0.104 and wR2(F2) = 0.212. For the subset of data with I > 2*sigma(I), the R1(F) value is 0.071 for 12301 reflections. The final difference electron density map contains maximum and minimum peak heights of 1.38 and –0.80 e/Å3. The top three peaks (1.30 to 1.38 e/Å3) are in the immediate vicinity of the two disordered CH_2Cl_2 and H_2O molecules. An attempt to obtain a reasonable model for these three peaks did not work. Neutral atom scattering factors were used and include terms for anomalous dispersion (5).

References

(1) Otwinowski, Z. & Minor, W., Methods in Enzymology, Vol 276: Macromolecular Crystallography, part A, 307-326, (1997), Carter, Jr., C. W. & Sweet, R. M., Eds., Academic Press. (2) SIR2004: M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Spagna, 2004. (3) SHELXL-2013: Sheldrick, G.M., Acta Cryst., (2008), A64, 112-122. (4) WinGX-Version 1.70.01: Farrugia, L. J., J. Appl. Cryst., (1999), 32, 837-838. (5) International Tables for Crystallography (1992). Volume C. Dordrecht: Kluwer Academic Publishers.

Table S1. Crystallographic details for hexaester **3**.

Formula	2(C51 H36 N6 O12), 2(C H2 Cl2), C4 H8 O2, H2 O	
Formula weight	2125.68	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 16.3360(2) Å	⟨= 67.123(1)°
	b = 17.1738(2) Å	®= 77.886(1)°
	c = 20.1389(2) Å	© = 77.704(1)°
Volume	5035.24(11) Å^3	
Z	2	
Density (calculated)	1.402 Mg/m^3	
Absorption coefficient	0.203 mm^{-1}	
F(000)	2204	
Crystal size	0.19 x 0.27 x 0.38 mm^3	
Theta range for data collection	1.301 to 25.009°	
Index ranges	-19<=h<=19, -20<=k<=20, -23<=l<=23	
Reflections collected	120874	
Independent reflections	17741 [R(int) = 0.041]	
Completeness to theta = 25.0°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17741 / 7 / 1397	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0705, wR2 = 0.1889	
R indices (all data)	R1 = 0.1036, wR2 = 0.2124	
Largest diff. peak and hole	1.384 and -0.802 e/Å^3	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for hexaester **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1C)	653(1)	1845(1)	6452(1)	64(1)
Cl(2C)	1379(1)	1403(1)	7782(1)	77(1)
C(1C)	461(3)	1815(3)	7357(2)	54(1)
Cl(1E)	6303(2)	2325(2)	2432(2)	81(1)*
Cl(2E)	5241(3)	1736(3)	1774(2)	153(2)*
C(1E)	5529(6)	1869(5)	2498(5)	63(3)*
O(1H)	5376(4)	1462(5)	2972(4)	71(2)*
Cl(1F)	5350(1)	5232(1)	4206(2)	208(2)
C(1F)	4643(6)	4867(7)	4839(7)	73(4)*
O(1D)	2822(3)	4827(3)	-694(3)	116(2)
O(2D)	3702(2)	3741(3)	-819(3)	99(1)
C(1D)	3255(6)	3713(4)	350(4)	127(3)
C(2D)	3214(3)	4170(3)	-431(3)	67(1)
C(3D)	3753(4)	4172(5)	-1633(5)	120(3)
C(4D)	4367(8)	3650(7)	-1941(7)	228(7)
O(1G)	5199(3)	458(3)	4408(3)	49(1)*
O(1A)	6875(4)	-102(4)	1480(2)	148(2)
O(2A)	6953(2)	264(2)	2377(2)	78(1)
O(3A)	6972(3)	-1925(6)	1563(3)	182(3)
O(4A)	5808(2)	-1121(2)	1192(2)	75(1)
O(5A)	2376(3)	-509(3)	630(2)	108(2)
O(6A)	1026(2)	-415(2)	562(2)	66(1)
O(7A)	766(2)	1233(2)	612(1)	52(1)
O(8A)	-441(2)	1201(2)	1392(1)	45(1)
O(9A)	2310(2)	3876(2)	2108(2)	57(1)
O(10A)	1142(2)	4102(2)	2858(1)	42(1)
O(11A)	4440(2)	3378(2)	2929(2)	67(1)
O(12A)	3275(2)	4352(2)	2856(1)	49(1)
N(1A)	5119(2)	-1482(2)	4526(2)	34(1)
N(2A)	4537(2)	-2583(2)	3998(2)	36(1)
N(3A)	1749(2)	-1905(2)	3494(1)	31(1)

N(4A)	552(2)	-526(2)	3786(1)	30(1)
N(5A)	1448(2)	1182(2)	4829(1)	29(1)
N(6A)	3212(2)	861(2)	5032(2)	33(1)
C(1A)	3225(2)	-1837(2)	5607(2)	30(1)
C(2A)	2930(2)	-2356(2)	5332(2)	30(1)
C(3A)	2111(2)	-2174(2)	5187(2)	28(1)
C(4A)	1553(2)	-1484(2)	5334(2)	26(1)
C(5A)	1837(2)	-1003(2)	5621(2)	29(1)
C(6A)	2689(2)	-1170(2)	5750(2)	30(1)
C(7A)	4157(2)	-2195(2)	5687(2)	36(1)
C(8A)	4588(2)	-2014(2)	4911(2)	34(1)
C(9A)	4294(2)	-2555(2)	4643(2)	32(1)
C(10A)	3671(2)	-3040(2)	5250(2)	34(1)
C(11A)	4112(2)	-3157(2)	5908(2)	40(1)
C(12A)	5382(2)	-1474(2)	3821(2)	35(1)
C(13A)	5920(2)	-899(2)	3342(2)	40(1)
C(14A)	6187(2)	-856(3)	2639(2)	45(1)
C(15A)	5945(2)	-1442(3)	2398(2)	54(1)
C(16A)	5410(2)	-2004(3)	2858(2)	50(1)
C(17A)	5107(2)	-2026(2)	3569(2)	36(1)
C(18A)	6699(3)	-200(3)	2122(3)	68(1)
C(19A)	7406(7)	931(6)	1827(4)	118(5)**
C(19C)	7042(14)	836(11)	1068(9)	89(8)**
C(20A)	6307(4)	-1520(5)	1680(3)	85(2)
C(21A)	6232(5)	-1160(5)	475(3)	110(2)
C(22A)	1603(2)	-2563(2)	4876(2)	28(1)
C(23A)	1449(2)	-1890(2)	4140(2)	28(1)
C(24A)	875(2)	-1196(2)	4289(2)	27(1)
C(25A)	709(2)	-1443(2)	5109(2)	27(1)
C(26A)	710(2)	-2414(2)	5307(2)	30(1)
C(27A)	1430(2)	-1186(2)	2943(2)	31(1)
C(28A)	1705(2)	-1131(2)	2218(2)	35(1)
C(29A)	1359(2)	-464(2)	1654(2)	35(1)
C(30A)	717(2)	169(2)	1804(2)	34(1)
C(31A)	461(2)	128(2)	2514(2)	32(1)
C(32A)	824(2)	-535(2)	3087(2)	29(1)

C(33A)	1653(3)	-453(3)	895(2)	54(1)
C(34A)	1261(5)	-275(4)	-211(3)	115(3)
C(35A)	371(2)	914(2)	1198(2)	36(1)
C(36A)	-813(3)	1950(2)	844(2)	53(1)
C(37A)	1398(2)	-256(2)	5861(2)	31(1)
C(38A)	1793(2)	504(2)	5314(2)	29(1)
C(39A)	2667(2)	347(2)	5420(2)	30(1)
C(40A)	2791(2)	-503(2)	6043(2)	33(1)
C(41A)	1896(2)	-441(2)	6499(2)	38(1)
C(42A)	2016(2)	1748(2)	4402(2)	27(1)
C(43A)	1711(2)	2493(2)	3844(2)	31(1)
C(44A)	2242(2)	3056(2)	3376(2)	32(1)
C(45A)	3099(2)	2918(2)	3490(2)	35(1)
C(46A)	3403(2)	2193(2)	4035(2)	35(1)
C(47A)	2875(2)	1592(2)	4493(2)	32(1)
C(48A)	1930(2)	3726(2)	2708(2)	37(1)
C(49A)	765(3)	4721(3)	2237(2)	56(1)
C(50A)	3689(3)	3557(3)	3056(2)	44(1)
C(51A)	3772(3)	5016(3)	2385(3)	70(1)
O(1B)	2314(2)	-112(2)	3753(2)	77(1)
O(2B)	3248(2)	762(2)	3088(2)	55(1)
O(3B)	3273(2)	1446(2)	1022(2)	76(1)
O(4B)	3072(2)	226(2)	1975(2)	60(1)
O(5B)	4290(2)	6098(2)	333(2)	78(1)
O(6B)	3753(2)	6253(3)	-644(2)	96(1)
O(7B)	3355(2)	7455(3)	1416(2)	83(1)
O(8B)	3694(2)	7874(2)	201(2)	80(1)
O(9B)	2679(2)	5691(2)	4587(1)	40(1)
O(10B)	2725(2)	6146(2)	3373(1)	40(1)
O(11B)	3061(2)	3961(2)	4589(1)	43(1)
O(12B)	2095(2)	3220(2)	5432(1)	40(1)
N(1B)	-198(2)	2359(2)	2966(1)	29(1)
N(2B)	288(2)	3071(2)	1400(1)	31(1)
N(3B)	716(2)	6012(2)	366(1)	32(1)
N(4B)	307(2)	7110(2)	1213(1)	32(1)
N(5B)	-389(2)	6111(2)	3411(1)	28(1)

N(6B)	-518(2)	4329(2)	4240(1)	27(1)
C(1B)	-1530(2)	4315(2)	2475(2)	27(1)
C(2B)	-1285(2)	4651(2)	1709(2)	27(1)
C(3B)	-1193(2)	5494(2)	1363(2)	29(1)
C(4B)	-1379(2)	6046(2)	1766(2)	27(1)
C(5B)	-1623(2)	5725(2)	2505(2)	27(1)
C(6B)	-1681(2)	4837(2)	2869(2)	26(1)
C(7B)	-1579(2)	3368(2)	2675(2)	30(1)
C(8B)	-678(2)	2946(2)	2518(2)	28(1)
C(9B)	-436(2)	3298(2)	1739(2)	28(1)
C(10B)	-1192(2)	3920(2)	1433(2)	30(1)
C(11B)	-1905(2)	3432(2)	1979(2)	34(1)
C(12B)	579(2)	2095(2)	2622(2)	30(1)
C(13B)	1140(2)	1451(2)	3056(2)	33(1)
C(14B)	1910(2)	1145(2)	2746(2)	35(1)
C(15B)	2131(2)	1460(2)	1980(2)	39(1)
C(16B)	1595(2)	2105(2)	1550(2)	37(1)
C(17B)	820(2)	2440(2)	1857(2)	31(1)
C(18B)	2497(2)	501(2)	3252(2)	40(1)
C(19B)	3887(3)	144(3)	3509(3)	72(1)
C(20B)	2895(3)	1059(3)	1602(2)	52(1)
C(21B)	3800(3)	-227(4)	1651(3)	84(2)
C(22B)	-885(2)	6040(2)	578(2)	32(1)
C(23B)	-48(2)	6256(2)	626(2)	30(1)
C(24B)	-245(2)	6813(2)	1042(2)	30(1)
C(25B)	-1207(2)	6928(2)	1240(2)	31(1)
C(26B)	-1449(2)	6909(2)	537(2)	35(1)
C(27B)	1333(2)	6354(2)	507(2)	31(1)
C(28B)	2174(2)	6185(2)	197(2)	37(1)
C(29B)	2807(2)	6525(2)	300(2)	43(1)
C(30B)	2609(2)	7042(2)	735(2)	44(1)
C(31B)	1791(2)	7203(2)	1047(2)	37(1)
C(32B)	1135(2)	6879(2)	929(2)	32(1)
C(33B)	3700(3)	6285(3)	8(3)	60(1)
C(34B)	4592(3)	5925(6)	-961(4)	130(3)
C(35B)	3267(3)	7458(3)	839(3)	59(1)

C(36B)	4360(4)	8303(5)	230(4)	123(3)
C(37B)	-1811(2)	6131(2)	3077(2)	28(1)
C(38B)	-1036(2)	5754(2)	3465(2)	27(1)
C(39B)	-1093(2)	4862(2)	3861(2)	25(1)
C(40B)	-1892(2)	4699(2)	3682(2)	28(1)
C(41B)	-2459(2)	5563(2)	3638(2)	31(1)
C(42B)	248(2)	5557(2)	3796(2)	28(1)
C(43B)	999(2)	5866(2)	3746(2)	31(1)
C(44B)	1663(2)	5335(2)	4093(2)	29(1)
C(45B)	1585(2)	4471(2)	4518(2)	30(1)
C(46B)	849(2)	4162(2)	4584(2)	29(1)
C(47B)	174(2)	4690(2)	4213(2)	26(1)
C(48B)	2415(2)	5724(2)	4056(2)	33(1)
C(49B)	3416(2)	6608(3)	3282(2)	51(1)
C(50B)	2334(2)	3874(2)	4837(2)	33(1)
C(51B)	2775(2)	2595(2)	5773(2)	46(1)

*Occupancy factor set to 0.5

**Occupancy factors for C(19A) and C(19C) refined to 0.71(1) and 0.29(1), respectively.

Table S3. Bond lengths [Å] and angles [°] for compound **3**.

Cl(1C)-C(1C)	1.766(4)
Cl(2C)-C(1C)	1.761(4)
C(1C)-H(1C1)	0.9900
C(1C)-H(1C2)	0.9900
Cl(1E)-C(1E)	1.581(9)
Cl(2E)-C(1E)	1.730(9)
C(1E)-H(1E)	0.9900
C(1E)-H(2E)	0.9900
Cl(1F)-C(1F)	1.556(13)
Cl(1F)-C(1F)#1	1.866(11)
C(1F)-Cl(1F)#1	1.865(11)
C(1F)-H(1F1)	0.9900
C(1F)-H(1F2)	0.9900
O(1D)-C(2D)	1.156(6)
O(2D)-C(2D)	1.314(6)
O(2D)-C(3D)	1.506(9)
C(1D)-C(2D)	1.468(9)
C(1D)-H(1D1)	0.9800
C(1D)-H(1D2)	0.9800
C(1D)-H(1D3)	0.9800
C(3D)-C(4D)	1.408(10)
C(3D)-H(3D1)	0.9900
C(3D)-H(3D2)	0.9900
C(4D)-H(4D1)	0.9800
C(4D)-H(4D2)	0.9800
C(4D)-H(4D3)	0.9800
O(1A)-C(18A)	1.217(6)
O(1A)-C(19C)	1.553(15)
O(2A)-C(18A)	1.271(6)
O(2A)-C(19A)	1.455(7)
O(3A)-C(20A)	1.191(8)
O(4A)-C(20A)	1.294(7)
O(4A)-C(21A)	1.486(6)
O(5A)-C(33A)	1.190(5)

O(6A)-C(33A)	1.314(5)
O(6A)-C(34A)	1.458(6)
O(7A)-C(35A)	1.200(4)
O(8A)-C(35A)	1.345(4)
O(8A)-C(36A)	1.444(4)
O(9A)-C(48A)	1.193(4)
O(10A)-C(48A)	1.342(4)
O(10A)-C(49A)	1.444(4)
O(11A)-C(50A)	1.198(5)
O(12A)-C(50A)	1.334(5)
O(12A)-C(51A)	1.445(5)
N(1A)-C(8A)	1.301(4)
N(1A)-C(12A)	1.391(4)
N(2A)-C(9A)	1.293(4)
N(2A)-C(17A)	1.389(5)
N(3A)-C(23A)	1.299(4)
N(3A)-C(27A)	1.390(4)
N(4A)-C(24A)	1.300(4)
N(4A)-C(32A)	1.391(4)
N(5A)-C(38A)	1.303(4)
N(5A)-C(42A)	1.393(4)
N(6A)-C(39A)	1.299(4)
N(6A)-C(47A)	1.397(4)
C(1A)-C(6A)	1.372(5)
C(1A)-C(2A)	1.419(5)
C(1A)-C(7A)	1.533(5)
C(2A)-C(3A)	1.374(5)
C(2A)-C(10A)	1.528(5)
C(3A)-C(4A)	1.421(4)
C(3A)-C(22A)	1.520(4)
C(4A)-C(5A)	1.371(4)
C(4A)-C(25A)	1.520(4)
C(5A)-C(6A)	1.417(5)
C(5A)-C(37A)	1.530(4)
C(6A)-C(40A)	1.529(5)
C(7A)-C(8A)	1.512(5)

C(7A)-C(11A)	1.550(5)
C(7A)-H(7A)	1.0000
C(8A)-C(9A)	1.441(5)
C(9A)-C(10A)	1.507(5)
C(10A)-C(11A)	1.566(5)
C(10A)-H(10A)	1.0000
C(11A)-H(11A)	0.9900
C(11A)-H(11B)	0.9900
C(12A)-C(13A)	1.398(5)
C(12A)-C(17A)	1.416(5)
C(13A)-C(14A)	1.370(5)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.426(6)
C(14A)-C(18A)	1.476(6)
C(15A)-C(16A)	1.371(6)
C(15A)-C(20A)	1.488(6)
C(16A)-C(17A)	1.400(5)
C(16A)-H(16A)	0.9500
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(19C)-H(19G)	0.9800
C(19C)-H(19H)	0.9800
C(19C)-H(19I)	0.9800
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(22A)-C(23A)	1.514(4)
C(22A)-C(26A)	1.559(4)
C(22A)-H(22A)	1.0000
C(23A)-C(24A)	1.440(4)
C(24A)-C(25A)	1.514(4)
C(25A)-C(26A)	1.556(4)
C(25A)-H(25A)	1.0000
C(26A)-H(26A)	0.9900
C(26A)-H(26B)	0.9900

C(27A)-C(32A)	1.405(5)
C(27A)-C(28A)	1.407(5)
C(28A)-C(29A)	1.379(5)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.418(5)
C(29A)-C(33A)	1.496(5)
C(30A)-C(31A)	1.382(5)
C(30A)-C(35A)	1.487(5)
C(31A)-C(32A)	1.399(5)
C(31A)-H(31A)	0.9500
C(34A)-H(34A)	0.9800
C(34A)-H(34B)	0.9800
C(34A)-H(34C)	0.9800
C(36A)-H(36A)	0.9800
C(36A)-H(36B)	0.9800
C(36A)-H(36C)	0.9800
C(37A)-C(38A)	1.509(5)
C(37A)-C(41A)	1.557(5)
C(37A)-H(37A)	1.0000
C(38A)-C(39A)	1.441(5)
C(39A)-C(40A)	1.518(5)
C(40A)-C(41A)	1.561(5)
C(40A)-H(40A)	1.0000
C(41A)-H(41A)	0.9900
C(41A)-H(41B)	0.9900
C(42A)-C(47A)	1.410(5)
C(42A)-C(43A)	1.411(5)
C(43A)-C(44A)	1.373(5)
C(43A)-H(43A)	0.9500
C(44A)-C(45A)	1.420(5)
C(44A)-C(48A)	1.492(5)
C(45A)-C(46A)	1.380(5)
C(45A)-C(50A)	1.500(5)
C(46A)-C(47A)	1.402(5)
C(46A)-H(46A)	0.9500
C(49A)-H(49A)	0.9800

C(49A)-H(49B)	0.9800
C(49A)-H(49C)	0.9800
C(51A)-H(51A)	0.9800
C(51A)-H(51B)	0.9800
C(51A)-H(51C)	0.9800
O(1B)-C(18B)	1.181(5)
O(2B)-C(18B)	1.328(5)
O(2B)-C(19B)	1.461(5)
O(3B)-C(20B)	1.207(5)
O(4B)-C(20B)	1.332(5)
O(4B)-C(21B)	1.455(5)
O(5B)-C(33B)	1.196(6)
O(6B)-C(33B)	1.320(6)
O(6B)-C(34B)	1.479(6)
O(7B)-C(35B)	1.199(5)
O(8B)-C(35B)	1.330(5)
O(8B)-C(36B)	1.459(6)
O(9B)-C(48B)	1.211(4)
O(10B)-C(48B)	1.327(4)
O(10B)-C(49B)	1.456(4)
O(11B)-C(50B)	1.206(4)
O(12B)-C(50B)	1.339(4)
O(12B)-C(51B)	1.448(4)
N(1B)-C(8B)	1.304(4)
N(1B)-C(12B)	1.389(4)
N(2B)-C(9B)	1.299(4)
N(2B)-C(17B)	1.392(4)
N(3B)-C(23B)	1.297(4)
N(3B)-C(27B)	1.394(4)
N(4B)-C(24B)	1.287(4)
N(4B)-C(32B)	1.393(4)
N(5B)-C(38B)	1.297(4)
N(5B)-C(42B)	1.391(4)
N(6B)-C(39B)	1.302(4)
N(6B)-C(47B)	1.383(4)
C(1B)-C(6B)	1.368(4)

C(1B)-C(2B)	1.420(4)
C(1B)-C(7B)	1.533(4)
C(2B)-C(3B)	1.368(5)
C(2B)-C(10B)	1.528(4)
C(3B)-C(4B)	1.420(4)
C(3B)-C(22B)	1.532(4)
C(4B)-C(5B)	1.373(4)
C(4B)-C(25B)	1.518(4)
C(5B)-C(6B)	1.426(4)
C(5B)-C(37B)	1.515(4)
C(6B)-C(40B)	1.534(4)
C(7B)-C(8B)	1.522(5)
C(7B)-C(11B)	1.557(5)
C(7B)-H(7B)	1.0000
C(8B)-C(9B)	1.445(4)
C(9B)-C(10B)	1.514(4)
C(10B)-C(11B)	1.558(5)
C(10B)-H(10B)	1.0000
C(11B)-H(11C)	0.9900
C(11B)-H(11D)	0.9900
C(12B)-C(13B)	1.408(5)
C(12B)-C(17B)	1.418(5)
C(13B)-C(14B)	1.376(5)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.416(5)
C(14B)-C(18B)	1.504(5)
C(15B)-C(16B)	1.379(5)
C(15B)-C(20B)	1.501(5)
C(16B)-C(17B)	1.398(5)
C(16B)-H(16B)	0.9500
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800

C(22B)-C(23B)	1.523(5)
C(22B)-C(26B)	1.560(5)
C(22B)-H(22B)	1.0000
C(23B)-C(24B)	1.449(5)
C(24B)-C(25B)	1.527(5)
C(25B)-C(26B)	1.562(5)
C(25B)-H(25B)	1.0000
C(26B)-H(26C)	0.9900
C(26B)-H(26D)	0.9900
C(27B)-C(28B)	1.405(5)
C(27B)-C(32B)	1.413(5)
C(28B)-C(29B)	1.377(5)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.422(5)
C(29B)-C(33B)	1.488(6)
C(30B)-C(31B)	1.371(5)
C(30B)-C(35B)	1.500(6)
C(31B)-C(32B)	1.405(5)
C(31B)-H(31B)	0.9500
C(34B)-H(34D)	0.9800
C(34B)-H(34E)	0.9800
C(34B)-H(34F)	0.9800
C(36B)-H(36D)	0.9800
C(36B)-H(36E)	0.9800
C(36B)-H(36F)	0.9800
C(37B)-C(38B)	1.518(4)
C(37B)-C(41B)	1.558(5)
C(37B)-H(37B)	1.0000
C(38B)-C(39B)	1.440(4)
C(39B)-C(40B)	1.529(4)
C(40B)-C(41B)	1.554(4)
C(40B)-H(40B)	1.0000
C(41B)-H(41C)	0.9900
C(41B)-H(41D)	0.9900
C(42B)-C(43B)	1.407(5)
C(42B)-C(47B)	1.413(4)

C(43B)-C(44B)	1.376(5)
C(43B)-H(43B)	0.9500
C(44B)-C(45B)	1.414(5)
C(44B)-C(48B)	1.496(5)
C(45B)-C(46B)	1.376(5)
C(45B)-C(50B)	1.498(5)
C(46B)-C(47B)	1.410(4)
C(46B)-H(46B)	0.9500
C(49B)-H(49D)	0.9800
C(49B)-H(49E)	0.9800
C(49B)-H(49F)	0.9800
C(51B)-H(51D)	0.9800
C(51B)-H(51E)	0.9800
C(51B)-H(51F)	0.9800

Cl(2C)-C(1C)-Cl(1C)	111.9(2)
Cl(2C)-C(1C)-H(1C1)	109.2
Cl(1C)-C(1C)-H(1C1)	109.2
Cl(2C)-C(1C)-H(1C2)	109.2
Cl(1C)-C(1C)-H(1C2)	109.2
H(1C1)-C(1C)-H(1C2)	107.9
Cl(1E)-C(1E)-Cl(2E)	123.9(7)
Cl(1E)-C(1E)-H(1E)	106.4
Cl(2E)-C(1E)-H(1E)	106.4
Cl(1E)-C(1E)-H(2E)	106.4
Cl(2E)-C(1E)-H(2E)	106.4
H(1E)-C(1E)-H(2E)	106.4
Cl(1F)-C(1F)-Cl(1F)#1	122.7(5)
Cl(1F)-C(1F)-H(1F1)	106.7
Cl(1F)#1-C(1F)-H(1F1)	106.7
Cl(1F)-C(1F)-H(1F2)	106.7
Cl(1F)#1-C(1F)-H(1F2)	106.7
H(1F1)-C(1F)-H(1F2)	106.6
C(2D)-O(2D)-C(3D)	116.1(5)
C(2D)-C(1D)-H(1D1)	109.5
C(2D)-C(1D)-H(1D2)	109.5

H(1D1)-C(1D)-H(1D2)	109.5
C(2D)-C(1D)-H(1D3)	109.5
H(1D1)-C(1D)-H(1D3)	109.5
H(1D2)-C(1D)-H(1D3)	109.5
O(1D)-C(2D)-O(2D)	122.3(6)
O(1D)-C(2D)-C(1D)	126.4(6)
O(2D)-C(2D)-C(1D)	111.3(5)
C(4D)-C(3D)-O(2D)	106.8(9)
C(4D)-C(3D)-H(3D1)	110.4
O(2D)-C(3D)-H(3D1)	110.4
C(4D)-C(3D)-H(3D2)	110.4
O(2D)-C(3D)-H(3D2)	110.4
H(3D1)-C(3D)-H(3D2)	108.6
C(3D)-C(4D)-H(4D1)	109.5
C(3D)-C(4D)-H(4D2)	109.5
H(4D1)-C(4D)-H(4D2)	109.5
C(3D)-C(4D)-H(4D3)	109.5
H(4D1)-C(4D)-H(4D3)	109.5
H(4D2)-C(4D)-H(4D3)	109.5
C(18A)-O(1A)-C(19C)	106.6(8)
C(18A)-O(2A)-C(19A)	113.8(5)
C(20A)-O(4A)-C(21A)	110.3(5)
C(33A)-O(6A)-C(34A)	114.6(4)
C(35A)-O(8A)-C(36A)	115.1(3)
C(48A)-O(10A)-C(49A)	115.6(3)
C(50A)-O(12A)-C(51A)	116.0(3)
C(8A)-N(1A)-C(12A)	114.0(3)
C(9A)-N(2A)-C(17A)	113.8(3)
C(23A)-N(3A)-C(27A)	112.9(3)
C(24A)-N(4A)-C(32A)	113.6(3)
C(38A)-N(5A)-C(42A)	113.3(3)
C(39A)-N(6A)-C(47A)	113.9(3)
C(6A)-C(1A)-C(2A)	120.3(3)
C(6A)-C(1A)-C(7A)	133.2(3)
C(2A)-C(1A)-C(7A)	106.5(3)
C(3A)-C(2A)-C(1A)	119.8(3)

C(3A)-C(2A)-C(10A)	133.1(3)
C(1A)-C(2A)-C(10A)	107.0(3)
C(2A)-C(3A)-C(4A)	120.0(3)
C(2A)-C(3A)-C(22A)	133.9(3)
C(4A)-C(3A)-C(22A)	106.0(3)
C(5A)-C(4A)-C(3A)	119.6(3)
C(5A)-C(4A)-C(25A)	133.0(3)
C(3A)-C(4A)-C(25A)	107.4(3)
C(4A)-C(5A)-C(6A)	120.6(3)
C(4A)-C(5A)-C(37A)	132.3(3)
C(6A)-C(5A)-C(37A)	107.1(3)
C(1A)-C(6A)-C(5A)	119.5(3)
C(1A)-C(6A)-C(40A)	133.8(3)
C(5A)-C(6A)-C(40A)	106.6(3)
C(8A)-C(7A)-C(1A)	103.8(3)
C(8A)-C(7A)-C(11A)	98.9(3)
C(1A)-C(7A)-C(11A)	99.2(3)
C(8A)-C(7A)-H(7A)	117.3
C(1A)-C(7A)-H(7A)	117.3
C(11A)-C(7A)-H(7A)	117.3
N(1A)-C(8A)-C(9A)	123.8(3)
N(1A)-C(8A)-C(7A)	129.5(3)
C(9A)-C(8A)-C(7A)	106.7(3)
N(2A)-C(9A)-C(8A)	124.3(3)
N(2A)-C(9A)-C(10A)	129.3(3)
C(8A)-C(9A)-C(10A)	106.5(3)
C(9A)-C(10A)-C(2A)	104.4(3)
C(9A)-C(10A)-C(11A)	98.4(3)
C(2A)-C(10A)-C(11A)	99.0(3)
C(9A)-C(10A)-H(10A)	117.3
C(2A)-C(10A)-H(10A)	117.3
C(11A)-C(10A)-H(10A)	117.3
C(7A)-C(11A)-C(10A)	95.3(3)
C(7A)-C(11A)-H(11A)	112.7
C(10A)-C(11A)-H(11A)	112.7
C(7A)-C(11A)-H(11B)	112.7

C(10A)-C(11A)-H(11B)	112.7
H(11A)-C(11A)-H(11B)	110.2
N(1A)-C(12A)-C(13A)	119.3(3)
N(1A)-C(12A)-C(17A)	121.8(3)
C(13A)-C(12A)-C(17A)	118.9(3)
C(14A)-C(13A)-C(12A)	121.6(3)
C(14A)-C(13A)-H(13A)	119.2
C(12A)-C(13A)-H(13A)	119.2
C(13A)-C(14A)-C(15A)	119.3(4)
C(13A)-C(14A)-C(18A)	121.0(4)
C(15A)-C(14A)-C(18A)	119.6(4)
C(16A)-C(15A)-C(14A)	119.6(4)
C(16A)-C(15A)-C(20A)	117.8(4)
C(14A)-C(15A)-C(20A)	122.4(4)
C(15A)-C(16A)-C(17A)	121.3(4)
C(15A)-C(16A)-H(16A)	119.4
C(17A)-C(16A)-H(16A)	119.4
N(2A)-C(17A)-C(16A)	118.5(3)
N(2A)-C(17A)-C(12A)	122.4(3)
C(16A)-C(17A)-C(12A)	119.2(3)
O(1A)-C(18A)-O(2A)	121.0(4)
O(1A)-C(18A)-C(14A)	121.9(5)
O(2A)-C(18A)-C(14A)	117.1(4)
O(2A)-C(19A)-H(19A)	109.5
O(2A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
O(2A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
O(1A)-C(19C)-H(19G)	109.5
O(1A)-C(19C)-H(19H)	109.5
H(19G)-C(19C)-H(19H)	109.5
O(1A)-C(19C)-H(19I)	109.5
H(19G)-C(19C)-H(19I)	109.5
H(19H)-C(19C)-H(19I)	109.5
O(3A)-C(20A)-O(4A)	122.7(5)

O(3A)-C(20A)-C(15A)	124.4(6)
O(4A)-C(20A)-C(15A)	112.9(5)
O(4A)-C(21A)-H(21A)	109.5
O(4A)-C(21A)-H(21B)	109.5
H(21A)-C(21A)-H(21B)	109.5
O(4A)-C(21A)-H(21C)	109.5
H(21A)-C(21A)-H(21C)	109.5
H(21B)-C(21A)-H(21C)	109.5
C(23A)-C(22A)-C(3A)	104.8(2)
C(23A)-C(22A)-C(26A)	98.4(2)
C(3A)-C(22A)-C(26A)	100.0(2)
C(23A)-C(22A)-H(22A)	116.9
C(3A)-C(22A)-H(22A)	116.9
C(26A)-C(22A)-H(22A)	116.9
N(3A)-C(23A)-C(24A)	124.9(3)
N(3A)-C(23A)-C(22A)	129.2(3)
C(24A)-C(23A)-C(22A)	105.9(3)
N(4A)-C(24A)-C(23A)	123.4(3)
N(4A)-C(24A)-C(25A)	129.6(3)
C(23A)-C(24A)-C(25A)	106.9(3)
C(24A)-C(25A)-C(4A)	105.5(2)
C(24A)-C(25A)-C(26A)	97.4(2)
C(4A)-C(25A)-C(26A)	99.2(2)
C(24A)-C(25A)-H(25A)	117.2
C(4A)-C(25A)-H(25A)	117.2
C(26A)-C(25A)-H(25A)	117.2
C(25A)-C(26A)-C(22A)	94.9(2)
C(25A)-C(26A)-H(26A)	112.8
C(22A)-C(26A)-H(26A)	112.8
C(25A)-C(26A)-H(26B)	112.8
C(22A)-C(26A)-H(26B)	112.8
H(26A)-C(26A)-H(26B)	110.2
N(3A)-C(27A)-C(32A)	122.4(3)
N(3A)-C(27A)-C(28A)	118.2(3)
C(32A)-C(27A)-C(28A)	119.3(3)
C(29A)-C(28A)-C(27A)	120.6(3)

C(29A)-C(28A)-H(28A)	119.7
C(27A)-C(28A)-H(28A)	119.7
C(28A)-C(29A)-C(30A)	119.9(3)
C(28A)-C(29A)-C(33A)	118.3(3)
C(30A)-C(29A)-C(33A)	121.7(3)
C(31A)-C(30A)-C(29A)	119.6(3)
C(31A)-C(30A)-C(35A)	119.7(3)
C(29A)-C(30A)-C(35A)	120.4(3)
C(30A)-C(31A)-C(32A)	120.7(3)
C(30A)-C(31A)-H(31A)	119.7
C(32A)-C(31A)-H(31A)	119.7
N(4A)-C(32A)-C(31A)	117.7(3)
N(4A)-C(32A)-C(27A)	122.5(3)
C(31A)-C(32A)-C(27A)	119.7(3)
O(5A)-C(33A)-O(6A)	123.4(4)
O(5A)-C(33A)-C(29A)	124.1(4)
O(6A)-C(33A)-C(29A)	112.5(4)
O(6A)-C(34A)-H(34A)	109.5
O(6A)-C(34A)-H(34B)	109.5
H(34A)-C(34A)-H(34B)	109.5
O(6A)-C(34A)-H(34C)	109.5
H(34A)-C(34A)-H(34C)	109.5
H(34B)-C(34A)-H(34C)	109.5
O(7A)-C(35A)-O(8A)	123.7(3)
O(7A)-C(35A)-C(30A)	124.6(4)
O(8A)-C(35A)-C(30A)	111.7(3)
O(8A)-C(36A)-H(36A)	109.5
O(8A)-C(36A)-H(36B)	109.5
H(36A)-C(36A)-H(36B)	109.5
O(8A)-C(36A)-H(36C)	109.5
H(36A)-C(36A)-H(36C)	109.5
H(36B)-C(36A)-H(36C)	109.5
C(38A)-C(37A)-C(5A)	104.6(3)
C(38A)-C(37A)-C(41A)	98.5(3)
C(5A)-C(37A)-C(41A)	99.0(3)
C(38A)-C(37A)-H(37A)	117.2

C(5A)-C(37A)-H(37A)	117.2
C(41A)-C(37A)-H(37A)	117.2
N(5A)-C(38A)-C(39A)	124.3(3)
N(5A)-C(38A)-C(37A)	129.2(3)
C(39A)-C(38A)-C(37A)	106.5(3)
N(6A)-C(39A)-C(38A)	123.9(3)
N(6A)-C(39A)-C(40A)	129.4(3)
C(38A)-C(39A)-C(40A)	106.7(3)
C(39A)-C(40A)-C(6A)	105.1(3)
C(39A)-C(40A)-C(41A)	98.4(3)
C(6A)-C(40A)-C(41A)	98.5(3)
C(39A)-C(40A)-H(40A)	117.2
C(6A)-C(40A)-H(40A)	117.2
C(41A)-C(40A)-H(40A)	117.2
C(37A)-C(41A)-C(40A)	95.3(3)
C(37A)-C(41A)-H(41A)	112.7
C(40A)-C(41A)-H(41A)	112.7
C(37A)-C(41A)-H(41B)	112.7
C(40A)-C(41A)-H(41B)	112.7
H(41A)-C(41A)-H(41B)	110.2
N(5A)-C(42A)-C(47A)	122.8(3)
N(5A)-C(42A)-C(43A)	117.7(3)
C(47A)-C(42A)-C(43A)	119.5(3)
C(44A)-C(43A)-C(42A)	121.1(3)
C(44A)-C(43A)-H(43A)	119.4
C(42A)-C(43A)-H(43A)	119.4
C(43A)-C(44A)-C(45A)	119.2(3)
C(43A)-C(44A)-C(48A)	118.5(3)
C(45A)-C(44A)-C(48A)	121.9(3)
C(46A)-C(45A)-C(44A)	120.0(3)
C(46A)-C(45A)-C(50A)	117.7(3)
C(44A)-C(45A)-C(50A)	122.2(3)
C(45A)-C(46A)-C(47A)	121.1(3)
C(45A)-C(46A)-H(46A)	119.5
C(47A)-C(46A)-H(46A)	119.5
N(6A)-C(47A)-C(46A)	119.3(3)

N(6A)-C(47A)-C(42A)	121.8(3)
C(46A)-C(47A)-C(42A)	118.9(3)
O(9A)-C(48A)-O(10A)	123.8(3)
O(9A)-C(48A)-C(44A)	124.6(3)
O(10A)-C(48A)-C(44A)	111.5(3)
O(10A)-C(49A)-H(49A)	109.5
O(10A)-C(49A)-H(49B)	109.5
H(49A)-C(49A)-H(49B)	109.5
O(10A)-C(49A)-H(49C)	109.5
H(49A)-C(49A)-H(49C)	109.5
H(49B)-C(49A)-H(49C)	109.5
O(11A)-C(50A)-O(12A)	124.3(3)
O(11A)-C(50A)-C(45A)	124.3(4)
O(12A)-C(50A)-C(45A)	111.4(3)
O(12A)-C(51A)-H(51A)	109.5
O(12A)-C(51A)-H(51B)	109.5
H(51A)-C(51A)-H(51B)	109.5
O(12A)-C(51A)-H(51C)	109.5
H(51A)-C(51A)-H(51C)	109.5
H(51B)-C(51A)-H(51C)	109.5
C(18B)-O(2B)-C(19B)	113.6(3)
C(20B)-O(4B)-C(21B)	115.7(4)
C(33B)-O(6B)-C(34B)	116.6(4)
C(35B)-O(8B)-C(36B)	116.0(4)
C(48B)-O(10B)-C(49B)	115.6(3)
C(50B)-O(12B)-C(51B)	115.7(3)
C(8B)-N(1B)-C(12B)	113.3(3)
C(9B)-N(2B)-C(17B)	113.8(3)
C(23B)-N(3B)-C(27B)	113.7(3)
C(24B)-N(4B)-C(32B)	113.5(3)
C(38B)-N(5B)-C(42B)	113.8(3)
C(39B)-N(6B)-C(47B)	114.0(3)
C(6B)-C(1B)-C(2B)	120.1(3)
C(6B)-C(1B)-C(7B)	133.5(3)
C(2B)-C(1B)-C(7B)	106.4(3)
C(3B)-C(2B)-C(1B)	120.3(3)

C(3B)-C(2B)-C(10B)	132.6(3)
C(1B)-C(2B)-C(10B)	107.1(3)
C(2B)-C(3B)-C(4B)	119.9(3)
C(2B)-C(3B)-C(22B)	133.8(3)
C(4B)-C(3B)-C(22B)	106.2(3)
C(5B)-C(4B)-C(3B)	119.8(3)
C(5B)-C(4B)-C(25B)	132.4(3)
C(3B)-C(4B)-C(25B)	107.7(3)
C(4B)-C(5B)-C(6B)	120.1(3)
C(4B)-C(5B)-C(37B)	132.1(3)
C(6B)-C(5B)-C(37B)	107.7(3)
C(1B)-C(6B)-C(5B)	119.6(3)
C(1B)-C(6B)-C(40B)	134.7(3)
C(5B)-C(6B)-C(40B)	105.6(3)
C(8B)-C(7B)-C(1B)	106.2(2)
C(8B)-C(7B)-C(11B)	97.8(2)
C(1B)-C(7B)-C(11B)	98.8(3)
C(8B)-C(7B)-H(7B)	117.0
C(1B)-C(7B)-H(7B)	117.0
C(11B)-C(7B)-H(7B)	117.0
N(1B)-C(8B)-C(9B)	124.1(3)
N(1B)-C(8B)-C(7B)	129.3(3)
C(9B)-C(8B)-C(7B)	106.5(3)
N(2B)-C(9B)-C(8B)	124.2(3)
N(2B)-C(9B)-C(10B)	129.5(3)
C(8B)-C(9B)-C(10B)	106.2(3)
C(9B)-C(10B)-C(2B)	105.8(2)
C(9B)-C(10B)-C(11B)	98.4(3)
C(2B)-C(10B)-C(11B)	98.8(2)
C(9B)-C(10B)-H(10B)	117.0
C(2B)-C(10B)-H(10B)	117.0
C(11B)-C(10B)-H(10B)	117.0
C(7B)-C(11B)-C(10B)	95.3(2)
C(7B)-C(11B)-H(11C)	112.7
C(10B)-C(11B)-H(11C)	112.7
C(7B)-C(11B)-H(11D)	112.7

C(10B)-C(11B)-H(11D)	112.7
H(11C)-C(11B)-H(11D)	110.2
N(1B)-C(12B)-C(13B)	117.9(3)
N(1B)-C(12B)-C(17B)	122.8(3)
C(13B)-C(12B)-C(17B)	119.3(3)
C(14B)-C(13B)-C(12B)	120.7(3)
C(14B)-C(13B)-H(13B)	119.6
C(12B)-C(13B)-H(13B)	119.6
C(13B)-C(14B)-C(15B)	119.8(3)
C(13B)-C(14B)-C(18B)	117.4(3)
C(15B)-C(14B)-C(18B)	122.8(3)
C(16B)-C(15B)-C(14B)	119.9(3)
C(16B)-C(15B)-C(20B)	117.5(3)
C(14B)-C(15B)-C(20B)	122.3(3)
C(15B)-C(16B)-C(17B)	121.0(3)
C(15B)-C(16B)-H(16B)	119.5
C(17B)-C(16B)-H(16B)	119.5
N(2B)-C(17B)-C(16B)	119.0(3)
N(2B)-C(17B)-C(12B)	121.9(3)
C(16B)-C(17B)-C(12B)	119.1(3)
O(1B)-C(18B)-O(2B)	124.3(4)
O(1B)-C(18B)-C(14B)	126.2(4)
O(2B)-C(18B)-C(14B)	109.3(3)
O(2B)-C(19B)-H(19D)	109.5
O(2B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
O(2B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
O(3B)-C(20B)-O(4B)	125.2(4)
O(3B)-C(20B)-C(15B)	123.5(4)
O(4B)-C(20B)-C(15B)	111.2(4)
O(4B)-C(21B)-H(21D)	109.5
O(4B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5
O(4B)-C(21B)-H(21F)	109.5

H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(23B)-C(22B)-C(3B)	103.8(3)
C(23B)-C(22B)-C(26B)	98.4(3)
C(3B)-C(22B)-C(26B)	99.4(3)
C(23B)-C(22B)-H(22B)	117.4
C(3B)-C(22B)-H(22B)	117.4
C(26B)-C(22B)-H(22B)	117.4
N(3B)-C(23B)-C(24B)	123.5(3)
N(3B)-C(23B)-C(22B)	129.7(3)
C(24B)-C(23B)-C(22B)	106.9(3)
N(4B)-C(24B)-C(23B)	124.8(3)
N(4B)-C(24B)-C(25B)	129.2(3)
C(23B)-C(24B)-C(25B)	105.9(3)
C(4B)-C(25B)-C(24B)	103.3(2)
C(4B)-C(25B)-C(26B)	99.5(3)
C(24B)-C(25B)-C(26B)	98.8(3)
C(4B)-C(25B)-H(25B)	117.4
C(24B)-C(25B)-H(25B)	117.4
C(26B)-C(25B)-H(25B)	117.4
C(22B)-C(26B)-C(25B)	95.4(2)
C(22B)-C(26B)-H(26C)	112.7
C(25B)-C(26B)-H(26C)	112.7
C(22B)-C(26B)-H(26D)	112.7
C(25B)-C(26B)-H(26D)	112.7
H(26C)-C(26B)-H(26D)	110.1
N(3B)-C(27B)-C(28B)	118.1(3)
N(3B)-C(27B)-C(32B)	122.4(3)
C(28B)-C(27B)-C(32B)	119.5(3)
C(29B)-C(28B)-C(27B)	120.8(3)
C(29B)-C(28B)-H(28B)	119.6
C(27B)-C(28B)-H(28B)	119.6
C(28B)-C(29B)-C(30B)	119.6(3)
C(28B)-C(29B)-C(33B)	119.3(3)
C(30B)-C(29B)-C(33B)	120.8(3)
C(31B)-C(30B)-C(29B)	120.1(3)

C(31B)-C(30B)-C(35B)	118.1(3)
C(29B)-C(30B)-C(35B)	121.7(3)
C(30B)-C(31B)-C(32B)	120.8(3)
C(30B)-C(31B)-H(31B)	119.6
C(32B)-C(31B)-H(31B)	119.6
N(4B)-C(32B)-C(31B)	118.7(3)
N(4B)-C(32B)-C(27B)	122.1(3)
C(31B)-C(32B)-C(27B)	119.1(3)
O(5B)-C(33B)-O(6B)	123.8(4)
O(5B)-C(33B)-C(29B)	125.0(4)
O(6B)-C(33B)-C(29B)	111.1(4)
O(6B)-C(34B)-H(34D)	109.5
O(6B)-C(34B)-H(34E)	109.5
H(34D)-C(34B)-H(34E)	109.5
O(6B)-C(34B)-H(34F)	109.5
H(34D)-C(34B)-H(34F)	109.5
H(34E)-C(34B)-H(34F)	109.5
O(7B)-C(35B)-O(8B)	125.1(4)
O(7B)-C(35B)-C(30B)	124.0(4)
O(8B)-C(35B)-C(30B)	110.7(4)
O(8B)-C(36B)-H(36D)	109.5
O(8B)-C(36B)-H(36E)	109.5
H(36D)-C(36B)-H(36E)	109.5
O(8B)-C(36B)-H(36F)	109.5
H(36D)-C(36B)-H(36F)	109.5
H(36E)-C(36B)-H(36F)	109.5
C(5B)-C(37B)-C(38B)	101.8(2)
C(5B)-C(37B)-C(41B)	99.6(2)
C(38B)-C(37B)-C(41B)	99.7(2)
C(5B)-C(37B)-H(37B)	117.5
C(38B)-C(37B)-H(37B)	117.5
C(41B)-C(37B)-H(37B)	117.5
N(5B)-C(38B)-C(39B)	124.2(3)
N(5B)-C(38B)-C(37B)	128.9(3)
C(39B)-C(38B)-C(37B)	106.6(3)
N(6B)-C(39B)-C(38B)	123.6(3)

N(6B)-C(39B)-C(40B)	130.1(3)
C(38B)-C(39B)-C(40B)	106.1(3)
C(39B)-C(40B)-C(6B)	103.6(2)
C(39B)-C(40B)-C(41B)	98.9(2)
C(6B)-C(40B)-C(41B)	99.7(2)
C(39B)-C(40B)-H(40B)	117.2
C(6B)-C(40B)-H(40B)	117.2
C(41B)-C(40B)-H(40B)	117.2
C(40B)-C(41B)-C(37B)	95.3(2)
C(40B)-C(41B)-H(41C)	112.7
C(37B)-C(41B)-H(41C)	112.7
C(40B)-C(41B)-H(41D)	112.7
C(37B)-C(41B)-H(41D)	112.7
H(41C)-C(41B)-H(41D)	110.2
N(5B)-C(42B)-C(43B)	118.6(3)
N(5B)-C(42B)-C(47B)	121.9(3)
C(43B)-C(42B)-C(47B)	119.4(3)
C(44B)-C(43B)-C(42B)	120.9(3)
C(44B)-C(43B)-H(43B)	119.5
C(42B)-C(43B)-H(43B)	119.5
C(43B)-C(44B)-C(45B)	119.8(3)
C(43B)-C(44B)-C(48B)	117.7(3)
C(45B)-C(44B)-C(48B)	122.3(3)
C(46B)-C(45B)-C(44B)	120.0(3)
C(46B)-C(45B)-C(50B)	120.0(3)
C(44B)-C(45B)-C(50B)	119.7(3)
C(45B)-C(46B)-C(47B)	120.9(3)
C(45B)-C(46B)-H(46B)	119.6
C(47B)-C(46B)-H(46B)	119.6
N(6B)-C(47B)-C(46B)	118.6(3)
N(6B)-C(47B)-C(42B)	122.4(3)
C(46B)-C(47B)-C(42B)	118.9(3)
O(9B)-C(48B)-O(10B)	124.6(3)
O(9B)-C(48B)-C(44B)	123.8(3)
O(10B)-C(48B)-C(44B)	111.5(3)
O(10B)-C(49B)-H(49D)	109.5

O(10B)-C(49B)-H(49E)	109.5
H(49D)-C(49B)-H(49E)	109.5
O(10B)-C(49B)-H(49F)	109.5
H(49D)-C(49B)-H(49F)	109.5
H(49E)-C(49B)-H(49F)	109.5
O(11B)-C(50B)-O(12B)	123.9(3)
O(11B)-C(50B)-C(45B)	124.7(3)
O(12B)-C(50B)-C(45B)	111.5(3)
O(12B)-C(51B)-H(51D)	109.5
O(12B)-C(51B)-H(51E)	109.5
H(51D)-C(51B)-H(51E)	109.5
O(12B)-C(51B)-H(51F)	109.5
H(51D)-C(51B)-H(51F)	109.5
H(51E)-C(51B)-H(51F)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1C)	73(1)	56(1)	66(1)	-21(1)	-12(1)	-19(1)
Cl(2C)	74(1)	74(1)	74(1)	-21(1)	-26(1)	11(1)
C(1C)	56(3)	39(2)	62(3)	-12(2)	-9(2)	-9(2)
Cl(1E)	84(2)	83(2)	72(2)	-24(1)	-18(1)	-4(1)
Cl(2E)	156(4)	191(4)	69(2)	-31(3)	-22(2)	40(3)
C(1E)	109(9)	26(4)	37(5)	-2(4)	-19(5)	17(5)
O(1H)	57(4)	87(5)	79(5)	-40(4)	-17(4)	-3(4)
Cl(1F)	82(1)	64(1)	413(5)	-20(2)	-42(2)	10(1)
C(1F)	52(6)	84(7)	130(9)	-84(7)	-69(6)	37(5)
O(1D)	140(4)	121(4)	99(3)	-70(3)	-50(3)	52(3)
O(2D)	76(3)	88(3)	138(4)	-61(3)	2(3)	-2(2)
C(1D)	181(8)	84(5)	108(6)	-12(4)	-39(5)	-30(5)
C(2D)	60(3)	61(3)	91(4)	-42(3)	-17(3)	-1(2)
C(3D)	91(5)	147(7)	135(7)	-85(6)	11(4)	-6(4)
C(4D)	237(12)	200(10)	278(14)	-181(11)	159(11)	-105(9)
O(1G)	46(3)	46(3)	56(3)	-22(3)	-5(3)	-5(2)
O(1A)	193(5)	231(6)	51(3)	-21(3)	-1(3)	-168(5)
O(2A)	111(3)	73(2)	55(2)	-19(2)	8(2)	-47(2)
O(3A)	57(3)	410(11)	127(4)	-178(6)	29(3)	-17(4)
O(4A)	95(3)	93(2)	44(2)	-32(2)	5(2)	-24(2)
O(5A)	85(3)	166(4)	30(2)	-19(2)	6(2)	27(3)
O(6A)	110(3)	59(2)	41(2)	-22(1)	-25(2)	-17(2)
O(7A)	81(2)	40(1)	26(1)	-1(1)	-4(1)	-16(1)
O(8A)	55(2)	35(1)	35(1)	2(1)	-15(1)	-5(1)
O(9A)	57(2)	69(2)	33(2)	-14(1)	1(1)	0(1)
O(10A)	41(1)	40(1)	34(1)	-4(1)	-4(1)	1(1)
O(11A)	42(2)	63(2)	85(2)	-18(2)	6(2)	-19(1)
O(12A)	56(2)	38(2)	47(2)	-13(1)	8(1)	-17(1)
N(1A)	28(2)	40(2)	38(2)	-20(1)	-12(1)	5(1)
N(2A)	27(2)	41(2)	45(2)	-23(1)	-6(1)	1(1)
N(3A)	36(2)	29(1)	24(2)	-8(1)	-2(1)	-2(1)

N(4A)	34(2)	28(1)	22(1)	-6(1)	-3(1)	-4(1)
N(5A)	30(1)	27(1)	31(2)	-13(1)	-6(1)	1(1)
N(6A)	35(2)	34(2)	37(2)	-18(1)	-13(1)	0(1)
C(1A)	34(2)	30(2)	24(2)	-7(1)	-9(1)	1(1)
C(2A)	35(2)	24(2)	26(2)	-6(1)	-4(1)	-2(1)
C(3A)	33(2)	25(2)	19(2)	-3(1)	-1(1)	-4(1)
C(4A)	28(2)	23(2)	19(2)	-2(1)	-1(1)	-2(1)
C(5A)	33(2)	25(2)	22(2)	-5(1)	-6(1)	1(1)
C(6A)	34(2)	30(2)	26(2)	-8(1)	-8(1)	-1(1)
C(7A)	36(2)	40(2)	34(2)	-16(2)	-13(2)	5(2)
C(8A)	26(2)	36(2)	42(2)	-18(2)	-12(2)	6(2)
C(9A)	29(2)	30(2)	39(2)	-18(2)	-11(2)	6(1)
C(10A)	36(2)	27(2)	38(2)	-12(2)	-10(2)	2(1)
C(11A)	41(2)	36(2)	40(2)	-11(2)	-16(2)	9(2)
C(12A)	24(2)	40(2)	44(2)	-21(2)	-9(2)	3(2)
C(13A)	33(2)	43(2)	48(2)	-20(2)	-13(2)	0(2)
C(14A)	28(2)	56(2)	50(2)	-20(2)	-5(2)	-6(2)
C(15A)	37(2)	85(3)	50(3)	-38(2)	0(2)	-11(2)
C(16A)	37(2)	73(3)	55(3)	-40(2)	2(2)	-16(2)
C(17A)	27(2)	46(2)	43(2)	-25(2)	-8(2)	1(2)
C(18A)	54(3)	84(3)	60(3)	-9(3)	-12(2)	-27(3)
C(19A)	205(11)	118(7)	52(5)	-5(5)	-17(6)	-116(8)
C(19C)	108(16)	118(17)	36(10)	-23(10)	25(9)	-48(13)
C(20A)	77(4)	144(5)	59(3)	-56(4)	20(3)	-60(4)
C(21A)	123(5)	160(7)	66(4)	-52(4)	7(4)	-58(5)
C(22A)	34(2)	24(2)	25(2)	-7(1)	-4(1)	-4(1)
C(23A)	31(2)	26(2)	27(2)	-8(1)	-5(1)	-6(1)
C(24A)	28(2)	27(2)	24(2)	-7(1)	-3(1)	-6(1)
C(25A)	30(2)	27(2)	22(2)	-7(1)	-1(1)	-4(1)
C(26A)	33(2)	30(2)	23(2)	-4(1)	-3(1)	-8(1)
C(27A)	35(2)	31(2)	25(2)	-7(1)	-3(1)	-5(1)
C(28A)	40(2)	36(2)	26(2)	-11(2)	-2(2)	-4(2)
C(29A)	41(2)	38(2)	24(2)	-10(2)	1(2)	-11(2)
C(30A)	42(2)	33(2)	24(2)	-5(1)	-6(2)	-12(2)
C(31A)	40(2)	28(2)	25(2)	-5(1)	-4(1)	-4(1)
C(32A)	34(2)	30(2)	22(2)	-5(1)	-1(1)	-8(1)

C(33A)	70(3)	51(2)	27(2)	-9(2)	-4(2)	4(2)
C(34A)	201(8)	113(5)	44(3)	-43(3)	-37(4)	0(5)
C(35A)	55(2)	27(2)	27(2)	-6(2)	-10(2)	-12(2)
C(36A)	75(3)	34(2)	45(2)	-3(2)	-33(2)	1(2)
C(37A)	31(2)	31(2)	26(2)	-10(1)	-2(1)	0(1)
C(38A)	32(2)	28(2)	29(2)	-16(1)	-5(1)	2(1)
C(39A)	32(2)	32(2)	32(2)	-20(2)	-8(1)	1(1)
C(40A)	36(2)	35(2)	30(2)	-14(2)	-14(2)	4(2)
C(41A)	47(2)	37(2)	30(2)	-15(2)	-9(2)	3(2)
C(42A)	29(2)	30(2)	29(2)	-18(1)	-5(1)	-2(1)
C(43A)	30(2)	32(2)	33(2)	-16(2)	-5(1)	-3(1)
C(44A)	36(2)	31(2)	32(2)	-17(2)	-3(2)	-3(1)
C(45A)	36(2)	38(2)	37(2)	-18(2)	-1(2)	-9(2)
C(46A)	31(2)	40(2)	42(2)	-22(2)	-7(2)	-4(2)
C(47A)	35(2)	33(2)	36(2)	-20(2)	-8(2)	-3(2)
C(48A)	43(2)	34(2)	33(2)	-14(2)	-2(2)	-7(2)
C(49A)	57(3)	50(2)	44(2)	-1(2)	-13(2)	1(2)
C(50A)	43(2)	53(2)	41(2)	-21(2)	1(2)	-17(2)
C(51A)	87(3)	54(3)	62(3)	-20(2)	22(3)	-31(2)
O(1B)	59(2)	76(2)	62(2)	12(2)	-18(2)	-3(2)
O(2B)	48(2)	55(2)	66(2)	-23(2)	-22(1)	3(1)
O(3B)	67(2)	85(2)	52(2)	-22(2)	6(2)	22(2)
O(4B)	64(2)	56(2)	60(2)	-34(2)	-11(2)	18(2)
O(5B)	42(2)	107(3)	104(3)	-63(2)	-7(2)	-6(2)
O(6B)	48(2)	186(4)	85(3)	-91(3)	21(2)	-29(2)
O(7B)	69(2)	133(3)	75(2)	-54(2)	-4(2)	-48(2)
O(8B)	77(2)	101(3)	85(2)	-59(2)	39(2)	-61(2)
O(9B)	39(1)	47(1)	44(2)	-25(1)	-12(1)	-4(1)
O(10B)	36(1)	49(1)	42(2)	-21(1)	1(1)	-17(1)
O(11B)	33(1)	48(2)	49(2)	-21(1)	-7(1)	2(1)
O(12B)	39(1)	36(1)	39(1)	-9(1)	-16(1)	5(1)
N(1B)	36(2)	27(1)	26(2)	-11(1)	-5(1)	-5(1)
N(2B)	36(2)	35(2)	26(2)	-14(1)	-7(1)	-3(1)
N(3B)	38(2)	33(2)	22(1)	-7(1)	-4(1)	-6(1)
N(4B)	38(2)	28(1)	26(2)	-8(1)	-6(1)	-3(1)
N(5B)	31(2)	26(1)	26(1)	-10(1)	-6(1)	0(1)

N(6B)	31(2)	28(1)	23(1)	-9(1)	-5(1)	-3(1)
C(1B)	24(2)	30(2)	26(2)	-10(1)	-5(1)	-1(1)
C(2B)	25(2)	33(2)	24(2)	-12(1)	-7(1)	1(1)
C(3B)	29(2)	32(2)	24(2)	-10(1)	-7(1)	1(1)
C(4B)	24(2)	29(2)	26(2)	-9(1)	-8(1)	2(1)
C(5B)	26(2)	31(2)	25(2)	-12(1)	-6(1)	1(1)
C(6B)	26(2)	30(2)	22(2)	-8(1)	-5(1)	-3(1)
C(7B)	31(2)	32(2)	27(2)	-11(1)	-1(1)	-9(1)
C(8B)	34(2)	27(2)	27(2)	-13(1)	-4(1)	-9(1)
C(9B)	34(2)	27(2)	27(2)	-13(1)	-8(1)	-5(1)
C(10B)	35(2)	34(2)	24(2)	-13(1)	-9(1)	0(1)
C(11B)	33(2)	38(2)	36(2)	-19(2)	-6(2)	-4(2)
C(12B)	37(2)	30(2)	28(2)	-14(1)	-7(1)	-4(1)
C(13B)	41(2)	35(2)	28(2)	-15(2)	-10(2)	-3(2)
C(14B)	39(2)	37(2)	35(2)	-17(2)	-14(2)	1(2)
C(15B)	38(2)	45(2)	36(2)	-19(2)	-8(2)	2(2)
C(16B)	38(2)	48(2)	29(2)	-20(2)	-5(2)	-2(2)
C(17B)	36(2)	33(2)	28(2)	-14(2)	-9(1)	-2(1)
C(18B)	33(2)	47(2)	40(2)	-20(2)	-6(2)	2(2)
C(19B)	52(3)	74(3)	88(4)	-27(3)	-33(3)	13(2)
C(20B)	49(2)	68(3)	40(2)	-28(2)	-13(2)	11(2)
C(21B)	85(4)	90(4)	74(4)	-52(3)	-19(3)	43(3)
C(22B)	40(2)	36(2)	20(2)	-9(1)	-7(1)	-4(2)
C(23B)	38(2)	30(2)	19(2)	-5(1)	-6(1)	-4(1)
C(24B)	37(2)	25(2)	21(2)	-2(1)	-5(1)	-2(1)
C(25B)	39(2)	30(2)	23(2)	-7(1)	-9(1)	-1(1)
C(26B)	38(2)	36(2)	26(2)	-6(2)	-8(2)	-3(2)
C(27B)	36(2)	32(2)	21(2)	-4(1)	-6(1)	-5(1)
C(28B)	38(2)	41(2)	31(2)	-14(2)	-3(2)	-5(2)
C(29B)	39(2)	51(2)	40(2)	-17(2)	-1(2)	-9(2)
C(30B)	45(2)	49(2)	39(2)	-16(2)	-2(2)	-14(2)
C(31B)	44(2)	37(2)	31(2)	-13(2)	-2(2)	-11(2)
C(32B)	40(2)	28(2)	22(2)	-3(1)	-4(1)	-6(1)
C(33B)	43(3)	81(3)	69(3)	-43(3)	7(2)	-20(2)
C(34B)	52(3)	242(9)	140(6)	-138(7)	35(4)	-28(4)
C(35B)	48(3)	77(3)	68(3)	-43(3)	7(2)	-24(2)

C(36B)	96(5)	159(6)	163(7)	-107(6)	57(4)	-94(5)
C(37B)	32(2)	26(2)	24(2)	-9(1)	-7(1)	2(1)
C(38B)	34(2)	30(2)	21(2)	-13(1)	-3(1)	-4(1)
C(39B)	29(2)	28(2)	20(2)	-12(1)	-2(1)	-3(1)
C(40B)	29(2)	32(2)	23(2)	-10(1)	-2(1)	-6(1)
C(41B)	30(2)	37(2)	29(2)	-17(2)	-2(1)	-1(1)
C(42B)	31(2)	30(2)	23(2)	-11(1)	-4(1)	-3(1)
C(43B)	38(2)	29(2)	26(2)	-11(1)	-4(1)	-6(1)
C(44B)	30(2)	35(2)	27(2)	-16(2)	-4(1)	-5(1)
C(45B)	34(2)	33(2)	27(2)	-14(1)	-7(1)	-1(1)
C(46B)	35(2)	28(2)	24(2)	-11(1)	-5(1)	-1(1)
C(47B)	31(2)	26(2)	23(2)	-10(1)	-6(1)	-3(1)
C(48B)	34(2)	33(2)	37(2)	-19(2)	-5(2)	-1(2)
C(49B)	37(2)	56(2)	66(3)	-30(2)	5(2)	-17(2)
C(50B)	36(2)	36(2)	33(2)	-20(2)	-9(2)	1(2)
C(51B)	48(2)	42(2)	48(2)	-18(2)	-25(2)	14(2)

Table S5. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for compound **3**.

	x	y	z	U(eq)
H(1C1)	252	2400	7358	65
H(1C2)	14	1456	7638	65
H(1E)	5024	2182	2703	76
H(2E)	5626	1292	2872	76
H(1F1)	4618	4288	4856	88
H(1F2)	4101	5221	4693	88
H(1D1)	3632	3169	423	190
H(1D2)	2688	3603	607	190
H(1D3)	3473	4061	541	190
H(3D1)	3197	4235	-1787	144
H(3D2)	3917	4747	-1792	144
H(4D1)	4419	3908	-2473	342
H(4D2)	4198	3083	-1777	342
H(4D3)	4914	3596	-1786	342
H(7A)	4420	-2028	6009	43
H(10A)	3533	-3566	5221	41
H(11A)	3758	-3392	6384	49
H(11B)	4678	-3507	5906	49
H(13A)	6106	-527	3509	48
H(16A)	5241	-2385	2693	60
H(19A)	7580	1264	2059	177
H(19B)	7034	1308	1469	177
H(19C)	7907	670	1582	177
H(19G)	7184	945	546	134
H(19H)	7513	931	1245	134
H(19I)	6532	1225	1155	134
H(21A)	5847	-859	111	165
H(21B)	6386	-1757	513	165
H(21C)	6745	-888	327	165
H(22A)	1821	-3159	4891	34

H(25A)	201	-1123	5314	33
H(26A)	255	-2530	5116	36
H(26B)	684	-2742	5836	36
H(28A)	2132	-1556	2115	42
H(31A)	34	555	2614	39
H(34A)	761	-258	-416	173
H(34B)	1696	-741	-273	173
H(34C)	1483	269	-463	173
H(36A)	-1403	2110	1029	79
H(36B)	-792	1824	405	79
H(36C)	-496	2422	725	79
H(37A)	766	-184	5971	37
H(40A)	3292	-623	6299	39
H(41A)	1797	-983	6906	46
H(41B)	1783	35	6683	46
H(43A)	1128	2606	3792	37
H(46A)	3980	2100	4101	42
H(49A)	194	4960	2401	84
H(49B)	733	4442	1903	84
H(49C)	1112	5181	1986	84
H(51A)	3409	5572	2270	105
H(51B)	4014	4911	1934	105
H(51C)	4229	5016	2632	105
H(7B)	-1912	3075	3154	36
H(10B)	-1214	4080	903	36
H(11C)	-2475	3770	1924	41
H(11D)	-1895	2866	1954	41
H(13B)	985	1225	3569	40
H(16B)	1755	2325	1038	45
H(19D)	4424	374	3360	107
H(19E)	3965	-391	3419	107
H(19F)	3702	34	4028	107
H(21D)	3876	-832	1964	125
H(21E)	4308	19	1603	125
H(21F)	3705	-173	1170	125
H(22B)	-892	5817	188	38

H(25B)	-1478	7425	1391	38
H(26C)	-2059	6886	579	42
H(26D)	-1273	7390	94	42
H(28B)	2308	5833	-87	44
H(31B)	1666	7537	1346	45
H(34D)	4556	5927	-1442	195
H(34E)	4772	5340	-641	195
H(34F)	5004	6290	-1010	195
H(36D)	4631	8592	-266	185
H(36E)	4784	7880	513	185
H(36F)	4114	8724	460	185
H(37B)	-1980	6764	2912	33
H(40B)	-2128	4165	4013	34
H(41C)	-2582	5651	4109	37
H(41D)	-2992	5637	3446	37
H(43B)	1049	6449	3470	37
H(46B)	795	3586	4883	35
H(49D)	3600	6897	2762	76
H(49E)	3891	6206	3507	76
H(49F)	3223	7033	3516	76
H(51D)	2536	2143	6199	69
H(51E)	3126	2874	5927	69
H(51F)	3122	2346	5425	69

Table S6. Hydrogen bonds for compound **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1C)-H(1C1)...N(5B)#2	0.99	2.45	3.272(5)	140.0
C(1E)-H(1E)...O(11A)	0.99	2.25	3.126(9)	147.3
C(1F)-H(1F2)...O(9B)	0.99	2.32	3.277(8)	163.2
C(22A)-H(22A)...O(9B)#3	1.00	2.37	3.332(4)	159.9
C(36A)-H(36C)...N(2B)	0.98	2.69	3.493(5)	139.1
C(37A)-H(37A)...N(4A)#4	1.00	2.30	3.229(4)	154.9
C(40A)-H(40A)...O(1G)#5	1.00	2.59	3.227(6)	121.7
C(10B)-H(10B)...N(3B)#6	1.00	2.57	3.503(4)	155.2
C(19B)-H(19D)...O(1H)	0.98	2.47	3.398(9)	157.4
C(25B)-H(25B)...O(3A)#7	1.00	2.55	3.292(6)	130.9
C(28B)-H(28B)...O(1D)	0.95	2.40	3.344(5)	171.1
C(34B)-H(34E)...O(5B)#8	0.98	2.53	3.442(10)	154.0
C(49B)-H(49D)...O(7B)	0.98	2.59	3.478(6)	151.0
C(49B)-H(49E)...Cl(1F)	0.98	2.89	3.859(5)	171.4
C(49B)-H(49F)...N(3A)#9	0.98	2.69	3.393(5)	129.0

Symmetry transformations used to generate equivalent atoms:

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

#4 -x,-y,-z+1 #5 -x+1,-y,-z+1 #6 -x,-y+1,-z

#7 x-1,y+1,z #8 -x+1,-y+1,-z #9 x,y+1,z

Computational Methods. A Monte Carlo computational protocol was used to generate random structures of basket **1** – each of which was subsequently optimized with the AMBER* force field included in the MacroModel software (6). From these structures, 10 were chosen for additional geometry optimizations: the five lowest energy structures that were unique were chosen first, then five additional unique conformations were chosen to adequately represent conformational space. Specifically, the orientations of the arms of the basket were examined. For each of the ten conformations, partial atomic charge calculations were performed using the Merz–Kollman scheme (B3LYP/6-31+G*//B3LYP/6-31+G*) utilizing the Gaussian 09 program (7-12); charges were averaged over all conformations. The basket conformations were prepared for MD simulations using the *antechamber* and *leap* modules of the AMBER 11 program (13). Each basket was solvated with explicit TIP3P water molecules within 10 Å of the basket in a periodic octahedral box. MD simulations of all baskets were carried out using the *sander* module in AMBER with the general AMBER force field (FF03) (14). A three-step equilibration scheme was performed: an initial minimization step where the basket was held fixed and the positions of solvent molecules were relaxed, followed by minimization of the system as a whole. Then, the system underwent a heating phase from 0 to 300 K with a small restraint on the basket to prevent drastic fluctuations in structure. The volume was kept constant, and the SHAKE algorithm (15) was used to constrain bonds involving hydrogen atoms. Production dynamics were run over 5 ns using NPT conditions. Long-range electrostatic interactions were calculated using the particle mesh Ewald (PME) algorithm (16) with a cutoff of 10 Å.

The resulting MD trajectories were aligned and combined, and a clustering analysis was done using the *ptraj* module of AMBER to obtain ten clusters. The cavity volumes were calculated using the Solvent Extraction module of the program 3V (17) with a 10 Å outer probe radius and 0.2 Å inner probe radius. Ten unique snapshots obtained from the clustering analysis were used for our docking simulations, which were completed using Autodock 4.0 (18-19); for these docking simulations, all rotatable bonds on the guest molecules were allowed to rotate, while the basket remained rigid.

Then, molecular dynamics simulations of the three lowest energy poses of each guest from each of the 10 docking simulations were performed for 8 ns in a box of TIP3P water molecules. We monitored the dynamics of the guest–basket complex as a function of time.

Computational Results. The conformational analysis and MD simulations of **1** suggest that the basket prefers to be very open with the arms oriented up and away from the base of the basket (Figure S11). The docking simulations of DMPP suggest that the guest will orient itself in the cavity of **1** with either the P–O or the P–C_6H_5 unit oriented towards the base of the basket. In most cases, the lowest energy docked conformation places the P–O toward the basket base, while in some cases, the most populated cluster (that is not the lowest energy cluster) has the P–C_6H_5 unit toward the basket base (Figure S12). From the MD simulations of the host-guest complex, the P–C_6H_5 unit is always situated inside the cavity of **1** and either the P–C_6H_5 unit or one of the OCH_3 substituents is oriented toward the base of the basket. This preferred orientation occurs regardless of the starting orientation of the guest, including when the guest starts the MD

simulation with the phosphoryl oxygen oriented toward the basket's base. As can be seen from Figure S13, the guest will rotate such that either the P–C_6H_5 unit or OCH_3 of the guest is situated toward the base of the basket.

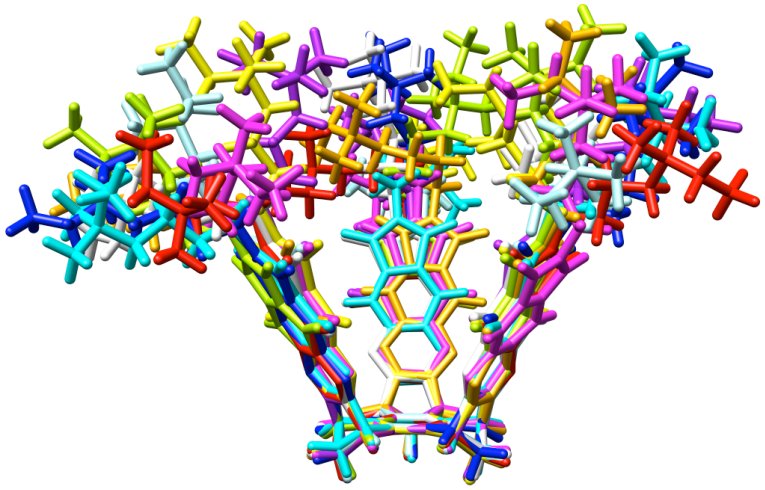


Figure S11. Ten major conformational states of **1** obtained from a clustering analysis of the MD simulations.

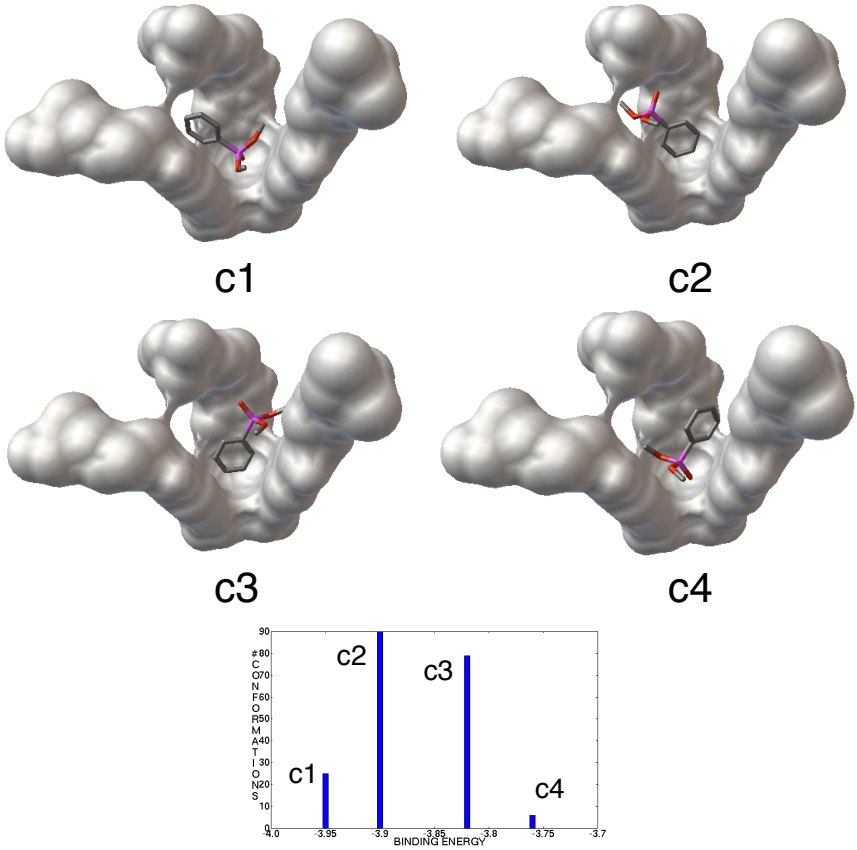


Figure S12. The docked clusters of DMPP in one of the snapshots from the MD simulation of **1**.

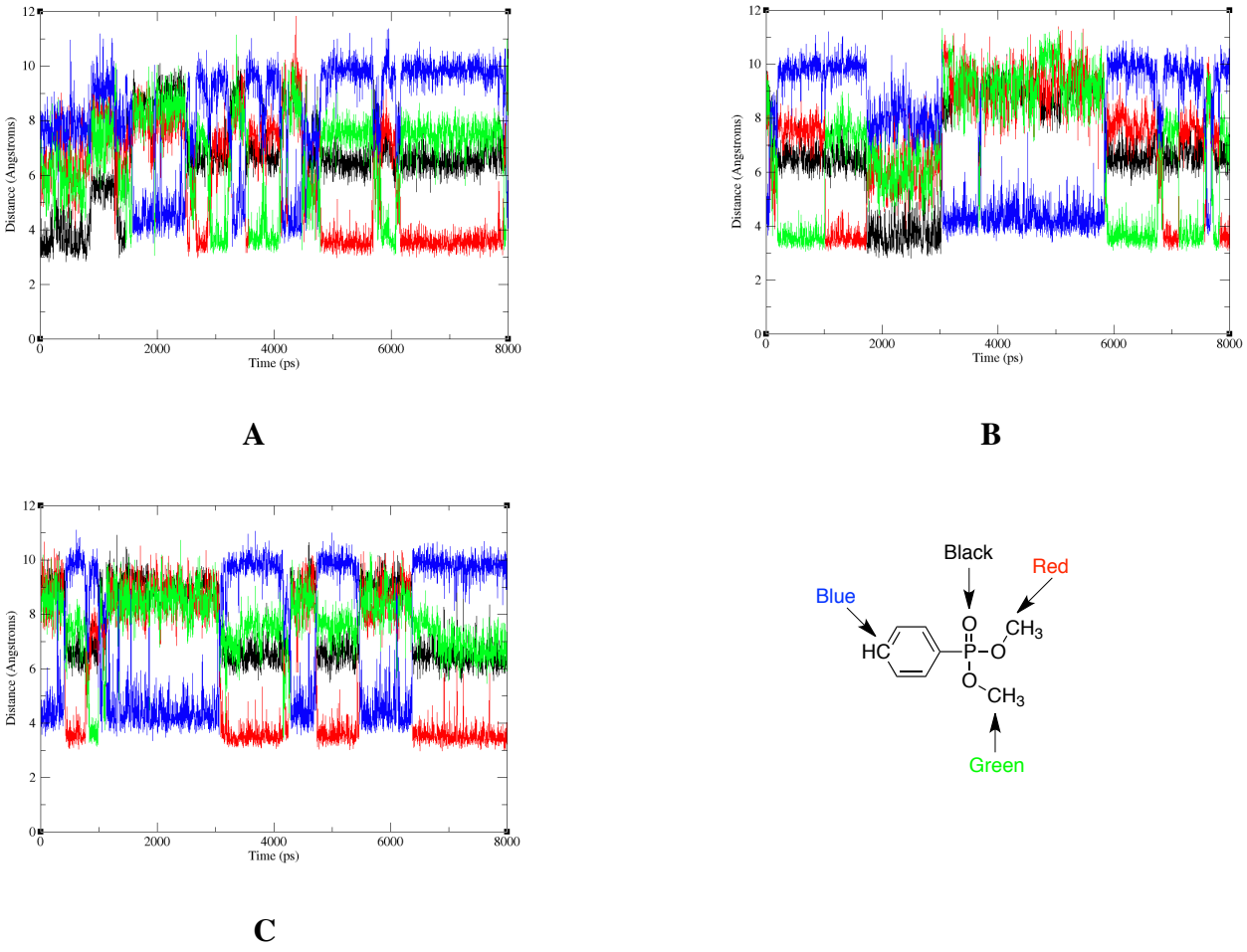


Figure S13. The plots of the distance from the center of mass of the benzene ring at the base of the basket to the phosphoryl oxygen (Black), one of the methoxy carbons (Red), the other methoxy carbon (Green), or the carbon at the *para*-position of the phenyl ring of the guest (Blue) throughout the course of the MD run for the lowest energy cluster (**A**), the second lowest energy cluster (**B**), and the third lowest energy cluster (**C**) for the snapshot shown in Figure S12.

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