Supplementary file

Table S1. Crystal data and details of refinements for the PCT and RCT complexes with betaine.

Complex	**[PCT·betaine]·2EtOH·5H$_2$O**	**[RCT·betaine]·EtOH·2H$_2$O**
	i	**ii**
Empirical formula	$C_{45}H_{73}NO_{21}$	$C_{43}H_{61}NO_{13}$
Formula weight	964.04	799.93
Crystal system	Triclinic	Triclinic
Space group	$P-1$	$P-1$
Unit cell dimensions		
a (Å)	12.0178(16)	12.1241(15)
b (Å)	12.275(2)	13.3655(19)
c (Å)	17.554(3)	13.964(2)
α (°)	109.887(4)	86.356(15)
β (°)	91.042(2)	82.010(15)
γ (°)	101.332(3)	73.242(10)
V (Å^3)	2377.4(6)	2145.1(5)
Z	2	2
F(000)	1,036	860
D_{calc} (g cm^{-3})	1.347	1.238
Crystal size (mm)	0.4 × 0.4 × 0.1	0.4 × 0.3 × 0.05
T (K)	120(2)	107(2)
μ (Mo Kα) (mm^{-1})	0.106	0.091
2θ Range (°)	4.08 − 54.0	4.30 − 54.0
Refractions collected	21,034	18,371
Independent refractions	9,860 [R_{int} = 0.0321]	8,883 [R_{int} = 0.0312]
Completeness (%) (2θ < 55.0)	94.9	94.8
Data/restraints/parameters	9,860/8/637	8,883/0/547
[a]Weighting scheme (w)	$1/[\sigma(F_o^2)^2 + (0.1482P)^2 + 1.6068P]$	$1/[\sigma(F_o^2)^2 + (0.1026P)^2 + 2.1000P]$
[b]R (for data with $I > 2\sigma(I)$)	R_1 = 0.093, wR_2 = 0.250 for 6,754 data	R_1 = 0.072, wR_2 = 0.197 for 7,067 data
[b]R (for all unique data)	R_1 = 0.124, wR_2 = 0.283 for 9,860 data	R_1 = 0.088, wR_2 = 0.211 for 8,883 data
goodness-of-fit on F^2	1.146	1.090
Max. shift/error	0.000	0.000
Max./min. residuals (e Å^{-3})	1.094/−0.741	0.551/−0.384

[a] $P = (F_o^2 + 2F_c^2)/3$; [b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Relevant bond lengths (Å) and angles (°) of non-hydrogen atoms in the PCT complex.

(i) PCT molecule

Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**
O(1)-C(2)	1.372(4)	C(5)-C(6)	1.391(5)	C(19)-C(20)	1.402(5)
O(2)-C(3)	1.382(4)	C(5)-C(7)	1.514(5)	C(19)-C(21)	1.531(5)
O(3)-C(4)	1.366(4)	C(7)-C(8)	1.525(5)	C(21)-C(33)	1.516(5)
O(4)-C(9)	1.383(4)	C(7)-C(29)	1.528(5)	C(21)-C(22)	1.528(4)
O(5)-C(10)	1.366(4)	C(8)-C(9)	1.382(5)	C(22)-C(23)	1.384(5)
O(6)-C(11)	1.380(4)	C(8)-C(13)	1.406(4)	C(22)-C(27)	1.391(5)
O(7)-C(16)	1.395(4)	C(9)-C(10)	1.398(5)	C(23)-C(24)	1.388(5)
O(8)-C(17)	1.362(4)	C(10)-C(11)	1.397(5)	C(24)-C(25)	1.401(5)
O(9)-C(18)	1.368(4)	C(11)-C(12)	1.389(5)	C(25)-C(26)	1.389(5)
O(10)-C(23)	1.379(4)	C(12)-C(13)	1.390(5)	C(26)-C(27)	1.404(5)
O(11)-C(24)	1.375(4)	C(12)-C(14)	1.533(4)	C(26)-C(28)	1.528(5)
O(12)-C(25)	1.378(4)	C(14)-C(31)	1.519(5)	C(28)-C(35)	1.560(5)
C(1)-C(6)	1.391(5)	C(14)-C(15)	1.529(5)	C(29)-C(30)	1.509(6)
C(1)-C(2)	1.400(4)	C(15)-C(16)	1.384(5)	C(31)-C(32)	1.526(5)
C(1)-C(28)	1.531(5)	C(15)-C(20)	1.401(5)	C(33)-C(34)	1.520(5)
C(2)-C(3)	1.387(5)	C(16)-C(17)	1.386(5)	C(35)-C(36)	1.530(5)
C(3)-C(4)	1.391(5)	C(17)-C(18)	1.405(5)	-	-
C(4)-C(5)	1.407(4)	C(18)-C(19)	1.395(5)	-	-
Atom1-Atom2-Atom3	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**
C(6)-C(1)-C(2)	117.3(3)	C(11)-C(10)-C(9)	120.0(3)	C(33)-C(21)-C(22)	111.7(3)
C(6)-C(1)-C(28)	122.0(3)	O(6)-C(11)-C(12)	120.0(3)	C(33)-C(21)-C(19)	113.8(3)
C(2)-C(1)-C(28)	120.7(3)	O(6)-C(11)-C(10)	119.1(3)	C(22)-C(21)-C(19)	112.0(3)
O(1)-C(2)-C(3)	120.7(3)	C(12)-C(11)-C(10)	120.8(3)	C(23)-C(22)-C(27)	118.3(3)
O(1)-C(2)-C(1)	118.6(3)	C(11)-C(12)-C(13)	117.7(3)	C(23)-C(22)-C(21)	120.0(3)
C(3)-C(2)-C(1)	120.6(3)	C(11)-C(12)-C(14)	119.5(3)	C(27)-C(22)-C(21)	121.7(3)
O(2)-C(3)-C(2)	117.8(3)	C(13)-C(12)-C(14)	122.9(3)	O(10)-C(23)-C(22)	118.9(3)
O(2)-C(3)-C(4)	121.6(3)	C(12)-C(13)-C(8)	123.1(3)	O(10)-C(23)-C(24)	120.6(3)
C(2)-C(3)-C(4)	120.6(3)	C(31)-C(14)-C(15)	113.3(3)	C(22)-C(23)-C(24)	120.4(3)
O(3)-C(4)-C(3)	121.4(3)	C(31)-C(14)-C(12)	113.1(3)	O(11)-C(24)-C(23)	117.7(3)
O(3)-C(4)-C(5)	118.2(3)	C(15)-C(14)-C(12)	109.8(3)	O(11)-C(24)-C(25)	122.0(3)
C(3)-C(4)-C(5)	120.3(3)	C(16)-C(15)-C(20)	117.4(3)	C(23)-C(24)-C(25)	120.3(3)
C(6)-C(5)-C(4)	117.2(3)	C(16)-C(15)-C(14)	120.9(3)	O(12)-C(25)-C(26)	124.2(3)
C(6)-C(5)-C(7)	121.7(3)	C(20)-C(15)-C(14)	121.7(3)	O(12)-C(25)-C(24)	114.8(3)
C(4)-C(5)-C(7)	121.0(3)	C(15)-C(16)-C(17)	121.8(3)	C(26)-C(25)-C(24)	121.0(3)
C(5)-C(6)-C(1)	123.8(3)	C(15)-C(16)-O(7)	122.6(3)	C(25)-C(26)-C(27)	116.9(3)
C(5)-C(7)-C(8)	112.0(3)	C(17)-C(16)-O(7)	115.6(3)	C(25)-C(26)-C(28)	121.1(3)
C(5)-C(7)-C(29)	112.7(3)	O(8)-C(17)-C(16)	121.8(3)	C(27)-C(26)-C(28)	122.0(3)
C(8)-C(7)-C(29)	112.5(3)	O(8)-C(17)-C(18)	118.2(3)	C(22)-C(27)-C(26)	123.1(3)
C(9)-C(8)-C(13)	117.6(3)	C(16)-C(17)-C(18)	120.0(3)	C(26)-C(28)-C(1)	111.1(3)
C(9)-C(8)-C(7)	121.0(3)	O(9)-C(18)-C(19)	125.1(3)	C(26)-C(28)-C(35)	113.4(3)
C(13)-C(8)-C(7)	121.4(3)	O(9)-C(18)-C(17)	115.0(3)	C(1)-C(28)-C(35)	110.8(3)
C(8)-C(9)-O(4)	124.7(3)	C(19)-C(18)-C(17)	119.8(3)	C(30)-C(29)-C(7)	113.2(3)
C(8)-C(9)-C(10)	120.7(3)	C(18)-C(19)-C(20)	118.3(3)	C(14)-C(31)-C(32)	112.4(3)
O(4)-C(9)-C(10)	114.6(3)	C(18)-C(19)-C(21)	121.3(3)	C(21)-C(33)-C(34)	113.4(3)
O(5)-C(10)-C(11)	118.6(3)	C(20)-C(19)-C(21)	120.5(3)	C(36)-C(35)-C(28)	113.6(3)
O(5)-C(10)-C(9)	121.4(3)	C(15)-C(20)-C(19)	122.6(3)	-	-

Table S2. *Cont.*

(ii) betaine molecule					
Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**
O(13)-C(37)	1.241(4)	C(38)-N(1)	1.499(5)	C(41)-N(1)	1.497(5)
O(14)-C(37)	1.255(4)	C(39)-N(1)	1.490(5)	-	-
C(37)-C(38)	1.527(5)	C(40)-N(1)	1.495(5)	-	-
Atom1-Atom2-Atom3	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**
O(13)-C(37)-O(14)	127.1(3)	C(39)-N(1)-C(40)	110.2(4)	C(40)-N(1)-C(38)	110.8(3)
O(13)-C(37)-C(38)	121.4(3)	C(39)-N(1)-C(41)	109.2(3)	C(41)-N(1)-C(38)	108.0(3)
O(14)-C(37)-C(38)	111.5(3)	C(40)-N(1)-C(41)	107.5(3)	-	-
N(1)-C(38)-C(37)	118.4(3)	C(39)-N(1)-C(38)	111.0(3)	-	-
(iii) ethanol molecule					
ethanol molecule 1		ethanol molecule 2			
Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**		
O(15)-C(42)	1.531(9)	O(161)-C(44)	1.378(7)		
C(42)-C(43)	1.438(10)	C(44)-O(162)	1.360(16)		
-	-	C(44)-C(45)	1.501(10)	-	
Atom1-Atom2-Atom3	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**		
C(43)-C(42)-O(15)	106.8(7)	O(162)-C(44)-O(161)	88.8(13)		
-	-	O(162)-C(44)-C(45)	133.0(12)		
-	-	O(161)-C(44)-C(45)	110.3(6)		

Symmetry transformations used to generate equivalent atoms:

Table S3. Relevant bond lengths (Å) and angles (°) of non-hydrogen atoms in the RCT complex.

(i) RCT molecule					
Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**
O(1)-C(2)	1.374(3)	C(7)-C(8)	1.525(4)	C(19)-C(20)	1.386(4)
O(2)-C(4)	1.379(3)	C(7)-C(29)	1.544(3)	C(19)-C(21)	1.529(3)
O(3)-C(9)	1.376(3)	C(8)-C(13)	1.389(3)	C(21)-C(22)	1.527(3)
O(4)-C(11)	1.374(3)	C(8)-C(9)	1.405(3)	C(21)-C(33)	1.531(3)
O(5)-C(16)	1.366(3)	C(9)-C(10)	1.380(4)	C(22)-C(27)	1.390(3)
O(6)-C(18)	1.375(3)	C(10)-C(11)	1.388(4)	C(22)-C(23)	1.395(3)
O(7)-C(23)	1.384(3)	C(11)-C(12)	1.395(3)	C(23)-C(24)	1.385(3)
O(8)-C(25)	1.374(3)	C(12)-C(13)	1.393(4)	C(24)-C(25)	1.391(3)
C(1)-C(6)	1.387(3)	C(12)-C(14)	1.524(3)	C(25)-C(26)	1.394(3)
C(1)-C(2)	1.401(3)	C(14)-C(15)	1.525(3)	C(26)-C(27)	1.404(3)
C(1)-C(28)	1.522(3)	C(14)-C(31)	1.538(3)	C(26)-C(28)	1.524(3)
C(2)-C(3)	1.385(3)	C(15)-C(20)	1.399(3)	C(28)-C(35)	1.544(3)
C(3)-C(4)	1.388(3)	C(15)-C(16)	1.408(3)	C(29)-C(30)	1.519(4)
C(4)-C(5)	1.398(3)	C(16)-C(17)	1.384(4)	C(31)-C(32)	1.520(4)
C(5)-C(6)	1.386(3)	C(17)-C(18)	1.387(4)	C(33)-C(34)	1.527(4)
C(5)-C(7)	1.524(3)	C(18)-C(19)	1.402(3)	C(35)-C(36)	1.514(4)

Table S3. *Cont.*

Atom1-Atom2-Atom3	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**
C(6)-C(1)-C(2)	116.8(2)	O(4)-C(11)-C(10)	121.3(2)	C(22)-C(21)-C(19)	110.91(19)
C(6)-C(1)-C(28)	122.0(2)	O(4)-C(11)-C(12)	118.0(2)	C(22)-C(21)-C(33)	113.2(2)
C(2)-C(1)-C(28)	121.2(2)	C(10)-C(11)-C(12)	120.7(2)	C(19)-C(21)-C(33)	112.9(2)
O(1)-C(2)-C(3)	121.1(2)	C(13)-C(12)-C(11)	117.2(2)	C(27)-C(22)-C(23)	116.9(2)
O(1)-C(2)-C(1)	117.7(2)	C(13)-C(12)-C(14)	122.8(2)	C(27)-C(22)-C(21)	122.8(2)
C(3)-C(2)-C(1)	121.2(2)	C(11)-C(12)-C(14)	119.9(2)	C(23)-C(22)-C(21)	120.3(2)
C(2)-C(3)-C(4)	119.6(2)	C(8)-C(13)-C(12)	124.0(2)	O(7)-C(23)-C(24)	120.2(2)
O(2)-C(4)-C(3)	116.6(2)	C(12)-C(14)-C(15)	111.5(2)	O(7)-C(23)-C(22)	118.2(2)
O(2)-C(4)-C(5)	122.1(2)	C(12)-C(14)-C(31)	112.6(2)	C(24)-C(23)-C(22)	121.6(2)
C(3)-C(4)-C(5)	121.3(2)	C(15)-C(14)-C(31)	112.7(2)	C(23)-C(24)-C(25)	119.9(2)
C(6)-C(5)-C(4)	116.9(2)	C(20)-C(15)-C(16)	116.6(2)	O(8)-C(25)-C(24)	116.6(2)
C(6)-C(5)-C(7)	120.9(2)	C(20)-C(15)-C(14)	121.3(2)	O(8)-C(25)-C(26)	122.4(2)
C(4)-C(5)-C(7)	122.2(2)	C(16)-C(15)-C(14)	122.1(2)	C(24)-C(25)-C(26)	121.0(2)
C(5)-C(6)-C(1)	124.2(2)	O(5)-C(16)-C(17)	116.3(2)	C(25)-C(26)-C(27)	117.0(2)
C(5)-C(7)-C(8)	110.45(19)	O(5)-C(16)-C(15)	122.9(2)	C(25)-C(26)-C(28)	121.3(2)
C(5)-C(7)-C(29)	112.4(2)	C(17)-C(16)-C(15)	120.8(2)	C(27)-C(26)-C(28)	121.7(2)
C(8)-C(7)-C(29)	112.8(2)	C(16)-C(17)-C(18)	120.6(2)	C(22)-C(27)-C(26)	123.6(2)
C(13)-C(8)-C(9)	116.5(2)	O(6)-C(18)-C(17)	116.8(2)	C(1)-C(28)-C(26)	110.49(19)
C(13)-C(8)-C(7)	123.0(2)	O(6)-C(18)-C(19)	122.5(2)	C(1)-C(28)-C(35)	112.6(2)
C(9)-C(8)-C(7)	120.5(2)	C(17)-C(18)-C(19)	120.7(2)	C(26)-C(28)-C(35)	112.70(19)
O(3)-C(9)-C(10)	120.1(2)	C(20)-C(19)-C(18)	117.2(2)	C(30)-C(29)-C(7)	112.9(2)
O(3)-C(9)-C(8)	118.7(2)	C(20)-C(19)-C(21)	120.9(2)	C(32)-C(31)-C(14)	112.7(2)
C(10)-C(9)-C(8)	121.2(2)	C(18)-C(19)-C(21)	121.9(2)	C(34)-C(33)-C(21)	112.2(2)
C(9)-C(10)-C(11)	120.4(2)	C(19)-C(20)-C(15)	124.1(2)	C(36)-C(35)-C(28)	112.7(2)
(ii) betaine molecule					
Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**
O(9)-C(37)	1.242(3)	C(38)-N(1)	1.503(3)	C(41)-N(1)	1.499(3)
O(10)-C(37)	1.234(3)	C(39)-N(1)	1.501(3)	-	-
C(37)-C(38)	1.534(4)	C(40)-N(1)	1.492(4)	-	-
Atom1-Atom2-Atom3	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**	**Atom1-Atom2-Atom3**	**Angle (°)**
O(10)-C(37)-O(9)	126.3(2)	C(40)-N(1)-C(41)	108.4(2)	C(41)-N(1)-C(38)	107.2(2)
O(10)-C(37)-C(38)	119.0(2)	C(40)-N(1)-C(39)	110.4(2)	C(39)-N(1)-C(38)	112.0(2)
O(9)-C(37)-C(38)	114.7(2)	C(41)-N(1)-C(39)	108.6(2)	-	-
N(1)-C(38)-C(37)	116.0(2)	C(40)-N(1)-C(38)	110.1(2)	-	-
(iii) ethanol molecules					
Atom1-Atom2	**Distance (Å)**	**Atom1-Atom2**	**Distance (Å)**		
O(11)-C(42)	1.426(4)	C(42)-C(43)	1.506(5)	-	
Atom1-Atom2-Atom3	**Angle (°)**	-	-		
O(11)-C(42)-C(43)	112.2(3)	-	-		

Symmetry transformations used to generate equivalent atoms:

Table S4. Torsion angles (°) of non-hydrogen atoms of the betaine molecules in the PCT and RCT complexes.

(i) betaine molecule in PCT complex	
Atom1-Atom2-Atom3-Atom4	**Angle (°)**
O(13)-C(37)-C(38)-N(1)	2.7(5)
O(14)-C(37)-C(38)-N(1)	179.7(3)
C(37)-C(38)-N(1)-C(39)	−62.2(4)
C(37)-C(38)-N(1)-C(40)	60.6(4)
C(37)-C(38)-N(1)-C(41)	178.1(3)
(ii) betaine molecule in RCT complex	
Atom1-Atom2-Atom3-Atom4	**Angle (°)**
O(10)-C(37)-C(38)-N(1)	35.5(4)
O(9)-C(37)-C(38)-N(1)	−146.5(2)
C(37)-C(38)-N(1)-C(40)	55.1(3)
C(37)-C(38)-N(1)-C(41)	172.8(2)
C(37)-C(38)-N(1)-C(39)	−68.2(3)

Symmetry transformations used to generate equivalent atoms:

Table S5. Intermolecular hydrogen bonds in the PCT complex.

Atom1	**Atom2**	**Distance (Å)**	**Atom1**	**Atom2**	**Distance (Å)**
O(1)	O(7)^{i}	2.692(4)	O(9)	O(162)^{vi}	3.10(2)
O(2)	O(7)^{i}	3.043(4)	O(10)	O(13)^{vii}	2.787(4)
O(2)	O(15)	2.652(6)	O(11)	O(161)	3.153(7)
O(2)	O(17)^{b}	3.031(4)	O(11)	O(13)^{vii}	3.177(4)
O(2)	O(14)^{ii}	2.880(4)	O(11)	O(19)$^{vii\ b}$	2.702(6)
O(3)	O(14)^{ii}	2.648(4)	O(12)	O(161)	2.908(6)
O(4)	O(17)$^{ii\ b}$	2.976(4)	O(12)	O(19)$^{vii\ b}$	3.172(6)
O(5)	O(21)	3.018(7)	O(13)	O(17)b	2.921(4)
O(5)	O(162)^{iii}	3.05(2)	O(14)	O(21)	2.794(5)
O(5)	O(17)$^{ii\ b}$	2.769(4)	O(14)	O(17)$^{ii\ b}$	3.167(4)
O(5)	O(21)$^{iv\ b}$	3.183(5)	O(15)	O(161)^{viii}	2.691(8)
O(6)	O(21)$^{iv\ b}$	2.562(6)	O(17)^{b}	O(18)$^{vii\ b}$	2.768(5)
O(7)	O(20)^{b}	3.121(6)	O(18)^{b}	O(19)^{b}	2.888(8)
O(7)	O(18)$^{v\ b}$	3.001(4)	O(18)^{b}	O(20)$^{v\ b}$	3.140(7)
O(8)	O(18)^{b}	2.803(5)	O(19)^{b}	O(20)^{b}	2.565(7)
O(8)	O(162)^{vi}	3.17(2)	O(20)^{b}	O(21)^{b}	2.693(8)
O(8)	O(18)$^{v\ b}$	2.763(5)	O(20)^{b}	O(162)^{vii}	2.581(19)
O(9)	O(18)^{b}	3.116(4)	O(21)^{b}	O(162)^{vii}	3.09(2)

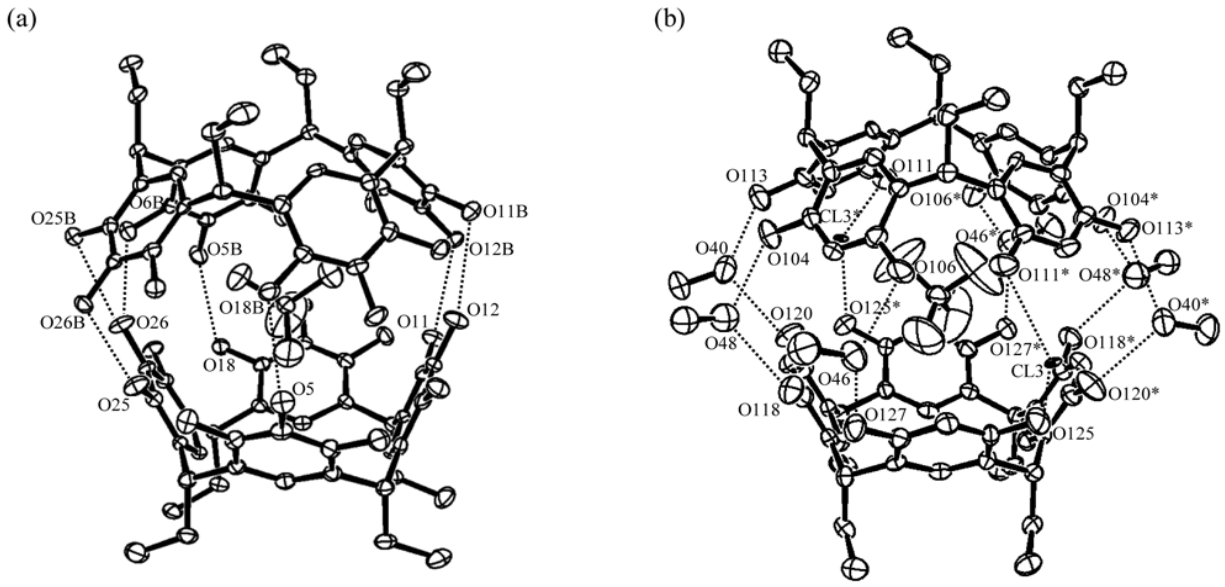
[a] Symmetry code: (none) x, y, z; (i) $x, y+1, z$; (ii) $-x, -y, -z+1$; (iii) $x-1, y-1, z$; (iv) $-x, -y-1, -z+1$; (v) $-x+1, -y-1, -z+1$; (vi) $x, y-1, z$; (vii) $-x+1, -y, -z+1$; (viii) $x-1, y, z$; [b] Water oxygens.

Table S6. Intermolecular hydrogen bonds in the RCT complex.

Atom1	Atom2	Distance (Å)	Atom1	Atom2	Distance (Å)
O(1)	O(4)[i]	3.111(3)	O(5)	O(12)iv b	3.097(3)
O(1)	O(10)[ii]	2.599(3)	O(7)	O(12)[v b]	2.649(3)
O(2)	O(11)[ii]	2.796(3)	O(8)	O(12)[b]	2.771(3)
O(3)	O(13)[b]	2.655(3)	O(9)	O(13)[b]	2.771(3)
O(4)	O(9)[iii]	2.639(3)	O(11)	O(12)[b]	2.711(3)
O(5)	O(8)[iv]	3.080(3)	O(12)[b]	O(13)[vi b]	2.835(3)

[a] Symmetry code: (none) x, y, z; (i) $x-1, y, z$; (ii) $-x, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+2$; (iv) $x+1, y, z$; (v) $-x, -y, -z+2$; (vi) $-x, -y+1, -z+2$; [b] Water oxygens.

Figure S1. Complete capsules formed with two upside-down molecules of PCT or RCT clathrating a tetramethylammonium molecule, depicted with structural data in CSD for comparison with Figure 2. (**a**) 2PCT-tetramethylammonium complex (CSD ID: JALFEI); (**b**) 2RCT-tetramethylammonium complex (CSD ID: XUSZOA) Intermolecular hydrogen bonds constructing the capsule forms are drawn with dotted lines. Solvent molecules without direct connections to two upside-down PCT or RCT molecules aren't drawn for clarity. The 2PCT-tetramethylammonium complex capsule keeps the shape with direct hydrogen bonds between two upside-down PCT molecules and cation−π interactions. The 2RCT-tetramethylammonium complex capsule is formed with two upside-down RCT molecules and sandwiched solvent molecules between two RCT molecules, that is, four methanol molecules and two chloride ions. Though no direct hydrogen bonds are observed between two upside-down RCT molecules, the capsule shape is maintained by cation−π interactions and hydrogen bonds with solvents.



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