Supplementary information:

Determination of complexation constants:

Initial concentrations of organic macrocycles were DOTP = 0.0912 mM and NOTP = 0.0973 mM. Complexation was determined at 0.25 mM $BaCl_2$ concentration. Using the graphs shown in Figure 2 of the main manuscript, the concentration of Ba^{2+} complexed was determined by the following procedure:

a) At 0.25mM Ba^{2+} the conductivity values of the DOTP and NOTP system were determined.

b) This value was used to determine the Ba^{2+} conc. in the absence of DOTP or NOTP by using the control linear regression.

c) 0.25 mM – Ba^{2+} conc. determined in b) = conc of Ba^{2+} complexed.

For NOTP the complexed $[Ba^{2+}] = 0.0001$ mM

While for DOTP the complexed $[Ba^{2+}] = 0.0444$ mM.

We then assumed

$$L^{4-} + 2Ba^{2+} \leftrightharpoons Ba_2L \qquad \text{Eqn. 1}$$

This was decided upon from the speciation information. We then calculated the K value, keeping in mind the stoichiometry of the complexed barium concentration to the complex concentration:

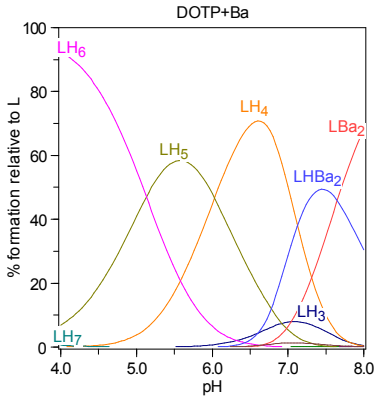
$$K = [Ba_2L]/([L^{4-}][Ba^{2+}]^2)$$

and the initial ligand and barium ion concentrations listed above.

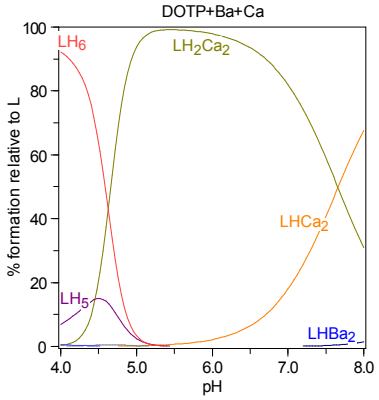
Using this method, we determined

	K	log K
DOTP	3,860,800	6.59
NOTP	2055.5	3.31

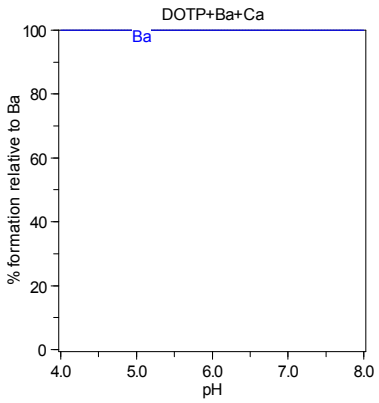
Speciation with barium present



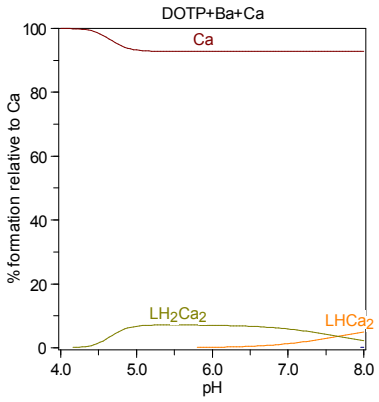
at 0.09mM DOTP and 0.25 mM Ba



Ca^{2+} at 2.5mM, Ba^{2+} at 0.25mM and DOTP at 0.09 mM



Ca^{2+} at 2.5mM, Ba^{2+} at 0.25mM and DOTP at 0.09 mM



Ca^{2+} at 2.5mM, Ba^{2+} at 0.25mM and DOTP at 0.09 mM

Interatomic potentials for describing the interactions between the organic molecule, DOTP and the barite lattice. C1 refers to that carbon bonded to the phosphorous atom or carboxylate carbon atom, C2 refers to that carbon on the backbone. O3 is the oxygen on the organic molecule while O is on the sulfate.

Lennard-Jones potentials (are 9 6 in form).

C1 core C1 core 77689.066061 22.932654

H1 core C1 core 4895.307763 5.719317

C1 core P core 142528.855995 46.742924

C1 core N core 87418.951402 34.993722

C1 core O3 core 30331.205624 22.281108

C2 core C2 core 77689.066061 22.932654

H1 core C2 core 4895.307763 5.719317

C2 core P core 142528.855995 46.742924

C2 core N core 87418.951402 34.993722

C2 core O3 core 30331.205624 22.281108

C1 core C2 core 77689.066061 22.932654

H1 core O3 core 1911.216003 5.556824

H1 core P core 8980.962838 11.657507

H1 core N core 5508.402831 8.727301

H1 core H1 core 308.460885 1.426376

O3 core O3 core 11841.847009 21.648074

O3 core P core 55645.823251 45.414898

N core O3 core 34129.927477 33.999506

P core P core 261484.348072 95.274665

N core P core 160379.365686 71.326627

N core N core 98367.420946 53.398117

harmonic

C1 core P core 21.618618 1.750000

O3 core P core 41.657715 1.530000

H1 core C1 core 29.561139 1.105000

H1 core C2 core 29.561139 1.105000

C1 core N core 30.948107 1.470000

C2 core N core 30.948107 1.470000

C2 core C2 core 28.007506 1.526000

three-body

C1 core H1 core P core 3.818624 109.500000

C1 core N core P core 4.339345 109.500000

P core C1 core O3 core 9.546560 120.000000

P core O3 core O3 core 9.546560 109.500000

C1 core H1 core N core 4.972890 109.500000

C2 core H1 core N core 4.972890 109.500000

N core C1 core C1 core 7.489710 110.250000

N core C1 core C2 core 7.489710 110.250000

C2 core C2 core N core 4.339345 109.500000

C2 core H1 core C2 core 3.853339 110.000000

C2 core H1 core H1 core 3.428083 106.400000

C1 core H1 core H1 core 3.428083 106.400000

four body

P core C1 core N core C1 core 0.005784 1 3

P core C1 core N core C2 core 0.005784 1 3

C1 core N core C1 core H1 core 0.005784 1 3

C1 core N core C2 core H1 core 0.005784 1 3

C2 core N core C1 core H1 core 0.005784 1 3

N core C2 core C2 core H1 core 0.006861 1 3

N core C2 core C2 core N core 0.006861 1 3

H1 core C2 core C2 core H1 core 0.006861 1 3

C2 core C2 core N core C1 core 0.005784 1 3

charges

O3 -1.19000

P 2.110000

C1 -0.595000

N -0.465000

C2 0.080000

H1 0.060000

organic-barium sulfate potentials

nine-six intermolecular

O3 core Ba core 1420.000 53.90000 0.000 15.000

P core Ba core 7210.000 173.0000 0.000 15.000

C2 core Ba core 2010.0000 64.7000 0.000 15.000

N core Ba core 1750.0000 62.4000 0.000 15.000

C1 core Ba core 2110.0000 66.5000 0.000 15.000

H1 core Ba core 301.0000 16.6000 0.000 15.000

H2 core Ba core 301.0000 16.6000 0.000 15.000

O3 core S core 2740.0000 62.2000 0.000 15.000

P core S core 1190.0000 199.0000 0.000 15.000

C2 core S core 3650.0000 74.6000 0.000 15.000

N core S core 3300.0000 71.9000 0.000 15.000

C1	core S	core	3800.0000	76.6000	0.000	15.000
H1	core S	core	688.0000	19.1000	0.000	15.000
H2	core S	core	688.0000	19.1000	0.000	15.000
O3	core O	core	673.0000	19.8000	0.000	15.000
P	core O	core	3140.0000	63.4000	0.000	15.000
C2	core O	core	921.0000	23.7000	0.000	15.000
N	core O	core	819.0000	22.9000	0.000	15.000
C1	core O	core	962.0000	24.4000	0.000	15.000
H1	core O	core	158.0000	6.09000	0.000	15.000
H2	core O	core	158.0000	6.09000	0.000	15.000

Solvation energies:

	Solvation energy (in $kJmol^{-1}$)
DOTP	-7489.1
DOTP complexed	-6791.4
EDTP	-7896.8
NTMP	-5472.2 (c/f -5770.6 from ref 27)

Initial energies:

	(in $kJmol^{-1}$)
DOTP	4890.6
DOTP complexed	-15.847
EDTP	5038.1
NTMP	2739.2